



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:23 AM UTC

PDB ID : 9CUL / pdb_00009cul
EMDB ID : EMD-45937
Title : Bacteriophage PhiTE mature capsid
Authors : Hodgkinson-Bean, J.; Ayala, R.
Deposited on : 2024-07-26
Resolution : 3.60 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

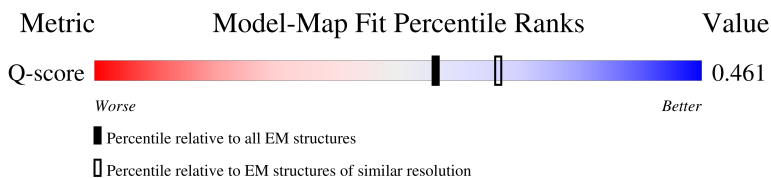
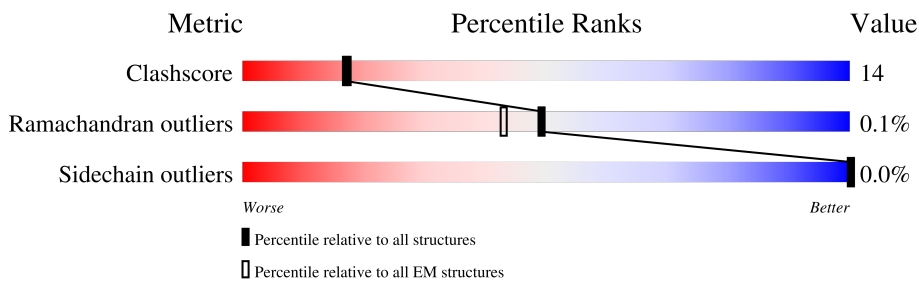
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 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.














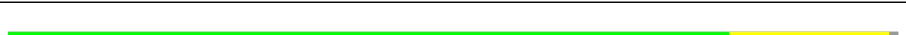

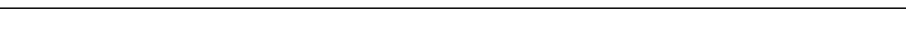
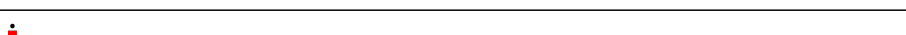
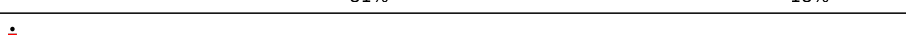
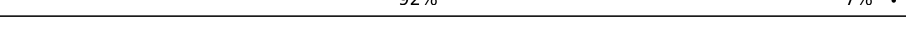
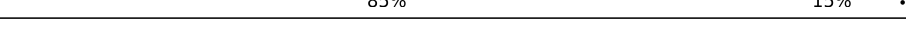




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	332	78% 21%
1	B	332	84% 16% .
1	C	332	82% 17% .
1	D	332	81% 18%

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Mol	Chain	Length	Quality of chain
1	E	332	 79% 21%
1	F	332	 80% 19%
1	G	332	 75% 24%
1	H	332	 77% 22%
1	I	332	 79% 20%
1	J	332	 81% 19%
1	K	332	 75% 24%
1	L	332	 80% 20%
1	M	332	 86% 12%
2	a	149	 88% 11%
2	b	149	 76% 23%
2	c	149	 81% 18%
2	d	149	 80% 19%
2	e	149	 77% 21%
2	f	149	 81% 18%
2	g	149	 92% 7%
2	h	149	 85% 15%
2	i	149	 86% 13%
2	j	149	 91% 8%
2	k	149	 85% 15%
2	l	149	 71% 27%
2	m	149	 83% 17%

2 Entry composition [\(i\)](#)

There are 2 unique types of molecules in this entry. The entry contains 48409 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	G	330	Total 2640	C 1664	N 468	O 502	S 6	0	0
1	M	327	Total 2624	C 1655	N 465	O 499	S 5	0	0
1	C	330	Total 2640	C 1664	N 468	O 502	S 6	0	0
1	B	330	Total 2640	C 1664	N 468	O 502	S 6	0	0
1	F	330	Total 2640	C 1664	N 468	O 502	S 6	0	0
1	I	330	Total 2640	C 1664	N 468	O 502	S 6	0	0
1	D	331	Total 2647	C 1668	N 469	O 504	S 6	0	0
1	E	330	Total 2640	C 1664	N 468	O 502	S 6	0	0
1	H	330	Total 2640	C 1664	N 468	O 502	S 6	0	0
1	K	330	Total 2640	C 1664	N 468	O 502	S 6	0	0
1	L	330	Total 2639	C 1664	N 468	O 501	S 6	0	0
1	J	331	Total 2647	C 1668	N 469	O 504	S 6	0	0
1	A	331	Total 2647	C 1668	N 469	O 504	S 6	0	0

- Molecule 2 is a protein called Head stabilization/decoration protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	e	145	Total 1066	C 682	N 176	O 206	S 2	0	0
2	b	148	Total 1087	C 693	N 179	O 213	S 2	0	0

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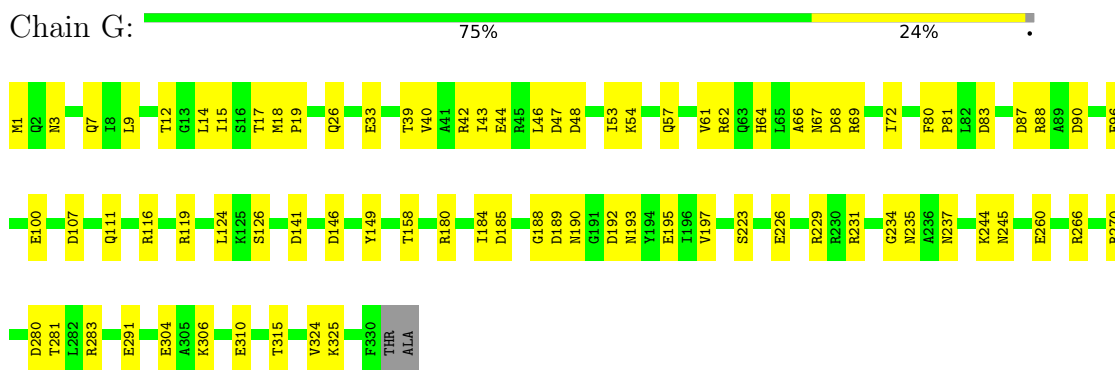
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	147	Total	C	N	O	S	0	0
			1078	687	178	211	2		
2	a	148	Total	C	N	O	S	0	0
			1087	693	179	213	2		
2	d	148	Total	C	N	O	S	0	0
			1087	693	179	213	2		
2	l	146	Total	C	N	O	S	0	0
			1071	682	177	210	2		
2	k	148	Total	C	N	O	S	0	0
			1087	693	179	213	2		
2	i	148	Total	C	N	O	S	0	0
			1087	693	179	213	2		
2	j	148	Total	C	N	O	S	0	0
			1087	693	179	213	2		
2	h	148	Total	C	N	O	S	0	0
			1087	693	179	213	2		
2	f	148	Total	C	N	O	S	0	0
			1087	693	179	213	2		
2	g	148	Total	C	N	O	S	0	0
			1087	693	179	213	2		
2	m	148	Total	C	N	O	S	0	0
			1087	693	179	213	2		

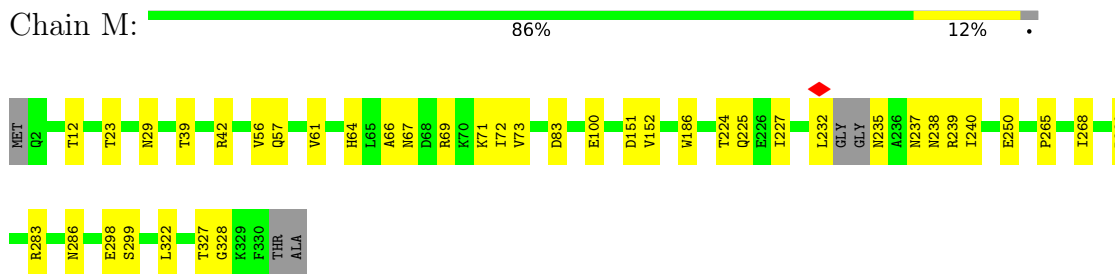
3 Residue-property plots [i](#)

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

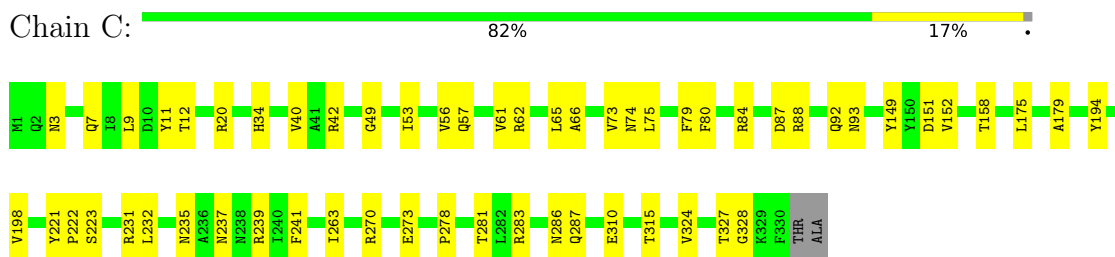
- Molecule 1: Major capsid protein



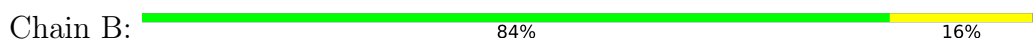
- Molecule 1: Major capsid protein

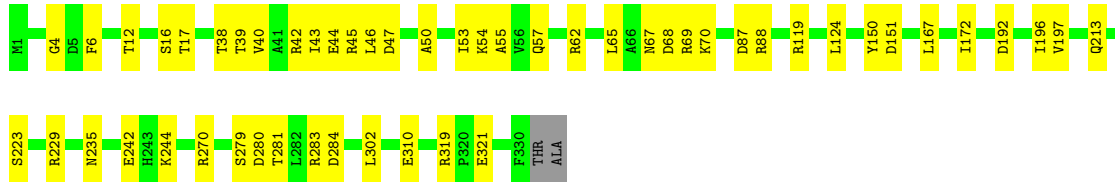


- Molecule 1: Major capsid protein

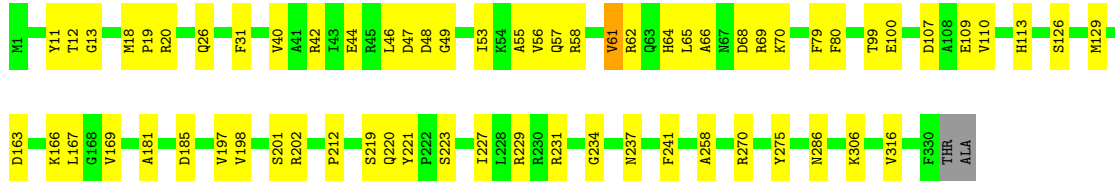
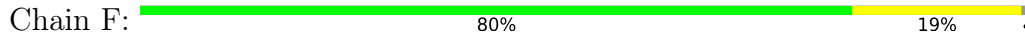


- Molecule 1: Major capsid protein

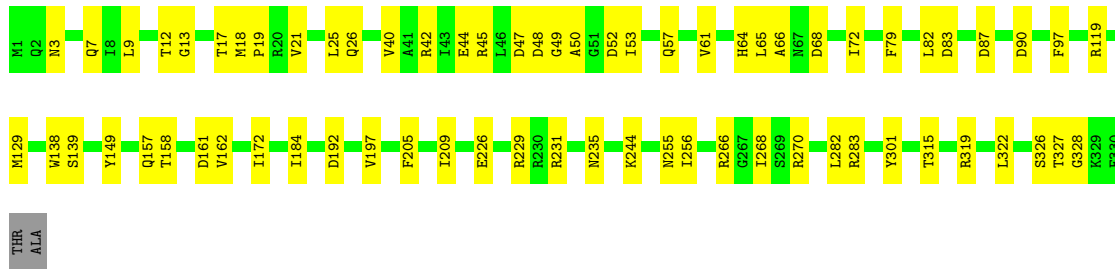
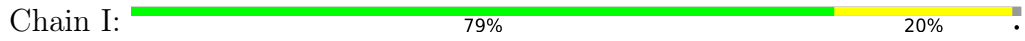




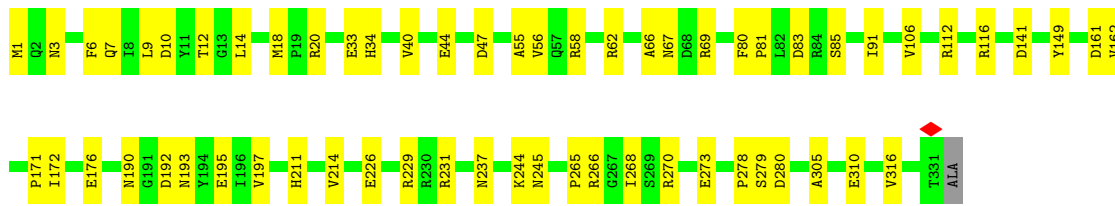
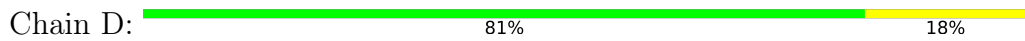
• Molecule 1: Major capsid protein



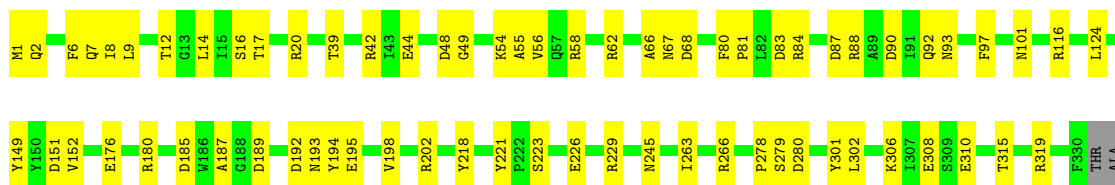
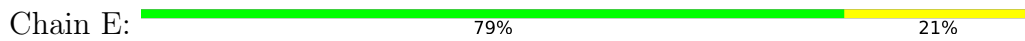
• Molecule 1: Major capsid protein




• Molecule 1: Major capsid protein

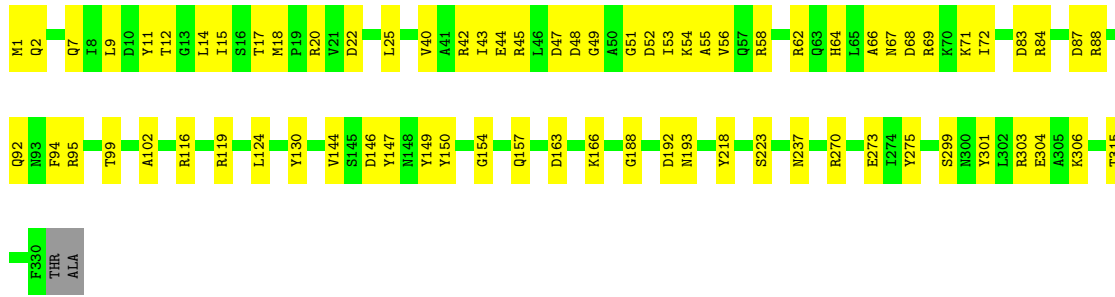


• Molecule 1: Major capsid protein




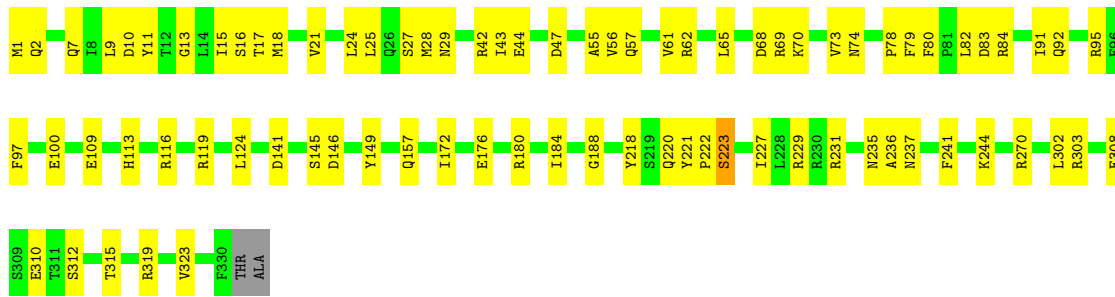
• Molecule 1: Major capsid protein

Chain H:  77% 22%




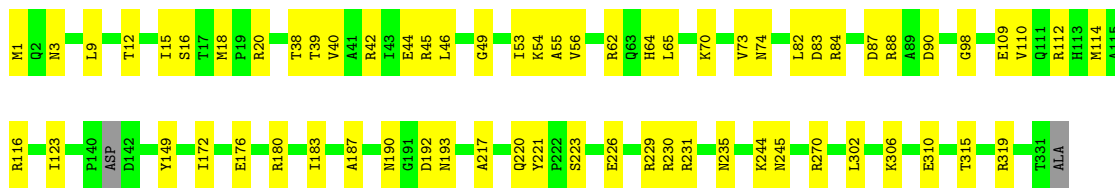
• Molecule 1: Major capsid protein

Chain K:  75% 24%




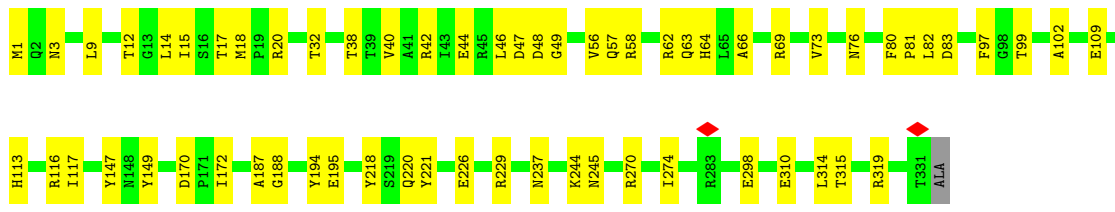
• Molecule 1: Major capsid protein

Chain L:  80% 20%

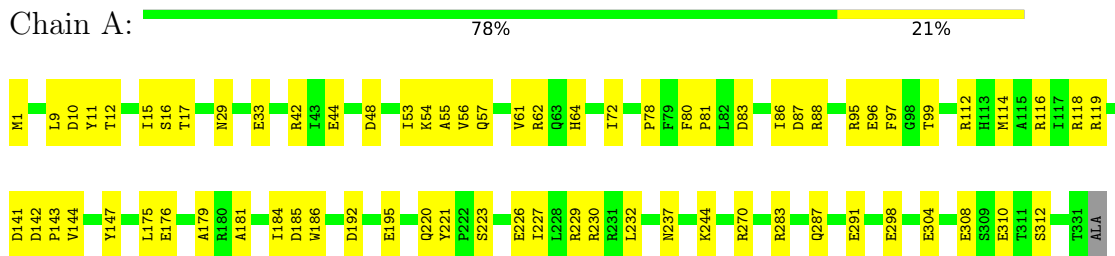


• Molecule 1: Major capsid protein

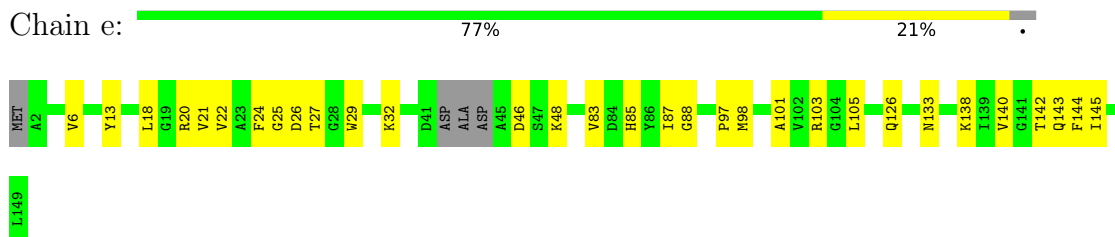
Chain J:  81% 19%



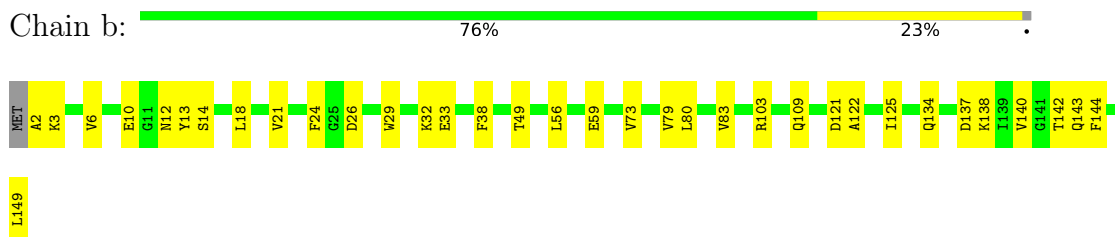
• Molecule 1: Major capsid protein



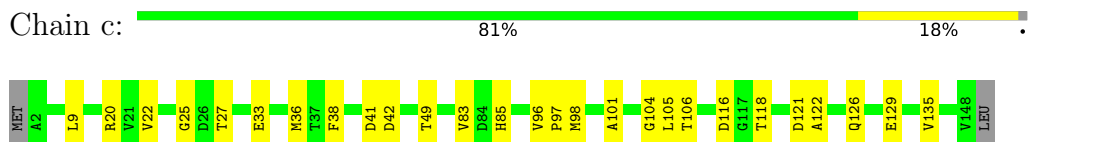
• Molecule 2: Head stabilization/decoration protein



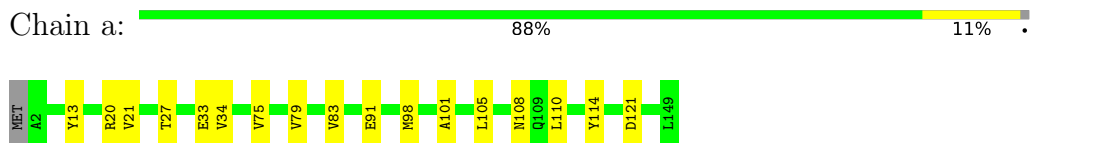
• Molecule 2: Head stabilization/decoration protein



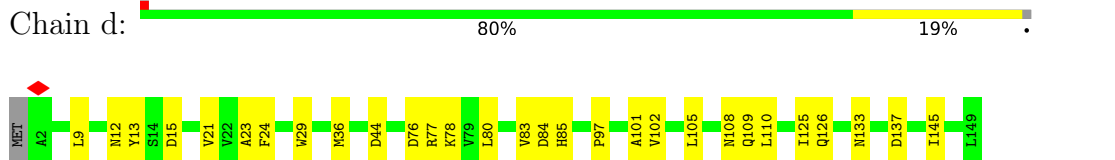
• Molecule 2: Head stabilization/decoration protein



• Molecule 2: Head stabilization/decoration protein

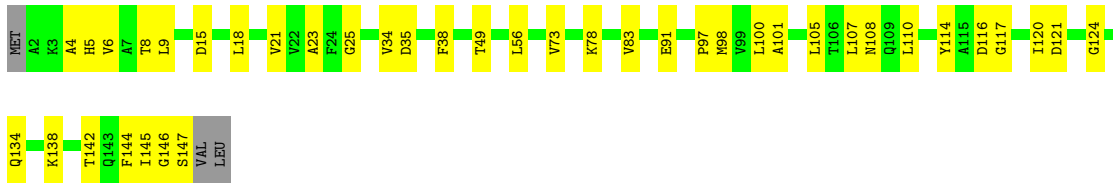


• Molecule 2: Head stabilization/decoration protein




- Molecule 2: Head stabilization/decoration protein

Chain l:  71% 27%




- Molecule 2: Head stabilization/decoration protein

Chain k:  85% 15%

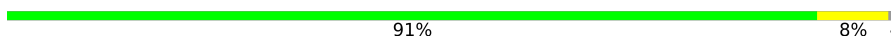


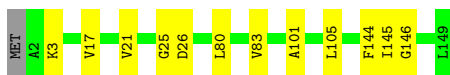
- Molecule 2: Head stabilization/decoration protein

Chain i:  86% 13%




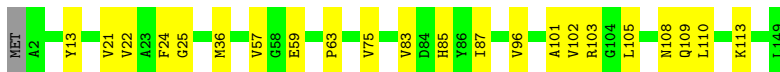
- Molecule 2: Head stabilization/decoration protein

Chain j:  91% 8%




- Molecule 2: Head stabilization/decoration protein

Chain h:  85% 15%



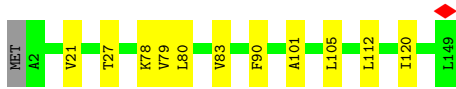
- Molecule 2: Head stabilization/decoration protein

Chain f:  81% 18%



- Molecule 2: Head stabilization/decoration protein

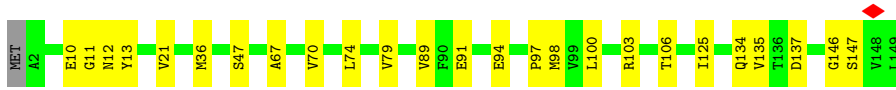
Chain g:  92% 7%



- Molecule 2: Head stabilization/decoration protein

Chain m: 83% 17%

A horizontal bar chart for Chain m showing 83% in green and 17% in yellow. A small red diamond is at the top left of the bar.



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	33053	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.673	Depositor
Minimum map value	-1.317	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.239	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	1248.2999, 1248.2999, 1248.2999	wwPDB
Map dimensions	808, 808, 808	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5449257, 1.5449257, 1.5449257	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/2704	0.35	0/3666
1	B	0.18	0/2697	0.48	0/3656
1	C	0.18	0/2697	0.47	0/3656
1	D	0.15	0/2704	0.35	0/3666
1	E	0.12	0/2697	0.31	0/3656
1	F	0.19	0/2697	0.48	0/3656
1	G	0.17	0/2697	0.35	0/3656
1	H	0.14	0/2697	0.33	0/3656
1	I	0.19	0/2697	0.50	0/3656
1	J	0.14	0/2704	0.33	0/3666
1	K	0.12	0/2697	0.34	1/3656 (0.0%)
1	L	0.13	0/2695	0.32	0/3652
1	M	0.11	0/2680	0.27	0/3633
2	a	0.16	0/1104	0.34	0/1500
2	b	0.12	0/1104	0.32	0/1500
2	c	0.16	0/1095	0.36	0/1489
2	d	0.16	0/1104	0.37	0/1500
2	e	0.14	0/1082	0.32	0/1468
2	f	0.16	0/1104	0.39	0/1500
2	g	0.16	0/1104	0.42	0/1500
2	h	0.17	0/1104	0.39	0/1500
2	i	0.16	0/1104	0.40	0/1500
2	j	0.16	0/1104	0.42	1/1500 (0.1%)
2	k	0.16	0/1104	0.40	0/1500
2	l	0.18	0/1088	0.45	0/1479
2	m	0.14	0/1104	0.37	0/1500
All	All	0.15	0/49368	0.38	2/66967 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	223	SER	CB-CA-C	-5.77	109.90	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	3	LYS	CB-CA-C	-5.26	110.50	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2647	0	2570	115	0
1	B	2640	0	2571	76	0
1	C	2640	0	2571	60	0
1	D	2647	0	2578	145	0
1	E	2640	0	2566	190	0
1	F	2640	0	2571	91	0
1	G	2640	0	2570	229	0
1	H	2640	0	2564	219	0
1	I	2640	0	2571	156	0
1	J	2647	0	2570	160	0
1	K	2640	0	2570	198	0
1	L	2639	0	2569	165	0
1	M	2624	0	2551	49	0
2	a	1087	0	1086	14	0
2	b	1087	0	1086	51	0
2	c	1078	0	1075	28	0
2	d	1087	0	1086	34	0
2	e	1066	0	1072	54	0
2	f	1087	0	1086	33	0
2	g	1087	0	1086	11	0
2	h	1087	0	1086	31	0
2	i	1087	0	1086	29	0
2	j	1087	0	1086	13	0
2	k	1087	0	1086	37	0
2	l	1071	0	1066	48	0
2	m	1087	0	1086	23	0
All	All	48409	0	47465	1319	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 14.

All (1319) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:MET:HE1	1:E:48:ASP:C	1.36	1.50
1:K:319:ARG:NH2	1:J:17:THR:CG2	1.78	1.46
1:D:18:MET:CE	1:E:48:ASP:C	1.86	1.46
1:D:229:ARG:NH2	1:E:221:TYR:CZ	1.85	1.45
1:G:1:MET:CE	1:H:42:ARG:HH11	1.28	1.44
1:D:80:PHE:CE1	1:E:55:ALA:HB2	1.53	1.41
1:G:141:ASP:CG	1:H:54:LYS:HD3	1.35	1.41
1:K:221:TYR:CE2	1:J:229:ARG:NH2	1.92	1.37
1:D:18:MET:HE1	1:E:49:GLY:N	1.08	1.37
1:F:11:TYR:HE1	1:A:44:GLU:OE2	1.07	1.35
1:K:319:ARG:HH22	1:J:17:THR:CG2	1.37	1.35
1:G:116:ARG:HH12	1:H:67:ASN:CA	1.37	1.34
2:e:13:TYR:HE1	1:H:87:ASP:OD2	1.07	1.34
1:D:18:MET:CE	1:E:49:GLY:N	1.85	1.33
1:G:1:MET:HE1	1:H:42:ARG:NH1	1.44	1.32
1:G:141:ASP:OD1	1:H:54:LYS:HD3	1.18	1.31
1:K:310:GLU:OE2	1:L:62:ARG:CZ	1.77	1.31
1:G:69:ARG:HD3	2:k:10:GLU:OE2	1.18	1.30
1:I:12:THR:O	1:J:270:ARG:NH2	1.63	1.29
1:K:42:ARG:O	1:J:12:THR:CG2	1.80	1.29
1:G:62:ARG:HD3	1:L:83:ASP:OD2	1.10	1.28
1:K:124:LEU:HD22	1:L:53:ILE:CG2	1.63	1.28
1:K:221:TYR:CZ	1:J:229:ARG:NH2	2.01	1.28
1:G:43:ILE:HG12	1:L:12:THR:CG2	1.64	1.28
1:G:69:ARG:CD	2:k:10:GLU:OE2	1.79	1.28
1:G:1:MET:CE	1:H:42:ARG:NH1	1.92	1.27
1:G:116:ARG:NH1	1:H:67:ASN:HA	1.47	1.27
1:D:229:ARG:NH2	1:E:221:TYR:CE1	2.01	1.27
1:D:229:ARG:CZ	1:E:221:TYR:CZ	2.16	1.27
1:K:44:GLU:HG3	1:J:14:LEU:CD1	1.64	1.27
1:F:62:ARG:NH1	1:E:310:GLU:OE2	1.69	1.25
1:I:18:MET:O	1:J:188:GLY:O	1.54	1.25
1:G:116:ARG:NH2	1:H:68:ASP:HB3	1.50	1.25
2:c:85:HIS:CD2	1:D:3:ASN:HD21	1.54	1.25
1:K:310:GLU:OE2	1:L:62:ARG:NE	1.68	1.25
1:C:310:GLU:OE2	1:D:62:ARG:NH2	1.68	1.25
1:I:283:ARG:NH2	1:E:302:LEU:HD12	1.50	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:TYR:CE1	1:A:44:GLU:OE2	1.91	1.23
1:G:12:THR:O	1:H:270:ARG:NH2	1.72	1.22
1:D:18:MET:SD	1:E:48:ASP:CB	2.26	1.22
1:D:1:MET:HE1	1:E:42:ARG:HD2	1.22	1.20
1:D:116:ARG:NH1	1:E:67:ASN:HA	1.56	1.20
1:K:62:ARG:NH2	1:J:310:GLU:OE2	1.74	1.20
2:e:13:TYR:CE1	1:H:87:ASP:OD2	1.94	1.20
1:K:68:ASP:CB	1:J:116:ARG:HH22	1.53	1.20
1:G:67:ASN:OD1	1:L:84:ARG:NH1	1.73	1.20
1:D:18:MET:SD	1:E:48:ASP:HB2	1.81	1.19
1:K:44:GLU:CG	1:J:14:LEU:HD13	1.72	1.19
1:G:237:ASN:ND2	1:H:192:ASP:CG	2.00	1.19
1:G:67:ASN:OD1	1:L:84:ARG:NH2	1.75	1.19
1:D:81:PRO:CD	1:E:56:VAL:HG22	1.72	1.18
1:I:9:LEU:CD1	1:J:42:ARG:HD2	1.73	1.18
1:G:62:ARG:NH2	1:L:310:GLU:OE2	1.75	1.18
1:I:283:ARG:CG	1:E:302:LEU:HD13	1.75	1.17
1:D:81:PRO:HD3	1:E:56:VAL:HG22	1.17	1.17
1:K:10:ASP:CG	1:L:38:THR:HG22	1.68	1.17
1:B:44:GLU:OE1	1:A:11:TYR:OH	1.62	1.17
1:K:124:LEU:HD22	1:L:53:ILE:HG23	1.25	1.17
1:K:184:ILE:O	1:J:20:ARG:CD	1.83	1.17
1:K:319:ARG:NH2	1:J:17:THR:HG22	1.42	1.17
1:G:310:GLU:OE2	1:H:62:ARG:NH2	1.77	1.15
1:I:231:ARG:HB3	1:J:245:ASN:ND2	1.61	1.15
1:D:81:PRO:CD	1:E:56:VAL:CG2	2.23	1.15
1:G:67:ASN:OD1	1:L:84:ARG:CZ	1.95	1.15
1:I:235:ASN:ND2	1:J:194:TYR:O	1.80	1.14
2:i:2:ALA:O	1:H:147:TYR:HE1	1.29	1.14
1:K:13:GLY:HA3	1:L:270:ARG:NH1	1.62	1.14
1:G:42:ARG:O	1:L:12:THR:HG22	1.47	1.14
2:i:11:GLY:HA2	1:H:67:ASN:HD21	1.05	1.14
1:G:116:ARG:HH21	1:H:68:ASP:HB3	0.98	1.13
1:G:7:GLN:NE2	2:h:83:VAL:HA	1.63	1.13
1:D:229:ARG:CZ	1:E:221:TYR:CE1	2.31	1.13
1:G:68:ASP:HB2	1:L:116:ARG:NH2	1.63	1.13
1:D:80:PHE:CE1	1:E:55:ALA:CB	2.31	1.12
1:G:12:THR:HG22	1:H:42:ARG:O	1.47	1.12
1:I:48:ASP:HB3	1:H:18:MET:SD	1.88	1.12
1:G:62:ARG:CD	1:L:83:ASP:OD2	1.96	1.12
1:K:17:THR:CG2	1:L:319:ARG:HH21	1.61	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:VAL:HG12	1:A:9:LEU:HD11	1.29	1.11
1:D:18:MET:HE3	1:E:48:ASP:C	1.73	1.11
1:D:226:GLU:OE2	1:E:221:TYR:OH	1.68	1.11
2:e:13:TYR:HE1	1:H:87:ASP:CG	1.57	1.11
1:G:43:ILE:HG12	1:L:12:THR:HG21	1.24	1.11
1:E:1:MET:HE1	1:H:2:GLN:HE22	0.97	1.10
1:D:116:ARG:HH12	1:E:67:ASN:CA	1.65	1.10
1:G:141:ASP:CG	1:H:54:LYS:CD	2.24	1.10
1:G:229:ARG:NH1	1:H:223:SER:OG	1.85	1.10
1:G:67:ASN:ND2	2:k:15:ASP:CG	2.10	1.09
1:D:237:ASN:HD21	1:E:192:ASP:HA	1.05	1.09
1:G:116:ARG:HH22	1:H:68:ASP:N	1.48	1.09
1:K:308:GLU:OE2	1:L:62:ARG:NH1	1.84	1.09
1:K:270:ARG:NH2	1:J:12:THR:O	1.84	1.09
1:G:69:ARG:CD	2:k:10:GLU:CD	2.25	1.08
1:K:68:ASP:HB2	1:J:116:ARG:HH22	0.95	1.08
1:D:237:ASN:ND2	1:E:192:ASP:CG	2.12	1.08
1:G:306:LYS:NZ	2:j:25:GLY:O	1.86	1.08
2:b:18:LEU:HD13	1:J:64:HIS:CD2	1.88	1.07
1:I:283:ARG:HG3	1:E:302:LEU:HD13	1.22	1.07
1:D:80:PHE:CD1	1:E:55:ALA:HA	1.90	1.07
1:D:81:PRO:HD3	1:E:56:VAL:CG2	1.84	1.07
1:K:319:ARG:NH2	1:J:17:THR:HG21	1.59	1.07
2:c:85:HIS:CD2	1:D:3:ASN:ND2	2.22	1.06
1:G:15:ILE:CD1	1:H:270:ARG:HH11	1.66	1.06
1:K:310:GLU:OE2	1:L:62:ARG:NH2	1.87	1.06
1:K:42:ARG:O	1:J:12:THR:HG22	0.90	1.05
1:G:62:ARG:HH22	1:L:310:GLU:CD	1.65	1.05
1:F:237:ASN:HB2	1:A:192:ASP:OD2	1.56	1.05
2:e:85:HIS:HE1	1:E:7:GLN:OE1	1.39	1.05
1:I:231:ARG:CB	1:J:245:ASN:HD21	1.70	1.05
2:k:26:ASP:OD2	2:m:106:THR:OG1	1.75	1.05
1:D:112:ARG:NH1	1:E:68:ASP:OD2	1.90	1.05
1:G:116:ARG:NH2	1:H:68:ASP:CB	2.20	1.04
1:G:141:ASP:OD1	1:H:54:LYS:CD	2.05	1.04
1:D:229:ARG:NH2	1:E:221:TYR:CE2	2.25	1.04
1:K:184:ILE:O	1:J:20:ARG:HD3	1.52	1.04
1:D:18:MET:HE3	1:E:48:ASP:O	1.57	1.04
1:M:57:GLN:NE2	2:m:97:PRO:O	1.90	1.03
1:C:12:THR:O	1:D:270:ARG:NH2	1.91	1.03
1:I:283:ARG:CD	1:E:302:LEU:HD12	1.87	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ARG:NH1	1:E:223:SER:OG	1.90	1.03
1:E:1:MET:CE	1:H:2:GLN:HE22	1.69	1.03
1:G:237:ASN:ND2	1:H:192:ASP:OD2	1.91	1.03
1:M:286:ASN:ND2	1:K:91:ILE:O	1.92	1.03
1:G:68:ASP:HB2	1:L:116:ARG:HH22	0.91	1.03
1:K:319:ARG:HH22	1:J:17:THR:HG22	0.93	1.03
1:D:18:MET:CE	1:E:49:GLY:CA	2.37	1.02
1:D:18:MET:SD	1:E:48:ASP:HB3	1.97	1.02
1:G:67:ASN:ND2	2:k:15:ASP:OD2	1.93	1.02
1:I:48:ASP:CB	1:H:18:MET:HE1	1.89	1.02
2:k:29:TRP:HA	2:m:134:GLN:OE1	1.60	1.01
1:G:15:ILE:HD11	1:H:270:ARG:NH1	1.75	1.00
1:G:83:ASP:OD2	1:H:62:ARG:HD3	1.60	1.00
1:D:141:ASP:OD2	1:E:54:LYS:HD3	1.59	1.00
1:E:1:MET:HE1	1:H:2:GLN:NE2	1.75	1.00
2:b:143:GLN:O	1:J:49:GLY:HA3	1.59	1.00
1:I:283:ARG:HD3	1:E:302:LEU:CD1	1.91	1.00
1:K:17:THR:HG21	1:L:319:ARG:HH21	1.23	1.00
1:K:68:ASP:HB2	1:J:116:ARG:NH2	1.76	1.00
1:I:283:ARG:HD3	1:E:302:LEU:HD12	1.39	1.00
1:I:184:ILE:HG23	1:H:20:ARG:NH2	1.76	0.99
1:E:2:GLN:NE2	1:H:1:MET:HE1	1.77	0.99
1:D:116:ARG:HH12	1:E:67:ASN:HA	0.83	0.99
1:K:188:GLY:O	1:J:18:MET:O	1.81	0.99
1:G:270:ARG:HD3	1:L:15:ILE:CD1	1.92	0.99
1:I:283:ARG:CD	1:E:302:LEU:CD1	2.40	0.99
1:E:2:GLN:HE22	1:H:1:MET:CE	1.76	0.99
2:i:2:ALA:O	1:H:147:TYR:CE1	2.14	0.98
1:G:67:ASN:ND2	2:k:15:ASP:OD1	1.94	0.98
1:G:83:ASP:OD2	1:H:62:ARG:CD	2.10	0.98
1:G:69:ARG:HD2	2:k:10:GLU:CD	1.87	0.98
1:I:283:ARG:HH21	1:E:302:LEU:CD1	1.76	0.98
1:K:308:GLU:CD	1:L:62:ARG:HH12	1.70	0.98
1:G:235:ASN:HB3	1:H:193:ASN:HA	1.43	0.98
1:C:20:ARG:HA	1:D:190:ASN:HD21	1.27	0.98
1:F:62:ARG:NH1	1:E:308:GLU:OE2	1.95	0.97
1:I:283:ARG:NH2	1:E:302:LEU:CD1	2.27	0.97
1:I:9:LEU:HD13	1:J:42:ARG:HD2	1.43	0.97
1:K:124:LEU:HD22	1:L:53:ILE:HG21	1.43	0.97
1:I:319:ARG:HH22	1:H:17:THR:CG2	1.78	0.97
1:G:270:ARG:HD3	1:L:15:ILE:HD11	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:270:ARG:HD3	1:H:15:ILE:HD11	1.45	0.96
1:I:283:ARG:CZ	1:E:302:LEU:HD12	1.93	0.96
1:K:68:ASP:CB	1:J:116:ARG:NH2	2.25	0.96
1:F:70:LYS:HD3	1:E:97:PHE:CE1	1.99	0.96
1:I:283:ARG:HH21	1:E:302:LEU:HD12	1.04	0.96
1:G:15:ILE:CD1	1:H:270:ARG:NH1	2.28	0.96
1:G:68:ASP:CB	1:L:116:ARG:HH22	1.79	0.96
1:D:1:MET:HE1	1:E:42:ARG:CD	1.95	0.95
2:l:134:GLN:OE1	2:m:103:ARG:NH2	1.99	0.95
1:K:44:GLU:CG	1:J:14:LEU:CD1	2.34	0.95
1:D:237:ASN:ND2	1:E:192:ASP:OD1	1.99	0.95
2:b:13:TYR:HE2	1:I:87:ASP:OD2	1.48	0.95
1:K:65:LEU:HD21	1:J:82:LEU:HD21	1.48	0.94
1:B:42:ARG:NH2	1:A:1:MET:SD	2.40	0.94
1:D:229:ARG:NE	1:E:221:TYR:OH	2.01	0.94
1:G:43:ILE:CG1	1:L:12:THR:HG21	1.98	0.94
1:F:220:GLN:OE1	1:A:220:GLN:NE2	2.00	0.94
1:I:48:ASP:HB2	1:H:18:MET:HE1	1.50	0.94
1:C:20:ARG:HA	1:D:190:ASN:ND2	1.81	0.94
1:K:44:GLU:HG2	1:J:14:LEU:HD13	1.46	0.94
1:B:270:ARG:HD3	1:A:15:ILE:HD11	1.47	0.93
1:G:68:ASP:CB	1:L:116:ARG:NH2	2.30	0.93
2:d:12:ASN:OD1	1:E:90:ASP:CG	2.12	0.93
1:K:319:ARG:HH21	1:J:17:THR:CG2	1.81	0.93
2:f:3:LYS:NZ	1:A:143:PRO:O	2.02	0.93
1:M:61:VAL:HG11	2:l:134:GLN:NE2	1.84	0.92
1:K:13:GLY:HA3	1:L:270:ARG:HH12	1.16	0.92
2:e:13:TYR:CE1	1:H:87:ASP:CG	2.42	0.91
1:G:1:MET:HE2	1:H:42:ARG:NH1	1.83	0.91
2:i:11:GLY:HA2	1:H:67:ASN:ND2	1.86	0.90
1:K:17:THR:CG2	1:L:319:ARG:NH2	2.33	0.90
1:I:9:LEU:HD13	1:J:42:ARG:CD	2.01	0.90
1:M:286:ASN:ND2	1:K:92:GLN:O	2.05	0.90
1:K:310:GLU:CD	1:L:62:ARG:NH2	2.29	0.90
2:e:85:HIS:CE1	1:E:7:GLN:OE1	2.25	0.90
1:G:9:LEU:HD13	1:H:40:VAL:CG1	2.02	0.90
1:B:40:VAL:HG12	1:A:9:LEU:CD1	2.02	0.90
1:I:40:VAL:CG1	1:H:9:LEU:HD22	2.01	0.90
1:D:237:ASN:HD21	1:E:192:ASP:CA	1.85	0.90
1:D:226:GLU:CD	1:E:221:TYR:HH	1.79	0.89
1:K:1:MET:CE	1:L:42:ARG:HD2	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:283:ARG:CG	1:E:302:LEU:CD1	2.50	0.89
1:G:116:ARG:HH12	1:H:67:ASN:HA	0.74	0.89
1:C:9:LEU:CD1	1:D:40:VAL:HG12	2.03	0.89
1:D:1:MET:CE	1:E:42:ARG:HD2	2.03	0.89
1:M:286:ASN:HD21	1:K:92:GLN:C	1.79	0.89
1:K:43:ILE:HG13	1:J:12:THR:HG21	1.53	0.89
1:G:15:ILE:HD13	1:H:270:ARG:HH11	1.36	0.89
2:b:10:GLU:OE2	1:J:69:ARG:HD3	1.72	0.89
2:d:13:TYR:HE2	1:E:87:ASP:OD2	1.54	0.89
1:G:180:ARG:NH1	1:L:231:ARG:HD2	1.88	0.88
1:G:17:THR:OG1	1:H:47:ASP:HA	1.71	0.88
1:D:80:PHE:CD1	1:E:55:ALA:CA	2.56	0.88
1:K:62:ARG:CZ	1:J:310:GLU:OE2	2.21	0.88
2:e:18:LEU:HD13	1:I:64:HIS:CD2	2.08	0.88
1:L:88:ARG:NH2	1:L:302:LEU:O	2.06	0.88
1:B:67:ASN:HA	1:A:116:ARG:HH12	1.36	0.88
1:D:80:PHE:HE1	1:E:55:ALA:HB2	1.14	0.87
1:D:237:ASN:ND2	1:E:192:ASP:HA	1.88	0.87
1:G:7:GLN:HE21	2:h:83:VAL:HA	1.33	0.87
2:b:138:LYS:NZ	1:J:56:VAL:HG22	1.90	0.87
1:K:13:GLY:CA	1:L:270:ARG:HH12	1.88	0.87
1:G:69:ARG:HD2	2:k:10:GLU:OE2	1.72	0.86
1:D:229:ARG:CZ	1:E:221:TYR:OH	2.21	0.86
1:K:62:ARG:CD	1:J:83:ASP:OD2	2.22	0.86
1:I:9:LEU:HD22	1:J:40:VAL:HG12	1.57	0.86
1:K:9:LEU:HA	1:L:38:THR:HG21	1.56	0.86
2:b:138:LYS:HZ2	1:J:56:VAL:HG22	1.41	0.86
1:K:84:ARG:HD2	1:L:65:LEU:HB3	1.55	0.86
1:K:221:TYR:OH	1:J:229:ARG:NH2	2.09	0.85
1:G:57:GLN:NE2	2:l:97:PRO:HB2	1.91	0.85
1:G:67:ASN:CG	1:L:84:ARG:HH22	1.84	0.85
2:b:26:ASP:OD2	2:c:106:THR:HG21	1.76	0.85
1:I:48:ASP:HB3	1:H:18:MET:CE	2.06	0.85
1:I:231:ARG:HB3	1:J:245:ASN:HD21	0.77	0.85
1:I:57:GLN:NE2	1:H:144:VAL:HG21	1.92	0.85
1:G:40:VAL:CG1	1:L:9:LEU:HD22	2.06	0.85
2:i:11:GLY:CA	1:H:67:ASN:HD21	1.88	0.85
1:K:10:ASP:OD2	1:L:38:THR:HG22	1.77	0.85
1:G:180:ARG:NH2	1:L:231:ARG:HH11	1.74	0.85
1:K:1:MET:SD	1:L:42:ARG:HD2	2.18	0.84
1:K:62:ARG:NH1	1:J:310:GLU:OE2	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:ASN:HD21	1:H:192:ASP:CG	1.79	0.84
2:d:13:TYR:CE2	1:E:87:ASP:OD2	2.29	0.84
2:e:140:VAL:HG13	1:I:52:ASP:O	1.78	0.84
1:K:184:ILE:HG22	1:J:20:ARG:NH1	1.92	0.84
2:e:32:LYS:NZ	2:f:129:GLU:OE2	2.11	0.84
1:F:44:GLU:O	1:E:14:LEU:HD12	1.77	0.84
1:E:2:GLN:HE22	1:H:1:MET:HE1	1.34	0.84
1:A:78:PRO:O	1:A:312:SER:OG	1.94	0.84
1:I:9:LEU:HD12	1:J:42:ARG:HD2	1.60	0.83
1:G:229:ARG:CZ	1:H:223:SER:OG	2.26	0.83
2:l:146:GLY:O	2:l:147:SER:OG	1.97	0.83
1:G:7:GLN:HE22	2:h:83:VAL:HG13	1.43	0.82
1:D:81:PRO:CD	1:E:56:VAL:HG21	2.09	0.82
1:H:17:THR:O	1:H:18:MET:HE2	1.77	0.82
1:G:48:ASP:HB3	1:L:18:MET:SD	2.19	0.82
1:G:195:GLU:N	1:G:195:GLU:OE2	2.12	0.82
1:K:17:THR:HG22	1:L:319:ARG:NH2	1.93	0.82
1:K:237:ASN:HB3	1:L:192:ASP:OD1	1.78	0.82
1:F:12:THR:O	1:A:270:ARG:NH2	2.12	0.82
1:I:270:ARG:CD	1:H:15:ILE:HD11	2.08	0.82
1:D:81:PRO:HG2	1:E:56:VAL:HG21	1.59	0.82
1:M:71:LYS:HG2	2:l:8:THR:CG2	2.09	0.82
1:B:62:ARG:NH2	1:A:83:ASP:OD2	2.12	0.82
1:I:25:LEU:HD22	1:I:129:MET:HE3	1.62	0.82
1:K:17:THR:HG22	1:L:319:ARG:HH21	1.43	0.82
1:G:12:THR:HG21	1:H:43:ILE:HG13	1.59	0.82
1:D:80:PHE:CE1	1:E:55:ALA:CA	2.63	0.81
1:K:56:VAL:HG22	1:J:81:PRO:CD	2.11	0.81
1:K:21:VAL:HG12	1:L:190:ASN:HD21	1.46	0.81
2:c:97:PRO:O	2:c:98:MET:HE2	1.81	0.81
2:a:33:GLU:OE2	1:K:57:GLN:HG2	1.80	0.81
1:G:12:THR:CG2	1:H:43:ILE:HG13	2.11	0.81
1:G:17:THR:HG21	1:H:45:ARG:HH21	1.45	0.81
1:F:237:ASN:CB	1:A:192:ASP:OD2	2.28	0.81
1:I:184:ILE:CG2	1:H:20:ARG:NH2	2.44	0.81
1:I:83:ASP:OD2	1:J:62:ARG:HD3	1.80	0.80
1:D:18:MET:CE	1:E:49:GLY:HA2	2.09	0.80
1:M:66:ALA:HB1	2:l:15:ASP:HB2	1.63	0.80
1:G:116:ARG:NH1	1:H:67:ASN:CA	2.22	0.80
1:M:286:ASN:CG	1:K:92:GLN:O	2.23	0.80
2:e:138:LYS:NZ	1:I:61:VAL:HG23	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:11:TYR:HE1	1:A:44:GLU:CD	1.89	0.80
2:e:25:GLY:O	1:F:306:LYS:NZ	2.13	0.80
1:I:9:LEU:CD1	1:J:42:ARG:CD	2.57	0.80
1:I:48:ASP:CB	1:H:18:MET:CE	2.60	0.80
1:G:26:GLN:OE1	1:G:126:SER:OG	1.99	0.80
1:B:40:VAL:CG1	1:A:9:LEU:HD11	2.11	0.79
1:K:44:GLU:HG3	1:J:14:LEU:HD12	1.63	0.79
1:A:298:GLU:N	1:A:298:GLU:OE1	2.15	0.79
1:G:116:ARG:HH12	1:H:67:ASN:C	1.89	0.79
2:e:26:ASP:OD2	2:f:106:THR:OG1	2.01	0.79
1:B:40:VAL:CG1	1:A:9:LEU:CD1	2.60	0.79
1:C:9:LEU:HD11	1:D:40:VAL:HG12	1.65	0.79
1:D:81:PRO:CG	1:E:56:VAL:HG21	2.12	0.79
2:b:134:GLN:OE1	2:d:29:TRP:HA	1.83	0.79
1:F:44:GLU:C	1:E:14:LEU:HD12	2.07	0.79
1:G:67:ASN:CG	1:L:84:ARG:NH2	2.41	0.79
1:I:47:ASP:OD1	1:H:17:THR:OG1	2.01	0.79
1:G:184:ILE:C	1:L:20:ARG:NH2	2.38	0.78
1:F:181:ALA:HB1	1:E:202:ARG:HH12	1.48	0.78
1:I:18:MET:O	1:J:188:GLY:C	2.26	0.78
1:K:84:ARG:CD	1:L:65:LEU:HB3	2.13	0.78
1:B:192:ASP:OD2	1:A:237:ASN:ND2	2.17	0.78
1:G:17:THR:OG1	1:H:47:ASP:OD1	1.98	0.78
1:G:40:VAL:HG11	1:L:9:LEU:HD22	1.64	0.78
1:I:40:VAL:HG11	1:H:9:LEU:CD2	2.14	0.78
1:M:71:LYS:HG2	2:l:8:THR:HG22	1.63	0.78
1:C:84:ARG:HH12	1:D:67:ASN:ND2	1.83	0.77
1:I:283:ARG:CZ	1:E:302:LEU:HB2	2.12	0.77
1:G:116:ARG:HH22	1:H:68:ASP:CA	1.97	0.77
1:I:42:ARG:O	1:H:12:THR:OG1	2.03	0.77
1:K:308:GLU:CD	1:L:62:ARG:NH1	2.37	0.77
1:G:192:ASP:OD2	1:G:193:ASN:N	2.18	0.77
1:M:286:ASN:OD1	1:K:92:GLN:O	2.02	0.77
1:D:229:ARG:NH1	1:E:221:TYR:CE1	2.53	0.77
1:K:184:ILE:CG2	1:J:20:ARG:NH1	2.48	0.77
1:M:283:ARG:HH21	1:K:302:LEU:CD1	1.98	0.76
1:I:9:LEU:CD2	1:J:40:VAL:CG1	2.62	0.76
1:I:48:ASP:OD1	1:I:49:GLY:N	2.18	0.76
2:m:91:GLU:OE1	2:m:91:GLU:N	2.18	0.76
1:F:47:ASP:OD2	1:F:69:ARG:NH1	2.19	0.76
1:D:47:ASP:OD2	1:D:69:ARG:NH1	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:PHE:HD1	1:E:55:ALA:HA	1.51	0.76
1:D:237:ASN:HD22	1:E:192:ASP:CG	1.86	0.76
1:G:83:ASP:OD2	1:H:62:ARG:HD2	1.84	0.76
1:M:186:TRP:CE2	2:l:147:SER:HB3	2.21	0.76
2:d:13:TYR:HB3	1:E:90:ASP:OD1	1.84	0.76
1:F:181:ALA:CB	1:E:202:ARG:HH12	1.99	0.76
1:K:55:ALA:HB2	1:J:80:PHE:CE1	2.20	0.76
2:e:6:VAL:HG23	1:I:72:ILE:O	1.85	0.76
2:i:2:ALA:CB	1:H:147:TYR:CE1	2.69	0.76
2:f:20:ARG:NH2	2:f:30:ASN:OD1	2.18	0.76
1:A:195:GLU:N	1:A:195:GLU:OE1	2.18	0.76
1:G:9:LEU:CD1	1:H:40:VAL:HG12	2.16	0.76
2:b:21:VAL:HG22	2:d:23:ALA:HB2	1.68	0.76
1:D:81:PRO:CG	1:E:56:VAL:CG2	2.63	0.76
1:K:62:ARG:HD3	1:J:83:ASP:OD2	1.85	0.76
1:G:306:LYS:NZ	2:j:26:ASP:HA	2.01	0.76
1:F:26:GLN:OE1	1:F:126:SER:OG	2.03	0.76
1:K:231:ARG:HB3	1:L:245:ASN:OD1	1.86	0.76
1:G:310:GLU:OE2	1:H:62:ARG:CZ	2.33	0.76
1:A:33:GLU:N	1:A:33:GLU:OE2	2.17	0.76
2:b:13:TYR:CE2	1:I:87:ASP:OD2	2.38	0.75
1:K:124:LEU:CD2	1:L:53:ILE:CG2	2.54	0.75
1:G:43:ILE:CG1	1:L:12:THR:CG2	2.55	0.75
1:B:47:ASP:OD1	1:A:17:THR:O	2.04	0.75
1:K:56:VAL:CG2	1:J:81:PRO:CD	2.65	0.75
1:C:237:ASN:CG	1:D:192:ASP:OD1	2.30	0.75
1:B:55:ALA:HB2	1:A:80:PHE:CE1	2.22	0.75
1:F:70:LYS:HD3	1:E:97:PHE:HE1	1.48	0.75
1:I:9:LEU:HD22	1:J:40:VAL:CG1	2.16	0.75
1:F:62:ARG:CZ	1:E:310:GLU:OE2	2.33	0.75
2:b:26:ASP:OD2	2:c:106:THR:CG2	2.34	0.75
1:D:81:PRO:HD2	1:E:56:VAL:CG2	2.15	0.75
1:D:81:PRO:HD2	1:E:56:VAL:HG22	1.66	0.75
1:F:270:ARG:NH1	1:E:12:THR:O	2.20	0.75
1:D:18:MET:CE	1:E:48:ASP:HB3	2.17	0.75
1:G:9:LEU:HD13	1:H:40:VAL:HG12	1.65	0.75
1:G:67:ASN:HD22	2:k:15:ASP:CG	1.84	0.75
1:G:304:GLU:OE2	2:i:20:ARG:NE	2.20	0.75
1:B:223:SER:OG	1:A:229:ARG:NH2	2.19	0.75
1:D:18:MET:HE1	1:E:49:GLY:H	1.40	0.75
1:G:1:MET:HE1	1:H:42:ARG:HH11	0.59	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:GLN:OE1	1:G:111:GLN:N	2.20	0.74
2:e:138:LYS:HZ3	1:I:61:VAL:HG23	1.49	0.74
1:G:17:THR:HG21	1:H:45:ARG:NH2	2.02	0.74
1:C:239:ARG:NH2	1:D:176:GLU:OE1	2.21	0.74
1:D:18:MET:HE1	1:E:48:ASP:CA	2.17	0.74
1:D:310:GLU:OE2	1:E:62:ARG:NH2	2.15	0.74
2:f:20:ARG:NH2	2:f:21:VAL:O	2.21	0.74
1:D:229:ARG:NH2	1:E:221:TYR:CD1	2.50	0.74
2:a:20:ARG:NH1	2:a:27:THR:O	2.20	0.74
2:j:80:LEU:O	2:j:83:VAL:HG12	1.88	0.74
1:F:231:ARG:CA	1:A:244:LYS:CE	2.61	0.74
1:D:226:GLU:OE2	1:E:221:TYR:CZ	2.40	0.73
1:G:69:ARG:HD3	2:k:10:GLU:CD	2.00	0.73
1:M:283:ARG:NH2	1:K:302:LEU:HD11	2.03	0.73
1:K:44:GLU:O	1:J:15:ILE:N	2.21	0.73
1:K:141:ASP:OD2	1:L:54:LYS:HD3	1.89	0.73
1:K:82:LEU:CD1	1:L:53:ILE:HD12	2.18	0.73
2:a:114:TYR:OH	2:a:121:ASP:OD1	2.04	0.73
2:l:144:PHE:O	2:l:146:GLY:N	2.21	0.73
1:B:55:ALA:HB2	1:A:80:PHE:HE1	1.51	0.73
1:G:43:ILE:HG12	1:L:12:THR:HG23	1.63	0.73
1:G:180:ARG:CZ	1:L:231:ARG:NH1	2.51	0.73
1:M:283:ARG:NH2	1:K:302:LEU:CD1	2.51	0.73
1:F:231:ARG:NH2	1:F:234:GLY:O	2.22	0.73
1:I:270:ARG:HD3	1:H:15:ILE:CD1	2.17	0.73
1:I:40:VAL:CG1	1:H:9:LEU:CD2	2.66	0.73
2:i:2:ALA:HB3	1:H:146:ASP:O	1.88	0.73
1:K:231:ARG:CB	1:L:245:ASN:OD1	2.37	0.73
1:H:83:ASP:OD1	1:H:84:ARG:N	2.22	0.72
1:G:116:ARG:NH2	1:H:68:ASP:N	2.32	0.72
1:B:67:ASN:HA	1:A:116:ARG:NH1	2.04	0.72
1:K:221:TYR:HE2	1:J:229:ARG:NH2	1.81	0.72
1:F:237:ASN:HD21	1:A:184:ILE:HG21	1.54	0.72
1:D:80:PHE:CZ	1:E:55:ALA:HB2	2.22	0.72
1:H:149:TYR:OH	1:H:315:THR:O	2.06	0.72
1:M:61:VAL:HG11	2:l:134:GLN:HE22	1.54	0.72
1:I:319:ARG:HH22	1:H:17:THR:HG22	1.53	0.72
1:M:186:TRP:CE2	2:l:147:SER:CB	2.72	0.72
2:e:97:PRO:HG2	1:A:57:GLN:NE2	2.04	0.72
2:d:109:GLN:NE2	2:d:137:ASP:OD1	2.22	0.72
2:k:23:ALA:HB2	2:m:21:VAL:HG22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:229:ARG:NH2	1:L:221:TYR:CE2	2.58	0.72
1:B:42:ARG:HH22	1:A:1:MET:HE1	1.55	0.71
1:K:124:LEU:CD2	1:L:53:ILE:HG21	2.18	0.71
1:G:42:ARG:HH11	1:L:1:MET:HE1	1.54	0.71
1:G:180:ARG:NH2	1:L:231:ARG:NH1	2.37	0.71
2:b:6:VAL:CG1	1:J:73:VAL:HG23	2.20	0.71
2:i:2:ALA:HB1	1:H:147:TYR:CE1	2.25	0.71
1:B:62:ARG:NH2	1:A:83:ASP:CG	2.48	0.71
1:K:229:ARG:NH1	1:L:223:SER:OG	2.24	0.71
1:G:310:GLU:CG	1:H:62:ARG:HH12	2.04	0.71
1:A:95:ARG:NH1	1:A:99:THR:O	2.23	0.71
1:C:151:ASP:OD1	1:C:152:VAL:N	2.24	0.70
1:D:20:ARG:NH1	1:E:185:ASP:OD1	2.19	0.70
1:G:180:ARG:CZ	1:L:231:ARG:HH11	2.04	0.70
2:d:101:ALA:HB1	2:d:105:LEU:HD11	1.73	0.70
1:G:245:ASN:ND2	1:L:231:ARG:H	1.89	0.70
2:h:101:ALA:HB1	2:h:105:LEU:HD11	1.73	0.70
1:F:231:ARG:HA	1:A:244:LYS:CE	2.19	0.70
1:G:306:LYS:CE	2:j:25:GLY:O	2.38	0.70
1:E:92:GLN:HE22	1:J:58:ARG:NH1	1.88	0.70
1:K:1:MET:CE	1:L:42:ARG:CD	2.69	0.70
1:K:80:PHE:CE1	1:L:55:ALA:HB2	2.25	0.70
1:I:119:ARG:NH1	1:J:48:ASP:OD2	2.22	0.70
2:b:26:ASP:OD2	2:c:106:THR:OG1	2.10	0.70
1:C:239:ARG:NH2	1:D:176:GLU:CD	2.50	0.70
1:F:12:THR:HG22	1:A:42:ARG:O	1.91	0.70
1:F:231:ARG:CA	1:A:244:LYS:HE3	2.21	0.70
1:C:287:GLN:OE1	1:C:287:GLN:N	2.24	0.70
1:K:83:ASP:OD2	1:L:62:ARG:HD2	1.91	0.70
2:l:25:GLY:O	1:L:306:LYS:CD	2.40	0.70
2:c:129:GLU:OE2	2:c:135:VAL:N	2.25	0.70
2:d:83:VAL:HG23	2:d:84:ASP:H	1.57	0.70
1:F:237:ASN:ND2	1:A:184:ILE:HG21	2.06	0.70
1:I:283:ARG:NE	1:E:302:LEU:HD12	2.05	0.70
1:M:71:LYS:CG	2:l:8:THR:HG22	2.21	0.69
1:I:283:ARG:NH2	1:E:302:LEU:CG	2.56	0.69
1:G:270:ARG:NH2	1:L:12:THR:O	2.26	0.69
1:C:198:VAL:HG22	1:C:263:ILE:HG22	1.73	0.69
1:I:205:PHE:CE1	1:I:209:ILE:HD11	2.28	0.69
1:H:87:ASP:OD1	1:H:88:ARG:N	2.25	0.69
1:G:310:GLU:OE2	1:H:62:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:49:GLY:O	1:H:119:ARG:NH2	2.26	0.69
2:l:25:GLY:O	1:L:306:LYS:HD2	1.92	0.69
1:I:40:VAL:HG12	1:H:9:LEU:HD22	1.74	0.69
1:D:237:ASN:ND2	1:E:192:ASP:CB	2.56	0.69
1:B:270:ARG:HD3	1:A:15:ILE:CD1	2.21	0.69
1:F:11:TYR:CE1	1:A:44:GLU:CD	2.68	0.69
1:F:237:ASN:N	1:A:192:ASP:OD1	2.25	0.69
2:b:10:GLU:HG2	1:J:69:ARG:HG2	1.75	0.69
1:B:40:VAL:HB	1:A:9:LEU:CD1	2.22	0.69
1:G:245:ASN:HD22	1:L:231:ARG:HG3	1.56	0.68
1:G:291:GLU:OE2	1:G:291:GLU:N	2.22	0.68
1:L:109:GLU:OE1	1:L:112:ARG:NH1	2.26	0.68
1:G:66:ALA:HB3	2:k:142:THR:HG23	1.75	0.68
2:i:56:LEU:HD11	2:i:120:ILE:HD13	1.74	0.68
1:G:15:ILE:HD11	1:H:270:ARG:HH11	1.37	0.68
1:K:62:ARG:HD2	1:J:83:ASP:OD2	1.93	0.68
1:I:68:ASP:OD1	1:H:116:ARG:NH2	2.24	0.68
1:K:56:VAL:HG22	1:J:81:PRO:HD3	1.75	0.68
2:e:22:VAL:CG2	1:H:304:GLU:OE1	2.42	0.68
2:l:91:GLU:N	2:l:91:GLU:OE1	2.27	0.68
1:D:18:MET:CE	1:E:48:ASP:CB	2.70	0.68
1:G:116:ARG:HH22	1:H:68:ASP:CB	1.98	0.68
2:b:6:VAL:HG12	1:J:73:VAL:HG23	1.76	0.68
1:I:184:ILE:CG2	1:H:20:ARG:CZ	2.72	0.68
1:K:218:TYR:CE2	1:J:229:ARG:CD	2.76	0.68
1:G:245:ASN:HD21	1:L:231:ARG:H	1.39	0.68
1:J:149:TYR:OH	1:J:315:THR:O	2.11	0.68
1:G:116:ARG:HH21	1:H:68:ASP:CB	1.88	0.68
1:G:270:ARG:CD	1:L:15:ILE:HD11	2.23	0.68
2:e:24:PHE:HD1	1:H:301:TYR:HH	1.42	0.68
1:C:237:ASN:ND2	1:D:192:ASP:OD1	2.27	0.68
1:K:218:TYR:CE2	1:J:229:ARG:HD2	2.28	0.68
1:D:231:ARG:HE	1:E:176:GLU:CD	2.02	0.67
1:E:2:GLN:NE2	1:H:1:MET:CE	2.45	0.67
1:C:310:GLU:CD	1:D:62:ARG:NH2	2.52	0.67
1:C:87:ASP:OD1	1:C:88:ARG:N	2.27	0.67
1:K:78:PRO:O	1:K:312:SER:OG	2.12	0.67
1:K:237:ASN:CB	1:L:192:ASP:OD1	2.39	0.67
1:G:185:ASP:HA	1:L:20:ARG:HE	1.58	0.67
1:G:237:ASN:CG	1:H:192:ASP:CG	2.62	0.67
1:E:195:GLU:OE1	1:E:266:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:ILE:O	1:L:187:ALA:N	2.28	0.67
1:B:270:ARG:NH1	1:A:12:THR:O	2.27	0.67
1:I:9:LEU:HD21	1:J:40:VAL:HG11	1.76	0.67
1:D:229:ARG:CZ	1:E:223:SER:OG	2.43	0.67
1:E:8:ILE:HG23	1:H:95:ARG:HG2	1.75	0.67
1:G:48:ASP:HB3	1:L:18:MET:CE	2.25	0.67
1:C:11:TYR:OH	1:D:44:GLU:OE1	2.12	0.67
1:B:40:VAL:HB	1:A:9:LEU:HD13	1.77	0.67
1:K:13:GLY:CA	1:L:270:ARG:NH1	2.48	0.67
1:D:229:ARG:NE	1:E:221:TYR:CZ	2.62	0.66
2:b:24:PHE:HE2	1:I:301:TYR:HH	1.42	0.66
2:d:97:PRO:HG2	1:J:57:GLN:HE21	1.59	0.66
2:g:112:LEU:HB2	2:g:120:ILE:HD11	1.77	0.66
1:G:7:GLN:NE2	2:h:83:VAL:CA	2.52	0.66
2:h:36:MET:CE	2:h:57:VAL:HG11	2.24	0.66
1:C:84:ARG:HH12	1:D:67:ASN:HD22	1.41	0.66
1:C:9:LEU:HD13	1:D:40:VAL:CG1	2.24	0.66
1:K:68:ASP:CA	1:J:116:ARG:HH22	2.06	0.66
1:D:18:MET:HE1	1:E:48:ASP:HB3	1.74	0.66
1:K:17:THR:HG21	1:L:319:ARG:NH2	2.04	0.66
1:K:62:ARG:HH12	1:J:310:GLU:CG	2.09	0.66
1:K:68:ASP:CG	1:J:116:ARG:NH2	2.53	0.66
2:e:97:PRO:HG2	1:A:57:GLN:HE21	1.61	0.66
1:B:62:ARG:NH2	1:A:83:ASP:OD1	2.29	0.66
1:I:283:ARG:HG3	1:E:302:LEU:CD1	2.10	0.66
1:F:58:ARG:NH1	1:E:278:PRO:O	2.28	0.65
2:h:36:MET:HE2	2:h:57:VAL:HG11	1.77	0.65
1:I:282:LEU:HD12	1:E:88:ARG:HG2	1.77	0.65
1:C:270:ARG:NH1	1:B:12:THR:O	2.30	0.65
1:K:56:VAL:CG2	1:J:81:PRO:HD3	2.27	0.65
1:K:124:LEU:HB2	1:L:53:ILE:HG22	1.78	0.65
1:G:116:ARG:NH2	1:H:68:ASP:CA	2.59	0.65
2:a:101:ALA:HB1	2:a:105:LEU:HD11	1.78	0.65
1:I:9:LEU:HD13	1:J:42:ARG:CG	2.26	0.65
1:K:42:ARG:HH11	1:J:1:MET:HE3	1.61	0.65
1:G:149:TYR:OH	1:G:315:THR:O	2.13	0.65
2:b:121:ASP:OD1	2:b:122:ALA:N	2.30	0.65
1:B:54:LYS:HD2	1:A:141:ASP:OD2	1.96	0.65
1:K:62:ARG:HH12	1:J:310:GLU:HG2	1.61	0.65
1:K:124:LEU:CD2	1:L:53:ILE:HG23	2.17	0.65
1:C:223:SER:OG	1:B:229:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:ASP:OD2	1:J:62:ARG:CD	2.45	0.65
1:I:319:ARG:HH22	1:H:17:THR:HG21	1.59	0.65
2:h:75:VAL:HG12	2:h:75:VAL:O	1.97	0.65
1:D:18:MET:HE2	1:E:49:GLY:CA	2.25	0.65
1:M:283:ARG:HH21	1:K:302:LEU:HD13	1.61	0.64
1:K:95:ARG:NH2	1:L:44:GLU:OE2	2.29	0.64
2:b:12:ASN:ND2	1:I:90:ASP:OD1	2.27	0.64
2:l:101:ALA:HB1	2:l:105:LEU:HD22	1.79	0.64
1:I:48:ASP:CB	1:H:18:MET:SD	2.78	0.64
1:G:270:ARG:NH2	1:L:12:THR:OG1	2.30	0.64
1:L:172:ILE:HG21	1:L:244:LYS:HD2	1.79	0.64
1:G:69:ARG:HD2	2:k:10:GLU:OE1	1.96	0.64
1:M:61:VAL:CG1	2:l:134:GLN:NE2	2.59	0.64
1:F:109:GLU:O	1:F:113:HIS:ND1	2.29	0.64
1:I:44:GLU:OE1	1:H:11:TYR:CE2	2.50	0.64
2:b:24:PHE:HE2	1:I:301:TYR:OH	1.81	0.64
1:C:9:LEU:CD1	1:D:40:VAL:CG1	2.76	0.64
1:K:1:MET:HE1	1:L:42:ARG:CD	2.27	0.64
1:K:62:ARG:HH12	1:J:310:GLU:CD	2.06	0.64
1:I:149:TYR:OH	1:I:315:THR:O	2.14	0.64
2:e:103:ARG:NH1	2:f:134:GLN:HB2	2.13	0.64
2:h:102:VAL:HG23	2:h:103:ARG:HE	1.63	0.64
1:B:40:VAL:CB	1:A:9:LEU:CD1	2.75	0.64
2:h:96:VAL:HG21	1:H:144:VAL:HG22	1.80	0.64
1:K:43:ILE:HG13	1:J:12:THR:CG2	2.26	0.64
1:G:12:THR:CG2	1:H:42:ARG:O	2.38	0.63
1:A:291:GLU:OE2	1:A:291:GLU:N	2.29	0.63
2:f:89:VAL:HG23	2:f:90:PHE:CD2	2.33	0.63
1:D:18:MET:HE1	1:E:48:ASP:CB	2.27	0.63
1:H:163:ASP:OD2	1:H:166:LYS:NZ	2.24	0.63
1:K:229:ARG:NH2	1:L:217:ALA:O	2.31	0.63
2:h:96:VAL:CG2	1:H:144:VAL:HG22	2.29	0.63
1:B:40:VAL:CG1	1:A:9:LEU:HD13	2.29	0.63
1:I:9:LEU:CD2	1:J:40:VAL:HG11	2.29	0.63
1:B:279:SER:OG	1:B:310:GLU:OE1	2.17	0.63
1:F:62:ARG:HH12	1:E:310:GLU:CD	1.98	0.63
1:K:220:GLN:HA	1:L:220:GLN:OE1	1.98	0.63
1:M:64:HIS:CD2	2:l:18:LEU:HD13	2.33	0.63
2:b:10:GLU:OE2	1:J:69:ARG:CD	2.47	0.63
1:F:185:ASP:HA	1:E:20:ARG:HD2	1.80	0.63
2:g:80:LEU:O	2:g:83:VAL:HG22	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:108:ASN:OD1	2:d:109:GLN:N	2.30	0.62
1:G:15:ILE:CD1	1:H:270:ARG:HD3	2.29	0.62
1:G:237:ASN:CG	1:H:192:ASP:OD1	2.42	0.62
2:b:21:VAL:HG22	2:d:23:ALA:CB	2.28	0.62
1:B:45:ARG:HA	1:A:15:ILE:O	1.99	0.62
1:B:68:ASP:OD2	1:A:112:ARG:HD3	1.99	0.62
1:D:80:PHE:HE1	1:E:55:ALA:CB	1.90	0.62
2:b:24:PHE:CE2	1:I:301:TYR:OH	2.51	0.62
1:G:245:ASN:ND2	1:L:231:ARG:HB2	2.15	0.62
2:d:97:PRO:HG2	1:J:57:GLN:NE2	2.14	0.62
2:g:101:ALA:HB1	2:g:105:LEU:CD1	2.30	0.62
1:G:245:ASN:HD22	1:L:231:ARG:CG	2.12	0.62
2:e:138:LYS:NZ	1:I:61:VAL:CG2	2.62	0.62
1:B:62:ARG:HH21	1:A:83:ASP:CG	2.08	0.62
1:K:56:VAL:HG22	1:J:81:PRO:HD2	1.81	0.62
1:K:1:MET:HE1	1:L:42:ARG:HD2	1.81	0.62
2:l:56:LEU:CD1	2:l:120:ILE:HD13	2.30	0.61
2:e:138:LYS:HZ2	1:I:61:VAL:CG2	2.13	0.61
1:D:14:LEU:HD12	1:E:44:GLU:O	1.99	0.61
2:j:83:VAL:HG13	2:j:83:VAL:O	1.98	0.61
1:B:270:ARG:NH2	1:A:12:THR:O	2.32	0.61
1:F:80:PHE:CD1	1:A:55:ALA:HA	2.35	0.61
1:K:56:VAL:HG21	1:J:81:PRO:CG	2.29	0.61
1:G:83:ASP:O	1:H:64:HIS:HA	2.01	0.61
1:C:278:PRO:O	1:D:58:ARG:NH2	2.27	0.61
1:K:68:ASP:CA	1:J:116:ARG:NH2	2.63	0.61
2:b:149:LEU:OXT	1:I:21:VAL:HA	2.00	0.61
1:B:42:ARG:NH2	1:A:1:MET:HE1	2.15	0.61
1:D:141:ASP:OD2	1:E:54:LYS:CD	2.43	0.61
1:G:80:PHE:CD1	1:H:55:ALA:HA	2.36	0.61
1:M:67:ASN:HD21	2:l:142:THR:HA	1.65	0.61
1:B:43:ILE:CG1	1:A:12:THR:OG1	2.49	0.61
2:c:20:ARG:NH2	2:c:27:THR:O	2.34	0.61
1:K:17:THR:O	1:K:18:MET:HE2	2.01	0.60
1:K:65:LEU:HD11	1:J:117:ILE:CG1	2.30	0.60
2:j:17:VAL:HG23	2:j:17:VAL:O	2.01	0.60
1:I:25:LEU:CD2	1:I:129:MET:HE3	2.31	0.60
2:b:144:PHE:CD2	1:J:69:ARG:NH2	2.63	0.60
1:G:310:GLU:CD	1:H:62:ARG:HH12	2.09	0.60
1:F:229:ARG:NH1	1:A:221:TYR:CE1	2.69	0.60
1:I:57:GLN:HE21	1:H:144:VAL:HG21	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:ASP:HB3	1:L:18:MET:HE1	1.82	0.60
1:K:9:LEU:CA	1:L:38:THR:HG21	2.29	0.60
2:h:25:GLY:HA2	1:H:306:LYS:HD2	1.84	0.60
1:D:237:ASN:ND2	1:E:192:ASP:CA	2.55	0.60
1:M:227:ILE:HG22	1:M:240:ILE:HD12	1.83	0.60
1:K:82:LEU:HG	1:L:53:ILE:HD12	1.84	0.60
1:G:42:ARG:HH11	1:L:1:MET:CE	2.15	0.60
2:e:24:PHE:HD1	1:H:301:TYR:OH	1.84	0.60
2:i:2:ALA:HB3	1:H:147:TYR:CE1	2.36	0.60
2:k:101:ALA:HB1	2:k:105:LEU:CD1	2.32	0.60
1:D:229:ARG:NH2	1:E:221:TYR:CD2	2.70	0.60
2:d:12:ASN:OD1	1:E:90:ASP:OD1	2.19	0.59
1:I:184:ILE:HG22	1:H:20:ARG:CZ	2.31	0.59
1:D:18:MET:CE	1:E:48:ASP:CA	2.76	0.59
1:K:236:ALA:HA	1:L:193:ASN:OD1	2.02	0.59
1:J:109:GLU:O	1:J:113:HIS:ND1	2.35	0.59
2:d:101:ALA:HB1	2:d:105:LEU:CD1	2.32	0.59
2:l:34:VAL:O	2:l:98:MET:N	2.35	0.59
2:l:56:LEU:HD11	2:l:120:ILE:HD13	1.84	0.59
1:F:169:VAL:HG23	1:F:169:VAL:O	2.02	0.59
1:I:13:GLY:HA3	1:J:270:ARG:NH2	2.16	0.59
2:e:22:VAL:HG22	1:H:304:GLU:CD	2.28	0.59
1:B:65:LEU:HD21	1:A:116:ARG:HG2	1.84	0.59
1:B:42:ARG:NH2	1:A:1:MET:CE	2.65	0.59
2:c:36:MET:HE3	2:c:98:MET:HG3	1.85	0.59
2:a:75:VAL:HG22	2:a:75:VAL:O	2.02	0.59
2:e:20:ARG:NH2	2:e:27:THR:O	2.35	0.59
2:c:121:ASP:OD1	2:c:122:ALA:N	2.36	0.59
1:B:62:ARG:NH2	1:A:308:GLU:OE1	2.34	0.59
1:I:40:VAL:HG11	1:H:9:LEU:HD21	1.83	0.59
2:e:26:ASP:OD2	2:f:106:THR:HG21	2.03	0.59
1:F:65:LEU:HB3	1:E:84:ARG:HD2	1.85	0.59
1:G:270:ARG:HD3	1:L:15:ILE:HD13	1.83	0.58
1:B:43:ILE:HA	1:A:12:THR:OG1	2.03	0.58
1:I:229:ARG:HH11	1:J:218:TYR:HA	1.67	0.58
1:E:6:PHE:O	1:H:94:PHE:HA	2.02	0.58
2:g:112:LEU:CB	2:g:120:ILE:HD11	2.34	0.58
1:G:158:THR:O	1:G:324:VAL:HG13	2.03	0.58
2:g:90:PHE:CZ	1:A:144:VAL:HG12	2.39	0.58
1:K:218:TYR:CD2	1:J:229:ARG:HD3	2.39	0.58
1:K:310:GLU:CD	1:L:62:ARG:CZ	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:52:ASP:OD1	1:H:53:ILE:N	2.36	0.58
1:G:9:LEU:CD1	1:H:40:VAL:CG1	2.77	0.58
1:G:68:ASP:CG	1:L:116:ARG:NH2	2.61	0.58
2:k:79:VAL:HG12	2:k:79:VAL:O	2.03	0.58
1:D:231:ARG:HB3	1:E:245:ASN:OD1	2.04	0.58
1:K:218:TYR:CE2	1:J:229:ARG:HD3	2.38	0.58
1:G:9:LEU:HD13	1:H:40:VAL:CB	2.34	0.58
1:G:188:GLY:O	1:L:18:MET:O	2.21	0.57
1:C:84:ARG:NH2	1:D:66:ALA:O	2.37	0.57
1:I:192:ASP:OD1	1:H:237:ASN:CG	2.34	0.57
2:c:38:PHE:O	2:c:49:THR:OG1	2.12	0.57
1:D:18:MET:HE3	1:E:49:GLY:HA2	1.85	0.57
1:D:172:ILE:HG21	1:D:244:LYS:HD2	1.86	0.57
1:E:39:THR:HG22	1:E:39:THR:O	2.03	0.57
1:A:87:ASP:OD1	1:A:88:ARG:N	2.38	0.57
1:G:116:ARG:NH1	1:H:66:ALA:O	2.37	0.57
1:K:55:ALA:HB2	1:J:80:PHE:HE1	1.67	0.57
1:A:226:GLU:OE1	1:A:230:ARG:NH1	2.37	0.57
1:B:87:ASP:OD1	1:B:88:ARG:N	2.37	0.57
1:I:268:ILE:HD13	1:I:322:LEU:HD13	1.87	0.57
1:G:116:ARG:HH22	1:H:67:ASN:C	2.10	0.57
2:b:18:LEU:CD1	1:J:64:HIS:CD2	2.78	0.57
1:K:109:GLU:O	1:K:113:HIS:ND1	2.38	0.57
1:G:80:PHE:CE1	1:H:55:ALA:HA	2.40	0.57
1:K:220:GLN:OE1	1:J:220:GLN:NE2	2.37	0.57
2:k:101:ALA:HB1	2:k:105:LEU:HD11	1.87	0.57
1:B:223:SER:HG	1:A:229:ARG:NH2	2.02	0.57
1:G:223:SER:OG	1:L:229:ARG:NH1	2.38	0.57
1:M:186:TRP:CZ2	2:l:147:SER:CB	2.88	0.57
2:a:108:ASN:OD1	2:a:110:LEU:N	2.38	0.57
1:M:283:ARG:NH2	1:K:302:LEU:HD13	2.18	0.56
1:H:22:ASP:OD2	1:H:130:TYR:OH	2.23	0.56
2:i:7:ALA:HB3	1:H:72:ILE:CG2	2.35	0.56
1:I:197:VAL:HG21	1:I:266:ARG:HE	1.70	0.56
1:G:223:SER:OG	1:L:229:ARG:CZ	2.53	0.56
1:M:61:VAL:HG11	2:l:134:GLN:HE21	1.66	0.56
2:a:101:ALA:HB1	2:a:105:LEU:CD1	2.35	0.56
2:d:108:ASN:OD1	2:d:110:LEU:N	2.38	0.56
1:I:9:LEU:HD13	1:J:42:ARG:HG3	1.87	0.56
1:D:226:GLU:OE2	1:E:221:TYR:CE1	2.59	0.56
1:K:56:VAL:HG21	1:J:81:PRO:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:218:TYR:CZ	1:J:229:ARG:CD	2.88	0.56
1:L:110:VAL:HG13	1:L:114:MET:HE2	1.87	0.56
2:i:2:ALA:HB3	1:H:147:TYR:CD1	2.40	0.56
1:F:237:ASN:HB2	1:A:192:ASP:CG	2.29	0.56
1:F:42:ARG:O	1:E:12:THR:HG22	2.05	0.56
1:I:283:ARG:CZ	1:E:302:LEU:CD1	2.78	0.56
1:G:69:ARG:CG	2:k:10:GLU:CD	2.79	0.56
1:C:286:ASN:N	1:C:287:GLN:OE1	2.38	0.56
1:I:53:ILE:CG2	1:H:124:LEU:HD22	2.36	0.56
2:l:25:GLY:O	1:L:306:LYS:NZ	2.36	0.56
1:F:46:LEU:O	1:E:16:SER:HA	2.05	0.56
2:e:22:VAL:HG22	1:H:304:GLU:OE2	2.07	0.55
2:b:79:VAL:O	2:b:79:VAL:HG12	2.06	0.55
1:C:53:ILE:HG21	1:B:124:LEU:HD22	1.87	0.55
1:C:80:PHE:CE1	1:D:55:ALA:HB2	2.41	0.55
1:K:44:GLU:HB3	1:J:14:LEU:HA	1.87	0.55
1:G:7:GLN:HE22	2:h:83:VAL:HA	1.67	0.55
1:F:62:ARG:NH2	1:E:310:GLU:OE2	2.38	0.55
1:I:255:ASN:OD1	1:I:256:ILE:N	2.39	0.55
1:E:8:ILE:CG2	1:H:95:ARG:HG2	2.36	0.55
1:K:70:LYS:HG2	1:J:97:PHE:CE1	2.42	0.55
1:G:7:GLN:HE22	2:h:83:VAL:CG1	2.16	0.55
1:M:239:ARG:NE	1:M:250:GLU:OE2	2.39	0.55
2:l:120:ILE:HD11	2:l:124:GLY:HA3	1.88	0.55
2:g:90:PHE:HZ	1:A:144:VAL:HG12	1.72	0.55
1:D:265:PRO:HG2	1:D:268:ILE:HD12	1.89	0.55
2:m:36:MET:HE2	2:m:100:LEU:HD21	1.87	0.55
1:C:49:GLY:O	1:B:119:ARG:NH1	2.39	0.55
1:A:29:ASN:ND2	1:A:29:ASN:O	2.39	0.55
2:e:26:ASP:OD2	2:f:106:THR:CB	2.55	0.55
2:e:145:ILE:HD11	1:H:17:THR:OG1	2.07	0.55
2:g:79:VAL:O	2:g:79:VAL:HG12	2.07	0.55
2:g:101:ALA:HB1	2:g:105:LEU:HD12	1.87	0.55
1:B:242:GLU:N	1:B:242:GLU:OE1	2.40	0.55
1:F:229:ARG:NH2	1:A:223:SER:OG	2.40	0.55
1:I:19:PRO:CD	1:J:48:ASP:O	2.54	0.55
1:K:119:ARG:NH1	1:L:49:GLY:O	2.39	0.55
2:m:36:MET:HE3	2:m:98:MET:CB	2.37	0.55
1:G:231:ARG:NH1	1:G:234:GLY:O	2.40	0.55
2:d:78:LYS:NZ	1:J:57:GLN:OE1	2.37	0.55
1:G:68:ASP:CG	1:L:116:ARG:HH21	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:SER:OG	1:D:280:ASP:N	2.40	0.55
2:m:146:GLY:O	2:m:147:SER:OG	2.22	0.55
2:l:116:ASP:OD1	2:l:117:GLY:N	2.39	0.55
1:B:302:LEU:HD12	1:B:302:LEU:O	2.07	0.55
1:F:40:VAL:HG12	1:E:9:LEU:HD22	1.89	0.55
1:I:42:ARG:HH11	1:H:9:LEU:CD1	2.20	0.55
1:G:9:LEU:HD13	1:H:40:VAL:HB	1.89	0.54
2:e:25:GLY:HA2	1:F:306:LYS:HD2	1.89	0.54
1:K:308:GLU:CG	1:L:62:ARG:NH1	2.71	0.54
1:A:142:ASP:OD1	1:A:144:VAL:HG22	2.07	0.54
2:e:83:VAL:HG22	1:E:7:GLN:NE2	2.22	0.54
1:E:279:SER:OG	1:E:280:ASP:N	2.41	0.54
1:M:83:ASP:N	1:M:83:ASP:OD2	2.37	0.54
2:e:32:LYS:HZ2	2:f:129:GLU:CD	2.09	0.54
2:h:102:VAL:HG23	2:h:103:ARG:NE	2.22	0.54
1:I:65:LEU:HB3	1:H:84:ARG:HD2	1.89	0.54
1:G:87:ASP:OD1	1:G:88:ARG:N	2.40	0.54
1:K:149:TYR:OH	1:K:315:THR:O	2.24	0.54
1:L:176:GLU:OE2	1:L:180:ARG:NH1	2.39	0.54
1:M:186:TRP:NE1	2:l:147:SER:HB3	2.23	0.54
1:F:68:ASP:CG	1:E:116:ARG:HH21	2.15	0.54
1:D:116:ARG:NH1	1:E:67:ASN:CA	2.43	0.54
1:C:34:HIS:NE2	1:C:273:GLU:OE2	2.41	0.54
2:m:137:ASP:OD2	2:m:137:ASP:C	2.51	0.54
1:M:56:VAL:HG12	2:l:138:LYS:NZ	2.23	0.54
2:b:3:LYS:HZ1	2:a:91:GLU:HB3	1.73	0.54
1:C:42:ARG:NE	1:C:74:ASN:OD1	2.40	0.54
1:C:232:LEU:HD23	1:C:241:PHE:HB2	1.89	0.54
1:D:112:ARG:HH12	1:E:68:ASP:CG	2.02	0.54
1:E:101:ASN:OD1	1:H:2:GLN:HG3	2.07	0.54
1:E:149:TYR:OH	1:E:315:THR:O	2.23	0.54
1:M:186:TRP:CZ2	2:l:147:SER:HB2	2.43	0.54
2:c:9:LEU:HD22	1:D:6:PHE:CD2	2.43	0.54
1:F:62:ARG:CZ	1:E:308:GLU:OE2	2.56	0.54
1:I:53:ILE:HG21	1:H:124:LEU:HD22	1.90	0.54
1:K:310:GLU:CD	1:L:62:ARG:HH21	2.14	0.54
1:J:298:GLU:N	1:J:298:GLU:OE1	2.41	0.54
1:G:180:ARG:NH2	1:L:235:ASN:OD1	2.40	0.54
1:M:57:GLN:NE2	2:m:97:PRO:C	2.64	0.54
2:b:59:GLU:OE1	2:c:126:GLN:NE2	2.41	0.54
2:c:33:GLU:OE2	1:F:57:GLN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:ALA:HB2	1:E:80:PHE:CE1	2.43	0.53
1:F:64:HIS:HA	1:E:83:ASP:O	2.08	0.53
1:K:44:GLU:C	1:J:14:LEU:HD12	2.33	0.53
1:M:232:LEU:O	1:M:235:ASN:N	2.42	0.53
2:i:101:ALA:HB1	2:i:105:LEU:CD1	2.38	0.53
1:C:239:ARG:HH22	1:D:176:GLU:CD	2.13	0.53
1:H:150:TYR:O	1:H:154:GLY:N	2.41	0.53
1:K:10:ASP:OD1	1:L:38:THR:HG22	2.06	0.53
1:G:19:PRO:HD3	1:H:48:ASP:O	2.08	0.53
1:G:96:GLU:HA	1:G:96:GLU:OE1	2.08	0.53
1:G:306:LYS:NZ	2:j:25:GLY:C	2.64	0.53
1:K:97:PHE:CD1	1:L:70:LYS:HD3	2.43	0.53
1:G:235:ASN:CB	1:H:193:ASN:HA	2.28	0.53
1:F:13:GLY:O	1:A:44:GLU:OE1	2.26	0.53
1:F:53:ILE:CG2	1:E:124:LEU:HD22	2.39	0.53
1:K:124:LEU:HB2	1:L:53:ILE:CG2	2.38	0.53
1:K:223:SER:HB3	1:J:229:ARG:CZ	2.38	0.53
1:B:319:ARG:NH1	1:B:321:GLU:OE1	2.41	0.53
1:F:40:VAL:CG1	1:E:9:LEU:HD22	2.39	0.53
2:i:79:VAL:HG12	2:i:79:VAL:O	2.08	0.53
2:f:30:ASN:ND2	2:f:103:ARG:O	2.40	0.53
1:B:40:VAL:O	1:A:10:ASP:OD2	2.25	0.53
2:d:78:LYS:HZ1	1:J:57:GLN:CD	2.16	0.53
2:l:105:LEU:HD23	2:l:107:LEU:HD21	1.91	0.53
1:B:16:SER:O	1:B:17:THR:OG1	2.22	0.53
1:G:197:VAL:HG21	1:G:266:ARG:HE	1.74	0.53
2:i:140:VAL:HG22	1:H:52:ASP:O	2.09	0.53
1:F:80:PHE:CE1	1:A:55:ALA:HB2	2.44	0.53
1:K:82:LEU:CG	1:L:53:ILE:HD12	2.38	0.53
2:b:3:LYS:NZ	2:a:91:GLU:HB3	2.24	0.52
2:d:102:VAL:O	2:d:133:ASN:ND2	2.36	0.52
1:F:31:PHE:CD1	1:F:129:MET:HE2	2.44	0.52
1:G:61:VAL:HG12	1:G:62:ARG:N	2.25	0.52
1:G:235:ASN:HB3	1:H:193:ASN:CA	2.29	0.52
1:F:220:GLN:CD	1:A:220:GLN:HE22	2.16	0.52
1:I:48:ASP:OD1	1:H:119:ARG:NH2	2.41	0.52
1:K:270:ARG:HH22	1:J:12:THR:HG23	1.74	0.52
1:G:146:ASP:O	2:k:2:ALA:HB2	2.09	0.52
2:e:26:ASP:OD1	1:A:64:HIS:NE2	2.36	0.52
1:D:116:ARG:NH1	1:E:66:ALA:O	2.42	0.52
1:F:18:MET:HG3	1:F:19:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:12:THR:C	1:J:270:ARG:HH22	2.01	0.52
1:B:62:ARG:HD2	1:A:81:PRO:HB2	1.92	0.52
1:B:223:SER:OG	1:A:229:ARG:CZ	2.58	0.52
1:G:15:ILE:HD11	1:H:270:ARG:HD3	1.90	0.52
2:k:29:TRP:CA	2:m:134:GLN:OE1	2.45	0.52
1:D:12:THR:HG23	1:D:12:THR:O	2.10	0.52
1:E:1:MET:CE	1:H:2:GLN:NE2	2.50	0.52
1:C:198:VAL:HG22	1:C:263:ILE:CG2	2.40	0.52
1:G:62:ARG:HD3	1:L:83:ASP:CG	2.16	0.52
2:h:101:ALA:HB1	2:h:105:LEU:CD1	2.38	0.52
2:f:7:ALA:HB3	1:A:72:ILE:CG2	2.40	0.52
1:B:46:LEU:HD12	1:B:69:ARG:O	2.10	0.52
1:K:82:LEU:HG	1:L:53:ILE:CD1	2.39	0.52
2:e:6:VAL:CG2	1:I:72:ILE:O	2.57	0.52
1:F:20:ARG:NH2	1:A:185:ASP:HB3	2.24	0.52
1:K:83:ASP:O	1:L:64:HIS:HA	2.10	0.52
1:G:15:ILE:HD11	1:H:270:ARG:CZ	2.38	0.52
1:G:116:ARG:NH1	1:H:67:ASN:C	2.57	0.52
1:B:40:VAL:CB	1:A:9:LEU:HD13	2.39	0.52
1:F:219:SER:O	1:A:221:TYR:HE2	1.93	0.52
1:I:79:PHE:HB3	1:J:56:VAL:O	2.10	0.51
1:K:116:ARG:HB3	1:L:65:LEU:HD21	1.92	0.51
1:J:99:THR:OG1	1:J:102:ALA:HB3	2.10	0.51
2:e:144:PHE:HE2	1:I:68:ASP:HA	1.74	0.51
1:C:194:TYR:O	1:B:235:ASN:ND2	2.41	0.51
1:B:42:ARG:HH22	1:A:1:MET:CE	2.21	0.51
1:F:70:LYS:HD3	1:E:97:PHE:CZ	2.45	0.51
1:I:268:ILE:CD1	1:I:322:LEU:HD13	2.41	0.51
1:K:229:ARG:CZ	1:L:221:TYR:CE2	2.93	0.51
1:G:100:GLU:OE2	1:G:100:GLU:N	2.38	0.51
2:b:109:GLN:NE2	2:b:137:ASP:OD1	2.42	0.51
2:i:6:VAL:HG21	1:H:71:LYS:HE3	1.93	0.51
1:C:84:ARG:NH1	1:D:67:ASN:HD22	2.07	0.51
1:I:68:ASP:CG	1:H:116:ARG:NH2	2.69	0.51
1:F:80:PHE:CE1	1:A:55:ALA:CA	2.92	0.51
1:F:275:TYR:CE2	1:F:316:VAL:HG21	2.45	0.51
1:G:53:ILE:HD11	1:L:82:LEU:CD1	2.41	0.51
2:b:29:TRP:O	2:b:103:ARG:NH1	2.43	0.51
1:C:3:ASN:N	1:C:7:GLN:O	2.43	0.51
1:F:163:ASP:OD2	1:F:166:LYS:NZ	2.40	0.51
1:M:12:THR:OG1	1:M:100:GLU:OE2	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:ASP:OD1	2:i:13:TYR:HB3	2.11	0.51
1:M:71:LYS:CG	2:l:8:THR:CG2	2.84	0.51
2:b:140:VAL:HG21	1:I:82:LEU:HD12	1.92	0.51
1:G:141:ASP:OD1	1:H:54:LYS:CE	2.59	0.51
2:b:80:LEU:O	2:b:83:VAL:HG12	2.11	0.51
2:c:9:LEU:HB2	1:D:6:PHE:CE2	2.45	0.51
1:G:17:THR:CG2	1:H:45:ARG:NH2	2.71	0.51
2:k:149:LEU:OXT	1:L:123:ILE:HD13	2.10	0.51
1:F:11:TYR:CZ	1:A:44:GLU:OE2	2.58	0.51
1:K:65:LEU:HD11	1:J:117:ILE:HG12	1.92	0.51
1:K:184:ILE:CB	1:J:20:ARG:NH1	2.48	0.51
1:L:39:THR:HG22	1:L:39:THR:O	2.11	0.51
2:a:21:VAL:O	2:a:21:VAL:HG13	2.10	0.50
1:B:172:ILE:HG21	1:B:244:LYS:HD3	1.93	0.50
1:B:50:ALA:HB2	1:A:119:ARG:NH2	2.27	0.50
1:I:18:MET:C	1:J:188:GLY:O	2.46	0.50
1:M:224:THR:OG1	1:M:225:GLN:N	2.44	0.50
2:c:85:HIS:NE2	1:D:3:ASN:ND2	2.60	0.50
2:m:125:ILE:CD1	2:m:135:VAL:HG11	2.41	0.50
1:G:9:LEU:CD1	1:H:40:VAL:HB	2.40	0.50
1:B:4:GLY:O	1:B:6:PHE:N	2.45	0.50
1:G:64:HIS:HA	1:L:83:ASP:O	2.12	0.50
1:I:283:ARG:NH2	1:E:302:LEU:HB2	2.26	0.50
1:K:319:ARG:HH21	1:J:17:THR:HG22	1.54	0.50
1:G:1:MET:CE	1:H:42:ARG:HH12	2.12	0.50
2:l:21:VAL:O	2:l:21:VAL:HG13	2.11	0.50
1:F:53:ILE:HG23	1:E:124:LEU:HD22	1.94	0.50
1:G:61:VAL:HG12	1:G:62:ARG:H	1.77	0.50
2:b:138:LYS:HZ3	1:J:56:VAL:HG22	1.74	0.50
1:G:146:ASP:O	2:k:2:ALA:CB	2.60	0.50
1:K:42:ARG:HG3	1:J:9:LEU:HD13	1.94	0.50
2:b:149:LEU:HB2	1:I:21:VAL:HG12	1.94	0.49
1:I:319:ARG:NH2	1:H:17:THR:HG22	2.25	0.49
1:K:44:GLU:HG3	1:J:14:LEU:HD11	1.80	0.49
1:L:226:GLU:OE1	1:L:230:ARG:NH2	2.45	0.49
2:b:6:VAL:HG12	1:J:73:VAL:CB	2.42	0.49
2:i:144:PHE:CD1	1:H:69:ARG:CZ	2.94	0.49
2:f:3:LYS:HB2	1:A:147:TYR:CE1	2.47	0.49
1:I:172:ILE:HG21	1:I:244:LYS:HD2	1.95	0.49
1:G:47:ASP:N	1:G:47:ASP:OD1	2.45	0.49
2:a:83:VAL:HG12	2:a:83:VAL:O	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:9:LEU:C	2:l:9:LEU:HD12	2.38	0.49
1:C:53:ILE:CG2	1:B:124:LEU:HD22	2.42	0.49
1:F:270:ARG:NH1	1:E:12:THR:HG23	2.27	0.49
1:H:25:LEU:HD11	1:H:130:TYR:CD1	2.47	0.49
1:K:84:ARG:CG	1:L:65:LEU:HB3	2.42	0.49
2:b:6:VAL:HG12	1:J:73:VAL:CG2	2.41	0.49
2:h:57:VAL:HG12	2:h:63:PRO:HA	1.95	0.49
1:I:44:GLU:OE1	1:H:11:TYR:HE2	1.95	0.49
2:i:101:ALA:HB1	2:i:105:LEU:HD12	1.95	0.49
2:m:94:GLU:HA	2:m:94:GLU:OE1	2.13	0.49
2:b:122:ALA:O	2:b:125:ILE:HG22	2.12	0.49
2:d:109:GLN:OE1	2:d:125:ILE:HD11	2.12	0.49
2:f:3:LYS:CB	1:A:147:TYR:HE1	2.25	0.49
1:B:279:SER:OG	1:B:280:ASP:N	2.45	0.49
1:I:48:ASP:H	1:H:18:MET:CE	2.26	0.49
1:K:44:GLU:CG	1:J:14:LEU:HD12	2.31	0.49
1:K:55:ALA:HA	1:J:80:PHE:CD1	2.48	0.49
2:b:142:THR:HB	1:J:66:ALA:HB3	1.95	0.49
2:j:21:VAL:O	2:j:21:VAL:HG13	2.11	0.49
2:h:108:ASN:OD1	2:h:109:GLN:N	2.46	0.49
1:A:283:ARG:O	1:A:287:GLN:NE2	2.46	0.49
2:l:114:TYR:OH	2:l:121:ASP:OD1	2.26	0.48
1:D:85:SER:OG	1:D:305:ALA:O	2.19	0.48
1:G:57:GLN:HE21	2:l:97:PRO:HB2	1.74	0.48
2:e:48:LYS:HG2	2:e:87:ILE:HD11	1.96	0.48
2:i:99:VAL:O	2:i:100:LEU:HD23	2.13	0.48
2:f:36:MET:HE1	2:f:57:VAL:HG12	1.94	0.48
1:K:21:VAL:HG12	1:L:190:ASN:ND2	2.23	0.48
1:G:14:LEU:HD12	1:H:44:GLU:O	2.13	0.48
1:G:189:ASP:OD1	1:G:189:ASP:C	2.57	0.48
2:e:29:TRP:HD1	2:f:106:THR:HG22	1.78	0.48
1:I:26:GLN:HG2	1:I:129:MET:HE1	1.94	0.48
2:k:21:VAL:O	2:k:21:VAL:HG13	2.14	0.48
1:D:18:MET:HE2	1:E:49:GLY:HA2	1.87	0.48
1:E:176:GLU:OE2	1:E:180:ARG:NE	2.46	0.48
1:J:187:ALA:O	1:J:319:ARG:NH1	2.45	0.48
1:F:202:ARG:NH2	1:A:181:ALA:HB2	2.29	0.48
1:F:221:TYR:OH	1:E:226:GLU:OE2	2.31	0.48
1:G:229:ARG:HH21	1:H:218:TYR:HA	1.77	0.48
2:e:27:THR:HG21	1:H:303:ARG:NH1	2.28	0.48
2:b:18:LEU:HD13	1:J:64:HIS:HD2	1.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:32:THR:O	1:J:274:ILE:HG22	2.13	0.48
1:G:245:ASN:ND2	1:L:231:ARG:CB	2.77	0.48
1:B:38:THR:HG22	1:B:39:THR:H	1.78	0.48
1:B:43:ILE:HG12	1:A:12:THR:OG1	2.12	0.48
1:I:157:GLN:O	1:I:158:THR:OG1	2.28	0.48
1:E:101:ASN:OD1	1:H:1:MET:O	2.31	0.48
1:K:21:VAL:CG1	1:L:190:ASN:HD21	2.20	0.48
1:G:17:THR:HG21	1:H:45:ARG:CZ	2.44	0.48
1:M:280:ASP:O	1:K:303:ARG:NH1	2.47	0.48
2:g:21:VAL:HG13	2:g:21:VAL:O	2.14	0.48
2:g:27:THR:HG22	2:g:27:THR:O	2.14	0.48
1:K:79:PHE:HB3	1:L:56:VAL:O	2.13	0.48
1:G:57:GLN:OE1	2:l:78:LYS:NZ	2.46	0.47
2:e:21:VAL:HG13	2:e:21:VAL:O	2.14	0.47
2:i:87:ILE:HG23	2:i:87:ILE:O	2.14	0.47
1:G:62:ARG:NH2	1:L:310:GLU:CD	2.49	0.47
2:b:138:LYS:HB3	1:J:63:GLN:HG2	1.96	0.47
2:f:102:VAL:O	2:f:133:ASN:ND2	2.46	0.47
1:F:79:PHE:HB3	1:A:56:VAL:O	2.14	0.47
1:D:83:ASP:OD2	1:E:62:ARG:HD2	2.14	0.47
1:G:237:ASN:HD21	1:H:192:ASP:CB	2.27	0.47
1:B:40:VAL:C	1:A:9:LEU:CD1	2.88	0.47
1:F:223:SER:OG	1:E:229:ARG:NH1	2.48	0.47
1:G:237:ASN:OD1	1:H:192:ASP:OD1	2.33	0.47
2:d:15:ASP:HB3	1:E:84:ARG:HH21	1.80	0.47
1:K:10:ASP:N	1:L:38:THR:HG21	2.29	0.47
1:G:188:GLY:HA2	2:k:145:ILE:HD12	1.96	0.47
1:G:280:ASP:HB2	1:H:58:ARG:NH1	2.28	0.47
2:d:126:GLN:N	2:d:126:GLN:OE1	2.47	0.47
2:f:79:VAL:HG12	2:f:79:VAL:O	2.14	0.47
1:D:278:PRO:O	1:E:58:ARG:NH2	2.41	0.47
1:A:96:GLU:OE1	1:A:96:GLU:HA	2.13	0.47
2:i:140:VAL:HG13	1:H:52:ASP:O	2.14	0.47
1:C:84:ARG:HH22	1:D:67:ASN:HD22	1.61	0.47
1:C:235:ASN:ND2	1:D:195:GLU:OE1	2.48	0.47
2:c:22:VAL:O	2:c:22:VAL:HG13	2.15	0.47
2:c:41:ASP:O	2:c:42:ASP:OD1	2.33	0.47
2:k:89:VAL:HG13	2:k:90:PHE:CD2	2.49	0.47
1:C:221:TYR:HB2	1:C:222:PRO:HD2	1.95	0.47
1:I:19:PRO:HD2	1:J:48:ASP:O	2.15	0.47
1:D:9:LEU:HD12	1:D:9:LEU:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:218:TYR:CE1	1:J:229:ARG:HG2	2.50	0.47
1:G:40:VAL:CB	1:L:9:LEU:HD22	2.45	0.47
1:G:80:PHE:CE1	1:H:55:ALA:CA	2.97	0.47
2:b:26:ASP:OD2	2:c:106:THR:CB	2.63	0.47
1:I:3:ASN:HB3	1:I:9:LEU:HD21	1.97	0.47
1:I:64:HIS:HA	1:H:83:ASP:O	2.14	0.47
1:A:114:MET:O	1:A:118:ARG:HG2	2.15	0.47
1:M:69:ARG:HD2	2:l:144:PHE:CE2	2.49	0.47
2:e:22:VAL:CG2	1:H:304:GLU:CD	2.88	0.47
1:K:16:SER:HA	1:L:46:LEU:O	2.15	0.47
2:e:22:VAL:HG22	1:H:304:GLU:OE1	2.14	0.47
2:b:2:ALA:HA	1:J:147:TYR:CD1	2.50	0.47
2:c:104:GLY:C	2:c:105:LEU:HD12	2.40	0.47
1:I:282:LEU:HD12	1:E:88:ARG:CG	2.45	0.47
2:l:38:PHE:O	2:l:49:THR:OG1	2.22	0.46
2:l:56:LEU:CD2	2:l:73:VAL:HG22	2.45	0.46
2:f:50:THR:HG22	2:f:50:THR:O	2.15	0.46
2:f:144:PHE:HA	1:A:48:ASP:O	2.15	0.46
1:B:270:ARG:CZ	1:A:12:THR:O	2.63	0.46
1:I:235:ASN:HD21	1:J:195:GLU:HA	1.80	0.46
2:d:12:ASN:CG	1:E:90:ASP:CG	2.82	0.46
1:C:11:TYR:CE1	1:D:44:GLU:OE1	2.68	0.46
1:L:149:TYR:OH	1:L:315:THR:O	2.29	0.46
1:M:72:ILE:O	2:l:6:VAL:HA	2.14	0.46
1:M:298:GLU:OE2	1:M:299:SER:O	2.33	0.46
2:e:26:ASP:OD2	2:f:106:THR:CG2	2.62	0.46
2:c:83:VAL:HA	1:D:7:GLN:NE2	2.29	0.46
2:d:44:ASP:OD1	2:d:44:ASP:N	2.47	0.46
1:F:40:VAL:CG1	1:E:9:LEU:CD2	2.93	0.46
1:K:65:LEU:HD21	1:J:82:LEU:CD2	2.34	0.46
1:K:227:ILE:HD11	1:K:241:PHE:CE1	2.50	0.46
1:G:17:THR:HG21	1:H:45:ARG:HE	1.81	0.46
1:G:180:ARG:HH12	1:L:231:ARG:HD2	1.76	0.46
2:c:25:GLY:O	1:E:306:LYS:CD	2.63	0.46
1:K:10:ASP:OD2	1:L:38:THR:N	2.25	0.46
1:K:24:LEU:HG	1:K:28:MET:HE2	1.97	0.46
1:G:17:THR:HG21	1:H:45:ARG:NE	2.31	0.46
1:G:67:ASN:ND2	1:L:84:ARG:NH2	2.64	0.46
1:F:201:SER:OG	1:F:258:ALA:O	2.32	0.46
1:I:3:ASN:OD1	1:I:7:GLN:HG3	2.16	0.46
1:K:310:GLU:OE1	1:L:62:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:ASP:HA	1:F:110:VAL:HG12	1.98	0.46
2:k:23:ALA:CB	2:m:21:VAL:HG22	2.45	0.46
1:H:273:GLU:OE1	1:H:275:TYR:OH	2.26	0.46
1:C:40:VAL:HG13	1:C:75:LEU:O	2.16	0.46
1:I:326:SER:O	1:I:327:THR:OG1	2.30	0.46
1:D:161:ASP:OD2	1:D:161:ASP:C	2.59	0.46
1:J:170:ASP:CG	1:J:172:ILE:HG22	2.41	0.46
1:G:46:LEU:O	1:L:16:SER:HA	2.15	0.46
2:i:145:ILE:HD12	1:H:188:GLY:HA2	1.97	0.46
1:I:40:VAL:HG11	1:H:9:LEU:HD22	1.78	0.46
1:G:9:LEU:CD1	1:H:40:VAL:CB	2.94	0.45
1:M:42:ARG:HH12	1:K:2:GLN:HE22	1.63	0.45
2:h:108:ASN:OD1	2:h:110:LEU:N	2.45	0.45
1:E:1:MET:SD	1:H:2:GLN:NE2	2.89	0.45
1:K:56:VAL:CG2	1:J:81:PRO:CG	2.93	0.45
2:h:96:VAL:CG2	1:H:144:VAL:CG2	2.94	0.45
1:D:229:ARG:NH2	1:E:221:TYR:CG	2.83	0.45
1:D:229:ARG:NH1	1:E:221:TYR:HE1	2.12	0.45
1:J:38:THR:HG23	1:J:40:VAL:H	1.81	0.45
1:A:227:ILE:HG13	1:A:232:LEU:HD21	1.98	0.45
1:B:40:VAL:C	1:A:9:LEU:HD11	2.42	0.45
2:e:143:GLN:O	1:I:49:GLY:CA	2.64	0.45
1:I:184:ILE:HD12	1:H:237:ASN:OD1	2.17	0.45
1:L:40:VAL:HG12	1:L:74:ASN:OD1	2.17	0.45
1:G:229:ARG:NH2	1:H:223:SER:OG	2.48	0.45
1:G:281:THR:HG22	1:G:283:ARG:H	1.80	0.45
2:e:142:THR:HG23	1:I:66:ALA:HB3	1.99	0.45
1:C:149:TYR:OH	1:C:315:THR:O	2.29	0.45
1:B:150:TYR:O	1:B:151:ASP:HB3	2.15	0.45
1:B:281:THR:HG22	1:B:283:ARG:HD3	1.97	0.45
1:F:231:ARG:HD2	1:A:176:GLU:OE2	2.17	0.45
1:F:237:ASN:ND2	1:A:184:ILE:CG2	2.75	0.45
1:D:162:VAL:HG13	1:D:171:PRO:HB3	1.98	0.45
1:G:53:ILE:HD11	1:L:82:LEU:HD11	1.97	0.45
1:G:72:ILE:O	2:k:6:VAL:HG23	2.16	0.45
1:G:107:ASP:O	1:G:111:GLN:OE1	2.34	0.45
1:G:244:LYS:HA	1:L:230:ARG:HA	1.97	0.45
2:k:13:TYR:HB3	1:L:90:ASP:OD1	2.16	0.45
1:F:65:LEU:HD23	1:F:66:ALA:O	2.17	0.45
1:I:229:ARG:O	1:J:244:LYS:HG3	2.17	0.45
1:E:193:ASN:O	1:E:193:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:46:ASP:OD1	2:e:88:GLY:N	2.50	0.45
2:f:3:LYS:CB	1:A:147:TYR:CE1	3.00	0.45
1:C:73:VAL:HG22	1:C:74:ASN:N	2.31	0.45
1:C:231:ARG:HB3	1:D:245:ASN:OD1	2.16	0.45
1:D:33:GLU:O	1:D:34:HIS:ND1	2.50	0.45
1:D:310:GLU:CD	1:E:62:ARG:HH22	2.18	0.45
1:E:187:ALA:O	1:E:319:ARG:NH1	2.50	0.45
1:G:39:THR:O	1:G:39:THR:HG22	2.17	0.45
2:e:103:ARG:HH12	2:f:134:GLN:HB2	1.79	0.45
1:F:62:ARG:HH11	1:E:308:GLU:CG	2.29	0.45
1:F:80:PHE:CE1	1:A:55:ALA:HA	2.51	0.45
1:D:1:MET:HE2	1:D:9:LEU:HD11	1.99	0.45
1:D:192:ASP:O	1:D:193:ASN:OD1	2.34	0.45
1:G:3:ASN:HD21	2:h:85:HIS:CD2	2.35	0.45
2:l:4:ALA:O	2:l:6:VAL:HG13	2.16	0.45
1:G:270:ARG:NH1	1:L:12:THR:O	2.50	0.45
2:e:27:THR:HG21	1:H:303:ARG:HH11	1.81	0.45
1:H:99:THR:HG21	1:H:102:ALA:HB3	1.99	0.45
1:B:70:LYS:HD3	1:A:97:PHE:CD2	2.52	0.44
1:I:50:ALA:HB2	1:H:119:ARG:HE	1.82	0.44
1:I:57:GLN:HE21	1:H:144:VAL:CG2	2.29	0.44
1:K:229:ARG:NH2	1:L:221:TYR:CZ	2.86	0.44
2:e:32:LYS:NZ	2:f:129:GLU:CD	2.71	0.44
2:e:101:ALA:HB1	2:e:105:LEU:CD1	2.47	0.44
2:l:23:ALA:HA	2:k:21:VAL:HG23	1.99	0.44
2:l:83:VAL:HG22	1:K:7:GLN:OE1	2.16	0.44
2:f:37:THR:HG23	2:f:37:THR:O	2.17	0.44
1:E:93:ASN:O	1:H:7:GLN:HA	2.17	0.44
1:K:218:TYR:CZ	1:J:229:ARG:HD2	2.51	0.44
1:G:40:VAL:HG11	1:L:9:LEU:CD2	2.39	0.44
1:G:81:PRO:CD	1:H:56:VAL:HB	2.48	0.44
1:G:310:GLU:HG3	1:H:62:ARG:HH12	1.81	0.44
2:b:56:LEU:HD23	2:b:73:VAL:HG22	2.00	0.44
2:e:98:MET:HE3	2:e:98:MET:HA	1.98	0.44
2:l:108:ASN:OD1	2:l:110:LEU:N	2.46	0.44
1:C:327:THR:HG22	1:C:328:GLY:N	2.32	0.44
1:I:226:GLU:OE2	1:J:221:TYR:OH	2.32	0.44
1:J:3:ASN:ND2	1:J:9:LEU:HD23	2.33	0.44
2:c:96:VAL:HG23	2:c:98:MET:HE3	2.00	0.44
2:a:79:VAL:HG12	2:a:79:VAL:O	2.18	0.44
2:d:83:VAL:HG23	2:d:84:ASP:N	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:22:VAL:O	2:f:22:VAL:HG23	2.18	0.44
1:G:119:ARG:NH2	1:H:49:GLY:O	2.46	0.44
2:b:2:ALA:HA	1:J:147:TYR:CE1	2.53	0.44
1:F:61:VAL:HG12	1:F:62:ARG:N	2.32	0.44
1:K:184:ILE:HD13	1:J:237:ASN:OD1	2.17	0.44
2:j:101:ALA:HB1	2:j:105:LEU:HD11	1.98	0.44
1:I:44:GLU:C	1:H:14:LEU:HD12	2.43	0.44
1:I:48:ASP:N	1:H:18:MET:HE1	2.33	0.44
1:D:149:TYR:CE1	1:D:316:VAL:HG23	2.52	0.44
1:K:68:ASP:CG	1:J:116:ARG:HH21	2.24	0.44
1:K:176:GLU:OE1	1:K:180:ARG:NE	2.51	0.44
1:K:222:PRO:C	1:K:223:SER:HG	2.20	0.44
1:M:39:THR:HG22	1:M:39:THR:O	2.18	0.44
2:d:85:HIS:CE1	1:H:7:GLN:HE22	2.35	0.44
2:f:19:GLY:N	2:f:106:THR:OG1	2.51	0.44
1:F:181:ALA:HB2	1:E:202:ARG:HH12	1.80	0.44
1:J:226:GLU:OE2	1:J:229:ARG:NE	2.38	0.44
1:G:9:LEU:HD21	1:H:42:ARG:HB2	2.00	0.44
1:G:44:GLU:OE1	1:L:98:GLY:N	2.51	0.44
1:G:229:ARG:NH2	1:H:218:TYR:HA	2.33	0.44
2:e:143:GLN:O	1:I:49:GLY:HA3	2.18	0.44
2:k:109:GLN:HG3	2:k:135:VAL:HG12	2.00	0.44
1:G:270:ARG:CZ	1:L:12:THR:O	2.66	0.43
2:f:76:ASP:OD1	2:f:77:ARG:N	2.51	0.43
1:M:283:ARG:HH21	1:K:302:LEU:HD11	1.68	0.43
2:d:76:ASP:OD1	2:d:77:ARG:N	2.52	0.43
2:f:101:ALA:HB1	2:f:105:LEU:CD1	2.48	0.43
1:I:161:ASP:OD1	1:I:162:VAL:N	2.51	0.43
1:K:223:SER:HB3	1:J:229:ARG:NH2	2.33	0.43
2:b:144:PHE:HB3	1:J:47:ASP:OD1	2.18	0.43
2:k:73:VAL:HG12	2:k:74:LEU:N	2.33	0.43
1:F:227:ILE:HD11	1:F:241:PHE:CE1	2.53	0.43
1:C:56:VAL:HG12	1:C:57:GLN:N	2.33	0.43
1:E:151:ASP:OD1	1:E:152:VAL:N	2.51	0.43
1:K:25:LEU:HA	1:K:28:MET:HE3	2.00	0.43
2:b:32:LYS:HG2	2:b:33:GLU:N	2.32	0.43
2:b:38:PHE:O	2:b:49:THR:OG1	2.27	0.43
2:c:101:ALA:HB1	2:c:105:LEU:HD22	2.00	0.43
2:f:83:VAL:O	2:f:83:VAL:HG13	2.18	0.43
2:g:78:LYS:NZ	1:B:57:GLN:OE1	2.42	0.43
1:C:61:VAL:HG12	1:C:62:ARG:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:231:ARG:HB2	1:L:245:ASN:OD1	2.18	0.43
1:M:23:THR:O	1:M:23:THR:HG22	2.19	0.43
1:I:283:ARG:NH1	1:E:302:LEU:HB2	2.34	0.43
1:D:9:LEU:HD12	1:D:10:ASP:N	2.33	0.43
1:A:175:LEU:O	1:A:179:ALA:HB3	2.18	0.43
2:c:25:GLY:O	1:E:306:LYS:HD2	2.19	0.43
1:K:157:GLN:NE2	1:K:323:VAL:O	2.52	0.43
1:L:87:ASP:OD1	1:L:88:ARG:N	2.52	0.43
1:A:86:ILE:HG22	1:A:87:ASP:N	2.34	0.43
1:G:17:THR:O	1:G:18:MET:HE2	2.18	0.43
1:G:116:ARG:NH2	1:H:67:ASN:C	2.73	0.43
2:e:133:ASN:O	2:h:103:ARG:NH2	2.52	0.43
2:l:34:VAL:HG21	2:l:100:LEU:CD1	2.49	0.43
2:i:2:ALA:O	2:i:3:LYS:C	2.62	0.43
2:i:22:VAL:HG23	2:i:22:VAL:O	2.18	0.43
1:C:158:THR:HG23	1:C:324:VAL:HG13	2.00	0.43
1:K:61:VAL:HG12	1:K:62:ARG:N	2.34	0.43
2:f:20:ARG:CZ	2:f:30:ASN:OD1	2.66	0.43
1:I:18:MET:N	1:J:188:GLY:O	2.52	0.43
1:I:327:THR:HG22	1:I:328:GLY:N	2.34	0.43
1:K:11:TYR:HE1	1:L:44:GLU:HG3	1.84	0.43
1:K:235:ASN:OD1	1:L:180:ARG:NH2	2.52	0.43
2:e:22:VAL:HG21	1:H:304:GLU:OE1	2.17	0.43
1:M:73:VAL:HA	2:l:5:HIS:O	2.19	0.42
2:h:110:LEU:O	2:h:113:LYS:NZ	2.52	0.42
1:I:283:ARG:NH2	1:E:302:LEU:HG	2.33	0.42
2:h:75:VAL:O	2:h:75:VAL:CG1	2.66	0.42
2:h:87:ILE:O	2:h:87:ILE:HG23	2.17	0.42
1:C:11:TYR:CZ	1:D:44:GLU:OE1	2.71	0.42
1:B:167:LEU:O	1:B:213:GLN:NE2	2.50	0.42
1:F:56:VAL:HG21	1:E:81:PRO:HG3	2.01	0.42
1:F:167:LEU:HD22	1:F:212:PRO:HG2	2.01	0.42
1:I:231:ARG:CB	1:J:245:ASN:ND2	2.50	0.42
1:E:83:ASP:OD1	1:E:84:ARG:N	2.52	0.42
1:M:151:ASP:OD1	1:M:152:VAL:N	2.52	0.42
2:l:34:VAL:HG12	2:l:35:ASP:N	2.34	0.42
1:F:48:ASP:OD1	1:F:49:GLY:N	2.52	0.42
1:A:283:ARG:CZ	1:A:283:ARG:HB3	2.50	0.42
1:C:87:ASP:OD1	1:C:88:ARG:HD3	2.19	0.42
1:K:44:GLU:O	1:J:14:LEU:HD12	2.19	0.42
1:L:3:ASN:ND2	1:L:9:LEU:HD21	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:HG22	1:A:54:LYS:N	2.33	0.42
1:G:185:ASP:N	1:L:20:ARG:NH2	2.68	0.42
2:k:26:ASP:OD2	2:m:106:THR:CB	2.65	0.42
1:C:175:LEU:O	1:C:179:ALA:HB3	2.20	0.42
1:B:46:LEU:O	1:A:16:SER:HA	2.19	0.42
1:B:284:ASP:OD1	1:B:284:ASP:N	2.52	0.42
1:I:57:GLN:NE2	1:H:144:VAL:CG2	2.72	0.42
2:m:12:ASN:OD1	2:m:13:TYR:N	2.48	0.42
1:I:17:THR:CG2	1:J:46:LEU:O	2.68	0.42
1:I:97:PHE:CD2	1:J:46:LEU:HD21	2.55	0.42
2:m:10:GLU:OE2	2:m:11:GLY:N	2.53	0.42
1:G:226:GLU:OE2	1:G:226:GLU:HA	2.20	0.42
1:G:306:LYS:NZ	2:j:26:ASP:CA	2.78	0.42
1:L:73:VAL:HG22	1:L:74:ASN:H	1.84	0.42
1:A:61:VAL:HG12	1:A:62:ARG:N	2.35	0.42
1:C:231:ARG:CB	1:D:245:ASN:OD1	2.68	0.42
1:F:56:VAL:HG22	1:E:81:PRO:CD	2.50	0.42
1:I:19:PRO:HD3	1:J:48:ASP:O	2.19	0.42
1:E:198:VAL:HG22	1:E:263:ILE:HG12	2.00	0.42
1:A:304:GLU:HA	1:A:304:GLU:OE1	2.19	0.42
1:G:100:GLU:H	1:G:100:GLU:CD	2.26	0.42
2:h:13:TYR:HE1	2:h:75:VAL:HG12	1.85	0.42
2:h:22:VAL:O	2:h:22:VAL:HG23	2.19	0.42
1:D:80:PHE:CE1	1:E:55:ALA:N	2.88	0.42
1:K:80:PHE:HE1	1:L:55:ALA:HB2	1.78	0.42
1:J:76:ASN:O	1:J:314:LEU:HD22	2.20	0.42
1:G:119:ARG:HH22	1:H:48:ASP:CG	2.27	0.42
1:G:189:ASP:OD1	1:G:190:ASN:N	2.52	0.42
1:M:327:THR:HG22	1:M:328:GLY:N	2.35	0.42
2:c:85:HIS:HD2	1:D:3:ASN:ND2	2.05	0.42
2:f:21:VAL:O	2:f:21:VAL:HG13	2.20	0.42
1:F:197:VAL:HG12	1:F:198:VAL:N	2.35	0.42
1:L:73:VAL:HG22	1:L:74:ASN:N	2.35	0.42
1:G:17:THR:CG2	1:H:45:ARG:HH21	2.24	0.41
1:G:19:PRO:HG3	1:H:49:GLY:HA2	2.02	0.41
1:G:53:ILE:HG22	1:G:54:LYS:N	2.35	0.41
2:i:11:GLY:CA	1:H:67:ASN:ND2	2.62	0.41
1:C:65:LEU:HG	1:C:66:ALA:H	1.85	0.41
1:C:327:THR:HG22	1:C:328:GLY:H	1.83	0.41
1:B:43:ILE:HG13	1:A:12:THR:OG1	2.18	0.41
1:I:45:ARG:HA	1:H:15:ILE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:VAL:HG22	1:K:74:ASN:N	2.35	0.41
2:m:36:MET:CE	2:m:74:LEU:HD13	2.49	0.41
1:G:69:ARG:HG3	2:k:10:GLU:CD	2.45	0.41
1:G:188:GLY:HA2	2:k:145:ILE:CD1	2.49	0.41
2:a:13:TYR:CE1	2:a:75:VAL:HG21	2.56	0.41
1:B:55:ALA:HA	1:A:80:PHE:CD1	2.55	0.41
1:D:80:PHE:CD1	1:E:55:ALA:N	2.88	0.41
1:D:229:ARG:HD3	1:E:218:TYR:CE1	2.55	0.41
1:K:100:GLU:OE1	1:K:100:GLU:N	2.52	0.41
1:A:185:ASP:OD1	1:A:186:TRP:N	2.52	0.41
2:m:89:VAL:HG12	2:m:89:VAL:O	2.20	0.41
1:C:151:ASP:OD1	1:C:151:ASP:C	2.63	0.41
1:E:189:ASP:O	1:E:194:TYR:OH	2.37	0.41
1:K:47:ASP:OD2	1:K:69:ARG:NE	2.52	0.41
1:K:65:LEU:HD11	1:J:117:ILE:HG13	2.01	0.41
1:G:9:LEU:HD12	1:H:40:VAL:O	2.20	0.41
2:k:79:VAL:O	2:k:79:VAL:CG1	2.67	0.41
1:I:53:ILE:CG2	1:H:124:LEU:HB2	2.51	0.41
1:I:97:PHE:CE2	1:J:44:GLU:OE1	2.73	0.41
1:I:138:TRP:O	1:I:139:SER:C	2.63	0.41
2:e:126:GLN:NE2	2:h:59:GLU:OE1	2.50	0.41
2:k:109:GLN:NE2	2:k:125:ILE:HD13	2.35	0.41
2:f:36:MET:HB3	2:f:98:MET:HG3	2.01	0.41
1:B:196:ILE:HG22	1:B:197:VAL:N	2.35	0.41
1:F:20:ARG:HH21	1:A:185:ASP:HB3	1.86	0.41
1:F:286:ASN:OD1	1:H:92:GLN:O	2.39	0.41
1:I:40:VAL:HB	1:H:9:LEU:CD2	2.51	0.41
1:D:3:ASN:HB2	1:D:9:LEU:HD23	2.02	0.41
1:K:84:ARG:HG3	1:L:65:LEU:HB3	2.02	0.41
1:G:306:LYS:HZ1	2:j:25:GLY:C	2.14	0.41
1:M:238:ASN:OD1	1:M:238:ASN:N	2.51	0.41
1:M:265:PRO:HG2	1:M:322:LEU:HD23	2.02	0.41
2:d:24:PHE:CD2	1:E:301:TYR:OH	2.73	0.41
2:d:80:LEU:O	2:d:83:VAL:HG22	2.21	0.41
1:C:92:GLN:O	1:C:93:ASN:HB2	2.21	0.41
1:I:68:ASP:HB3	1:H:116:ARG:NH2	2.36	0.41
1:D:197:VAL:CG2	1:D:266:ARG:HE	2.34	0.41
1:K:42:ARG:HH11	1:J:1:MET:CE	2.32	0.41
1:K:172:ILE:HG21	1:K:244:LYS:HD2	2.03	0.41
1:G:124:LEU:HD22	1:H:53:ILE:HB	2.01	0.41
1:G:260:GLU:OE2	1:G:325:LYS:NZ	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:83:VAL:O	2:i:83:VAL:HG12	2.19	0.41
2:i:140:VAL:CG1	1:H:51:GLY:HA3	2.51	0.41
2:h:21:VAL:O	2:h:21:VAL:HG13	2.20	0.41
1:F:56:VAL:HG22	1:E:81:PRO:HD3	2.02	0.41
1:K:27:SER:O	1:K:29:ASN:ND2	2.54	0.41
1:K:82:LEU:HD12	1:L:53:ILE:HD12	2.01	0.41
1:K:188:GLY:O	1:J:18:MET:N	2.41	0.41
1:G:33:GLU:OE2	1:G:33:GLU:HA	2.21	0.41
1:G:40:VAL:HB	1:L:9:LEU:HD22	2.02	0.41
2:b:14:SER:HB3	1:I:90:ASP:OD2	2.21	0.41
2:c:116:ASP:OD2	2:c:118:THR:OG1	2.35	0.41
2:a:34:VAL:O	2:a:98:MET:N	2.43	0.41
2:d:36:MET:HE2	2:d:36:MET:HB3	1.98	0.41
1:B:53:ILE:HG22	1:B:54:LYS:N	2.36	0.41
1:I:283:ARG:NH2	1:E:302:LEU:CB	2.84	0.41
1:D:91:ILE:HD12	1:D:106:VAL:HA	2.02	0.41
1:K:15:ILE:O	1:L:45:ARG:HA	2.21	0.41
1:K:44:GLU:HG3	1:J:14:LEU:HD13	1.38	0.41
2:m:79:VAL:O	2:m:79:VAL:CG1	2.69	0.41
2:m:91:GLU:N	2:m:91:GLU:CD	2.79	0.41
2:e:140:VAL:HG23	1:I:64:HIS:O	2.20	0.41
2:c:33:GLU:OE2	1:F:57:GLN:CB	2.68	0.41
2:d:12:ASN:OD1	1:E:90:ASP:CB	2.69	0.41
1:I:53:ILE:HG23	1:H:124:LEU:HD22	2.03	0.41
1:M:29:ASN:OD1	1:M:29:ASN:N	2.54	0.40
2:b:83:VAL:O	2:b:83:VAL:HG13	2.22	0.40
2:j:83:VAL:O	2:j:83:VAL:CG1	2.69	0.40
1:I:68:ASP:HB3	1:H:116:ARG:HH21	1.86	0.40
1:H:150:TYR:CZ	1:H:157:GLN:HG2	2.56	0.40
1:K:62:ARG:HD3	1:J:83:ASP:CG	2.46	0.40
1:G:15:ILE:HD13	1:H:270:ARG:NH1	2.13	0.40
1:G:192:ASP:OD2	1:G:192:ASP:C	2.62	0.40
2:b:12:ASN:HD22	1:I:90:ASP:CG	2.24	0.40
2:d:145:ILE:HD12	1:E:17:THR:HB	2.03	0.40
1:C:237:ASN:CB	1:D:192:ASP:OD1	2.69	0.40
1:K:68:ASP:OD1	1:J:116:ARG:NH2	2.50	0.40
2:m:67:ALA:O	2:m:70:VAL:HG22	2.22	0.40
2:d:21:VAL:O	2:d:21:VAL:HG13	2.21	0.40
2:j:144:PHE:O	2:j:146:GLY:N	2.54	0.40
1:C:281:THR:HG22	1:C:283:ARG:H	1.86	0.40
1:I:44:GLU:OE1	1:H:11:TYR:CZ	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:145:SER:O	1:K:146:ASP:C	2.65	0.40
2:h:25:GLY:HA2	1:H:306:LYS:CD	2.51	0.40
1:B:38:THR:HG22	1:B:39:THR:N	2.36	0.40
1:B:62:ARG:NH1	1:A:310:GLU:OE2	2.54	0.40
1:K:221:TYR:HB2	1:K:222:PRO:HD2	2.04	0.40
2:d:9:LEU:HD23	1:F:70:LYS:HD2	2.04	0.40
2:h:24:PHE:CE2	1:H:299:SER:HB3	2.57	0.40
1:C:79:PHE:HB3	1:D:56:VAL:O	2.21	0.40
1:F:99:THR:HG22	1:F:100:GLU:N	2.37	0.40
1:D:211:HIS:O	1:D:214:VAL:HG22	2.21	0.40
1:D:270:ARG:NE	1:D:273:GLU:OE2	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/332 (99%)	321 (98%)	8 (2%)	0	100	100
1	B	328/332 (99%)	314 (96%)	14 (4%)	0	100	100
1	C	328/332 (99%)	314 (96%)	14 (4%)	0	100	100
1	D	329/332 (99%)	309 (94%)	20 (6%)	0	100	100
1	E	328/332 (99%)	318 (97%)	10 (3%)	0	100	100
1	F	328/332 (99%)	312 (95%)	15 (5%)	1 (0%)	36	65
1	G	328/332 (99%)	313 (95%)	15 (5%)	0	100	100
1	H	328/332 (99%)	320 (98%)	8 (2%)	0	100	100
1	I	328/332 (99%)	313 (95%)	15 (5%)	0	100	100
1	J	329/332 (99%)	314 (95%)	15 (5%)	0	100	100
1	K	328/332 (99%)	312 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	326/332 (98%)	313 (96%)	13 (4%)	0	100	100
1	M	323/332 (97%)	310 (96%)	12 (4%)	1 (0%)	36	65
2	a	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
2	b	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
2	c	145/149 (97%)	136 (94%)	9 (6%)	0	100	100
2	d	146/149 (98%)	137 (94%)	9 (6%)	0	100	100
2	e	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
2	f	146/149 (98%)	138 (94%)	8 (6%)	0	100	100
2	g	146/149 (98%)	131 (90%)	15 (10%)	0	100	100
2	h	146/149 (98%)	135 (92%)	11 (8%)	0	100	100
2	i	146/149 (98%)	137 (94%)	9 (6%)	0	100	100
2	j	146/149 (98%)	137 (94%)	8 (6%)	1 (1%)	18	51
2	k	146/149 (98%)	134 (92%)	12 (8%)	0	100	100
2	l	144/149 (97%)	129 (90%)	14 (10%)	1 (1%)	18	51
2	m	146/149 (98%)	141 (97%)	5 (3%)	0	100	100
All	All	6150/6253 (98%)	5849 (95%)	297 (5%)	4 (0%)	49	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	61	VAL
2	l	145	ILE
2	j	145	ILE
1	M	268	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/280 (100%)	280 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	279/280 (100%)	279 (100%)	0	100	100
1	C	279/280 (100%)	279 (100%)	0	100	100
1	D	280/280 (100%)	280 (100%)	0	100	100
1	E	279/280 (100%)	279 (100%)	0	100	100
1	F	279/280 (100%)	279 (100%)	0	100	100
1	G	279/280 (100%)	279 (100%)	0	100	100
1	H	279/280 (100%)	279 (100%)	0	100	100
1	I	279/280 (100%)	279 (100%)	0	100	100
1	J	280/280 (100%)	280 (100%)	0	100	100
1	K	279/280 (100%)	279 (100%)	0	100	100
1	L	279/280 (100%)	279 (100%)	0	100	100
1	M	278/280 (99%)	277 (100%)	1 (0%)	84	81
2	a	111/112 (99%)	111 (100%)	0	100	100
2	b	111/112 (99%)	111 (100%)	0	100	100
2	c	110/112 (98%)	110 (100%)	0	100	100
2	d	111/112 (99%)	111 (100%)	0	100	100
2	e	109/112 (97%)	109 (100%)	0	100	100
2	f	111/112 (99%)	111 (100%)	0	100	100
2	g	111/112 (99%)	111 (100%)	0	100	100
2	h	111/112 (99%)	111 (100%)	0	100	100
2	i	111/112 (99%)	111 (100%)	0	100	100
2	j	111/112 (99%)	111 (100%)	0	100	100
2	k	111/112 (99%)	111 (100%)	0	100	100
2	l	109/112 (97%)	109 (100%)	0	100	100
2	m	111/112 (99%)	110 (99%)	1 (1%)	70	76
All	All	5067/5096 (99%)	5065 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	237	ASN
2	m	47	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	3	ASN
1	G	7	GLN
1	G	237	ASN
1	G	245	ASN
1	M	64	HIS
1	M	286	ASN
2	e	131	GLN
2	e	143	GLN
2	c	85	HIS
2	a	143	GLN
2	l	133	ASN
2	k	12	ASN
2	h	85	HIS
2	f	134	GLN
2	g	109	GLN
2	g	133	ASN
1	C	63	GLN
1	C	67	ASN
1	C	182	HIS
1	C	193	ASN
1	C	211	HIS
1	F	64	HIS
1	F	182	HIS
1	F	190	ASN
1	F	211	HIS
1	F	237	ASN
1	I	26	GLN
1	I	64	HIS
1	I	211	HIS
1	D	3	ASN
1	D	63	GLN
1	D	67	ASN
1	D	74	ASN
1	D	190	ASN
1	D	237	ASN
1	E	2	GLN
1	E	92	GLN
1	E	211	HIS
1	E	238	ASN
1	E	243	HIS
1	E	255	ASN

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Mol	Chain	Res	Type
1	H	2	GLN
1	H	7	GLN
1	H	34	HIS
1	H	67	ASN
1	H	182	HIS
1	H	286	ASN
1	K	2	GLN
1	K	76	ASN
1	K	92	GLN
1	K	243	HIS
1	L	182	HIS
1	L	255	ASN
1	J	64	HIS
1	J	92	GLN
1	J	93	ASN
1	J	157	GLN
1	J	245	ASN
1	A	26	GLN
1	A	57	GLN
1	A	157	GLN
1	A	220	GLN
1	A	287	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

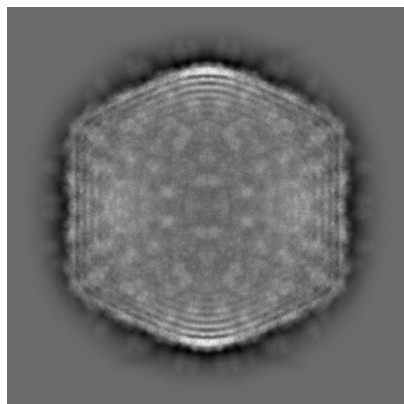
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45937. These allow visual inspection of the internal detail of the map and identification of artifacts.

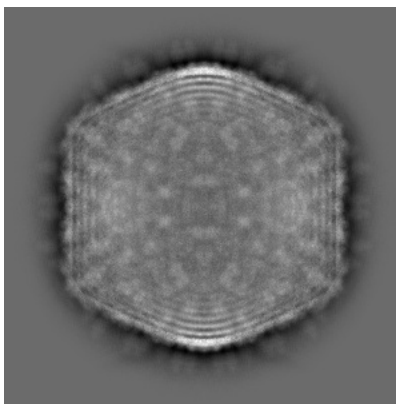
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

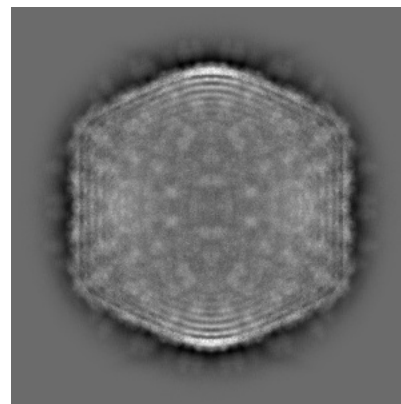
6.1.1 Primary map



X

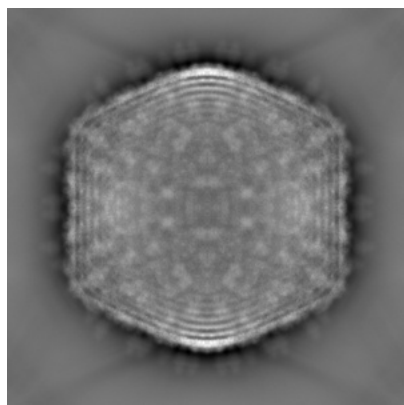


Y

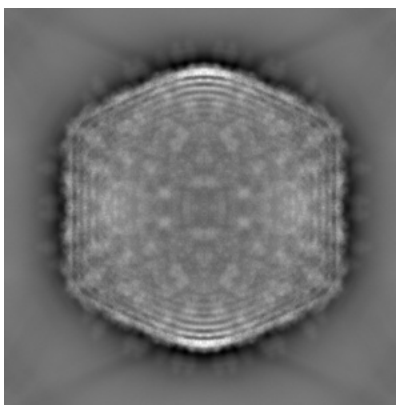


Z

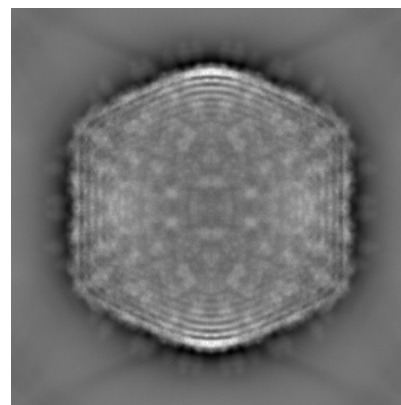
6.1.2 Raw map



X



Y

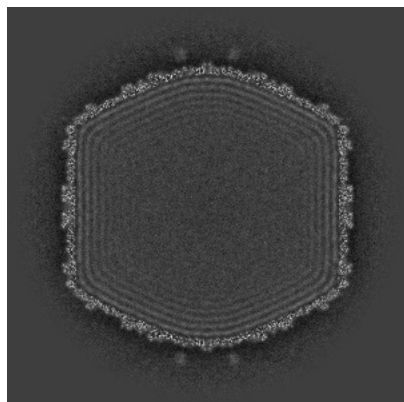


Z

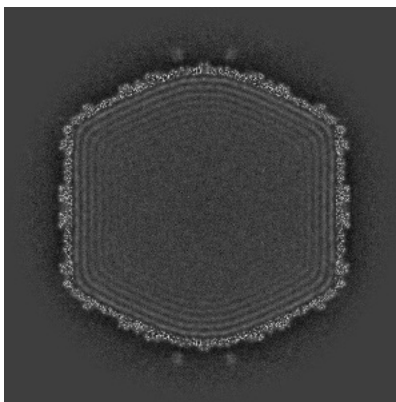
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

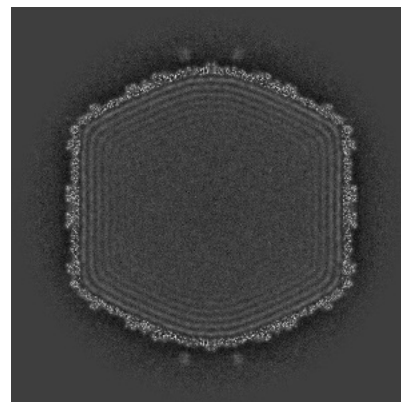
6.2.1 Primary map



X Index: 404

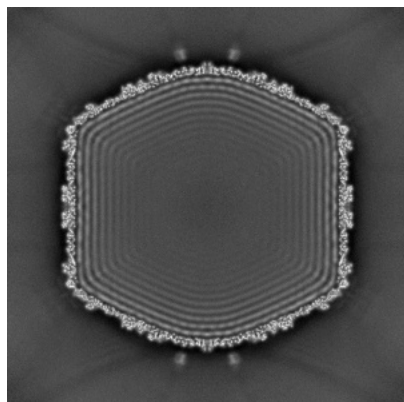


Y Index: 404

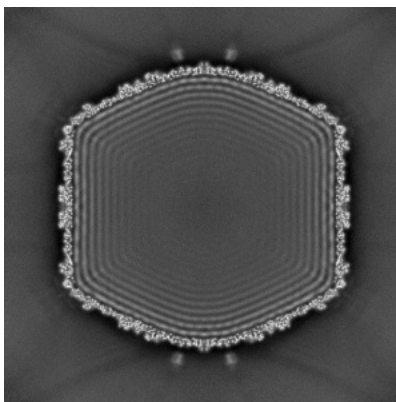


Z Index: 404

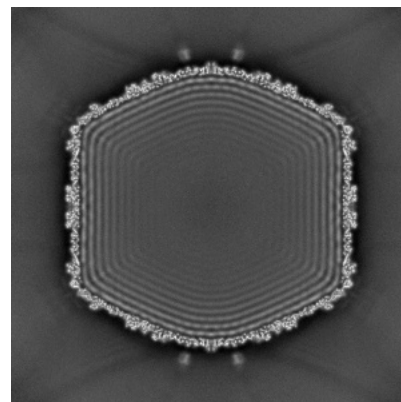
6.2.2 Raw map



X Index: 404



Y Index: 404

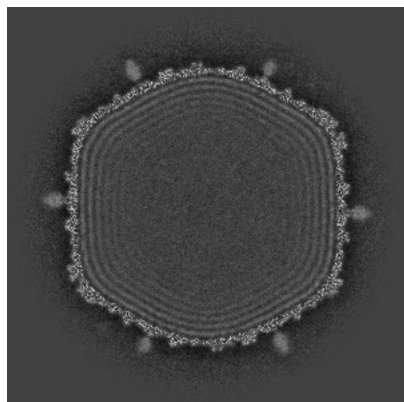


Z Index: 404

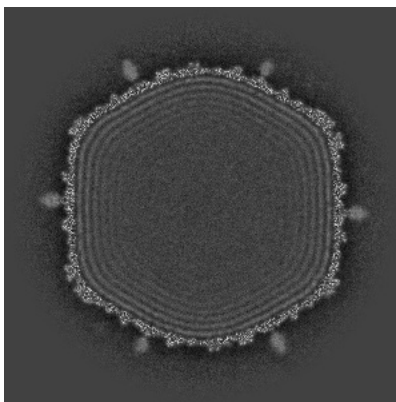
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

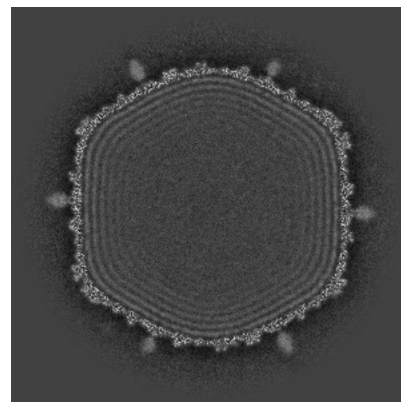
6.3.1 Primary map



X Index: 354

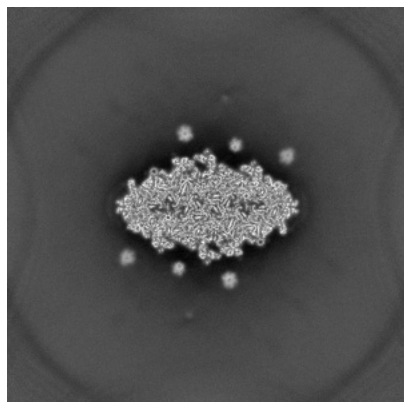


Y Index: 354

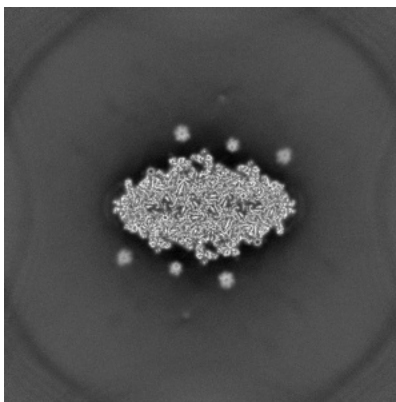


Z Index: 354

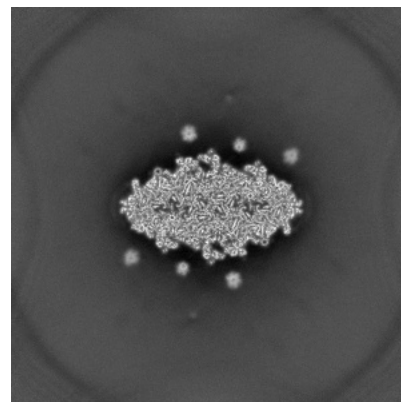
6.3.2 Raw map



X Index: 135



Y Index: 135

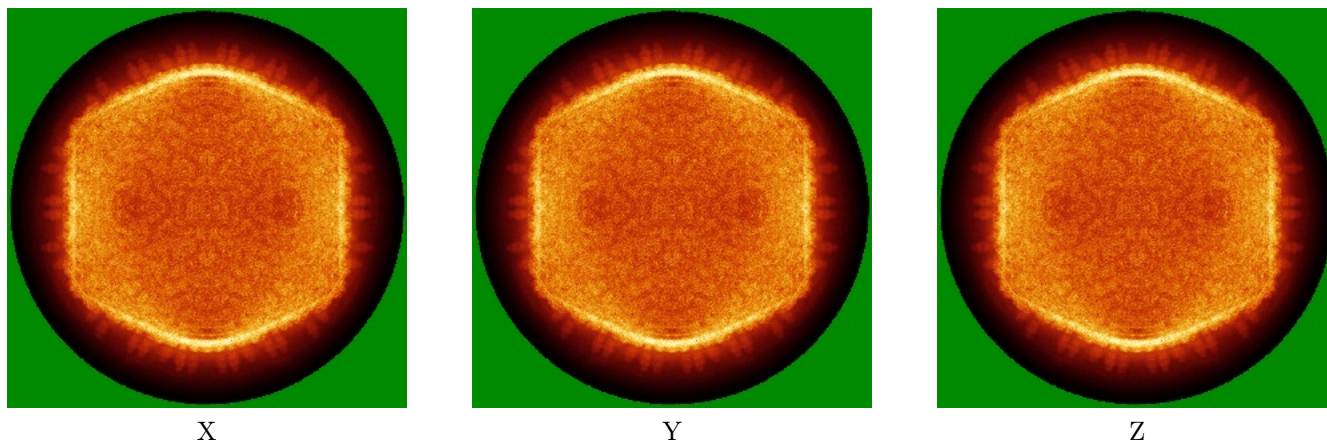


Z Index: 135

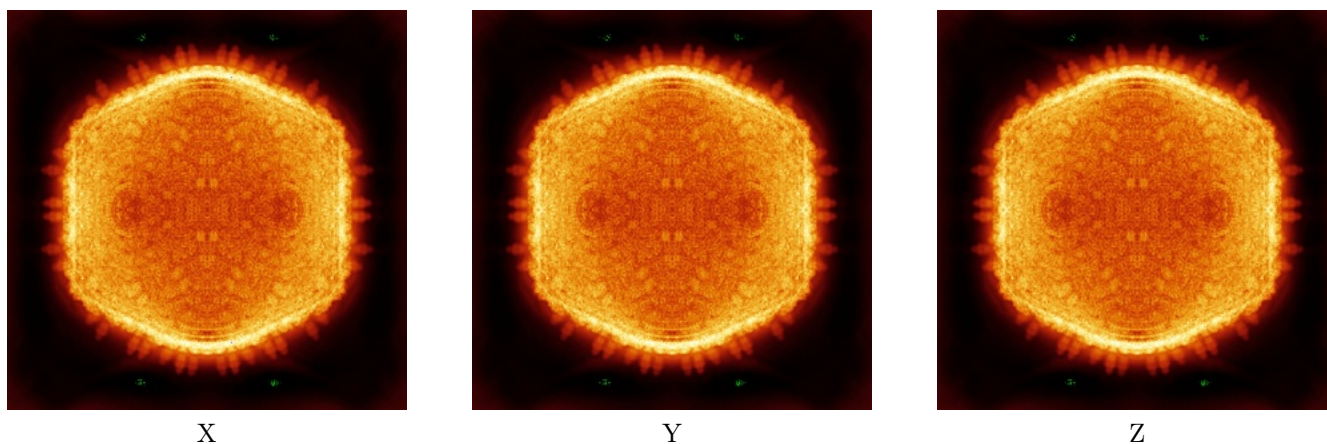
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

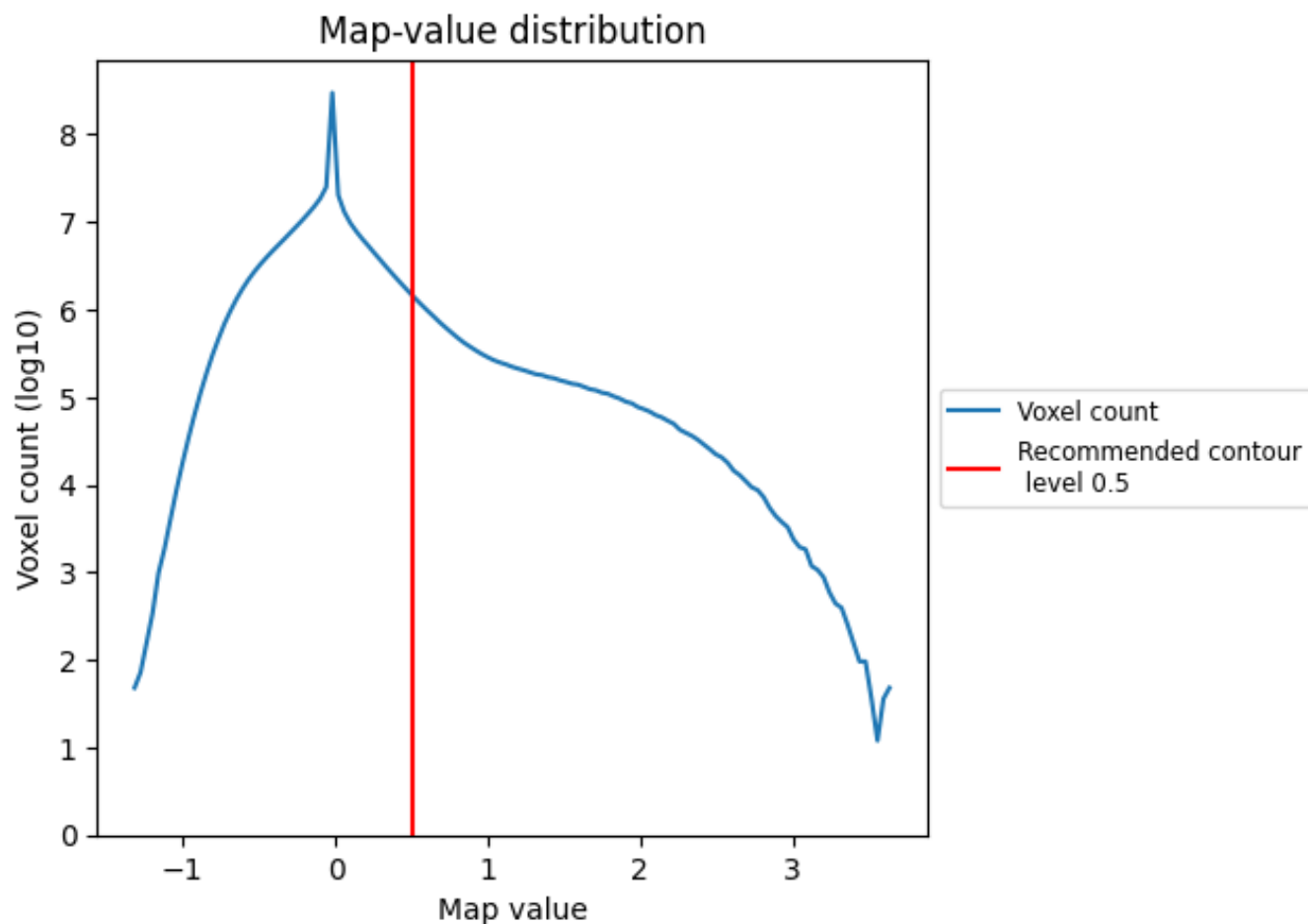
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

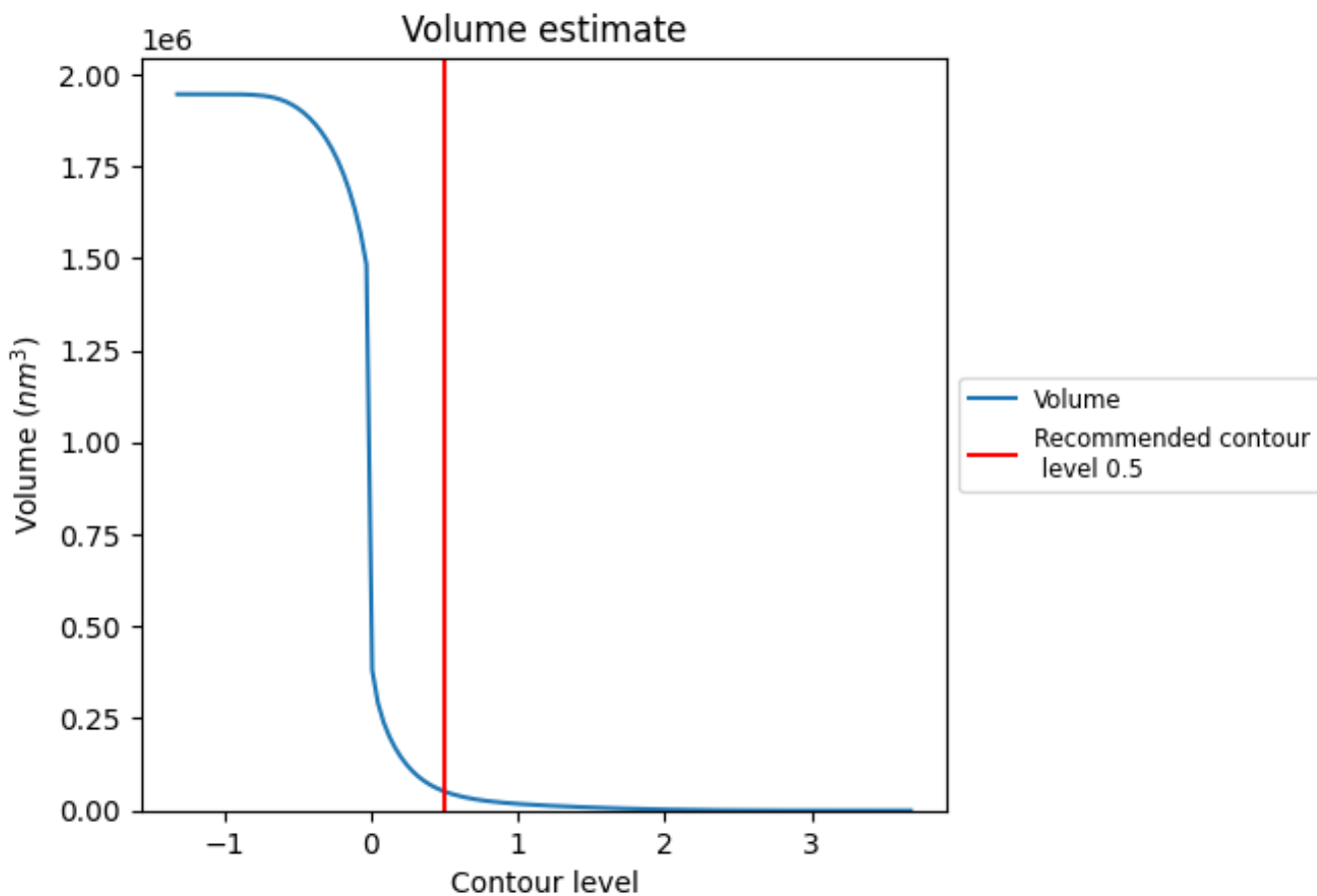
This section contains the results of statistical analysis of the map.

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.

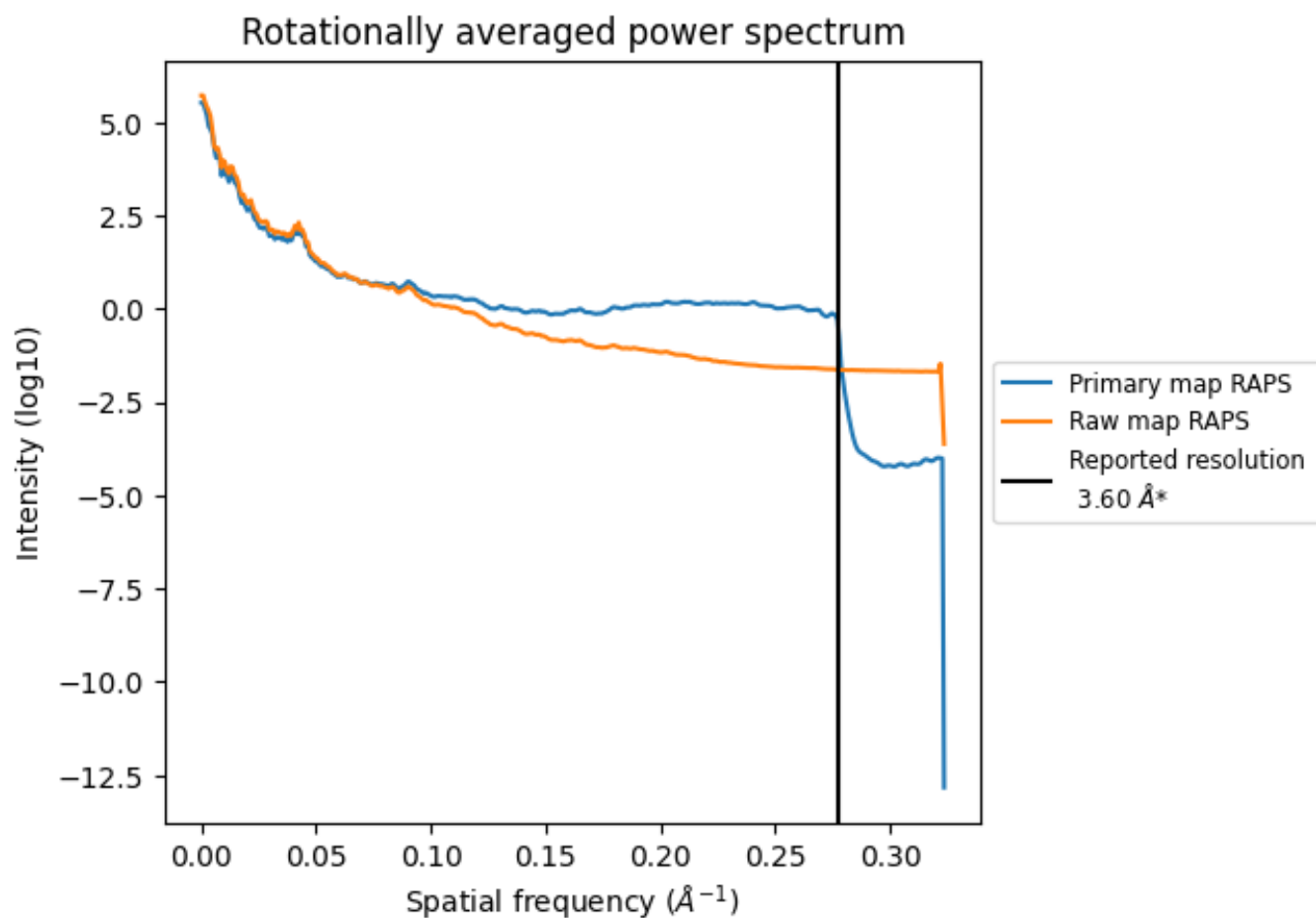
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 51983 nm^3 ; this corresponds to an approximate mass of 46958 kDa.

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

7.3 Rotationally averaged power spectrum i

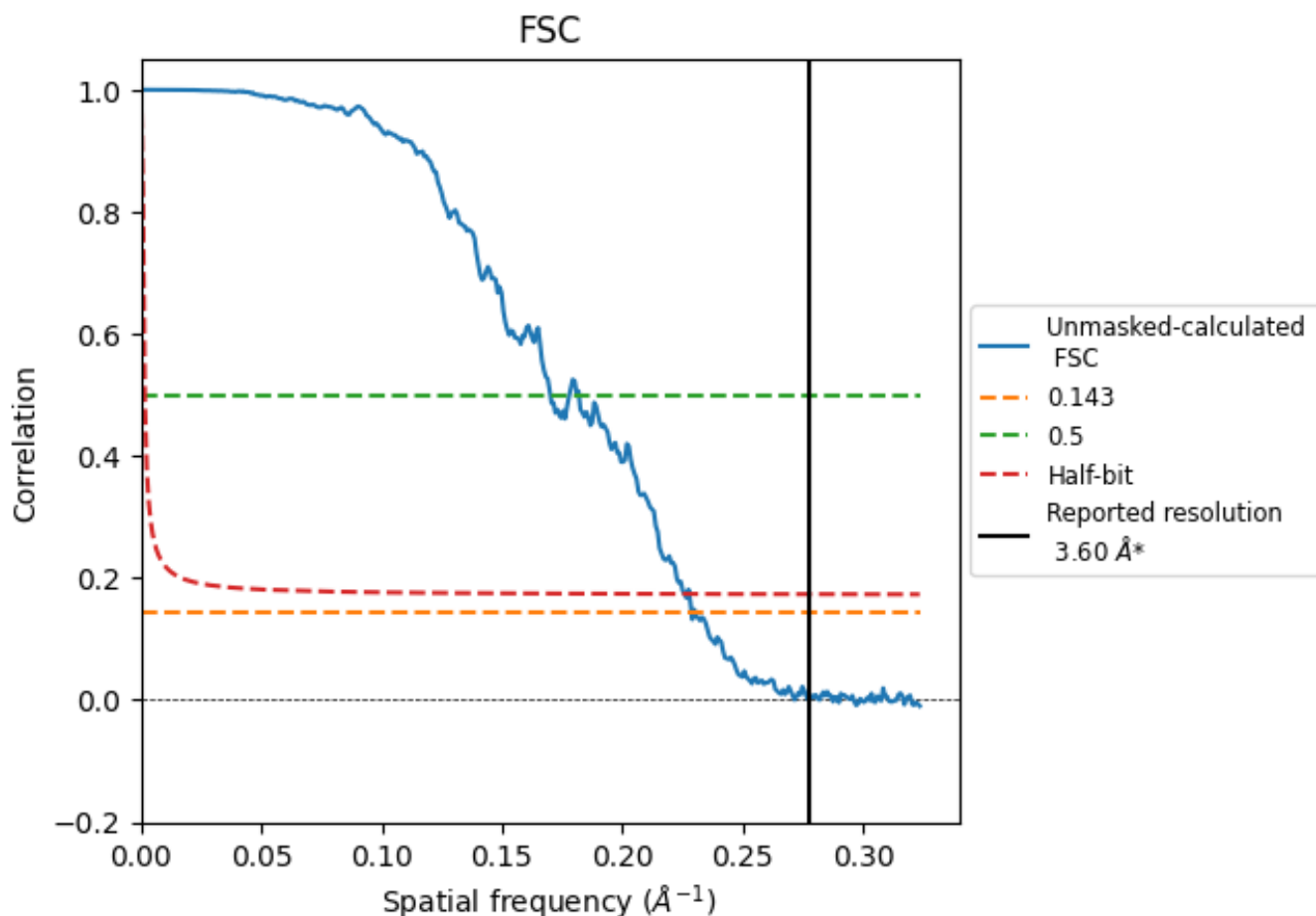


*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

8 Fourier-Shell correlation [\(i\)](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.37	5.88	4.43

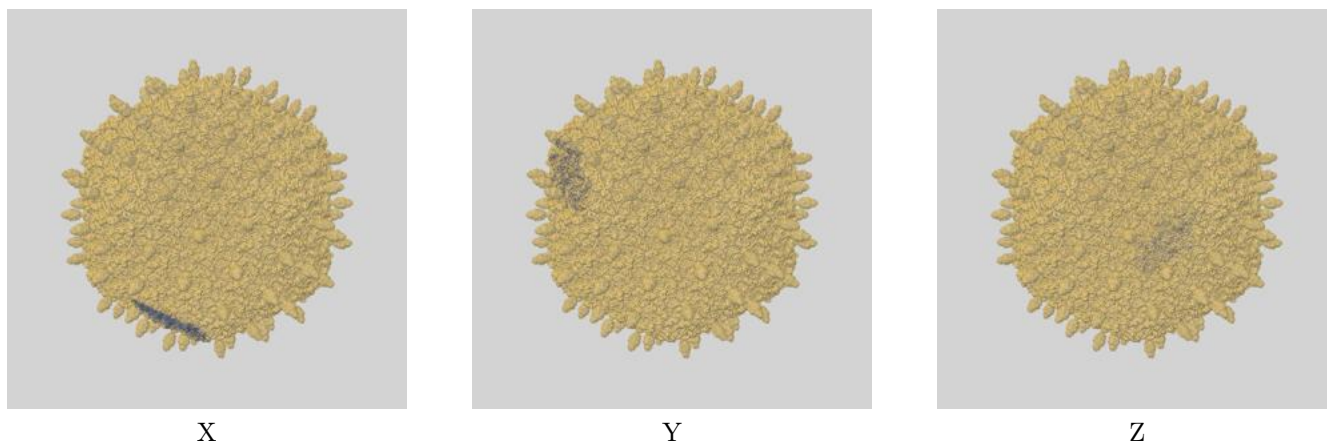
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.37 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

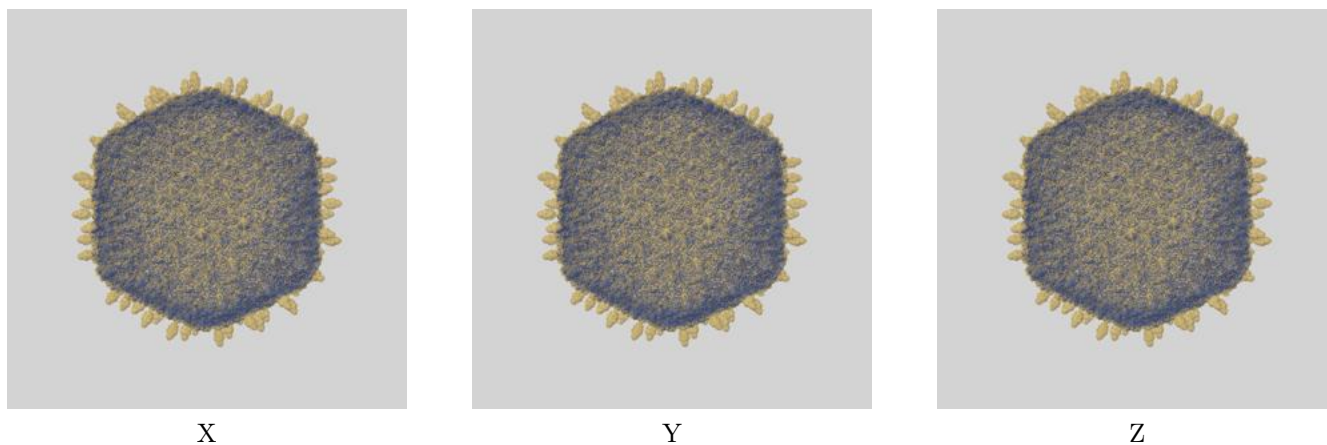
This section contains information regarding the fit between EMDB map EMD-45937 and PDB model 9CUL. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

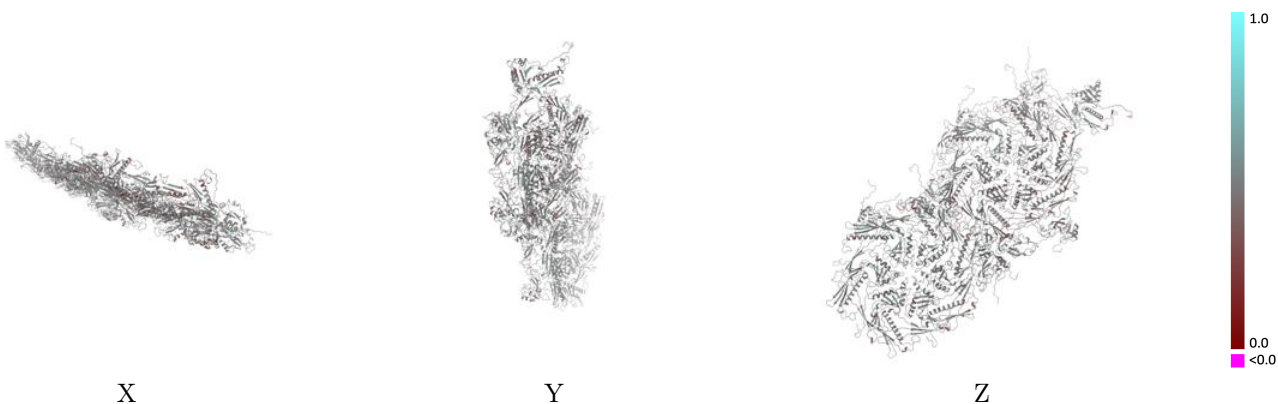


9.1.2 Map-model assembly overlay [i](#)



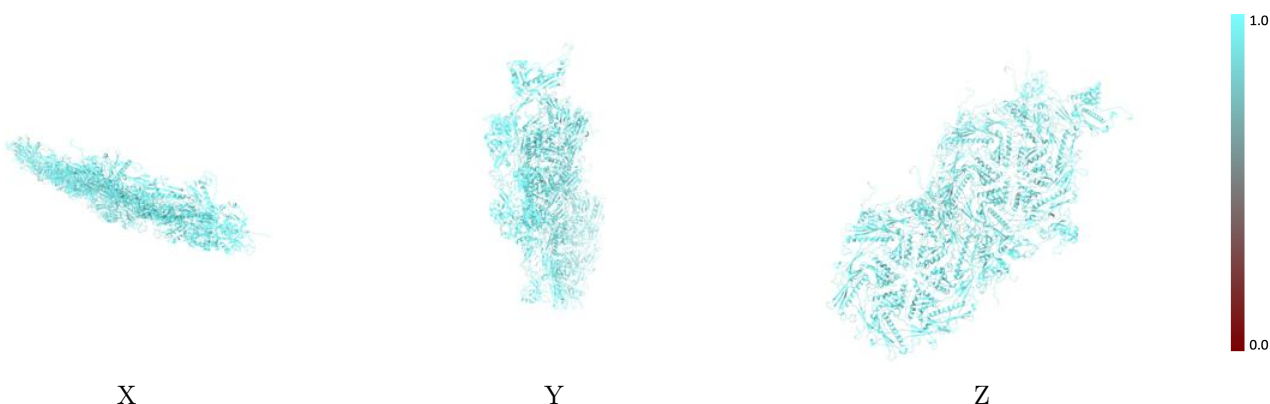
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



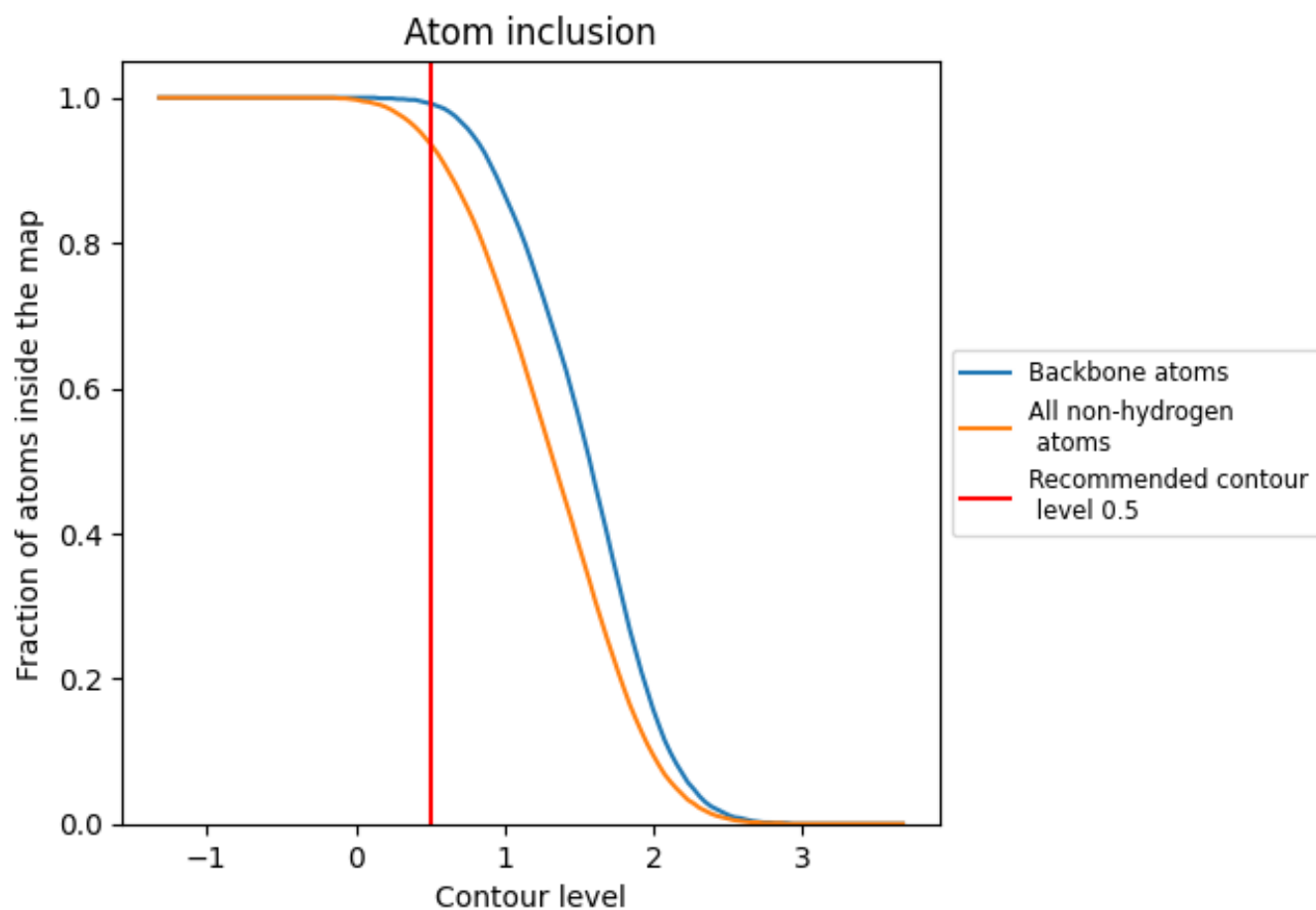
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9370	 0.4610
A	 0.9570	 0.5030
B	 0.9270	 0.4720
C	 0.9270	 0.4620
D	 0.9330	 0.4550
E	 0.9230	 0.4520
F	 0.9310	 0.4720
G	 0.9540	 0.4960
H	 0.9250	 0.4590
I	 0.9320	 0.4600
J	 0.9180	 0.4430
K	 0.9280	 0.4450
L	 0.9240	 0.4480
M	 0.9440	 0.4540
a	 0.9490	 0.4600
b	 0.9380	 0.4600
c	 0.9580	 0.4590
d	 0.9450	 0.4640
e	 0.9500	 0.4540
f	 0.9300	 0.4510
g	 0.9280	 0.4440
h	 0.9420	 0.4590
i	 0.9420	 0.4540
j	 0.9530	 0.4510
k	 0.9380	 0.4390
l	 0.9580	 0.4450
m	 0.9770	 0.4810

