



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:39 AM UTC

PDB ID : 9ILP / pdb_00009ilp
EMDB ID : EMD-60672
Title : Structure of the bacteriophage T5 portal complex
Authors : Peng, Y.N.; Liu, H.R.
Deposited on : 2024-07-01
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

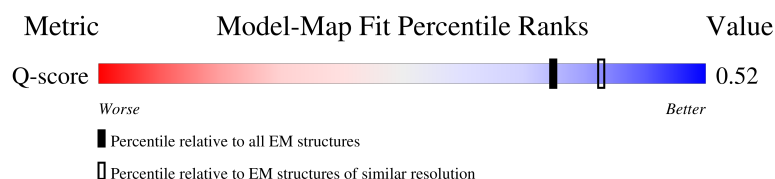
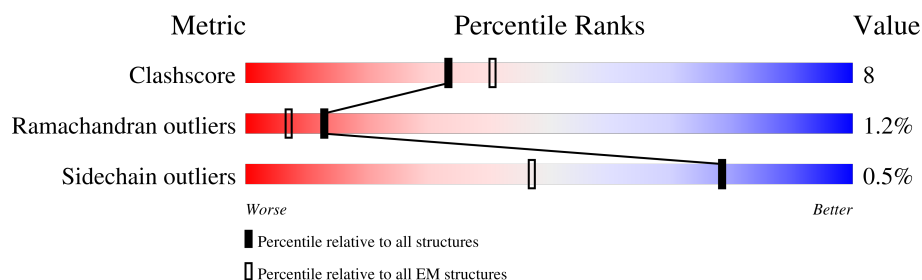
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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



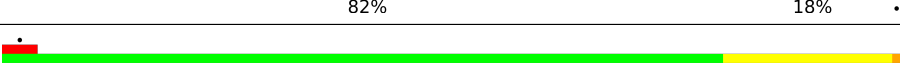
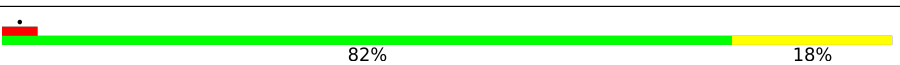
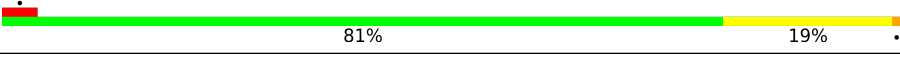
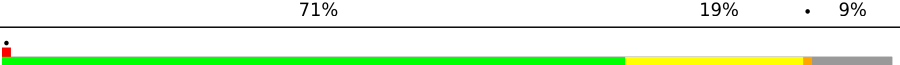
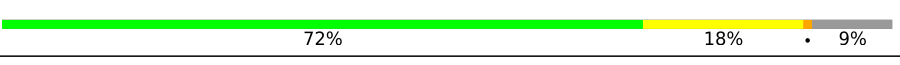
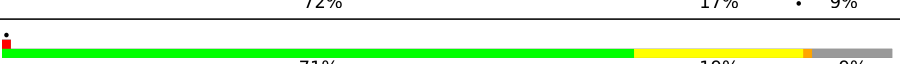
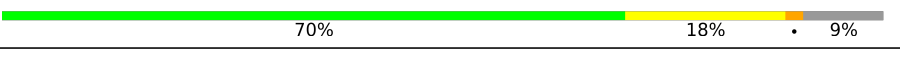
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	a	170	 84% 16%
1	b	170	 78% 22%
1	c	170	 81% 19%
1	d	170	 80% 19%

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Mol	Chain	Length	Quality of chain
1	e	170	
1	f	170	
1	g	170	
1	h	170	
1	i	170	
1	j	170	
1	k	170	
1	l	170	
2	A	403	
2	B	403	
2	C	403	
2	D	403	
2	E	403	
2	F	403	
2	G	403	
2	H	403	
2	I	403	
2	J	403	
2	K	403	
2	L	403	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 51180 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 Head completion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	170	Total	C	N	O	S	0	0
			1347	853	224	262	8		
1	b	170	Total	C	N	O	S	0	0
			1347	853	224	262	8		
1	c	170	Total	C	N	O	S	0	0
			1347	853	224	262	8		
1	d	170	Total	C	N	O	S	0	0
			1347	853	224	262	8		
1	e	170	Total	C	N	O	S	0	0
			1347	853	224	262	8		
1	f	170	Total	C	N	O	S	0	0
			1347	853	224	262	8		
1	g	170	Total	C	N	O	S	0	0
			1347	853	224	262	8		
1	h	170	Total	C	N	O	S	0	0
			1347	853	224	262	8		
1	i	170	Total	C	N	O	S	0	0
			1347	853	224	262	8		
1	j	170	Total	C	N	O	S	0	0
			1347	853	224	262	8		
1	k	170	Total	C	N	O	S	0	0
			1347	853	224	262	8		
1	l	170	Total	C	N	O	S	0	0
			1347	853	224	262	8		

- Molecule 2 is a protein called Portal protein pb7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	367	Total	C	N	O	S	0	0
			2918	1853	491	561	13		
2	B	367	Total	C	N	O	S	0	0
			2918	1853	491	561	13		
2	C	367	Total	C	N	O	S	0	0
			2918	1853	491	561	13		

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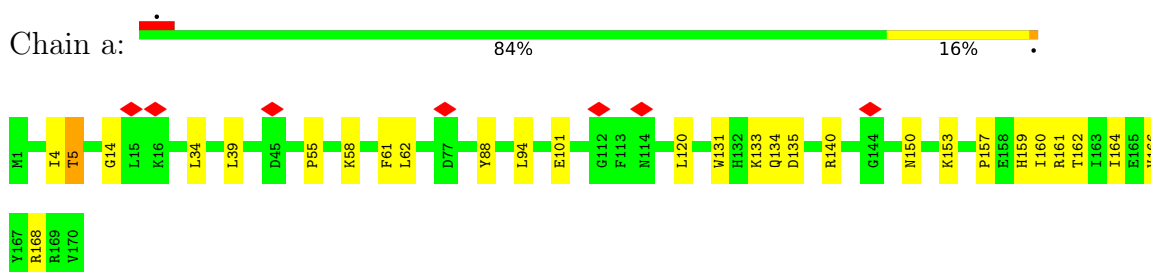
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	367	Total 2918	C 1853	N 491	O 561	S 13	0	0
2	E	367	Total 2918	C 1853	N 491	O 561	S 13	0	0
2	F	367	Total 2918	C 1853	N 491	O 561	S 13	0	0
2	G	367	Total 2918	C 1853	N 491	O 561	S 13	0	0
2	H	367	Total 2918	C 1853	N 491	O 561	S 13	0	0
2	I	367	Total 2918	C 1853	N 491	O 561	S 13	0	0
2	J	367	Total 2918	C 1853	N 491	O 561	S 13	0	0
2	K	367	Total 2918	C 1853	N 491	O 561	S 13	0	0
2	L	367	Total 2918	C 1853	N 491	O 561	S 13	0	0

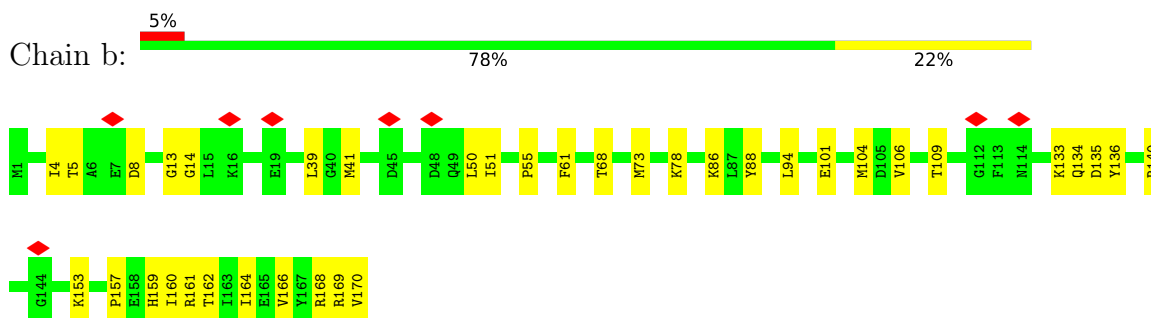
3 Residue-property plots [i](#)

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.

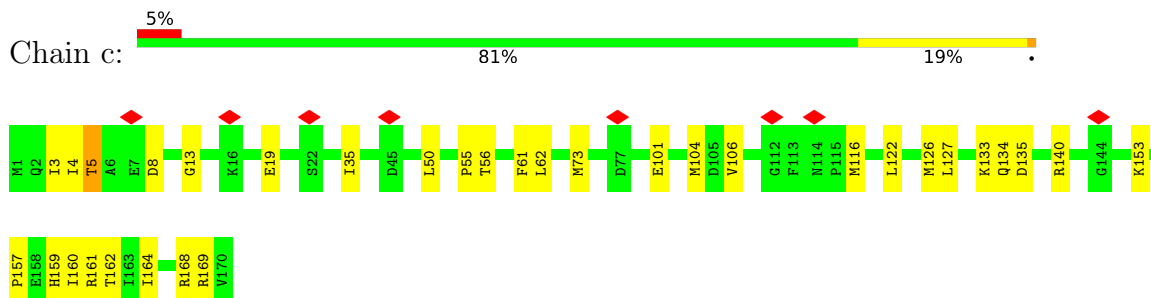
- Molecule 1: Head completion protein



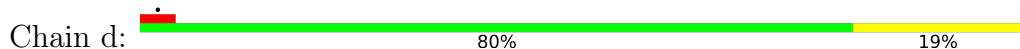
- Molecule 1: Head completion protein

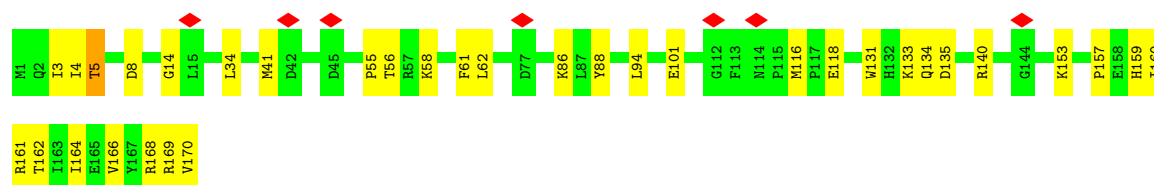


- Molecule 1: Head completion protein

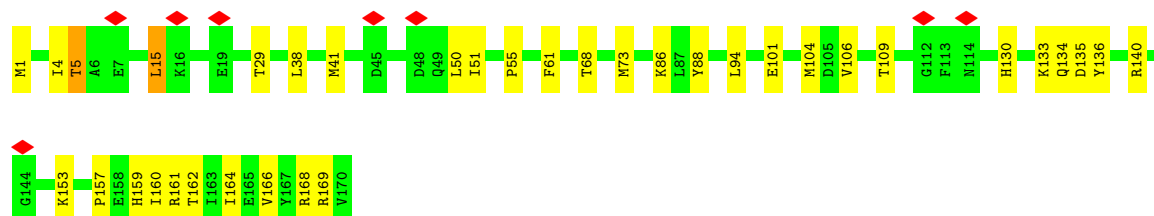
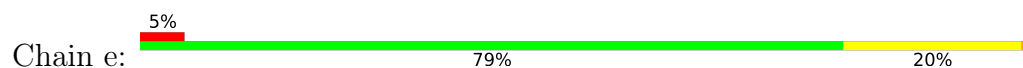


- Molecule 1: Head completion protein

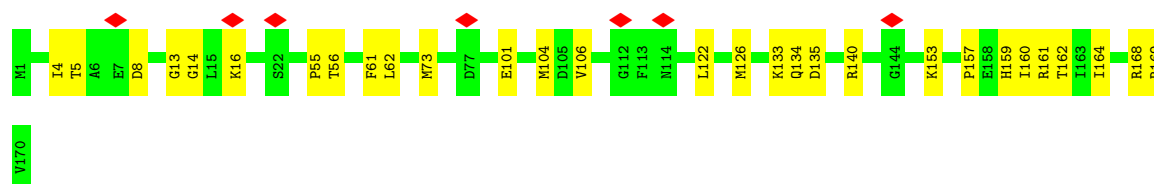
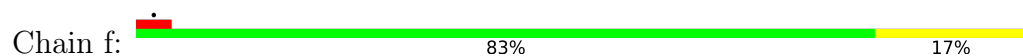




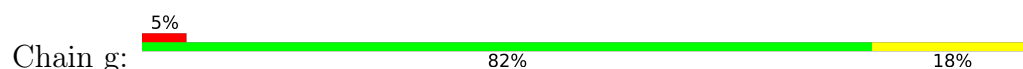
- Molecule 1: Head completion protein



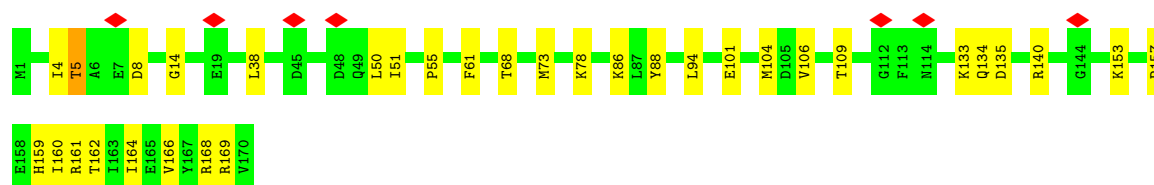
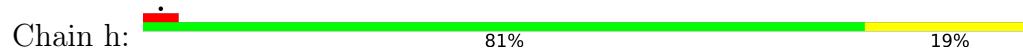
- Molecule 1: Head completion protein



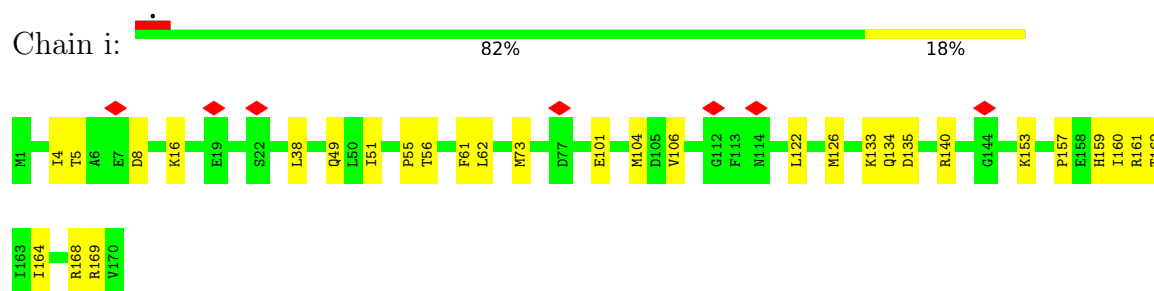
- Molecule 1: Head completion protein



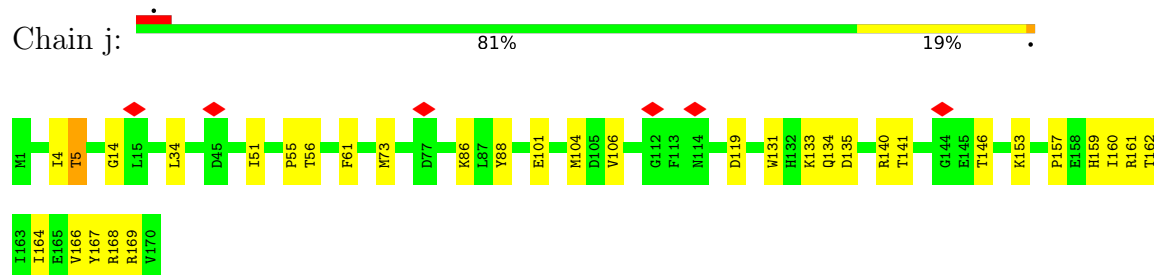
- Molecule 1: Head completion protein



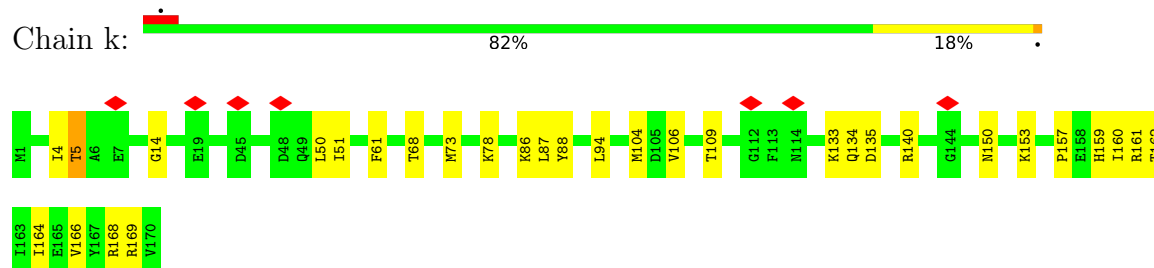
- Molecule 1: Head completion protein



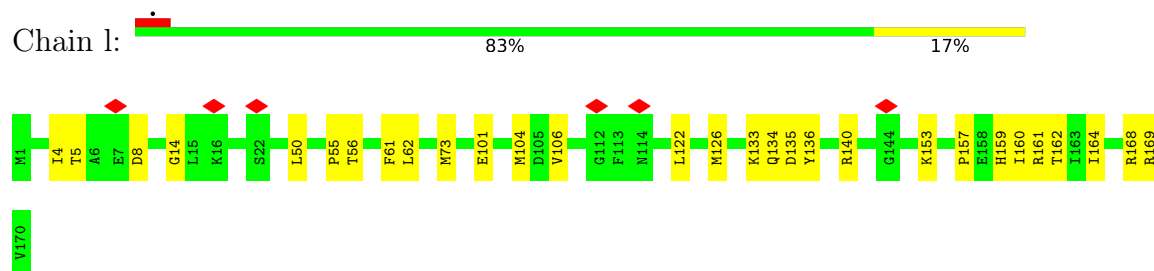
- Molecule 1: Head completion protein



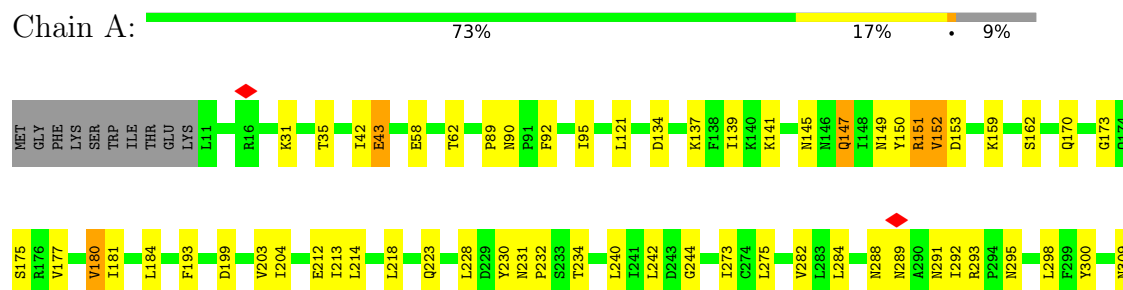
- Molecule 1: Head completion protein

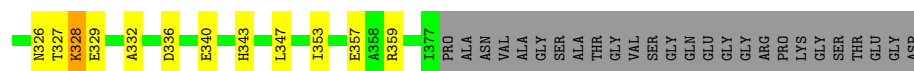


- Molecule 1: Head completion protein

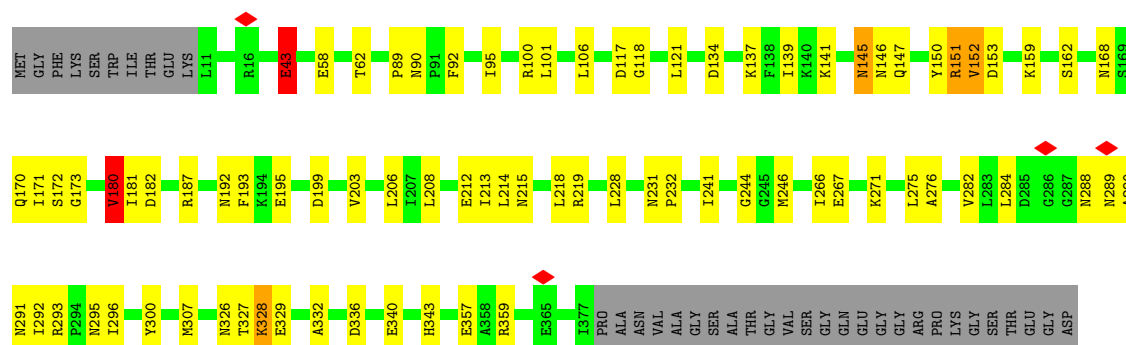


- Molecule 2: Portal protein pb7

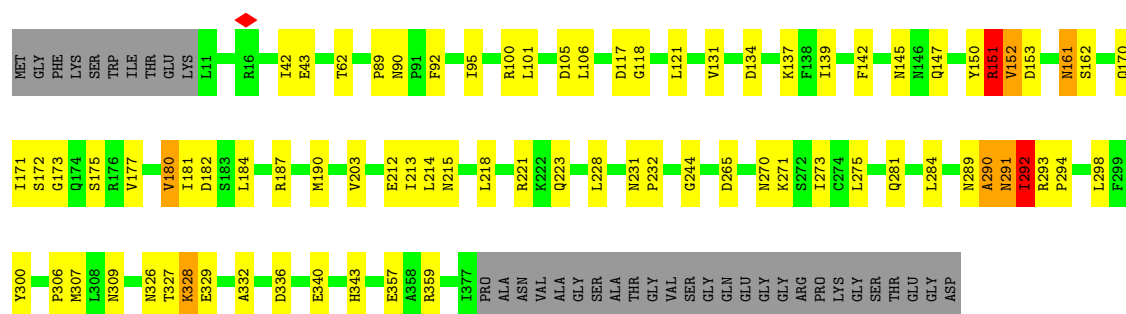




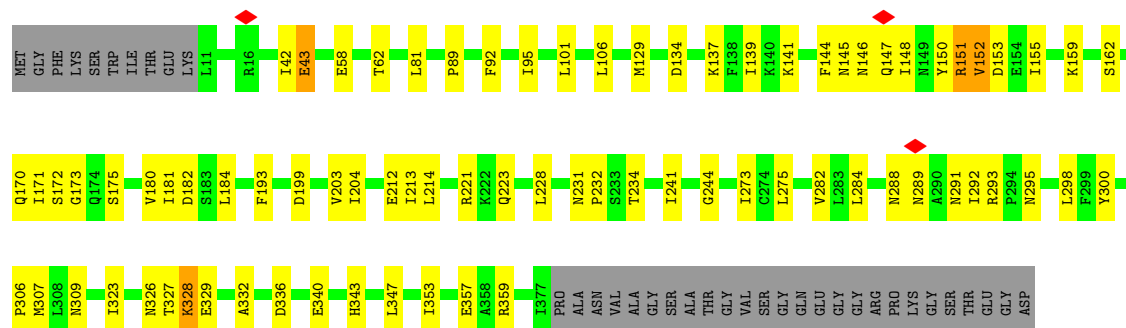
• Molecule 2: Portal protein pb7



• Molecule 2: Portal protein pb7

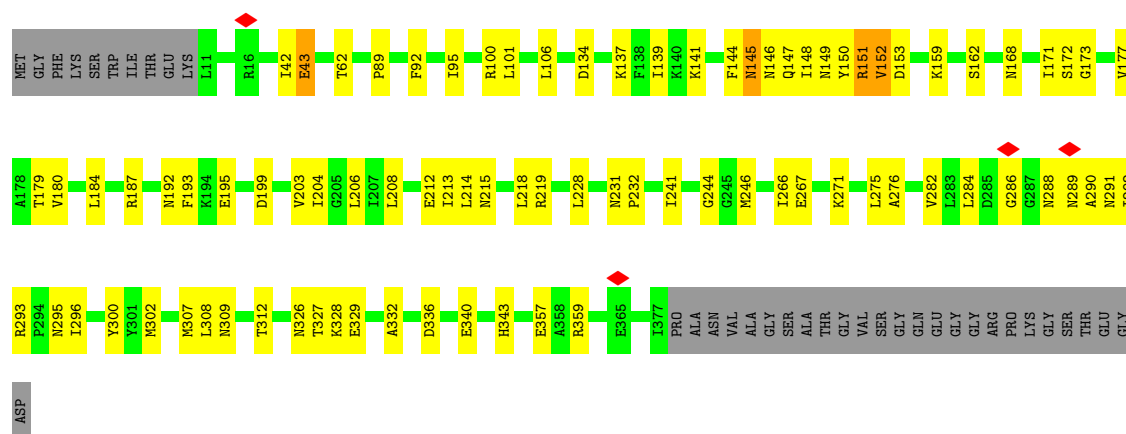


• Molecule 2: Portal protein pb7



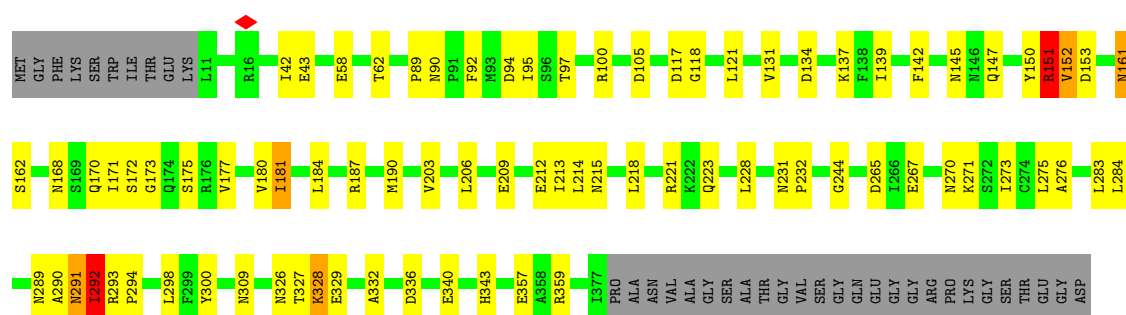
• Molecule 2: Portal protein pb7





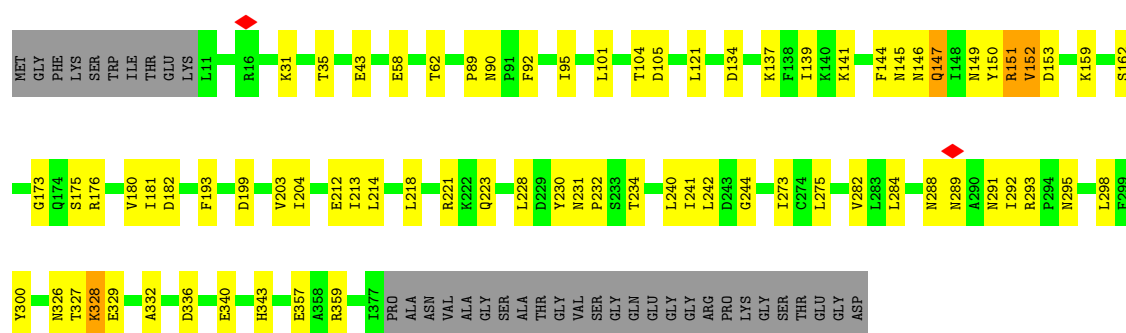
• Molecule 2: Portal protein pb7

Chain F: 71% 19% 9%



• Molecule 2: Portal protein pb7

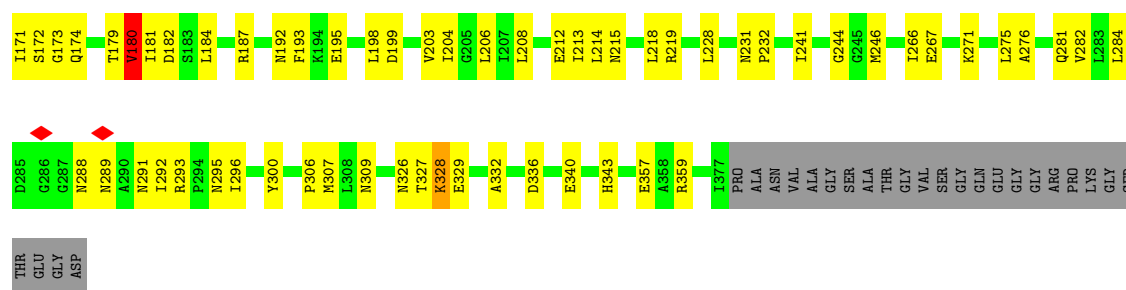
Chain G: 72% 18% 9%



• Molecule 2: Portal protein pb7

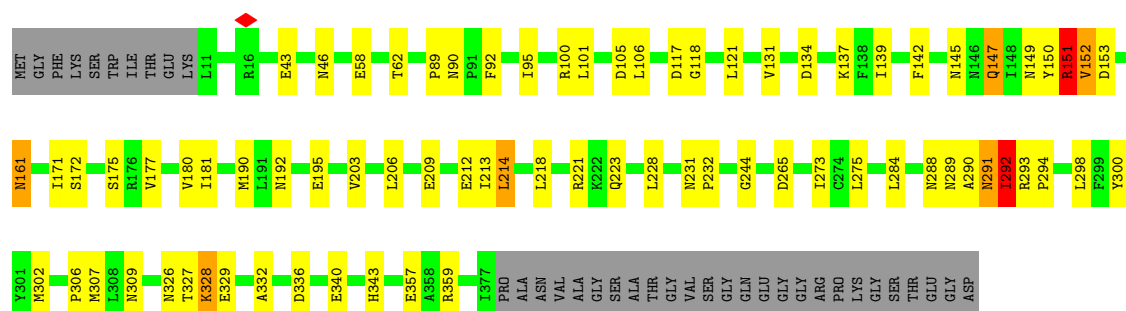
Chain H: 69% 21% 9%





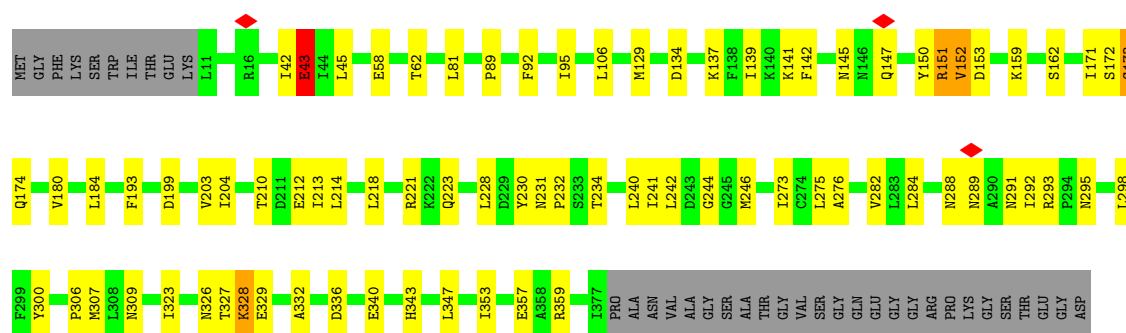
• Molecule 2: Portal protein pb7

Chain I: 72% 17% 9%



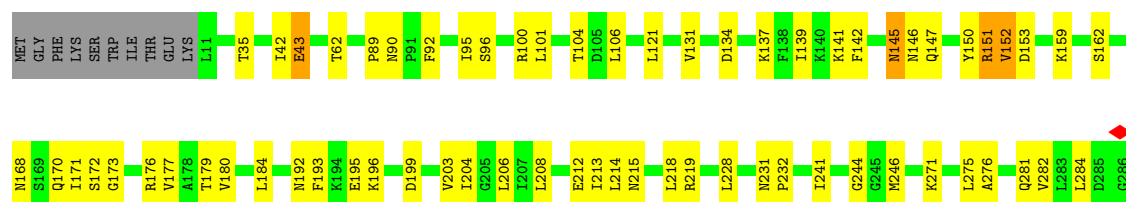
• Molecule 2: Portal protein pb7

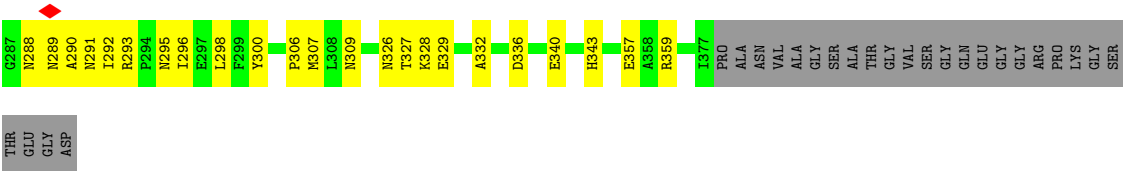
Chain J: 71% 19% 9%



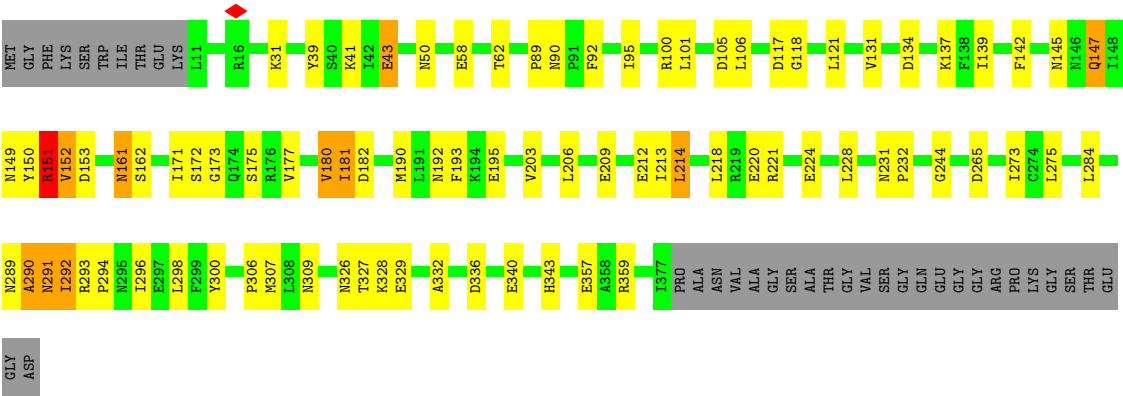
• Molecule 2: Portal protein pb7

Chain K: 69% 21% 9%





● Molecule 2: Portal protein pb7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18398	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	43.535	Depositor
Minimum map value	-26.861	Depositor
Average map value	0.007	Depositor
Map value standard deviation	2.338	Depositor
Recommended contour level	6	Depositor
Map size ($\text{\AA}$)	489.6, 489.6, 489.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.36, 1.36, 1.36	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	a	0.27	0/1373	0.54	2/1860 (0.1%)
1	b	0.27	0/1373	0.52	3/1860 (0.2%)
1	c	0.25	0/1373	0.52	2/1860 (0.1%)
1	d	0.25	0/1373	0.53	2/1860 (0.1%)
1	e	0.33	1/1373 (0.1%)	0.51	0/1860
1	f	0.25	0/1373	0.51	0/1860
1	g	0.27	0/1373	0.50	0/1860
1	h	0.28	0/1373	0.55	2/1860 (0.1%)
1	i	0.29	0/1373	0.51	0/1860
1	j	0.26	0/1373	0.53	2/1860 (0.1%)
1	k	0.28	0/1373	0.55	2/1860 (0.1%)
1	l	0.26	0/1373	0.53	2/1860 (0.1%)
2	A	0.35	1/2968 (0.0%)	0.49	1/4012 (0.0%)
2	B	0.37	0/2968	0.52	2/4012 (0.0%)
2	C	0.42	3/2968 (0.1%)	0.55	4/4012 (0.1%)
2	D	0.36	2/2968 (0.1%)	0.47	0/4012
2	E	0.35	0/2968	0.49	1/4012 (0.0%)
2	F	0.40	3/2968 (0.1%)	0.55	4/4012 (0.1%)
2	G	0.33	1/2968 (0.0%)	0.46	1/4012 (0.0%)
2	H	0.34	0/2968	0.47	1/4012 (0.0%)
2	I	0.45	3/2968 (0.1%)	0.58	5/4012 (0.1%)
2	J	0.41	2/2968 (0.1%)	0.52	2/4012 (0.0%)
2	K	0.19	0/2968	0.42	0/4012
2	L	0.48	3/2968 (0.1%)	0.60	6/4012 (0.1%)
All	All	0.35	19/52092 (0.0%)	0.52	44/70464 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	43	GLU	C-O	-7.51	1.15	1.24
1	e	15	LEU	C-O	-6.78	1.15	1.23
2	D	175	SER	CA-C	-6.21	1.45	1.52
2	A	175	SER	CA-C	-6.19	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	175	SER	CA-C	-6.00	1.45	1.52
2	L	290	ALA	C-O	-5.50	1.17	1.24
2	I	290	ALA	C-O	-5.37	1.17	1.24
2	D	43	GLU	CA-C	-5.29	1.45	1.52
2	C	290	ALA	C-O	-5.26	1.17	1.24
2	L	177	VAL	CA-CB	-5.19	1.48	1.54
2	F	290	ALA	C-O	-5.19	1.18	1.24
2	J	173	GLY	C-O	-5.14	1.19	1.23
2	F	177	VAL	CA-CB	-5.12	1.48	1.54
2	L	175	SER	CA-C	-5.11	1.46	1.52
2	I	177	VAL	CA-CB	-5.11	1.48	1.54
2	C	177	VAL	CA-CB	-5.11	1.48	1.54
2	I	175	SER	CA-C	-5.04	1.46	1.52
2	F	175	SER	CA-C	-5.03	1.46	1.52
2	C	175	SER	CA-C	-5.02	1.46	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	43	GLU	N-CA-C	10.70	122.94	111.28
2	I	214	LEU	N-CA-C	10.06	123.32	110.65
2	L	292	ILE	N-CA-C	8.86	122.12	111.05
2	I	292	ILE	N-CA-C	8.79	122.07	111.09
2	A	180	VAL	N-CA-C	8.26	118.30	110.53
2	J	45	LEU	N-CA-C	-8.22	103.70	114.31
2	L	214	LEU	N-CA-C	8.15	122.72	111.55
2	I	181	ILE	N-CA-C	7.37	118.13	110.62
2	F	181	ILE	N-CA-C	7.08	117.84	110.62
2	C	292	ILE	N-CA-C	6.85	121.62	112.04
2	F	292	ILE	N-CA-C	6.75	121.61	111.89
2	J	43	GLU	N-CA-C	6.64	118.18	111.07
2	B	180	VAL	N-CA-C	6.53	117.32	110.72
1	j	14	GLY	CA-C-N	-6.31	114.21	123.05
1	j	14	GLY	C-N-CA	-6.31	114.21	123.05
1	d	14	GLY	CA-C-N	-6.30	114.23	123.05
1	d	14	GLY	C-N-CA	-6.30	114.23	123.05
2	H	180	VAL	N-CA-C	6.28	117.06	110.72
2	F	151	ARG	CA-C-N	6.21	133.14	121.97
2	F	151	ARG	C-N-CA	6.21	133.14	121.97
2	C	151	ARG	CA-C-N	6.17	133.08	121.97
2	C	151	ARG	C-N-CA	6.17	133.08	121.97
2	I	151	ARG	CA-C-N	6.08	132.91	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	151	ARG	C-N-CA	6.08	132.91	121.97
2	L	151	ARG	CA-C-N	6.07	132.89	121.97
2	L	151	ARG	C-N-CA	6.07	132.89	121.97
2	L	180	VAL	N-CA-C	5.98	116.76	110.72
2	C	180	VAL	N-CA-C	5.97	116.75	110.72
1	k	14	GLY	CA-C-N	-5.94	114.62	123.00
1	k	14	GLY	C-N-CA	-5.94	114.62	123.00
1	a	14	GLY	CA-C-N	-5.91	114.67	123.00
1	a	14	GLY	C-N-CA	-5.91	114.67	123.00
1	h	14	GLY	CA-C-N	-5.90	114.68	123.00
1	h	14	GLY	C-N-CA	-5.90	114.68	123.00
1	l	14	GLY	CA-C-N	-5.87	114.83	123.05
1	l	14	GLY	C-N-CA	-5.87	114.83	123.05
1	c	13	GLY	O-C-N	-5.41	115.49	122.80
1	c	19	GLU	N-CA-C	5.38	117.24	109.07
2	L	39	TYR	O-C-N	-5.25	115.56	122.39
2	E	177	VAL	N-CA-C	5.19	117.54	111.05
1	b	14	GLY	CA-C-N	-5.18	114.76	122.74
1	b	14	GLY	C-N-CA	-5.18	114.76	122.74
2	G	176	ARG	N-CA-C	5.07	116.80	111.28
1	b	13	GLY	O-C-N	-5.05	117.47	122.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	1347	0	1347	22	0
1	b	1347	0	1347	30	0
1	c	1347	0	1347	28	0
1	d	1347	0	1347	28	0
1	e	1347	0	1347	29	0
1	f	1347	0	1347	23	0
1	g	1347	0	1347	25	0
1	h	1347	0	1347	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	i	1347	0	1347	26	0
1	j	1347	0	1347	25	0
1	k	1347	0	1347	26	0
1	l	1347	0	1347	27	0
2	A	2918	0	2940	58	0
2	B	2918	0	2940	64	0
2	C	2918	0	2940	64	0
2	D	2918	0	2940	59	0
2	E	2918	0	2940	65	0
2	F	2918	0	2940	64	0
2	G	2918	0	2940	64	0
2	H	2918	0	2940	70	0
2	I	2918	0	2940	60	0
2	J	2918	0	2940	64	0
2	K	2918	0	2940	74	0
2	L	2918	0	2940	67	0
All	All	51180	0	51444	852	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 8.

All (852) 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)
2:I:151:ARG:O	2:I:152:VAL:HG13	1.81	0.81
2:L:151:ARG:O	2:L:152:VAL:HG13	1.81	0.81
2:C:151:ARG:O	2:C:152:VAL:HG13	1.81	0.81
2:F:151:ARG:O	2:F:152:VAL:HG13	1.81	0.80
2:B:291:ASN:O	2:B:295:ASN:ND2	2.21	0.73
2:E:291:ASN:O	2:E:295:ASN:ND2	2.21	0.73
2:K:291:ASN:O	2:K:295:ASN:ND2	2.20	0.73
1:c:134:GLN:O	1:c:140:ARG:NH2	2.21	0.73
1:l:134:GLN:O	1:l:140:ARG:NH2	2.21	0.73
2:H:291:ASN:O	2:H:295:ASN:ND2	2.21	0.72
1:b:134:GLN:O	1:b:140:ARG:NH2	2.23	0.71
2:B:145:ASN:O	2:B:146:ASN:ND2	2.23	0.71
1:i:134:GLN:O	1:i:140:ARG:NH2	2.23	0.71
1:k:134:GLN:O	1:k:140:ARG:NH2	2.24	0.71
2:B:199:ASP:O	2:C:231:ASN:ND2	2.24	0.71
2:J:291:ASN:O	2:J:295:ASN:ND2	2.24	0.71
2:E:199:ASP:O	2:F:231:ASN:ND2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:199:ASP:O	2:I:231:ASN:ND2	2.24	0.70
2:E:145:ASN:O	2:E:146:ASN:ND2	2.24	0.70
2:D:291:ASN:O	2:D:295:ASN:ND2	2.24	0.70
2:A:291:ASN:O	2:A:295:ASN:ND2	2.24	0.70
1:f:134:GLN:O	1:f:140:ARG:NH2	2.24	0.69
2:G:291:ASN:O	2:G:295:ASN:ND2	2.25	0.69
2:K:145:ASN:O	2:K:146:ASN:ND2	2.26	0.69
1:e:134:GLN:O	1:e:140:ARG:NH2	2.25	0.69
2:K:199:ASP:O	2:L:231:ASN:ND2	2.24	0.69
1:d:134:GLN:O	1:d:140:ARG:NH2	2.26	0.68
1:h:134:GLN:O	1:h:140:ARG:NH2	2.25	0.68
1:g:134:GLN:O	1:g:140:ARG:NH2	2.27	0.68
1:k:73:MET:HG3	1:k:106:VAL:HG22	1.75	0.68
2:H:145:ASN:O	2:H:146:ASN:ND2	2.26	0.68
2:A:309:ASN:ND2	2:B:58:GLU:OE1	2.27	0.68
1:a:134:GLN:O	1:a:140:ARG:NH2	2.27	0.67
2:K:276:ALA:HB2	2:L:43:GLU:HB3	1.76	0.67
1:e:73:MET:HG3	1:e:106:VAL:HG22	1.76	0.66
1:j:134:GLN:O	1:j:140:ARG:NH2	2.28	0.66
2:K:290:ALA:HB1	2:L:289:ASN:HB2	1.79	0.64
1:g:161:ARG:NH2	2:J:244:GLY:O	2.30	0.64
2:H:42:ILE:HG13	2:H:184:LEU:HD23	1.80	0.63
1:j:161:ARG:NH2	2:A:244:GLY:O	2.32	0.62
2:D:62:THR:HG21	2:D:326:ASN:HD22	1.65	0.62
2:J:62:THR:HG21	2:J:326:ASN:HD22	1.65	0.62
2:A:62:THR:HG21	2:A:326:ASN:HD22	1.66	0.61
2:L:106:LEU:HD22	2:L:307:MET:HE2	1.83	0.61
2:H:357:GLU:OE1	2:I:359:ARG:NH2	2.34	0.61
1:a:88:TYR:HE2	1:b:50:LEU:HD21	1.66	0.61
1:d:161:ARG:NH2	2:G:244:GLY:O	2.33	0.61
1:k:153:LYS:NZ	2:B:212:GLU:OE2	2.33	0.61
2:C:309:ASN:ND2	2:D:58:GLU:OE1	2.34	0.61
2:B:62:THR:HG21	2:B:326:ASN:HD22	1.66	0.61
2:D:171:ILE:HG22	2:D:172:SER:H	1.66	0.60
2:D:199:ASP:O	2:E:231:ASN:ND2	2.33	0.60
2:C:271:LYS:NZ	2:C:281:GLN:HE22	1.98	0.60
2:E:357:GLU:OE1	2:F:359:ARG:NH2	2.34	0.60
2:G:62:THR:HG21	2:G:326:ASN:HD22	1.66	0.60
2:I:106:LEU:HD22	2:I:307:MET:HE2	1.83	0.60
1:c:169:ARG:HH22	2:F:214:LEU:HD13	1.66	0.60
1:l:161:ARG:NH2	2:C:244:GLY:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:61:PHE:HE1	2:L:228:LEU:HD12	1.67	0.60
2:B:357:GLU:OE1	2:C:359:ARG:NH2	2.34	0.60
2:I:309:ASN:ND2	2:J:58:GLU:OE1	2.34	0.60
2:J:171:ILE:HG22	2:J:172:SER:H	1.65	0.60
2:H:162:SER:HB3	2:H:173:GLY:HA2	1.83	0.60
2:K:90:ASN:ND2	2:K:121:LEU:O	2.34	0.60
1:l:126:MET:HE3	1:l:159:HIS:HD2	1.67	0.60
1:d:169:ARG:HB3	2:G:218:LEU:HD13	1.82	0.60
2:B:90:ASN:ND2	2:B:121:LEU:O	2.35	0.60
2:C:62:THR:HG21	2:C:326:ASN:HD22	1.67	0.60
2:C:106:LEU:HD22	2:C:307:MET:HE2	1.84	0.60
1:l:169:ARG:HH22	2:C:214:LEU:HD13	1.65	0.60
2:K:62:THR:HG21	2:K:326:ASN:HD22	1.67	0.60
2:F:309:ASN:ND2	2:G:58:GLU:OE1	2.35	0.59
2:I:151:ARG:NH2	2:I:153:ASP:OD2	2.35	0.59
2:I:62:THR:HG21	2:I:326:ASN:HD22	1.68	0.59
2:K:171:ILE:HG22	2:K:172:SER:H	1.68	0.59
2:A:199:ASP:O	2:B:231:ASN:ND2	2.32	0.59
2:L:62:THR:HG21	2:L:326:ASN:HD22	1.68	0.59
1:j:169:ARG:HB3	2:A:218:LEU:HD13	1.85	0.59
1:g:169:ARG:HB3	2:J:218:LEU:HD13	1.83	0.59
2:A:58:GLU:OE1	2:L:309:ASN:ND2	2.36	0.59
2:C:357:GLU:OE2	2:D:359:ARG:NH2	2.35	0.59
2:B:151:ARG:NH2	2:B:153:ASP:OD2	2.35	0.59
2:E:203:VAL:HG22	2:F:232:PRO:HD3	1.85	0.59
2:G:199:ASP:O	2:H:231:ASN:ND2	2.33	0.59
2:K:357:GLU:OE1	2:L:359:ARG:NH2	2.34	0.58
2:B:171:ILE:HG22	2:B:172:SER:H	1.68	0.58
2:H:62:THR:HG21	2:H:326:ASN:HD22	1.67	0.58
1:b:153:LYS:NZ	2:E:212:GLU:OE2	2.32	0.58
1:i:38:LEU:HD22	2:K:213:ILE:HD12	1.85	0.58
2:E:62:THR:HG21	2:E:326:ASN:HD22	1.67	0.58
2:K:42:ILE:HG13	2:K:184:LEU:HD23	1.85	0.58
2:B:203:VAL:HG22	2:C:232:PRO:HD3	1.85	0.58
2:C:151:ARG:NH2	2:C:153:ASP:OD2	2.37	0.58
2:K:282:VAL:HG11	2:K:291:ASN:HB3	1.84	0.58
1:c:126:MET:HE3	1:c:159:HIS:HD2	1.68	0.58
2:E:171:ILE:HG22	2:E:172:SER:H	1.68	0.58
2:F:62:THR:HG21	2:F:326:ASN:HD22	1.68	0.58
2:H:171:ILE:HG22	2:H:172:SER:H	1.67	0.58
2:H:203:VAL:HG22	2:I:232:PRO:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:161:ARG:NH2	2:F:244:GLY:O	2.37	0.58
2:A:180:VAL:HG13	2:A:273:ILE:HG12	1.85	0.58
2:A:359:ARG:NH2	2:L:357:GLU:OE2	2.35	0.57
2:I:171:ILE:HG22	2:I:172:SER:H	1.69	0.57
1:c:159:HIS:CD2	1:c:160:ILE:HG13	2.40	0.57
2:C:161:ASN:C	2:C:161:ASN:HD22	2.11	0.57
2:L:171:ILE:HG22	2:L:172:SER:H	1.69	0.57
2:K:203:VAL:HG22	2:L:232:PRO:HD3	1.86	0.57
1:i:126:MET:HE3	1:i:159:HIS:HD2	1.69	0.57
2:B:106:LEU:HD22	2:B:307:MET:HE2	1.86	0.57
2:F:90:ASN:ND2	2:F:121:LEU:O	2.37	0.57
2:F:161:ASN:C	2:F:161:ASN:HD22	2.12	0.57
1:k:86:LYS:HE2	1:k:88:TYR:CE1	2.40	0.57
1:l:159:HIS:CD2	1:l:160:ILE:HG13	2.40	0.57
2:I:150:TYR:O	2:I:151:ARG:HG3	2.05	0.57
1:i:55:PRO:HD3	1:i:101:GLU:HG2	1.87	0.57
2:A:242:LEU:HB2	2:L:209:GLU:HA	1.85	0.57
2:L:150:TYR:O	2:L:151:ARG:HG3	2.04	0.57
1:f:61:PHE:HE1	2:I:228:LEU:HD12	1.69	0.57
2:C:171:ILE:HG22	2:C:172:SER:H	1.70	0.57
2:F:357:GLU:OE2	2:G:359:ARG:NH2	2.36	0.57
2:J:199:ASP:O	2:K:231:ASN:ND2	2.32	0.57
1:c:61:PHE:HE1	2:F:228:LEU:HD12	1.69	0.57
2:H:180:VAL:C	2:H:182:ASP:H	2.13	0.57
2:E:106:LEU:HD22	2:E:307:MET:HE2	1.87	0.56
1:f:126:MET:HE3	1:f:159:HIS:HD2	1.70	0.56
1:i:168:ARG:HD2	2:K:213:ILE:HD13	1.86	0.56
2:D:275:LEU:HD11	2:E:284:LEU:HD13	1.87	0.56
2:D:282:VAL:HG11	2:D:291:ASN:HB3	1.87	0.56
1:e:153:LYS:NZ	2:H:212:GLU:OE2	2.33	0.56
1:k:61:PHE:HE2	2:B:228:LEU:HD12	1.70	0.56
1:l:61:PHE:HE1	2:C:228:LEU:HD12	1.69	0.56
2:B:340:GLU:HA	2:B:343:HIS:CD2	2.40	0.56
2:D:340:GLU:HA	2:D:343:HIS:CD2	2.41	0.56
2:D:357:GLU:OE2	2:E:359:ARG:NH2	2.37	0.56
2:K:340:GLU:HA	2:K:343:HIS:CD2	2.40	0.56
1:i:159:HIS:CD2	1:i:160:ILE:HG13	2.40	0.56
1:f:159:HIS:CD2	1:f:160:ILE:HG13	2.40	0.56
2:A:340:GLU:HA	2:A:343:HIS:CD2	2.41	0.56
2:A:282:VAL:HG11	2:A:291:ASN:HB3	1.88	0.56
2:B:180:VAL:C	2:B:182:ASP:H	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:151:ARG:NH2	2:F:153:ASP:OD2	2.37	0.56
2:F:171:ILE:HG22	2:F:172:SER:H	1.70	0.56
2:G:340:GLU:HA	2:G:343:HIS:CD2	2.41	0.56
2:J:340:GLU:HA	2:J:343:HIS:CD2	2.41	0.56
1:l:55:PRO:HD3	1:l:101:GLU:HG2	1.86	0.56
2:E:208:LEU:HD23	2:E:246:MET:SD	2.46	0.56
2:E:340:GLU:HA	2:E:343:HIS:CD2	2.40	0.56
2:G:282:VAL:HG11	2:G:291:ASN:HB3	1.88	0.56
2:C:203:VAL:HG22	2:D:232:PRO:HD3	1.88	0.56
2:H:340:GLU:HA	2:H:343:HIS:CD2	2.40	0.56
1:h:38:LEU:HD22	2:J:213:ILE:HD12	1.87	0.56
2:G:357:GLU:OE2	2:H:359:ARG:NH2	2.38	0.56
1:h:61:PHE:HE2	2:K:228:LEU:HD12	1.71	0.55
2:A:232:PRO:HD3	2:L:203:VAL:HG22	1.88	0.55
2:B:276:ALA:HB2	2:C:43:GLU:HB3	1.88	0.55
2:H:208:LEU:HD23	2:H:246:MET:SD	2.46	0.55
1:e:133:LYS:O	1:e:135:ASP:N	2.37	0.55
2:E:290:ALA:HB1	2:F:289:ASN:HB2	1.88	0.55
2:I:340:GLU:HA	2:I:343:HIS:CD2	2.41	0.55
2:L:340:GLU:HA	2:L:343:HIS:CD2	2.41	0.55
2:B:290:ALA:HB1	2:C:289:ASN:HB2	1.88	0.55
2:F:340:GLU:HA	2:F:343:HIS:CD2	2.41	0.55
2:H:276:ALA:HB2	2:I:43:GLU:HB3	1.87	0.55
2:J:357:GLU:OE2	2:K:359:ARG:NH2	2.38	0.55
1:a:161:ARG:NH2	2:D:244:GLY:O	2.39	0.55
2:C:340:GLU:HA	2:C:343:HIS:CD2	2.41	0.55
2:A:357:GLU:OE2	2:B:359:ARG:NH2	2.37	0.55
2:B:208:LEU:HD23	2:B:246:MET:SD	2.46	0.55
2:H:151:ARG:NH2	2:H:153:ASP:OD2	2.37	0.55
2:F:150:TYR:O	2:F:151:ARG:HG3	2.06	0.55
2:K:208:LEU:HD23	2:K:246:MET:SD	2.46	0.55
2:L:151:ARG:NH2	2:L:153:ASP:OD2	2.35	0.55
1:b:161:ARG:NH2	2:E:244:GLY:O	2.40	0.55
2:I:357:GLU:OE2	2:J:359:ARG:NH2	2.35	0.55
2:J:162:SER:HB3	2:J:173:GLY:HA2	1.89	0.55
2:J:282:VAL:HG11	2:J:291:ASN:HB3	1.89	0.55
1:h:133:LYS:O	1:h:135:ASP:N	2.38	0.55
2:E:276:ALA:HB2	2:F:43:GLU:HB3	1.88	0.55
2:J:275:LEU:HD11	2:K:284:LEU:HD13	1.88	0.55
2:L:117:ASP:OD1	2:L:118:GLY:N	2.36	0.55
2:L:147:GLN:O	2:L:149:ASN:ND2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:150:TYR:O	2:C:151:ARG:HG3	2.07	0.55
2:D:106:LEU:HD22	2:D:307:MET:HE2	1.89	0.55
2:G:180:VAL:C	2:G:182:ASP:H	2.13	0.55
2:J:151:ARG:HH21	2:J:153:ASP:HB2	1.72	0.55
1:b:61:PHE:HE2	2:E:228:LEU:HD12	1.71	0.54
2:F:94:ASP:HB2	2:F:97:THR:HG23	1.88	0.54
1:e:38:LEU:HD22	2:G:213:ILE:HD12	1.88	0.54
2:F:203:VAL:HG22	2:G:232:PRO:HD3	1.88	0.54
1:d:157:PRO:HD2	1:d:160:ILE:HD12	1.88	0.54
1:e:61:PHE:HE2	2:H:228:LEU:HD12	1.71	0.54
1:c:62:LEU:O	2:F:221:ARG:NH2	2.41	0.54
2:D:151:ARG:HH21	2:D:153:ASP:HB2	1.73	0.54
2:H:293:ARG:HH12	2:H:336:ASP:HB2	1.73	0.54
2:I:203:VAL:HG22	2:J:232:PRO:HD3	1.89	0.54
1:d:61:PHE:HE2	2:G:228:LEU:HD12	1.73	0.54
2:K:293:ARG:HH12	2:K:336:ASP:HB2	1.73	0.54
1:j:153:LYS:NZ	2:A:212:GLU:OE1	2.39	0.54
2:E:151:ARG:NH2	2:E:153:ASP:OD2	2.37	0.54
2:L:161:ASN:O	2:L:161:ASN:ND2	2.39	0.54
1:c:4:ILE:O	1:c:5:THR:HG22	2.07	0.54
1:h:153:LYS:NZ	2:K:212:GLU:OE2	2.36	0.54
2:B:267:GLU:O	2:B:271:LYS:HG2	2.08	0.54
2:F:180:VAL:HG13	2:F:273:ILE:HG12	1.88	0.54
2:G:204:ILE:HD11	2:H:206:LEU:HD22	1.90	0.54
2:I:180:VAL:HG13	2:I:273:ILE:HG12	1.90	0.54
2:L:90:ASN:ND2	2:L:121:LEU:O	2.41	0.54
2:L:180:VAL:C	2:L:182:ASP:H	2.16	0.54
1:a:61:PHE:HE2	2:D:228:LEU:HD12	1.73	0.54
2:H:168:ASN:ND2	2:I:105:ASP:OD1	2.41	0.54
2:J:293:ARG:HH12	2:J:336:ASP:HB2	1.73	0.54
1:l:126:MET:HE3	1:l:159:HIS:CD2	2.44	0.53
2:A:204:ILE:HD11	2:B:206:LEU:HD22	1.90	0.53
2:C:90:ASN:ND2	2:C:121:LEU:O	2.41	0.53
2:D:204:ILE:HD11	2:E:206:LEU:HD22	1.90	0.53
1:c:126:MET:HE3	1:c:159:HIS:CD2	2.43	0.53
2:E:267:GLU:O	2:E:271:LYS:HG2	2.08	0.53
1:j:157:PRO:HD2	1:j:160:ILE:HD12	1.91	0.53
1:k:161:ARG:NH2	2:B:244:GLY:O	2.41	0.53
1:j:61:PHE:HE2	2:A:228:LEU:HD12	1.72	0.53
2:I:90:ASN:ND2	2:I:121:LEU:O	2.41	0.53
1:i:62:LEU:O	2:L:221:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:293:ARG:HH12	2:E:336:ASP:HB2	1.73	0.53
1:g:157:PRO:HD2	1:g:160:ILE:HD12	1.90	0.53
1:f:122:LEU:O	1:f:126:MET:HG3	2.09	0.53
1:b:159:HIS:CD2	1:b:160:ILE:HG13	2.44	0.53
1:i:126:MET:HE3	1:i:159:HIS:CD2	2.44	0.53
1:l:122:LEU:O	1:l:126:MET:HG3	2.09	0.53
2:J:106:LEU:HD22	2:J:307:MET:HE2	1.90	0.53
1:c:122:LEU:O	1:c:126:MET:HG3	2.09	0.53
1:g:153:LYS:NZ	2:J:212:GLU:OE1	2.37	0.53
2:D:180:VAL:C	2:D:182:ASP:H	2.16	0.53
2:G:203:VAL:HG22	2:H:232:PRO:HD3	1.90	0.53
2:I:293:ARG:HH12	2:I:336:ASP:HB2	1.74	0.53
1:g:133:LYS:O	1:g:135:ASP:N	2.42	0.52
2:C:271:LYS:HZ2	2:C:281:GLN:HE22	1.57	0.52
1:g:61:PHE:HE2	2:J:228:LEU:HD12	1.74	0.52
1:h:159:HIS:CD2	1:h:160:ILE:HG13	2.44	0.52
2:A:203:VAL:HG22	2:B:232:PRO:HD3	1.90	0.52
2:C:180:VAL:C	2:C:182:ASP:H	2.16	0.52
2:K:168:ASN:ND2	2:L:105:ASP:OD1	2.41	0.52
1:a:157:PRO:HD2	1:a:160:ILE:HD12	1.91	0.52
2:D:203:VAL:HG22	2:E:232:PRO:HD3	1.90	0.52
2:I:275:LEU:HD11	2:J:284:LEU:HD13	1.91	0.52
2:J:204:ILE:HD11	2:K:206:LEU:HD22	1.91	0.52
1:h:4:ILE:O	1:h:5:THR:HG22	2.09	0.52
2:L:180:VAL:O	2:L:182:ASP:N	2.42	0.52
1:d:3:ILE:HG23	1:d:116:MET:HE2	1.91	0.52
1:f:126:MET:HE3	1:f:159:HIS:CD2	2.44	0.52
2:E:300:TYR:HE2	2:E:332:ALA:HB3	1.75	0.52
1:j:133:LYS:O	1:j:135:ASP:N	2.42	0.52
1:l:157:PRO:HD2	1:l:160:ILE:HD12	1.92	0.52
2:B:293:ARG:HH12	2:B:336:ASP:HB2	1.74	0.52
2:F:293:ARG:HH12	2:F:336:ASP:HB2	1.75	0.52
2:H:150:TYR:O	2:H:151:ARG:HG3	2.09	0.52
2:G:293:ARG:HH12	2:G:336:ASP:HB2	1.75	0.52
1:a:4:ILE:O	1:a:5:THR:HG22	2.10	0.52
1:i:122:LEU:O	1:i:126:MET:HG3	2.09	0.52
1:i:133:LYS:O	1:i:135:ASP:N	2.43	0.52
2:C:275:LEU:HD11	2:D:284:LEU:HD13	1.92	0.52
2:J:203:VAL:HG22	2:K:232:PRO:HD3	1.90	0.52
2:K:150:TYR:O	2:K:151:ARG:HG3	2.09	0.52
2:K:151:ARG:NH2	2:K:153:ASP:OD2	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:4:ILE:O	1:j:5:THR:HG22	2.10	0.52
2:A:293:ARG:HH12	2:A:336:ASP:HB2	1.74	0.52
2:D:293:ARG:HH12	2:D:336:ASP:HB2	1.74	0.52
2:K:176:ARG:O	2:K:179:THR:OG1	2.20	0.52
1:k:159:HIS:CD2	1:k:160:ILE:HG13	2.45	0.51
2:C:162:SER:HB3	2:C:173:GLY:HA2	1.92	0.51
2:F:161:ASN:O	2:F:161:ASN:ND2	2.39	0.51
2:G:151:ARG:HH21	2:G:153:ASP:HB2	1.76	0.51
2:K:106:LEU:HD22	2:K:307:MET:HE2	1.92	0.51
1:e:159:HIS:CD2	1:e:160:ILE:HG13	2.44	0.51
1:e:161:ARG:NH2	2:H:244:GLY:O	2.42	0.51
1:i:73:MET:HG3	1:i:106:VAL:HG22	1.91	0.51
1:d:133:LYS:O	1:d:135:ASP:N	2.43	0.51
1:f:73:MET:HG3	1:f:106:VAL:HG22	1.92	0.51
2:C:180:VAL:O	2:C:182:ASP:N	2.42	0.51
2:G:180:VAL:O	2:G:182:ASP:N	2.41	0.51
1:a:133:LYS:O	1:a:135:ASP:N	2.42	0.51
2:A:284:LEU:HD13	2:L:275:LEU:HD11	1.92	0.51
2:B:168:ASN:ND2	2:C:105:ASP:OD1	2.41	0.51
2:L:293:ARG:HH12	2:L:336:ASP:HB2	1.75	0.51
1:i:157:PRO:HD2	1:i:160:ILE:HD12	1.93	0.51
2:B:150:TYR:O	2:B:151:ARG:HG3	2.10	0.51
2:E:168:ASN:ND2	2:F:105:ASP:OD1	2.43	0.51
2:L:161:ASN:C	2:L:161:ASN:HD22	2.11	0.51
1:c:133:LYS:O	1:c:135:ASP:N	2.43	0.51
1:c:169:ARG:HB3	2:F:218:LEU:HD23	1.93	0.51
2:C:293:ARG:HH12	2:C:336:ASP:HB2	1.75	0.51
2:D:180:VAL:O	2:D:182:ASP:N	2.42	0.51
1:e:4:ILE:O	1:e:5:THR:HG22	2.11	0.51
2:B:300:TYR:HE2	2:B:332:ALA:HB3	1.76	0.51
1:h:73:MET:HG3	1:h:106:VAL:HG22	1.93	0.51
1:i:153:LYS:NZ	2:L:212:GLU:OE2	2.28	0.51
2:A:92:PHE:CD2	2:L:137:LYS:HB3	2.46	0.51
2:I:161:ASN:C	2:I:161:ASN:HD22	2.12	0.51
1:j:73:MET:SD	1:j:104:MET:HE3	2.50	0.51
1:e:55:PRO:HD3	1:e:101:GLU:HG2	1.93	0.51
1:h:55:PRO:HD3	1:h:101:GLU:HG2	1.93	0.51
1:h:161:ARG:NH2	2:K:244:GLY:O	2.44	0.51
1:k:4:ILE:O	1:k:5:THR:HG22	2.10	0.51
2:A:151:ARG:HH21	2:A:153:ASP:HB2	1.76	0.51
1:b:41:MET:HE2	1:b:170:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:157:PRO:HD2	1:f:160:ILE:HD12	1.92	0.50
2:B:275:LEU:HD11	2:C:284:LEU:HD13	1.94	0.50
1:e:169:ARG:NH2	2:H:246:MET:HE1	2.27	0.50
2:A:275:LEU:HD11	2:B:284:LEU:HD13	1.92	0.50
2:E:150:TYR:O	2:E:151:ARG:HG3	2.11	0.50
1:b:169:ARG:NH2	2:E:246:MET:HE1	2.26	0.50
1:d:153:LYS:HD3	1:d:161:ARG:HG2	1.94	0.50
2:A:230:TYR:HE2	2:A:240:LEU:HD12	1.76	0.50
2:D:148:ILE:HD12	2:D:148:ILE:H	1.74	0.50
2:H:106:LEU:HD22	2:H:307:MET:HE2	1.92	0.50
2:H:180:VAL:O	2:H:182:ASP:N	2.44	0.50
1:b:55:PRO:HD3	1:b:101:GLU:HG2	1.93	0.50
1:i:73:MET:SD	1:i:104:MET:HE3	2.52	0.50
2:B:288:ASN:O	2:B:292:ILE:HG12	2.12	0.50
2:F:168:ASN:ND2	2:G:105:ASP:OD1	2.42	0.50
2:J:288:ASN:O	2:J:292:ILE:HG12	2.12	0.50
2:I:147:GLN:O	2:I:149:ASN:ND2	2.32	0.50
1:a:153:LYS:NZ	2:D:212:GLU:OE1	2.40	0.50
1:d:159:HIS:ND1	1:d:160:ILE:HG13	2.27	0.50
1:h:168:ARG:HD2	2:J:213:ILE:HD13	1.93	0.50
1:k:169:ARG:NH2	2:B:246:MET:HE1	2.27	0.50
2:B:180:VAL:O	2:B:182:ASP:N	2.44	0.50
1:d:88:TYR:HE2	1:e:50:LEU:HD21	1.77	0.50
1:l:169:ARG:HB3	2:C:218:LEU:HD23	1.94	0.50
2:K:141:LYS:HA	2:K:151:ARG:O	2.12	0.50
2:K:288:ASN:O	2:K:292:ILE:HG12	2.12	0.50
1:c:73:MET:HG3	1:c:106:VAL:HG22	1.92	0.50
1:l:73:MET:SD	1:l:104:MET:HE3	2.52	0.50
2:H:141:LYS:HA	2:H:151:ARG:O	2.12	0.50
2:J:230:TYR:HE2	2:J:240:LEU:HD12	1.76	0.50
2:K:35:THR:HG23	2:K:177:VAL:HG11	1.93	0.50
1:d:160:ILE:O	1:d:164:ILE:HG12	2.12	0.49
2:I:302:MET:SD	2:J:300:TYR:OH	2.66	0.49
1:a:159:HIS:ND1	1:a:160:ILE:HG13	2.27	0.49
1:b:86:LYS:HE2	1:b:88:TYR:CE1	2.47	0.49
1:e:1:MET:SD	1:e:41:MET:HE1	2.52	0.49
1:l:133:LYS:O	1:l:135:ASP:N	2.43	0.49
2:E:275:LEU:HD11	2:F:284:LEU:HD13	1.94	0.49
2:E:288:ASN:O	2:E:292:ILE:HG12	2.12	0.49
1:c:157:PRO:HD2	1:c:160:ILE:HD12	1.93	0.49
1:f:4:ILE:O	1:f:8:ASP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:73:MET:SD	1:f:104:MET:HE3	2.52	0.49
2:D:288:ASN:O	2:D:292:ILE:HG12	2.13	0.49
2:F:137:LYS:HB3	2:G:92:PHE:CD2	2.47	0.49
2:F:209:GLU:HA	2:G:242:LEU:HB2	1.94	0.49
1:f:169:ARG:HB3	2:I:218:LEU:HD23	1.94	0.49
1:g:160:ILE:O	1:g:164:ILE:HG12	2.12	0.49
2:C:137:LYS:HB3	2:D:92:PHE:CD2	2.47	0.49
2:F:275:LEU:HD11	2:G:284:LEU:HD13	1.93	0.49
1:f:153:LYS:NZ	2:I:212:GLU:OE2	2.29	0.49
1:i:161:ARG:NH2	2:L:244:GLY:O	2.45	0.49
2:E:137:LYS:HB3	2:F:92:PHE:CD2	2.48	0.49
2:D:180:VAL:HG13	2:D:273:ILE:HG12	1.95	0.49
1:d:4:ILE:O	1:d:5:THR:HG22	2.13	0.49
1:c:73:MET:SD	1:c:104:MET:HE3	2.52	0.49
1:e:168:ARG:HD2	2:G:213:ILE:HD13	1.94	0.49
2:B:137:LYS:HB3	2:C:92:PHE:CE2	2.48	0.49
2:J:230:TYR:CE2	2:J:240:LEU:HD12	2.48	0.49
1:a:159:HIS:O	1:a:162:THR:HG22	2.13	0.49
1:g:159:HIS:ND1	1:g:160:ILE:HG13	2.28	0.49
1:k:87:LEU:HD23	1:k:88:TYR:O	2.13	0.49
2:D:89:PRO:HD3	2:D:95:ILE:HD13	1.95	0.49
2:E:141:LYS:HA	2:E:151:ARG:O	2.13	0.49
1:h:169:ARG:NH2	2:K:246:MET:HE1	2.27	0.48
2:G:288:ASN:O	2:G:292:ILE:HG12	2.12	0.48
2:J:231:ASN:HD22	2:J:234:THR:HG22	1.77	0.48
2:K:137:LYS:HB3	2:L:92:PHE:CE2	2.48	0.48
1:a:164:ILE:O	1:a:168:ARG:N	2.45	0.48
1:g:161:ARG:NH1	2:I:213:ILE:HD11	2.27	0.48
2:A:288:ASN:O	2:A:292:ILE:HG12	2.12	0.48
2:I:288:ASN:OD1	2:I:289:ASN:N	2.45	0.48
2:B:141:LYS:HA	2:B:151:ARG:O	2.13	0.48
2:H:89:PRO:HD3	2:H:95:ILE:HD13	1.94	0.48
2:I:137:LYS:HB3	2:J:92:PHE:CD2	2.47	0.48
2:I:161:ASN:O	2:I:161:ASN:ND2	2.39	0.48
2:K:89:PRO:HD3	2:K:95:ILE:HD13	1.94	0.48
1:d:153:LYS:NZ	2:G:212:GLU:OE1	2.36	0.48
1:g:88:TYR:HE2	1:h:50:LEU:HD21	1.77	0.48
2:A:141:LYS:HA	2:A:151:ARG:O	2.13	0.48
2:A:231:ASN:HD22	2:A:234:THR:HG22	1.78	0.48
2:F:267:GLU:O	2:F:271:LYS:HG2	2.13	0.48
2:C:161:ASN:O	2:C:161:ASN:ND2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:271:LYS:HE3	2:H:281:GLN:NE2	2.28	0.48
1:g:4:ILE:O	1:g:5:THR:HG22	2.13	0.48
2:G:230:TYR:HE2	2:G:240:LEU:HD12	1.79	0.48
2:G:230:TYR:CE2	2:G:240:LEU:HD12	2.49	0.48
2:G:275:LEU:HD11	2:H:284:LEU:HD13	1.95	0.48
1:g:162:THR:O	1:g:166:VAL:HG23	2.14	0.48
2:F:117:ASP:OD1	2:F:118:GLY:N	2.36	0.48
2:H:137:LYS:HB3	2:I:92:PHE:CD2	2.49	0.48
2:H:300:TYR:HE2	2:H:332:ALA:HB3	1.78	0.48
1:a:162:THR:O	1:a:166:VAL:HG23	2.13	0.48
1:b:133:LYS:O	1:b:135:ASP:N	2.44	0.48
1:i:164:ILE:O	1:i:168:ARG:HB2	2.14	0.48
2:I:117:ASP:OD1	2:I:118:GLY:N	2.36	0.48
1:a:160:ILE:O	1:a:164:ILE:HG12	2.14	0.48
1:f:133:LYS:O	1:f:135:ASP:N	2.43	0.48
2:C:180:VAL:HG13	2:C:273:ILE:HG12	1.95	0.48
2:G:141:LYS:HA	2:G:151:ARG:O	2.13	0.48
2:J:89:PRO:HD3	2:J:95:ILE:HD13	1.95	0.48
2:K:309:ASN:ND2	2:L:58:GLU:OE1	2.47	0.48
1:b:73:MET:HG3	1:b:106:VAL:HG22	1.94	0.48
1:b:159:HIS:O	1:b:162:THR:HG22	2.14	0.48
1:k:157:PRO:HD2	1:k:160:ILE:HD12	1.96	0.48
2:C:187:ARG:NH1	2:C:270:ASN:OD1	2.47	0.48
2:D:150:TYR:O	2:D:151:ARG:HB2	2.14	0.48
2:H:288:ASN:O	2:H:292:ILE:HG12	2.12	0.48
2:L:180:VAL:HG13	2:L:273:ILE:HG12	1.96	0.48
1:e:162:THR:O	1:e:166:VAL:HG23	2.14	0.47
1:l:153:LYS:HD3	1:l:161:ARG:HG2	1.96	0.47
2:B:137:LYS:HB3	2:C:92:PHE:CD2	2.49	0.47
1:h:162:THR:O	1:h:166:VAL:HG23	2.14	0.47
2:G:231:ASN:HD22	2:G:234:THR:HG22	1.79	0.47
2:H:137:LYS:HB3	2:I:92:PHE:CE2	2.48	0.47
1:e:157:PRO:HD2	1:e:160:ILE:HD12	1.96	0.47
1:f:164:ILE:O	1:f:168:ARG:HB2	2.14	0.47
1:h:4:ILE:O	1:h:8:ASP:HB2	2.14	0.47
1:h:157:PRO:HD2	1:h:160:ILE:HD12	1.96	0.47
1:i:169:ARG:HB3	2:L:218:LEU:HD23	1.96	0.47
1:j:159:HIS:ND1	1:j:160:ILE:HG13	2.29	0.47
2:G:150:TYR:O	2:G:151:ARG:HB2	2.14	0.47
2:J:150:TYR:O	2:J:151:ARG:HB2	2.14	0.47
1:b:164:ILE:O	1:b:168:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:4:ILE:O	1:c:8:ASP:HB2	2.14	0.47
1:j:86:LYS:HE2	1:j:88:TYR:CE1	2.49	0.47
1:l:4:ILE:O	1:l:5:THR:OG1	2.29	0.47
2:A:137:LYS:HB3	2:B:92:PHE:CD2	2.49	0.47
2:G:89:PRO:HD3	2:G:95:ILE:HD13	1.96	0.47
2:H:309:ASN:ND2	2:I:58:GLU:OE1	2.47	0.47
2:J:137:LYS:HB3	2:K:92:PHE:CD2	2.50	0.47
1:a:34:LEU:HD12	1:a:131:TRP:CH2	2.49	0.47
1:d:55:PRO:HD3	1:d:101:GLU:HG2	1.96	0.47
1:h:159:HIS:O	1:h:162:THR:HG22	2.15	0.47
2:A:89:PRO:HD3	2:A:95:ILE:HD13	1.97	0.47
2:A:230:TYR:CE2	2:A:240:LEU:HD12	2.48	0.47
2:H:90:ASN:OD1	2:H:121:LEU:O	2.33	0.47
1:b:157:PRO:HD2	1:b:160:ILE:HD12	1.95	0.47
1:g:55:PRO:HD3	1:g:101:GLU:HG2	1.95	0.47
1:j:34:LEU:HD12	1:j:131:TRP:CH2	2.49	0.47
2:A:150:TYR:O	2:A:151:ARG:HB2	2.14	0.47
2:E:42:ILE:HG13	2:E:184:LEU:HD23	1.97	0.47
2:E:309:ASN:ND2	2:F:58:GLU:OE1	2.47	0.47
2:F:300:TYR:HE2	2:F:332:ALA:HB3	1.80	0.47
2:G:137:LYS:HB3	2:H:92:PHE:CD2	2.49	0.47
2:G:180:VAL:HG13	2:G:273:ILE:HG12	1.96	0.47
1:i:49:GLN:HG2	1:i:51:ILE:HG13	1.95	0.47
1:k:88:TYR:HE2	1:l:50:LEU:HD21	1.79	0.47
1:k:162:THR:O	1:k:166:VAL:HG23	2.14	0.47
2:D:231:ASN:HD22	2:D:234:THR:HG22	1.80	0.47
2:E:144:PHE:HD2	2:E:148:ILE:HD12	1.80	0.47
2:H:275:LEU:HD11	2:I:284:LEU:HD13	1.97	0.47
2:L:300:TYR:HE2	2:L:332:ALA:HB3	1.80	0.47
2:C:300:TYR:HE2	2:C:332:ALA:HB3	1.80	0.47
2:H:170:GLN:HG2	2:I:101:LEU:HD21	1.97	0.47
2:J:81:LEU:HD21	2:J:323:ILE:HD11	1.96	0.47
2:K:271:LYS:HE3	2:K:281:GLN:NE2	2.29	0.47
1:e:159:HIS:O	1:e:162:THR:HG22	2.15	0.47
2:B:89:PRO:HD3	2:B:95:ILE:HD13	1.97	0.47
2:K:137:LYS:HB3	2:L:92:PHE:CD2	2.49	0.47
2:K:300:TYR:HE2	2:K:332:ALA:HB3	1.79	0.47
1:c:153:LYS:HD3	1:c:161:ARG:HG2	1.96	0.47
1:h:164:ILE:O	1:h:168:ARG:HB2	2.15	0.47
1:j:51:ILE:O	1:j:104:MET:HB3	2.15	0.47
1:j:161:ARG:NH1	2:L:213:ILE:HD11	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:164:ILE:O	1:k:168:ARG:N	2.48	0.47
2:A:289:ASN:HB2	2:L:294:PRO:HG3	1.97	0.47
2:B:170:GLN:HG2	2:C:101:LEU:HD21	1.98	0.47
2:I:294:PRO:HG3	2:J:289:ASN:HB2	1.96	0.47
2:L:220:GLU:O	2:L:224:GLU:HG3	2.15	0.47
1:f:161:ARG:NH2	2:I:244:GLY:O	2.48	0.46
1:k:159:HIS:O	1:k:162:THR:HG22	2.15	0.46
2:K:170:GLN:HG2	2:L:101:LEU:HD21	1.97	0.46
2:A:300:TYR:HE2	2:A:332:ALA:HB3	1.81	0.46
2:F:276:ALA:HB2	2:G:43:GLU:HB3	1.97	0.46
2:H:187:ARG:HD2	2:H:266:ILE:HG23	1.97	0.46
2:I:300:TYR:HE2	2:I:332:ALA:HB3	1.79	0.46
1:c:55:PRO:O	1:c:56:THR:OG1	2.28	0.46
1:d:34:LEU:HD12	1:d:131:TRP:CH2	2.51	0.46
1:k:164:ILE:O	1:k:168:ARG:HB2	2.16	0.46
1:l:55:PRO:O	1:l:56:THR:OG1	2.28	0.46
2:B:43:GLU:H	2:B:43:GLU:HG2	1.17	0.46
2:C:223:GLN:HG2	2:D:241:ILE:HG12	1.98	0.46
2:F:187:ARG:NH1	2:F:270:ASN:OD1	2.48	0.46
2:L:151:ARG:HH12	2:L:153:ASP:HB2	1.81	0.46
1:d:161:ARG:NH1	2:F:213:ILE:HD11	2.30	0.46
2:E:89:PRO:HD3	2:E:95:ILE:HD13	1.96	0.46
2:G:300:TYR:HE2	2:G:332:ALA:HB3	1.81	0.46
2:I:223:GLN:HG2	2:J:241:ILE:HG12	1.97	0.46
1:a:58:LYS:O	1:a:94:LEU:HD12	2.16	0.46
2:D:300:TYR:HE2	2:D:332:ALA:HB3	1.81	0.46
2:K:179:THR:HG22	2:L:41:LYS:HA	1.98	0.46
1:b:162:THR:O	1:b:166:VAL:HG23	2.14	0.46
1:e:164:ILE:O	1:e:168:ARG:N	2.47	0.46
1:d:159:HIS:O	1:d:162:THR:HG22	2.16	0.46
1:l:164:ILE:O	1:l:168:ARG:HB2	2.16	0.46
2:D:81:LEU:HD21	2:D:323:ILE:HD11	1.96	0.46
2:E:137:LYS:HB3	2:F:92:PHE:CE2	2.51	0.46
2:J:180:VAL:HG13	2:J:273:ILE:HG12	1.98	0.46
2:K:179:THR:HG22	2:L:41:LYS:CA	2.46	0.46
1:g:34:LEU:HD12	1:g:131:TRP:CH2	2.51	0.46
1:k:133:LYS:O	1:k:135:ASP:N	2.44	0.46
2:H:282:VAL:HG11	2:H:291:ASN:HB3	1.97	0.46
1:a:161:ARG:NH1	2:C:213:ILE:HD11	2.31	0.46
1:e:51:ILE:HB	1:e:104:MET:HE2	1.98	0.46
1:i:161:ARG:NH1	2:K:213:ILE:HD11	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:73:MET:HG3	1:j:106:VAL:HG22	1.98	0.46
1:k:51:ILE:HB	1:k:104:MET:HE2	1.97	0.46
1:k:68:THR:OG1	1:k:109:THR:OG1	2.34	0.46
2:E:288:ASN:OD1	2:E:289:ASN:N	2.49	0.46
2:I:151:ARG:HH12	2:I:153:ASP:HB2	1.81	0.46
2:C:294:PRO:HG3	2:D:289:ASN:HB2	1.98	0.45
2:F:294:PRO:HG3	2:G:289:ASN:HB2	1.98	0.45
2:L:291:ASN:OD1	2:L:291:ASN:N	2.49	0.45
1:b:4:ILE:O	1:b:8:ASP:HB2	2.16	0.45
1:b:88:TYR:CZ	1:b:94:LEU:HD12	2.52	0.45
2:C:151:ARG:HH12	2:C:153:ASP:HB2	1.81	0.45
2:J:43:GLU:H	2:J:43:GLU:HG2	1.03	0.45
1:h:164:ILE:O	1:h:168:ARG:N	2.49	0.45
2:D:141:LYS:HA	2:D:151:ARG:O	2.16	0.45
1:c:164:ILE:O	1:c:168:ARG:HB2	2.16	0.45
1:j:159:HIS:O	1:j:162:THR:HG22	2.17	0.45
2:D:137:LYS:HB3	2:E:92:PHE:CD2	2.52	0.45
2:D:298:LEU:HD12	2:E:296:ILE:HD11	1.98	0.45
2:H:288:ASN:OD1	2:H:289:ASN:N	2.49	0.45
1:e:164:ILE:O	1:e:168:ARG:HB2	2.16	0.45
1:g:159:HIS:O	1:g:162:THR:HG22	2.17	0.45
1:h:51:ILE:HB	1:h:104:MET:HE2	1.98	0.45
2:A:223:GLN:HG2	2:B:241:ILE:HG12	1.98	0.45
2:A:298:LEU:HD12	2:B:296:ILE:HD11	1.99	0.45
2:J:141:LYS:HA	2:J:151:ARG:O	2.15	0.45
2:L:292:ILE:HD13	2:L:292:ILE:HA	1.79	0.45
1:a:55:PRO:HD3	1:a:101:GLU:HG2	1.98	0.45
2:D:170:GLN:HG2	2:E:101:LEU:HD21	1.98	0.45
2:I:288:ASN:O	2:I:292:ILE:N	2.48	0.45
1:b:51:ILE:HB	1:b:104:MET:HE2	1.98	0.45
1:b:68:THR:OG1	1:b:109:THR:OG1	2.34	0.45
1:l:159:HIS:O	1:l:162:THR:HG22	2.17	0.45
2:C:117:ASP:OD1	2:C:118:GLY:N	2.36	0.45
2:E:327:THR:O	2:E:329:GLU:N	2.50	0.45
2:H:327:THR:O	2:H:329:GLU:N	2.50	0.45
2:J:134:ASP:HB2	2:J:139:ILE:C	2.42	0.45
1:c:159:HIS:O	1:c:162:THR:HG22	2.17	0.45
1:g:86:LYS:HG3	1:g:88:TYR:HE1	1.81	0.45
2:B:282:VAL:HG11	2:B:291:ASN:HB3	1.99	0.45
2:F:89:PRO:HD3	2:F:95:ILE:HD13	1.99	0.45
2:J:300:TYR:HE2	2:J:332:ALA:HB3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:162:SER:HB3	2:D:173:GLY:HA2	1.99	0.44
2:F:151:ARG:HH12	2:F:153:ASP:HB2	1.81	0.44
2:F:223:GLN:HG2	2:G:241:ILE:HG12	1.98	0.44
2:K:151:ARG:O	2:K:152:VAL:HB	2.17	0.44
2:K:275:LEU:HD11	2:L:284:LEU:HD13	1.99	0.44
1:d:41:MET:HE2	1:d:170:VAL:HB	2.00	0.44
2:C:161:ASN:C	2:C:161:ASN:ND2	2.76	0.44
2:B:288:ASN:OD1	2:B:289:ASN:N	2.49	0.44
2:E:192:ASN:HA	2:E:195:GLU:HG2	1.98	0.44
2:G:288:ASN:OD1	2:G:289:ASN:N	2.51	0.44
2:I:298:LEU:HD13	2:J:292:ILE:HD12	1.99	0.44
1:g:41:MET:HE2	1:g:170:VAL:HB	1.99	0.44
1:k:161:ARG:NH1	2:A:213:ILE:HD11	2.32	0.44
1:l:4:ILE:HG22	1:l:5:THR:O	2.18	0.44
2:B:327:THR:O	2:B:329:GLU:N	2.50	0.44
2:K:192:ASN:HA	2:K:195:GLU:HG2	1.99	0.44
1:j:55:PRO:HD3	1:j:101:GLU:HG2	1.99	0.44
1:j:119:ASP:OD2	1:j:167:TYR:OH	2.28	0.44
2:B:187:ARG:HD2	2:B:266:ILE:HG23	1.99	0.44
2:G:223:GLN:HG2	2:H:241:ILE:HG12	1.99	0.44
2:H:192:ASN:HA	2:H:195:GLU:HG2	1.99	0.44
2:K:288:ASN:OD1	2:K:289:ASN:N	2.49	0.44
2:K:327:THR:O	2:K:329:GLU:N	2.50	0.44
1:a:164:ILE:O	1:a:168:ARG:HB2	2.17	0.44
1:b:164:ILE:O	1:b:168:ARG:N	2.51	0.44
1:j:55:PRO:O	1:j:56:THR:OG1	2.30	0.44
2:D:327:THR:O	2:D:329:GLU:N	2.51	0.44
2:G:327:THR:O	2:G:329:GLU:N	2.51	0.44
2:I:292:ILE:HD13	2:I:292:ILE:HA	1.69	0.44
1:a:34:LEU:HD12	1:a:131:TRP:HH2	1.82	0.44
1:b:161:ARG:NH1	2:D:213:ILE:HD11	2.32	0.44
1:j:34:LEU:HD12	1:j:131:TRP:HH2	1.81	0.44
2:C:190:MET:HE1	2:C:265:ASP:HB2	2.00	0.44
1:d:55:PRO:O	1:d:56:THR:OG1	2.28	0.44
1:k:88:TYR:CZ	1:k:94:LEU:HD12	2.52	0.44
2:A:31:LYS:O	2:A:35:THR:OG1	2.28	0.44
2:B:151:ARG:O	2:B:152:VAL:HB	2.18	0.44
2:B:192:ASN:HA	2:B:195:GLU:HG2	1.99	0.44
2:F:214:LEU:O	2:F:214:LEU:HD12	2.18	0.44
2:F:327:THR:O	2:F:329:GLU:N	2.51	0.44
2:I:161:ASN:C	2:I:161:ASN:ND2	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:134:ASP:HB2	2:K:139:ILE:C	2.43	0.44
2:L:134:ASP:HB2	2:L:139:ILE:C	2.43	0.44
2:C:170:GLN:HG2	2:D:101:LEU:HD21	1.99	0.44
2:C:327:THR:O	2:C:329:GLU:N	2.51	0.44
2:D:223:GLN:HG2	2:E:241:ILE:HG12	1.99	0.44
2:E:282:VAL:HG11	2:E:291:ASN:HB3	2.00	0.44
2:I:134:ASP:HB2	2:I:139:ILE:C	2.43	0.44
2:L:89:PRO:HD3	2:L:95:ILE:HD13	2.00	0.44
2:L:327:THR:O	2:L:329:GLU:N	2.51	0.44
1:d:86:LYS:HG3	1:d:88:TYR:HE1	1.81	0.43
1:e:88:TYR:CZ	1:e:94:LEU:HD12	2.53	0.43
1:g:164:ILE:O	1:g:168:ARG:N	2.51	0.43
1:l:62:LEU:O	2:C:221:ARG:NH2	2.51	0.43
2:A:327:THR:O	2:A:329:GLU:N	2.51	0.43
2:E:187:ARG:HD2	2:E:266:ILE:HG23	2.00	0.43
2:F:161:ASN:C	2:F:161:ASN:ND2	2.76	0.43
1:c:153:LYS:NZ	2:F:212:GLU:OE2	2.41	0.43
1:e:169:ARG:HH21	2:H:246:MET:HE1	1.82	0.43
2:A:151:ARG:O	2:A:152:VAL:HB	2.18	0.43
2:C:89:PRO:HD3	2:C:95:ILE:HD13	2.00	0.43
2:D:288:ASN:OD1	2:D:289:ASN:N	2.51	0.43
2:D:298:LEU:HD13	2:E:292:ILE:HD12	2.00	0.43
2:E:162:SER:HB3	2:E:173:GLY:HA2	2.00	0.43
2:E:282:VAL:O	2:E:286:GLY:N	2.49	0.43
2:F:134:ASP:HB2	2:F:139:ILE:C	2.43	0.43
2:G:298:LEU:HD13	2:H:292:ILE:HD12	2.01	0.43
2:I:327:THR:O	2:I:329:GLU:N	2.51	0.43
2:J:223:GLN:HG2	2:K:241:ILE:HG12	1.98	0.43
2:K:214:LEU:O	2:K:214:LEU:HD12	2.18	0.43
1:b:160:ILE:O	1:b:164:ILE:HG12	2.18	0.43
1:f:55:PRO:HD3	1:f:101:GLU:HG2	2.00	0.43
1:i:4:ILE:O	1:i:8:ASP:HB2	2.18	0.43
1:j:164:ILE:O	1:j:168:ARG:HB2	2.19	0.43
2:D:193:PHE:CE2	2:F:232:PRO:HG2	2.54	0.43
2:H:134:ASP:HB2	2:H:139:ILE:C	2.43	0.43
2:J:288:ASN:OD1	2:J:289:ASN:N	2.51	0.43
1:d:164:ILE:O	1:d:168:ARG:HB2	2.19	0.43
2:C:328:LYS:HB3	2:C:328:LYS:HE2	1.80	0.43
2:H:151:ARG:O	2:H:152:VAL:HB	2.17	0.43
2:I:291:ASN:OD1	2:I:291:ASN:N	2.51	0.43
2:J:327:THR:O	2:J:329:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:153:LYS:NZ	2:C:212:GLU:OE2	2.41	0.43
2:A:298:LEU:HD13	2:B:292:ILE:HD12	2.00	0.43
2:D:159:LYS:O	2:E:100:ARG:NH2	2.52	0.43
2:E:151:ARG:O	2:E:152:VAL:HB	2.18	0.43
1:f:55:PRO:O	1:f:56:THR:OG1	2.28	0.43
1:h:88:TYR:CZ	1:h:94:LEU:HD12	2.53	0.43
2:B:214:LEU:HD12	2:B:214:LEU:O	2.18	0.43
2:B:328:LYS:HB3	2:B:328:LYS:HE2	1.79	0.43
2:E:214:LEU:HD12	2:E:214:LEU:O	2.18	0.43
2:G:151:ARG:HG2	2:G:152:VAL:HG12	2.00	0.43
2:H:215:ASN:ND2	2:H:218:LEU:HD13	2.33	0.43
2:K:215:ASN:ND2	2:K:218:LEU:HD13	2.34	0.43
1:c:161:ARG:NH1	2:E:213:ILE:HD11	2.32	0.43
1:f:4:ILE:HG22	1:f:5:THR:O	2.18	0.43
1:g:58:LYS:O	1:g:94:LEU:HD12	2.19	0.43
2:A:288:ASN:OD1	2:A:289:ASN:N	2.51	0.43
2:B:134:ASP:HB2	2:B:139:ILE:C	2.44	0.43
2:C:134:ASP:HB2	2:C:139:ILE:C	2.44	0.43
2:C:298:LEU:HD13	2:D:292:ILE:HD12	2.01	0.43
2:K:180:VAL:HG12	2:K:184:LEU:HD13	2.00	0.43
1:b:169:ARG:HH21	2:E:246:MET:HE1	1.83	0.43
1:h:169:ARG:HH21	2:K:246:MET:HE1	1.84	0.43
1:l:161:ARG:NH1	2:B:213:ILE:HD11	2.32	0.43
2:C:292:ILE:HD13	2:C:292:ILE:HA	1.68	0.43
2:D:151:ARG:O	2:D:152:VAL:HB	2.17	0.43
2:E:134:ASP:HB2	2:E:139:ILE:C	2.44	0.43
2:G:151:ARG:O	2:G:152:VAL:HB	2.18	0.43
2:H:214:LEU:HD12	2:H:214:LEU:O	2.19	0.43
2:J:151:ARG:O	2:J:152:VAL:HB	2.18	0.43
1:d:118:GLU:HG3	1:e:29:THR:HG22	2.01	0.43
2:A:90:ASN:OD1	2:A:121:LEU:O	2.36	0.43
2:A:134:ASP:HB2	2:A:139:ILE:C	2.43	0.43
2:A:292:ILE:HD12	2:L:298:LEU:HD13	2.01	0.43
2:F:298:LEU:HD13	2:G:292:ILE:HD12	2.01	0.43
2:K:159:LYS:O	2:L:100:ARG:NH2	2.52	0.43
1:f:13:GLY:O	1:f:14:GLY:C	2.59	0.43
1:i:55:PRO:O	1:i:56:THR:OG1	2.28	0.43
2:A:147:GLN:O	2:A:149:ASN:ND2	2.38	0.43
2:L:161:ASN:ND2	2:L:161:ASN:C	2.76	0.43
2:C:291:ASN:OD1	2:C:291:ASN:N	2.52	0.42
2:H:193:PHE:CE2	2:J:232:PRO:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:89:PRO:HD3	2:I:95:ILE:HD13	2.01	0.42
2:I:306:PRO:HA	2:I:309:ASN:HB2	2.01	0.42
1:d:58:LYS:O	1:d:94:LEU:HD12	2.19	0.42
1:g:62:LEU:O	2:J:221:ARG:NH2	2.51	0.42
2:A:232:PRO:HG2	2:K:193:PHE:CE2	2.54	0.42
2:F:170:GLN:HG2	2:G:101:LEU:HD21	2.00	0.42
2:F:292:ILE:HD13	2:F:292:ILE:HA	1.69	0.42
2:L:190:MET:HE1	2:L:265:ASP:HB2	2.01	0.42
1:i:4:ILE:HG22	1:i:5:THR:O	2.19	0.42
2:A:151:ARG:HG2	2:A:152:VAL:HG12	2.00	0.42
2:A:193:PHE:CE2	2:C:232:PRO:HG2	2.54	0.42
2:A:328:LYS:HB3	2:A:328:LYS:HE2	1.79	0.42
2:A:347:LEU:HD13	2:A:353:ILE:HD12	2.02	0.42
2:F:190:MET:HE1	2:F:265:ASP:HB2	2.00	0.42
2:F:291:ASN:OD1	2:F:291:ASN:N	2.52	0.42
2:G:162:SER:HB3	2:G:173:GLY:HA2	2.01	0.42
2:J:129:MET:SD	2:J:142:PHE:HB3	2.60	0.42
2:J:298:LEU:HD13	2:K:292:ILE:HD12	2.01	0.42
2:K:162:SER:HB3	2:K:173:GLY:HA2	2.01	0.42
1:e:86:LYS:HE2	1:e:88:TYR:CE1	2.55	0.42
1:g:3:ILE:HG23	1:g:116:MET:HE2	2.01	0.42
1:j:141:THR:HG22	1:j:146:THR:HG23	2.00	0.42
1:j:164:ILE:O	1:j:168:ARG:N	2.52	0.42
2:B:162:SER:HB3	2:B:173:GLY:HA2	2.01	0.42
2:E:193:PHE:CE2	2:G:232:PRO:HG2	2.55	0.42
2:G:134:ASP:HB2	2:G:139:ILE:C	2.44	0.42
1:b:169:ARG:NH1	2:E:219:ARG:HA	2.35	0.42
1:e:130:HIS:CE1	1:e:136:TYR:HB3	2.53	0.42
2:C:214:LEU:HD12	2:C:214:LEU:O	2.18	0.42
2:D:347:LEU:HD13	2:D:353:ILE:HD12	2.01	0.42
2:E:179:THR:H	2:E:179:THR:HG23	1.51	0.42
2:E:215:ASN:ND2	2:E:218:LEU:HD13	2.35	0.42
2:H:267:GLU:O	2:H:271:LYS:HG2	2.19	0.42
2:K:196:LYS:HD3	2:K:196:LYS:HA	1.92	0.42
1:b:4:ILE:HG22	1:b:5:THR:O	2.19	0.42
2:I:209:GLU:HG2	2:J:242:LEU:HD12	2.00	0.42
1:d:34:LEU:HD12	1:d:131:TRP:HH2	1.84	0.42
2:E:159:LYS:O	2:F:100:ARG:NH2	2.53	0.42
2:J:347:LEU:HD13	2:J:353:ILE:HD12	2.01	0.42
2:L:43:GLU:H	2:L:43:GLU:HG3	1.24	0.42
1:h:161:ARG:NH1	2:J:213:ILE:HD11	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:ASP:HB2	2:D:139:ILE:C	2.43	0.42
2:G:31:LYS:O	2:G:35:THR:OG1	2.27	0.42
2:H:198:LEU:HD23	2:H:198:LEU:HA	1.90	0.42
2:H:306:PRO:HA	2:H:309:ASN:HB2	2.02	0.42
2:I:190:MET:HE1	2:I:265:ASP:HB2	2.01	0.42
2:J:193:PHE:CE2	2:L:232:PRO:HG2	2.54	0.42
2:L:327:THR:C	2:L:329:GLU:H	2.28	0.42
1:g:34:LEU:HD12	1:g:131:TRP:HH2	1.85	0.42
1:g:164:ILE:O	1:g:168:ARG:HB2	2.19	0.42
1:k:169:ARG:HH21	2:B:246:MET:HE1	1.84	0.42
2:B:327:THR:C	2:B:329:GLU:H	2.28	0.42
2:D:129:MET:HE1	2:D:155:ILE:HD13	2.02	0.42
2:F:42:ILE:HG21	2:F:184:LEU:HD22	2.02	0.42
2:J:298:LEU:HD12	2:K:296:ILE:HD11	2.02	0.42
2:J:306:PRO:HA	2:J:309:ASN:HB2	2.02	0.42
2:K:96:SER:O	2:K:100:ARG:HG3	2.20	0.42
1:d:164:ILE:O	1:d:168:ARG:N	2.52	0.42
1:h:160:ILE:O	1:h:164:ILE:HG12	2.18	0.42
2:B:159:LYS:O	2:C:100:ARG:NH2	2.53	0.42
2:C:306:PRO:HA	2:C:309:ASN:HB2	2.02	0.42
2:E:141:LYS:HD3	2:E:149:ASN:OD1	2.20	0.42
2:H:131:VAL:HG22	2:H:142:PHE:CD2	2.55	0.42
1:e:161:ARG:NH1	2:G:213:ILE:HD11	2.36	0.41
1:f:160:ILE:O	1:f:164:ILE:HG12	2.20	0.41
2:E:43:GLU:H	2:E:43:GLU:HG2	1.36	0.41
2:G:159:LYS:O	2:H:100:ARG:NH2	2.53	0.41
2:K:101:LEU:HA	2:K:104:THR:HG22	2.02	0.41
1:h:68:THR:OG1	1:h:109:THR:OG1	2.37	0.41
1:h:86:LYS:HE2	1:h:88:TYR:CE1	2.55	0.41
2:D:328:LYS:HB3	2:D:328:LYS:HE2	1.80	0.41
2:F:131:VAL:HG22	2:F:142:PHE:CD2	2.55	0.41
2:G:193:PHE:CE2	2:I:232:PRO:HG2	2.55	0.41
2:H:151:ARG:HH12	2:H:153:ASP:HB2	1.85	0.41
2:L:290:ALA:O	2:L:294:PRO:HD2	2.20	0.41
1:c:55:PRO:HD3	1:c:101:GLU:HG2	2.03	0.41
1:i:160:ILE:O	1:i:164:ILE:HG12	2.20	0.41
2:A:214:LEU:HD12	2:A:214:LEU:O	2.20	0.41
2:C:131:VAL:HG22	2:C:142:PHE:CD2	2.55	0.41
2:H:96:SER:O	2:H:100:ARG:HG3	2.20	0.41
2:H:159:LYS:O	2:I:100:ARG:NH2	2.52	0.41
2:I:192:ASN:HA	2:I:195:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:327:THR:C	2:I:329:GLU:H	2.28	0.41
2:J:210:THR:HG22	2:J:212:GLU:H	1.86	0.41
2:L:192:ASN:HA	2:L:195:GLU:HG2	2.02	0.41
2:L:306:PRO:HA	2:L:309:ASN:HB2	2.01	0.41
1:c:35:ILE:HD11	1:c:127:LEU:HD12	2.01	0.41
1:k:150:ASN:ND2	1:l:136:TYR:O	2.54	0.41
2:A:159:LYS:O	2:B:100:ARG:NH2	2.54	0.41
2:D:42:ILE:HG21	2:D:184:LEU:HD22	2.03	0.41
2:D:306:PRO:HA	2:D:309:ASN:HB2	2.01	0.41
2:F:162:SER:HB3	2:F:173:GLY:HA2	2.02	0.41
2:G:327:THR:C	2:G:329:GLU:H	2.29	0.41
2:H:101:LEU:HA	2:H:104:THR:HG22	2.01	0.41
2:H:328:LYS:HE2	2:H:328:LYS:HB3	1.79	0.41
2:L:131:VAL:HG22	2:L:142:PHE:CD2	2.56	0.41
1:c:164:ILE:O	1:c:168:ARG:N	2.53	0.41
1:l:73:MET:HG3	1:l:106:VAL:HG22	2.01	0.41
2:A:162:SER:HB3	2:A:173:GLY:HA2	2.01	0.41
2:B:215:ASN:ND2	2:B:218:LEU:HD13	2.35	0.41
2:C:290:ALA:O	2:C:294:PRO:HD2	2.21	0.41
2:D:214:LEU:O	2:D:214:LEU:HD12	2.21	0.41
2:J:242:LEU:HD22	2:J:246:MET:HB3	2.02	0.41
2:J:328:LYS:HE2	2:J:328:LYS:HB3	1.80	0.41
1:d:162:THR:O	1:d:166:VAL:HG23	2.20	0.41
1:i:164:ILE:O	1:i:168:ARG:N	2.54	0.41
1:j:162:THR:O	1:j:166:VAL:HG23	2.20	0.41
1:l:4:ILE:O	1:l:8:ASP:HB2	2.20	0.41
2:A:170:GLN:HG2	2:B:101:LEU:HD21	2.03	0.41
2:B:193:PHE:CE2	2:D:232:PRO:HG2	2.55	0.41
2:C:42:ILE:HG21	2:C:184:LEU:HD22	2.03	0.41
2:K:327:THR:C	2:K:329:GLU:H	2.28	0.41
1:e:169:ARG:NH1	2:H:219:ARG:HA	2.36	0.41
1:f:159:HIS:O	1:f:162:THR:HG22	2.21	0.41
1:i:159:HIS:O	1:i:162:THR:HG22	2.21	0.41
1:k:78:LYS:HE2	1:k:78:LYS:HB2	1.86	0.41
2:A:42:ILE:HG21	2:A:184:LEU:HD22	2.03	0.41
2:C:327:THR:C	2:C:329:GLU:H	2.28	0.41
2:E:180:VAL:H	2:E:180:VAL:HG23	1.64	0.41
2:F:215:ASN:ND2	2:F:218:LEU:HD13	2.36	0.41
2:K:204:ILE:HD11	2:L:206:LEU:HD22	2.01	0.41
1:b:88:TYR:HE2	1:c:50:LEU:HD21	1.85	0.41
1:f:62:LEU:O	2:I:221:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:214:LEU:O	2:G:214:LEU:HD12	2.21	0.41
2:H:204:ILE:HD11	2:I:206:LEU:HD22	2.02	0.41
2:I:131:VAL:HG22	2:I:142:PHE:CD2	2.56	0.41
2:I:328:LYS:HE2	2:I:328:LYS:HB3	1.80	0.41
1:f:161:ARG:NH1	2:H:213:ILE:HD11	2.36	0.41
1:k:169:ARG:NH1	2:B:219:ARG:HA	2.35	0.41
2:D:144:PHE:O	2:D:146:ASN:N	2.54	0.41
2:F:168:ASN:HD22	2:G:104:THR:HG23	1.86	0.41
2:G:147:GLN:O	2:G:149:ASN:ND2	2.38	0.41
2:H:179:THR:HG21	2:I:46:ASN:ND2	2.36	0.41
2:K:131:VAL:HG22	2:K:142:PHE:CD2	2.56	0.41
2:K:151:ARG:HH12	2:K:153:ASP:HB2	1.85	0.41
1:d:62:LEU:O	2:G:221:ARG:NH2	2.54	0.41
1:g:4:ILE:O	1:g:8:ASP:HB2	2.20	0.41
1:h:169:ARG:NH1	2:K:219:ARG:HA	2.35	0.41
2:D:327:THR:C	2:D:329:GLU:H	2.29	0.41
2:E:302:MET:HE1	2:F:283:LEU:HD13	2.03	0.41
1:a:62:LEU:O	2:D:221:ARG:NH2	2.54	0.40
1:e:68:THR:OG1	1:e:109:THR:OG1	2.39	0.40
1:h:86:LYS:HG3	1:h:88:TYR:HE1	1.86	0.40
1:j:88:TYR:CE2	1:k:50:LEU:HD21	2.55	0.40
2:A:43:GLU:H	2:A:43:GLU:HG2	1.20	0.40
2:G:328:LYS:HE2	2:G:328:LYS:HB3	1.80	0.40
2:J:159:LYS:O	2:K:100:ARG:NH2	2.54	0.40
2:J:327:THR:C	2:J:329:GLU:H	2.29	0.40
2:K:306:PRO:HA	2:K:309:ASN:HB2	2.02	0.40
1:a:39:LEU:HD21	1:a:120:LEU:HD21	2.03	0.40
1:b:39:LEU:HD23	1:b:164:ILE:HG23	2.03	0.40
1:c:160:ILE:O	1:c:164:ILE:HG12	2.20	0.40
2:A:177:VAL:H	2:A:177:VAL:HG23	1.69	0.40
2:A:327:THR:C	2:A:329:GLU:H	2.28	0.40
2:G:137:LYS:HB3	2:H:92:PHE:CE2	2.56	0.40
2:G:144:PHE:O	2:G:146:ASN:N	2.54	0.40
2:J:214:LEU:HD12	2:J:214:LEU:O	2.21	0.40
2:L:162:SER:HB3	2:L:173:GLY:HA2	2.03	0.40
1:b:78:LYS:HE2	1:b:78:LYS:HB2	1.86	0.40
1:c:3:ILE:HA	1:c:116:MET:HE2	2.03	0.40
1:d:4:ILE:O	1:d:8:ASP:HB2	2.20	0.40
2:B:117:ASP:OD1	2:B:118:GLY:N	2.52	0.40
2:E:308:LEU:O	2:E:312:THR:HG23	2.21	0.40
2:G:298:LEU:HD12	2:H:296:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:327:THR:C	2:H:329:GLU:H	2.28	0.40
2:L:31:LYS:HB2	2:L:181:ILE:HD13	2.03	0.40
1:a:150:ASN:ND2	1:b:136:TYR:O	2.55	0.40
1:e:160:ILE:O	1:e:164:ILE:HG12	2.21	0.40
2:C:215:ASN:ND2	2:C:218:LEU:HD13	2.36	0.40
2:F:328:LYS:HB3	2:F:328:LYS:HE2	1.80	0.40
2:J:276:ALA:HB2	2:K:43:GLU:HB3	2.03	0.40
2:K:176:ARG:NH2	2:L:50:ASN:HD22	2.20	0.40
2:K:298:LEU:HD12	2:L:296:ILE:HD11	2.04	0.40
1:h:78:LYS:HE2	1:h:78:LYS:HB2	1.86	0.40
1:l:164:ILE:O	1:l:168:ARG:N	2.54	0.40
2:B:232:PRO:HG2	2:L:193:PHE:CE2	2.56	0.40
2:E:204:ILE:HD11	2:F:206:LEU:HD22	2.04	0.40
2:G:90:ASN:OD1	2:G:121:LEU:O	2.38	0.40
2:J:42:ILE:HG21	2:J:184:LEU:HD22	2.03	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	168/170 (99%)	154 (92%)	13 (8%)	1 (1%)	21	50
1	b	168/170 (99%)	155 (92%)	13 (8%)	0	100	100
1	c	168/170 (99%)	157 (94%)	10 (6%)	1 (1%)	21	50
1	d	168/170 (99%)	157 (94%)	10 (6%)	1 (1%)	21	50
1	e	168/170 (99%)	157 (94%)	10 (6%)	1 (1%)	21	50
1	f	168/170 (99%)	156 (93%)	12 (7%)	0	100	100
1	g	168/170 (99%)	156 (93%)	11 (6%)	1 (1%)	21	50
1	h	168/170 (99%)	155 (92%)	12 (7%)	1 (1%)	21	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	i	168/170 (99%)	157 (94%)	11 (6%)	0	100	100
1	j	168/170 (99%)	157 (94%)	10 (6%)	1 (1%)	21	50
1	k	168/170 (99%)	156 (93%)	11 (6%)	1 (1%)	21	50
1	l	168/170 (99%)	155 (92%)	13 (8%)	0	100	100
2	A	365/403 (91%)	335 (92%)	24 (7%)	6 (2%)	7	29
2	B	365/403 (91%)	331 (91%)	28 (8%)	6 (2%)	7	29
2	C	365/403 (91%)	332 (91%)	27 (7%)	6 (2%)	7	29
2	D	365/403 (91%)	333 (91%)	26 (7%)	6 (2%)	7	29
2	E	365/403 (91%)	332 (91%)	28 (8%)	5 (1%)	9	31
2	F	365/403 (91%)	333 (91%)	27 (7%)	5 (1%)	9	31
2	G	365/403 (91%)	334 (92%)	25 (7%)	6 (2%)	7	29
2	H	365/403 (91%)	334 (92%)	25 (7%)	6 (2%)	7	29
2	I	365/403 (91%)	334 (92%)	26 (7%)	5 (1%)	9	31
2	J	365/403 (91%)	332 (91%)	28 (8%)	5 (1%)	9	31
2	K	365/403 (91%)	334 (92%)	26 (7%)	5 (1%)	9	31
2	L	365/403 (91%)	333 (91%)	26 (7%)	6 (2%)	7	29
All	All	6396/6876 (93%)	5869 (92%)	452 (7%)	75 (1%)	13	35

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	151	ARG
2	A	152	VAL
2	B	151	ARG
2	B	152	VAL
2	B	181	ILE
2	C	151	ARG
2	C	152	VAL
2	C	181	ILE
2	D	151	ARG
2	D	152	VAL
2	D	181	ILE
2	E	151	ARG
2	E	152	VAL
2	F	151	ARG
2	F	152	VAL

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Mol	Chain	Res	Type
2	G	151	ARG
2	G	152	VAL
2	G	181	ILE
2	H	151	ARG
2	H	152	VAL
2	H	181	ILE
2	I	151	ARG
2	I	152	VAL
2	J	151	ARG
2	J	152	VAL
2	K	151	ARG
2	K	152	VAL
2	L	151	ARG
2	L	152	VAL
2	L	181	ILE
1	a	5	THR
1	d	5	THR
1	e	5	THR
1	g	5	THR
1	h	5	THR
1	j	5	THR
1	k	5	THR
1	c	5	THR
2	B	145	ASN
2	H	145	ASN
2	I	147	GLN
2	K	145	ASN
2	L	147	GLN
2	A	147	GLN
2	B	147	GLN
2	C	145	ASN
2	C	147	GLN
2	D	145	ASN
2	D	147	GLN
2	E	145	ASN
2	E	147	GLN
2	F	145	ASN
2	F	147	GLN
2	G	147	GLN
2	H	147	GLN
2	J	145	ASN
2	J	147	GLN

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Mol	Chain	Res	Type
2	K	147	GLN
2	A	328	LYS
2	B	328	LYS
2	C	328	LYS
2	D	328	LYS
2	E	328	LYS
2	G	328	LYS
2	H	328	LYS
2	J	328	LYS
2	K	328	LYS
2	A	145	ASN
2	A	181	ILE
2	F	328	LYS
2	G	145	ASN
2	I	145	ASN
2	I	328	LYS
2	L	145	ASN
2	L	328	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	149/149 (100%)	149 (100%)	0	100	100
1	b	149/149 (100%)	149 (100%)	0	100	100
1	c	149/149 (100%)	149 (100%)	0	100	100
1	d	149/149 (100%)	149 (100%)	0	100	100
1	e	149/149 (100%)	148 (99%)	1 (1%)	76	78
1	f	149/149 (100%)	148 (99%)	1 (1%)	76	78
1	g	149/149 (100%)	149 (100%)	0	100	100
1	h	149/149 (100%)	149 (100%)	0	100	100
1	i	149/149 (100%)	148 (99%)	1 (1%)	76	78
1	j	149/149 (100%)	149 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	k	149/149 (100%)	149 (100%)	0	100	100
1	l	149/149 (100%)	149 (100%)	0	100	100
2	A	328/353 (93%)	327 (100%)	1 (0%)	86	84
2	B	328/353 (93%)	326 (99%)	2 (1%)	78	80
2	C	328/353 (93%)	325 (99%)	3 (1%)	70	76
2	D	328/353 (93%)	327 (100%)	1 (0%)	86	84
2	E	328/353 (93%)	327 (100%)	1 (0%)	86	84
2	F	328/353 (93%)	324 (99%)	4 (1%)	63	72
2	G	328/353 (93%)	328 (100%)	0	100	100
2	H	328/353 (93%)	326 (99%)	2 (1%)	78	80
2	I	328/353 (93%)	324 (99%)	4 (1%)	63	72
2	J	328/353 (93%)	326 (99%)	2 (1%)	78	80
2	K	328/353 (93%)	327 (100%)	1 (0%)	86	84
2	L	328/353 (93%)	324 (99%)	4 (1%)	63	72
All	All	5724/6024 (95%)	5696 (100%)	28 (0%)	78	81

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	15	LEU
1	f	16	LYS
1	i	16	LYS
2	A	43	GLU
2	B	43	GLU
2	B	180	VAL
2	C	161	ASN
2	C	291	ASN
2	C	292	ILE
2	D	43	GLU
2	E	43	GLU
2	F	161	ASN
2	F	181	ILE
2	F	291	ASN
2	F	292	ILE
2	H	174	GLN
2	H	180	VAL
2	I	161	ASN

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Mol	Chain	Res	Type
2	I	214	LEU
2	I	291	ASN
2	I	292	ILE
2	J	43	GLU
2	J	174	GLN
2	K	43	GLU
2	L	43	GLU
2	L	161	ASN
2	L	214	LEU
2	L	291	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	84	GLN
1	a	132	HIS
1	b	84	GLN
1	b	130	HIS
1	c	159	HIS
1	d	84	GLN
1	d	132	HIS
1	e	130	HIS
1	e	132	HIS
1	e	150	ASN
1	e	159	HIS
1	f	138	GLN
1	f	159	HIS
1	g	84	GLN
1	g	132	HIS
1	h	159	HIS
1	i	159	HIS
1	j	84	GLN
1	l	159	HIS
2	A	15	GLN
2	A	231	ASN
2	A	270	ASN
2	B	15	GLN
2	B	90	ASN
2	B	146	ASN
2	B	223	GLN
2	B	270	ASN
2	B	281	GLN

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Mol	Chain	Res	Type
2	B	291	ASN
2	B	356	ASN
2	C	15	GLN
2	C	46	ASN
2	C	161	ASN
2	C	174	GLN
2	C	227	GLN
2	C	281	GLN
2	C	288	ASN
2	D	15	GLN
2	D	149	ASN
2	D	231	ASN
2	E	15	GLN
2	E	46	ASN
2	E	146	ASN
2	E	270	ASN
2	E	281	GLN
2	E	291	ASN
2	F	15	GLN
2	F	46	ASN
2	F	161	ASN
2	F	174	GLN
2	F	288	ASN
2	G	15	GLN
2	G	46	ASN
2	G	231	ASN
2	G	270	ASN
2	H	15	GLN
2	H	46	ASN
2	H	146	ASN
2	H	174	GLN
2	H	223	GLN
2	H	270	ASN
2	H	356	ASN
2	I	15	GLN
2	I	46	ASN
2	I	161	ASN
2	I	174	GLN
2	I	227	GLN
2	J	15	GLN
2	J	149	ASN
2	J	174	GLN

Continued on next page...

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Mol	Chain	Res	Type
2	J	231	ASN
2	J	270	ASN
2	J	289	ASN
2	K	15	GLN
2	K	90	ASN
2	K	146	ASN
2	K	223	GLN
2	K	270	ASN
2	K	356	ASN
2	L	15	GLN
2	L	46	ASN
2	L	161	ASN
2	L	174	GLN
2	L	227	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.

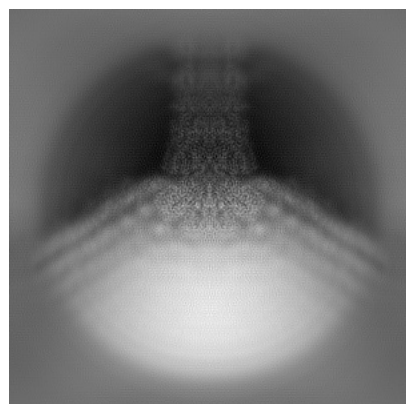
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60672. These allow visual inspection of the internal detail of the map and identification of artifacts.

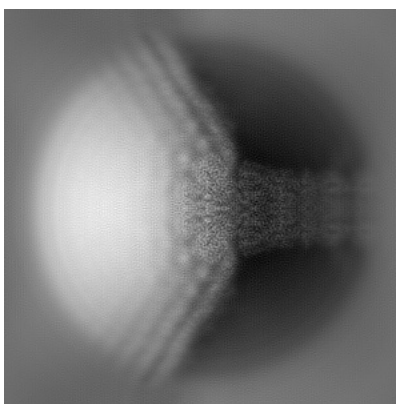
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

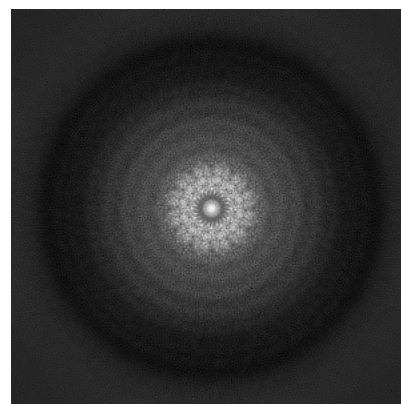
6.1.1 Primary map



X

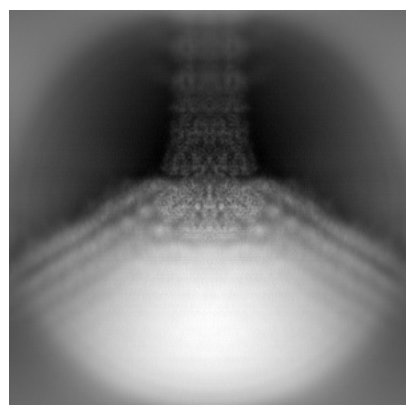


Y

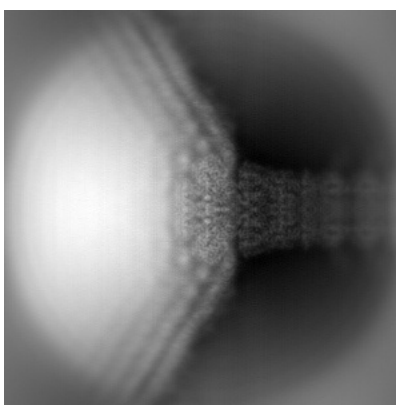


Z

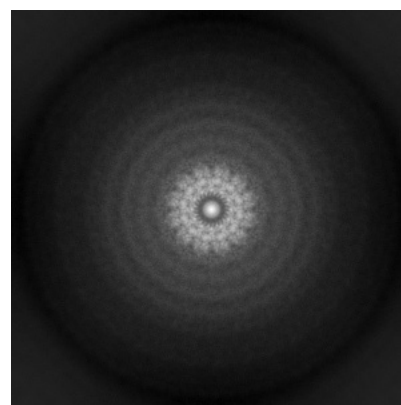
6.1.2 Raw map



X



Y

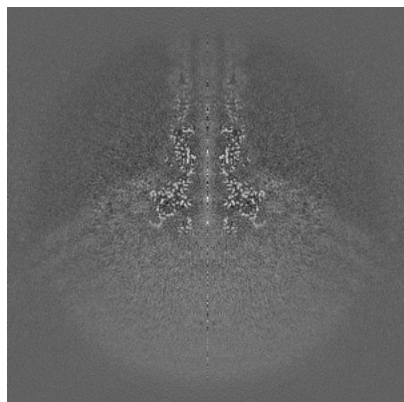


Z

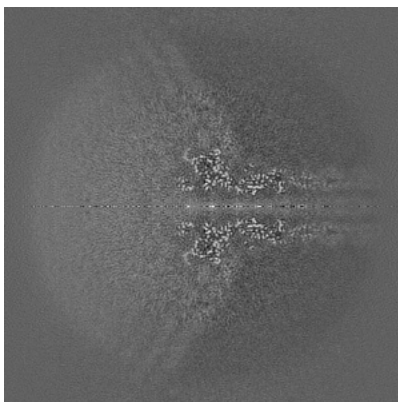
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

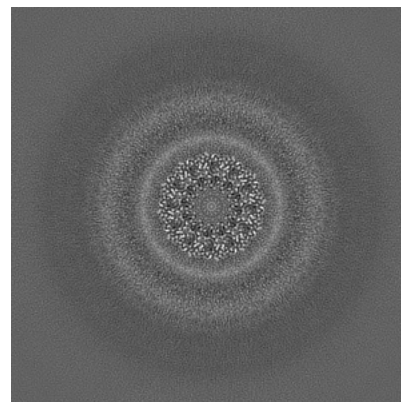
6.2.1 Primary map



X Index: 180

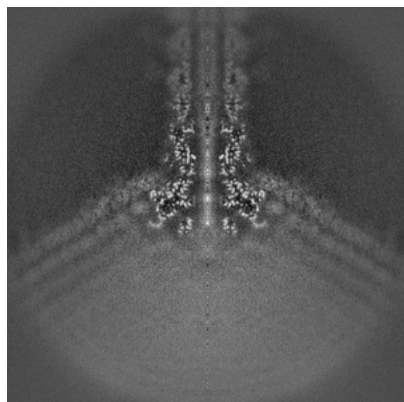


Y Index: 180

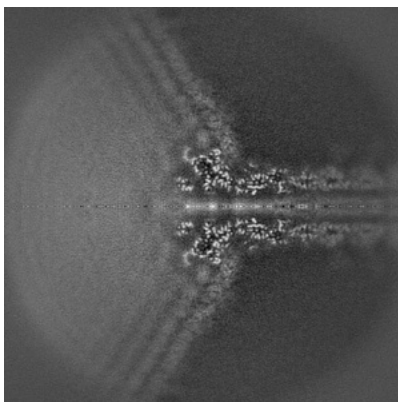


Z Index: 180

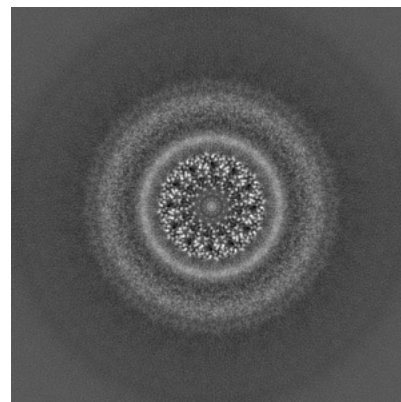
6.2.2 Raw map



X Index: 180



Y Index: 180

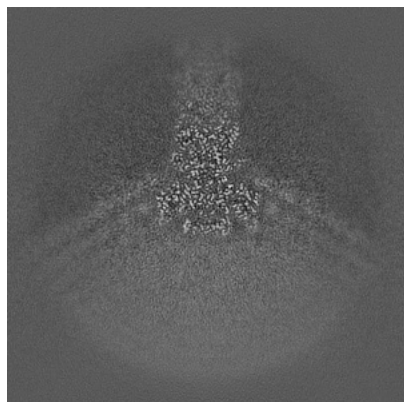


Z Index: 180

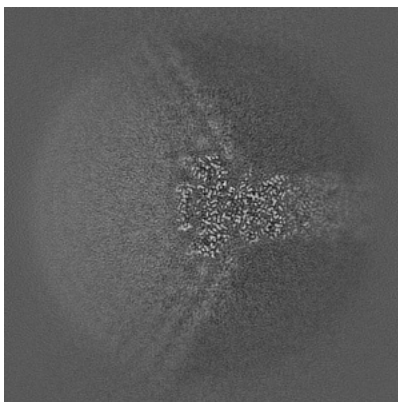
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

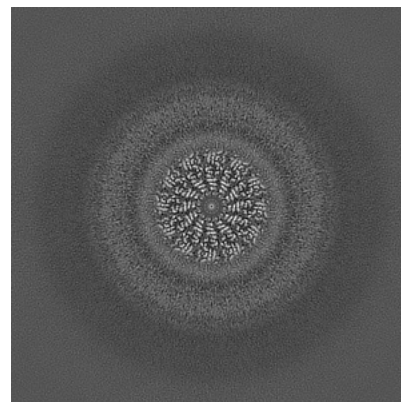
6.3.1 Primary map



X Index: 161

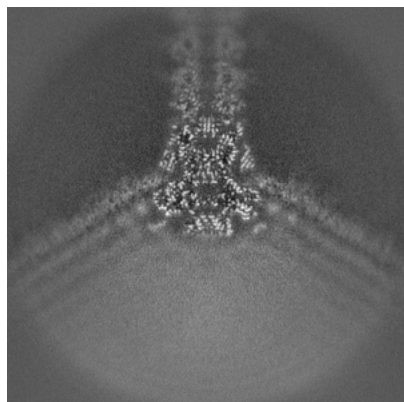


Y Index: 199

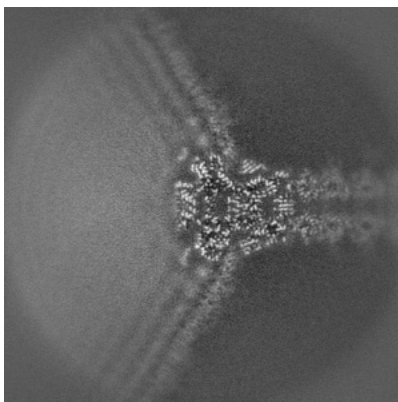


Z Index: 182

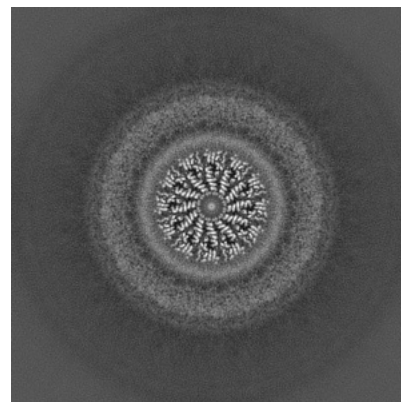
6.3.2 Raw map



X Index: 194



Y Index: 166

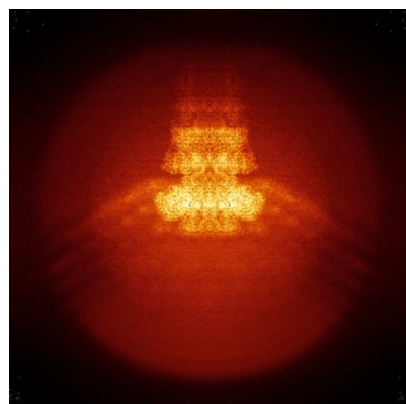


Z Index: 182

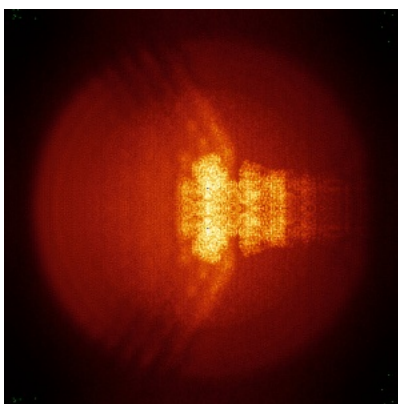
The images above show the largest variance slices of the map in three orthogonal directions.

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

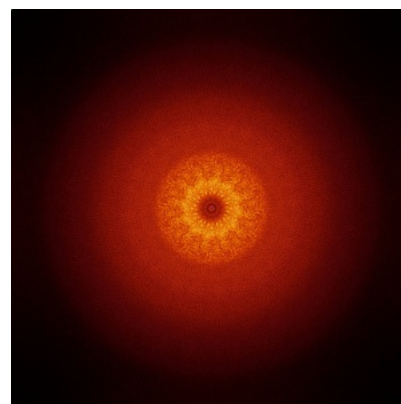
6.4.1 Primary map



X

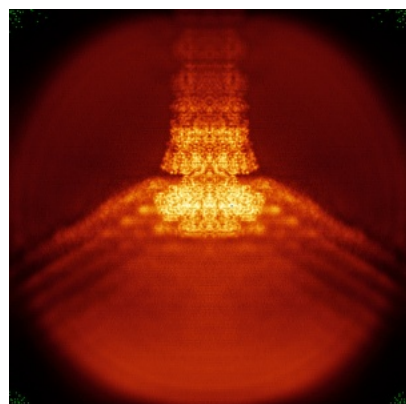


Y

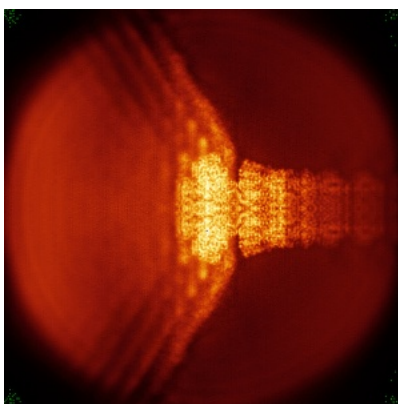


Z

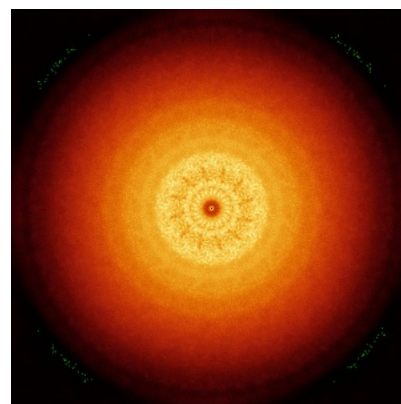
6.4.2 Raw map



X



Y

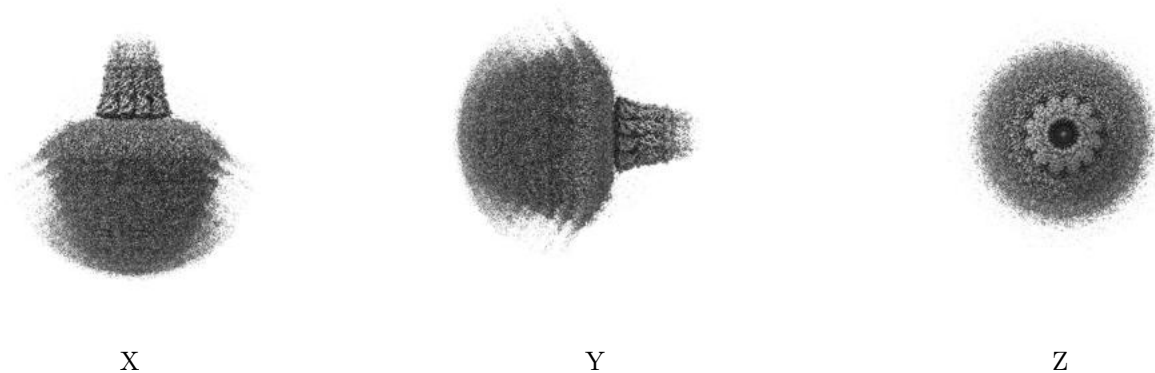


Z

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

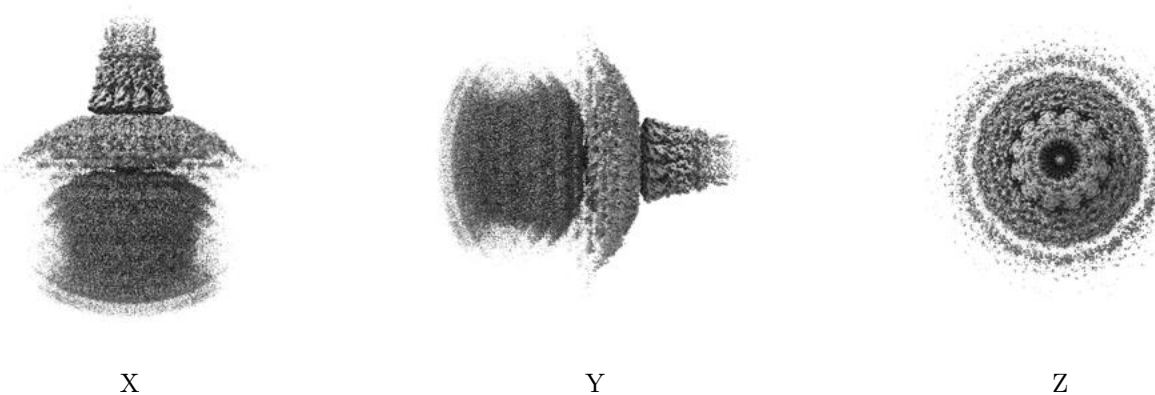
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

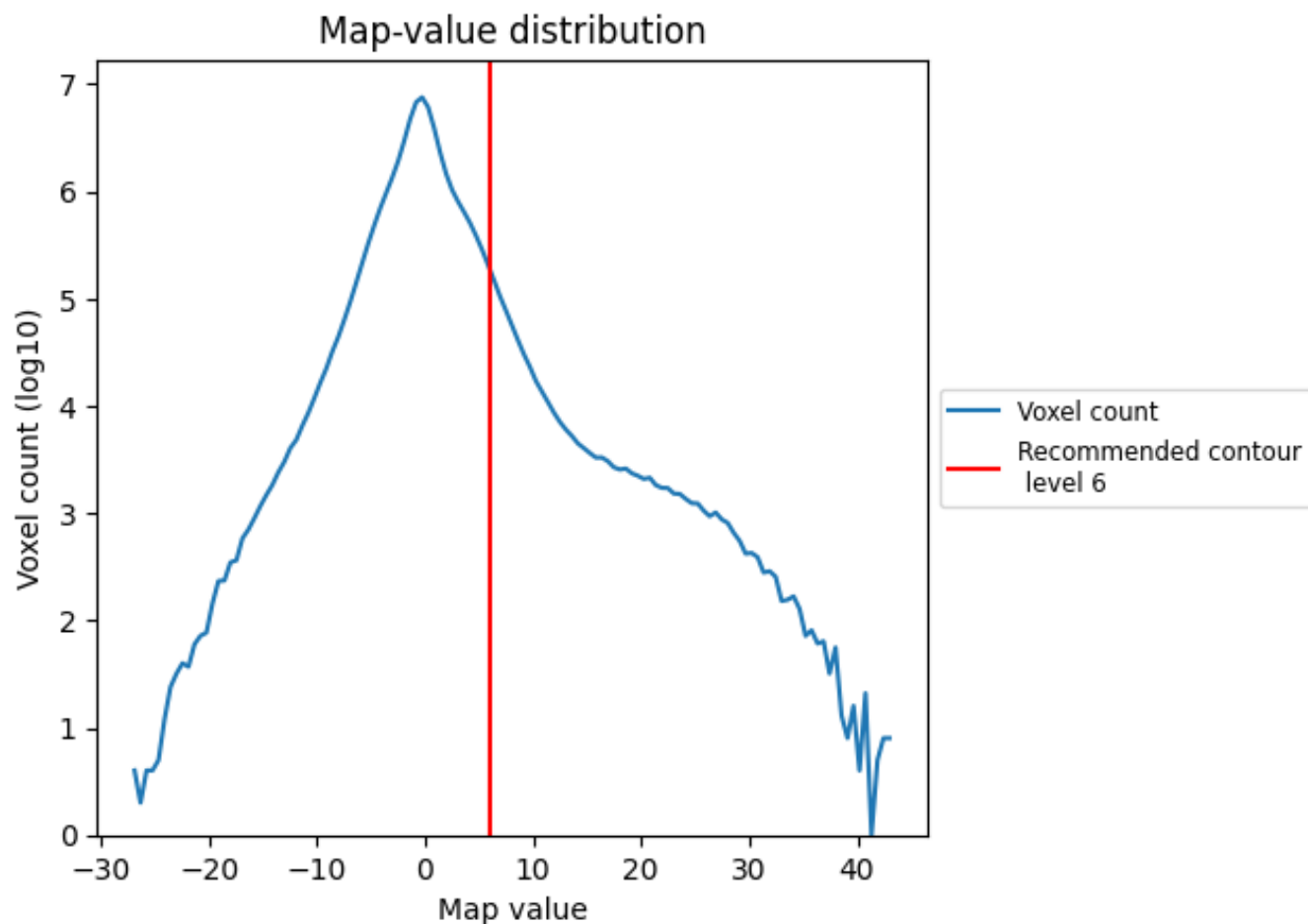
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

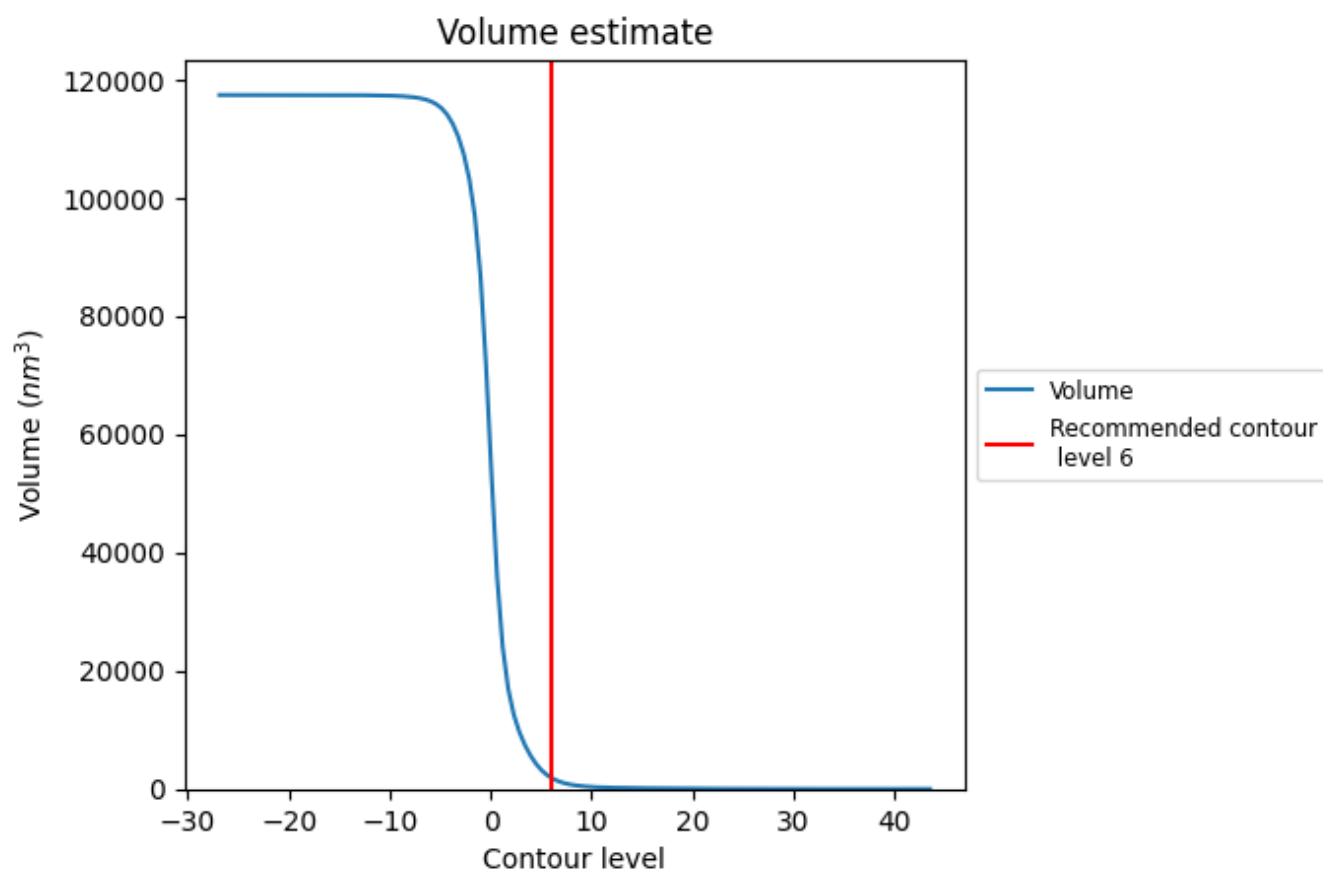
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

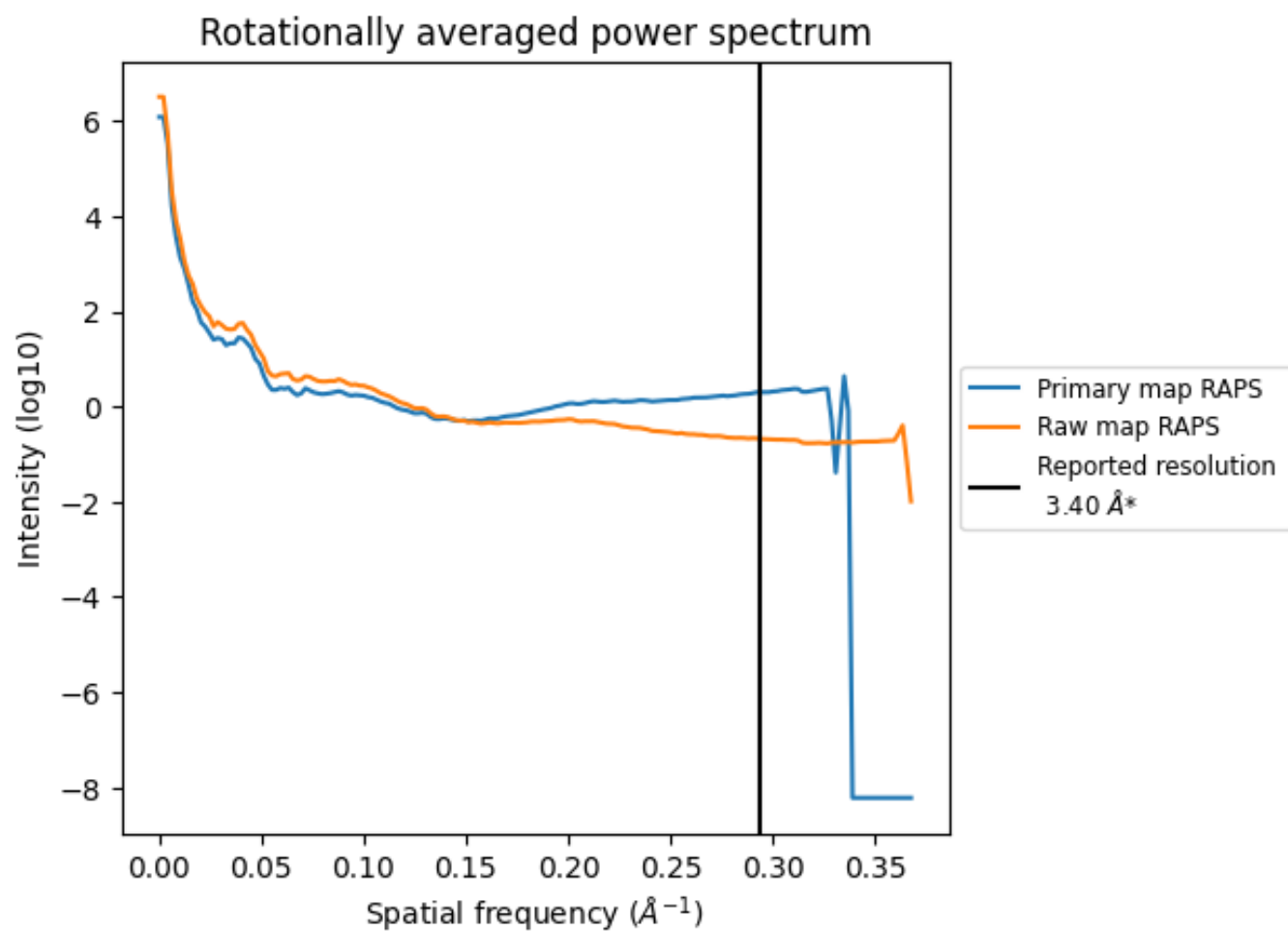
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1905 nm³; this corresponds to an approximate mass of 1720 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

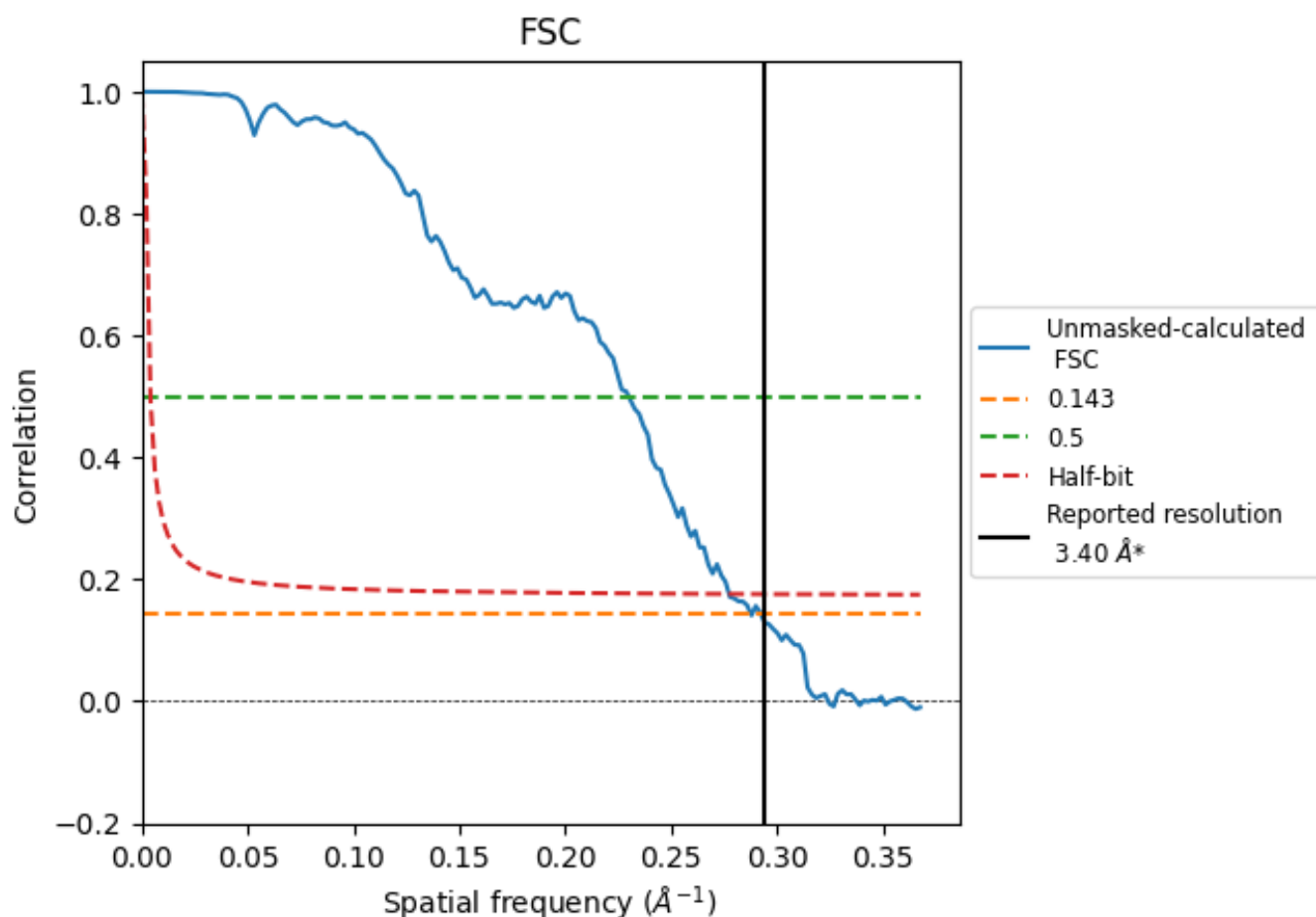


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.48	4.35	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

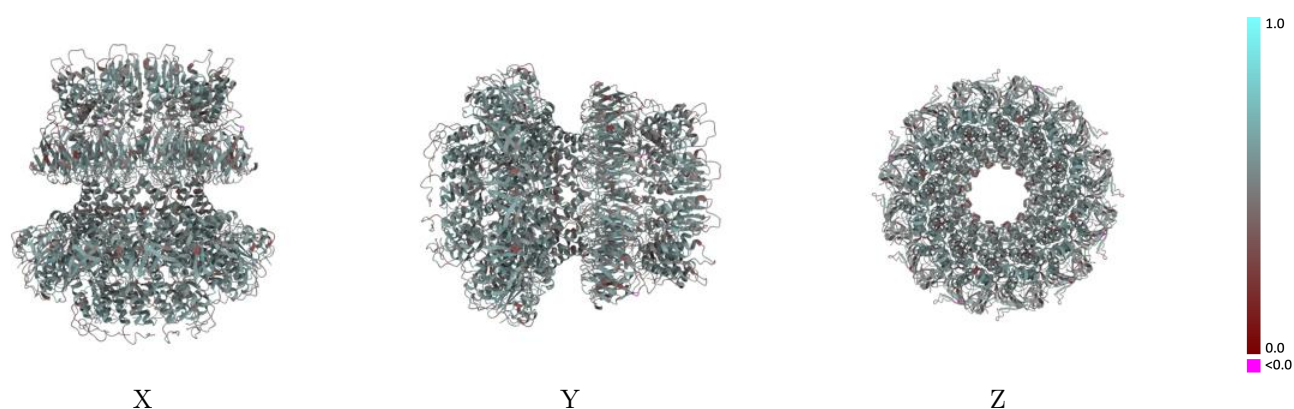
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60672 and PDB model 9ILP. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

This section was not generated.

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

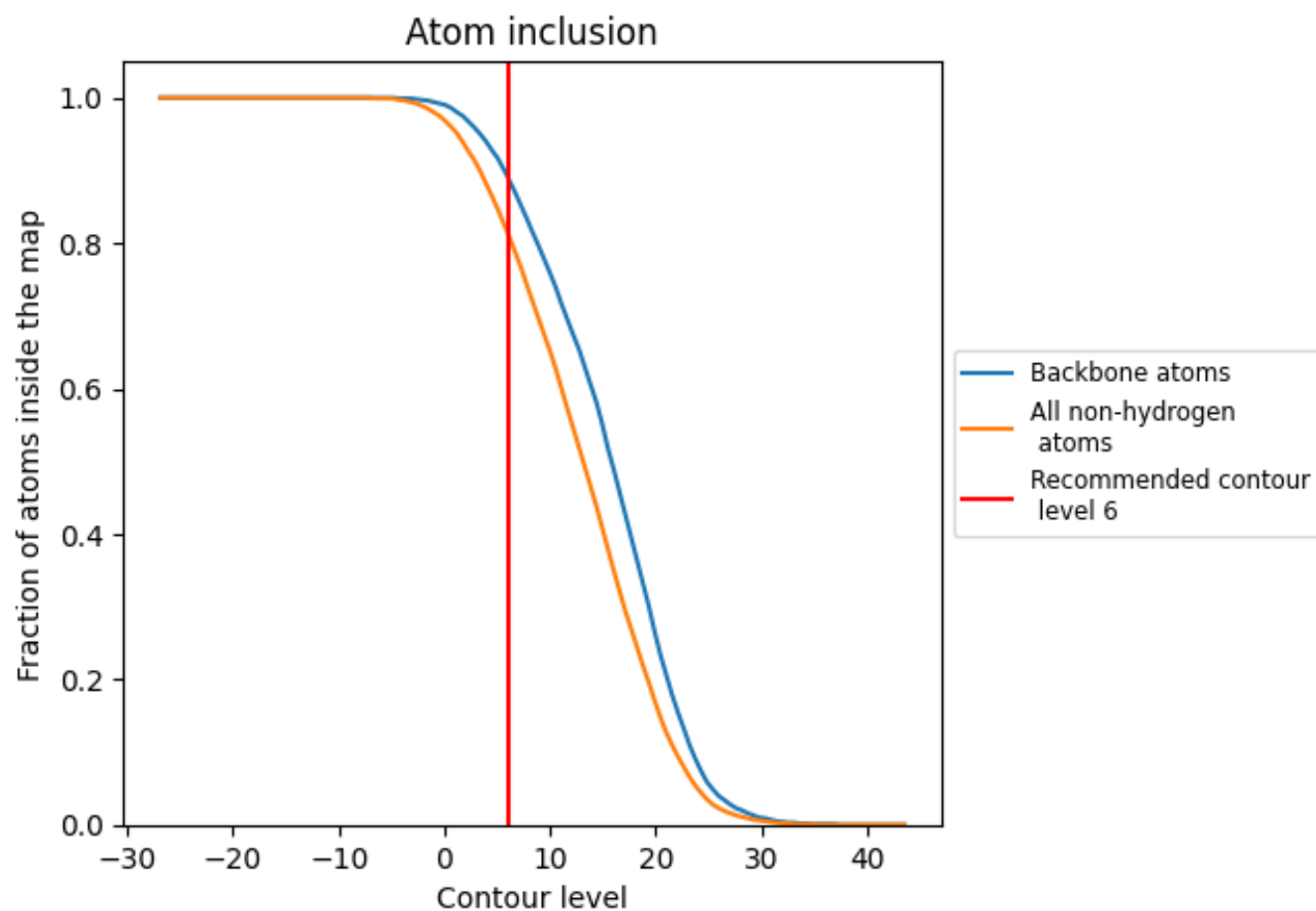


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 81% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8140	 0.5200
A	 0.8430	 0.5250
B	 0.8450	 0.5260
C	 0.8400	 0.5290
D	 0.8420	 0.5270
E	 0.8420	 0.5250
F	 0.8410	 0.5280
G	 0.8420	 0.5270
H	 0.8430	 0.5270
I	 0.8420	 0.5300
J	 0.8450	 0.5280
K	 0.8380	 0.5220
L	 0.8420	 0.5280
a	 0.7510	 0.5000
b	 0.7490	 0.5040
c	 0.7610	 0.5060
d	 0.7500	 0.5070
e	 0.7430	 0.5010
f	 0.7590	 0.5080
g	 0.7470	 0.5040
h	 0.7450	 0.4990
i	 0.7630	 0.5080
j	 0.7520	 0.5040
k	 0.7490	 0.5010
l	 0.7610	 0.5070

