



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 05:01 AM UTC

PDB ID : 6M99 / pdb_00006m99
EMDB ID : EMD-9050
Title : In situ structure of transcriptional enzyme complex and asymmetric inner capsid protein of aquareovirus at primed state
Authors : Ding, K.; Zhou, Z.H.
Deposited on : 2018-08-23
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

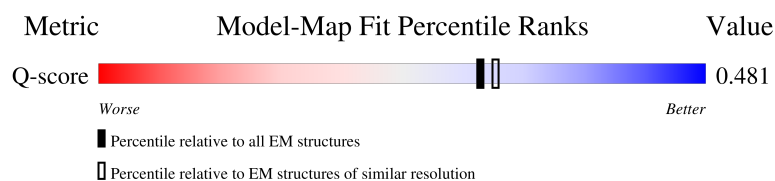
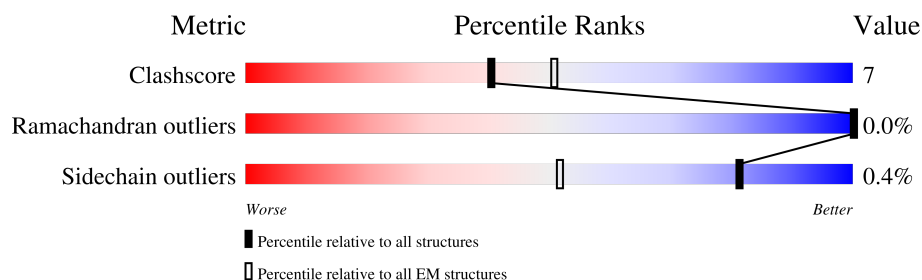
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	1274	25% 83% 17%
2	B	728	17% 66% 16% 17%
3	C	1214	7% 72% 18% 10%
3	D	1214	12% 81% 16% .

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Mol	Chain	Length	Quality of chain
3	E	1214	 69% 19% 12%
3	F	1214	 82% 16%
3	G	1214	 72% 16% 13%
3	H	1214	 82% 16%
3	I	1214	 71% 16% 13%
3	J	1214	 81% 16%
3	K	1214	 73% 14% 13%
3	L	1214	 81% 17%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 101389 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 VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1273	Total	C	N	O	S	0	0
			9974	6376	1733	1820	45		

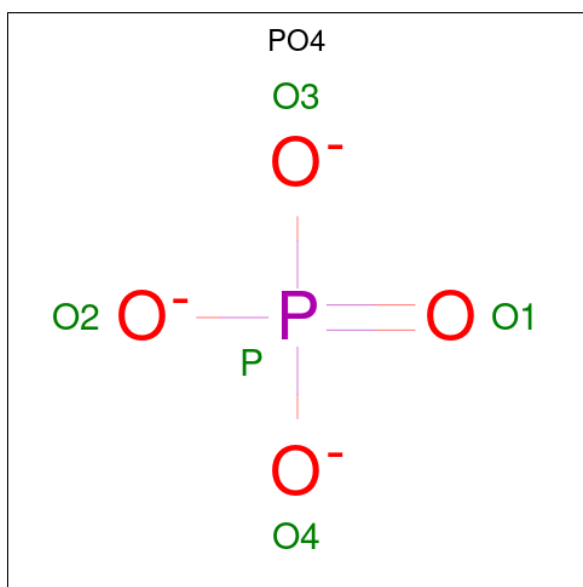
- Molecule 2 is a protein called Putative core protein NTPase/VP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	601	Total	C	N	O	S	0	0
			4667	2991	809	852	15		

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1096	Total	C	N	O	S	0	0
			8474	5404	1456	1563	51		
3	D	1187	Total	C	N	O	S	0	0
			9088	5763	1565	1709	51		
3	E	1064	Total	C	N	O	S	0	0
			8222	5251	1407	1516	48		
3	F	1187	Total	C	N	O	S	0	0
			9088	5763	1565	1709	51		
3	G	1061	Total	C	N	O	S	0	0
			8202	5238	1404	1512	48		
3	H	1187	Total	C	N	O	S	0	0
			9088	5763	1565	1709	51		
3	I	1061	Total	C	N	O	S	0	0
			8202	5238	1404	1512	48		
3	J	1187	Total	C	N	O	S	0	0
			9088	5763	1565	1709	51		
3	K	1061	Total	C	N	O	S	0	0
			8202	5238	1404	1512	48		
3	L	1187	Total	C	N	O	S	0	0
			9088	5763	1565	1709	51		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
4	B	1	Total	O	P	0
			5	4	1	

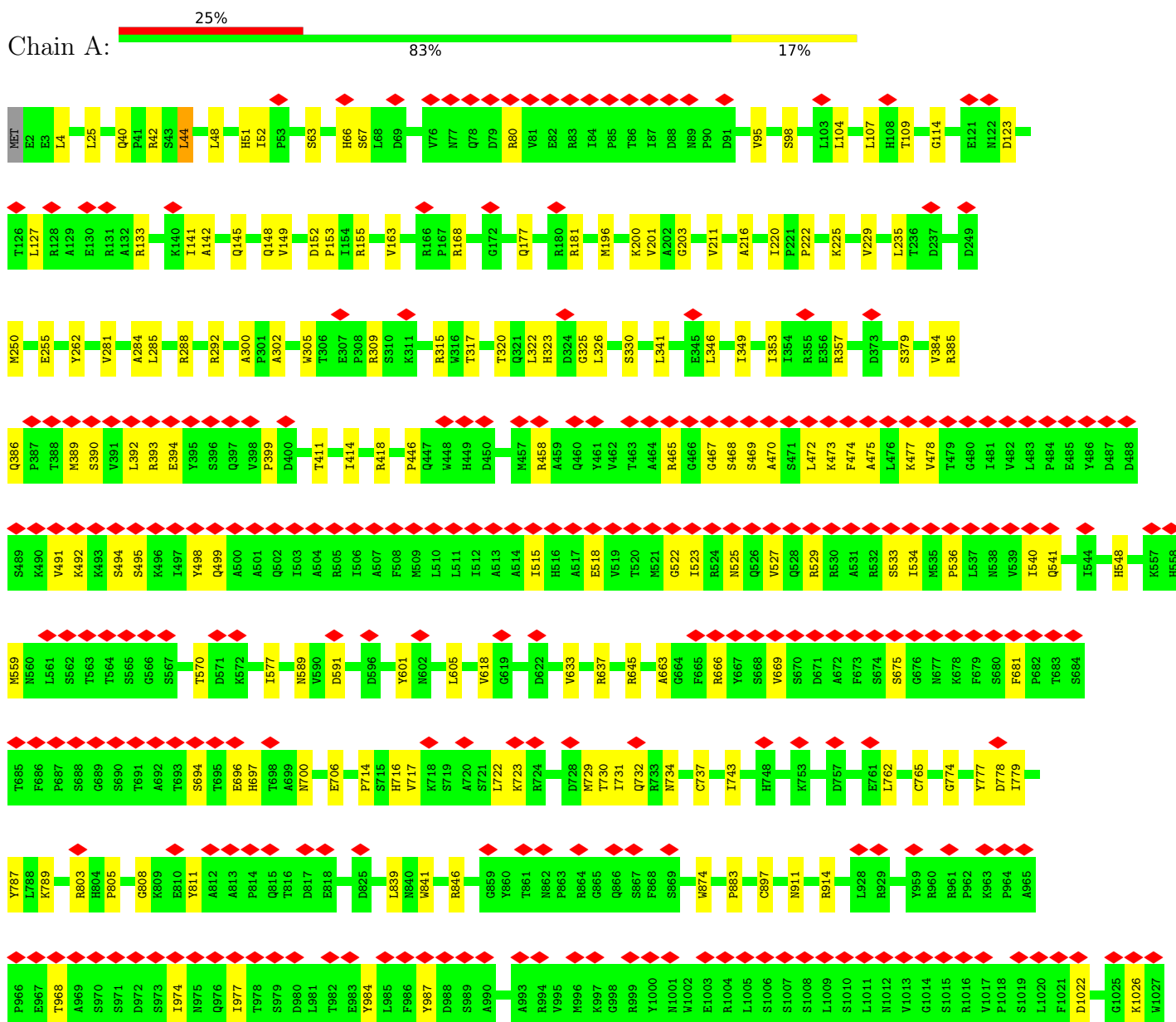
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

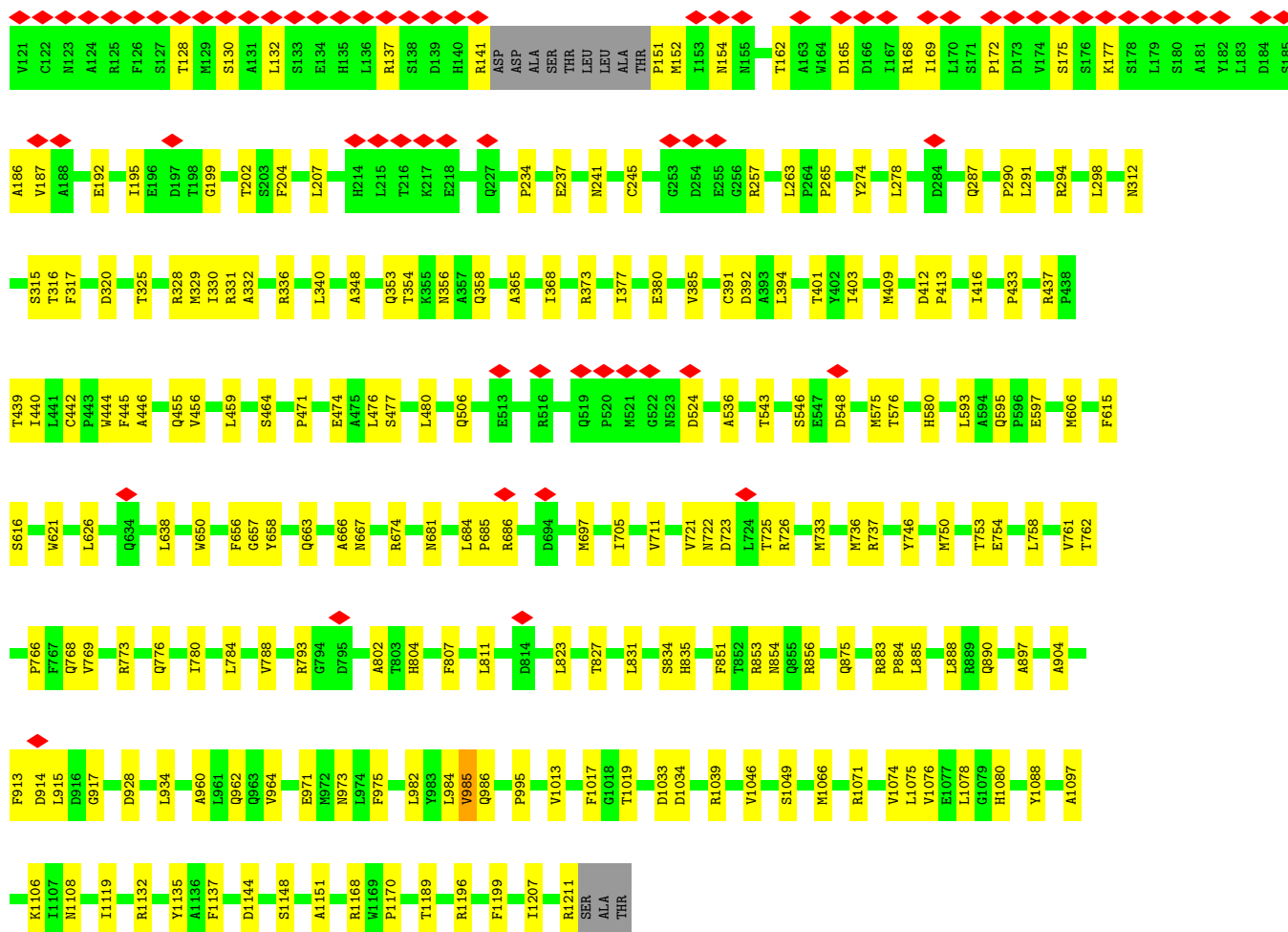
Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Zn	0
			1	1	

3 Residue-property plots

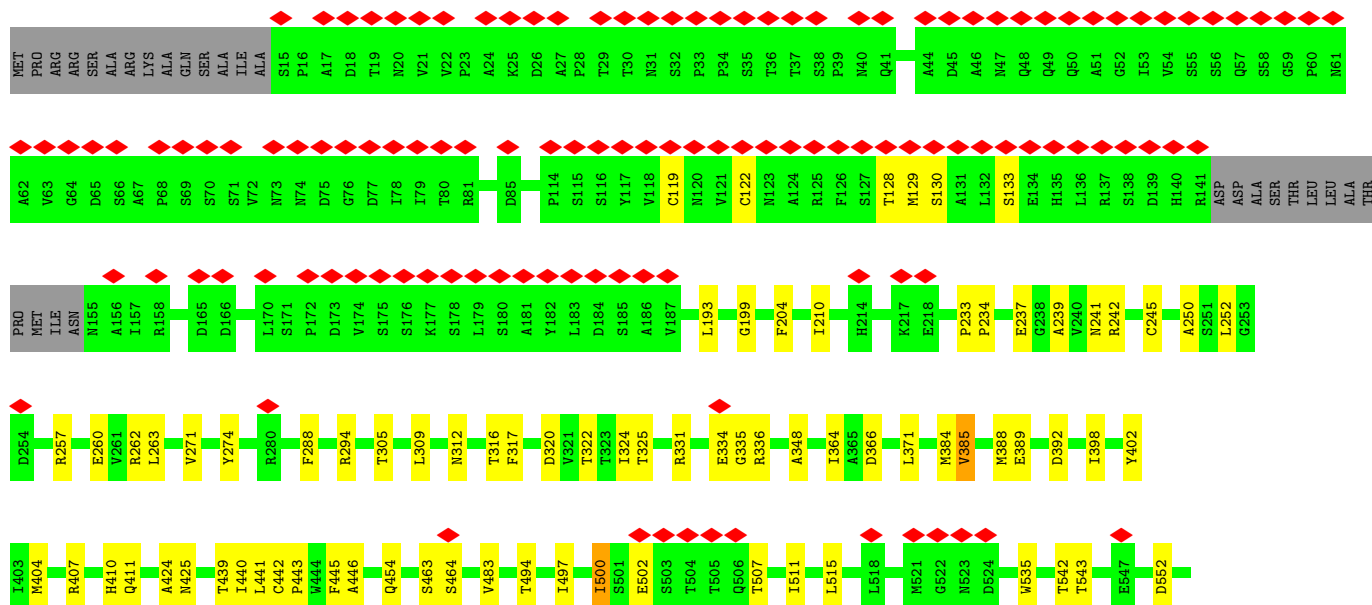
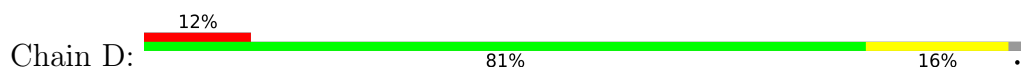
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

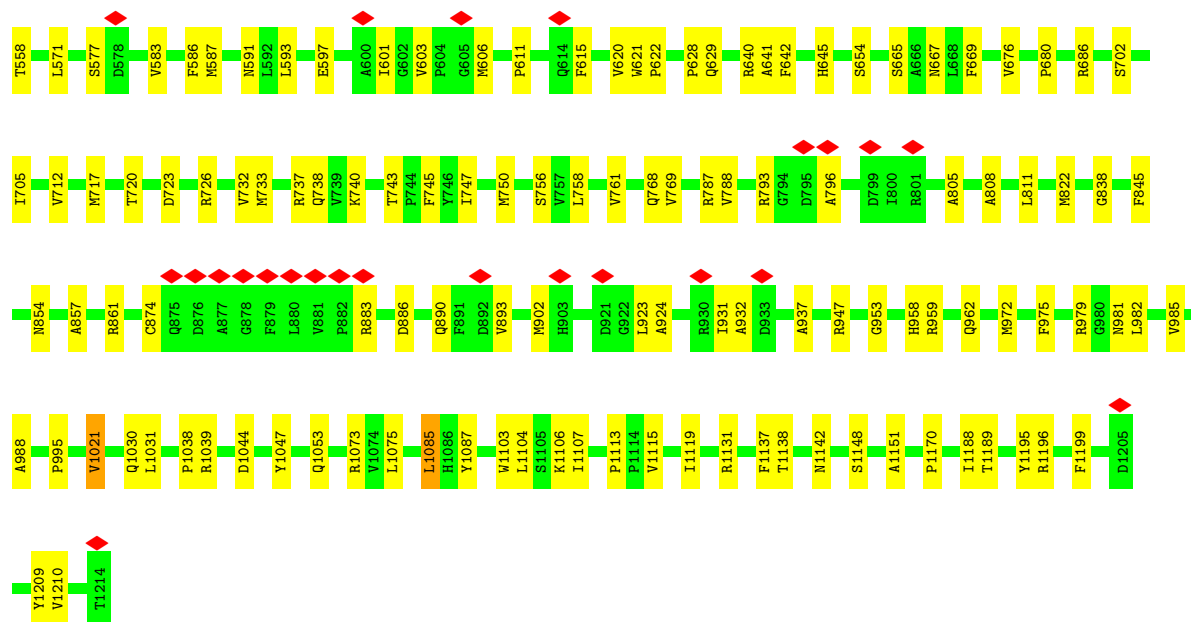
• Molecule 1: VP2





• Molecule 3: VP3





• Molecule 3: VP3

Chain E: 69% 19% 12%

MET PRO ARG GLY SER ALA ARG LYS VAL GLN SER SER ILE ALA SER PRO ASP THR ASN VAL PRO THR THR SER PRO GLN ALA ASP MET ALA GLN GLN ALA GLY VAL SER GLY PRO

ASN ALA VAL GLY ASP SER ALA PRO SER SER VAL ASN ASN ASP GLY ASP ILE THR ARG THR THR ASP SER ILE ALA VAL THR ASN VAL VAL ASP PRO GLN SER MET LYS VAL THR ILE VAL ASP THR VAL CYS ASN

VAL CYS ASN ARG PHE SER MET THR LEU LEU GLU HIS LEU ARG SER ASP HIS ARG ASP ASP ALA SER THR LEU A149 T150 A156 S159 F160 L161 T162 D165 D166 I167 L170 V174 K177 D184 S186 A186 V187 A188 I189 L193 E196 D197

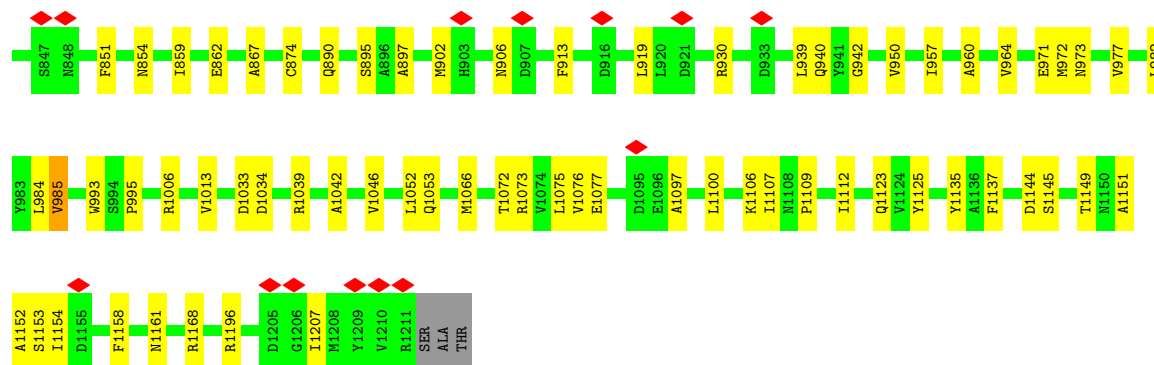
S203 T210 A213 H214 L215 T216 K217 F221 G221 T223 W224 P234 E237 G238 A239 R242 M246 T247 A250 E255 E260 V261 R262 H272 L278 S279 T283 D294 Q287 R294 M300 F304 K313 S314 S315 F317 T323

R328 M329 I330 R331 A332 F333 E334 G335 R336 L339 A348 Q353 T354 A357 Q358 I364 R367 I368 G369 R370 L371 D372 R373 A374 N375 I377 E380 C387 M388 E389 D392 A393 L394 R399 E400 T401 Y402 T403 L406 D412 P413 T416 V417 C423

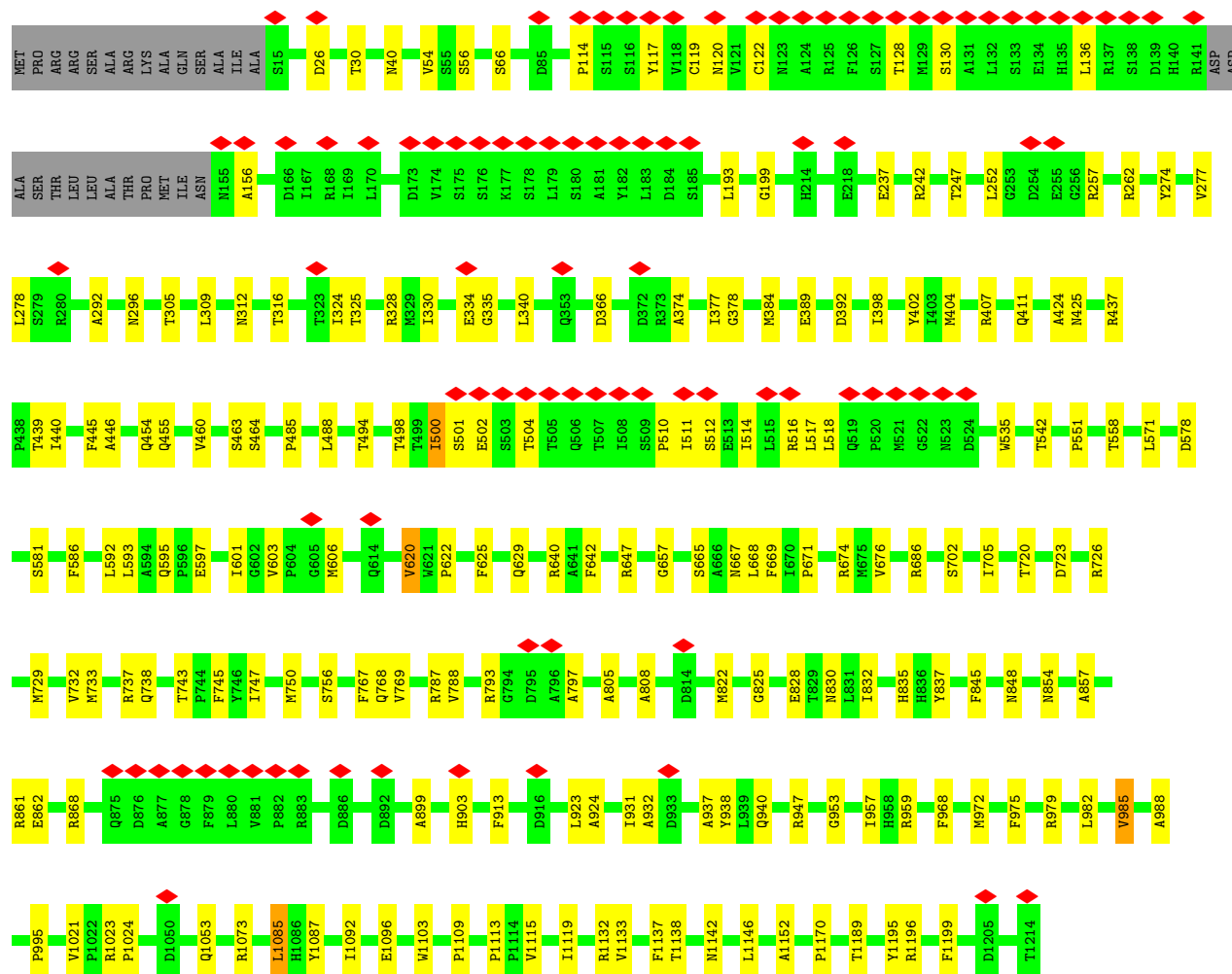
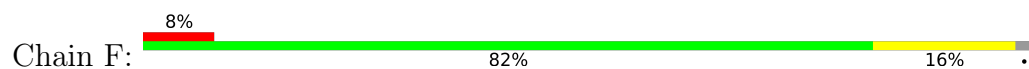
M429 S430 T431 I432 P433 I434 S435 L436 L441 Q442 P443 A446 D450 V456 P471 L472 V473 L479 L480 R481 P485 D489 P490 L493 S501 R516 P520 M521 D524 Y525 A526 A527 W535 A536 G539 T543 D548 A549 P550 P551 D552 S556

L569 T570 L571 T576 H580 A590 L593 E597 V603 M606 T610 P611 A612 F615 S616 V620 W621 L626 L639 W650 P651 G659 M667 L668 F669 T670 S672 V676 P678 L684 P685 R686 M697 I705 N716 N722

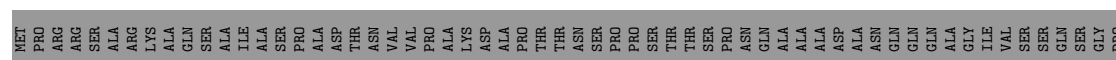
D723 L724 T725 R726 R727 M733 Q738 T743 I747 C751 P752 T753 E754 L758 P766 F767 Q768 F771 T772 R773 Q776 M777 D778 V783 A786 R793 G794 D795 R801 H804 L811 P812 V813 D814 P815 V819 V820 A821 M822 Q826 H830 L831

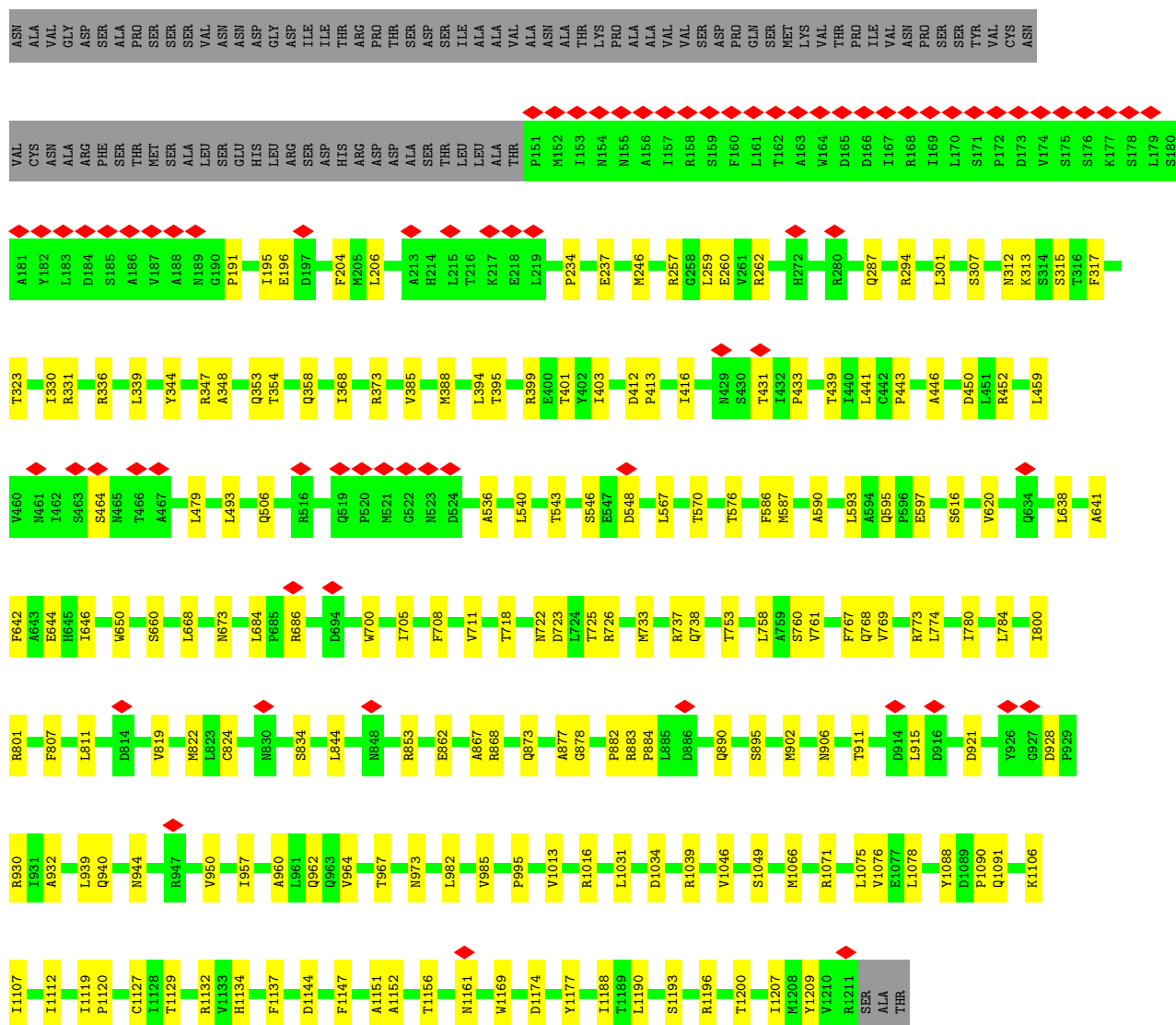


• Molecule 3: VP3

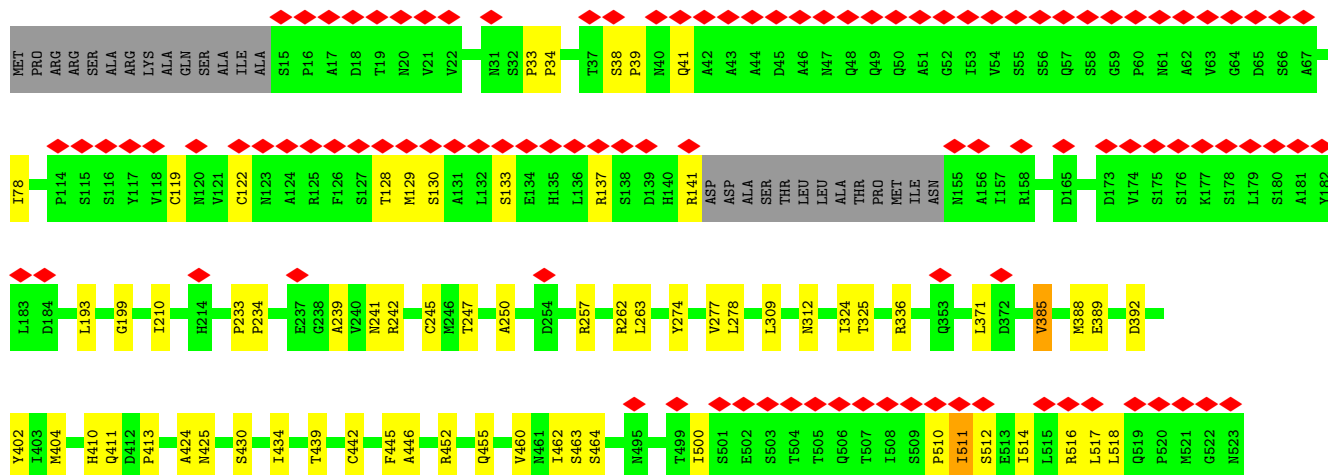
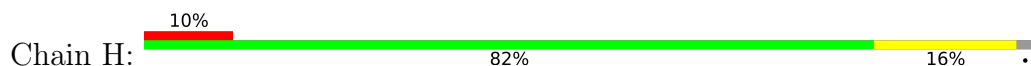


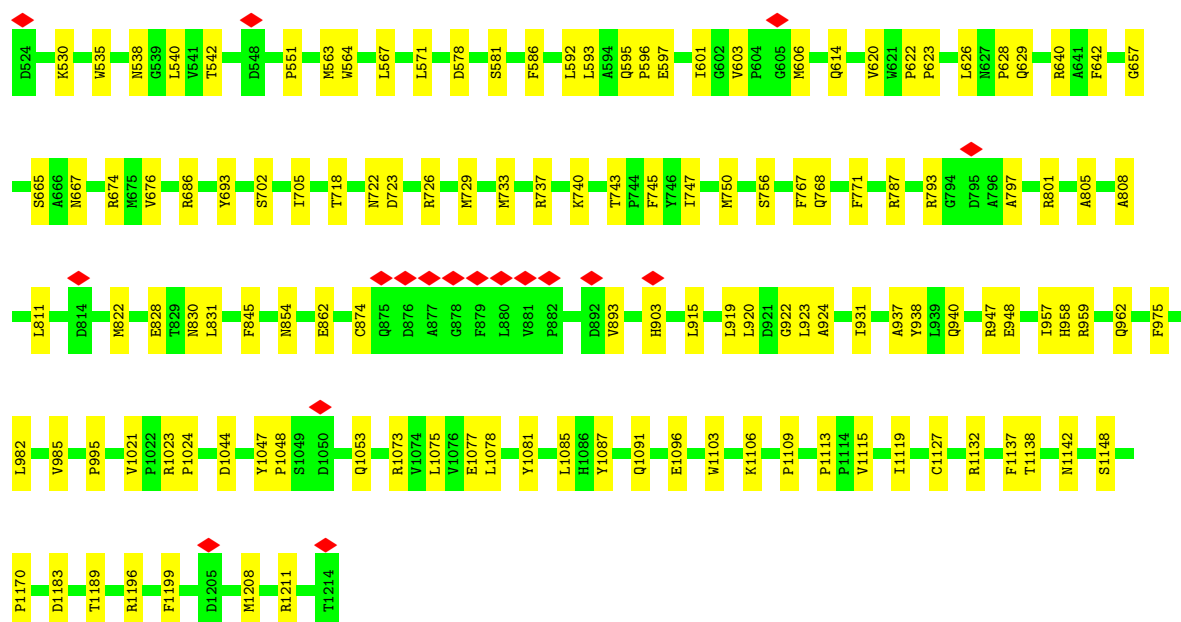
• Molecule 3: VP3



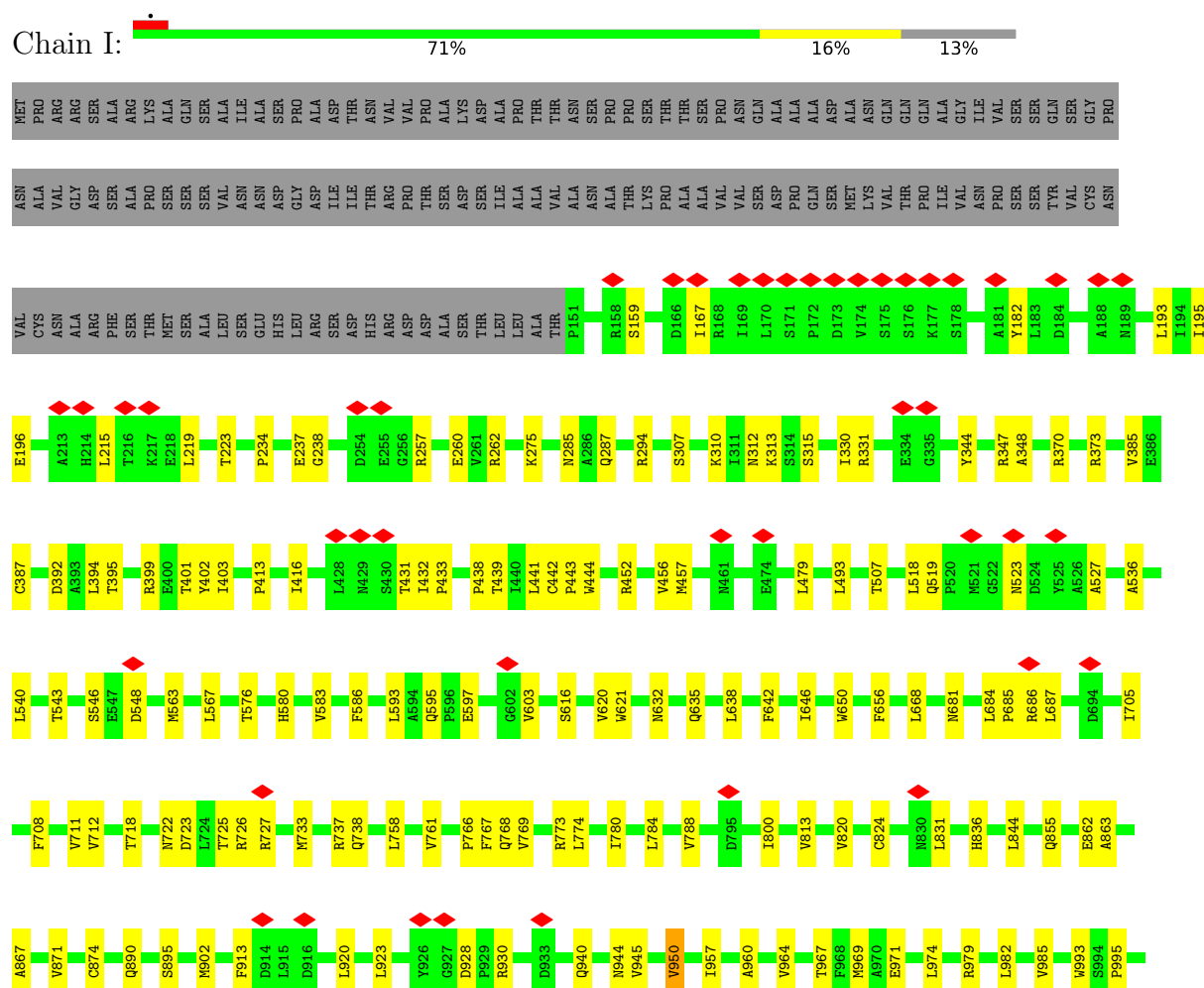


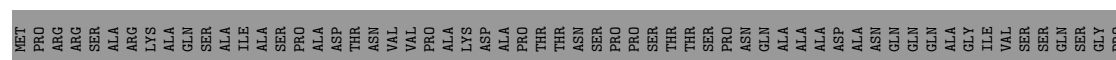
• Molecule 3: VP3

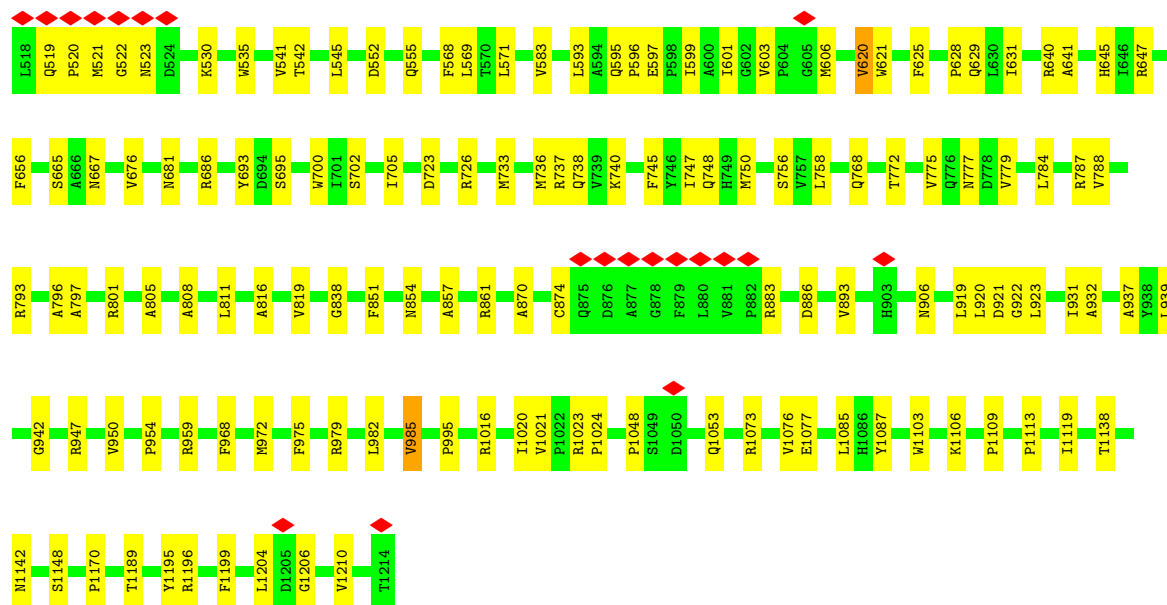




- Molecule 3: VP3







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73472	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.102	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0194	Depositor
Map size (Å)	399.0, 399.0, 399.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZN

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	0.24	0/10258	0.50	1/14016 (0.0%)
2	B	0.29	0/4775	0.59	5/6533 (0.1%)
3	C	0.29	0/8692	0.53	2/11907 (0.0%)
3	D	0.29	0/9316	0.54	0/12771
3	E	0.30	0/8435	0.54	0/11561
3	F	0.28	0/9316	0.53	2/12771 (0.0%)
3	G	0.29	0/8415	0.52	0/11532
3	H	0.28	0/9316	0.54	2/12771 (0.0%)
3	I	0.29	0/8415	0.52	3/11532 (0.0%)
3	J	0.28	0/9316	0.54	0/12771
3	K	0.28	0/8415	0.53	2/11532 (0.0%)
3	L	0.29	0/9316	0.56	4/12771 (0.0%)
All	All	0.28	0/103985	0.53	21/142468 (0.0%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	671	ALA	CA-C-N	-5.89	114.32	120.38
2	B	671	ALA	C-N-CA	-5.89	114.32	120.38
2	B	674	LEU	CA-C-N	-5.67	113.92	119.76
2	B	674	LEU	C-N-CA	-5.67	113.92	119.76
3	C	913	PHE	CA-C-N	5.55	132.13	121.54
3	C	913	PHE	C-N-CA	5.55	132.13	121.54
3	L	1020	ILE	CA-C-N	-5.54	117.94	123.04
3	L	1020	ILE	C-N-CA	-5.54	117.94	123.04
3	K	913	PHE	CA-C-N	5.46	131.98	121.54
3	K	913	PHE	C-N-CA	5.46	131.98	121.54
3	L	522	GLY	CA-C-N	5.42	131.88	121.54
3	L	522	GLY	C-N-CA	5.42	131.88	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	913	PHE	CA-C-N	5.35	131.77	121.54
3	I	913	PHE	C-N-CA	5.35	131.77	121.54
3	I	219	LEU	CA-CB-CG	5.19	134.46	116.30
3	F	913	PHE	CA-C-N	5.19	131.45	121.54
3	F	913	PHE	C-N-CA	5.19	131.45	121.54
2	B	676	LEU	N-CA-C	-5.09	105.73	111.28
3	H	1183	ASP	CA-C-N	5.08	126.10	120.06
3	H	1183	ASP	C-N-CA	5.08	126.10	120.06
1	A	201	VAL	N-CA-C	-5.01	108.62	113.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9974	0	9892	124	0
2	B	4667	0	4778	91	0
3	C	8474	0	8445	141	0
3	D	9088	0	9019	126	0
3	E	8222	0	8201	146	0
3	F	9088	0	9019	125	0
3	G	8202	0	8179	123	0
3	H	9088	0	9019	127	0
3	I	8202	0	8179	127	0
3	J	9088	0	9019	129	0
3	K	8202	0	8179	116	0
3	L	9088	0	9019	128	0
4	B	5	0	0	0	0
5	C	1	0	0	0	0
All	All	101389	0	100948	1410	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 7.

All (1410) 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:J:593:LEU:CD1	3:J:597:GLU:HB2	1.66	1.24
3:L:593:LEU:CD1	3:L:597:GLU:HB2	1.69	1.22
3:J:593:LEU:HD13	3:J:597:GLU:CB	1.69	1.21
3:L:593:LEU:HD13	3:L:597:GLU:CB	1.68	1.21
3:L:593:LEU:HD13	3:L:597:GLU:CG	1.68	1.20
3:G:593:LEU:HD13	3:G:597:GLU:HG3	1.18	1.17
3:H:915:LEU:HD22	3:H:919:LEU:HD23	1.19	1.16
3:F:593:LEU:HD13	3:F:597:GLU:CB	1.76	1.15
3:G:593:LEU:HD13	3:G:597:GLU:CG	1.76	1.15
3:H:593:LEU:HD13	3:H:597:GLU:CG	1.78	1.14
3:C:1019:THR:HG22	3:D:1209:TYR:CD2	1.84	1.13
3:I:593:LEU:HD13	3:I:597:GLU:CG	1.78	1.12
3:F:593:LEU:HD13	3:F:597:GLU:CG	1.81	1.10
3:L:593:LEU:HD13	3:L:597:GLU:HB2	1.22	1.10
3:F:593:LEU:HD13	3:F:597:GLU:HB2	1.24	1.09
3:K:593:LEU:HD13	3:K:597:GLU:CG	1.82	1.09
3:F:593:LEU:CD1	3:F:597:GLU:HB2	1.81	1.08
3:E:593:LEU:HD13	3:E:597:GLU:HB2	1.36	1.06
3:I:593:LEU:HD13	3:I:597:GLU:HG3	1.08	1.06
3:G:593:LEU:CD1	3:G:597:GLU:HB2	1.86	1.04
3:K:593:LEU:HD13	3:K:597:GLU:HG3	1.05	1.04
3:H:593:LEU:CD1	3:H:597:GLU:HB2	1.88	1.03
3:H:593:LEU:HD13	3:H:597:GLU:CB	1.90	1.02
3:I:593:LEU:CD1	3:I:597:GLU:HB2	1.94	0.96
3:K:593:LEU:CD1	3:K:597:GLU:HG3	1.94	0.96
3:I:593:LEU:CD1	3:I:597:GLU:HG3	1.96	0.94
3:G:593:LEU:CD1	3:G:597:GLU:HG3	1.99	0.93
2:B:674:LEU:HD23	2:B:674:LEU:H	1.34	0.92
3:H:593:LEU:HD13	3:H:597:GLU:HB2	1.42	0.92
3:J:593:LEU:HD13	3:J:597:GLU:HB2	0.95	0.91
2:B:654:SER:HB2	2:B:672:PRO:HG2	1.53	0.90
2:B:654:SER:CB	2:B:672:PRO:HG2	2.04	0.88
3:G:593:LEU:HD12	3:G:597:GLU:HB2	1.55	0.87
3:H:915:LEU:HD22	3:H:919:LEU:CD2	2.04	0.86
3:G:593:LEU:CD1	3:G:597:GLU:CB	2.55	0.84
3:E:593:LEU:CD1	3:E:597:GLU:HB2	2.06	0.84
3:I:593:LEU:HD12	3:I:597:GLU:HB2	1.56	0.84
3:J:593:LEU:HD13	3:J:597:GLU:CG	2.09	0.81
3:K:593:LEU:CD1	3:K:597:GLU:HB2	2.12	0.80
2:B:654:SER:HA	2:B:672:PRO:HG3	1.62	0.80
2:B:654:SER:HA	2:B:672:PRO:CG	2.12	0.79
3:L:593:LEU:HD12	3:L:593:LEU:O	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:593:LEU:HD13	3:L:597:GLU:HG3	1.62	0.79
3:I:593:LEU:CD1	3:I:597:GLU:CB	2.60	0.79
3:G:593:LEU:HD13	3:G:597:GLU:CB	2.12	0.78
3:G:593:LEU:CD1	3:G:597:GLU:CG	2.61	0.78
3:K:593:LEU:HD12	3:K:597:GLU:HB2	1.67	0.75
3:H:593:LEU:HD13	3:H:597:GLU:HG3	1.65	0.75
3:C:1019:THR:CG2	3:D:1209:TYR:CD2	2.69	0.75
3:F:593:LEU:O	3:F:593:LEU:HD12	1.87	0.74
3:J:593:LEU:HD12	3:J:593:LEU:O	1.88	0.73
3:I:593:LEU:HD13	3:I:597:GLU:CB	2.18	0.73
3:L:1085:LEU:HD13	3:L:1087:TYR:CE1	2.24	0.73
2:B:26:ARG:HD3	2:B:245:LEU:HD11	1.70	0.73
3:C:593:LEU:CD1	3:C:597:GLU:HB2	2.20	0.72
1:A:518:GLU:HB3	2:B:673:PRO:HG3	1.72	0.72
3:I:593:LEU:CD1	3:I:597:GLU:CG	2.63	0.72
2:B:674:LEU:H	2:B:674:LEU:CD2	2.02	0.72
3:L:593:LEU:HD13	3:L:597:GLU:HG2	1.71	0.71
3:E:593:LEU:HD13	3:E:597:GLU:OE1	1.91	0.71
3:I:616:SER:HB3	3:J:723:ASP:HB2	1.73	0.70
3:F:593:LEU:HD13	3:F:597:GLU:HG3	1.70	0.70
3:C:1049:SER:HB2	3:C:1078:LEU:HB3	1.74	0.70
3:H:593:LEU:HD13	3:H:597:GLU:HG2	1.74	0.69
1:A:477:LYS:HD2	2:B:675:PRO:HB3	1.74	0.69
3:K:1078:LEU:HD13	3:K:1081:TYR:HB3	1.75	0.69
3:L:787:ARG:HH12	3:L:923:LEU:HA	1.57	0.68
3:G:593:LEU:HD12	3:G:593:LEU:O	1.94	0.68
3:C:593:LEU:HD13	3:C:597:GLU:CG	2.24	0.68
2:B:62:LEU:HB2	2:B:224:LEU:HD11	1.75	0.67
3:F:787:ARG:HH12	3:F:923:LEU:HA	1.60	0.67
3:H:38:SER:HB2	3:H:41:GLN:HB2	1.77	0.67
3:H:629:GLN:HA	3:H:640:ARG:HH12	1.59	0.67
3:I:416:ILE:HD11	3:I:1207:ILE:HG21	1.75	0.67
3:H:593:LEU:HD12	3:H:593:LEU:O	1.95	0.67
1:A:284:ALA:HA	1:A:288:ARG:HB2	1.77	0.66
3:D:982:LEU:HD11	3:D:1115:VAL:HG11	1.77	0.66
3:L:378:GLY:HA3	3:L:437:ARG:HH22	1.59	0.66
3:I:536:ALA:HA	3:I:768:GLN:HE21	1.58	0.66
3:G:416:ILE:HD11	3:G:1207:ILE:HG21	1.77	0.66
3:K:593:LEU:CD1	3:K:597:GLU:CB	2.73	0.66
3:K:616:SER:HB3	3:L:723:ASP:HB2	1.77	0.66
3:C:616:SER:HB3	3:D:723:ASP:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:705:ILE:HG23	3:E:733:MET:HG2	1.77	0.66
3:H:538:ASN:HD22	3:H:771:PHE:HE1	1.44	0.65
3:I:593:LEU:HD12	3:I:593:LEU:O	1.95	0.65
3:L:995:PRO:HD2	3:L:1119:ILE:HG12	1.79	0.65
3:I:800:ILE:HG13	3:I:945:VAL:HG21	1.78	0.65
3:K:593:LEU:CD1	3:K:597:GLU:CG	2.66	0.65
3:C:416:ILE:HD11	3:C:1207:ILE:HG21	1.79	0.65
3:F:312:ASN:HB3	3:F:1196:ARG:HD3	1.79	0.65
3:G:616:SER:HB3	3:H:723:ASP:HB2	1.80	0.64
3:G:195:ILE:HD12	3:G:257:ARG:HH11	1.63	0.64
3:L:593:LEU:HD12	3:L:597:GLU:HB2	1.72	0.64
2:B:26:ARG:HH21	2:B:385:CYS:HB2	1.62	0.64
2:B:293:ILE:HG12	2:B:313:THR:HG22	1.80	0.64
3:J:787:ARG:HH12	3:J:923:LEU:HA	1.63	0.64
3:J:982:LEU:HD11	3:J:1115:VAL:HG11	1.80	0.64
3:K:877:ALA:H	3:K:883:ARG:HH12	1.46	0.64
1:A:1122:PHE:O	1:A:1172:ARG:NH2	2.31	0.63
3:F:676:VAL:O	3:F:768:GLN:NE2	2.32	0.63
3:D:995:PRO:HD2	3:D:1119:ILE:HG12	1.80	0.63
3:F:404:MET:SD	3:F:959:ARG:NH2	2.71	0.63
3:C:536:ALA:HA	3:C:768:GLN:HE21	1.62	0.63
3:G:761:VAL:HG11	3:G:844:LEU:HD13	1.81	0.63
2:B:654:SER:HB2	2:B:672:PRO:CG	2.28	0.63
2:B:26:ARG:NH2	2:B:385:CYS:O	2.32	0.63
3:I:761:VAL:HG11	3:I:844:LEU:HD13	1.81	0.62
3:K:593:LEU:HD12	3:K:593:LEU:O	1.98	0.62
3:G:536:ALA:HA	3:G:768:GLN:HE21	1.64	0.62
3:I:890:GLN:O	3:J:686:ARG:NH2	2.33	0.62
3:H:119:CYS:SG	3:H:122:CYS:N	2.73	0.62
3:C:593:LEU:HD13	3:C:597:GLU:HG2	1.81	0.62
3:H:676:VAL:O	3:H:768:GLN:NE2	2.33	0.62
1:A:1052:CYS:SG	1:A:1055:ARG:NH1	2.73	0.62
3:L:593:LEU:CD1	3:L:597:GLU:CB	2.46	0.62
3:C:316:THR:HG23	3:C:332:ALA:HB3	1.81	0.62
3:J:241:ASN:HD22	3:J:1148:SER:HB3	1.65	0.62
3:C:298:LEU:HD12	3:C:885:LEU:HD12	1.82	0.62
3:D:676:VAL:O	3:D:768:GLN:NE2	2.33	0.62
3:C:287:GLN:NE2	3:C:1106:LYS:O	2.33	0.62
3:G:315:SER:HB2	3:G:331:ARG:HD2	1.81	0.62
3:E:786:ALA:HB2	3:E:804:HIS:HA	1.80	0.61
1:A:1077:SER:HA	1:A:1249:ARG:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:676:VAL:O	3:J:768:GLN:NE2	2.33	0.61
3:E:616:SER:HB3	3:F:723:ASP:HB2	1.83	0.61
3:H:514:ILE:HA	3:H:517:LEU:HB3	1.81	0.61
3:F:411:GLN:HB2	3:F:445:PHE:HB2	1.81	0.61
1:A:181:ARG:NH2	1:A:255:GLU:OE2	2.34	0.61
3:J:425:ASN:ND2	3:J:756:SER:OG	2.32	0.61
3:C:117:TYR:HB3	3:C:132:LEU:HD22	1.83	0.61
3:J:629:GLN:HA	3:J:640:ARG:HH12	1.64	0.61
3:E:982:LEU:HB3	3:E:1076:VAL:HB	1.82	0.61
3:G:1091:GLN:NE2	3:G:1127:CYS:SG	2.74	0.61
1:A:63:SER:HA	1:A:66:HIS:HD2	1.67	0.60
1:A:42:ARG:NH2	1:A:152:ASP:OD2	2.34	0.60
3:I:413:PRO:HA	3:I:416:ILE:HG12	1.82	0.60
3:L:676:VAL:O	3:L:768:GLN:NE2	2.35	0.60
3:D:119:CYS:SG	3:D:122:CYS:N	2.75	0.60
3:F:995:PRO:HD2	3:F:1119:ILE:HG12	1.82	0.60
3:K:684:LEU:HD22	3:K:753:THR:HG21	1.84	0.60
1:A:591:ASP:HB2	1:A:778:ASP:HB3	1.83	0.60
3:J:242:ARG:HH12	3:J:1085:LEU:HD21	1.66	0.60
3:L:404:MET:SD	3:L:959:ARG:NH2	2.75	0.60
3:I:1049:SER:HB2	3:I:1078:LEU:HB3	1.84	0.60
3:K:416:ILE:HD11	3:K:1207:ILE:HG21	1.83	0.60
3:L:521:MET:HB2	3:L:523:ASN:HB3	1.84	0.60
1:A:559:MET:HE1	1:A:737:CYS:H	1.67	0.60
3:H:542:THR:HG23	3:H:808:ALA:HB3	1.84	0.60
1:A:570:THR:HG21	1:A:1196:MET:HB3	1.83	0.59
3:D:242:ARG:HH12	3:D:1085:LEU:HD21	1.67	0.59
3:D:787:ARG:HH12	3:D:923:LEU:HA	1.66	0.59
3:G:940:GLN:HE21	3:G:944:ASN:HB3	1.67	0.59
3:C:616:SER:O	3:D:726:ARG:NH2	2.35	0.59
3:E:862:GLU:HG2	3:E:957:ILE:HD12	1.83	0.59
3:I:603:VAL:HG21	3:I:620:VAL:HG12	1.84	0.59
3:K:940:GLN:HE21	3:K:944:ASN:HB3	1.66	0.59
2:B:674:LEU:HD23	2:B:674:LEU:N	2.11	0.59
3:K:800:ILE:HG13	3:K:945:VAL:HG21	1.83	0.59
3:E:287:GLN:NE2	3:E:1106:LYS:O	2.35	0.59
3:H:199:GLY:O	3:H:1196:ARG:NH2	2.35	0.59
3:H:1048:PRO:HA	3:H:1077:GLU:HB2	1.85	0.59
3:H:404:MET:SD	3:H:959:ARG:NH2	2.75	0.59
3:I:315:SER:HB2	3:I:331:ARG:HD2	1.84	0.59
3:K:1091:GLN:NE2	3:K:1127:CYS:SG	2.76	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ILE:O	1:A:541:GLN:NE2	2.35	0.59
3:L:241:ASN:HD22	3:L:1148:SER:HB3	1.67	0.59
1:A:107:LEU:HB2	1:A:114:GLY:HA2	1.85	0.59
3:H:324:ILE:HG23	3:H:325:THR:HG23	1.84	0.59
2:B:336:ARG:NH1	2:B:369:THR:O	2.34	0.59
3:I:784:LEU:HD22	3:I:800:ILE:HG22	1.84	0.59
3:K:593:LEU:HD13	3:K:597:GLU:CB	2.33	0.59
3:K:1045:TRP:HB2	3:K:1074:VAL:HG12	1.84	0.59
2:B:654:SER:CA	2:B:672:PRO:CG	2.81	0.58
3:E:1053:GLN:HB3	3:E:1109:PRO:HA	1.85	0.58
3:F:407:ARG:NH1	3:F:440:ILE:O	2.36	0.58
3:H:995:PRO:HD2	3:H:1119:ILE:HG12	1.84	0.58
3:K:294:ARG:HB3	3:K:890:GLN:HB2	1.85	0.58
1:A:468:SER:HB2	1:A:522:GLY:H	1.68	0.58
3:D:629:GLN:HA	3:D:640:ARG:HH12	1.67	0.58
3:L:312:ASN:HB3	3:L:1196:ARG:HD3	1.84	0.58
3:J:119:CYS:SG	3:J:122:CYS:N	2.76	0.58
1:A:42:ARG:HG2	1:A:155:ARG:HE	1.66	0.58
2:B:397:PRO:O	2:B:535:GLN:NE2	2.36	0.58
3:C:762:THR:O	3:C:853:ARG:NH2	2.36	0.58
3:G:877:ALA:H	3:G:883:ARG:HH12	1.51	0.58
3:H:425:ASN:ND2	3:H:756:SER:OG	2.36	0.58
3:D:241:ASN:HD22	3:D:1148:SER:HB3	1.68	0.58
3:D:1170:PRO:HD2	3:D:1189:THR:HG23	1.86	0.58
3:H:511:ILE:HA	3:H:514:ILE:HG22	1.84	0.58
3:C:971:GLU:OE2	3:C:1168:ARG:NH1	2.36	0.58
3:E:237:GLU:HB3	3:E:1152:ALA:HB2	1.86	0.58
3:F:657:GLY:HA2	3:F:674:ARG:HA	1.86	0.58
3:D:389:GLU:OE2	3:D:1196:ARG:NH2	2.34	0.58
3:C:328:ARG:HG2	3:C:368:ILE:HG23	1.85	0.58
3:E:603:VAL:HG11	3:E:620:VAL:HG12	1.84	0.58
3:C:409:MET:HB2	3:C:445:PHE:H	1.68	0.57
3:D:404:MET:SD	3:D:959:ARG:NH2	2.77	0.57
3:I:705:ILE:HG21	3:I:737:ARG:HB2	1.86	0.57
3:K:1053:GLN:HB3	3:K:1109:PRO:HA	1.85	0.57
3:L:459:LEU:O	3:L:801:ARG:NH2	2.34	0.57
1:A:1229:MET:HE1	1:A:1267:LEU:HD12	1.86	0.57
2:B:254:LYS:HB3	3:C:336:ARG:HH12	1.70	0.57
2:B:461:LEU:HD12	2:B:462:ASP:HB2	1.85	0.57
3:F:500:ILE:HD13	3:F:732:VAL:HG22	1.86	0.57
3:G:705:ILE:HG21	3:G:737:ARG:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:542:THR:HG23	3:J:808:ALA:HB3	1.86	0.57
3:C:175:SER:OG	3:C:177:LYS:NZ	2.38	0.57
3:C:856:ARG:HH12	3:C:915:LEU:HD13	1.69	0.57
3:E:890:GLN:O	3:F:686:ARG:NH2	2.37	0.57
3:G:294:ARG:HB3	3:G:890:GLN:HB2	1.85	0.57
3:H:919:LEU:HD12	3:H:920:LEU:CB	2.34	0.57
1:A:1137:ALA:HA	1:A:1186:VAL:HG12	1.86	0.57
3:C:593:LEU:HD12	3:C:593:LEU:O	2.04	0.57
3:K:705:ILE:HG21	3:K:737:ARG:HB2	1.87	0.57
3:E:416:ILE:HD11	3:E:1207:ILE:HG21	1.85	0.57
2:B:655:ARG:HB3	2:B:671:ALA:HB3	1.87	0.57
3:K:760:SER:O	3:K:853:ARG:NH1	2.38	0.57
3:L:705:ILE:HG21	3:L:737:ARG:HB2	1.86	0.57
2:B:461:LEU:HD12	2:B:462:ASP:N	2.19	0.57
3:F:389:GLU:OE2	3:F:1196:ARG:NH2	2.36	0.57
3:J:1048:PRO:HA	3:J:1077:GLU:HB2	1.86	0.57
3:F:805:ALA:HB2	3:G:433:PRO:HB3	1.86	0.56
3:J:324:ILE:HG23	3:J:325:THR:HG23	1.87	0.56
3:K:513:GLU:OE1	3:K:516:ARG:NH1	2.38	0.56
3:K:784:LEU:HD22	3:K:800:ILE:HG22	1.88	0.56
3:C:165:ASP:O	3:C:168:ARG:NH2	2.38	0.56
3:E:1033:ASP:OD2	3:E:1039:ARG:NH1	2.38	0.56
3:F:242:ARG:HH12	3:F:1085:LEU:HD21	1.70	0.56
3:G:705:ILE:HG23	3:G:733:MET:HB3	1.86	0.56
3:G:890:GLN:O	3:H:686:ARG:NH2	2.38	0.56
1:A:1204:ILE:HG12	1:A:1238:THR:HG21	1.85	0.56
3:K:315:SER:HB2	3:K:331:ARG:HD2	1.87	0.56
3:L:324:ILE:HG23	3:L:325:THR:HG23	1.88	0.56
3:E:616:SER:O	3:F:726:ARG:NH2	2.39	0.56
3:I:527:ALA:HB1	3:I:813:VAL:HG13	1.87	0.56
3:F:705:ILE:HG21	3:F:737:ARG:HB2	1.88	0.56
3:H:371:LEU:HD11	3:H:388:MET:HE2	1.87	0.56
3:F:514:ILE:HA	3:F:517:LEU:HB3	1.88	0.56
3:I:518:LEU:HD23	3:I:820:VAL:HG22	1.88	0.56
3:C:195:ILE:HD12	3:C:257:ARG:HH11	1.71	0.56
3:C:1019:THR:HG22	3:D:1209:TYR:CG	2.38	0.56
3:F:571:LEU:HD11	3:F:705:ILE:HD11	1.88	0.56
3:G:413:PRO:HA	3:G:416:ILE:HG12	1.87	0.56
3:L:1048:PRO:HA	3:L:1077:GLU:HB2	1.87	0.56
3:C:439:THR:HB	3:C:1199:PHE:HA	1.88	0.56
3:F:1096:GLU:OE2	3:F:1132:ARG:NH2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:535:TRP:HH2	3:L:747:ILE:HD11	1.69	0.56
1:A:1120:SER:O	1:A:1182:GLN:NE2	2.39	0.55
2:B:256:THR:HG21	3:C:315:SER:HB3	1.88	0.55
3:D:723:ASP:OD1	3:D:726:ARG:NH2	2.39	0.55
3:I:723:ASP:OD1	3:I:726:ARG:NH2	2.40	0.55
3:J:257:ARG:NH1	3:J:309:LEU:O	2.37	0.55
3:C:506:GLN:NE2	3:E:501:SER:OG	2.39	0.55
3:C:1033:ASP:OD2	3:C:1039:ARG:NH1	2.39	0.55
3:J:245:CYS:HB3	3:J:263:LEU:HD12	1.88	0.55
3:K:616:SER:O	3:L:726:ARG:NH2	2.40	0.55
3:C:433:PRO:HB3	3:L:805:ALA:HB2	1.87	0.55
3:E:479:LEU:HD23	3:E:758:LEU:HD22	1.87	0.55
3:H:128:THR:HG22	3:H:130:SER:H	1.71	0.55
3:H:312:ASN:HB3	3:H:1196:ARG:HD3	1.87	0.55
3:C:684:LEU:HD22	3:C:753:THR:HG21	1.88	0.55
3:D:425:ASN:ND2	3:D:756:SER:OG	2.37	0.55
3:G:452:ARG:HE	3:G:668:LEU:HD23	1.71	0.55
3:J:995:PRO:HD2	3:J:1119:ILE:HG12	1.88	0.55
1:A:839:LEU:O	1:A:1096:ASN:ND2	2.40	0.55
3:F:1170:PRO:HD2	3:F:1189:THR:HG23	1.88	0.55
3:H:245:CYS:HB3	3:H:263:LEU:HD12	1.87	0.55
3:I:871:VAL:HG11	3:I:930:ARG:HA	1.88	0.55
3:K:1049:SER:HB2	3:K:1078:LEU:HB3	1.89	0.55
2:B:654:SER:CA	2:B:672:PRO:HG2	2.36	0.55
3:C:331:ARG:HH22	3:C:1196:ARG:HG3	1.71	0.55
3:D:439:THR:HB	3:D:1199:PHE:HD1	1.72	0.55
3:I:1012:ARG:NH1	3:I:1040:ASP:OD1	2.40	0.55
3:J:705:ILE:HG21	3:J:737:ARG:HB2	1.87	0.55
3:L:628:PRO:O	3:L:640:ARG:NH1	2.40	0.55
3:E:723:ASP:OD1	3:E:726:ARG:NH2	2.40	0.55
3:H:257:ARG:NH1	3:H:309:LEU:O	2.40	0.55
1:A:717:VAL:HG21	1:A:722:LEU:HD23	1.88	0.55
3:C:186:ALA:HB1	3:C:917:GLY:HA2	1.89	0.55
3:C:444:TRP:HB3	3:C:851:PHE:HB3	1.88	0.55
3:D:324:ILE:HG23	3:D:325:THR:HG23	1.88	0.55
3:F:425:ASN:ND2	3:F:756:SER:OG	2.38	0.55
3:H:514:ILE:HG12	3:H:518:LEU:HB2	1.88	0.55
3:I:616:SER:O	3:J:726:ARG:NH2	2.40	0.55
3:E:1046:VAL:HG13	3:E:1075:LEU:HD22	1.88	0.55
3:L:242:ARG:NH2	3:L:1087:TYR:OH	2.40	0.55
3:L:702:SER:OG	3:L:737:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1017:PHE:CB	3:C:1019:THR:HG23	2.37	0.55
3:H:705:ILE:HG21	3:H:737:ARG:HB2	1.88	0.55
3:E:684:LEU:HD22	3:E:753:THR:HG21	1.88	0.54
3:E:795:ASP:OD1	3:F:737:ARG:NH1	2.38	0.54
1:A:714:PRO:O	1:A:723:LYS:NZ	2.40	0.54
3:F:988:ALA:HA	3:F:1133:VAL:HG12	1.90	0.54
3:G:395:THR:HG22	3:G:399:ARG:HE	1.73	0.54
3:H:595:GLN:HB2	3:I:686:ARG:HB2	1.88	0.54
3:L:874:CYS:HB3	3:L:893:VAL:HG21	1.89	0.54
2:B:291:ASP:O	2:B:386:ALA:N	2.36	0.54
3:K:536:ALA:HA	3:K:768:GLN:HE21	1.72	0.54
3:D:316:THR:OG1	3:D:334:GLU:OE2	2.26	0.54
3:G:353:GLN:NE2	3:G:358:GLN:OE1	2.41	0.54
3:G:878:GLY:H	3:G:883:ARG:HH22	1.55	0.54
3:I:159:SER:O	3:I:519:GLN:NE2	2.41	0.54
3:K:195:ILE:HD12	3:K:257:ARG:HH11	1.73	0.54
3:L:625:PHE:O	3:L:647:ARG:NH2	2.40	0.54
3:C:595:GLN:HB3	3:E:738:GLN:HG3	1.90	0.54
2:B:668:VAL:HG23	2:B:691:VAL:HG21	1.89	0.54
3:D:193:LEU:O	3:D:402:TYR:OH	2.24	0.54
3:D:407:ARG:NH1	3:D:440:ILE:O	2.37	0.54
3:E:667:ASN:HB2	3:E:672:SER:HA	1.88	0.54
3:F:119:CYS:SG	3:F:122:CYS:N	2.76	0.54
3:J:389:GLU:OE2	3:J:1196:ARG:NH2	2.33	0.54
3:L:119:CYS:SG	3:L:122:CYS:N	2.80	0.54
2:B:352:MET:O	2:B:586:LYS:NZ	2.41	0.54
2:B:540:SER:HB3	2:B:578:PRO:HB2	1.90	0.54
3:E:485:PRO:HB3	3:E:831:LEU:HD21	1.89	0.54
3:G:1046:VAL:HA	3:G:1075:LEU:HB3	1.90	0.54
3:K:543:THR:O	3:K:576:THR:OG1	2.26	0.54
3:C:137:ARG:NH1	3:C:162:THR:OG1	2.40	0.54
3:D:705:ILE:HG21	3:D:737:ARG:HB2	1.90	0.54
3:E:626:LEU:HD21	3:E:776:GLN:HE21	1.73	0.54
3:H:1091:GLN:NE2	3:H:1127:CYS:SG	2.78	0.54
3:L:629:GLN:HA	3:L:640:ARG:HH12	1.72	0.54
2:B:432:GLU:H	2:B:688:THR:HG23	1.73	0.54
3:C:287:GLN:NE2	3:C:1108:ASN:OD1	2.40	0.54
3:F:384:MET:SD	3:F:1195:TYR:OH	2.62	0.54
3:K:1147:PHE:HE1	3:K:1169:TRP:HE1	1.56	0.54
3:D:593:LEU:HD13	3:D:597:GLU:OE2	2.08	0.53
3:G:620:VAL:HG11	3:H:718:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1147:PHE:HE1	3:G:1169:TRP:HE1	1.56	0.53
3:J:411:GLN:HB2	3:J:445:PHE:HB2	1.90	0.53
3:L:793:ARG:HD3	3:L:797:ALA:H	1.73	0.53
3:L:1170:PRO:HD2	3:L:1189:THR:HG23	1.89	0.53
1:A:133:ARG:HG3	1:A:675:SER:HB3	1.89	0.53
1:A:211:VAL:HA	1:A:216:ALA:HA	1.88	0.53
3:D:665:SER:OG	3:D:667:ASN:OD1	2.26	0.53
3:E:867:ALA:HB1	3:E:902:MET:HG3	1.90	0.53
3:K:1078:LEU:CD1	3:K:1081:TYR:HB3	2.37	0.53
1:A:163:VAL:O	1:A:846:ARG:NH2	2.42	0.53
3:C:187:VAL:HG13	3:C:856:ARG:HG3	1.91	0.53
3:I:257:ARG:HG2	3:I:310:LYS:HZ2	1.73	0.53
3:J:330:ILE:HD12	3:J:340:LEU:HD11	1.90	0.53
3:K:353:GLN:NE2	3:K:358:GLN:OE1	2.41	0.53
2:B:655:ARG:H	2:B:672:PRO:HD3	1.74	0.53
3:E:556:SER:OG	3:G:738:GLN:O	2.27	0.53
3:J:745:PHE:HE2	3:J:750:MET:HE3	1.74	0.53
1:A:618:VAL:HG12	3:C:471:PRO:HG3	1.91	0.53
3:C:1017:PHE:HB3	3:C:1019:THR:HG23	1.91	0.53
3:H:439:THR:HB	3:H:1199:PHE:HD1	1.73	0.53
3:H:593:LEU:HD12	3:H:597:GLU:HB2	1.84	0.53
3:I:260:GLU:OE1	3:I:262:ARG:NH2	2.41	0.53
3:I:982:LEU:HB3	3:I:1076:VAL:HB	1.90	0.53
3:L:193:LEU:O	3:L:402:TYR:OH	2.27	0.53
3:C:580:HIS:HD2	3:C:621:TRP:HE1	1.57	0.53
3:C:1046:VAL:HG13	3:C:1075:LEU:HD22	1.90	0.53
3:F:982:LEU:HD11	3:F:1115:VAL:HG11	1.90	0.53
3:I:294:ARG:HB3	3:I:890:GLN:HB2	1.90	0.53
3:J:657:GLY:HA2	3:J:674:ARG:HA	1.91	0.53
3:I:705:ILE:HG23	3:I:733:MET:HB3	1.90	0.53
3:J:460:VAL:HG11	3:J:923:LEU:HD12	1.90	0.53
3:E:392:ASP:N	3:E:392:ASP:OD1	2.37	0.53
3:H:578:ASP:HB3	3:H:581:SER:HB2	1.91	0.53
2:B:6:VAL:HG23	2:B:209:LEU:HD11	1.91	0.53
3:F:439:THR:HB	3:F:1199:PHE:HD1	1.74	0.53
3:G:431:THR:HB	3:G:1209:TYR:HB3	1.91	0.53
1:A:458:ARG:HH22	1:A:987:TYR:HB2	1.74	0.53
1:A:492:LYS:HE2	1:A:494:SER:HB2	1.91	0.53
2:B:629:LEU:HD13	2:B:698:ARG:HD3	1.90	0.53
3:E:543:THR:HG22	3:E:811:LEU:HB2	1.89	0.53
3:E:550:PHE:HA	3:E:569:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:745:PHE:HE2	3:L:750:MET:HE3	1.74	0.53
3:C:543:THR:O	3:C:576:THR:OG1	2.26	0.52
3:C:721:VAL:O	3:E:727:ARG:NH2	2.42	0.52
3:D:628:PRO:O	3:D:640:ARG:NH1	2.41	0.52
3:K:890:GLN:O	3:L:686:ARG:NH2	2.42	0.52
3:E:580:HIS:HD2	3:E:621:TRP:HE1	1.56	0.52
3:E:722:ASN:HB2	3:E:725:THR:HG22	1.91	0.52
3:H:665:SER:OG	3:H:667:ASN:OD1	2.27	0.52
3:I:441:LEU:HD23	3:I:443:PRO:HD3	1.90	0.52
3:I:940:GLN:HE21	3:I:944:ASN:HB3	1.74	0.52
3:J:392:ASP:OD1	3:J:392:ASP:N	2.39	0.52
1:A:285:LEU:O	1:A:357:ARG:NH2	2.43	0.52
2:B:287:LEU:HD21	2:B:318:PRO:HB3	1.91	0.52
3:E:417:VAL:HG11	3:E:432:ILE:HG12	1.91	0.52
3:L:571:LEU:HA	3:L:700:TRP:HE1	1.73	0.52
1:A:80:ARG:O	1:A:133:ARG:NH2	2.42	0.52
3:F:193:LEU:O	3:F:402:TYR:OH	2.26	0.52
3:G:196:GLU:HB3	3:G:313:LYS:HB2	1.91	0.52
3:G:260:GLU:OE1	3:G:262:ARG:NH2	2.43	0.52
3:L:542:THR:HG23	3:L:808:ALA:HB3	1.91	0.52
1:A:411:THR:O	1:A:418:ARG:NH1	2.40	0.52
3:C:890:GLN:O	3:D:686:ARG:NH2	2.42	0.52
3:H:564:TRP:NE1	3:H:729:MET:SD	2.80	0.52
3:H:1170:PRO:HD2	3:H:1189:THR:HG23	1.91	0.52
3:J:702:SER:OG	3:J:737:ARG:NH1	2.42	0.52
3:K:1078:LEU:HD11	3:K:1081:TYR:CD1	2.44	0.52
3:E:413:PRO:HB3	3:E:1207:ILE:HG23	1.91	0.52
3:F:392:ASP:OD1	3:F:392:ASP:N	2.41	0.52
3:F:745:PHE:HE2	3:F:750:MET:HE3	1.74	0.52
3:G:330:ILE:HG21	3:G:347:ARG:HD2	1.91	0.52
3:I:1053:GLN:HE21	3:I:1112:ILE:HG23	1.74	0.52
3:J:277:VAL:HG12	3:J:278:LEU:HG	1.91	0.52
3:K:884:PRO:HD3	3:K:962:GLN:HE22	1.75	0.52
3:L:425:ASN:ND2	3:L:756:SER:OG	2.42	0.52
3:L:631:ILE:O	3:L:640:ARG:NH1	2.43	0.52
1:A:181:ARG:NH1	1:A:250:MET:O	2.39	0.52
1:A:1161:MET:HE3	1:A:1165:GLU:HB3	1.90	0.52
2:B:666:MET:HE3	2:B:691:VAL:HG12	1.92	0.52
3:F:985:VAL:HG12	3:F:1073:ARG:HB3	1.92	0.52
3:J:413:PRO:HB2	3:J:434:ILE:HD13	1.91	0.52
3:L:139:ASP:OD1	3:L:158:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1170:PRO:HD2	3:C:1189:THR:HG23	1.92	0.52
3:F:593:LEU:HD13	3:F:597:GLU:HG2	1.85	0.52
3:F:937:ALA:HB2	3:F:947:ARG:HG3	1.92	0.52
2:B:297:GLU:HB3	2:B:379:HIS:HB2	1.92	0.52
3:C:626:LEU:HD21	3:C:776:GLN:HE21	1.75	0.52
3:E:394:LEU:HD11	3:E:964:VAL:HG22	1.92	0.52
3:I:1047:TYR:N	3:I:1075:LEU:O	2.39	0.52
3:K:527:ALA:HB1	3:K:813:VAL:HG13	1.92	0.52
3:L:906:ASN:ND2	3:L:921:ASP:OD1	2.42	0.52
3:C:353:GLN:NE2	3:C:358:GLN:OE1	2.43	0.52
3:C:982:LEU:HB3	3:C:1076:VAL:HB	1.92	0.52
3:E:353:GLN:NE2	3:E:358:GLN:OE1	2.43	0.52
3:F:985:VAL:HG22	3:F:1137:PHE:HE1	1.75	0.52
3:G:543:THR:HG22	3:G:811:LEU:HB2	1.92	0.52
3:G:616:SER:O	3:H:726:ARG:NH2	2.43	0.52
3:J:446:ALA:HB3	3:J:854:ASN:HD22	1.75	0.52
3:J:628:PRO:O	3:J:640:ARG:NH1	2.43	0.52
1:A:142:ALA:HB1	1:A:229:VAL:HG21	1.92	0.51
1:A:305:TRP:HE1	1:A:309:ARG:HA	1.73	0.51
2:B:288:PRO:HD2	2:B:594:MET:HE1	1.92	0.51
3:E:1046:VAL:HA	3:E:1075:LEU:HB3	1.92	0.51
3:G:459:LEU:HB3	3:G:807:PHE:HZ	1.75	0.51
3:E:535:TRP:O	3:E:768:GLN:NE2	2.38	0.51
3:F:510:PRO:HG2	3:F:511:ILE:HD12	1.93	0.51
3:G:906:ASN:ND2	3:G:921:ASP:OD1	2.43	0.51
3:H:452:ARG:NH2	3:H:948:GLU:OE1	2.43	0.51
3:H:464:SER:HB2	3:H:801:ARG:HG2	1.92	0.51
3:H:512:SER:O	3:H:516:ARG:NH1	2.43	0.51
3:H:571:LEU:HD11	3:H:705:ILE:HD11	1.92	0.51
3:I:196:GLU:HB3	3:I:313:LYS:HB2	1.92	0.51
3:D:454:GLN:HE21	3:D:857:ALA:HA	1.74	0.51
3:D:571:LEU:HD11	3:D:705:ILE:HD11	1.92	0.51
3:F:512:SER:O	3:F:516:ARG:NH1	2.43	0.51
3:J:250:ALA:HA	3:J:336:ARG:HH21	1.76	0.51
3:L:883:ARG:HB3	3:L:886:ASP:HB2	1.91	0.51
3:E:778:ASP:HA	3:E:940:GLN:HB3	1.91	0.51
3:G:928:ASP:HB2	3:H:740:LYS:HB2	1.93	0.51
3:H:250:ALA:HA	3:H:336:ARG:HH21	1.75	0.51
3:H:919:LEU:HD12	3:H:920:LEU:N	2.25	0.51
3:I:638:LEU:HD21	3:I:711:VAL:HG13	1.93	0.51
3:L:665:SER:OG	3:L:667:ASN:OD1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:GLY:O	2:B:548:ASN:ND2	2.43	0.51
3:D:587:MET:HE3	3:D:615:PHE:HE2	1.75	0.51
3:E:906:ASN:ND2	3:E:919:LEU:O	2.38	0.51
3:I:370:ARG:HA	3:I:387:CYS:HA	1.92	0.51
3:I:543:THR:O	3:I:576:THR:OG1	2.28	0.51
3:K:543:THR:HG22	3:K:811:LEU:HB2	1.93	0.51
3:L:446:ALA:HB3	3:L:854:ASN:HD22	1.74	0.51
2:B:416:THR:O	2:B:420:THR:OG1	2.27	0.51
3:C:593:LEU:HD13	3:C:597:GLU:HB2	1.92	0.51
3:C:758:LEU:HA	3:C:761:VAL:HG22	1.92	0.51
3:D:441:LEU:HG	3:D:443:PRO:HD3	1.91	0.51
3:E:246:MET:HA	3:E:262:ARG:HA	1.92	0.51
3:E:413:PRO:HA	3:E:416:ILE:HG12	1.92	0.51
3:G:982:LEU:HB3	3:G:1076:VAL:HB	1.93	0.51
3:K:1047:TYR:O	3:K:1077:GLU:N	2.41	0.51
1:A:465:ARG:HH21	1:A:536:PRO:HD3	1.75	0.51
1:A:1143:LYS:HE2	1:A:1174:SER:HA	1.93	0.51
3:E:401:THR:HG21	3:E:960:ALA:HB2	1.93	0.51
3:F:199:GLY:O	3:F:1196:ARG:NH2	2.40	0.51
3:G:769:VAL:HG11	3:G:780:ILE:HG21	1.93	0.51
3:C:392:ASP:OD1	3:C:392:ASP:N	2.40	0.51
3:L:454:GLN:HE21	3:L:857:ALA:HA	1.76	0.51
3:E:1013:VAL:O	3:E:1034:ASP:N	2.44	0.51
3:I:312:ASN:HB3	3:I:1196:ARG:HG2	1.92	0.51
3:J:483:VAL:HG21	3:J:758:LEU:HD11	1.92	0.51
3:L:245:CYS:HB3	3:L:263:LEU:HD12	1.93	0.51
3:C:446:ALA:H	3:C:854:ASN:HB3	1.76	0.51
3:C:1097:ALA:HB2	3:C:1135:TYR:HE2	1.76	0.51
3:E:972:MET:HB3	3:E:977:VAL:HG23	1.92	0.51
3:H:793:ARG:HD3	3:H:797:ALA:H	1.76	0.51
3:I:1147:PHE:HE1	3:I:1169:TRP:HE1	1.57	0.51
3:J:646:ILE:HG22	3:J:774:LEU:HD21	1.92	0.51
3:K:1053:GLN:HE21	3:K:1112:ILE:HG23	1.75	0.51
3:L:1085:LEU:HD13	3:L:1087:TYR:CZ	2.44	0.51
1:A:523:ILE:HD11	1:A:529:ARG:HB2	1.92	0.50
3:E:597:GLU:OE2	3:E:716:ASN:ND2	2.45	0.50
3:F:542:THR:HG23	3:F:808:ALA:HB3	1.92	0.50
3:G:567:LEU:HA	3:G:708:PHE:HE2	1.76	0.50
3:K:723:ASP:OD1	3:K:726:ARG:NH2	2.44	0.50
3:K:1012:ARG:NH1	3:K:1040:ASP:OD1	2.38	0.50
3:L:257:ARG:NH1	3:L:309:LEU:O	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:593:LEU:CD1	3:L:593:LEU:O	2.55	0.50
2:B:654:SER:HA	2:B:672:PRO:HG2	1.88	0.50
3:C:373:ARG:HG3	3:C:385:VAL:HG12	1.93	0.50
3:H:1106:LYS:HB2	3:H:1113:PRO:HG3	1.92	0.50
3:L:439:THR:HB	3:L:1199:PHE:HD1	1.76	0.50
3:L:985:VAL:HG12	3:L:1073:ARG:HB3	1.93	0.50
1:A:148:GLN:HE22	1:A:811:TYR:H	1.60	0.50
1:A:1071:HIS:HD2	1:A:1255:GLU:HG3	1.77	0.50
3:D:392:ASP:OD1	3:D:392:ASP:N	2.44	0.50
3:D:593:LEU:CD1	3:D:597:GLU:OE2	2.59	0.50
3:E:210:ILE:O	3:E:239:ALA:N	2.44	0.50
3:E:751:CYS:HA	3:E:754:GLU:HB3	1.93	0.50
3:H:424:ALA:HB2	3:H:845:PHE:HE2	1.76	0.50
3:F:593:LEU:HD12	3:F:597:GLU:HB2	1.83	0.50
3:F:788:VAL:O	3:F:793:ARG:NH2	2.45	0.50
3:I:223:THR:HA	3:I:1153:SER:HA	1.92	0.50
3:J:312:ASN:HB3	3:J:1196:ARG:HD3	1.92	0.50
3:L:571:LEU:HD11	3:L:705:ILE:HD11	1.94	0.50
1:A:696:GLU:OE2	1:A:700:ASN:ND2	2.42	0.50
1:A:1203:TYR:OH	1:A:1249:ARG:O	2.28	0.50
3:D:542:THR:HG23	3:D:808:ALA:HB3	1.93	0.50
3:D:586:PHE:HA	3:D:642:PHE:HE2	1.76	0.50
3:F:903:HIS:HD2	3:F:924:ALA:HB1	1.77	0.50
3:H:745:PHE:HE2	3:H:750:MET:HE3	1.76	0.50
3:H:874:CYS:HB3	3:H:893:VAL:HG21	1.94	0.50
3:K:412:ASP:N	3:K:412:ASP:OD1	2.42	0.50
3:L:198:THR:O	3:L:331:ARG:NH2	2.42	0.50
1:A:200:LYS:HD2	1:A:203:GLY:HA2	1.94	0.50
1:A:386:GLN:O	1:A:390:SER:N	2.43	0.50
3:G:1046:VAL:HG13	3:G:1075:LEU:HD22	1.93	0.50
3:I:167:ILE:HD12	3:I:523:ASN:HA	1.93	0.50
3:J:787:ARG:HB3	3:J:931:ILE:HG22	1.93	0.50
3:L:392:ASP:N	3:L:392:ASP:OD1	2.43	0.50
3:L:1106:LYS:HB2	3:L:1113:PRO:HG3	1.93	0.50
1:A:805:PRO:HB2	1:A:808:GLY:H	1.77	0.50
3:H:277:VAL:HG12	3:H:278:LEU:HG	1.94	0.50
3:L:176:SER:HA	3:L:179:LEU:HD13	1.93	0.50
1:A:67:SER:HB2	1:A:98:SER:HA	1.93	0.50
3:C:312:ASN:HB3	3:C:1196:ARG:HD2	1.94	0.50
3:C:413:PRO:HA	3:C:416:ILE:HG12	1.94	0.50
3:E:223:THR:HA	3:E:1153:SER:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:278:LEU:HD11	3:E:897:ALA:HA	1.93	0.50
3:H:603:VAL:HG21	3:H:620:VAL:HG13	1.93	0.50
3:I:493:LEU:HB2	3:I:824:CYS:HB2	1.92	0.50
3:J:805:ALA:HB2	3:K:433:PRO:HB3	1.94	0.50
3:J:985:VAL:HG22	3:J:1137:PHE:HE1	1.76	0.50
3:C:412:ASP:N	3:C:412:ASP:OD1	2.45	0.50
3:C:746:TYR:OH	3:C:754:GLU:OE2	2.24	0.50
3:D:543:THR:HA	3:D:811:LEU:HB3	1.93	0.50
3:K:438:PRO:HB2	3:K:439:THR:HG23	1.93	0.50
1:A:694:SER:HA	1:A:697:HIS:HD2	1.77	0.49
2:B:587:GLN:NE2	2:B:676:LEU:HD21	2.27	0.49
3:C:464:SER:HB2	3:D:500:ILE:HG22	1.94	0.49
3:H:446:ALA:HB3	3:H:854:ASN:HD22	1.75	0.49
3:J:793:ARG:HD3	3:J:797:ALA:H	1.76	0.49
3:J:1096:GLU:OE2	3:J:1132:ARG:NH2	2.36	0.49
3:K:928:ASP:HB2	3:L:740:LYS:HB2	1.93	0.49
1:A:469:SER:O	1:A:499:GLN:NE2	2.46	0.49
3:C:536:ALA:HB1	3:C:766:PRO:HB3	1.93	0.49
3:E:1052:LEU:HD21	3:E:1107:ILE:HD13	1.94	0.49
3:H:389:GLU:OE2	3:H:1196:ARG:NH2	2.36	0.49
3:I:769:VAL:HG11	3:I:780:ILE:HG21	1.94	0.49
3:J:198:THR:O	3:J:331:ARG:NH2	2.43	0.49
3:L:838:GLY:HA3	3:L:1210:VAL:HG23	1.93	0.49
3:F:1092:ILE:O	3:F:1132:ARG:NH1	2.44	0.49
3:H:985:VAL:HG12	3:H:1073:ARG:HB3	1.94	0.49
3:K:330:ILE:HG21	3:K:347:ARG:HD2	1.93	0.49
1:A:222:PRO:HG2	1:A:225:LYS:HB2	1.94	0.49
1:A:458:ARG:NH2	1:A:984:TYR:O	2.45	0.49
2:B:655:ARG:N	2:B:672:PRO:HD3	2.27	0.49
3:C:546:SER:OG	3:C:548:ASP:OD1	2.28	0.49
3:D:502:GLU:HB3	3:D:507:THR:HG21	1.95	0.49
3:F:324:ILE:HG23	3:F:325:THR:HG23	1.94	0.49
3:G:1049:SER:HB2	3:G:1078:LEU:HB3	1.95	0.49
3:H:787:ARG:HH12	3:H:923:LEU:HA	1.78	0.49
3:J:874:CYS:HB3	3:J:893:VAL:HG21	1.95	0.49
3:K:793:ARG:HH12	3:L:738:GLN:HG2	1.78	0.49
1:A:1223:ARG:NH1	3:G:506:GLN:O	2.45	0.49
3:I:438:PRO:HB2	3:I:439:THR:HG23	1.92	0.49
3:E:446:ALA:HB1	3:E:450:ASP:HB2	1.93	0.49
3:E:569:LEU:HD23	3:E:815:PRO:HG2	1.95	0.49
3:E:571:LEU:HD22	3:E:819:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:787:ARG:HB3	3:F:931:ILE:HG22	1.95	0.49
3:G:1013:VAL:O	3:G:1034:ASP:N	2.46	0.49
3:H:919:LEU:HD12	3:H:920:LEU:HB2	1.95	0.49
3:J:535:TRP:HH2	3:J:747:ILE:HD11	1.77	0.49
3:J:1138:THR:HG21	3:J:1142:ASN:HD22	1.78	0.49
3:K:1013:VAL:O	3:K:1034:ASP:N	2.46	0.49
3:C:663:GLN:NE2	3:C:854:ASN:OD1	2.46	0.49
3:D:199:GLY:O	3:D:1196:ARG:NH2	2.44	0.49
3:D:874:CYS:HB3	3:D:893:VAL:HG21	1.95	0.49
3:J:384:MET:SD	3:J:1195:TYR:OH	2.63	0.49
1:A:392:LEU:HD23	1:A:393:ARG:HE	1.78	0.49
3:C:769:VAL:HG11	3:C:780:ILE:HG21	1.95	0.49
3:D:861:ARG:HD2	3:D:953:GLY:H	1.78	0.49
3:E:389:GLU:OE2	3:E:1196:ARG:NH2	2.45	0.49
3:F:128:THR:HG22	3:F:130:SER:H	1.76	0.49
3:F:502:GLU:OE2	3:F:504:THR:OG1	2.30	0.49
3:H:462:ILE:HG21	3:H:540:LEU:HD11	1.95	0.49
3:H:805:ALA:HB2	3:I:433:PRO:HB3	1.94	0.49
3:I:1013:VAL:O	3:I:1034:ASP:N	2.46	0.49
3:J:193:LEU:O	3:J:402:TYR:OH	2.27	0.49
3:F:629:GLN:HA	3:F:640:ARG:HH12	1.78	0.49
3:G:441:LEU:HD23	3:G:443:PRO:HD3	1.94	0.49
3:H:702:SER:OG	3:H:737:ARG:NH1	2.46	0.49
3:I:394:LEU:HD11	3:I:964:VAL:HG22	1.93	0.49
3:J:603:VAL:HG13	3:J:606:MET:HB2	1.95	0.49
3:K:761:VAL:HG11	3:K:844:LEU:HD13	1.95	0.49
2:B:363:ARG:NH1	3:C:169:ILE:O	2.41	0.49
2:B:527:LEU:HD23	2:B:532:ILE:HD11	1.93	0.49
3:C:1088:TYR:OH	3:C:1132:ARG:NE	2.43	0.49
3:G:867:ALA:HB1	3:G:902:MET:HG3	1.94	0.49
3:G:895:SER:HA	3:G:930:ARG:HD2	1.94	0.49
3:H:1096:GLU:OE2	3:H:1132:ARG:NH2	2.35	0.49
3:I:546:SER:OG	3:I:548:ASP:OD1	2.31	0.49
3:L:128:THR:HG22	3:L:130:SER:H	1.78	0.49
3:D:787:ARG:HB3	3:D:931:ILE:HG22	1.95	0.48
3:F:120:ASN:HB2	3:F:136:LEU:HD11	1.95	0.48
3:F:446:ALA:HB3	3:F:854:ASN:HD22	1.78	0.48
3:F:498:THR:HA	3:F:501:SER:HB3	1.95	0.48
3:F:603:VAL:HG13	3:F:606:MET:HB2	1.95	0.48
3:G:394:LEU:HD11	3:G:964:VAL:HG22	1.94	0.48
3:G:1046:VAL:HG22	3:G:1075:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1170:PRO:HD2	3:J:1189:THR:HG23	1.95	0.48
3:K:452:ARG:HE	3:K:668:LEU:HD23	1.78	0.48
3:K:906:ASN:ND2	3:K:921:ASP:OD1	2.46	0.48
3:L:456:VAL:HG21	3:L:950:VAL:HG11	1.95	0.48
1:A:1078:ILE:HD11	1:A:1105:CYS:HB3	1.95	0.48
3:E:539:GLY:HA2	3:E:783:VAL:HG21	1.94	0.48
3:E:793:ARG:HG2	3:E:795:ASP:HB2	1.95	0.48
3:F:595:GLN:HB2	3:G:686:ARG:HB2	1.95	0.48
3:H:411:GLN:HB2	3:H:445:PHE:HB2	1.94	0.48
3:J:404:MET:SD	3:J:959:ARG:NH2	2.86	0.48
1:A:467:GLY:HA3	1:A:495:SER:HB2	1.94	0.48
1:A:469:SER:O	1:A:495:SER:OG	2.28	0.48
3:C:1211:ARG:HH11	3:L:552:ASP:HA	1.77	0.48
3:E:525:TYR:HE1	3:E:820:VAL:HG13	1.79	0.48
3:E:668:LEU:HD22	3:E:767:PHE:HE1	1.78	0.48
3:F:601:ILE:HG23	3:F:622:PRO:HB3	1.96	0.48
3:G:760:SER:O	3:G:853:ARG:NH1	2.46	0.48
3:H:603:VAL:HG13	3:H:606:MET:HB2	1.94	0.48
3:H:985:VAL:HG22	3:H:1137:PHE:HE1	1.78	0.48
3:J:294:ARG:HB3	3:J:890:GLN:HB2	1.95	0.48
3:J:595:GLN:HB2	3:K:686:ARG:HB2	1.95	0.48
3:C:827:THR:HG21	3:C:831:LEU:HD22	1.94	0.48
3:D:937:ALA:HB2	3:D:947:ARG:HG3	1.94	0.48
3:E:793:ARG:HH12	3:F:738:GLN:HA	1.78	0.48
3:E:985:VAL:HG22	3:E:1137:PHE:HE1	1.78	0.48
3:G:985:VAL:HG22	3:G:1137:PHE:HE1	1.78	0.48
3:K:705:ILE:HG23	3:K:733:MET:HB3	1.94	0.48
1:A:911:ASN:OD1	1:A:914:ARG:NH2	2.39	0.48
2:B:654:SER:CB	2:B:672:PRO:CG	2.85	0.48
3:C:543:THR:HG22	3:C:811:LEU:HB2	1.95	0.48
3:C:606:MET:HB3	3:C:615:PHE:HE1	1.77	0.48
3:G:638:LEU:HD21	3:G:711:VAL:HG13	1.95	0.48
3:H:628:PRO:O	3:H:640:ARG:NH1	2.47	0.48
3:J:547:GLU:O	3:K:1211:ARG:NH2	2.47	0.48
3:K:790:PRO:HG3	3:K:803:THR:HB	1.96	0.48
3:K:867:ALA:HB1	3:K:902:MET:HG3	1.95	0.48
1:A:386:GLN:HB2	1:A:389:MET:HB2	1.96	0.48
3:G:439:THR:O	3:G:1200:THR:N	2.45	0.48
3:H:937:ALA:HB2	3:H:947:ARG:HG3	1.96	0.48
3:I:595:GLN:HG2	3:K:738:GLN:HG2	1.94	0.48
3:J:586:PHE:HA	3:J:642:PHE:HE2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LEU:HA	1:A:475:ALA:HB3	1.94	0.48
3:C:320:ASP:OD2	3:C:325:THR:OG1	2.29	0.48
3:F:316:THR:OG1	3:F:334:GLU:OE2	2.31	0.48
3:F:938:TYR:HE2	3:F:940:GLN:HE21	1.62	0.48
3:I:1045:TRP:HB2	3:I:1074:VAL:HG12	1.95	0.48
3:J:903:HIS:HD2	3:J:924:ALA:HB1	1.78	0.48
3:L:530:LYS:HD3	3:L:811:LEU:HD21	1.96	0.48
1:A:841:TRP:NE1	1:A:1097:ASP:OD1	2.44	0.48
3:E:777:ASN:O	3:E:942:GLY:N	2.38	0.48
3:E:851:PHE:HA	3:E:854:ASN:HD22	1.78	0.48
3:E:1013:VAL:HG22	3:E:1046:VAL:HB	1.94	0.48
3:F:535:TRP:HH2	3:F:747:ILE:HD11	1.79	0.48
3:G:928:ASP:OD2	3:H:693:TYR:OH	2.25	0.48
3:H:193:LEU:O	3:H:402:TYR:OH	2.30	0.48
3:H:430:SER:HA	3:H:1208:MET:HA	1.95	0.48
3:H:828:GLU:HB3	3:H:831:LEU:HB2	1.96	0.48
3:C:394:LEU:HD11	3:C:964:VAL:HG22	1.95	0.48
3:D:410:HIS:CD2	3:D:442:CYS:H	2.31	0.48
3:I:985:VAL:HG22	3:I:1137:PHE:HE1	1.79	0.48
3:J:1021:VAL:HG12	3:K:353:GLN:HB2	1.95	0.48
3:E:423:CYS:HA	3:E:659:GLY:HA2	1.96	0.48
3:E:895:SER:HA	3:E:930:ARG:HD2	1.96	0.48
3:G:246:MET:HA	3:G:262:ARG:HA	1.96	0.48
3:G:1066:MET:HE1	3:G:1071:ARG:HE	1.79	0.48
3:I:928:ASP:HB2	3:J:740:LYS:HB2	1.96	0.48
3:K:413:PRO:HA	3:K:416:ILE:HG12	1.96	0.48
3:L:982:LEU:HB3	3:L:1076:VAL:HB	1.96	0.48
1:A:716:HIS:HD1	1:A:765:CYS:HG	1.61	0.47
3:C:141:ARG:HA	3:C:154:ASN:HB3	1.96	0.47
3:D:237:GLU:HA	3:D:1151:ALA:HB3	1.96	0.47
3:E:315:SER:HB2	3:E:331:ARG:HD2	1.96	0.47
3:F:374:ALA:HB1	3:F:377:ILE:HD11	1.95	0.47
3:H:551:PRO:HB2	3:H:592:LEU:HD21	1.96	0.47
3:I:392:ASP:N	3:I:392:ASP:OD1	2.47	0.47
3:L:202:THR:HG22	3:L:391:CYS:HA	1.96	0.47
1:A:883:PRO:HG3	1:A:897:CYS:HA	1.96	0.47
2:B:437:ILE:HB	2:B:519:ALA:HA	1.96	0.47
3:C:686:ARG:HG2	3:C:834:SER:HB3	1.94	0.47
3:G:234:PRO:HG3	3:G:348:ALA:HB2	1.96	0.47
3:G:546:SER:OG	3:G:548:ASP:OD1	2.31	0.47
3:G:873:GLN:NE2	3:G:882:PRO:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:596:PRO:HD3	3:I:687:LEU:HD21	1.96	0.47
3:I:567:LEU:HA	3:I:708:PHE:HE2	1.79	0.47
3:I:863:ALA:HB1	3:I:920:LEU:HD22	1.95	0.47
3:K:257:ARG:HG2	3:K:310:LYS:HZ1	1.79	0.47
3:F:793:ARG:HD3	3:F:797:ALA:H	1.79	0.47
3:I:401:THR:HG21	3:I:960:ALA:HB2	1.96	0.47
3:C:985:VAL:HG22	3:C:1137:PHE:HE1	1.79	0.47
3:D:128:THR:HG22	3:D:130:SER:H	1.80	0.47
3:D:411:GLN:HB2	3:D:445:PHE:HB2	1.96	0.47
3:D:1138:THR:HG21	3:D:1142:ASN:HD22	1.78	0.47
3:E:1042:ALA:HA	3:E:1072:THR:HB	1.96	0.47
3:F:1021:VAL:HG12	3:G:353:GLN:HB2	1.96	0.47
3:J:665:SER:OG	3:J:667:ASN:OD1	2.29	0.47
3:K:862:GLU:HB3	3:K:957:ILE:HD12	1.96	0.47
3:L:222:PHE:HE1	3:L:351:PRO:HD3	1.79	0.47
1:A:168:ARG:NH2	1:A:177:GLN:O	2.36	0.47
3:C:204:PHE:HE1	3:C:975:PHE:HE1	1.62	0.47
3:C:723:ASP:OD1	3:C:726:ARG:NH2	2.47	0.47
3:G:543:THR:O	3:G:576:THR:OG1	2.31	0.47
1:A:633:VAL:HG12	1:A:645:ARG:HB3	1.95	0.47
3:D:958:HIS:CE1	3:D:962:GLN:HE21	2.33	0.47
3:E:1042:ALA:HB2	3:E:1066:MET:HE2	1.95	0.47
3:F:578:ASP:HB3	3:F:581:SER:HB2	1.95	0.47
3:F:743:THR:OG1	3:F:822:MET:O	2.33	0.47
3:G:204:PHE:HE2	3:G:1188:ILE:HG21	1.80	0.47
3:I:431:THR:HB	3:I:1209:TYR:HB3	1.96	0.47
3:K:439:THR:O	3:K:1200:THR:N	2.44	0.47
3:K:769:VAL:HG11	3:K:780:ILE:HG21	1.97	0.47
3:L:222:PHE:HE2	3:L:348:ALA:HB1	1.79	0.47
3:F:156:ALA:H	3:F:848:ASN:HD22	1.62	0.47
3:F:463:SER:OG	3:F:464:SER:N	2.44	0.47
3:F:625:PHE:O	3:F:647:ARG:NH2	2.47	0.47
3:G:723:ASP:OD1	3:G:726:ARG:NH2	2.48	0.47
3:H:392:ASP:OD1	3:H:392:ASP:N	2.46	0.47
3:H:958:HIS:CE1	3:H:962:GLN:HE21	2.32	0.47
3:I:237:GLU:HB3	3:I:1152:ALA:HB2	1.96	0.47
3:I:238:GLY:H	3:I:1151:ALA:HB3	1.80	0.47
3:I:330:ILE:HG21	3:I:347:ARG:HD2	1.97	0.47
3:I:373:ARG:HG3	3:I:385:VAL:HG12	1.97	0.47
3:I:867:ALA:HB1	3:I:902:MET:HG3	1.97	0.47
3:J:618:PRO:O	3:J:776:GLN:NE2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:417:VAL:O	3:K:421:ASN:ND2	2.48	0.47
3:K:650:TRP:HD1	3:K:773:ARG:HG3	1.80	0.47
3:L:384:MET:SD	3:L:1195:TYR:OH	2.67	0.47
3:L:413:PRO:HB2	3:L:434:ILE:HD13	1.97	0.47
3:L:1085:LEU:CD1	3:L:1087:TYR:CZ	2.98	0.47
1:A:353:ILE:O	1:A:357:ARG:N	2.46	0.47
2:B:645:THR:HA	2:B:648:ILE:HG22	1.97	0.47
3:E:196:GLU:HB3	3:E:313:LYS:HB2	1.96	0.47
3:F:488:LEU:HA	3:F:825:GLY:HA2	1.96	0.47
3:G:646:ILE:HG22	3:G:774:LEU:HD21	1.95	0.47
3:G:650:TRP:HD1	3:G:773:ARG:HG3	1.78	0.47
3:J:439:THR:HB	3:J:1199:PHE:HD1	1.80	0.47
3:K:395:THR:HG22	3:K:399:ARG:HE	1.80	0.47
3:L:274:TYR:OH	3:L:975:PHE:O	2.28	0.47
1:A:601:TYR:HA	1:A:605:LEU:HB2	1.96	0.47
2:B:11:HIS:HB2	2:B:391:ILE:HD12	1.97	0.47
3:E:234:PRO:HG3	3:E:348:ALA:HB2	1.96	0.47
3:E:328:ARG:HG2	3:E:368:ILE:HG23	1.95	0.47
3:H:210:ILE:HB	3:H:239:ALA:HB3	1.97	0.47
3:H:601:ILE:HG22	3:H:603:VAL:HG12	1.97	0.47
3:L:603:VAL:HG13	3:L:606:MET:HB2	1.97	0.47
3:D:424:ALA:HB2	3:D:845:PHE:HE2	1.80	0.47
3:D:535:TRP:HH2	3:D:747:ILE:HD11	1.80	0.47
3:E:250:ALA:HB1	3:E:339:LEU:HD21	1.97	0.47
3:J:274:TYR:OH	3:J:975:PHE:O	2.29	0.47
3:K:394:LEU:HD11	3:K:964:VAL:HG22	1.96	0.47
3:L:371:LEU:HD11	3:L:388:MET:HE2	1.96	0.47
3:L:777:ASN:O	3:L:942:GLY:N	2.45	0.47
1:A:589:ASN:OD1	1:A:589:ASN:N	2.46	0.46
1:A:777:TYR:HB3	1:A:779:ILE:HG13	1.96	0.46
2:B:669:GLU:CD	2:B:670:TYR:N	2.73	0.46
3:C:128:THR:HG22	3:C:130:SER:H	1.80	0.46
3:C:888:LEU:HA	3:C:1080:HIS:HD2	1.80	0.46
1:A:491:VAL:HG11	1:A:977:ILE:HG21	1.96	0.46
3:C:658:TYR:HE1	3:C:667:ASN:HD21	1.63	0.46
3:D:305:THR:HA	3:D:398:ILE:HD13	1.97	0.46
3:F:378:GLY:HA3	3:F:437:ARG:HH22	1.80	0.46
3:I:1170:PRO:HD2	3:I:1189:THR:HG23	1.96	0.46
3:L:599:ILE:HD11	3:L:631:ILE:HG12	1.97	0.46
1:A:40:GLN:HE21	1:A:44:LEU:HB3	1.79	0.46
1:A:262:TYR:HE1	1:A:379:SER:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:199:GLY:O	3:C:1196:ARG:NH2	2.47	0.46
3:F:667:ASN:ND2	3:F:671:PRO:O	2.48	0.46
3:G:344:TYR:HB3	3:G:368:ILE:HD11	1.98	0.46
3:G:862:GLU:HB3	3:G:957:ILE:HD12	1.97	0.46
3:H:129:MET:O	3:H:133:SER:N	2.45	0.46
3:H:563:MET:O	3:H:567:LEU:N	2.48	0.46
3:L:199:GLY:O	3:L:1196:ARG:NH2	2.45	0.46
1:A:474:PHE:CE1	2:B:675:PRO:HG3	2.50	0.46
3:C:593:LEU:HD13	3:C:597:GLU:CB	2.45	0.46
3:C:1013:VAL:O	3:C:1034:ASP:N	2.48	0.46
3:D:988:ALA:O	3:D:1131:ARG:NH1	2.49	0.46
3:D:1047:TYR:N	3:D:1075:LEU:O	2.45	0.46
3:G:312:ASN:HB3	3:G:1196:ARG:HG2	1.96	0.46
3:J:1103:TRP:CD1	3:J:1113:PRO:HG2	2.50	0.46
3:K:287:GLN:NE2	3:K:1106:LYS:O	2.48	0.46
3:K:697:MET:HG2	3:K:744:PRO:HA	1.98	0.46
3:L:787:ARG:HB3	3:L:931:ILE:HG22	1.97	0.46
2:B:285:SER:HA	2:B:393:VAL:HB	1.97	0.46
2:B:396:SER:OG	2:B:398:ALA:O	2.34	0.46
2:B:399:MET:N	2:B:535:GLN:OE1	2.40	0.46
2:B:637:TYR:HB2	2:B:684:LEU:HB3	1.98	0.46
3:C:884:PRO:HD3	3:C:962:GLN:HE22	1.81	0.46
3:D:252:LEU:HD11	3:D:335:GLY:HA3	1.98	0.46
3:D:1106:LYS:HB2	3:D:1113:PRO:HG3	1.96	0.46
3:E:364:ILE:HG13	3:E:367:ARG:HE	1.80	0.46
3:E:441:LEU:HD23	3:E:443:PRO:HD3	1.97	0.46
3:F:252:LEU:HD11	3:F:335:GLY:HA3	1.98	0.46
3:F:551:PRO:HB2	3:F:592:LEU:HD21	1.96	0.46
3:I:650:TRP:HD1	3:I:773:ARG:HG3	1.81	0.46
3:J:988:ALA:HA	3:J:1133:VAL:HG12	1.98	0.46
3:K:234:PRO:HG3	3:K:348:ALA:HB2	1.97	0.46
3:K:638:LEU:HD21	3:K:711:VAL:HG13	1.96	0.46
3:L:568:PHE:HE1	3:L:736:MET:HE1	1.79	0.46
2:B:24:ASP:HB3	2:B:27:LEU:HD13	1.97	0.46
3:C:476:LEU:O	3:C:480:LEU:N	2.49	0.46
3:D:242:ARG:NH2	3:D:1087:TYR:OH	2.49	0.46
3:D:981:ASN:HB3	3:D:1075:LEU:HD11	1.96	0.46
3:E:370:ARG:HA	3:E:387:CYS:HA	1.97	0.46
3:I:456:VAL:HG21	3:I:950:VAL:HG11	1.98	0.46
3:J:120:ASN:HB2	3:J:136:LEU:HD11	1.97	0.46
3:K:425:ASN:HD21	3:K:756:SER:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:SER:HA	2:B:390:ILE:HB	1.97	0.46
2:B:588:LEU:HD22	2:B:687:VAL:HG13	1.98	0.46
3:C:442:CYS:HB2	3:C:444:TRP:CZ3	2.51	0.46
3:D:312:ASN:HB3	3:D:1196:ARG:HD3	1.98	0.46
3:D:1103:TRP:CD1	3:D:1113:PRO:HG2	2.51	0.46
3:E:161:LEU:O	3:E:165:ASP:N	2.41	0.46
3:G:464:SER:HB2	3:H:500:ILE:HG22	1.97	0.46
3:K:995:PRO:HD2	3:K:1119:ILE:HG12	1.98	0.46
1:A:722:LEU:HD21	1:A:762:LEU:HB2	1.98	0.46
3:D:384:MET:SD	3:D:1195:TYR:OH	2.64	0.46
3:D:1030:GLN:HG3	3:D:1038:PRO:HB2	1.98	0.46
3:E:219:LEU:N	3:E:1125:TYR:OH	2.43	0.46
3:E:412:ASP:OD1	3:E:412:ASP:N	2.47	0.46
3:F:514:ILE:HG12	3:F:518:LEU:HB2	1.98	0.46
3:G:259:LEU:HD23	3:G:911:THR:HB	1.96	0.46
3:H:657:GLY:HA2	3:H:674:ARG:HA	1.97	0.46
3:I:234:PRO:HG3	3:I:348:ALA:HB2	1.97	0.46
1:A:1182:GLN:HG2	1:A:1185:ARG:HH21	1.81	0.46
2:B:669:GLU:OE1	2:B:670:TYR:N	2.49	0.46
3:D:260:GLU:OE1	3:D:262:ARG:NH2	2.49	0.46
3:E:985:VAL:HG12	3:E:1073:ARG:HB3	1.98	0.46
3:G:493:LEU:HB2	3:G:824:CYS:HB2	1.98	0.46
3:H:601:ILE:HG23	3:H:622:PRO:HB3	1.97	0.46
1:A:548:HIS:CE1	1:A:696:GLU:HG3	2.51	0.46
2:B:292:ILE:HG22	2:B:314:ILE:HB	1.98	0.46
2:B:675:PRO:HD2	2:B:678:SER:HB2	1.98	0.46
3:C:234:PRO:HG3	3:C:348:ALA:HB2	1.98	0.46
3:C:928:ASP:HB2	3:D:740:LYS:HB2	1.97	0.46
3:F:460:VAL:HG11	3:F:923:LEU:HD12	1.97	0.46
3:I:275:LYS:HZ2	3:I:285:ASN:HA	1.81	0.46
1:A:1074:LEU:HD21	1:A:1241:ALA:HA	1.98	0.45
3:C:650:TRP:HD1	3:C:773:ARG:HG3	1.81	0.45
3:D:745:PHE:HE2	3:D:750:MET:HE3	1.81	0.45
3:E:167:ILE:HD12	3:E:170:LEU:HD12	1.98	0.45
3:E:527:ALA:HB1	3:E:813:VAL:HG13	1.97	0.45
3:G:373:ARG:HG3	3:G:385:VAL:HG12	1.98	0.45
3:I:260:GLU:HG2	3:I:307:SER:HB2	1.98	0.45
3:J:861:ARG:HD2	3:J:953:GLY:H	1.80	0.45
2:B:352:MET:HE1	2:B:589:PHE:HB2	1.97	0.45
3:D:805:ALA:HB2	3:E:433:PRO:HB3	1.98	0.45
3:F:242:ARG:NH2	3:F:1087:TYR:OH	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1012:ARG:HH11	3:I:1039:ARG:HB3	1.81	0.45
2:B:21:ASN:HB3	2:B:390:ILE:HG13	1.97	0.45
3:C:456:VAL:HG11	3:C:934:LEU:HB3	1.98	0.45
3:D:371:LEU:HD11	3:D:388:MET:HE2	1.97	0.45
3:E:174:VAL:HG21	3:E:471:PRO:HG3	1.98	0.45
3:E:489:ASP:OD2	3:E:826:GLN:NE2	2.39	0.45
3:E:1006:ARG:NH1	3:E:1077:GLU:OE1	2.49	0.45
3:G:722:ASN:HB3	3:G:725:THR:HG22	1.99	0.45
3:K:392:ASP:OD1	3:K:392:ASP:N	2.48	0.45
1:A:533:SER:HB3	1:A:669:VAL:HA	1.98	0.45
3:C:237:GLU:HA	3:C:1151:ALA:HB3	1.98	0.45
3:C:802:ALA:O	3:D:737:ARG:NH2	2.49	0.45
3:E:197:ASP:OD2	3:E:399:ARG:NH1	2.49	0.45
3:J:188:ALA:HB3	3:J:763:VAL:HG11	1.98	0.45
3:L:1138:THR:HG21	3:L:1142:ASN:HD22	1.81	0.45
1:A:1249:ARG:HD3	3:E:156:ALA:HB2	1.99	0.45
2:B:321:LEU:HD11	2:B:348:LEU:HB3	1.99	0.45
3:C:401:THR:HG21	3:C:960:ALA:HB2	1.99	0.45
3:C:656:PHE:HB3	3:C:681:ASN:HD21	1.82	0.45
3:D:712:VAL:HA	3:D:717:MET:HG3	1.98	0.45
3:E:260:GLU:OE1	3:E:262:ARG:NH2	2.50	0.45
3:F:328:ARG:NH2	3:F:366:ASP:OD1	2.49	0.45
3:F:558:THR:O	3:F:720:THR:OG1	2.32	0.45
3:G:237:GLU:HA	3:G:1151:ALA:HB3	1.97	0.45
3:G:336:ARG:HD2	3:G:339:LEU:HD22	1.99	0.45
3:H:241:ASN:HD22	3:H:1148:SER:HB3	1.81	0.45
3:I:536:ALA:HB1	3:I:766:PRO:HB3	1.97	0.45
3:L:723:ASP:OD1	3:L:726:ARG:NH2	2.50	0.45
1:A:292:ARG:NH2	1:A:330:SER:OG	2.49	0.45
3:E:1123:GLN:HB2	3:E:1158:PHE:HB3	1.98	0.45
3:F:593:LEU:CD1	3:F:593:LEU:O	2.63	0.45
3:F:1053:GLN:HB3	3:F:1109:PRO:HA	1.98	0.45
3:F:1138:THR:HG21	3:F:1142:ASN:HD22	1.82	0.45
3:I:395:THR:HG22	3:I:399:ARG:HE	1.81	0.45
3:L:793:ARG:HG2	3:L:796:ALA:HA	1.97	0.45
3:L:1053:GLN:HB3	3:L:1109:PRO:HA	1.97	0.45
1:A:743:ILE:HG12	1:A:787:TYR:HD1	1.82	0.45
3:E:221:GLY:O	3:E:224:TRP:NE1	2.50	0.45
3:G:995:PRO:HD2	3:G:1119:ILE:HG12	1.98	0.45
3:J:838:GLY:HA3	3:J:1210:VAL:HG23	1.99	0.45
1:A:320:THR:HA	3:E:481:ARG:HH12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:PHE:HD2	2:B:531:ASN:HB3	1.82	0.45
3:E:743:THR:HG21	3:E:822:MET:HA	1.98	0.45
3:H:903:HIS:HD2	3:H:924:ALA:HB1	1.82	0.45
3:H:1138:THR:HG21	3:H:1142:ASN:HD22	1.82	0.45
3:I:193:LEU:O	3:I:402:TYR:OH	2.29	0.45
3:L:1103:TRP:CD1	3:L:1113:PRO:HG2	2.52	0.45
1:A:346:LEU:HB3	1:A:349:ILE:HD12	1.98	0.45
3:C:413:PRO:HB3	3:C:1207:ILE:HG23	1.99	0.45
3:D:611:PRO:HD3	3:E:429:ASN:HB2	1.98	0.45
3:F:601:ILE:HG22	3:F:603:VAL:HG12	1.98	0.45
3:I:758:LEU:HA	3:I:761:VAL:HG22	1.98	0.45
3:K:973:ASN:HB2	3:K:1144:ASP:HB3	1.99	0.45
3:L:601:ILE:HG22	3:L:603:VAL:HG12	1.99	0.45
3:C:657:GLY:HA2	3:C:674:ARG:HA	1.99	0.45
3:C:705:ILE:HG23	3:C:733:MET:HB3	1.98	0.45
3:D:838:GLY:HA3	3:D:1210:VAL:HG23	1.99	0.45
3:F:257:ARG:NH1	3:F:309:LEU:O	2.44	0.45
3:F:702:SER:OG	3:F:737:ARG:NH1	2.50	0.45
3:I:969:MET:O	3:I:979:ARG:NH2	2.50	0.45
3:J:571:LEU:HD11	3:J:705:ILE:HD11	1.99	0.45
3:J:899:ALA:O	3:J:903:HIS:N	2.45	0.45
3:J:985:VAL:HG12	3:J:1073:ARG:HB3	1.99	0.45
2:B:407:THR:HG22	2:B:521:ALA:HB3	1.99	0.44
3:C:354:THR:HG22	3:C:356:ASN:H	1.83	0.44
3:E:193:LEU:O	3:E:402:TYR:OH	2.26	0.44
3:H:743:THR:OG1	3:H:822:MET:O	2.34	0.44
3:J:26:ASP:O	3:J:30:THR:OG1	2.29	0.44
3:J:237:GLU:HB3	3:J:1152:ALA:HB2	1.98	0.44
1:A:729:MET:HA	1:A:734:ASN:HD22	1.81	0.44
2:B:233:LEU:HD22	3:C:192:GLU:HG2	1.98	0.44
3:C:995:PRO:HD2	3:C:1119:ILE:HG12	1.97	0.44
3:D:654:SER:HB3	3:D:680:PRO:HA	1.99	0.44
3:F:665:SER:OG	3:F:667:ASN:OD1	2.29	0.44
3:F:903:HIS:CD2	3:F:924:ALA:HB1	2.53	0.44
3:F:1103:TRP:CD1	3:F:1113:PRO:HG2	2.53	0.44
3:H:242:ARG:NH2	3:H:1087:TYR:OH	2.50	0.44
3:J:650:TRP:HD1	3:J:773:ARG:HG3	1.82	0.44
3:L:937:ALA:HB2	3:L:947:ARG:HG3	1.98	0.44
3:C:984:LEU:HB2	3:C:1074:VAL:HG13	1.98	0.44
3:D:271:VAL:HG23	3:D:288:PHE:HB3	1.99	0.44
3:F:330:ILE:HD12	3:F:340:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:595:GLN:OE1	3:I:686:ARG:N	2.50	0.44
3:I:656:PHE:HB3	3:I:681:ASN:HD22	1.83	0.44
3:J:413:PRO:HG2	3:J:440:ILE:HD11	1.99	0.44
3:J:514:ILE:HA	3:J:517:LEU:HB2	1.99	0.44
3:J:530:LYS:HD3	3:J:811:LEU:HD21	1.99	0.44
3:K:983:TYR:HE2	3:K:1139:SER:HB3	1.82	0.44
2:B:357:THR:HG22	2:B:364:SER:HA	1.98	0.44
3:D:883:ARG:HB3	3:D:886:ASP:HB2	1.98	0.44
3:E:493:LEU:HD13	3:E:820:VAL:HA	2.00	0.44
3:E:543:THR:O	3:E:576:THR:OG1	2.35	0.44
3:F:26:ASP:O	3:F:30:THR:OG1	2.30	0.44
3:J:788:VAL:HG23	3:J:932:ALA:HB3	1.99	0.44
3:L:277:VAL:HG12	3:L:278:LEU:HG	1.98	0.44
3:L:816:ALA:HA	3:L:819:VAL:HG12	1.99	0.44
1:A:477:LYS:HG3	1:A:478:VAL:HG13	1.99	0.44
1:A:1182:GLN:HA	1:A:1185:ARG:HE	1.82	0.44
3:C:245:CYS:HB3	3:C:263:LEU:HD13	2.00	0.44
3:D:446:ALA:HB3	3:D:854:ASN:HD22	1.81	0.44
3:D:601:ILE:HG22	3:D:603:VAL:HG12	2.00	0.44
3:D:758:LEU:HA	3:D:761:VAL:HG22	2.00	0.44
3:L:784:LEU:HD13	3:L:939:LEU:HD13	2.00	0.44
3:G:479:LEU:HD23	3:G:758:LEU:HD22	1.98	0.44
3:G:973:ASN:HB2	3:G:1144:ASP:HB2	2.00	0.44
3:H:1078:LEU:HD22	3:H:1081:TYR:HB3	1.99	0.44
3:J:439:THR:HB	3:J:1199:PHE:HA	2.00	0.44
3:L:260:GLU:OE1	3:L:262:ARG:NH2	2.51	0.44
1:A:123:ASP:O	1:A:127:LEU:N	2.41	0.44
3:C:330:ILE:HD11	3:C:340:LEU:HD11	1.99	0.44
3:C:746:TYR:HD1	3:C:750:MET:HE3	1.83	0.44
3:D:543:THR:HG23	3:D:577:SER:H	1.83	0.44
3:E:650:TRP:HD1	3:E:773:ARG:HG3	1.83	0.44
3:G:595:GLN:HG2	3:I:738:GLN:HG2	1.99	0.44
3:I:195:ILE:HD12	3:I:257:ARG:HH11	1.82	0.44
3:I:995:PRO:HD2	3:I:1119:ILE:HG12	1.99	0.44
3:J:705:ILE:HG23	3:J:733:MET:HB3	2.00	0.44
3:J:1053:GLN:HB3	3:J:1109:PRO:HA	1.99	0.44
3:L:861:ARG:NH1	3:L:954:PRO:O	2.50	0.44
3:D:245:CYS:HB3	3:D:263:LEU:HD12	2.00	0.44
3:G:317:PHE:HD2	3:G:373:ARG:HH21	1.64	0.44
3:I:452:ARG:HE	3:I:668:LEU:HD23	1.82	0.44
3:K:238:GLY:H	3:K:1151:ALA:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1019:THR:HG23	3:K:1032:ILE:HB	2.00	0.44
3:L:593:LEU:HB2	3:L:596:PRO:HG2	1.99	0.44
3:L:641:ALA:O	3:L:645:HIS:N	2.50	0.44
1:A:706:GLU:HB2	1:A:731:ILE:HD13	1.99	0.44
2:B:608:VAL:HG13	2:B:630:GLU:HB2	2.00	0.44
3:D:641:ALA:O	3:D:645:HIS:N	2.49	0.44
3:E:203:SER:HB3	3:E:247:THR:HG22	1.99	0.44
3:E:670:ILE:HG12	3:E:676:VAL:HG13	2.00	0.44
3:G:412:ASP:OD1	3:G:412:ASP:N	2.50	0.44
3:G:819:VAL:HA	3:G:822:MET:HB3	1.99	0.44
3:H:903:HIS:CD2	3:H:924:ALA:HB1	2.53	0.44
3:J:995:PRO:HB3	3:J:1137:PHE:HA	2.00	0.44
1:A:281:VAL:HG11	1:A:341:LEU:HD21	1.99	0.43
1:A:1022:ASP:O	1:A:1026:LYS:N	2.51	0.43
3:D:985:VAL:HG22	3:D:1137:PHE:HE1	1.83	0.43
3:E:473:VAL:HG11	3:E:811:LEU:HD11	1.99	0.43
3:E:801:ARG:HG3	3:E:939:LEU:HD13	2.00	0.43
3:F:669:PHE:HD2	3:F:769:VAL:HG12	1.83	0.43
3:G:586:PHE:HA	3:G:642:PHE:HE2	1.83	0.43
3:G:1174:ASP:HB3	3:G:1177:TYR:HB2	2.00	0.43
3:I:287:GLN:NE2	3:I:1106:LYS:O	2.50	0.43
3:I:507:THR:HG21	3:K:153:ILE:HD13	1.99	0.43
1:A:322:LEU:HA	1:A:326:LEU:HD12	1.99	0.43
1:A:473:LYS:NZ	1:A:525:ASN:O	2.47	0.43
3:D:1104:LEU:HD23	3:D:1107:ILE:HD12	1.99	0.43
3:E:148:LEU:HG	3:E:150:THR:H	1.83	0.43
3:E:279:SER:HB3	3:E:283:ILE:HD11	2.01	0.43
3:E:294:ARG:NH2	3:E:874:CYS:O	2.49	0.43
3:F:305:THR:HA	3:F:398:ILE:HD13	2.00	0.43
3:F:828:GLU:HG2	3:F:830:ASN:H	1.81	0.43
3:F:1023:ARG:HA	3:F:1024:PRO:HD3	1.77	0.43
3:G:191:PRO:HB3	3:G:915:LEU:HD23	2.00	0.43
3:G:587:MET:HA	3:G:590:ALA:HB3	2.00	0.43
3:G:1016:ARG:HB3	3:H:1211:ARG:HG3	1.98	0.43
3:I:1150:ASN:HB3	3:I:1153:SER:HB3	2.01	0.43
1:A:145:GLN:OE1	1:A:384:VAL:N	2.48	0.43
2:B:456:GLU:O	2:B:460:ASN:ND2	2.51	0.43
2:B:475:SER:OG	2:B:477:THR:O	2.34	0.43
3:C:172:PRO:HB3	3:C:904:ALA:HB2	2.01	0.43
3:C:973:ASN:HB2	3:C:1144:ASP:HB3	2.00	0.43
3:D:511:ILE:HG22	3:D:515:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:277:VAL:HG12	3:F:278:LEU:HG	2.00	0.43
3:H:938:TYR:HE2	3:H:940:GLN:HE21	1.67	0.43
3:I:831:LEU:HD11	3:I:836:HIS:HB2	2.00	0.43
3:I:928:ASP:OD2	3:J:693:TYR:OH	2.26	0.43
3:I:971:GLU:HB3	3:I:974:LEU:HD13	2.00	0.43
3:J:593:LEU:CD1	3:J:593:LEU:O	2.63	0.43
3:K:871:VAL:HG11	3:K:930:ARG:HA	2.00	0.43
1:A:48:LEU:HA	1:A:51:HIS:HD2	1.83	0.43
1:A:300:ALA:O	1:A:320:THR:N	2.49	0.43
2:B:268:LEU:HD12	2:B:329:GLU:HB3	2.00	0.43
2:B:362:ARG:HH12	3:C:914:ASP:HB2	1.83	0.43
2:B:604:LYS:HG3	2:B:637:TYR:HE1	1.84	0.43
3:I:1088:TYR:OH	3:I:1134:HIS:NE2	2.52	0.43
3:I:1149:THR:HB	3:I:1162:ALA:HB3	2.01	0.43
3:J:601:ILE:HG22	3:J:603:VAL:HG12	2.00	0.43
3:K:646:ILE:HG22	3:K:774:LEU:HD21	2.00	0.43
3:L:298:LEU:HD21	3:L:870:ALA:HA	1.99	0.43
1:A:315:ARG:HG3	3:E:490:PRO:HD2	1.99	0.43
2:B:524:ASP:OD2	2:B:574:SER:OG	2.34	0.43
3:C:437:ARG:HB3	3:C:440:ILE:HG21	2.01	0.43
3:C:705:ILE:HG21	3:C:737:ARG:HB2	1.98	0.43
3:D:129:MET:O	3:D:133:SER:N	2.48	0.43
3:D:385:VAL:HG13	3:D:1196:ARG:HB2	2.00	0.43
3:F:603:VAL:HG21	3:F:620:VAL:HG13	1.99	0.43
3:H:413:PRO:HB2	3:H:434:ILE:HD13	2.01	0.43
3:H:1053:GLN:HB3	3:H:1109:PRO:HA	2.00	0.43
3:I:586:PHE:HA	3:I:642:PHE:HE2	1.82	0.43
3:L:407:ARG:NH1	3:L:440:ILE:O	2.50	0.43
1:A:527:VAL:HB	2:B:671:ALA:HB1	2.01	0.43
1:A:663:ALA:O	1:A:666:ARG:NH2	2.51	0.43
2:B:674:LEU:CD2	2:B:674:LEU:N	2.73	0.43
3:C:241:ASN:HD22	3:C:1148:SER:HG	1.61	0.43
3:H:455:GLN:NE2	3:H:767:PHE:HB2	2.34	0.43
3:H:1047:TYR:N	3:H:1075:LEU:O	2.44	0.43
3:I:540:LEU:HD12	3:I:767:PHE:HD2	1.83	0.43
3:I:684:LEU:HD12	3:I:685:PRO:HD2	1.99	0.43
3:L:545:LEU:HD13	3:L:569:LEU:HD11	2.00	0.43
1:A:25:LEU:HD22	1:A:874:TRP:CD1	2.54	0.43
3:C:377:ILE:HB	3:C:380:GLU:HB3	2.01	0.43
3:E:859:ILE:HG23	3:E:913:PHE:HD2	1.84	0.43
3:E:971:GLU:OE2	3:E:1168:ARG:NH1	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1153:SER:OG	3:E:1154:ILE:N	2.52	0.43
3:H:1044:ASP:OD1	3:H:1044:ASP:N	2.48	0.43
3:I:331:ARG:H	3:I:344:TYR:HE2	1.67	0.43
3:J:1023:ARG:HA	3:J:1024:PRO:HD3	1.79	0.43
3:J:1030:GLN:HG3	3:J:1038:PRO:HB2	2.01	0.43
3:L:157:ILE:HD13	3:L:1204:LEU:HB2	2.00	0.43
1:A:446:PRO:HG2	3:C:524:ASP:HA	1.99	0.43
3:C:686:ARG:HB2	3:L:595:GLN:HB2	1.99	0.43
3:F:54:VAL:HG12	3:F:56:SER:H	1.84	0.43
3:H:233:PRO:HA	3:H:234:PRO:HD3	1.91	0.43
3:H:828:GLU:HG2	3:H:830:ASN:H	1.84	0.43
3:J:129:MET:HG3	3:J:132:LEU:HD23	2.01	0.43
3:K:237:GLU:HB3	3:K:1152:ALA:HB2	2.00	0.43
3:L:26:ASP:O	3:L:30:THR:OG1	2.28	0.43
3:L:460:VAL:HG12	3:L:922:GLY:HA3	2.00	0.43
3:L:603:VAL:HG21	3:L:620:VAL:HG13	2.00	0.43
3:L:695:SER:HA	3:L:748:GLN:HE21	1.84	0.43
2:B:9:THR:HG21	2:B:389:ARG:HD3	2.00	0.43
3:D:669:PHE:HD2	3:D:769:VAL:HG12	1.84	0.43
3:G:686:ARG:HG2	3:G:834:SER:HB3	2.01	0.43
3:H:982:LEU:HD11	3:H:1115:VAL:HG11	2.01	0.43
3:I:1122:PRO:HB3	3:I:1159:GLY:HA3	1.99	0.43
3:J:463:SER:OG	3:J:464:SER:N	2.51	0.43
3:C:784:LEU:HB3	3:C:804:HIS:HB3	2.01	0.43
3:D:603:VAL:HG21	3:D:620:VAL:HG13	2.01	0.43
3:E:406:LEU:HB3	3:E:441:LEU:HD21	2.01	0.43
3:E:593:LEU:HD12	3:E:593:LEU:O	2.18	0.43
3:F:237:GLU:HB3	3:F:1152:ALA:HB2	2.00	0.43
3:F:494:THR:O	3:F:498:THR:OG1	2.31	0.43
3:F:668:LEU:HD12	3:F:767:PHE:HE1	1.84	0.43
3:G:388:MET:HG2	3:G:1193:SER:HB3	2.01	0.43
3:G:884:PRO:HD3	3:G:962:GLN:HE22	1.84	0.43
3:G:1013:VAL:HG22	3:G:1046:VAL:HB	2.00	0.43
3:J:385:VAL:HG13	3:J:1196:ARG:HB2	2.00	0.43
3:J:502:GLU:OE2	3:J:504:THR:OG1	2.32	0.43
3:J:511:ILE:HA	3:J:514:ILE:HG22	1.99	0.43
3:J:868:ARG:HG3	3:J:931:ILE:HG13	2.01	0.43
3:L:583:VAL:HG21	3:L:621:TRP:CD1	2.53	0.43
1:A:104:LEU:HD13	1:A:220:ILE:HG22	2.01	0.42
1:A:323:HIS:CD2	1:A:325:GLY:H	2.37	0.42
2:B:670:TYR:N	2:B:670:TYR:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:805:ALA:HA	3:E:435:SER:HB3	2.00	0.42
3:E:1107:ILE:HG23	3:E:1112:ILE:HG22	2.00	0.42
3:G:1088:TYR:OH	3:G:1134:HIS:NE2	2.45	0.42
3:H:39:PRO:HG2	3:H:78:ILE:HG12	2.01	0.42
3:H:137:ARG:HA	3:H:141:ARG:HD3	1.99	0.42
3:I:294:ARG:NH2	3:I:874:CYS:O	2.48	0.42
3:I:580:HIS:HD2	3:I:621:TRP:HE1	1.66	0.42
3:K:182:TYR:CG	3:K:479:LEU:HD11	2.54	0.42
3:K:563:MET:HE1	3:K:712:VAL:HG23	2.01	0.42
3:K:727:ARG:O	3:K:731:GLY:N	2.48	0.42
3:D:322:THR:HG21	3:D:348:ALA:HB2	2.00	0.42
3:F:899:ALA:O	3:F:903:HIS:N	2.49	0.42
3:G:570:THR:O	3:G:700:TRP:NE1	2.47	0.42
3:G:684:LEU:HD22	3:G:753:THR:HG21	2.00	0.42
3:I:620:VAL:HG11	3:J:718:THR:HG21	2.00	0.42
3:J:198:THR:HB	3:J:315:SER:HB2	2.02	0.42
3:J:371:LEU:HD11	3:J:388:MET:HE2	2.00	0.42
3:J:903:HIS:CD2	3:J:924:ALA:HB1	2.53	0.42
3:K:802:ALA:O	3:L:737:ARG:NH2	2.52	0.42
3:D:552:ASP:OD1	3:D:552:ASP:N	2.51	0.42
3:G:641:ALA:HA	3:G:644:GLU:HB2	2.00	0.42
3:H:623:PRO:HA	3:H:626:LEU:HB2	2.00	0.42
3:J:937:ALA:HB2	3:J:947:ARG:HG3	2.01	0.42
1:A:789:LYS:HD3	1:A:803:ARG:HH22	1.83	0.42
3:C:290:PRO:HG2	3:C:291:LEU:HD12	2.01	0.42
3:C:455:GLN:HB2	3:C:666:ALA:HB1	2.01	0.42
3:D:274:TYR:OH	3:D:975:PHE:O	2.29	0.42
3:E:456:VAL:HG22	3:E:668:LEU:HD21	2.01	0.42
3:F:861:ARG:HD2	3:F:953:GLY:H	1.85	0.42
3:J:455:GLN:NE2	3:J:767:PHE:HB2	2.35	0.42
3:J:650:TRP:CD1	3:J:773:ARG:HG3	2.55	0.42
3:K:354:THR:HG22	3:K:356:ASN:H	1.83	0.42
1:A:1189:LEU:HB3	1:A:1235:LEU:HD22	2.01	0.42
2:B:541:ILE:H	2:B:541:ILE:HG13	1.61	0.42
3:C:575:MET:HE2	3:C:697:MET:HE1	2.02	0.42
3:C:793:ARG:HH12	3:D:738:GLN:HA	1.85	0.42
3:D:558:THR:O	3:D:720:THR:OG1	2.35	0.42
3:J:242:ARG:HD3	3:J:1146:LEU:HA	2.01	0.42
3:K:524:ASP:OD1	3:K:524:ASP:N	2.53	0.42
1:A:577:ILE:HD11	1:A:787:TYR:H	1.85	0.42
2:B:4:ILE:HB	2:B:195:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:202:THR:HB	3:C:391:CYS:HA	2.00	0.42
3:C:722:ASN:HB3	3:C:725:THR:HG22	2.01	0.42
3:G:801:ARG:HG3	3:G:939:LEU:HD13	2.01	0.42
3:H:33:PRO:HA	3:H:34:PRO:HD3	1.83	0.42
3:L:252:LEU:HD11	3:L:335:GLY:HA3	2.01	0.42
3:L:919:LEU:HD23	3:L:920:LEU:HB2	2.01	0.42
1:A:385:ARG:HH22	1:A:394:GLU:HG3	1.84	0.42
3:E:242:ARG:NH1	3:E:1145:SER:OG	2.51	0.42
3:E:317:PHE:HB3	3:E:329:MET:HE3	2.02	0.42
3:F:114:PRO:HA	3:F:117:TYR:CZ	2.54	0.42
3:F:274:TYR:OH	3:F:975:PHE:O	2.30	0.42
3:F:485:PRO:HD3	3:F:837:TYR:HE1	1.84	0.42
3:H:705:ILE:HG23	3:H:733:MET:HB3	2.02	0.42
3:I:444:TRP:HD1	3:I:855:GLN:HE21	1.68	0.42
3:J:500:ILE:HD13	3:J:732:VAL:HG22	2.01	0.42
3:K:444:TRP:HD1	3:K:855:GLN:HE21	1.67	0.42
3:K:684:LEU:HD12	3:K:685:PRO:HD2	2.01	0.42
3:K:982:LEU:HD11	3:K:1115:VAL:HG11	2.02	0.42
3:L:1023:ARG:HA	3:L:1024:PRO:HD3	1.77	0.42
1:A:107:LEU:HD23	1:A:109:THR:H	1.85	0.42
1:A:498:TYR:HA	1:A:977:ILE:HD11	2.02	0.42
1:A:968:THR:HG22	1:A:974:ILE:HG13	2.01	0.42
3:C:684:LEU:HD12	3:C:685:PRO:HD2	2.01	0.42
3:D:1053:GLN:HB2	3:E:323:THR:HG21	2.02	0.42
3:E:606:MET:HG2	3:E:610:THR:HG21	2.02	0.42
3:E:984:LEU:HD22	3:E:1100:LEU:HD21	2.00	0.42
3:F:705:ILE:HG23	3:F:733:MET:HB3	2.01	0.42
3:G:1107:ILE:HG23	3:G:1112:ILE:HG22	2.02	0.42
3:H:460:VAL:HG12	3:H:922:GLY:HA3	2.01	0.42
3:H:593:LEU:CD1	3:H:593:LEU:O	2.66	0.42
3:H:614:GLN:NE2	3:I:432:ILE:O	2.50	0.42
3:I:287:GLN:HA	3:I:1113:PRO:HA	2.01	0.42
3:I:457:MET:HE1	3:I:923:LEU:HD11	2.01	0.42
3:J:233:PRO:HA	3:J:234:PRO:HD3	1.91	0.42
3:J:292:ALA:O	3:J:296:ASN:ND2	2.53	0.42
3:J:579:PRO:HG3	3:J:807:PHE:HE2	1.84	0.42
3:J:623:PRO:HA	3:J:626:LEU:HD12	2.01	0.42
3:J:668:LEU:HD12	3:J:767:PHE:HE1	1.84	0.42
3:K:928:ASP:OD2	3:L:693:TYR:OH	2.24	0.42
1:A:196:MET:HE3	1:A:235:LEU:HD11	2.02	0.42
3:C:151:PRO:HB2	3:C:152:MET:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:506:GLN:HE21	3:E:501:SER:HG	1.66	0.42
3:D:788:VAL:HG23	3:D:932:ALA:HB3	2.02	0.42
3:E:354:THR:HB	3:E:357:ALA:H	1.84	0.42
3:F:292:ALA:O	3:F:296:ASN:ND2	2.53	0.42
3:F:968:PHE:HD1	3:F:975:PHE:HD2	1.66	0.42
3:I:567:LEU:HD13	3:I:708:PHE:HD2	1.85	0.42
3:J:432:ILE:HG12	3:J:1206:GLY:HA3	2.02	0.42
3:K:167:ILE:HG22	3:K:525:TYR:HB2	2.02	0.42
2:B:33:ILE:HD11	2:B:245:LEU:HA	2.01	0.42
3:C:274:TYR:OH	3:C:975:PHE:O	2.33	0.42
3:C:353:GLN:HB2	3:L:1021:VAL:HG12	2.02	0.42
3:C:986:GLN:HG3	3:C:1135:TYR:HE1	1.85	0.42
3:D:463:SER:OG	3:D:464:SER:N	2.45	0.42
3:D:705:ILE:HG23	3:D:733:MET:HB3	2.01	0.42
3:E:973:ASN:HB2	3:E:1144:ASP:HB2	2.02	0.42
3:F:455:GLN:NE2	3:F:767:PHE:HB2	2.35	0.42
3:G:287:GLN:NE2	3:G:1106:LYS:O	2.52	0.42
3:K:317:PHE:HE1	3:K:331:ARG:HD3	1.85	0.42
3:K:1078:LEU:CD1	3:K:1081:TYR:CD1	3.02	0.42
3:K:1156:THR:HG21	3:K:1161:ASN:HA	2.02	0.42
3:L:483:VAL:HG21	3:L:758:LEU:HD11	2.02	0.42
1:A:399:PRO:O	2:B:497:ARG:NH2	2.53	0.41
1:A:470:ALA:HB3	1:A:525:ASN:HB3	2.02	0.41
3:D:793:ARG:HG2	3:D:796:ALA:HA	2.01	0.41
3:E:284:ASP:OD1	3:E:284:ASP:N	2.53	0.41
3:E:300:MET:O	3:E:304:PHE:N	2.51	0.41
3:F:454:GLN:HE21	3:F:857:ALA:HA	1.85	0.41
3:G:650:TRP:CD1	3:G:773:ARG:HG3	2.55	0.41
3:H:410:HIS:CD2	3:H:442:CYS:H	2.37	0.41
3:I:331:ARG:HH22	3:I:1196:ARG:CZ	2.33	0.41
3:J:441:LEU:HD23	3:J:1201:TYR:HE1	1.85	0.41
3:K:580:HIS:HD2	3:K:621:TRP:HE1	1.66	0.41
3:K:626:LEU:HD21	3:K:776:GLN:HE21	1.85	0.41
3:L:656:PHE:HB3	3:L:681:ASN:HD21	1.85	0.41
1:A:1149:PRO:HA	1:A:1152:PHE:HD2	1.84	0.41
3:D:233:PRO:HA	3:D:234:PRO:HD3	1.92	0.41
3:E:294:ARG:HB3	3:E:890:GLN:HB2	2.02	0.41
3:E:697:MET:HE2	3:E:747:ILE:HG21	2.02	0.41
3:G:718:THR:O	3:I:727:ARG:NH1	2.53	0.41
3:H:510:PRO:HG2	3:H:511:ILE:HD12	2.01	0.41
3:H:614:GLN:HA	3:I:431:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1006:ARG:NH2	3:K:1077:GLU:OE1	2.46	0.41
3:C:278:LEU:HD21	3:C:897:ALA:HB1	2.03	0.41
3:C:365:ALA:HB2	3:L:1016:ARG:HH22	1.84	0.41
3:D:985:VAL:HG12	3:D:1073:ARG:HB3	2.02	0.41
3:E:237:GLU:HA	3:E:1151:ALA:HB3	2.01	0.41
3:E:590:ALA:HB2	3:E:639:LEU:HD11	2.02	0.41
3:E:650:TRP:HA	3:E:651:PRO:HD3	1.94	0.41
3:J:1053:GLN:HB2	3:K:323:THR:HG21	2.02	0.41
3:K:746:TYR:HD1	3:K:750:MET:HE3	1.85	0.41
3:K:910:LYS:NZ	3:K:921:ASP:OD2	2.53	0.41
2:B:40:TYR:CZ	2:B:71:PRO:HG3	2.55	0.41
2:B:489:LEU:HD21	2:B:571:THR:HG21	2.02	0.41
3:C:459:LEU:HB3	3:C:807:PHE:HZ	1.85	0.41
3:C:1046:VAL:HA	3:C:1075:LEU:HB3	2.03	0.41
3:D:320:ASP:OD2	3:D:325:THR:OG1	2.37	0.41
3:D:483:VAL:HG21	3:D:758:LEU:HD11	2.02	0.41
3:D:972:MET:HE3	3:D:979:ARG:HH21	1.86	0.41
3:E:548:ASP:OD1	3:E:548:ASP:N	2.53	0.41
3:E:1149:THR:HG21	3:E:1161:ASN:HA	2.02	0.41
3:G:301:LEU:HD22	3:G:964:VAL:HG12	2.03	0.41
3:G:401:THR:HG21	3:G:960:ALA:HB2	2.01	0.41
3:G:1031:LEU:N	3:G:1039:ARG:O	2.52	0.41
3:J:191:PRO:HD2	3:J:855:GLN:HB3	2.03	0.41
3:D:257:ARG:NH1	3:D:309:LEU:O	2.41	0.41
3:D:583:VAL:HG21	3:D:621:TRP:CD1	2.56	0.41
3:D:1031:LEU:N	3:D:1039:ARG:O	2.48	0.41
3:H:862:GLU:HB3	3:H:957:ILE:HD12	2.03	0.41
3:I:182:TYR:CG	3:I:479:LEU:HD11	2.55	0.41
3:I:632:ASN:HB3	3:I:635:GLN:HB2	2.03	0.41
3:I:1096:GLU:OE1	3:I:1135:TYR:N	2.47	0.41
3:K:401:THR:HG21	3:K:960:ALA:HB2	2.02	0.41
3:K:863:ALA:HB1	3:K:920:LEU:HD22	2.02	0.41
3:L:54:VAL:HG12	3:L:56:SER:H	1.85	0.41
3:L:772:THR:HG21	3:L:779:VAL:HB	2.03	0.41
1:A:477:LYS:HB3	2:B:675:PRO:HG2	2.01	0.41
2:B:337:GLN:HE21	2:B:343:VAL:HA	1.85	0.41
3:C:474:GLU:HA	3:C:477:SER:HB3	2.02	0.41
3:D:294:ARG:HB3	3:D:890:GLN:HB2	2.02	0.41
3:D:593:LEU:HD13	3:D:597:GLU:CD	2.46	0.41
3:D:743:THR:OG1	3:D:822:MET:O	2.38	0.41
3:E:159:SER:HA	3:E:162:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:257:ARG:HG2	3:G:307:SER:HA	2.03	0.41
3:H:274:TYR:OH	3:H:975:PHE:O	2.36	0.41
3:J:596:PRO:HD3	3:K:687:LEU:HD21	2.03	0.41
3:K:546:SER:OG	3:K:548:ASP:OD1	2.31	0.41
3:F:586:PHE:HA	3:F:642:PHE:HE2	1.86	0.41
3:G:1090:PRO:HB2	3:G:1129:THR:HG23	2.02	0.41
3:I:718:THR:HG23	3:I:726:ARG:HH12	1.85	0.41
3:I:862:GLU:HB3	3:I:957:ILE:HD12	2.02	0.41
3:J:364:ILE:HG22	3:J:366:ASP:H	1.85	0.41
3:J:494:THR:O	3:J:498:THR:OG1	2.30	0.41
3:K:455:GLN:HB2	3:K:666:ALA:HB1	2.03	0.41
3:K:1012:ARG:HH11	3:K:1039:ARG:HB3	1.85	0.41
3:L:330:ILE:HD12	3:L:340:LEU:HD11	2.03	0.41
3:L:788:VAL:HG23	3:L:932:ALA:HB3	2.02	0.41
1:A:1192:PRO:HD2	1:A:1195:TRP:CD2	2.56	0.41
3:C:317:PHE:HB3	3:C:329:MET:HE3	2.02	0.41
3:D:500:ILE:HD13	3:D:732:VAL:HA	2.02	0.41
3:D:1021:VAL:HG12	3:E:353:GLN:HB2	2.03	0.41
3:E:1097:ALA:HB2	3:E:1135:TYR:HE2	1.86	0.41
3:F:242:ARG:HD3	3:F:1146:LEU:HA	2.02	0.41
3:F:788:VAL:HG23	3:F:932:ALA:HB3	2.02	0.41
3:G:718:THR:HG23	3:G:726:ARG:HH12	1.85	0.41
3:J:758:LEU:HA	3:J:761:VAL:HG22	2.03	0.41
3:J:1087:TYR:HE1	3:J:1119:ILE:HB	1.84	0.41
3:L:972:MET:HE3	3:L:979:ARG:HH21	1.86	0.41
1:A:149:VAL:HG21	1:A:153:PRO:HD3	2.03	0.41
2:B:431:LEU:HB2	2:B:688:THR:HG22	2.02	0.41
2:B:627:PRO:O	2:B:698:ARG:NH2	2.54	0.41
3:C:294:ARG:HB3	3:C:890:GLN:HB2	2.02	0.41
3:C:638:LEU:HD21	3:C:711:VAL:HG13	2.03	0.41
3:C:736:MET:HB3	3:C:823:LEU:HD21	2.03	0.41
3:C:1066:MET:HE3	3:C:1071:ARG:HB2	2.03	0.41
3:D:204:PHE:CE2	3:D:1188:ILE:HD13	2.56	0.41
3:D:250:ALA:HA	3:D:336:ARG:HH21	1.84	0.41
3:D:593:LEU:HD13	3:D:597:GLU:HG2	2.03	0.41
3:D:603:VAL:HG13	3:D:606:MET:HB2	2.02	0.41
3:D:702:SER:OG	3:D:737:ARG:NH1	2.54	0.41
3:F:595:GLN:OE1	3:G:686:ARG:N	2.50	0.41
3:F:1053:GLN:HB2	3:G:323:THR:HG21	2.03	0.41
3:G:540:LEU:HD12	3:G:767:PHE:HD2	1.85	0.41
3:G:784:LEU:HD22	3:G:800:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:868:ARG:NH2	3:G:932:ALA:O	2.49	0.41
3:G:1156:THR:HG21	3:G:1161:ASN:HA	2.02	0.41
3:H:247:THR:O	3:H:262:ARG:NE	2.53	0.41
3:H:530:LYS:HD3	3:H:811:LEU:HD21	2.02	0.41
3:H:1103:TRP:CD1	3:H:1113:PRO:HG2	2.56	0.41
3:I:646:ILE:HG22	3:I:774:LEU:HD21	2.02	0.41
3:I:722:ASN:HB3	3:I:725:THR:HG22	2.02	0.41
3:I:895:SER:HA	3:I:930:ARG:HD2	2.02	0.41
3:I:993:TRP:NE1	3:I:995:PRO:HG3	2.36	0.41
3:I:1064:TRP:HE1	3:I:1068:LYS:HE3	1.86	0.41
3:I:1189:THR:HG22	3:I:1191:TYR:H	1.86	0.41
3:J:684:LEU:HA	3:J:749:HIS:HB3	2.03	0.41
3:K:650:TRP:CD1	3:K:773:ARG:HG3	2.56	0.41
2:B:591:PRO:HA	2:B:594:MET:HG2	2.03	0.41
3:C:875:GLN:O	3:C:883:ARG:NH2	2.47	0.41
3:D:424:ALA:HB2	3:D:845:PHE:CE2	2.56	0.41
3:E:536:ALA:HB1	3:E:766:PRO:HB3	2.03	0.41
3:E:1046:VAL:HG22	3:E:1075:LEU:HD13	2.03	0.41
3:F:40:ASN:HB3	3:F:66:SER:HB3	2.03	0.41
3:F:832:ILE:HG21	3:F:835:HIS:HD2	1.85	0.41
3:H:460:VAL:O	3:H:463:SER:OG	2.31	0.41
3:I:442:CYS:HB2	3:I:444:TRP:CD2	2.56	0.41
3:I:583:VAL:HG21	3:I:621:TRP:CE2	2.56	0.41
3:J:424:ALA:HB2	3:J:845:PHE:HE2	1.85	0.41
3:K:223:THR:HA	3:K:1153:SER:HA	2.02	0.41
3:L:411:GLN:HB2	3:L:445:PHE:HB2	2.03	0.41
3:L:705:ILE:HG23	3:L:733:MET:HB3	2.02	0.41
3:L:968:PHE:HD1	3:L:975:PHE:HD2	1.69	0.41
1:A:95:VAL:HG22	1:A:141:ILE:HG22	2.03	0.40
1:A:414:ILE:HD11	1:A:637:ARG:HD3	2.03	0.40
3:C:207:LEU:HD23	3:C:265:PRO:HB3	2.03	0.40
3:D:587:MET:O	3:D:591:ASN:N	2.50	0.40
3:D:621:TRP:HA	3:D:622:PRO:HD3	1.93	0.40
3:D:902:MET:HB3	3:D:924:ALA:HB2	2.02	0.40
3:F:868:ARG:HG3	3:F:931:ILE:HG13	2.03	0.40
3:G:354:THR:HG23	3:G:1152:ALA:HA	2.03	0.40
3:G:660:SER:O	3:G:673:ASN:ND2	2.54	0.40
3:J:128:THR:HG22	3:J:130:SER:H	1.85	0.40
3:J:459:LEU:O	3:J:801:ARG:NH2	2.46	0.40
3:K:344:TYR:HB3	3:K:368:ILE:HD11	2.02	0.40
1:A:1209:TYR:OH	3:E:516:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:449:SER:HB3	2:B:452:THR:HG23	2.03	0.40
3:C:705:ILE:HD12	3:C:733:MET:HB3	2.03	0.40
3:C:835:HIS:HB2	3:L:555:GLN:HA	2.03	0.40
3:E:612:ALA:HA	3:E:615:PHE:HD2	1.86	0.40
3:G:446:ALA:HB1	3:G:450:ASP:HB2	2.01	0.40
3:G:1120:PRO:HG3	3:G:1132:ARG:HH21	1.86	0.40
3:J:119:CYS:HA	3:J:132:LEU:HD21	2.04	0.40
3:J:915:LEU:HD22	3:J:919:LEU:HD13	2.04	0.40
1:A:399:PRO:HB2	1:A:774:GLY:HA3	2.03	0.40
1:A:716:HIS:ND1	1:A:765:CYS:SG	2.92	0.40
2:B:296:LEU:HD13	2:B:312:LEU:HD12	2.04	0.40
3:D:317:PHE:CE1	3:D:331:ARG:HG2	2.57	0.40
3:E:377:ILE:HB	3:E:380:GLU:HB3	2.03	0.40
3:F:424:ALA:HB2	3:F:845:PHE:HE2	1.86	0.40
3:F:510:PRO:HB3	3:F:729:MET:HE1	2.04	0.40
3:H:722:ASN:O	3:H:726:ARG:N	2.39	0.40
3:I:394:LEU:HD13	3:I:967:THR:HG21	2.04	0.40
3:I:638:LEU:HD11	3:I:711:VAL:HG22	2.02	0.40
3:J:558:THR:O	3:J:720:THR:OG1	2.32	0.40
3:J:593:LEU:HB2	3:J:596:PRO:HG2	2.02	0.40
3:J:741:THR:OG1	3:J:824:CYS:O	2.36	0.40
3:K:718:THR:HG23	3:K:726:ARG:HH12	1.87	0.40
3:L:515:LEU:HA	3:L:519:GLN:HB3	2.04	0.40
1:A:4:LEU:HD22	1:A:52:ILE:HD11	2.02	0.40
3:D:210:ILE:HB	3:D:239:ALA:HB3	2.04	0.40
3:D:364:ILE:HG22	3:D:366:ASP:H	1.86	0.40
3:D:494:THR:HA	3:D:497:ILE:HG22	2.03	0.40
3:D:1044:ASP:N	3:D:1044:ASP:OD1	2.54	0.40
3:E:193:LEU:HD21	3:E:859:ILE:HD11	2.02	0.40
3:E:333:PHE:HD2	3:E:339:LEU:HB3	1.85	0.40
3:E:535:TRP:CE2	3:E:678:PRO:HG3	2.56	0.40
3:E:993:TRP:NE1	3:E:995:PRO:HG3	2.37	0.40
3:F:247:THR:O	3:F:262:ARG:NE	2.54	0.40
3:G:394:LEU:HD13	3:G:967:THR:HG21	2.03	0.40
3:H:385:VAL:HG13	3:H:1196:ARG:HB2	2.04	0.40
3:H:923:LEU:HD21	3:H:931:ILE:HD13	2.02	0.40
3:H:1023:ARG:HA	3:H:1024:PRO:HD3	1.77	0.40
3:I:718:THR:O	3:K:727:ARG:NH1	2.54	0.40
3:K:658:TYR:CD1	3:K:675:MET:HG3	2.56	0.40
3:L:156:ALA:HB1	3:L:851:PHE:HD2	1.87	0.40
3:L:385:VAL:HG13	3:L:1196:ARG:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:410:HIS:CD2	3:L:442:CYS:H	2.39	0.40
3:L:432:ILE:HG12	3:L:1206:GLY:HA3	2.03	0.40
1:A:302:ALA:O	1:A:317:THR:OG1	2.32	0.40
1:A:730:THR:HG22	1:A:732:GLN:H	1.85	0.40
2:B:292:ILE:HD12	2:B:292:ILE:HA	1.98	0.40
3:E:524:ASP:OD1	3:E:524:ASP:N	2.52	0.40
3:F:862:GLU:HB3	3:F:957:ILE:HD12	2.03	0.40
3:F:972:MET:HE3	3:F:979:ARG:HH21	1.85	0.40
3:G:206:LEU:HD11	3:G:1190:LEU:HD13	2.04	0.40
3:H:535:TRP:HH2	3:H:747:ILE:HD11	1.86	0.40
3:H:586:PHE:HA	3:H:642:PHE:HE2	1.87	0.40
3:I:563:MET:HE1	3:I:712:VAL:HG23	2.03	0.40
3:J:973:ASN:HD22	3:J:1144:ASP:HB3	1.86	0.40
3:J:1044:ASP:OD1	3:J:1044:ASP:N	2.46	0.40
3:K:493:LEU:HB2	3:K:824:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1271/1274 (100%)	1206 (95%)	65 (5%)	0	100	100
2	B	597/728 (82%)	561 (94%)	35 (6%)	1 (0%)	43	71
3	C	1092/1214 (90%)	1021 (94%)	71 (6%)	0	100	100
3	D	1183/1214 (97%)	1112 (94%)	71 (6%)	0	100	100
3	E	1062/1214 (88%)	999 (94%)	63 (6%)	0	100	100
3	F	1183/1214 (97%)	1100 (93%)	83 (7%)	0	100	100
3	G	1059/1214 (87%)	1014 (96%)	45 (4%)	0	100	100
3	H	1183/1214 (97%)	1105 (93%)	78 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	1059/1214 (87%)	1011 (96%)	48 (4%)	0	100	100
3	J	1183/1214 (97%)	1115 (94%)	68 (6%)	0	100	100
3	K	1059/1214 (87%)	1007 (95%)	52 (5%)	0	100	100
3	L	1183/1214 (97%)	1106 (94%)	76 (6%)	1 (0%)	48	78
All	All	13114/14142 (93%)	12357 (94%)	755 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	672	PRO
3	L	520	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1090/1091 (100%)	1086 (100%)	4 (0%)	84	83
2	B	518/626 (83%)	517 (100%)	1 (0%)	87	85
3	C	939/1030 (91%)	936 (100%)	3 (0%)	86	84
3	D	1009/1030 (98%)	1005 (100%)	4 (0%)	84	83
3	E	908/1030 (88%)	904 (100%)	4 (0%)	84	83
3	F	1009/1030 (98%)	1005 (100%)	4 (0%)	84	83
3	G	906/1030 (88%)	904 (100%)	2 (0%)	87	85
3	H	1009/1030 (98%)	1005 (100%)	4 (0%)	84	83
3	I	906/1030 (88%)	902 (100%)	4 (0%)	84	83
3	J	1009/1030 (98%)	1004 (100%)	5 (0%)	81	81
3	K	906/1030 (88%)	904 (100%)	2 (0%)	87	85
3	L	1009/1030 (98%)	1003 (99%)	6 (1%)	78	80
All	All	11218/12017 (93%)	11175 (100%)	43 (0%)	81	83

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	534	ILE
1	A	540	ILE
1	A	1215	ILE
2	B	541	ILE
3	C	403	ILE
3	C	788	VAL
3	C	985	VAL
3	D	385	VAL
3	D	500	ILE
3	D	1021	VAL
3	D	1085	LEU
3	E	403	ILE
3	E	670	ILE
3	E	950	VAL
3	E	985	VAL
3	F	500	ILE
3	F	620	VAL
3	F	985	VAL
3	F	1085	LEU
3	G	403	ILE
3	G	950	VAL
3	H	385	VAL
3	H	511	ILE
3	H	1021	VAL
3	H	1085	LEU
3	I	215	LEU
3	I	403	ILE
3	I	788	VAL
3	I	950	VAL
3	J	385	VAL
3	J	500	ILE
3	J	775	VAL
3	J	985	VAL
3	J	1085	LEU
3	K	403	ILE
3	K	1194	LEU
3	L	385	VAL
3	L	500	ILE
3	L	541	VAL
3	L	620	VAL
3	L	775	VAL

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Mol	Chain	Res	Type
3	L	985	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (248) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	40	GLN
1	A	51	HIS
1	A	66	HIS
1	A	148	GLN
1	A	197	GLN
1	A	323	HIS
1	A	360	HIS
1	A	444	GLN
1	A	499	GLN
1	A	548	HIS
1	A	734	ASN
1	A	1012	ASN
1	A	1088	GLN
1	A	1207	HIS
2	B	48	GLN
2	B	227	GLN
2	B	337	GLN
2	B	379	HIS
2	B	460	ASN
2	B	504	GLN
2	B	514	GLN
2	B	587	GLN
3	C	154	ASN
3	C	272	HIS
3	C	285	ASN
3	C	455	GLN
3	C	461	ASN
3	C	506	GLN
3	C	580	HIS
3	C	591	ASN
3	C	607	HIS
3	C	663	GLN
3	C	749	HIS
3	C	776	GLN
3	C	782	ASN
3	C	835	HIS

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Mol	Chain	Res	Type
3	C	854	ASN
3	C	940	GLN
3	C	962	GLN
3	C	973	ASN
3	C	986	GLN
3	C	1080	HIS
3	C	1134	HIS
3	C	1141	ASN
3	C	1192	ASN
3	C	1198	ASN
3	D	31	ASN
3	D	41	GLN
3	D	140	HIS
3	D	241	ASN
3	D	289	ASN
3	D	312	ASN
3	D	353	GLN
3	D	375	ASN
3	D	410	HIS
3	D	425	ASN
3	D	454	GLN
3	D	458	HIS
3	D	555	GLN
3	D	559	HIS
3	D	595	GLN
3	D	617	HIS
3	D	649	ASN
3	D	748	GLN
3	D	768	GLN
3	D	854	ASN
3	D	958	HIS
3	D	962	GLN
3	D	963	GLN
3	D	1142	ASN
3	D	1192	ASN
3	E	248	ASN
3	E	272	HIS
3	E	289	ASN
3	E	411	GLN
3	E	455	GLN
3	E	523	ASN
3	E	580	HIS

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Mol	Chain	Res	Type
3	E	649	ASN
3	E	663	GLN
3	E	776	GLN
3	E	854	ASN
3	E	903	HIS
3	E	906	ASN
3	E	958	HIS
3	E	963	GLN
3	E	1141	ASN
3	E	1142	ASN
3	F	31	ASN
3	F	113	ASN
3	F	353	GLN
3	F	454	GLN
3	F	458	HIS
3	F	519	GLN
3	F	559	HIS
3	F	607	HIS
3	F	617	HIS
3	F	663	GLN
3	F	713	ASN
3	F	748	GLN
3	F	836	HIS
3	F	854	ASN
3	F	873	GLN
3	F	903	HIS
3	F	940	GLN
3	F	958	HIS
3	F	962	GLN
3	F	963	GLN
3	F	973	ASN
3	F	976	ASN
3	F	990	ASN
3	F	1123	GLN
3	F	1182	ASN
3	G	248	ASN
3	G	308	ASN
3	G	356	ASN
3	G	415	GLN
3	G	425	ASN
3	G	458	HIS
3	G	519	GLN

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Mol	Chain	Res	Type
3	G	645	HIS
3	G	652	GLN
3	G	663	GLN
3	G	682	GLN
3	G	776	GLN
3	G	875	GLN
3	G	940	GLN
3	G	962	GLN
3	G	973	ASN
3	G	1091	GLN
3	G	1141	ASN
3	H	41	GLN
3	H	123	ASN
3	H	140	HIS
3	H	241	ASN
3	H	506	GLN
3	H	519	GLN
3	H	555	GLN
3	H	559	HIS
3	H	591	ASN
3	H	607	HIS
3	H	663	GLN
3	H	713	ASN
3	H	748	GLN
3	H	836	HIS
3	H	854	ASN
3	H	873	GLN
3	H	903	HIS
3	H	949	HIS
3	H	958	HIS
3	H	973	ASN
3	H	976	ASN
3	H	1080	HIS
3	H	1091	GLN
3	H	1134	HIS
3	H	1142	ASN
3	I	227	GLN
3	I	248	ASN
3	I	285	ASN
3	I	353	GLN
3	I	455	GLN
3	I	458	HIS

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Mol	Chain	Res	Type
3	I	506	GLN
3	I	645	HIS
3	I	652	GLN
3	I	663	GLN
3	I	673	ASN
3	I	738	GLN
3	I	776	GLN
3	I	835	HIS
3	I	855	GLN
3	I	875	GLN
3	I	940	GLN
3	I	973	ASN
3	I	986	GLN
3	I	1091	GLN
3	I	1141	ASN
3	I	1150	ASN
3	I	1192	ASN
3	J	31	ASN
3	J	120	ASN
3	J	123	ASN
3	J	241	ASN
3	J	353	GLN
3	J	425	ASN
3	J	454	GLN
3	J	458	HIS
3	J	649	ASN
3	J	663	GLN
3	J	854	ASN
3	J	855	GLN
3	J	873	GLN
3	J	890	GLN
3	J	903	HIS
3	J	949	HIS
3	J	958	HIS
3	J	962	GLN
3	J	963	GLN
3	J	973	ASN
3	J	976	ASN
3	J	1030	GLN
3	J	1086	HIS
3	J	1123	GLN
3	J	1142	ASN

Continued on next page...

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Mol	Chain	Res	Type
3	J	1150	ASN
3	J	1192	ASN
3	K	425	ASN
3	K	458	HIS
3	K	506	GLN
3	K	559	HIS
3	K	591	ASN
3	K	595	GLN
3	K	645	HIS
3	K	652	GLN
3	K	663	GLN
3	K	748	GLN
3	K	776	GLN
3	K	906	ASN
3	K	940	GLN
3	K	963	GLN
3	K	973	ASN
3	K	986	GLN
3	K	1053	GLN
3	K	1091	GLN
3	K	1123	GLN
3	K	1141	ASN
3	L	31	ASN
3	L	40	ASN
3	L	241	ASN
3	L	353	GLN
3	L	411	GLN
3	L	425	ASN
3	L	455	GLN
3	L	465	ASN
3	L	617	HIS
3	L	663	GLN
3	L	713	ASN
3	L	768	GLN
3	L	854	ASN
3	L	873	GLN
3	L	903	HIS
3	L	962	GLN
3	L	976	ASN
3	L	1123	GLN
3	L	1142	ASN
3	L	1182	ASN

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Mol	Chain	Res	Type
3	L	1192	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	B	801	-	4,4,4	1.05	0	6,6,6	0.45	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

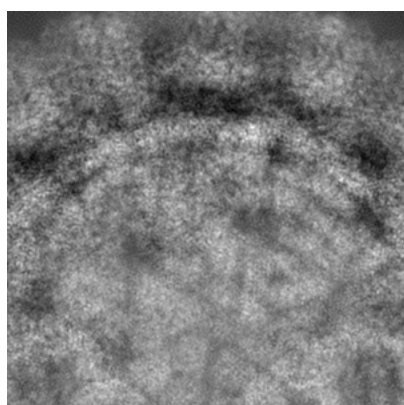
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9050. These allow visual inspection of the internal detail of the map and identification of artifacts.

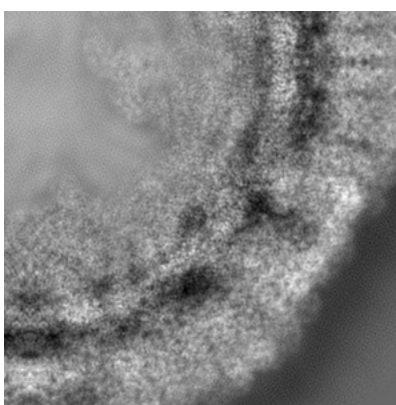
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

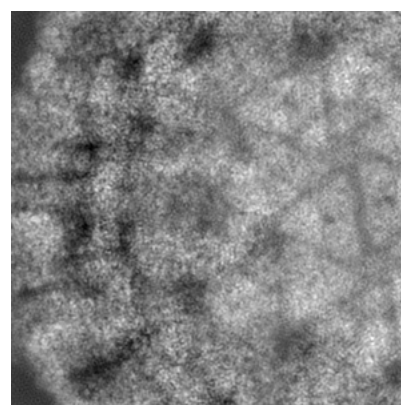
6.1.1 Primary map



X



Y

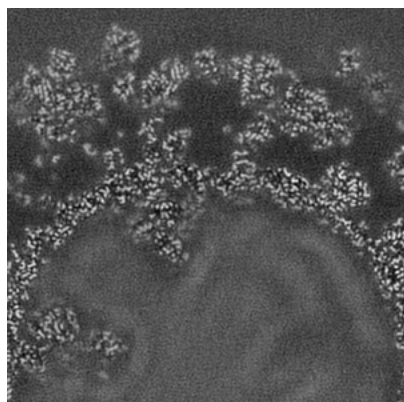


Z

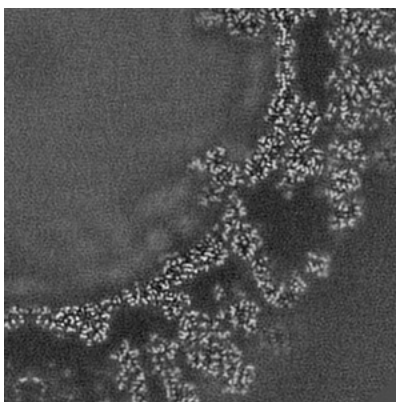
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

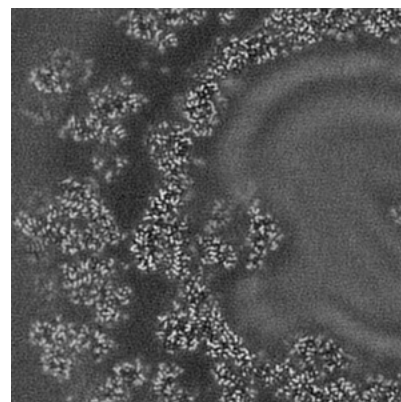
6.2.1 Primary map



X Index: 150



Y Index: 150

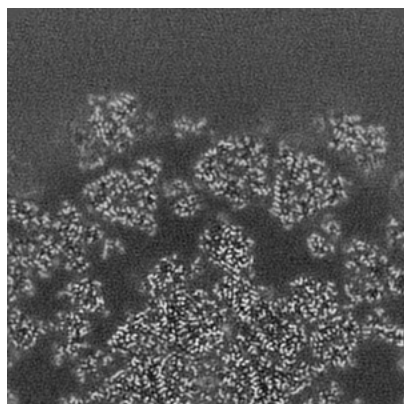


Z Index: 150

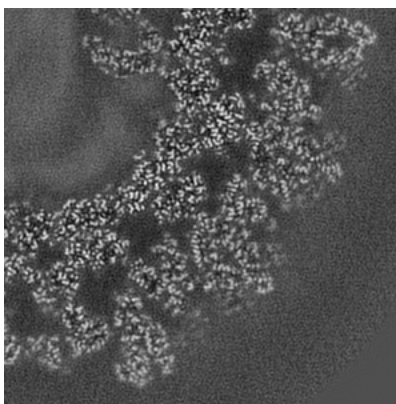
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

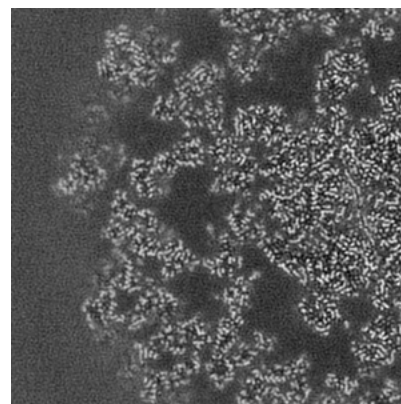
6.3.1 Primary map



X Index: 74



Y Index: 296

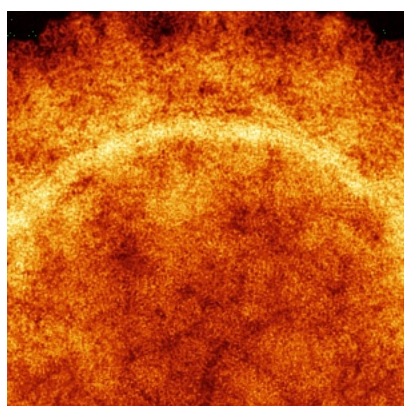


Z Index: 208

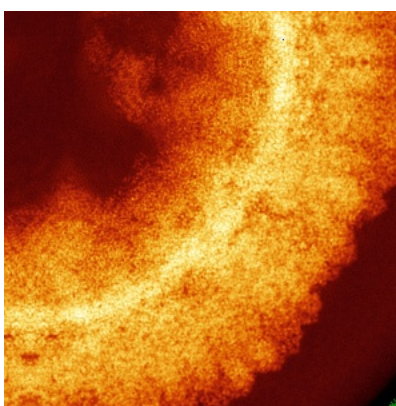
The images above show the largest variance slices of the map in three orthogonal directions.

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

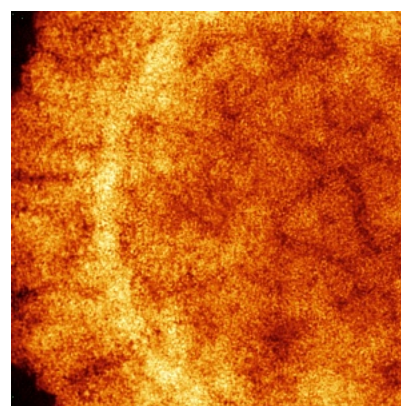
6.4.1 Primary map



X



Y

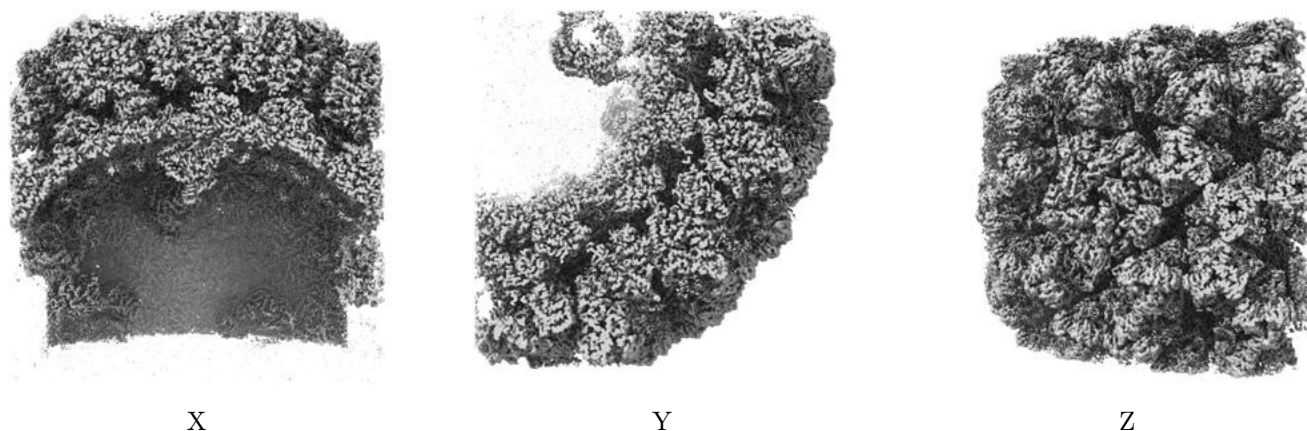


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0194. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

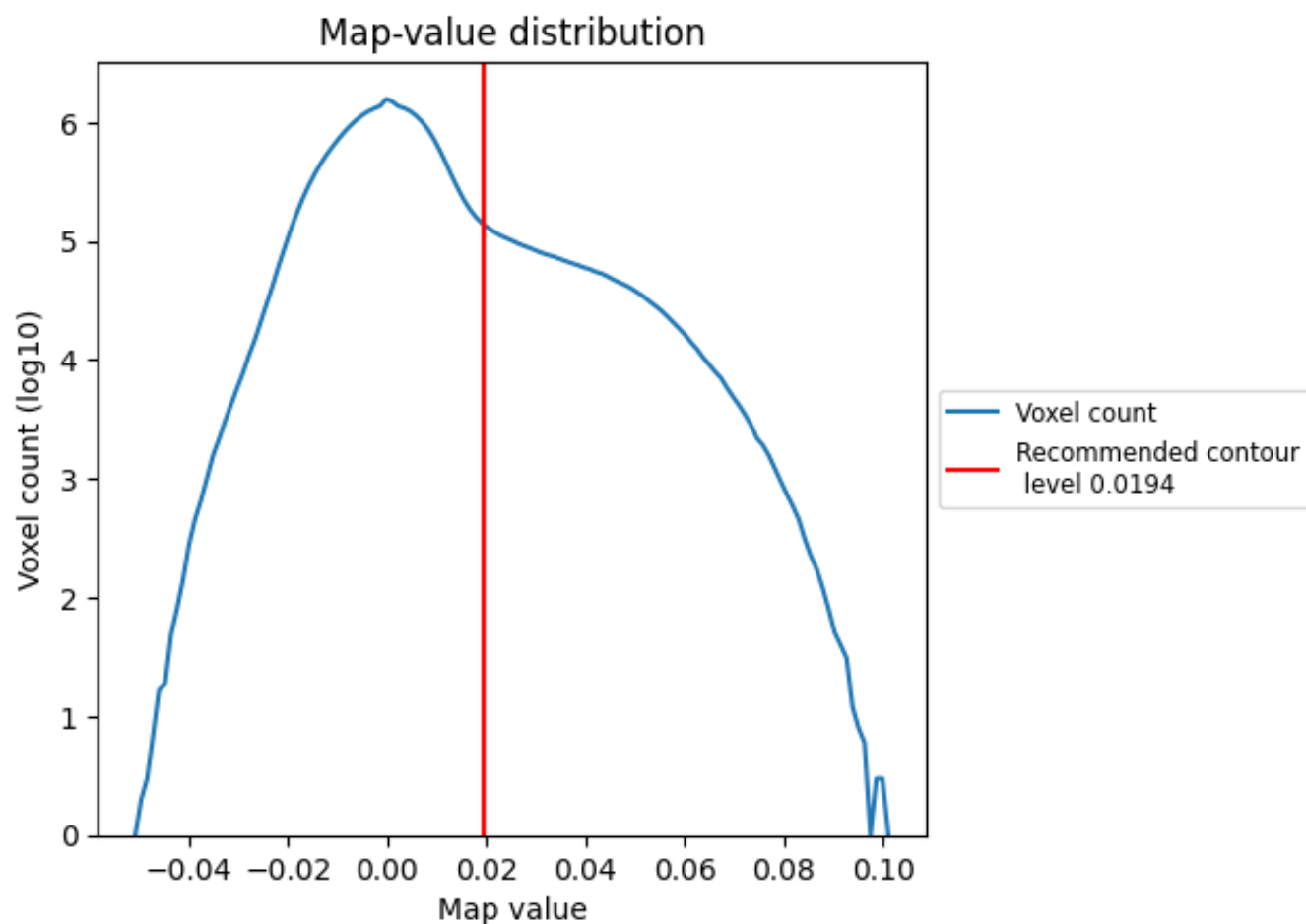
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

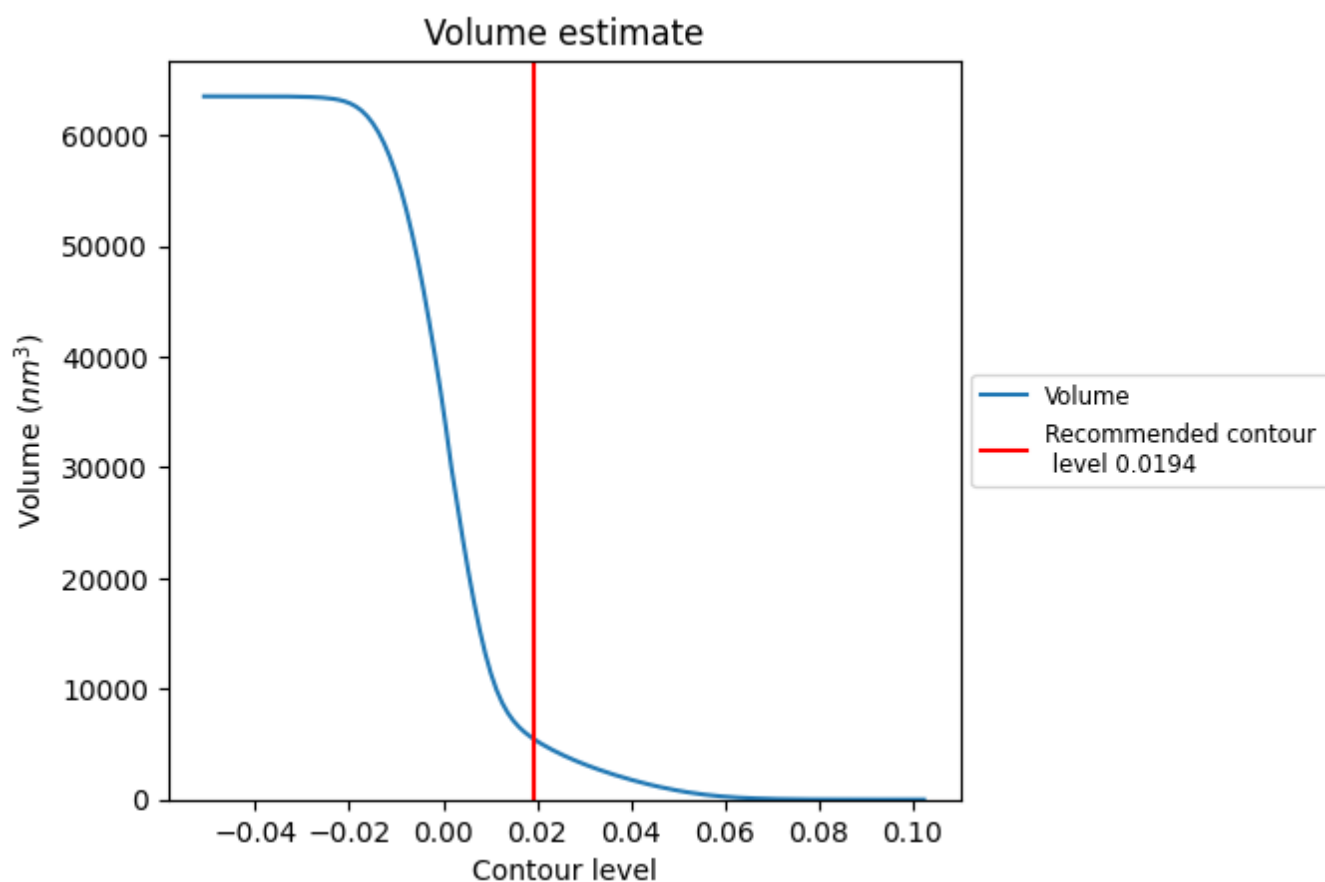
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

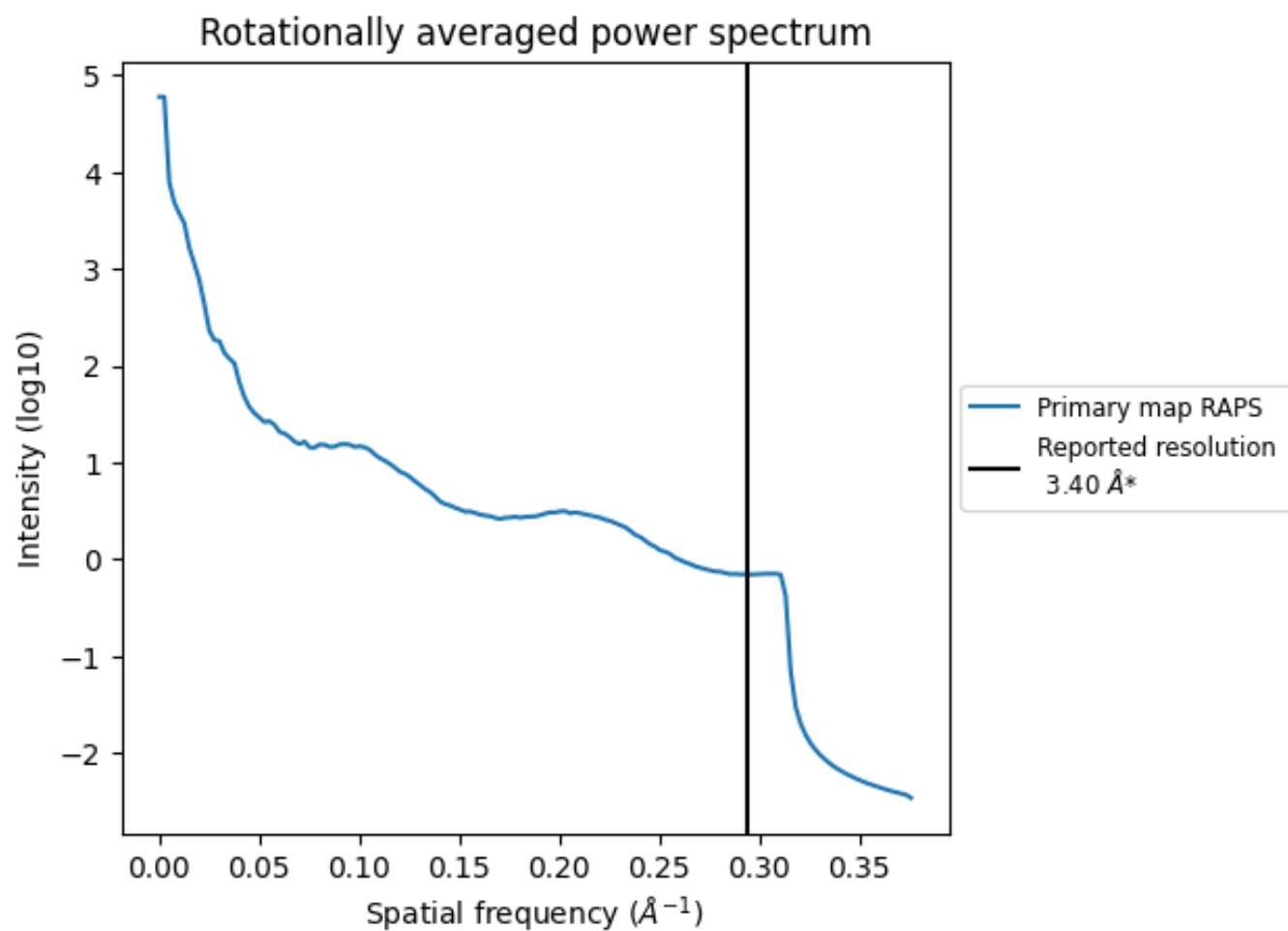
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5446 nm³; this corresponds to an approximate mass of 4919 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

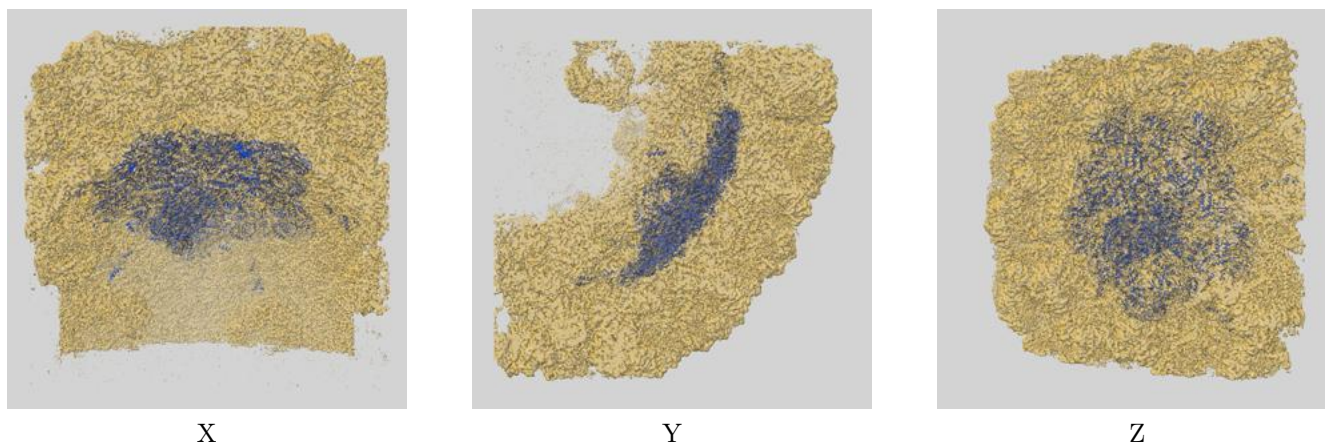
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

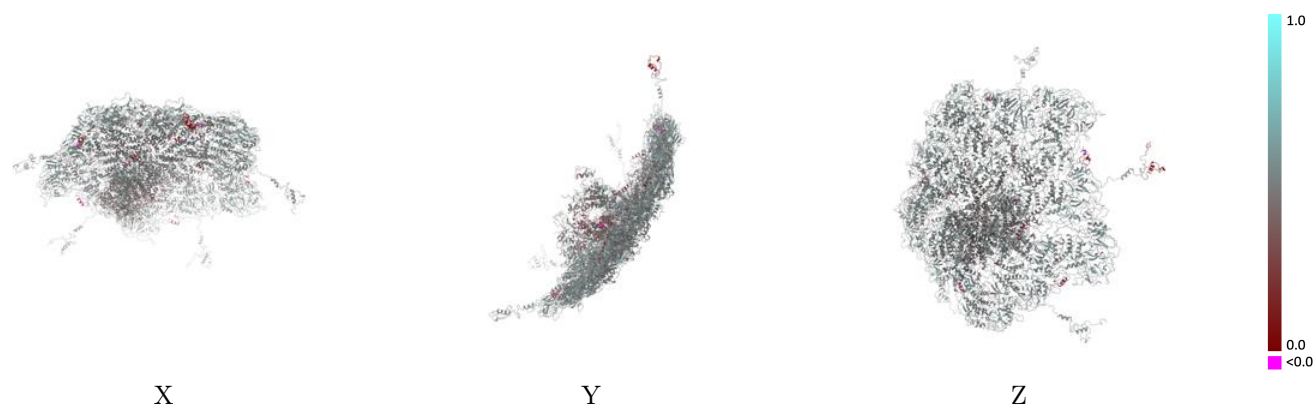
This section contains information regarding the fit between EMDB map EMD-9050 and PDB model 6M99. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



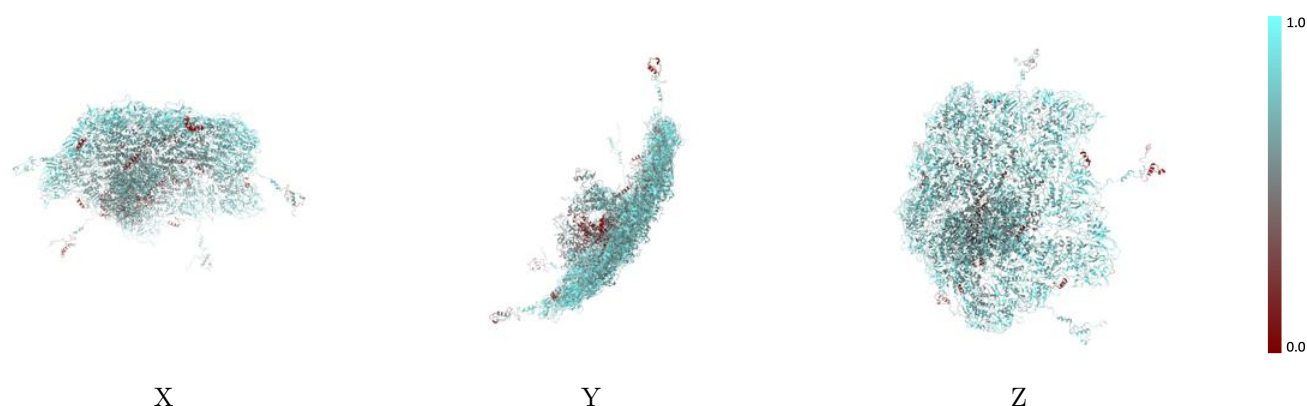
The images above show the 3D surface view of the map at the recommended contour level 0.0194 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



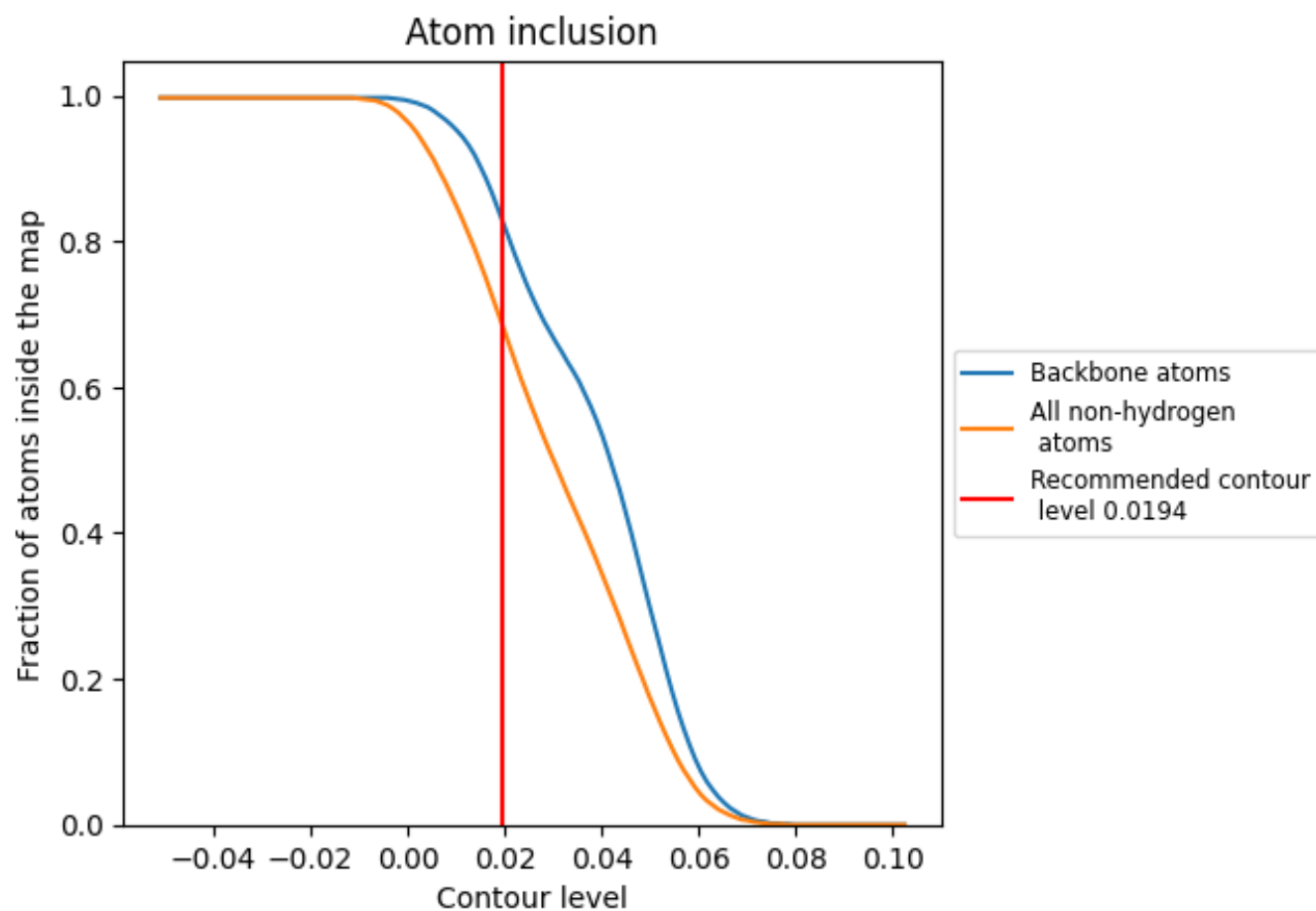
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0194).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 69% 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 (0.0194) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6880	0.4810
A	0.5590	0.4400
B	0.5730	0.4550
C	0.7000	0.4940
D	0.6850	0.4850
E	0.7260	0.4860
F	0.7140	0.4860
G	0.7120	0.4870
H	0.6900	0.4690
I	0.7320	0.4970
J	0.7000	0.4840
K	0.7280	0.4980
L	0.7020	0.4860

