



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 07:51 PM UTC

PDB ID : 8HEY / pdb_00008hey
EMDB ID : EMD-34704
Title : One CVSC-binding penton vertex in HCMV B-capsid
Authors : Li, Z.; Yu, X.
Deposited on : 2022-11-09
Resolution : 4.10 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

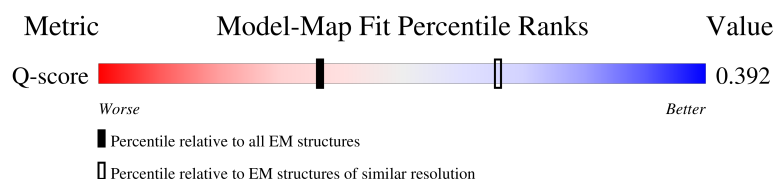
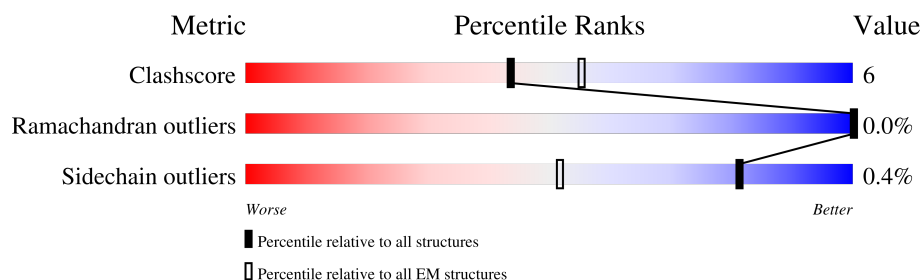
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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.



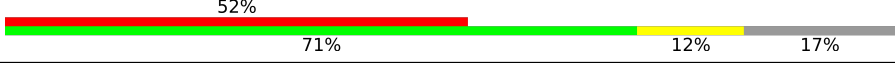
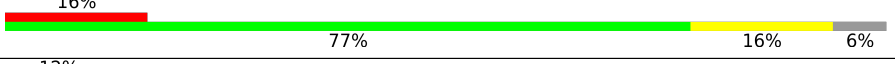
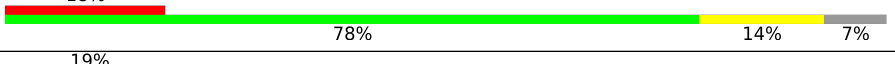
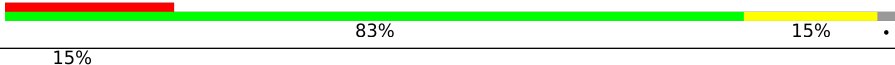
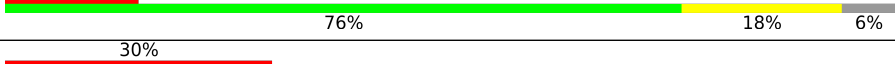
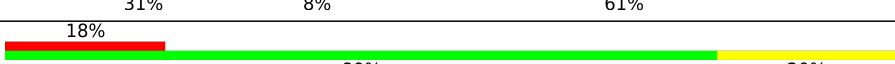
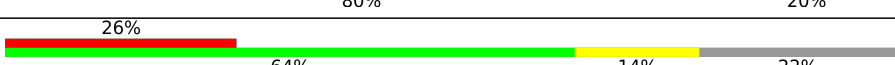
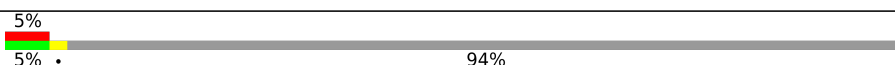
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	Q	75	56% 52% 7% 41%
1	R	75	53% 60% 13% 27%
1	S	75	51% 64% 8% 27%
1	T	75	19% 31% 69%

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Mol	Chain	Length	Quality of chain
1	i	75	
1	j	75	
2	A	1370	
2	B	1370	
2	C	1370	
2	D	1370	
2	Y	1370	
2	Z	1370	
2	a	1370	
3	I	306	
3	h	306	
3	n	306	
3	o	306	
4	g	290	
4	m	290	
5	M	594	
6	N	642	
6	O	642	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 90223 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 Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	T	23	Total	C	N	O	S	0	0
			192	121	38	31	2		
1	i	56	Total	C	N	O	S	0	0
			446	282	80	80	4		
1	j	58	Total	C	N	O	S	0	0
			467	294	87	82	4		
1	Q	44	Total	C	N	O	S	0	0
			352	221	65	62	4		
1	R	55	Total	C	N	O	S	0	0
			436	276	77	79	4		
1	S	55	Total	C	N	O	S	0	0
			436	276	77	79	4		

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	1281	Total	C	N	O	S	0	0
			10125	6444	1760	1864	57		
2	D	1270	Total	C	N	O	S	0	0
			10054	6409	1745	1843	57		
2	Y	1347	Total	C	N	O	S	0	0
			10676	6799	1850	1966	61		
2	Z	1326	Total	C	N	O	S	0	0
			10498	6687	1820	1933	58		
2	A	1142	Total	C	N	O	S	0	0
			9105	5832	1576	1648	49		
2	B	1282	Total	C	N	O	S	0	0
			10164	6479	1760	1866	59		
2	C	1300	Total	C	N	O	S	0	0
			10291	6562	1785	1885	59		

- Molecule 3 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	h	290	Total	C	N	O	S	0	0
			2304	1481	397	409	17		
3	I	277	Total	C	N	O	S	0	0
			2209	1418	381	393	17		
3	n	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
3	o	289	Total	C	N	O	S	0	0
			2291	1473	393	407	18		

- Molecule 4 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	112	Total	C	N	O	S	0	0
			929	596	164	165	4		
4	m	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 5 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	464	Total	C	N	O	S	0	0
			3813	2388	733	678	14		

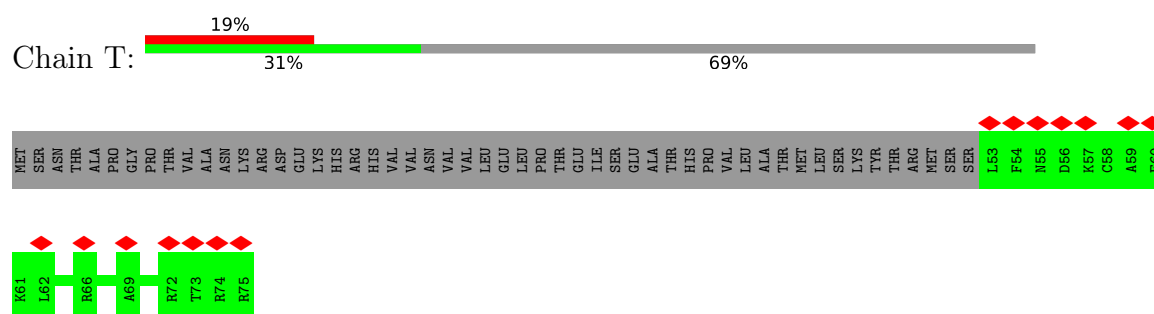
- Molecule 6 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	51	Total	C	N	O	S	0	0
			432	269	87	73	3		
6	O	41	Total	C	N	O	S	0	0
			344	223	62	57	2		

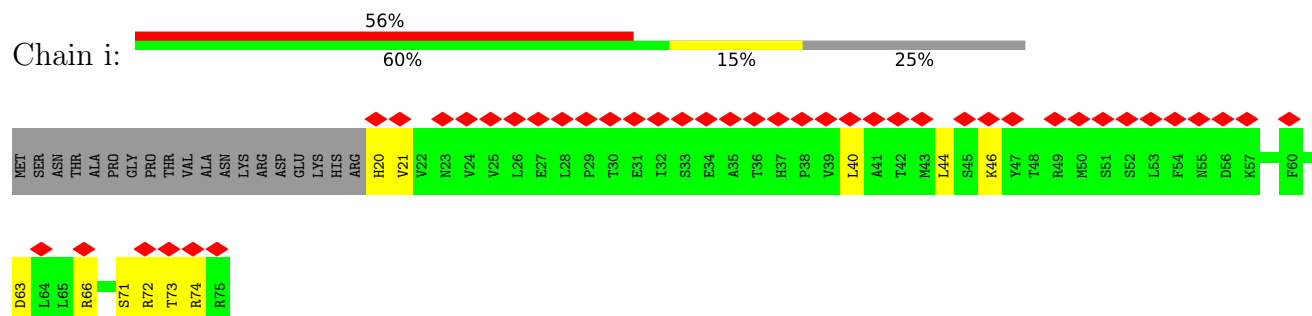
3 Residue-property plots [i](#)

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.

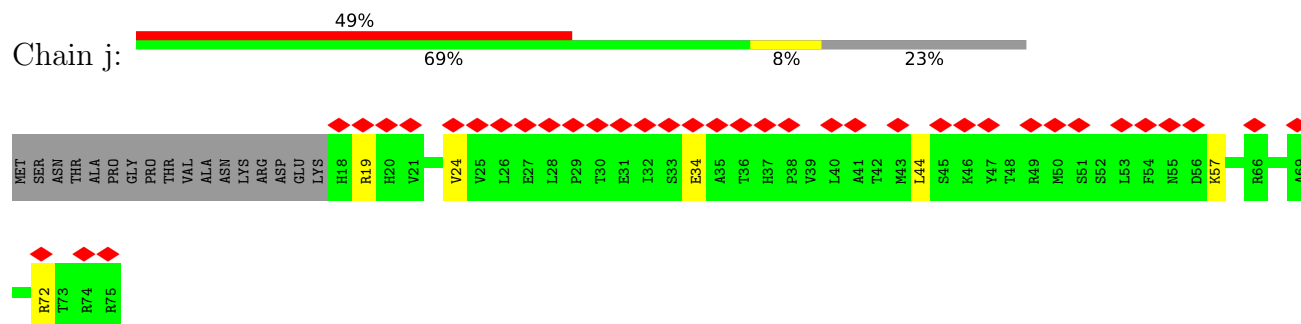
- Molecule 1: Small capsomere-interacting protein



- Molecule 1: Small capsomere-interacting protein

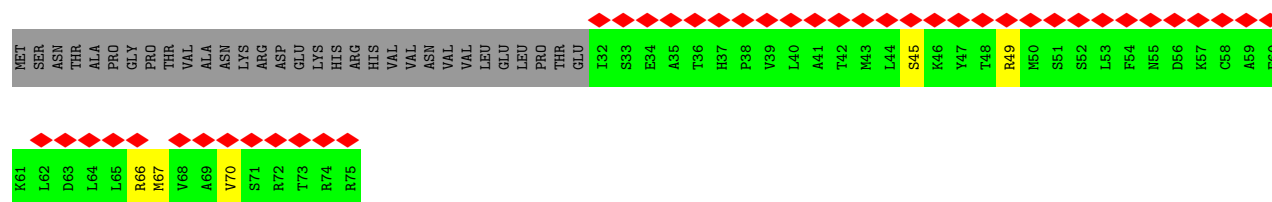


- Molecule 1: Small capsomere-interacting protein

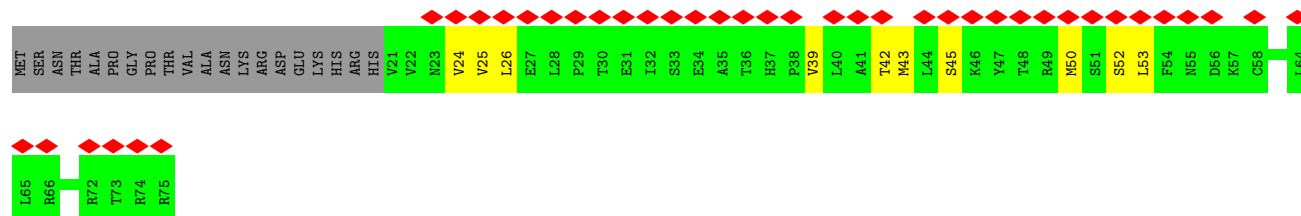


- Molecule 1: Small capsomere-interacting protein

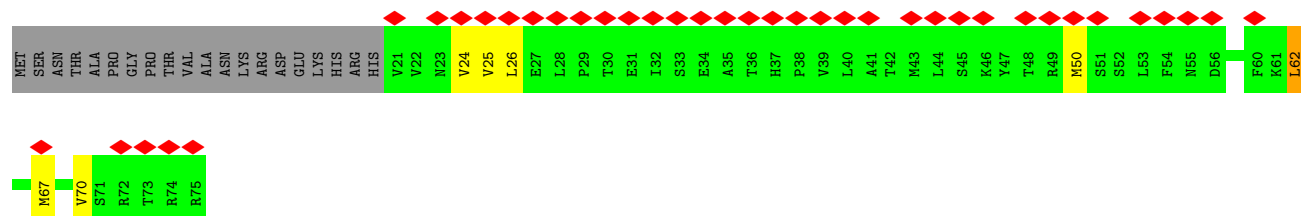




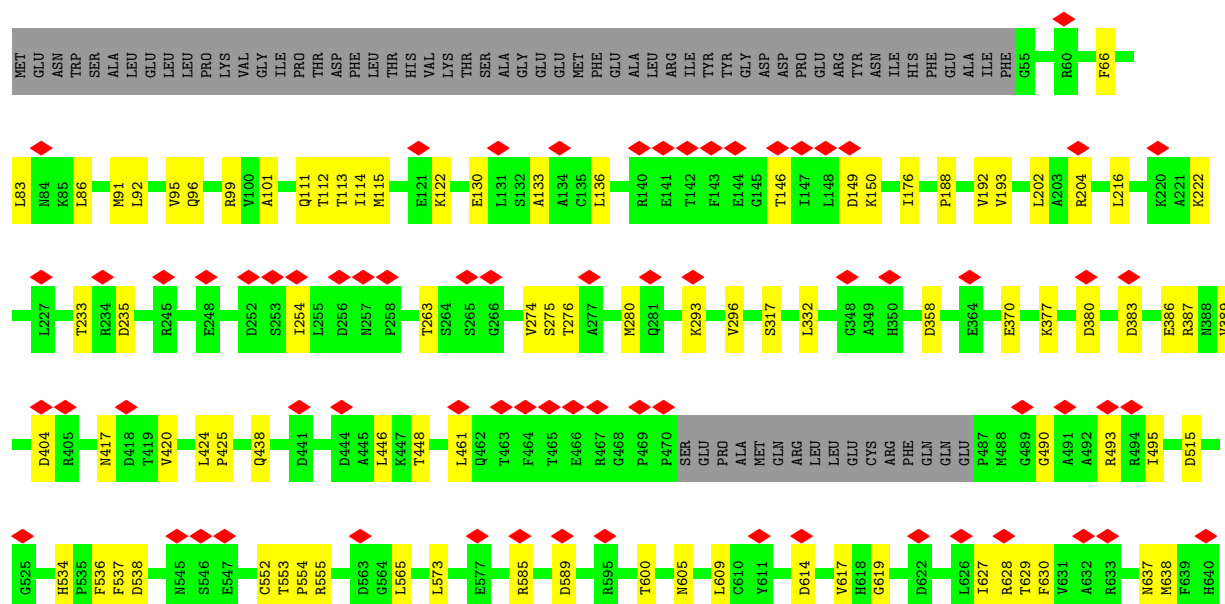
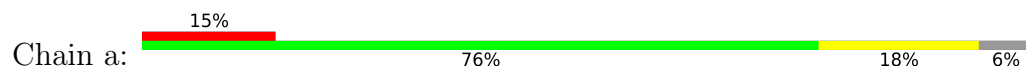
• Molecule 1: Small capsomere-interacting protein

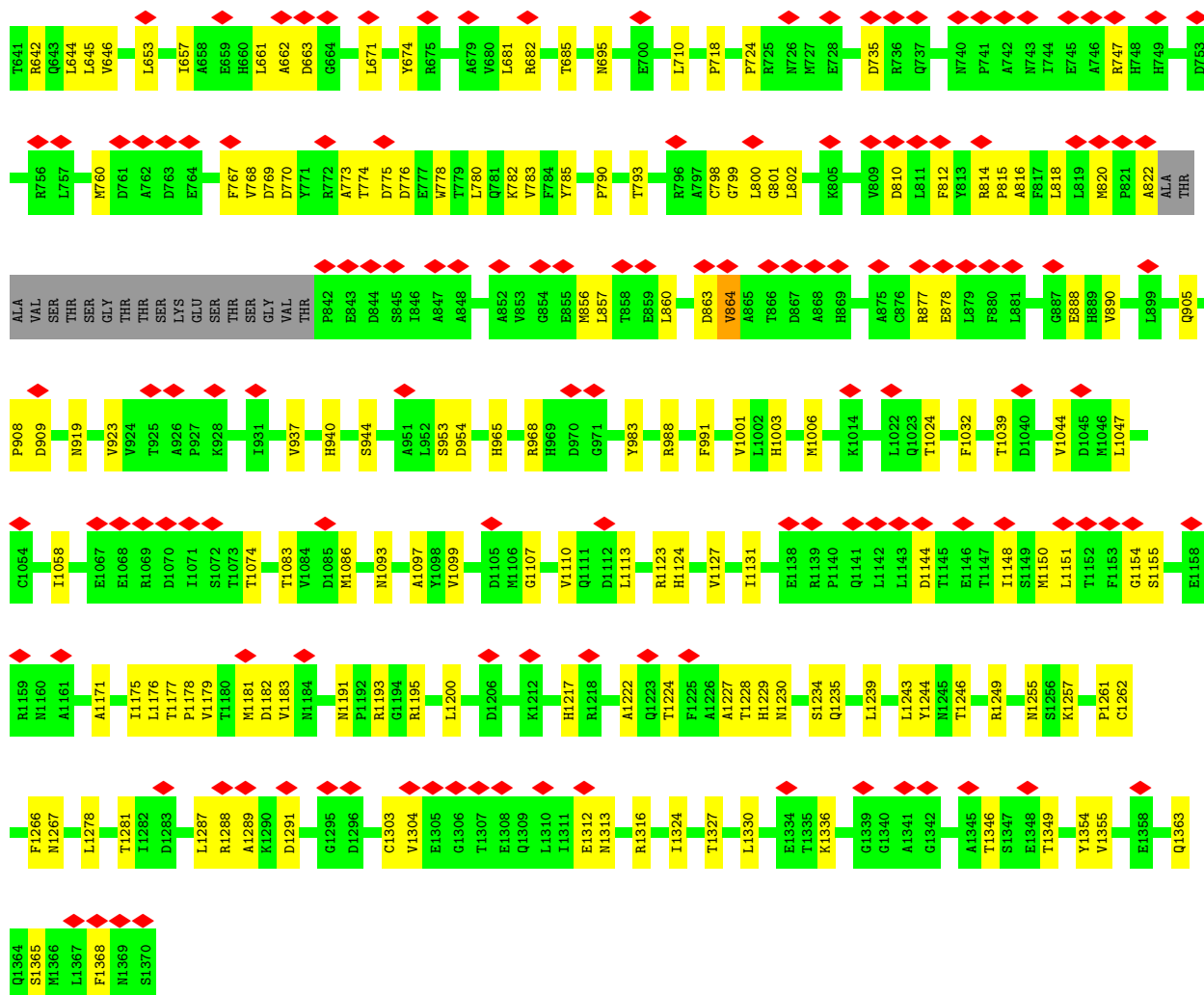


• Molecule 1: Small capsomere-interacting protein

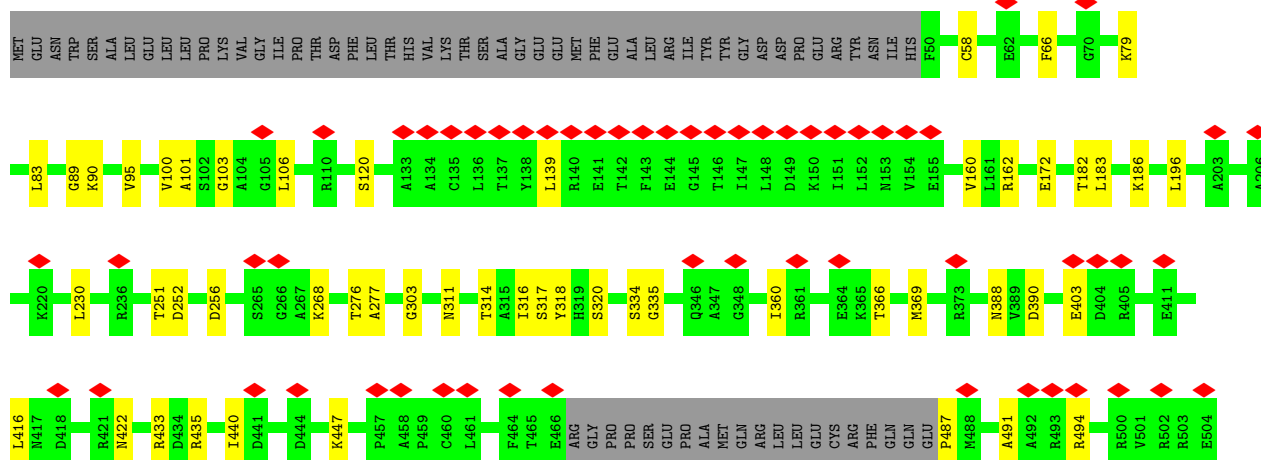
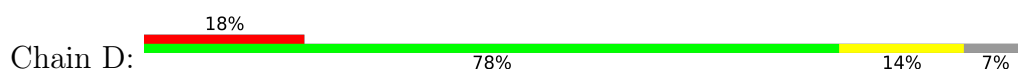


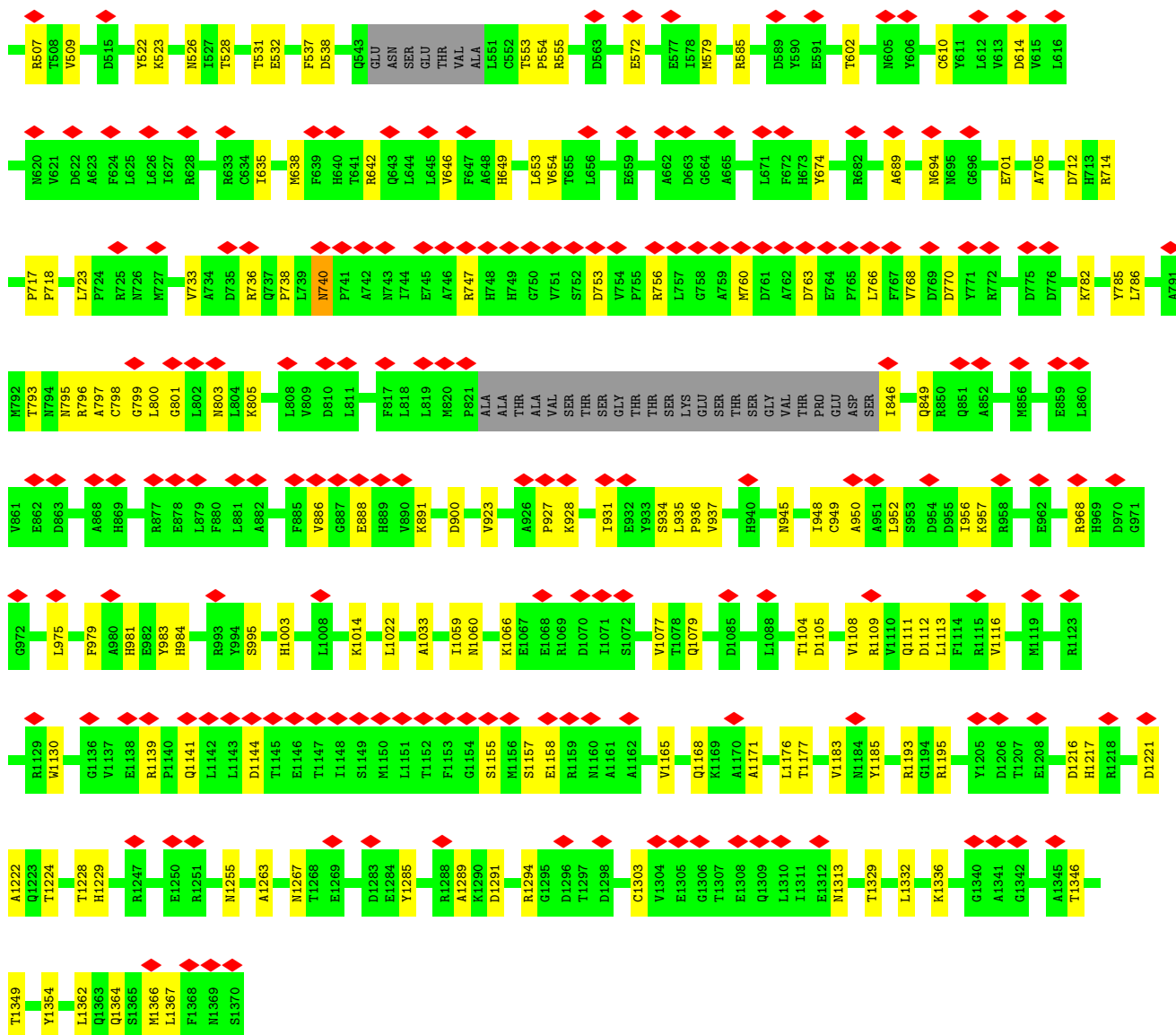
• Molecule 2: Major capsid protein





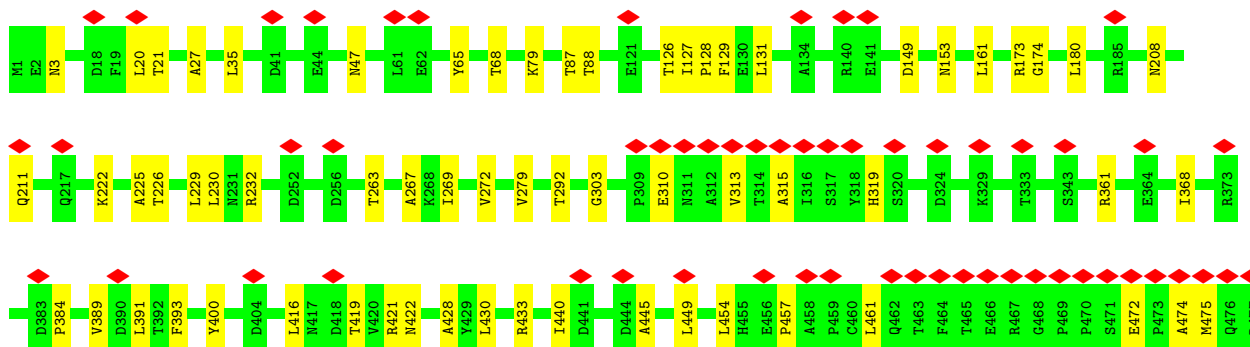
• Molecule 2: Major capsid protein

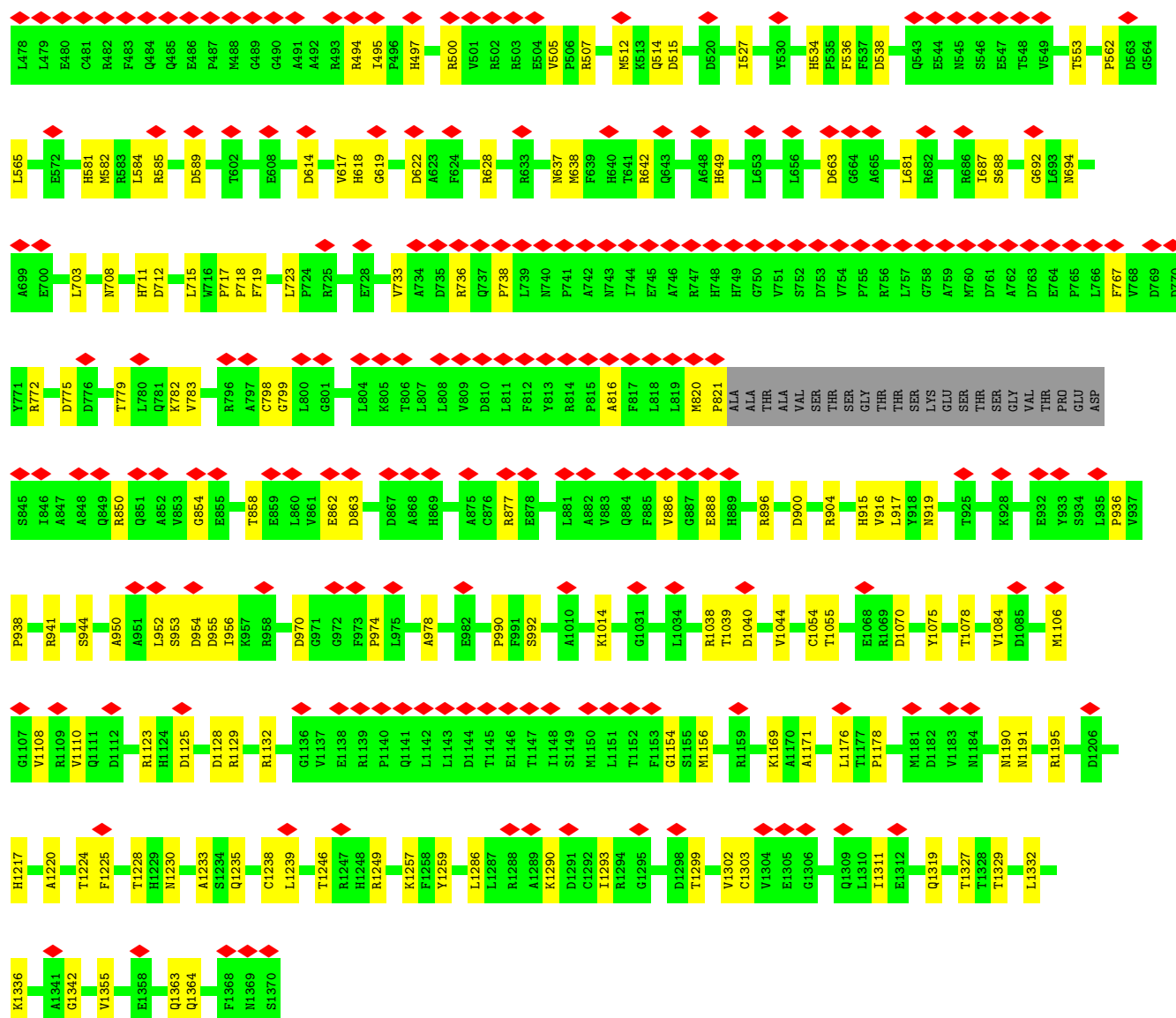




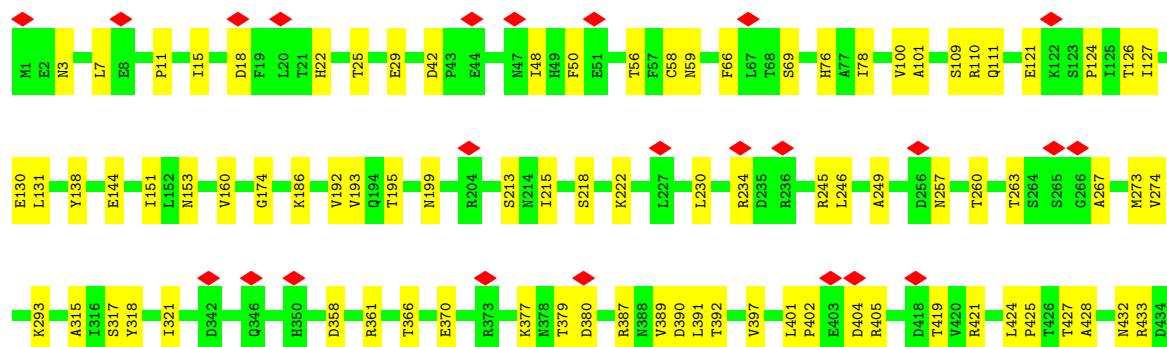
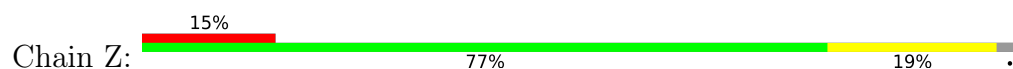
• Molecule 2: Major capsid protein

Chain Y: 19% 83% 15%

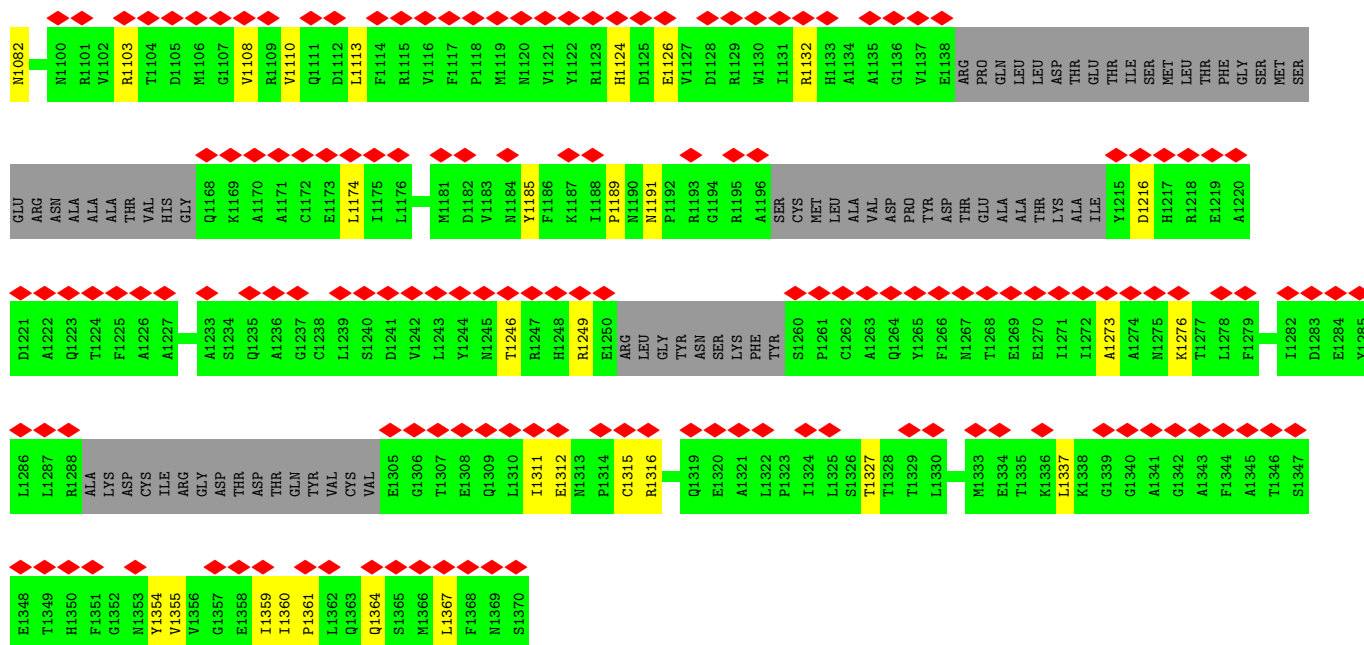




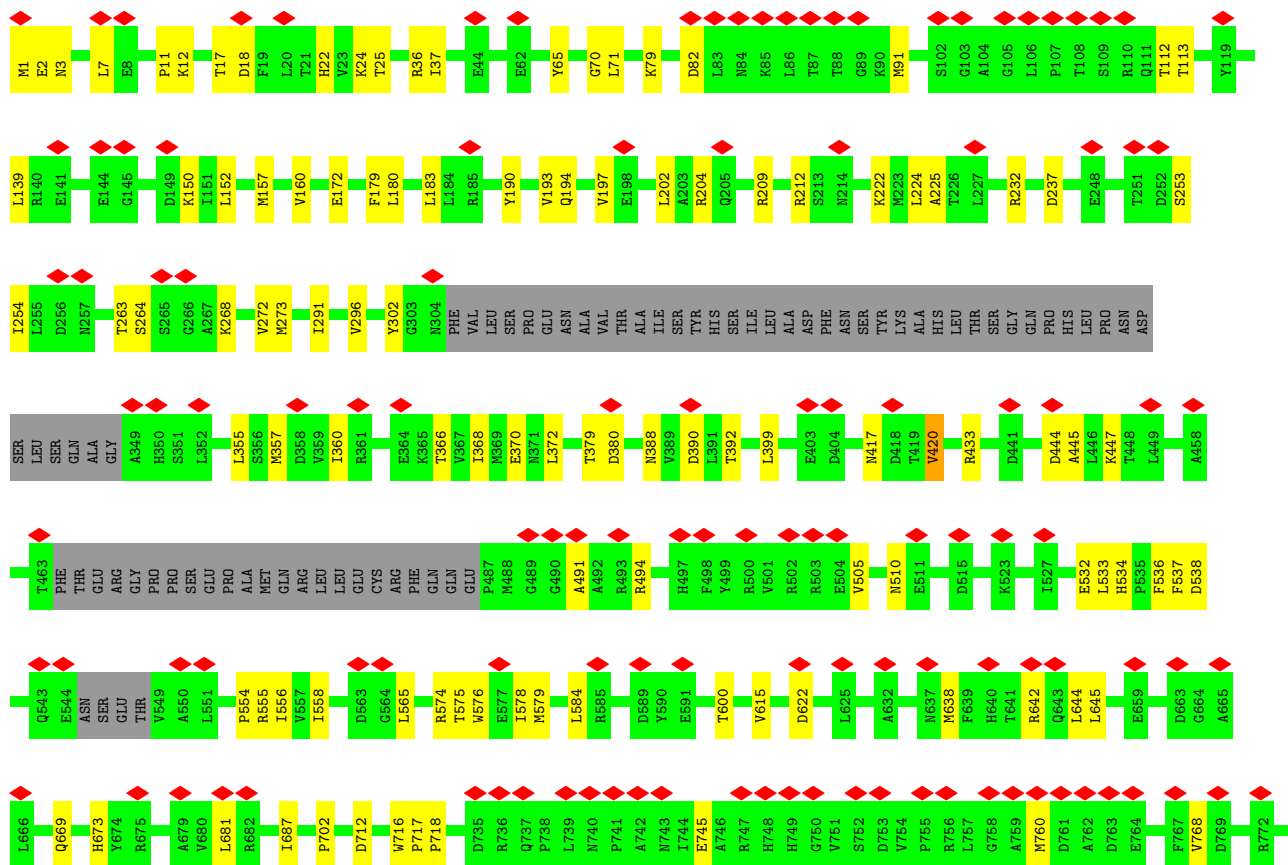
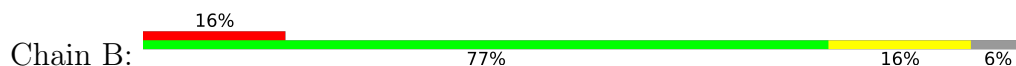
• Molecule 2: Major capsid protein

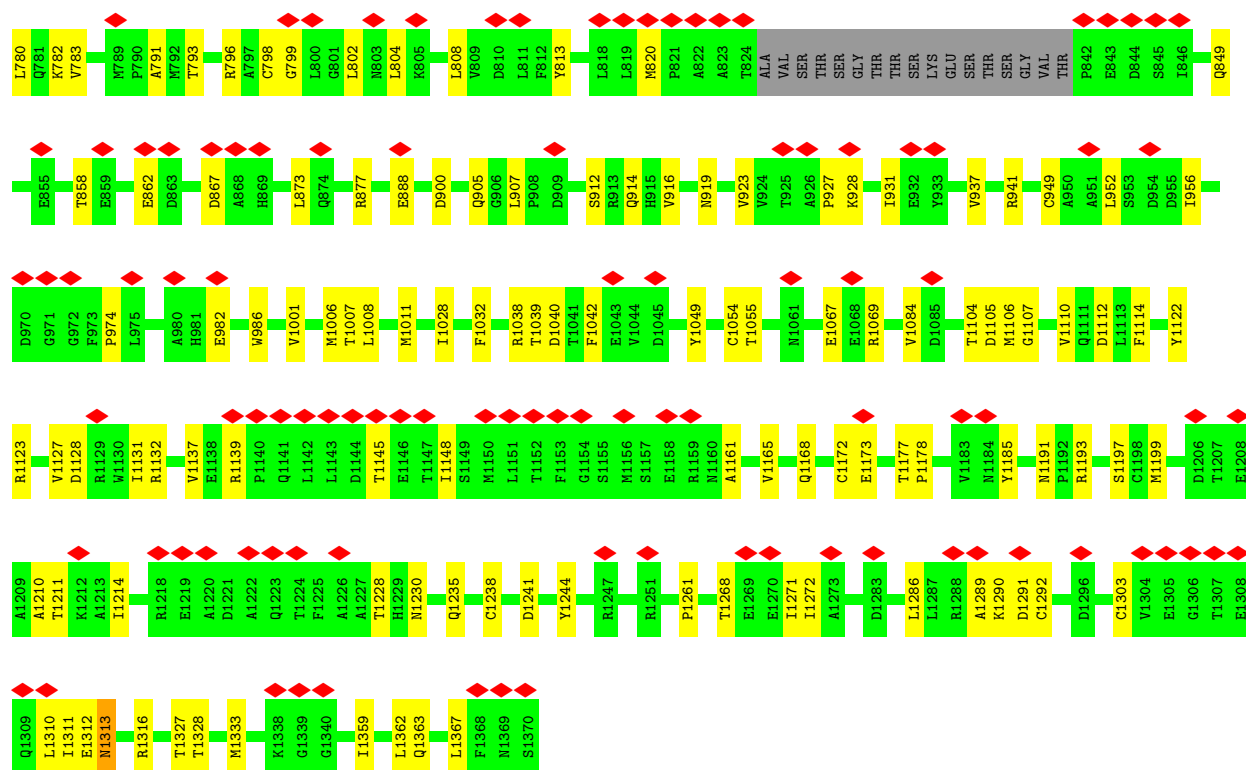




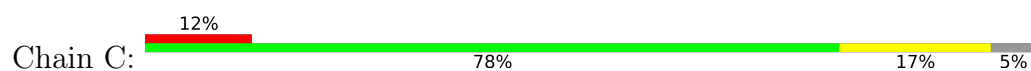


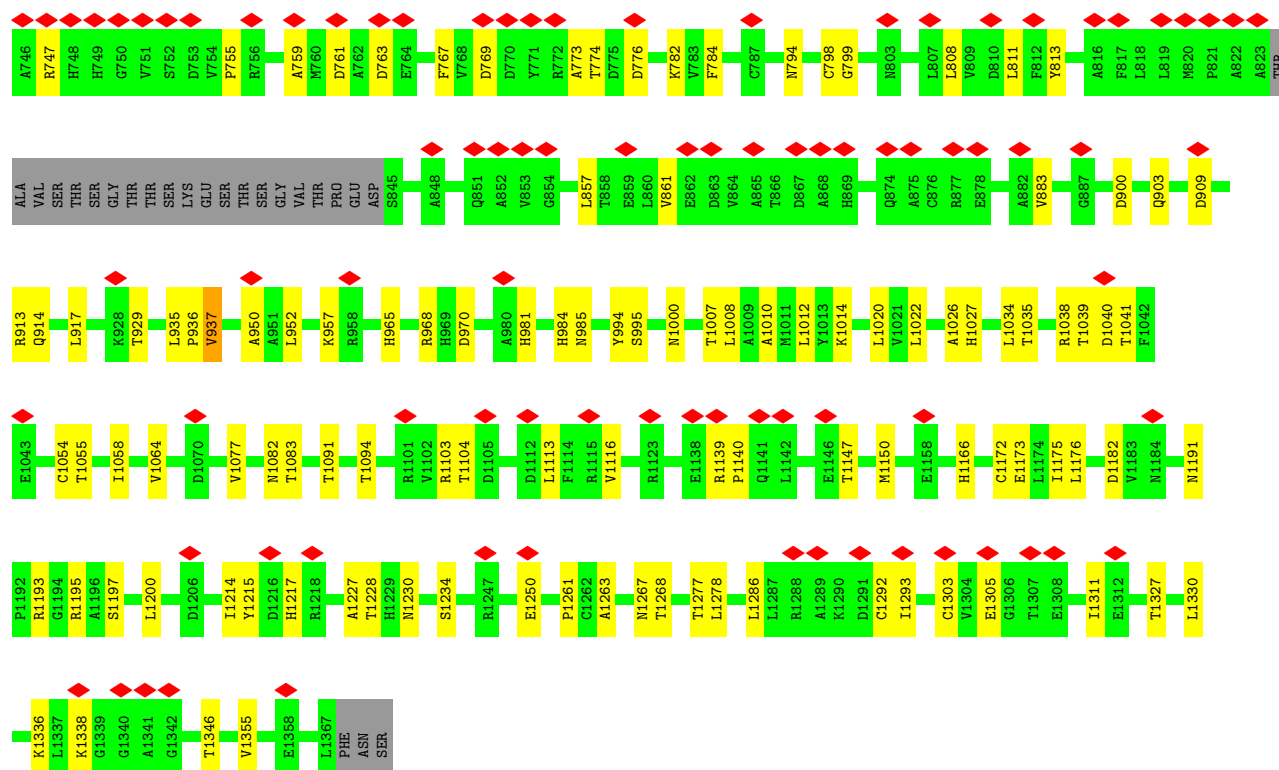
• Molecule 2: Major capsid protein



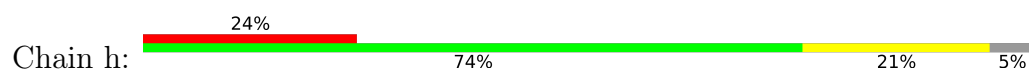


• Molecule 2: Major capsid protein

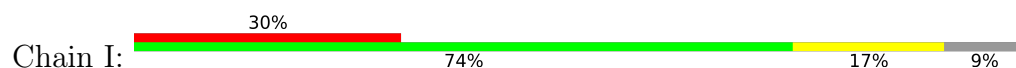


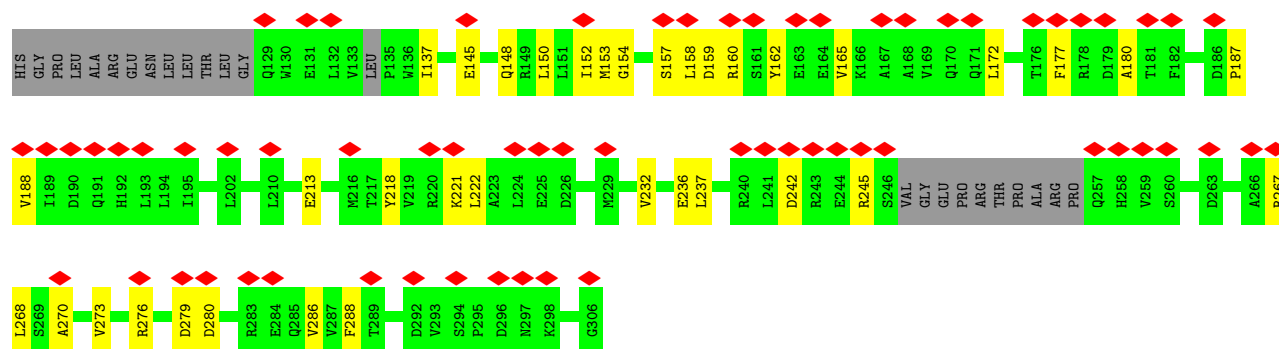


• Molecule 3: Triplex capsid protein 2

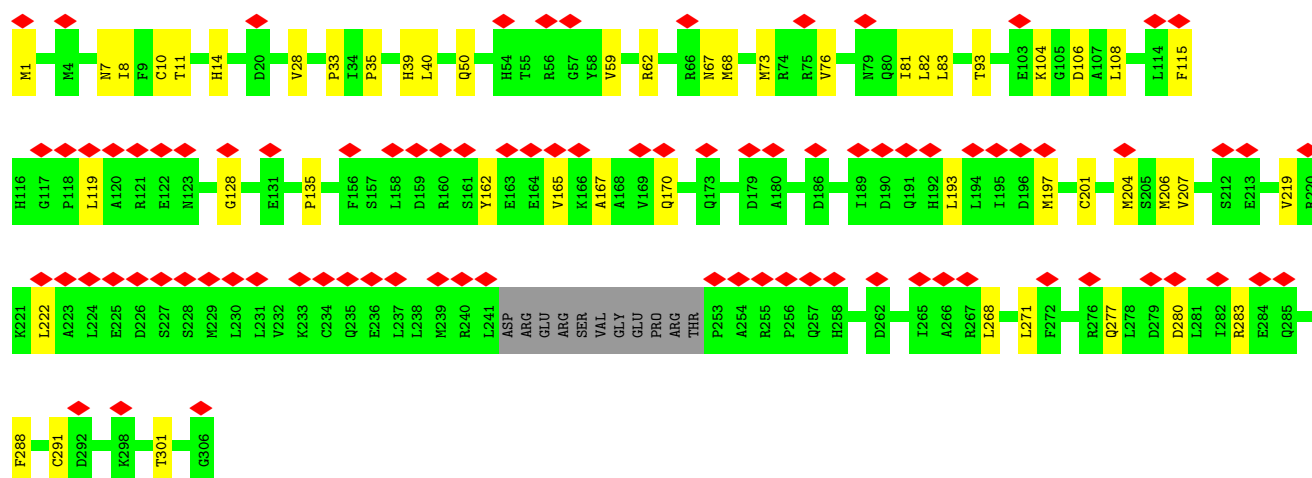
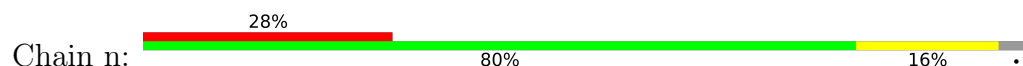


• Molecule 3: Triplex capsid protein 2

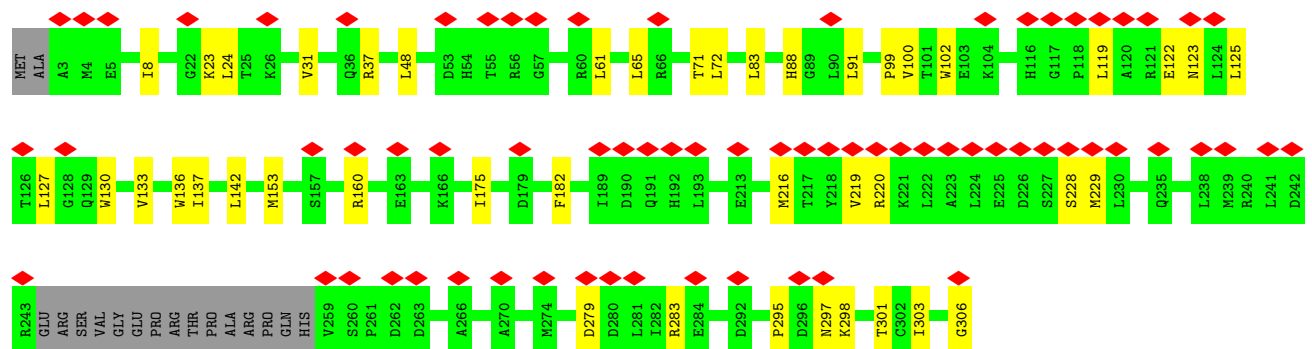
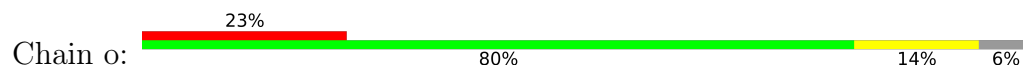




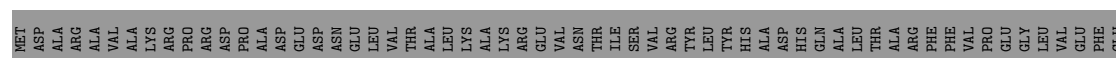
- Molecule 3: Triplex capsid protein 2

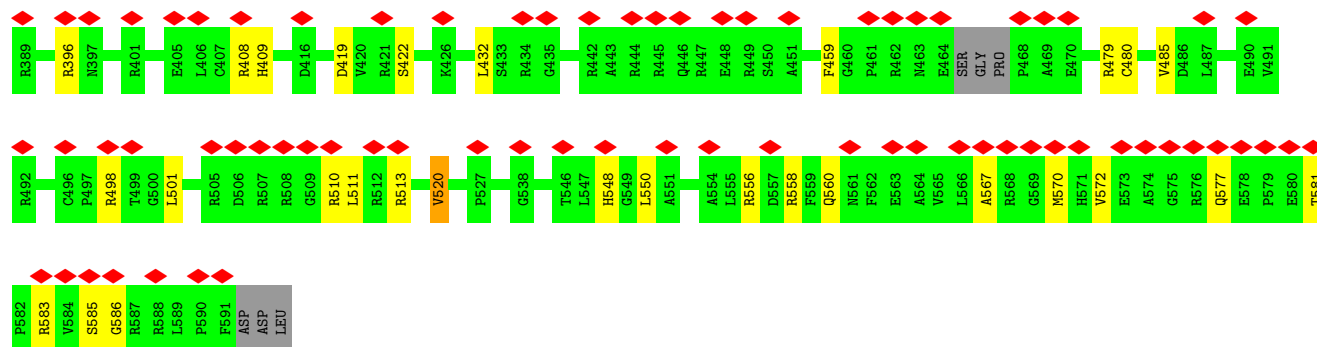


- Molecule 3: Triplex capsid protein 2

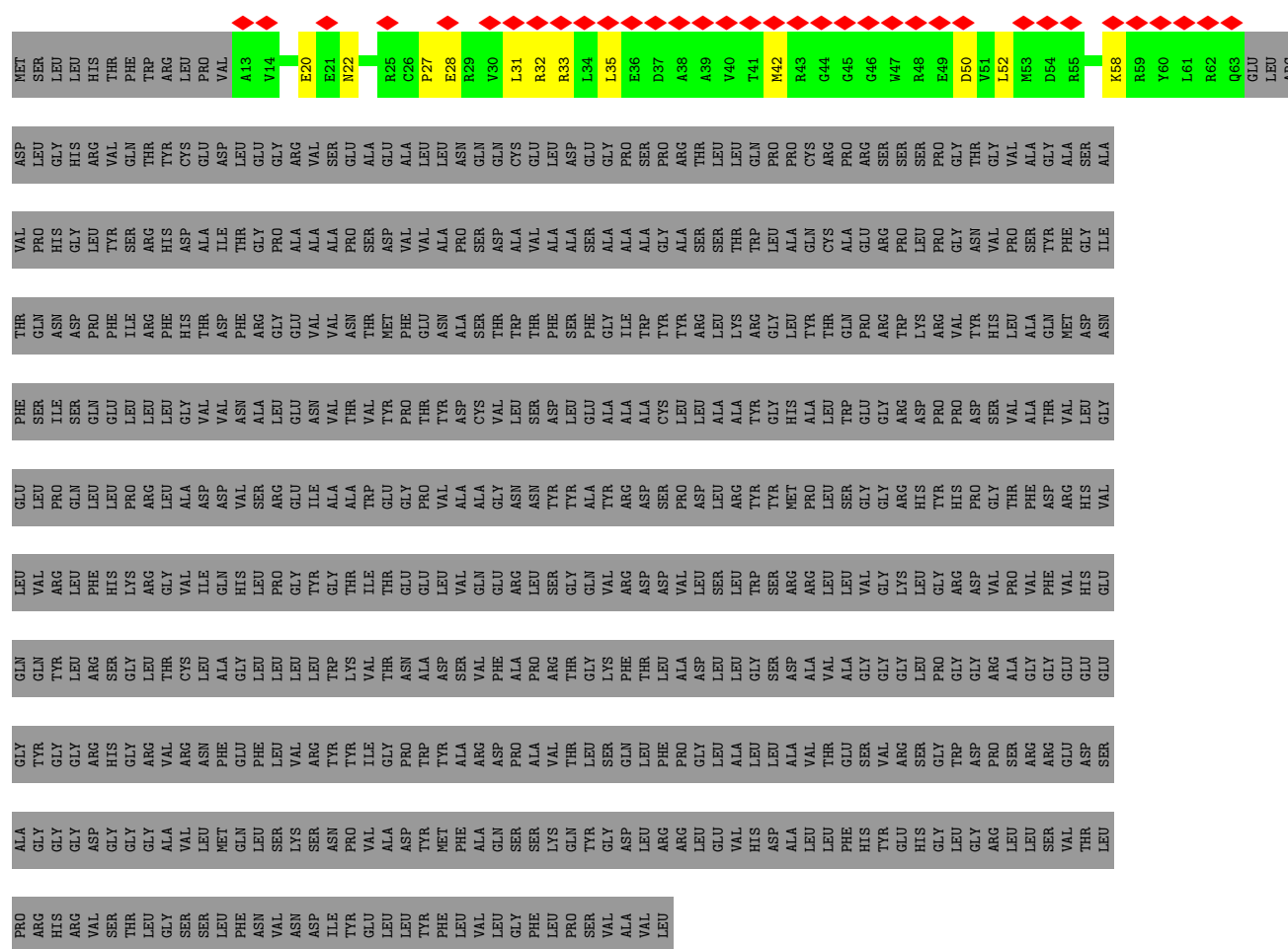


- Molecule 4: Triplex capsid protein 1

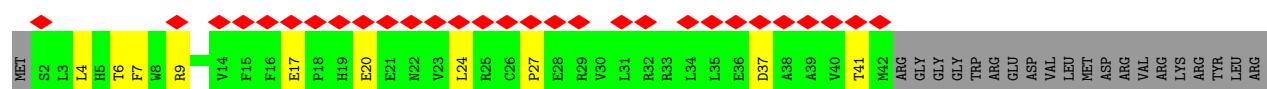




• Molecule 6: Capsid vertex component 2



• Molecule 6: Capsid vertex component 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40903	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.625, 1.625, 1.625	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	Q	0.17	0/356	0.48	0/475
1	R	0.20	0/441	0.54	0/594
1	S	0.20	0/441	0.56	0/594
1	T	0.20	0/193	0.56	0/254
1	i	0.19	0/452	0.49	0/609
1	j	0.18	0/474	0.48	0/638
2	A	0.22	0/9319	0.55	0/12686
2	B	0.27	0/10403	0.57	3/14166 (0.0%)
2	C	0.26	0/10533	0.54	0/14346
2	D	0.25	0/10292	0.53	2/14019 (0.0%)
2	Y	0.25	0/10932	0.55	2/14892 (0.0%)
2	Z	0.26	0/10750	0.53	3/14644 (0.0%)
2	a	0.27	0/10365	0.55	0/14122
3	I	0.23	0/2248	0.56	0/3046
3	h	0.25	0/2348	0.58	0/3189
3	n	0.25	0/2379	0.54	0/3230
3	o	0.24	0/2333	0.52	0/3167
4	g	0.20	0/951	0.49	0/1288
4	m	0.26	0/2374	0.58	0/3221
5	M	0.24	0/3900	0.63	2/5284 (0.0%)
6	N	0.25	0/439	0.76	2/588 (0.3%)
6	O	0.22	0/353	0.64	0/480
All	All	0.25	0/92276	0.55	14/125532 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	D	0	1
2	Y	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	M	0	2
All	All	0	5

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	1127	VAL	N-CA-C	-7.33	106.34	113.53
2	Z	753	ASP	CA-C-N	6.35	124.24	120.24
2	Z	753	ASP	C-N-CA	6.35	124.24	120.24
6	N	28	GLU	CA-C-N	6.31	133.60	121.54
6	N	28	GLU	C-N-CA	6.31	133.60	121.54
2	B	1127	VAL	N-CA-C	-5.84	107.17	111.90
2	B	760	MET	CA-C-N	5.46	135.82	126.32
2	B	760	MET	C-N-CA	5.46	135.82	126.32
2	Y	944	SER	CA-C-N	5.42	128.37	120.51
2	Y	944	SER	C-N-CA	5.42	128.37	120.51
5	M	498	ARG	CA-C-N	5.20	129.79	122.46
5	M	498	ARG	C-N-CA	5.20	129.79	122.46
2	D	760	MET	CA-C-N	5.04	131.17	121.54
2	D	760	MET	C-N-CA	5.04	131.17	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1303	CYS	Peptide
2	D	585	ARG	Peptide
5	M	511	LEU	Peptide
5	M	66	ALA	Peptide
2	Y	585	ARG	Peptide

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	Q	352	0	373	3	0
1	R	436	0	463	7	0
1	S	436	0	463	5	0
1	T	192	0	207	0	0
1	i	446	0	470	8	0
1	j	467	0	490	5	0
2	A	9105	0	9096	99	0
2	B	10164	0	10131	148	0
2	C	10291	0	10265	152	0
2	D	10054	0	10026	123	0
2	Y	10676	0	10618	131	0
2	Z	10498	0	10431	179	0
2	a	10125	0	10087	159	0
3	I	2209	0	2289	36	0
3	h	2304	0	2391	48	0
3	n	2334	0	2431	34	0
3	o	2291	0	2383	25	0
4	g	929	0	922	12	0
4	m	2325	0	2363	39	0
5	M	3813	0	3741	52	0
6	N	432	0	436	10	0
6	O	344	0	346	6	0
All	All	90223	0	90422	1175	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 6.

All (1175) 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:C:324:ASP:HB2	2:C:343:SER:HB3	1.73	0.71
5:M:170:ARG:HB3	5:M:315:ARG:HH22	1.57	0.70
2:Z:144:GLU:H	4:m:36:ARG:HH21	1.40	0.69
2:Y:820:MET:HE3	2:Y:821:PRO:HD2	1.76	0.67
2:A:553:THR:HG21	2:A:983:TYR:HB3	1.76	0.66
2:Z:574:ARG:HG3	2:Z:1028:ILE:HD11	1.77	0.66
4:m:142:ILE:HG21	2:C:1305:GLU:HB3	1.78	0.66
2:Z:1324:ILE:HD11	2:Z:1363:GLN:HE21	1.61	0.65
2:Y:581:HIS:ND1	2:Y:582:MET:SD	2.69	0.65
3:h:209:ASN:HB2	3:I:237:LEU:HD21	1.79	0.65
2:A:778:TRP:HA	2:A:781:GLN:HE21	1.62	0.65
2:A:1312:GLU:HB3	2:A:1315:CYS:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1139:ARG:HE	2:C:1140:PRO:HD2	1.62	0.65
3:I:75:ARG:HB2	3:I:82:LEU:HD12	1.79	0.64
2:Y:798:CYS:SG	2:Y:799:GLY:N	2.70	0.64
6:N:32:ARG:HH22	6:N:33:ARG:HE	1.45	0.64
2:B:388:ASN:HB2	2:B:1311:ILE:HD12	1.79	0.63
4:m:179:ARG:HD2	4:m:183:GLN:HE22	1.64	0.63
2:Y:534:HIS:HD2	2:Y:536:PHE:H	1.44	0.63
4:m:188:ILE:HG12	4:m:248:ILE:HG12	1.80	0.63
2:A:630:PHE:HA	2:A:633:ARG:HH21	1.64	0.63
3:n:1:MET:SD	4:m:181:ARG:NH1	2.72	0.63
2:Y:638:MET:SD	2:Y:642:ARG:NH2	2.72	0.62
3:I:232:VAL:HG22	5:M:6:TYR:HB2	1.80	0.62
2:C:575:THR:HG21	2:C:1007:THR:HA	1.80	0.62
2:C:433:ARG:HH12	2:C:1166:HIS:HA	1.64	0.62
2:B:681:LEU:HD12	2:B:783:VAL:HG13	1.81	0.62
5:M:513:ARG:NH1	6:O:17:GLU:O	2.33	0.61
2:B:858:THR:O	2:B:862:GLU:HB3	1.99	0.61
2:B:291:ILE:HG12	2:B:360:ILE:HG22	1.82	0.61
2:C:798:CYS:SG	2:C:799:GLY:N	2.73	0.61
2:D:416:LEU:HD22	2:D:422:ASN:HD21	1.66	0.61
2:B:1228:THR:HG22	2:B:1230:ASN:H	1.65	0.61
2:C:392:THR:HA	2:C:1039:THR:HA	1.81	0.61
2:a:193:VAL:HG11	2:a:1093:ASN:HD22	1.66	0.61
2:Y:180:LEU:HD23	2:Y:384:PRO:HG2	1.81	0.61
3:o:102:TRP:H	3:o:297:ASN:HD21	1.49	0.61
2:D:58:CYS:SG	2:D:162:ARG:NH1	2.74	0.61
3:n:67:ASN:HD21	4:m:214:THR:HG21	1.66	0.61
2:D:950:ALA:HB1	2:D:957:LYS:HD3	1.83	0.60
2:B:578:ILE:HG12	2:B:1028:ILE:HD12	1.82	0.60
2:Z:895:VAL:HB	2:Z:914:GLN:HB2	1.82	0.60
2:Y:1235:GLN:HB2	2:Y:1238:CYS:HB3	1.83	0.60
2:A:461:LEU:HD13	2:A:552:CYS:HB2	1.84	0.60
2:B:420:VAL:HG11	2:B:576:TRP:HB3	1.83	0.60
2:B:798:CYS:SG	2:B:799:GLY:N	2.73	0.60
2:D:800:LEU:HD22	2:D:923:VAL:HB	1.83	0.60
3:h:37:ARG:HG2	3:h:69:THR:HG21	1.84	0.60
2:a:534:HIS:HD2	2:a:536:PHE:H	1.47	0.60
2:a:768:VAL:HG23	2:a:770:ASP:H	1.67	0.60
4:m:254:CYS:SG	4:m:255:LEU:N	2.75	0.60
2:Y:263:THR:HB	2:Y:267:ALA:H	1.67	0.59
2:B:1007:THR:O	2:B:1011:MET:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:617:VAL:HG13	2:Y:619:GLY:H	1.66	0.59
2:a:122:LYS:NZ	3:h:77:GLU:O	2.35	0.59
2:a:317:SER:O	2:Z:3:ASN:ND2	2.35	0.59
2:Y:1110:VAL:HA	2:Y:1171:ALA:HB3	1.85	0.59
2:Z:56:THR:HG22	2:B:12:LYS:HG3	1.85	0.59
2:a:642:ARG:NH2	2:Z:662:ALA:O	2.36	0.59
2:C:1293:ILE:H	2:C:1311:ILE:HD13	1.67	0.59
1:j:34:GLU:HG2	1:j:44:LEU:HD11	1.83	0.59
2:Z:138:TYR:O	2:Z:153:ASN:ND2	2.36	0.59
2:Z:694:ASN:HD22	2:Z:704:SER:HB2	1.67	0.59
2:B:575:THR:HG21	2:B:1007:THR:HA	1.84	0.58
2:D:1155:SER:HA	2:D:1255:ASN:HD21	1.68	0.58
2:B:804:LEU:O	2:B:808:LEU:HB2	2.03	0.58
2:C:241:LYS:HG3	2:C:245:ARG:HH21	1.68	0.58
2:Y:618:HIS:NE2	2:Y:886:VAL:O	2.36	0.58
2:Y:915:HIS:NE2	2:Y:978:ALA:O	2.35	0.58
2:A:890:VAL:HA	2:A:919:ASN:HB3	1.85	0.58
2:B:433:ARG:NH1	2:C:214:ASN:OD1	2.37	0.58
2:B:849:GLN:HB2	2:B:873:LEU:HD23	1.85	0.58
2:a:438:GLN:HE22	2:a:1107:GLY:HA2	1.69	0.58
2:Z:1196:ALA:HB3	2:Z:1222:ALA:HB3	1.84	0.58
2:B:900:ASP:OD1	2:B:900:ASP:N	2.37	0.58
5:M:501:LEU:HD21	6:N:20:GLU:HA	1.86	0.58
4:m:66:LEU:HB3	4:m:84:LEU:HB2	1.86	0.58
2:B:1161:ALA:O	2:C:209:ARG:NH2	2.37	0.58
2:a:1291:ASP:OD2	2:a:1313:ASN:ND2	2.36	0.57
3:h:240:ARG:HG3	3:I:267:ARG:HH21	1.68	0.57
2:Y:970:ASP:OD1	2:Y:970:ASP:N	2.38	0.57
2:a:637:ASN:ND2	2:a:863:ASP:O	2.36	0.57
3:I:177:PHE:HB3	3:I:180:ALA:HB3	1.86	0.57
2:Z:126:THR:HG21	3:n:39:HIS:HD2	1.70	0.57
2:C:747:ARG:NH1	2:C:769:ASP:OD1	2.36	0.57
2:A:357:MET:HE3	2:A:358:ASP:H	1.70	0.57
2:Y:129:PHE:HB2	2:Z:111:GLN:HE21	1.69	0.57
4:g:220:ARG:NH1	4:g:290:VAL:OXT	2.37	0.57
1:Q:66:ARG:NH2	2:A:884:GLN:O	2.37	0.57
2:A:445:ALA:HA	2:A:1110:VAL:HG21	1.85	0.57
2:B:82:ASP:OD1	2:B:82:ASP:N	2.38	0.57
2:D:766:LEU:HD13	2:D:891:LYS:HD2	1.86	0.57
2:Z:1132:ARG:NH2	2:Z:1138:GLU:O	2.38	0.57
4:g:176:GLU:HG3	4:g:178:THR:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:LYS:H	2:B:302:TYR:HB3	1.68	0.57
2:Z:58:CYS:SG	2:Z:59:ASN:N	2.77	0.57
2:A:783:VAL:O	2:A:787:CYS:HB2	2.05	0.57
2:C:225:ALA:O	2:C:232:ARG:NH1	2.38	0.57
2:a:1336:LYS:NZ	2:a:1346:THR:OG1	2.38	0.57
2:Y:1191:ASN:ND2	2:Y:1319:GLN:O	2.38	0.57
2:B:3:ASN:ND2	2:C:317:SER:O	2.36	0.57
2:B:390:ASP:HB2	2:B:1313:ASN:HB3	1.86	0.57
2:B:1211:THR:HA	2:B:1214:ILE:HG22	1.86	0.57
2:a:968:ARG:NH1	2:Z:694:ASN:O	2.38	0.56
2:C:215:ILE:HG21	2:C:1278:LEU:HD11	1.87	0.56
2:B:392:THR:HG22	2:B:1039:THR:HG22	1.87	0.56
2:C:375:VAL:HG13	2:C:376:TYR:HD1	1.70	0.56
3:I:31:VAL:HG21	3:I:137:ILE:HD11	1.87	0.56
4:g:183:GLN:NE2	4:g:208:SER:OG	2.38	0.56
2:A:557:VAL:HA	2:A:1014:LYS:HA	1.87	0.56
2:B:532:GLU:OE1	2:B:555:ARG:NH2	2.39	0.56
2:B:1132:ARG:HD3	2:B:1139:ARG:HG2	1.87	0.56
2:C:291:ILE:HG12	2:C:360:ILE:HG22	1.86	0.56
2:C:534:HIS:HD2	2:C:536:PHE:H	1.51	0.56
2:Y:208:ASN:OD1	2:Y:211:GLN:NE2	2.38	0.56
2:Z:1292:CYS:HB3	2:Z:1310:LEU:HD13	1.86	0.56
2:C:811:LEU:HD21	2:C:857:LEU:HD13	1.88	0.56
2:a:589:ASP:OD1	2:a:589:ASP:N	2.38	0.56
2:Z:532:GLU:OE1	2:Z:555:ARG:NH1	2.38	0.56
3:n:108:LEU:HB2	3:n:288:PHE:HB2	1.87	0.56
5:M:23:LEU:HD11	5:M:134:LEU:HD23	1.88	0.56
2:a:446:LEU:HD21	2:a:1024:THR:HG21	1.87	0.56
2:a:202:LEU:O	2:a:204:ARG:NH1	2.39	0.56
2:Y:1329:THR:HG23	2:Y:1332:LEU:H	1.70	0.56
3:h:108:LEU:HD22	3:h:137:ILE:HG22	1.88	0.56
2:B:1122:TYR:HB2	2:B:1128:ASP:HB3	1.88	0.56
5:M:27:LEU:HB3	5:M:31:VAL:HG21	1.88	0.56
2:a:798:CYS:SG	2:a:799:GLY:N	2.79	0.56
2:A:850:ARG:HA	2:A:858:THR:HG21	1.88	0.56
2:B:1327:THR:HG21	2:B:1333:MET:HB2	1.86	0.56
5:M:48:VAL:HG13	5:M:146:THR:HG23	1.87	0.56
2:D:756:ARG:NH2	2:D:886:VAL:O	2.38	0.56
2:Z:667:PRO:HD2	2:Z:670:LEU:HD23	1.89	0.55
3:I:108:LEU:HB2	3:I:288:PHE:HB2	1.86	0.55
3:n:283:ARG:NH1	3:o:279:ASP:OD2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:533:LEU:HB3	2:B:1235:GLN:HE21	1.71	0.55
2:D:1336:LYS:NZ	2:D:1346:THR:OG1	2.40	0.55
1:S:62:LEU:HD11	2:C:808:LEU:HB3	1.88	0.55
2:Y:1054:CYS:SG	2:Y:1055:THR:N	2.79	0.55
2:Z:377:LYS:NZ	2:B:17:THR:O	2.40	0.55
2:B:579:MET:HE2	2:B:1006:MET:HG2	1.88	0.55
2:B:669:GLN:O	2:B:673:HIS:ND1	2.37	0.55
2:B:1038:ARG:NH1	2:B:1107:GLY:O	2.39	0.55
2:D:654:VAL:HG13	2:D:674:TYR:HD1	1.72	0.55
2:B:712:ASP:O	2:B:782:LYS:NZ	2.39	0.55
2:D:798:CYS:SG	2:D:799:GLY:N	2.80	0.55
2:Y:904:ARG:O	2:Y:1123:ARG:NH2	2.40	0.55
3:I:109:CYS:SG	3:I:110:VAL:N	2.79	0.55
3:n:104:LYS:NZ	3:n:291:CYS:O	2.40	0.55
3:n:268:LEU:HD13	3:n:271:LEU:HD23	1.89	0.55
2:B:716:TRP:H	2:B:914:GLN:HE22	1.55	0.55
2:C:641:THR:HG23	2:C:642:ARG:HG3	1.89	0.55
2:a:293:LYS:HD2	2:a:358:ASP:HB3	1.88	0.55
2:D:491:ALA:HA	2:D:494:ARG:HB2	1.88	0.55
2:Y:230:LEU:HD22	2:Y:279:VAL:HG23	1.88	0.55
2:A:1064:VAL:HG12	2:A:1077:VAL:HG22	1.88	0.55
2:B:273:MET:HB3	2:B:1049:TYR:HB2	1.89	0.55
2:Y:500:ARG:NH1	2:Y:955:ASP:OD2	2.40	0.55
3:I:77:GLU:OE1	3:I:79:ASN:ND2	2.39	0.55
2:B:237:ASP:OD1	2:B:237:ASP:N	2.40	0.55
2:a:1044:VAL:HG12	2:a:1099:VAL:HG12	1.88	0.55
2:D:610:CYS:O	2:D:614:ASP:HB2	2.07	0.55
3:h:109:CYS:HA	3:h:287:VAL:HG22	1.89	0.55
2:C:1191:ASN:ND2	2:C:1197:SER:OG	2.39	0.55
2:D:949:CYS:HB3	2:D:956:ILE:HD13	1.88	0.55
2:B:1327:THR:OG1	2:B:1328:THR:N	2.39	0.55
5:M:46:ARG:HE	5:M:148:HIS:HD2	1.53	0.55
2:Z:1095:CYS:SG	2:Z:1096:VAL:N	2.80	0.54
2:B:745:GLU:HB3	2:B:768:VAL:HG22	1.89	0.54
1:j:72:ARG:NH2	2:a:820:MET:O	2.41	0.54
2:a:495:ILE:HD13	2:a:937:VAL:HG12	1.89	0.54
2:a:1155:SER:HG	2:a:1255:ASN:HD21	1.52	0.54
2:D:1228:THR:OG1	2:D:1229:HIS:N	2.41	0.54
2:Y:3:ASN:ND2	2:Z:317:SER:O	2.40	0.54
2:Z:581:HIS:ND1	2:Z:582:MET:SD	2.80	0.54
2:C:950:ALA:HB1	2:C:957:LYS:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:115:MET:HB2	2:B:36:ARG:HB3	1.90	0.54
2:a:1124:HIS:HB3	2:a:1127:VAL:HG12	1.89	0.54
2:a:1150:MET:O	3:h:36:GLN:NE2	2.34	0.54
2:a:1324:ILE:HD11	2:a:1363:GLN:HE21	1.72	0.54
2:Y:225:ALA:O	2:Y:232:ARG:NH1	2.40	0.54
2:A:1189:PRO:HG3	2:A:1359:ILE:HG21	1.90	0.54
2:Y:472:GLU:HG3	2:Y:474:ALA:H	1.72	0.54
2:C:1035:THR:HG22	2:C:1176:LEU:HB2	1.87	0.54
2:a:905:GLN:O	2:a:1123:ARG:NH1	2.41	0.54
2:A:981:HIS:HB3	2:A:984:HIS:HB2	1.89	0.54
2:C:275:SER:OG	2:C:276:THR:N	2.41	0.54
2:C:716:TRP:H	2:C:914:GLN:HE22	1.55	0.54
2:a:747:ARG:NH2	2:a:767:PHE:O	2.38	0.54
2:Z:379:THR:O	2:B:22:HIS:NE2	2.38	0.54
2:Z:454:LEU:HD13	2:Z:1239:LEU:HD11	1.90	0.54
3:h:17:SER:OG	3:h:20:ASP:OD1	2.26	0.54
6:O:37:ASP:O	6:O:41:THR:OG1	2.25	0.54
2:a:968:ARG:NH2	2:Z:691:PRO:O	2.41	0.54
3:o:175:ILE:HG23	3:o:182:PHE:HB3	1.89	0.54
4:m:258:ASP:HB2	4:m:277:ASP:HB3	1.90	0.54
2:a:424:LEU:HD12	2:a:425:PRO:HD2	1.89	0.54
2:a:1239:LEU:O	2:a:1243:LEU:HB2	2.07	0.54
2:Z:1234:SER:OG	2:Z:1235:GLN:NE2	2.40	0.54
2:A:787:CYS:HB3	2:A:1005:VAL:HG13	1.90	0.54
2:B:202:LEU:HD11	2:B:204:ARG:HE	1.71	0.54
2:B:225:ALA:O	2:B:232:ARG:NH1	2.41	0.54
1:j:24:VAL:O	1:j:57:LYS:NZ	2.41	0.54
2:D:927:PRO:HD2	2:D:952:LEU:HD21	1.90	0.54
2:Y:20:LEU:HG	2:Y:21:THR:HG23	1.90	0.54
2:Y:584:LEU:HD12	2:Y:687:ILE:HD12	1.90	0.54
2:Y:628:ARG:NH2	2:Y:663:ASP:OD2	2.40	0.54
2:Z:379:THR:OG1	2:Z:380:ASP:N	2.39	0.54
2:Z:575:THR:HG21	2:Z:1007:THR:HA	1.90	0.54
2:D:763:ASP:OD1	2:D:763:ASP:N	2.41	0.53
2:Z:263:THR:HB	2:Z:267:ALA:HB3	1.90	0.53
3:o:153:MET:O	3:o:160:ARG:NH1	2.39	0.53
2:Y:1156:MET:HG3	2:Y:1257:LYS:HD3	1.89	0.53
3:h:152:ILE:HD12	3:I:268:LEU:HB3	1.90	0.53
3:o:91:LEU:HA	3:o:303:ILE:HA	1.90	0.53
4:m:90:ARG:HH22	4:m:199:ARG:HA	1.73	0.53
2:C:713:HIS:ND1	2:C:726:ASN:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:714:ARG:NH1	2:C:900:ASP:OD1	2.40	0.53
6:N:50:ASP:OD1	6:N:50:ASP:N	2.39	0.53
2:a:646:VAL:O	2:a:674:TYR:OH	2.25	0.53
2:a:965:HIS:NE2	2:Z:697:GLN:OE1	2.42	0.53
2:D:800:LEU:HD12	2:D:934:SER:HB2	1.90	0.53
2:C:421:ARG:NH2	2:C:1027:HIS:O	2.40	0.53
2:C:663:ASP:OD1	2:C:663:ASP:N	2.40	0.53
2:a:111:GLN:NE2	2:Z:130:GLU:O	2.41	0.53
3:I:157:SER:HA	3:I:160:ARG:HE	1.73	0.53
3:n:291:CYS:SG	3:o:37:ARG:NH2	2.82	0.53
1:S:24:VAL:HG13	1:S:25:VAL:HG23	1.91	0.53
2:B:927:PRO:HD2	2:B:952:LEU:HD11	1.90	0.53
2:D:139:LEU:HD22	2:D:160:VAL:HG21	1.91	0.53
2:Z:193:VAL:HG11	2:Z:1093:ASN:HD22	1.74	0.53
3:h:59:VAL:HG22	3:h:150:LEU:HD21	1.89	0.53
2:A:232:ARG:HH21	2:A:1360:ILE:HB	1.73	0.53
2:D:1195:ARG:NH2	2:D:1216:ASP:O	2.41	0.53
2:Z:29:GLU:OE1	2:C:1277:THR:OG1	2.26	0.53
2:C:574:ARG:NH2	2:C:1010:ALA:O	2.41	0.53
2:D:701:GLU:OE1	2:D:714:ARG:NH1	2.42	0.53
4:m:91:ALA:O	4:m:99:ARG:NH2	2.42	0.53
2:A:587:PRO:HD3	2:A:683:LEU:HD13	1.90	0.53
2:C:1336:LYS:NZ	2:C:1346:THR:OG1	2.41	0.53
2:D:100:VAL:HG12	2:C:173:ARG:HB3	1.91	0.53
2:B:510:ASN:ND2	2:B:538:ASP:OD2	2.41	0.53
2:D:83:LEU:HD23	2:D:1060:ASN:HB3	1.91	0.53
2:a:130:GLU:HG2	2:a:1074:THR:HG22	1.91	0.53
2:Y:900:ASP:N	2:Y:900:ASP:OD1	2.42	0.53
2:Z:1199:MET:HB3	2:Z:1275:ASN:HB3	1.90	0.53
4:m:185:VAL:HG23	4:m:251:LEU:HB3	1.91	0.53
3:I:145:GLU:HA	3:I:148:GLN:HE21	1.74	0.52
2:C:1054:CYS:HG	2:C:1091:THR:HG1	1.54	0.52
2:D:1104:THR:HG23	2:D:1168:GLN:HB2	1.90	0.52
2:Y:775:ASP:N	2:Y:775:ASP:OD1	2.42	0.52
2:Z:1292:CYS:HA	2:Z:1311:ILE:HG12	1.91	0.52
6:O:7:PHE:O	6:O:9:ARG:NH1	2.43	0.52
2:a:1246:THR:HG23	2:a:1267:ASN:HD21	1.74	0.52
2:Y:1342:GLY:H	2:Y:1364:GLN:HE22	1.57	0.52
3:n:167:ALA:O	3:n:170:GLN:NE2	2.36	0.52
4:g:187:LEU:HB2	4:g:251:LEU:HD11	1.90	0.52
5:M:32:LEU:O	5:M:126:TYR:OH	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:816:ALA:O	2:a:877:ARG:NH1	2.42	0.52
2:D:487:PRO:HB3	2:D:736:ARG:HE	1.74	0.52
2:B:1172:CYS:SG	2:B:1173:GLU:N	2.72	0.52
2:B:1290:LYS:HB3	2:B:1310:LEU:HB3	1.91	0.52
2:C:968:ARG:HG3	2:C:970:ASP:H	1.75	0.52
2:C:1228:THR:HG22	2:C:1230:ASN:H	1.73	0.52
2:a:114:ILE:HG12	2:B:37:ILE:HG22	1.91	0.52
2:Y:174:GLY:HA3	2:Z:101:ALA:HB3	1.91	0.52
2:Z:1105:ASP:HB3	2:Z:1166:HIS:HB3	1.91	0.52
2:a:275:SER:HB3	2:a:280:MET:HE2	1.90	0.52
2:a:461:LEU:HD13	2:a:552:CYS:HB2	1.91	0.52
3:h:291:CYS:SG	3:I:37:ARG:NH1	2.82	0.52
2:a:222:LYS:NZ	2:Z:1370:SER:O	2.43	0.52
3:o:88:HIS:ND1	3:o:306:GLY:OXT	2.43	0.52
4:m:131:THR:OG1	4:m:249:GLN:NE2	2.37	0.52
2:A:1060:ASN:ND2	2:A:1061:ASN:O	2.43	0.52
2:C:747:ARG:HE	2:C:767:PHE:HB3	1.74	0.52
2:D:705:ALA:HB1	2:D:712:ASP:HB3	1.91	0.52
3:n:14:HIS:HE1	3:n:128:GLY:HA3	1.75	0.52
2:B:1032:PHE:HA	2:B:1178:PRO:HD3	1.91	0.52
2:Y:622:ASP:N	2:Y:622:ASP:OD1	2.42	0.52
2:B:622:ASP:OD1	2:B:622:ASP:N	2.40	0.52
5:M:345:ASP:N	5:M:345:ASP:OD1	2.42	0.52
2:a:1144:ASP:HB2	2:a:1148:ILE:HG23	1.92	0.52
2:D:95:VAL:HG12	2:C:59:ASN:HB2	1.91	0.52
2:Y:1176:LEU:HD21	2:Y:1233:ALA:HB2	1.91	0.52
2:Z:230:LEU:O	2:Z:234:ARG:NH2	2.43	0.52
2:Z:955:ASP:HA	2:Z:958:ARG:HB2	1.92	0.52
2:Z:274:VAL:HG12	2:Z:370:GLU:HB3	1.92	0.51
3:h:221:LYS:HD3	3:I:158:LEU:HD11	1.92	0.51
3:I:242:ASP:OD1	3:I:245:ARG:NH1	2.43	0.51
3:I:280:ASP:OD2	3:I:280:ASP:N	2.43	0.51
4:m:166:MET:HE1	4:m:275:ARG:HE	1.74	0.51
2:B:1290:LYS:HE3	2:B:1312:GLU:HB3	1.92	0.51
2:C:557:VAL:HG21	2:C:1012:LEU:HD13	1.92	0.51
2:C:1064:VAL:HG22	2:C:1077:VAL:HG12	1.90	0.51
2:D:447:LYS:HE3	2:D:1112:ASP:HB3	1.93	0.51
2:D:1329:THR:HG23	2:D:1332:LEU:H	1.74	0.51
2:Y:953:SER:OG	2:Y:954:ASP:N	2.43	0.51
3:n:219:VAL:HA	3:n:222:LEU:HD12	1.93	0.51
2:A:534:HIS:HD2	2:A:536:PHE:H	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:444:ASP:OD1	2:B:444:ASP:N	2.42	0.51
2:a:1193:ARG:NH2	2:a:1234:SER:O	2.43	0.51
2:Y:723:LEU:HD21	2:Y:772:ARG:HH21	1.74	0.51
2:Z:392:THR:HA	2:Z:1039:THR:HA	1.91	0.51
3:I:108:LEU:HD22	3:I:137:ILE:HG22	1.92	0.51
2:A:261:TYR:HB3	2:A:269:ILE:HD12	1.93	0.51
2:B:70:GLY:N	2:B:370:GLU:OE2	2.40	0.51
5:M:82:PHE:HB2	5:M:556:ARG:HH22	1.75	0.51
2:a:1191:ASN:ND2	2:a:1195:ARG:O	2.39	0.51
2:D:1105:ASP:OD1	2:D:1109:ARG:NH2	2.42	0.51
2:Y:507:ARG:HB2	2:Y:512:MET:HE2	1.92	0.51
3:n:115:PHE:HB2	3:n:119:LEU:HD21	1.92	0.51
4:m:285:ASP:OD1	4:m:285:ASP:N	2.44	0.51
2:B:1199:MET:HE2	2:B:1272:ILE:HA	1.93	0.51
2:a:681:LEU:HB3	2:a:780:LEU:HD22	1.91	0.51
2:a:1001:VAL:HG12	2:a:1003:HIS:H	1.75	0.51
2:Y:208:ASN:HB2	2:Y:211:GLN:HG3	1.93	0.51
2:Y:1129:ARG:O	2:Y:1129:ARG:NH1	2.44	0.51
2:Z:199:ASN:HD22	2:Z:215:ILE:HD13	1.75	0.51
2:B:224:LEU:HD21	2:B:1359:ILE:HG13	1.93	0.51
2:C:763:ASP:OD1	2:C:763:ASP:N	2.43	0.51
2:a:146:THR:O	2:a:150:LYS:NZ	2.39	0.51
2:D:103:GLY:H	2:D:106:LEU:HD12	1.75	0.51
2:Y:269:ILE:HD13	2:Y:368:ILE:HD11	1.93	0.51
2:Z:121:GLU:O	2:Z:1082:ASN:ND2	2.44	0.51
3:h:62:ARG:NH1	3:h:147:ASN:OD1	2.44	0.51
2:A:401:LEU:HD11	2:A:1354:TYR:HB3	1.92	0.51
2:C:717:PRO:HB3	2:C:782:LYS:HA	1.93	0.51
2:D:1060:ASN:O	2:D:1079:GLN:NE2	2.38	0.51
2:Y:736:ARG:HH12	2:Y:896:ARG:HH12	1.59	0.51
2:C:981:HIS:O	2:C:985:ASN:ND2	2.43	0.51
2:a:380:ASP:N	2:a:380:ASP:OD1	2.40	0.51
2:a:490:GLY:HA2	2:a:493:ARG:HH21	1.76	0.51
2:Z:11:PRO:HD3	2:C:332:LEU:HD13	1.93	0.51
2:Z:390:ASP:OD1	2:Z:1039:THR:OG1	2.28	0.51
3:o:127:LEU:HB2	3:o:130:TRP:HB3	1.92	0.51
4:g:188:ILE:HG22	4:g:248:ILE:HG12	1.93	0.51
2:B:1145:THR:HA	2:B:1148:ILE:HG12	1.93	0.51
2:a:424:LEU:HD13	2:a:573:LEU:HD23	1.92	0.50
2:Y:1106:MET:HE3	2:Y:1363:GLN:HE22	1.76	0.50
2:Z:615:VAL:HG21	2:Z:802:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1216:ASP:OD1	2:A:1216:ASP:N	2.44	0.50
2:A:1327:THR:HG23	2:A:1355:VAL:HG12	1.93	0.50
2:B:1172:CYS:HB2	2:B:1261:PRO:HG2	1.93	0.50
5:M:102:GLU:OE2	5:M:121:ARG:NH1	2.40	0.50
2:D:1022:LEU:HD21	2:D:1130:TRP:HH2	1.76	0.50
5:M:171:GLU:OE2	5:M:313:ARG:NH2	2.44	0.50
2:a:420:VAL:HG23	2:a:585:ARG:HE	1.76	0.50
2:a:810:ASP:OD1	2:a:810:ASP:N	2.44	0.50
2:D:796:ARG:O	2:D:945:ASN:ND2	2.45	0.50
2:A:375:VAL:HG13	2:A:376:TYR:HD1	1.75	0.50
2:B:445:ALA:HA	2:B:1110:VAL:HG11	1.93	0.50
2:B:1193:ARG:HH22	2:B:1197:SER:HB3	1.77	0.50
5:M:20:GLN:HE22	5:M:90:GLN:HE22	1.57	0.50
2:a:657:ILE:HA	2:a:661:LEU:HD13	1.93	0.50
2:D:638:MET:SD	2:D:642:ARG:NH1	2.85	0.50
4:m:234:ARG:NH1	4:m:240:GLN:O	2.44	0.50
2:A:448:THR:HG22	2:A:1113:LEU:HB2	1.94	0.50
2:B:554:PRO:HD3	2:B:907:LEU:HD22	1.92	0.50
2:C:556:ILE:HD11	2:C:903:GLN:HE21	1.76	0.50
2:Z:1040:ASP:OD1	2:Z:1104:THR:OG1	2.26	0.50
4:m:35:VAL:HG12	2:C:1064:VAL:HG21	1.93	0.50
2:A:240:LEU:HD12	2:A:287:LEU:HD21	1.92	0.50
2:B:209:ARG:HG3	2:B:212:ARG:HH22	1.75	0.50
2:B:867:ASP:OD1	2:B:867:ASP:N	2.44	0.50
2:B:1289:ALA:HB1	2:B:1316:ARG:HD3	1.93	0.50
2:C:1193:ARG:NH2	2:C:1214:ILE:O	2.41	0.50
2:Y:47:ASN:ND2	3:n:76:VAL:O	2.39	0.50
3:n:280:ASP:OD2	3:o:283:ARG:NH2	2.44	0.50
2:D:718:PRO:HD2	2:D:785:TYR:HB3	1.93	0.50
2:D:1112:ASP:N	2:D:1112:ASP:OD1	2.45	0.50
2:Z:1103:ARG:HH21	2:Z:1168:GLN:HE22	1.57	0.50
3:I:159:ASP:OD1	3:I:159:ASP:N	2.44	0.50
3:I:236:GLU:OE2	5:M:302:ARG:N	2.44	0.50
2:A:442:PHE:HA	2:A:445:ALA:HB3	1.93	0.50
2:B:417:ASN:ND2	2:C:406:GLY:O	2.45	0.50
2:B:1104:THR:OG1	2:B:1105:ASP:N	2.45	0.50
2:C:78:ILE:HB	2:C:1058:ILE:HG22	1.94	0.50
5:M:585:SER:OG	5:M:586:GLY:N	2.45	0.50
1:i:40:LEU:O	1:i:44:LEU:HB2	2.12	0.50
2:a:609:LEU:HD21	2:a:864:VAL:HG11	1.94	0.50
2:Z:1263:ALA:O	2:Z:1267:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:n:8:ILE:HB	3:n:83:LEU:HB2	1.92	0.50
2:C:572:GLU:OE1	2:C:994:TYR:OH	2.29	0.50
2:a:614:ASP:HB3	2:a:653:LEU:HD11	1.93	0.50
2:Z:798:CYS:SG	2:Z:799:GLY:N	2.84	0.50
2:Z:1110:VAL:HA	2:Z:1171:ALA:HB3	1.94	0.50
5:M:344:ASP:OD1	5:M:344:ASP:N	2.41	0.50
2:a:149:ASP:OD1	2:a:149:ASP:N	2.42	0.49
2:Y:1195:ARG:NH1	2:Y:1220:ALA:O	2.45	0.49
2:Z:888:GLU:O	2:Z:919:ASN:ND2	2.45	0.49
3:n:106:ASP:OD1	3:n:106:ASP:N	2.45	0.49
3:n:162:TYR:HA	3:n:165:VAL:HG12	1.94	0.49
2:B:537:PHE:HA	2:B:555:ARG:H	1.77	0.49
2:C:724:PRO:HA	2:C:773:ALA:HB3	1.93	0.49
5:M:41:ARG:NH1	5:M:570:MET:SD	2.85	0.49
3:h:189:ILE:HA	3:h:193:LEU:HD23	1.94	0.49
2:A:1050:SER:OG	2:A:1051:GLY:N	2.45	0.49
2:B:565:LEU:HD22	2:B:1177:THR:HG21	1.94	0.49
2:C:216:LEU:HD13	2:C:1200:LEU:HD23	1.93	0.49
3:n:10:CYS:HB3	3:n:81:ILE:HB	1.93	0.49
3:o:228:SER:OG	3:o:229:MET:N	2.45	0.49
2:C:311:ASN:ND2	2:C:322:LEU:O	2.41	0.49
2:C:1147:THR:OG1	2:C:1150:MET:SD	2.69	0.49
2:a:1239:LEU:O	2:a:1243:LEU:CB	2.59	0.49
2:Z:7:LEU:HD13	2:C:92:LEU:HB3	1.94	0.49
2:C:1172:CYS:SG	2:C:1173:GLU:N	2.85	0.49
2:C:1113:LEU:HA	2:C:1116:VAL:HG12	1.92	0.49
2:a:1195:ARG:NH1	2:a:1227:ALA:O	2.46	0.49
2:Z:655:THR:O	2:Z:659:GLU:HB2	2.12	0.49
2:Z:756:ARG:HH22	2:Z:887:GLY:HA2	1.77	0.49
2:B:1173:GLU:O	2:B:1244:TYR:OH	2.30	0.49
2:C:995:SER:HB2	2:C:1008:LEU:HD11	1.94	0.49
2:C:1182:ASP:N	2:C:1182:ASP:OD1	2.39	0.49
5:M:409:HIS:ND1	5:M:480:CYS:SG	2.81	0.49
2:D:733:VAL:HG12	2:D:738:PRO:HA	1.94	0.49
2:A:87:THR:OG1	2:A:88:THR:N	2.46	0.49
2:A:579:MET:HG2	2:A:584:LEU:HD11	1.94	0.49
2:C:535:PRO:HG3	2:C:1175:ILE:HG21	1.94	0.49
2:Z:186:LYS:NZ	2:Z:1054:CYS:SG	2.82	0.49
2:C:693:LEU:HD11	2:C:1026:ALA:HB2	1.94	0.49
2:a:1154:GLY:HA3	2:a:1257:LYS:HE2	1.95	0.49
2:D:770:ASP:OD1	2:D:770:ASP:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:795:ASN:ND2	2:D:995:SER:OG	2.37	0.49
2:Z:1191:ASN:HD21	2:Z:1193:ARG:HB2	1.78	0.49
2:A:287:LEU:HD23	2:A:360:ILE:HD11	1.95	0.49
2:B:71:LEU:HD11	2:B:180:LEU:HD13	1.94	0.49
5:M:44:TYR:HB2	5:M:150:ARG:HB3	1.95	0.49
2:a:1181:MET:HG3	2:a:1183:VAL:HG12	1.94	0.49
2:D:532:GLU:OE1	2:D:555:ARG:NH1	2.39	0.49
2:Z:599:THR:O	2:Z:603:SER:OG	2.31	0.49
3:h:155:LEU:HG	3:h:197:MET:HE3	1.94	0.49
2:A:714:ARG:O	2:A:914:GLN:NE2	2.34	0.49
2:C:731:GLN:HG2	2:C:740:ASN:HD21	1.77	0.49
2:a:1039:THR:HG23	2:a:1261:PRO:HB3	1.94	0.48
2:a:1262:CYS:HB3	2:a:1266:PHE:HD2	1.78	0.48
2:Z:614:ASP:OD2	2:Z:649:HIS:NE2	2.46	0.48
4:m:75:ASP:O	4:m:78:ARG:NE	2.46	0.48
2:B:702:PRO:HB3	2:C:965:HIS:HB3	1.95	0.48
2:D:182:THR:O	2:D:186:LYS:NZ	2.44	0.48
3:o:23:LYS:NZ	3:o:123:ASN:O	2.38	0.48
1:R:50:MET:N	1:R:50:MET:SD	2.84	0.48
2:a:275:SER:OG	2:a:276:THR:N	2.45	0.48
2:D:435:ARG:NH2	2:D:1364:GLN:OE1	2.43	0.48
2:D:712:ASP:OD1	2:D:712:ASP:N	2.44	0.48
2:D:1185:TYR:OH	2:D:1193:ARG:O	2.31	0.48
2:Y:692:GLY:HA2	2:Z:993:ARG:HH12	1.78	0.48
2:Z:694:ASN:HA	2:Z:703:LEU:HD22	1.95	0.48
2:Z:903:GLN:HE22	2:Z:1014:LYS:HD3	1.78	0.48
2:A:634:CYS:HB2	2:A:864:VAL:HG22	1.94	0.48
2:C:442:PHE:HE1	2:C:1034:LEU:HD23	1.78	0.48
2:C:538:ASP:HB3	2:C:555:ARG:HH21	1.79	0.48
5:M:11:PHE:O	5:M:15:PHE:HB2	2.13	0.48
2:a:812:PHE:HE1	2:a:857:LEU:HD11	1.76	0.48
2:a:1032:PHE:HA	2:a:1178:PRO:HD3	1.95	0.48
2:D:1144:ASP:OD1	2:D:1144:ASP:N	2.46	0.48
2:Y:495:ILE:HG21	2:Y:938:PRO:HD2	1.96	0.48
2:Y:850:ARG:NH2	2:Y:862:GLU:OE2	2.46	0.48
1:R:52:SER:OG	1:R:53:LEU:N	2.47	0.48
2:A:612:LEU:O	2:A:616:LEU:HB2	2.14	0.48
2:a:101:ALA:HB3	2:Z:174:GLY:HA3	1.94	0.48
2:D:646:VAL:O	2:D:674:TYR:OH	2.29	0.48
2:Y:454:LEU:HD22	2:Y:1239:LEU:HD11	1.94	0.48
2:Z:48:ILE:HD11	2:B:152:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:437:VAL:HG21	2:Z:1330:LEU:HD21	1.96	0.48
3:n:204:MET:HA	3:n:207:VAL:HG12	1.95	0.48
2:A:243:LEU:HB3	2:A:362:LEU:HD21	1.96	0.48
2:A:663:ASP:N	2:A:663:ASP:OD1	2.46	0.48
5:M:4:HIS:ND1	5:M:331:TYR:OH	2.41	0.48
2:a:66:PHE:HA	2:a:176:ILE:HD11	1.96	0.48
2:D:801:GLY:O	2:D:935:LEU:N	2.45	0.48
2:D:1059:ILE:HB	2:D:1079:GLN:HE21	1.78	0.48
2:Y:126:THR:HG22	2:Y:1078:THR:HG23	1.95	0.48
2:A:507:ARG:HG3	2:A:511:GLU:HB2	1.95	0.48
3:n:277:GLN:HG2	4:m:290:VAL:HB	1.95	0.48
2:A:958:ARG:HA	2:A:961:THR:HG22	1.94	0.48
2:C:532:GLU:OE2	2:C:555:ARG:NH2	2.36	0.48
2:C:632:ALA:HB2	2:C:661:LEU:HD11	1.96	0.48
2:D:740:ASN:OD1	2:D:740:ASN:N	2.35	0.48
2:Y:1128:ASP:OD1	2:Y:1132:ARG:NH2	2.47	0.48
2:Y:1217:HIS:ND1	2:Y:1228:THR:OG1	2.38	0.48
2:Z:941:ARG:NH2	2:Z:982:GLU:OE1	2.46	0.48
2:Z:968:ARG:HE	2:Z:972:GLY:HA3	1.78	0.48
2:A:1246:THR:HA	2:A:1249:ARG:HG2	1.95	0.48
2:B:1165:VAL:HG23	2:C:216:LEU:HD23	1.96	0.48
2:Z:874:GLN:HA	2:Z:877:ARG:HG3	1.95	0.48
4:g:250:LYS:HZ3	4:g:284:GLY:HA3	1.79	0.48
2:B:112:THR:HG23	2:B:113:THR:HG23	1.96	0.48
2:B:1128:ASP:N	2:B:1128:ASP:OD2	2.44	0.48
2:D:1113:LEU:HA	2:D:1116:VAL:HG22	1.96	0.48
2:Y:1327:THR:HG22	2:Y:1355:VAL:HG22	1.96	0.48
2:Z:1285:TYR:HA	2:Z:1289:ALA:HB3	1.95	0.48
4:g:169:LYS:HG3	4:g:273:VAL:HA	1.96	0.48
2:a:1222:ALA:HB1	2:Z:1165:VAL:HG22	1.95	0.47
2:D:717:PRO:HB3	2:D:782:LYS:HA	1.95	0.47
2:Z:558:ILE:HB	2:Z:1015:ILE:HD11	1.96	0.47
2:Z:785:TYR:O	2:Z:943:TYR:OH	2.30	0.47
2:A:403:GLU:OE2	2:A:422:ASN:ND2	2.47	0.47
2:B:556:ILE:HD11	2:B:986:TRP:HA	1.96	0.47
2:a:1144:ASP:OD1	2:a:1144:ASP:N	2.46	0.47
2:Z:218:SER:OG	2:Z:222:LYS:NZ	2.46	0.47
3:h:305:LYS:NZ	3:h:306:GLY:OXT	2.47	0.47
2:C:493:ARG:NH2	2:C:761:ASP:OD1	2.47	0.47
5:M:396:ARG:NH1	6:O:4:LEU:O	2.42	0.47
2:Z:954:ASP:OD1	2:Z:954:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:1093:ASN:N	2:Z:1093:ASN:OD1	2.46	0.47
2:Z:1195:ARG:NH2	2:Z:1216:ASP:O	2.47	0.47
4:g:261:THR:HA	4:g:274:VAL:HG22	1.95	0.47
2:A:1273:ALA:HA	2:A:1276:LYS:HG2	1.97	0.47
2:C:1054:CYS:SG	2:C:1091:THR:OG1	2.65	0.47
6:O:6:THR:OG1	6:O:7:PHE:N	2.46	0.47
2:a:83:LEU:HD11	2:a:1058:ILE:HG22	1.96	0.47
2:D:553:THR:HG21	2:D:983:TYR:HB3	1.96	0.47
2:Z:439:LYS:HB2	2:Z:439:LYS:HE3	1.73	0.47
2:a:417:ASN:OD1	2:a:417:ASN:N	2.46	0.47
2:a:801:GLY:HA3	2:a:890:VAL:HG21	1.95	0.47
2:Z:18:ASP:N	2:Z:18:ASP:OD1	2.48	0.47
2:Z:245:ARG:O	2:Z:249:ALA:HB2	2.15	0.47
2:Z:534:HIS:HE1	2:Z:1239:LEU:HD13	1.78	0.47
2:Y:816:ALA:O	2:Y:877:ARG:NH2	2.48	0.47
2:Z:990:PRO:HA	2:Z:993:ARG:HB2	1.97	0.47
2:A:122:LYS:HG2	2:A:1082:ASN:HB3	1.97	0.47
5:M:479:ARG:HG2	5:M:520:VAL:HG12	1.96	0.47
2:a:628:ARG:NH1	2:a:663:ASP:OD1	2.48	0.47
2:D:360:ILE:HG21	2:D:369:MET:HE2	1.97	0.47
2:D:635:ILE:HG22	2:D:646:VAL:HB	1.96	0.47
2:Z:404:ASP:OD2	2:Z:404:ASP:N	2.45	0.47
2:Z:510:ASN:N	2:Z:983:TYR:OH	2.47	0.47
3:I:153:MET:HE3	3:I:187:PRO:HD3	1.96	0.47
2:A:173:ARG:HG2	2:A:375:VAL:HG23	1.96	0.47
2:B:355:LEU:HD11	2:B:357:MET:HE3	1.96	0.47
2:B:888:GLU:O	2:B:919:ASN:ND2	2.47	0.47
2:B:1132:ARG:HH21	2:B:1139:ARG:HG2	1.79	0.47
2:B:1291:ASP:OD1	2:B:1313:ASN:ND2	2.47	0.47
2:D:390:ASP:HB2	2:D:1313:ASN:HB3	1.96	0.47
2:C:1217:HIS:NE2	2:C:1234:SER:OG	2.41	0.47
2:a:383:ASP:HB3	2:a:386:GLU:HG3	1.97	0.47
2:a:790:PRO:HA	2:a:793:THR:HG22	1.95	0.47
2:Y:1176:LEU:HD22	2:Y:1230:ASN:HB3	1.97	0.47
2:Z:257:ASN:ND2	2:Z:260:THR:OG1	2.47	0.47
2:Z:537:PHE:O	2:Z:555:ARG:NH2	2.48	0.47
3:h:42:LYS:HD2	3:h:42:LYS:HA	1.71	0.47
3:h:209:ASN:HD22	3:h:210:LEU:HD22	1.79	0.47
3:n:193:LEU:O	3:n:197:MET:HG3	2.15	0.47
4:m:49:ARG:HD3	4:m:145:LEU:HD11	1.96	0.47
2:B:91:MET:HE3	2:B:91:MET:HB2	1.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:791:ALA:HB2	2:B:1008:LEU:HD12	1.96	0.47
2:D:101:ALA:HB3	2:C:174:GLY:HA3	1.96	0.47
2:Y:430:LEU:HD12	2:Y:1108:VAL:HG12	1.97	0.47
2:Z:537:PHE:HA	2:Z:554:PRO:HA	1.97	0.47
3:h:292:ASP:OD2	2:B:1069:ARG:NH2	2.47	0.47
2:C:681:LEU:O	2:C:685:THR:OG1	2.32	0.47
2:C:900:ASP:OD2	2:C:1014:LYS:NZ	2.47	0.47
2:D:1033:ALA:HB3	2:D:1176:LEU:HB3	1.95	0.46
2:Z:387:ARG:HG2	2:Z:1046:MET:HE2	1.97	0.46
2:Z:953:SER:OG	2:Z:955:ASP:OD1	2.27	0.46
4:m:77:PRO:HD3	2:C:1150:MET:HE3	1.97	0.46
2:A:275:SER:OG	2:A:276:THR:N	2.47	0.46
2:B:268:LYS:O	2:B:366:THR:OG1	2.33	0.46
2:B:447:LYS:HE3	2:B:1112:ASP:HB3	1.96	0.46
1:i:66:ARG:NH2	2:Z:884:GLN:O	2.48	0.46
2:Y:79:LYS:N	2:Y:303:GLY:O	2.47	0.46
2:Z:317:SER:OG	2:Z:318:TYR:N	2.48	0.46
4:m:236:THR:HG23	4:m:237:ARG:HG3	1.98	0.46
2:A:976:PRO:O	2:A:980:ALA:N	2.48	0.46
2:C:445:ALA:HB1	2:C:449:LEU:HD23	1.98	0.46
2:Y:863:ASP:OD1	2:Y:863:ASP:N	2.48	0.46
2:Z:78:ILE:HB	2:Z:1058:ILE:HG22	1.96	0.46
2:B:534:HIS:HD2	2:B:536:PHE:H	1.63	0.46
2:B:1168:GLN:HE21	2:C:210:ILE:HD13	1.80	0.46
2:a:662:ALA:HA	2:a:671:LEU:HD21	1.96	0.46
2:D:1217:HIS:HE1	2:D:1228:THR:HB	1.81	0.46
3:o:31:VAL:HG11	3:o:137:ILE:HD11	1.96	0.46
2:C:180:LEU:HD23	2:C:384:PRO:HG2	1.97	0.46
2:Y:715:LEU:HB3	2:Y:782:LYS:HD3	1.98	0.46
2:Y:854:GLY:O	2:Y:858:THR:OG1	2.34	0.46
2:Z:361:ARG:HB3	2:Z:366:THR:HG22	1.97	0.46
2:Z:663:ASP:N	2:Z:663:ASP:OD1	2.48	0.46
3:h:145:GLU:OE1	3:I:276:ARG:NH2	2.42	0.46
3:h:241:LEU:HD13	3:I:213:GLU:HG2	1.98	0.46
4:m:183:GLN:HE21	4:m:256:ALA:HA	1.81	0.46
2:A:554:PRO:O	2:A:988:ARG:NH2	2.49	0.46
2:B:491:ALA:HA	2:B:494:ARG:HG2	1.96	0.46
2:Y:681:LEU:HD22	2:Y:783:VAL:HG13	1.97	0.46
2:Z:528:THR:O	2:Z:531:THR:OG1	2.33	0.46
2:Z:793:THR:HB	2:Z:796:ARG:H	1.80	0.46
3:h:91:LEU:HD13	3:h:303:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:61:LEU:O	3:o:65:LEU:HB2	2.16	0.46
4:m:231:VAL:O	4:m:235:ILE:HB	2.16	0.46
2:a:91:MET:HE2	2:a:91:MET:HB3	1.75	0.46
2:a:953:SER:OG	2:a:954:ASP:N	2.48	0.46
2:a:1327:THR:HG23	2:a:1355:VAL:HG22	1.97	0.46
2:D:579:MET:SD	2:D:1003:HIS:ND1	2.82	0.46
3:n:93:THR:HA	3:n:301:THR:HA	1.97	0.46
3:o:99:PRO:HG2	3:o:100:VAL:HG23	1.97	0.46
2:A:598:LYS:O	2:A:602:THR:OG1	2.31	0.46
2:C:1263:ALA:O	2:C:1267:ASN:ND2	2.49	0.46
1:i:71:SER:OG	1:i:72:ARG:NH1	2.48	0.46
2:a:92:LEU:HD12	2:B:7:LEU:HD22	1.98	0.46
2:a:630:PHE:HB2	2:a:878:GLU:HG2	1.98	0.46
2:A:1364:GLN:HA	2:A:1367:LEU:HG	1.98	0.46
2:B:1106:MET:HE1	2:B:1363:GLN:HE22	1.81	0.46
2:C:177:HIS:ND1	2:C:376:TYR:OH	2.44	0.46
2:C:1195:ARG:NH1	2:C:1227:ALA:O	2.48	0.46
2:a:888:GLU:OE1	2:a:919:ASN:ND2	2.48	0.46
2:D:638:MET:HB2	2:D:638:MET:HE2	1.85	0.46
2:Y:1336:LYS:HE3	2:Y:1355:VAL:HG11	1.98	0.46
2:A:388:ASN:HD22	2:A:1103:ARG:HH12	1.64	0.46
2:B:558:ILE:HG21	2:B:574:ARG:HH22	1.81	0.46
2:B:941:ARG:NH2	2:B:982:GLU:OE2	2.49	0.46
2:B:1185:TYR:OH	2:B:1191:ASN:O	2.26	0.46
2:a:724:PRO:HA	2:a:773:ALA:HB3	1.98	0.46
2:Y:272:VAL:HG12	2:Y:368:ILE:HB	1.98	0.46
2:Y:717:PRO:HB3	2:Y:782:LYS:HA	1.98	0.46
2:Z:131:LEU:HD21	2:Z:160:VAL:HG22	1.98	0.46
2:Z:955:ASP:OD1	2:Z:955:ASP:N	2.48	0.46
1:S:50:MET:HE3	1:S:50:MET:HB2	1.86	0.46
2:B:194:GLN:HG3	2:B:222:LYS:HE3	1.97	0.46
2:D:256:ASP:OD1	2:D:256:ASP:N	2.49	0.45
2:Y:292:THR:HG21	2:Y:361:ARG:HH22	1.81	0.45
2:Z:637:ASN:ND2	2:Z:864:VAL:O	2.49	0.45
3:h:58:TYR:CZ	3:h:112:PRO:HG2	2.51	0.45
1:R:39:VAL:HA	1:R:42:THR:HG22	1.97	0.45
2:B:820:MET:HG2	2:B:877:ARG:HD3	1.98	0.45
2:C:913:ARG:N	2:C:984:HIS:O	2.47	0.45
2:a:776:ASP:OD2	2:a:776:ASP:N	2.47	0.45
2:a:815:PRO:HA	2:a:818:LEU:HB2	1.98	0.45
2:Z:315:ALA:HB2	2:Z:321:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:800:LEU:HD22	2:Z:952:LEU:HD21	1.98	0.45
4:m:118:LEU:HD23	4:m:118:LEU:HA	1.86	0.45
2:A:431:LEU:HD21	2:A:1337:LEU:HD21	1.97	0.45
2:A:638:MET:HE1	2:A:642:ARG:HD2	1.98	0.45
2:a:86:LEU:HA	2:Z:50:PHE:HB2	1.98	0.45
2:a:332:LEU:HD13	2:B:11:PRO:HD3	1.97	0.45
2:a:810:ASP:O	2:a:814:ARG:NH1	2.49	0.45
2:D:793:THR:HG21	2:D:797:ALA:HB2	1.98	0.45
2:D:803:ASN:HD21	2:D:935:LEU:HD23	1.81	0.45
2:Y:27:ALA:HB1	2:Y:35:LEU:HD13	1.97	0.45
2:Z:1174:LEU:HB3	2:Z:1176:LEU:HD13	1.99	0.45
3:I:279:ASP:OD1	3:I:279:ASP:N	2.46	0.45
1:Q:67:MET:HA	1:Q:70:VAL:HG12	1.98	0.45
2:A:257:ASN:HB3	2:A:260:THR:HG22	1.97	0.45
2:A:532:GLU:OE2	2:A:555:ARG:NH1	2.49	0.45
2:C:188:PRO:HA	2:C:1286:LEU:HD21	1.97	0.45
2:C:315:ALA:HB2	2:C:321:ILE:HD11	1.98	0.45
2:A:991:PHE:HE1	2:A:1011:MET:HG3	1.81	0.45
2:A:1185:TYR:OH	2:A:1191:ASN:O	2.33	0.45
2:B:263:THR:OG1	2:B:264:SER:N	2.50	0.45
2:B:1054:CYS:SG	2:B:1055:THR:N	2.89	0.45
2:D:522:TYR:OH	2:D:1177:THR:OG1	2.33	0.45
2:D:1263:ALA:O	2:D:1267:ASN:ND2	2.45	0.45
2:Y:310:GLU:HA	2:Y:313:VAL:HG22	1.99	0.45
3:n:28:VAL:HA	3:n:73:MET:HE2	1.99	0.45
1:S:26:LEU:O	2:C:813:TYR:OH	2.33	0.45
1:S:67:MET:HA	1:S:70:VAL:HG12	1.98	0.45
2:a:565:LEU:HD22	2:a:1177:THR:HG21	1.99	0.45
2:D:1139:ARG:NH2	2:D:1141:GLN:OE1	2.40	0.45
2:Y:733:VAL:HG12	2:Y:738:PRO:HA	1.97	0.45
2:Y:1154:GLY:HA3	2:Y:1257:LYS:HB2	1.97	0.45
2:Z:433:ARG:HD3	2:Z:1105:ASP:HA	1.97	0.45
3:I:150:LEU:HA	3:I:153:MET:HE2	1.98	0.45
2:B:139:LEU:HD11	2:B:160:VAL:HG21	1.99	0.45
2:C:965:HIS:O	2:C:968:ARG:NH1	2.48	0.45
2:C:1041:THR:HG23	2:C:1103:ARG:HB3	1.98	0.45
5:M:319:ASP:OD2	5:M:322:HIS:N	2.50	0.45
2:a:778:TRP:CD1	2:a:782:LYS:HZ2	2.35	0.45
2:Y:688:SER:OG	2:Y:708:ASN:ND2	2.47	0.45
2:C:449:LEU:HD21	2:C:1034:LEU:HD11	1.99	0.45
2:a:600:THR:OG1	2:a:645:LEU:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:119:LEU:HB2	3:o:122:GLU:HB2	1.98	0.45
2:C:308:SER:OG	2:C:310:GLU:OE1	2.33	0.45
2:a:553:THR:HG21	2:a:983:TYR:HB3	1.98	0.45
2:a:735:ASP:OD1	2:a:735:ASP:N	2.50	0.45
2:D:602:THR:HG23	2:C:675:ARG:HH22	1.82	0.45
2:Y:534:HIS:CD2	2:Y:536:PHE:H	2.30	0.45
2:Y:1070:ASP:OD1	2:Y:1070:ASP:N	2.50	0.45
2:Z:397:VAL:HG23	2:Z:428:ALA:HB2	1.98	0.45
2:Z:756:ARG:NH1	2:Z:886:VAL:O	2.42	0.45
3:I:162:TYR:HB2	3:I:165:VAL:HG22	1.99	0.45
2:B:1114:PHE:HB3	2:B:1137:VAL:HG21	1.98	0.45
2:C:1022:LEU:HD23	2:C:1022:LEU:HA	1.87	0.45
2:a:537:PHE:HA	2:a:554:PRO:HA	1.98	0.45
2:a:909:ASP:OD1	2:a:909:ASP:N	2.39	0.45
2:Y:173:ARG:HB3	2:Z:100:VAL:HG12	1.99	0.45
2:Y:416:LEU:HD13	2:Y:422:ASN:HB3	1.99	0.45
2:Y:494:ARG:HA	2:Y:497:HIS:HB2	1.99	0.45
2:Y:505:VAL:HG11	2:Y:974:PRO:HG3	1.97	0.45
2:Y:900:ASP:OD2	2:Y:1014:LYS:NZ	2.50	0.45
2:Z:774:THR:HG23	2:Z:777:GLU:H	1.82	0.45
4:m:224:ALA:HA	4:m:227:ARG:HG3	1.99	0.45
2:A:901:HIS:CD2	2:A:904:ARG:HE	2.35	0.45
2:A:993:ARG:HD2	2:A:993:ARG:HA	1.73	0.45
2:B:1:MET:HG2	2:B:2:GLU:HG2	1.99	0.45
2:D:538:ASP:N	2:D:553:THR:O	2.48	0.44
2:Y:428:ALA:HB3	2:Y:440:ILE:HG23	1.98	0.44
2:Y:888:GLU:HB2	2:Y:919:ASN:HD22	1.82	0.44
2:Z:42:ASP:OD1	2:Z:42:ASP:N	2.50	0.44
3:h:70:LEU:HD21	3:h:110:VAL:HG21	1.99	0.44
2:A:1045:ASP:N	2:A:1045:ASP:OD1	2.50	0.44
2:C:591:GLU:OE1	2:C:595:ARG:NH2	2.50	0.44
2:Y:1246:THR:HA	2:Y:1249:ARG:HB3	1.99	0.44
1:i:63:ASP:HA	1:i:66:ARG:HG2	2.00	0.44
2:a:1287:LEU:HB3	2:a:1288:ARG:HD3	1.99	0.44
2:D:507:ARG:HD2	2:C:695:ASN:HB3	1.97	0.44
2:Y:515:ASP:OD1	2:Y:515:ASP:N	2.49	0.44
2:Y:589:ASP:OD1	2:Y:589:ASP:N	2.50	0.44
2:Z:273:MET:HE2	2:Z:273:MET:HB3	1.83	0.44
2:a:92:LEU:HG	2:B:7:LEU:HD13	1.99	0.44
2:a:293:LYS:HB3	2:a:293:LYS:HE3	1.81	0.44
2:Z:856:MET:HE2	2:Z:856:MET:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:1183:VAL:HA	2:Z:1187:LYS:HE2	1.98	0.44
3:h:270:ALA:HB2	4:g:241:ILE:HD11	1.99	0.44
2:C:182:THR:HG21	2:C:1083:THR:HG21	1.99	0.44
2:a:448:THR:HG23	2:a:1113:LEU:HG	1.99	0.44
2:a:629:THR:OG1	2:a:878:GLU:OE1	2.36	0.44
2:a:1244:TYR:HA	2:a:1249:ARG:HH11	1.83	0.44
2:D:526:ASN:HB2	2:D:528:THR:HG22	1.99	0.44
2:D:1111:GLN:HG2	2:D:1171:ALA:H	1.81	0.44
2:Y:1286:LEU:O	2:Y:1290:LYS:NZ	2.50	0.44
2:Z:509:VAL:O	2:Z:513:LYS:HB2	2.17	0.44
3:h:161:SER:OG	3:h:164:GLU:OE1	2.35	0.44
2:B:180:LEU:HD12	2:B:180:LEU:HA	1.87	0.44
2:C:234:ARG:HH22	2:C:282:ILE:HD13	1.82	0.44
5:M:363:VAL:HG23	5:M:550:LEU:HD12	1.98	0.44
2:D:276:THR:OG1	2:D:277:ALA:N	2.51	0.44
2:D:614:ASP:OD2	2:D:649:HIS:NE2	2.50	0.44
2:D:782:LYS:O	2:D:786:LEU:HB2	2.17	0.44
3:o:8:ILE:HB	3:o:83:LEU:HB2	1.99	0.44
1:R:24:VAL:HG23	1:R:25:VAL:HG23	1.99	0.44
2:A:264:SER:HG	2:A:295:THR:HG1	1.57	0.44
2:B:793:THR:HG23	2:B:796:ARG:H	1.82	0.44
2:C:936:PRO:HB3	2:C:952:LEU:HD23	1.99	0.44
5:M:513:ARG:NH1	6:O:20:GLU:O	2.51	0.44
2:D:90:LYS:HD2	2:C:53:ILE:HG12	1.99	0.44
2:Z:25:THR:OG1	2:C:203:ALA:O	2.35	0.44
2:Z:858:THR:HA	2:Z:862:GLU:HB3	1.98	0.44
3:h:56:ARG:HG3	3:h:60:ARG:HD3	2.00	0.44
3:I:152:ILE:HG13	3:I:172:LEU:HD21	1.99	0.44
2:B:71:LEU:HD13	2:B:179:PHE:HD2	1.81	0.44
2:B:272:VAL:HG23	2:B:368:ILE:HB	1.99	0.44
2:C:635:ILE:HD13	2:C:646:VAL:HG12	2.00	0.44
2:C:1055:THR:HG1	2:C:1083:THR:HG1	1.59	0.44
2:C:1250:GLU:HB3	5:M:459:PHE:CG	2.53	0.44
1:j:72:ARG:HD2	2:a:822:ALA:HB2	2.00	0.44
2:D:1294:ARG:HG2	2:D:1303:CYS:HB3	2.00	0.44
2:Z:7:LEU:HB2	2:C:92:LEU:HD23	2.00	0.44
2:Z:358:ASP:OD1	2:Z:358:ASP:N	2.43	0.44
3:h:99:PRO:HG2	3:h:116:HIS:CE1	2.52	0.44
3:n:204:MET:HE2	3:n:204:MET:HB3	1.90	0.44
3:o:24:LEU:HD13	3:o:125:LEU:HD12	2.00	0.44
4:m:234:ARG:HA	4:m:234:ARG:HD2	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:m:249:GLN:HB3	4:m:286:PHE:HA	1.99	0.44
2:A:440:ILE:HB	2:A:1108:VAL:HG11	2.00	0.44
2:A:958:ARG:HE	2:A:958:ARG:HB3	1.67	0.44
2:C:1215:TYR:OH	2:C:1268:THR:OG1	2.34	0.44
5:M:364:GLU:OE1	5:M:558:ARG:NH2	2.51	0.44
2:a:1234:SER:OG	2:a:1235:GLN:OE1	2.35	0.44
2:D:1291:ASP:OD1	2:D:1313:ASN:ND2	2.45	0.44
2:Z:714:ARG:HH21	2:Z:900:ASP:HA	1.83	0.44
3:n:59:VAL:HG23	3:n:62:ARG:HH21	1.81	0.44
2:A:575:THR:HA	2:A:578:ILE:HG12	1.98	0.44
2:A:718:PRO:HG2	2:A:943:TYR:HE2	1.83	0.44
2:A:1124:HIS:HE1	2:A:1126:GLU:HB2	1.83	0.44
2:B:399:LEU:HD23	2:B:399:LEU:HA	1.82	0.44
2:B:1268:THR:HA	2:B:1271:ILE:HB	2.00	0.44
2:a:99:ARG:HH21	2:Z:127:ILE:HG21	1.83	0.43
2:a:404:ASP:HB2	2:Z:421:ARG:HB2	2.00	0.43
2:D:318:TYR:O	2:D:320:SER:N	2.52	0.43
2:D:403:GLU:OE2	2:C:417:ASN:ND2	2.51	0.43
2:Y:637:ASN:ND2	2:Y:863:ASP:O	2.51	0.43
2:Y:719:PHE:HD1	2:Y:917:LEU:HD22	1.80	0.43
2:Z:66:PHE:O	2:Z:69:SER:OG	2.35	0.43
2:Z:124:PRO:HG2	3:n:40:LEU:HD21	2.00	0.43
2:B:1238:CYS:SG	2:B:1241:ASP:N	2.91	0.43
2:C:131:LEU:HD21	2:C:160:VAL:HG22	2.00	0.43
2:D:433:ARG:N	2:D:1105:ASP:O	2.50	0.43
2:Y:127:ILE:HD12	2:Y:128:PRO:HD2	2.00	0.43
2:Y:475:MET:HE2	2:Y:527:ILE:HG22	2.00	0.43
2:Y:717:PRO:HA	2:Y:718:PRO:HD3	1.85	0.43
2:Y:1169:LYS:HD3	2:Y:1299:THR:HG22	1.99	0.43
2:Z:538:ASP:HB3	2:Z:553:THR:HG23	2.00	0.43
2:Z:635:ILE:HG22	2:Z:670:LEU:HD21	1.99	0.43
3:h:298:LYS:HA	3:h:298:LYS:HD2	1.86	0.43
2:B:584:LEU:HD12	2:B:687:ILE:HD11	2.00	0.43
2:B:600:THR:HA	2:B:644:LEU:HD12	1.99	0.43
2:C:909:ASP:OD1	2:C:909:ASP:N	2.46	0.43
2:a:216:LEU:HD12	2:a:1200:LEU:HB2	2.00	0.43
2:a:263:THR:HG22	2:a:296:VAL:HG22	2.00	0.43
2:D:723:LEU:HD23	2:D:768:VAL:HG11	2.00	0.43
2:D:747:ARG:NH2	2:D:888:GLU:OE1	2.51	0.43
2:Y:1257:LYS:HA	2:Y:1302:VAL:HG12	1.99	0.43
2:Z:898:PRO:HG3	2:Z:911:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:o:71:THR:OG1	3:o:72:LEU:N	2.51	0.43
3:o:88:HIS:HD1	3:o:306:GLY:H	1.65	0.43
4:g:234:ARG:HH21	4:g:238:PRO:HA	1.83	0.43
2:B:1040:ASP:HA	2:B:1104:THR:HG21	2.00	0.43
2:C:433:ARG:NH2	2:C:1166:HIS:O	2.51	0.43
2:D:440:ILE:HD13	2:D:1108:VAL:HB	2.01	0.43
2:Y:180:LEU:HD12	2:Y:180:LEU:HA	1.88	0.43
2:Z:424:LEU:HD12	2:Z:425:PRO:HD2	2.01	0.43
2:Z:970:ASP:OD1	2:Z:970:ASP:N	2.46	0.43
2:Z:1327:THR:HG21	2:Z:1333:MET:HB2	2.01	0.43
2:A:657:ILE:HA	2:A:661:LEU:HD13	2.01	0.43
2:B:928:LYS:HA	2:B:931:ILE:HD11	2.00	0.43
2:C:273:MET:HE3	2:C:273:MET:HB2	1.81	0.43
2:a:96:GLN:HA	2:a:113:THR:HA	2.01	0.43
2:a:617:VAL:HG13	2:a:619:GLY:H	1.84	0.43
2:D:1221:ASP:OD2	2:D:1222:ALA:N	2.51	0.43
2:D:1362:LEU:HA	2:D:1366:MET:HG2	1.99	0.43
2:Y:65:TYR:HB2	2:Y:68:THR:HG22	2.00	0.43
2:Y:131:LEU:HD23	2:Y:131:LEU:HA	1.84	0.43
2:Y:428:ALA:N	2:Y:440:ILE:O	2.52	0.43
2:Y:717:PRO:HD3	2:Y:782:LYS:HG3	2.00	0.43
2:Z:538:ASP:N	2:Z:553:THR:O	2.49	0.43
2:Z:1191:ASN:HD22	2:Z:1196:ALA:HA	1.83	0.43
2:A:626:LEU:HD11	2:A:881:LEU:HB3	2.00	0.43
2:B:263:THR:HA	2:B:296:VAL:HA	2.01	0.43
2:C:617:VAL:HG23	2:C:619:GLY:H	1.84	0.43
2:D:79:LYS:N	2:D:303:GLY:O	2.50	0.43
2:D:1349:THR:HA	2:D:1354:TYR:HA	1.99	0.43
2:Y:419:THR:HG21	2:Z:404:ASP:HA	2.01	0.43
3:h:102:TRP:H	3:h:297:ASN:HD21	1.67	0.43
2:A:457:PRO:O	2:A:461:LEU:N	2.48	0.43
2:C:322:LEU:HD12	2:C:322:LEU:HA	1.84	0.43
2:a:274:VAL:HG12	2:a:370:GLU:HB3	1.99	0.43
2:a:638:MET:HE3	2:a:644:LEU:HD21	2.00	0.43
2:a:1047:LEU:HD22	2:a:1097:ALA:HB2	2.01	0.43
2:a:1110:VAL:HA	2:a:1171:ALA:HB3	2.00	0.43
2:D:523:LYS:HE3	2:D:523:LYS:HB3	1.91	0.43
2:D:936:PRO:HB3	2:D:952:LEU:HD12	2.00	0.43
2:Y:562:PRO:HD2	2:Y:565:LEU:HD12	2.01	0.43
2:Y:1176:LEU:HD23	2:Y:1176:LEU:HA	1.85	0.43
2:Z:22:HIS:NE2	2:B:379:THR:O	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:690:LEU:HD23	2:Z:690:LEU:HA	1.92	0.43
2:Z:927:PRO:HD2	2:Z:952:LEU:HD11	2.01	0.43
2:Z:1336:LYS:NZ	2:Z:1346:THR:OG1	2.52	0.43
3:h:106:ASP:H	3:h:290:VAL:HG22	1.84	0.43
3:n:7:ASN:HB3	3:n:82:LEU:HD11	2.01	0.43
2:B:615:VAL:HG11	2:B:802:LEU:HD12	2.01	0.43
5:M:40:LEU:HD11	5:M:151:LEU:HB3	1.99	0.43
2:a:387:ARG:HD3	2:a:387:ARG:HA	1.86	0.43
2:Y:941:ARG:HG3	2:Y:992:SER:HB3	2.01	0.43
2:Y:1039:THR:HG21	2:Y:1259:TYR:HE2	1.83	0.43
2:Z:391:LEU:HB2	2:Z:1042:PHE:HE2	1.83	0.43
2:Z:427:THR:HG22	2:Z:441:ASP:HB3	2.00	0.43
3:h:55:THR:HG21	5:M:577:GLN:HB3	1.99	0.43
3:I:26:LYS:HA	3:I:26:LYS:HD3	1.80	0.43
2:C:278:ASN:OD1	2:C:278:ASN:N	2.51	0.43
2:C:432:ASN:HD22	2:C:436:ALA:HB3	1.83	0.43
2:C:538:ASP:OD1	2:C:538:ASP:N	2.52	0.43
2:C:597:PHE:HA	2:C:600:THR:HG22	2.01	0.43
2:C:719:PHE:HD1	2:C:917:LEU:HD22	1.84	0.43
2:C:1038:ARG:HE	2:C:1038:ARG:HB3	1.72	0.43
5:M:147:LEU:O	5:M:148:HIS:ND1	2.52	0.43
6:N:42:MET:HE3	6:N:42:MET:HB3	1.86	0.43
2:Y:1125:ASP:OD1	2:Y:1125:ASP:N	2.50	0.43
2:Z:428:ALA:HB3	2:Z:440:ILE:HG23	2.01	0.43
2:Z:1224:THR:OG1	2:Z:1225:PHE:N	2.51	0.43
3:I:76:VAL:HG22	3:I:81:ILE:HG23	2.00	0.43
3:o:48:LEU:HB2	3:o:133:VAL:HG13	2.00	0.43
2:A:232:ARG:HG3	2:A:1361:PRO:HG2	2.01	0.43
2:C:427:THR:HG22	2:C:441:ASP:HB3	2.01	0.43
3:h:238:LEU:HD23	3:h:241:LEU:HD12	2.01	0.43
3:n:35:PRO:HB3	3:n:68:MET:HE2	2.00	0.43
4:m:148:CYS:SG	4:m:149:VAL:N	2.92	0.43
2:B:22:HIS:O	2:B:25:THR:OG1	2.36	0.43
2:B:36:ARG:HD2	2:B:36:ARG:HA	1.80	0.43
2:B:71:LEU:HD23	2:B:71:LEU:HA	1.87	0.43
2:B:681:LEU:HB3	2:B:780:LEU:HD22	1.99	0.43
2:B:912:SER:OG	2:B:986:TRP:NE1	2.51	0.43
2:B:1367:LEU:HD23	2:B:1367:LEU:HA	1.90	0.43
2:C:646:VAL:O	2:C:674:TYR:OH	2.31	0.43
5:M:321:GLN:HE22	6:N:52:LEU:HD12	1.83	0.43
2:a:1150:MET:HE1	3:h:67:ASN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:h:64:LEU:HA	3:h:67:ASN:HD22	1.84	0.42
2:A:269:ILE:HD13	2:A:368:ILE:HD11	2.01	0.42
2:A:428:ALA:HB3	2:A:440:ILE:HG23	2.01	0.42
2:A:433:ARG:HE	2:A:433:ARG:HB3	1.58	0.42
2:A:1316:ARG:HD3	2:A:1316:ARG:HA	1.87	0.42
2:B:157:MET:HE3	2:B:157:MET:HB2	1.85	0.42
2:B:1042:PHE:HZ	2:B:1362:LEU:HD21	1.83	0.42
2:C:624:PHE:HZ	2:C:653:LEU:HG	1.84	0.42
2:a:389:VAL:HG22	2:a:1312:GLU:HB3	2.01	0.42
2:a:1349:THR:HA	2:a:1354:TYR:HA	2.00	0.42
2:D:968:ARG:HD2	2:D:968:ARG:HA	1.79	0.42
2:D:1285:TYR:HA	2:D:1289:ALA:HB3	2.01	0.42
2:Z:1156:MET:HE2	2:Z:1257:LYS:HD3	2.01	0.42
3:o:100:VAL:HG21	3:o:142:LEU:HD21	2.02	0.42
2:A:388:ASN:OD1	2:A:388:ASN:N	2.50	0.42
2:A:515:ASP:OD1	2:A:515:ASP:N	2.40	0.42
2:A:575:THR:HG21	2:A:1007:THR:HA	2.00	0.42
2:A:638:MET:SD	2:A:642:ARG:NH2	2.91	0.42
2:B:600:THR:OG1	2:B:645:LEU:O	2.28	0.42
2:C:263:THR:HG22	2:C:296:VAL:HG12	2.00	0.42
2:C:709:ALA:HB3	2:C:1012:LEU:HD12	2.00	0.42
2:a:404:ASP:HA	2:Z:419:THR:HG21	2.01	0.42
2:a:682:ARG:HA	2:a:685:THR:HG22	2.01	0.42
2:D:537:PHE:HA	2:D:554:PRO:HA	2.01	0.42
2:Y:1293:ILE:HG12	2:Y:1311:ILE:HD11	2.00	0.42
2:Z:1282:ILE:HA	2:Z:1285:TYR:HB3	2.01	0.42
3:I:11:THR:OG1	3:I:12:PHE:N	2.52	0.42
3:n:206:MET:HE3	3:n:206:MET:HB2	1.78	0.42
4:m:168:PRO:HA	4:m:273:VAL:HA	2.00	0.42
2:A:820:MET:HE3	2:A:877:ARG:HG3	2.01	0.42
2:A:1070:ASP:OD1	2:A:1070:ASP:N	2.52	0.42
5:M:338:SER:O	5:M:338:SER:OG	2.37	0.42
2:a:1291:ASP:OD1	2:a:1316:ARG:NH2	2.53	0.42
2:Y:694:ASN:HA	2:Y:703:LEU:HD23	2.01	0.42
2:Z:321:ILE:HD13	2:Z:321:ILE:HA	1.93	0.42
2:Z:401:LEU:HA	2:Z:402:PRO:HD3	1.91	0.42
2:Z:432:ASN:HD22	2:Z:436:ALA:HB3	1.84	0.42
2:Z:1264:GLN:HB2	2:Z:1316:ARG:HD3	2.00	0.42
3:h:161:SER:OG	3:h:163:GLU:OE2	2.33	0.42
4:m:48:ALA:N	4:m:148:CYS:O	2.52	0.42
2:A:110:ARG:HH22	2:A:114:ILE:HG23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:435:ARG:HD3	2:A:1367:LEU:HD22	2.01	0.42
2:A:585:ARG:HA	2:A:585:ARG:HD3	1.78	0.42
2:B:1067:GLU:OE1	2:B:1069:ARG:NH1	2.52	0.42
2:C:449:LEU:HD12	2:C:1020:LEU:HD21	2.01	0.42
2:C:1172:CYS:HB2	2:C:1261:PRO:HD2	2.02	0.42
5:M:3:THR:O	5:M:7:SER:OG	2.32	0.42
5:M:408:ARG:HD3	6:N:35:LEU:HD23	2.02	0.42
2:a:555:ARG:HA	2:a:988:ARG:HH12	1.84	0.42
2:a:718:PRO:HD2	2:a:785:TYR:HB3	2.02	0.42
2:a:1175:ILE:HB	2:a:1239:LEU:HD21	2.00	0.42
2:D:975:LEU:HB3	2:D:979:PHE:HB2	2.02	0.42
2:Z:459:PRO:HB2	2:Z:1242:VAL:HG21	2.00	0.42
2:Z:651:TYR:HA	2:Z:654:VAL:HG22	2.00	0.42
3:I:218:TYR:HA	3:I:221:LYS:HB2	2.01	0.42
2:B:505:VAL:HG11	2:B:974:PRO:HB3	2.01	0.42
2:B:905:GLN:O	2:B:1123:ARG:NH2	2.53	0.42
2:C:608:GLU:OE1	2:C:929:THR:OG1	2.32	0.42
2:a:774:THR:OG1	2:a:775:ASP:N	2.53	0.42
2:D:311:ASN:HA	2:D:314:THR:HG22	2.01	0.42
2:D:805:LYS:HB3	2:D:805:LYS:HE3	1.81	0.42
2:D:1014:LYS:HE3	2:D:1014:LYS:HB3	1.86	0.42
2:Y:767:PHE:HD1	2:Y:888:GLU:HG2	1.84	0.42
3:o:295:PRO:O	3:o:298:LYS:NZ	2.52	0.42
2:A:941:ARG:HH11	2:A:985:ASN:HD21	1.67	0.42
2:C:188:PRO:HA	2:C:189:PRO:HD3	1.93	0.42
2:C:448:THR:HG22	2:C:1113:LEU:HD13	2.01	0.42
5:M:5:LEU:HD13	5:M:306:TRP:CD2	2.54	0.42
2:a:112:THR:HG21	2:B:24:LYS:HE3	2.01	0.42
2:a:133:ALA:HA	2:a:136:LEU:HD12	2.01	0.42
2:a:605:ASN:OD1	2:a:605:ASN:N	2.49	0.42
2:a:1006:MET:HE2	2:a:1006:MET:HB2	1.89	0.42
2:a:1224:THR:HG21	2:a:1229:HIS:HD2	1.84	0.42
2:a:1278:LEU:HA	2:a:1281:THR:HG22	2.02	0.42
2:a:1289:ALA:HB1	2:a:1316:ARG:HD2	2.02	0.42
2:D:183:LEU:HD23	2:D:183:LEU:HA	1.89	0.42
2:D:268:LYS:O	2:D:366:THR:OG1	2.35	0.42
2:D:602:THR:HG23	2:C:675:ARG:NH2	2.35	0.42
2:Z:124:PRO:HG3	3:n:11:THR:HG21	2.01	0.42
2:Z:695:ASN:OD1	2:Z:695:ASN:N	2.50	0.42
2:Z:717:PRO:HA	2:Z:718:PRO:HD3	1.86	0.42
2:Z:1349:THR:HA	2:Z:1354:TYR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:949:CYS:HB2	2:B:956:ILE:HG21	2.02	0.42
2:C:187:ALA:HB1	2:C:1094:THR:HG23	2.02	0.42
1:i:46:LYS:HD3	1:i:46:LYS:HA	1.83	0.42
2:a:122:LYS:HE2	2:a:122:LYS:HB3	1.79	0.42
2:a:1365:SER:HA	2:a:1368:PHE:HB2	2.02	0.42
2:Z:1327:THR:OG1	2:Z:1328:THR:N	2.53	0.42
2:C:495:ILE:HG13	2:C:937:VAL:HG12	2.02	0.42
2:C:755:PRO:O	2:C:759:ALA:N	2.52	0.42
5:M:309:ALA:HB1	5:M:332:VAL:HG23	2.02	0.42
5:M:567:ALA:H	5:M:570:MET:HG3	1.84	0.42
1:i:72:ARG:HD3	1:i:72:ARG:HA	1.78	0.42
2:D:509:VAL:HG21	2:D:531:THR:HG21	2.02	0.42
2:D:572:GLU:OE1	2:C:583:ARG:NH2	2.49	0.42
2:D:1183:VAL:HG21	2:C:1330:LEU:HD22	2.02	0.42
2:Z:538:ASP:HB2	2:Z:555:ARG:HG3	2.01	0.42
3:h:127:LEU:HD12	3:h:130:TRP:HE3	1.84	0.42
3:h:187:PRO:HG2	5:M:572:VAL:HB	2.02	0.42
3:n:35:PRO:HG3	3:n:50:GLN:HE22	1.84	0.42
4:m:245:THR:OG1	4:m:246:GLY:N	2.53	0.42
2:C:704:SER:HA	2:C:707:VAL:HG12	2.01	0.42
5:M:419:ASP:O	5:M:422:SER:OG	2.31	0.42
2:a:377:LYS:HE3	2:a:377:LYS:HB2	1.83	0.42
2:D:1157:SER:OG	2:D:1158:GLU:N	2.52	0.42
2:Y:514:GLN:NE2	2:Y:990:PRO:HG3	2.34	0.42
2:A:125:ILE:HD11	2:A:178:SER:HB2	2.01	0.42
2:B:380:ASP:OD1	2:B:380:ASP:N	2.42	0.42
2:B:638:MET:HE1	2:B:642:ARG:HD2	2.02	0.42
2:B:718:PRO:HA	2:B:916:VAL:HG23	2.02	0.42
5:M:172:GLU:OE1	5:M:313:ARG:NH1	2.48	0.42
2:a:111:GLN:HE21	2:Z:130:GLU:HG2	1.83	0.41
2:a:940:HIS:O	2:a:944:SER:OG	2.29	0.41
2:Y:718:PRO:HA	2:Y:916:VAL:HG23	2.01	0.41
2:Y:936:PRO:HB3	2:Y:952:LEU:HD23	2.01	0.41
2:Z:1271:ILE:HD13	2:Z:1271:ILE:HA	1.91	0.41
3:h:197:MET:HE2	3:I:222:LEU:HD12	2.02	0.41
3:I:13:ASP:OD2	3:I:13:ASP:N	2.53	0.41
2:a:908:PRO:HB2	5:M:34:ASN:HD22	1.85	0.41
2:a:1131:ILE:HD13	2:a:1131:ILE:HA	1.95	0.41
2:a:1182:ASP:OD1	2:a:1182:ASP:N	2.49	0.41
2:D:196:LEU:HD23	2:D:196:LEU:HA	1.90	0.41
2:Y:131:LEU:HD12	2:Y:1075:TYR:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:950:ALA:HA	2:Y:956:ILE:HB	2.02	0.41
2:Y:1190:ASN:OD1	2:Y:1191:ASN:N	2.52	0.41
2:Z:192:VAL:O	2:Z:195:THR:OG1	2.35	0.41
2:Z:389:VAL:HG23	2:Z:1312:GLU:HB3	2.02	0.41
2:A:451:HIS:HD2	2:A:453:VAL:H	1.68	0.41
5:M:89:TRP:HZ3	5:M:560:GLN:HE21	1.67	0.41
6:N:22:ASN:OD1	6:N:22:ASN:N	2.51	0.41
2:a:235:ASP:OD1	2:a:235:ASP:N	2.43	0.41
2:D:314:THR:HA	2:D:317:SER:HB3	2.01	0.41
2:D:928:LYS:HA	2:D:931:ILE:HD11	2.02	0.41
2:Z:1228:THR:OG1	2:Z:1229:HIS:N	2.54	0.41
2:A:555:ARG:HB3	2:A:560:ASN:HB2	2.01	0.41
2:A:656:LEU:HD23	2:A:656:LEU:HA	1.93	0.41
2:A:726:ASN:OD1	2:A:726:ASN:N	2.53	0.41
2:C:681:LEU:HD11	2:C:784:PHE:HD1	1.85	0.41
5:M:97:LEU:HD23	5:M:97:LEU:HA	1.94	0.41
2:a:233:THR:OG1	2:a:235:ASP:OD1	2.39	0.41
2:a:856:MET:O	2:a:860:LEU:HB2	2.21	0.41
2:D:689:ALA:O	2:D:694:ASN:ND2	2.53	0.41
2:D:1362:LEU:HD13	2:D:1366:MET:HG3	2.02	0.41
2:Y:87:THR:OG1	2:Y:88:THR:N	2.53	0.41
2:Y:457:PRO:O	2:Y:461:LEU:N	2.49	0.41
2:Z:753:ASP:OD1	2:Z:753:ASP:N	2.42	0.41
2:Z:981:HIS:HB3	2:Z:984:HIS:HB2	2.02	0.41
2:Z:1182:ASP:OD1	2:Z:1182:ASP:N	2.52	0.41
3:n:33:PRO:HD3	3:n:135:PRO:HG3	2.02	0.41
2:A:182:THR:HG23	2:A:185:ARG:HH21	1.86	0.41
2:B:183:LEU:HD23	2:B:183:LEU:HA	1.86	0.41
2:B:1199:MET:HE1	2:B:1210:ALA:HB1	2.01	0.41
2:C:1058:ILE:HD11	2:C:1082:ASN:HD21	1.84	0.41
6:N:27:PRO:HB2	6:N:31:LEU:HD12	2.01	0.41
2:Y:389:VAL:HG13	2:Y:1044:VAL:HG11	2.02	0.41
2:Z:293:LYS:HG2	2:Z:358:ASP:HB3	2.03	0.41
2:Z:1032:PHE:HA	2:Z:1178:PRO:HD3	2.01	0.41
3:n:201:CYS:HB2	3:o:219:VAL:HG22	2.03	0.41
4:m:222:LYS:HA	4:m:222:LYS:HD3	1.74	0.41
2:B:150:LYS:H	2:B:150:LYS:HG2	1.72	0.41
5:M:124:MET:HE2	5:M:124:MET:HB3	1.87	0.41
2:a:538:ASP:OD1	2:a:555:ARG:NE	2.53	0.41
2:D:948:ILE:HD13	2:D:948:ILE:HA	1.90	0.41
2:D:981:HIS:HB3	2:D:984:HIS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:393:PHE:N	2:Y:1038:ARG:O	2.51	0.41
2:Y:433:ARG:NH1	2:Z:213:SER:OG	2.54	0.41
2:Y:445:ALA:HB1	2:Y:449:LEU:HD13	2.02	0.41
2:Z:109:SER:OG	2:Z:110:ARG:N	2.52	0.41
4:g:192:ASP:HB3	4:g:199:ARG:HB3	2.03	0.41
2:B:18:ASP:OD1	2:B:18:ASP:N	2.54	0.41
2:B:190:TYR:HA	2:B:193:VAL:HG12	2.03	0.41
2:B:253:SER:OG	2:B:254:ILE:N	2.54	0.41
2:B:1286:LEU:O	2:B:1290:LYS:NZ	2.43	0.41
2:Y:315:ALA:HA	2:Y:319:HIS:HA	2.01	0.41
3:I:154:GLY:O	3:I:157:SER:OG	2.32	0.41
3:o:136:TRP:HZ3	3:o:182:PHE:HZ	1.68	0.41
4:m:239:ARG:O	4:m:240:GLN:NE2	2.53	0.41
2:C:534:HIS:CD2	2:C:536:PHE:H	2.35	0.41
2:a:802:LEU:HD23	2:a:802:LEU:HA	1.86	0.41
2:a:1176:LEU:HD22	2:a:1230:ASN:HB3	2.03	0.41
2:D:251:THR:OG1	2:D:252:ASP:N	2.54	0.41
2:Y:638:MET:HE2	2:Y:638:MET:HB2	1.83	0.41
2:A:608:GLU:H	2:A:608:GLU:HG2	1.70	0.41
2:B:194:GLN:HA	2:B:197:VAL:HG12	2.02	0.41
2:B:372:LEU:HD23	2:B:372:LEU:HA	1.91	0.41
2:B:716:TRP:O	2:B:914:GLN:NE2	2.54	0.41
2:C:307:LEU:HD23	2:C:307:LEU:HA	1.90	0.41
2:C:776:ASP:OD1	2:C:776:ASP:N	2.51	0.41
2:C:1338:LYS:HE2	2:C:1338:LYS:HB3	1.86	0.41
5:M:432:LEU:HD23	5:M:556:ARG:HE	1.85	0.41
5:M:510:ARG:HD2	5:M:510:ARG:HA	1.76	0.41
2:a:515:ASP:OD1	2:a:515:ASP:N	2.45	0.41
2:a:710:LEU:HD21	2:a:783:VAL:HG22	2.02	0.41
2:a:760:MET:HE2	2:a:888:GLU:HA	2.03	0.41
2:D:753:ASP:HB3	2:D:756:ARG:HB3	2.03	0.41
2:Y:149:ASP:O	2:Y:153:ASN:ND2	2.54	0.41
2:Y:400:TYR:N	2:Y:1178:PRO:O	2.51	0.41
2:Z:76:HIS:HD2	2:Z:78:ILE:HD11	1.84	0.41
2:Z:625:LEU:HD22	2:Z:628:ARG:HH11	1.86	0.41
2:Z:638:MET:HE3	2:Z:864:VAL:HG23	2.03	0.41
2:Z:1112:ASP:N	2:Z:1112:ASP:OD1	2.49	0.41
3:h:229:MET:HE1	2:B:1139:ARG:HH21	1.86	0.41
3:I:107:ALA:HB1	3:I:286:VAL:HG13	2.03	0.41
3:n:14:HIS:CE1	3:n:128:GLY:HA3	2.55	0.41
3:o:216:MET:O	3:o:220:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:m:51:PHE:HE1	4:m:145:LEU:HD12	1.85	0.41
4:m:80:LEU:HD12	4:m:80:LEU:HA	1.87	0.41
4:m:183:GLN:HG2	4:m:256:ALA:HB2	2.02	0.41
1:Q:45:SER:O	1:Q:49:ARG:HB2	2.21	0.41
1:R:42:THR:O	1:R:45:SER:OG	2.38	0.41
2:A:307:LEU:HG	2:A:311:ASN:HD21	1.86	0.41
2:A:1034:LEU:HB3	2:A:1174:LEU:HD12	2.03	0.41
2:A:1132:ARG:HA	2:A:1132:ARG:HD3	1.91	0.41
2:B:1292:CYS:HB3	2:B:1310:LEU:HD23	2.03	0.41
2:C:127:ILE:HD13	2:C:127:ILE:HA	1.89	0.41
2:C:328:TYR:O	2:C:332:LEU:HB2	2.21	0.41
2:C:441:ASP:OD1	2:C:441:ASP:N	2.47	0.41
2:C:703:LEU:HG	2:C:1022:LEU:HD11	2.03	0.41
2:a:95:VAL:HG23	2:Z:59:ASN:HD22	1.86	0.41
2:a:188:PRO:HB2	2:a:192:VAL:HG21	2.02	0.41
2:a:358:ASP:OD1	2:a:358:ASP:N	2.54	0.41
2:D:66:PHE:N	2:D:172:GLU:OE2	2.53	0.41
2:D:89:GLY:H	2:D:120:SER:HB2	1.85	0.41
2:D:230:LEU:HD23	2:D:230:LEU:HA	1.94	0.41
2:Y:229:LEU:HB3	2:Y:230:LEU:HD12	2.01	0.41
2:Y:538:ASP:N	2:Y:553:THR:O	2.48	0.41
2:Y:711:HIS:HA	2:Y:779:THR:HG22	2.01	0.41
3:h:101:THR:HA	3:h:297:ASN:HD21	1.86	0.41
1:R:39:VAL:O	1:R:43:MET:HB2	2.21	0.41
2:B:65:TYR:HA	2:B:172:GLU:HG2	2.02	0.41
2:C:1035:THR:HB	2:C:1176:LEU:HD22	2.03	0.41
2:C:1040:ASP:HA	2:C:1104:THR:HG21	2.03	0.41
5:M:68:ALA:HB3	5:M:548:HIS:HA	2.03	0.41
5:M:318:TRP:HA	5:M:325:ARG:HA	2.04	0.41
2:a:254:ILE:HB	2:a:1086:MET:HG3	2.03	0.40
2:a:627:ILE:HD12	2:a:627:ILE:HG23	1.89	0.40
2:Y:391:LEU:O	2:Y:1040:ASP:N	2.52	0.40
2:Y:614:ASP:OD2	2:Y:649:HIS:NE2	2.54	0.40
3:h:5:GLU:HB3	3:h:6:ALA:H	1.69	0.40
2:A:110:ARG:NE	2:A:111:GLN:OE1	2.53	0.40
2:A:227:LEU:HD23	2:A:227:LEU:HA	1.90	0.40
2:B:1131:ILE:HD13	2:B:1131:ILE:HA	1.95	0.40
2:C:161:LEU:HD23	2:C:161:LEU:HA	1.96	0.40
2:C:399:LEU:HD23	2:C:399:LEU:HA	1.90	0.40
2:C:794:ASN:OD1	2:C:1000:ASN:ND2	2.54	0.40
1:i:20:HIS:CD2	1:i:21:VAL:HG13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:1151:LEU:HD23	4:g:209:ILE:HA	2.03	0.40
2:D:900:ASP:OD1	2:D:900:ASP:N	2.47	0.40
2:D:1066:LYS:HB2	2:D:1066:LYS:HE2	1.94	0.40
2:D:1224:THR:OG1	2:D:1229:HIS:NE2	2.47	0.40
2:Y:222:LYS:O	2:Y:226:THR:OG1	2.37	0.40
2:Y:421:ARG:HH21	2:Z:405:ARG:HH21	1.69	0.40
2:Y:953:SER:HB3	2:Y:956:ILE:HD12	2.03	0.40
2:Z:582:MET:HE2	2:Z:691:PRO:HD2	2.04	0.40
3:h:281:LEU:HD23	3:h:281:LEU:HA	1.91	0.40
2:A:387:ARG:HH21	2:A:1311:ILE:HG21	1.85	0.40
2:C:935:LEU:HD12	2:C:936:PRO:HD2	2.03	0.40
6:N:32:ARG:HA	6:N:35:LEU:HG	2.03	0.40
2:a:695:ASN:OD1	2:a:695:ASN:N	2.55	0.40
2:a:1217:HIS:HE1	2:a:1228:THR:HB	1.86	0.40
2:D:846:ILE:O	2:D:849:GLN:NE2	2.55	0.40
3:h:56:ARG:HD2	3:h:56:ARG:HA	1.85	0.40
3:h:108:LEU:N	3:h:288:PHE:O	2.51	0.40
3:h:197:MET:HE2	3:h:197:MET:HB3	1.80	0.40
3:I:270:ALA:HA	3:I:273:VAL:HG12	2.01	0.40
2:B:717:PRO:HA	2:B:718:PRO:HD3	1.93	0.40
6:N:58:LYS:HB3	6:N:58:LYS:HE3	1.93	0.40
2:a:332:LEU:HG	2:Z:151:ILE:HD12	2.02	0.40
2:a:769:ASP:OD1	2:a:769:ASP:N	2.47	0.40
2:a:800:LEU:HD23	2:a:923:VAL:HG21	2.04	0.40
2:a:991:PHE:HD1	2:a:991:PHE:HA	1.78	0.40
2:a:1330:LEU:HD23	2:a:1330:LEU:HA	1.88	0.40
2:D:334:SER:OG	2:D:335:GLY:N	2.54	0.40
2:D:435:ARG:HH21	2:D:1364:GLN:HA	1.85	0.40
2:Y:538:ASP:HB3	2:Y:553:THR:HG23	2.02	0.40
2:Z:15:ILE:HD13	2:Z:15:ILE:HA	1.93	0.40
2:Z:246:LEU:HD23	2:Z:246:LEU:HA	1.93	0.40
2:Z:709:ALA:O	2:Z:782:LYS:NZ	2.45	0.40
3:h:15:LYS:HD2	3:h:15:LYS:HA	1.94	0.40
3:h:265:ILE:HD13	3:h:265:ILE:HA	1.94	0.40
3:I:157:SER:HB2	3:I:188:VAL:HB	2.03	0.40
4:m:70:MET:HE3	4:m:70:MET:HB2	1.86	0.40
1:R:26:LEU:O	2:B:813:TYR:OH	2.33	0.40
2:A:233:THR:OG1	2:A:235:ASP:OD1	2.30	0.40
2:A:572:GLU:O	2:A:575:THR:OG1	2.39	0.40
2:B:780:LEU:HA	2:B:783:VAL:HG12	2.02	0.40
5:M:312:SER:HB3	5:M:332:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:73:THR:OG1	1:i:74:ARG:N	2.54	0.40
1:j:19:ARG:H	1:j:19:ARG:HG3	1.74	0.40
2:D:653:LEU:HD23	2:D:653:LEU:HA	1.85	0.40
2:D:1313:ASN:OD1	2:D:1313:ASN:N	2.51	0.40
2:Y:161:LEU:HD23	2:Y:161:LEU:HA	1.95	0.40
2:Y:712:ASP:O	2:Y:782:LYS:NZ	2.49	0.40
2:Y:1224:THR:OG1	2:Y:1225:PHE:N	2.55	0.40
2:Z:627:ILE:HG22	2:Z:630:PHE:HB3	2.03	0.40
2:Z:1172:CYS:HB2	2:Z:1261:PRO:HG2	2.04	0.40
4:m:126:HIS:CE1	4:m:127:ARG:HG3	2.57	0.40
2:A:264:SER:OG	2:A:295:THR:OG1	2.32	0.40
2:B:798:CYS:O	2:B:923:VAL:N	2.54	0.40
2:C:774:THR:OG1	2:C:776:ASP:OD1	2.31	0.40
2:C:1327:THR:HG22	2:C:1355:VAL:HG22	2.02	0.40
5:M:581:THR:HG23	5:M:583:ARG:HB2	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	Q	42/75 (56%)	42 (100%)	0	0	100	100
1	R	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
1	S	53/75 (71%)	53 (100%)	0	0	100	100
1	T	21/75 (28%)	20 (95%)	1 (5%)	0	100	100
1	i	54/75 (72%)	54 (100%)	0	0	100	100
1	j	56/75 (75%)	55 (98%)	1 (2%)	0	100	100
2	A	1118/1370 (82%)	1058 (95%)	60 (5%)	0	100	100
2	B	1272/1370 (93%)	1192 (94%)	80 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	1288/1370 (94%)	1216 (94%)	72 (6%)	0	100	100
2	D	1262/1370 (92%)	1184 (94%)	78 (6%)	0	100	100
2	Y	1343/1370 (98%)	1262 (94%)	81 (6%)	0	100	100
2	Z	1318/1370 (96%)	1235 (94%)	83 (6%)	0	100	100
2	a	1275/1370 (93%)	1202 (94%)	73 (6%)	0	100	100
3	I	269/306 (88%)	261 (97%)	8 (3%)	0	100	100
3	h	286/306 (94%)	266 (93%)	20 (7%)	0	100	100
3	n	291/306 (95%)	271 (93%)	20 (7%)	0	100	100
3	o	285/306 (93%)	268 (94%)	17 (6%)	0	100	100
4	g	108/290 (37%)	102 (94%)	6 (6%)	0	100	100
4	m	288/290 (99%)	268 (93%)	20 (7%)	0	100	100
5	M	458/594 (77%)	417 (91%)	41 (9%)	0	100	100
6	N	49/642 (8%)	44 (90%)	5 (10%)	0	100	100
6	O	39/642 (6%)	32 (82%)	6 (15%)	1 (3%)	4	28
All	All	11228/13722 (82%)	10554 (94%)	673 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	O	27	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	40/68 (59%)	40 (100%)	0	100	100
1	R	51/68 (75%)	51 (100%)	0	100	100
1	S	51/68 (75%)	50 (98%)	1 (2%)	48	66
1	T	21/68 (31%)	21 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	i	52/68 (76%)	52 (100%)	0	100	100
1	j	54/68 (79%)	54 (100%)	0	100	100
2	A	1001/1192 (84%)	999 (100%)	2 (0%)	87	87
2	B	1116/1192 (94%)	1110 (100%)	6 (0%)	81	82
2	C	1130/1192 (95%)	1124 (100%)	6 (0%)	81	82
2	D	1106/1192 (93%)	1099 (99%)	7 (1%)	78	80
2	Y	1174/1192 (98%)	1172 (100%)	2 (0%)	87	87
2	Z	1152/1192 (97%)	1145 (99%)	7 (1%)	78	80
2	a	1115/1192 (94%)	1110 (100%)	5 (0%)	84	83
3	I	251/273 (92%)	251 (100%)	0	100	100
3	h	261/273 (96%)	260 (100%)	1 (0%)	84	83
3	n	263/273 (96%)	263 (100%)	0	100	100
3	o	259/273 (95%)	258 (100%)	1 (0%)	84	83
4	g	101/252 (40%)	101 (100%)	0	100	100
4	m	252/252 (100%)	252 (100%)	0	100	100
5	M	391/500 (78%)	388 (99%)	3 (1%)	73	77
6	N	45/526 (9%)	45 (100%)	0	100	100
6	O	38/526 (7%)	37 (97%)	1 (3%)	40	61
All	All	9924/11900 (83%)	9882 (100%)	42 (0%)	81	83

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	a	864	VAL
2	a	1083	THR
2	a	1179	VAL
2	a	1303	CYS
2	a	1304	VAL
2	D	316	ILE
2	D	388	ASN
2	D	740	ASN
2	D	937	VAL
2	D	1077	VAL
2	D	1165	VAL
2	D	1367	LEU
2	Y	1084	VAL

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Mol	Chain	Res	Type
2	Y	1303	CYS
2	Z	653	LEU
2	Z	695	ASN
2	Z	710	LEU
2	Z	730	VAL
2	Z	1179	VAL
2	Z	1221	ASP
2	Z	1303	CYS
3	h	38	LEU
3	o	301	THR
1	S	62	LEU
2	A	609	LEU
2	A	1001	VAL
2	B	420	VAL
2	B	937	VAL
2	B	1001	VAL
2	B	1084	VAL
2	B	1303	CYS
2	B	1313	ASN
2	C	97	VAL
2	C	518	VAL
2	C	861	VAL
2	C	883	VAL
2	C	937	VAL
2	C	1292	CYS
5	M	76	VAL
5	M	485	VAL
5	M	520	VAL
6	O	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (206) such sidechains are listed below:

Mol	Chain	Res	Type
1	i	23	ASN
1	i	37	HIS
2	a	194	GLN
2	a	388	ASN
2	a	438	GLN
2	a	510	ASN
2	a	534	HIS
2	a	541	HIS
2	a	643	GLN

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Mol	Chain	Res	Type
2	a	673	HIS
2	a	794	ASN
2	a	919	ASN
2	a	945	ASN
2	a	969	HIS
2	a	981	HIS
2	a	1000	ASN
2	a	1023	GLN
2	a	1111	GLN
2	a	1166	HIS
2	a	1248	HIS
2	a	1255	ASN
2	a	1267	ASN
2	a	1319	GLN
2	a	1363	GLN
2	D	96	GLN
2	D	199	ASN
2	D	290	HIS
2	D	326	ASN
2	D	422	ASN
2	D	514	GLN
2	D	637	ASN
2	D	676	ASN
2	D	711	HIS
2	D	743	ASN
2	D	794	ASN
2	D	901	HIS
2	D	914	GLN
2	D	967	HIS
2	D	1027	HIS
2	D	1060	ASN
2	D	1080	ASN
2	D	1120	ASN
2	D	1168	GLN
2	D	1223	GLN
2	D	1350	HIS
2	Y	76	HIS
2	Y	81	HIS
2	Y	84	ASN
2	Y	153	ASN
2	Y	181	GLN
2	Y	199	ASN

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Mol	Chain	Res	Type
2	Y	205	GLN
2	Y	208	ASN
2	Y	211	GLN
2	Y	278	ASN
2	Y	484	GLN
2	Y	510	ASN
2	Y	534	HIS
2	Y	543	GLN
2	Y	560	ASN
2	Y	660	HIS
2	Y	748	HIS
2	Y	794	ASN
2	Y	795	ASN
2	Y	903	GLN
2	Y	940	HIS
2	Y	945	ASN
2	Y	984	HIS
2	Y	1029	HIS
2	Y	1060	ASN
2	Y	1061	ASN
2	Y	1079	GLN
2	Y	1080	ASN
2	Y	1093	ASN
2	Y	1141	GLN
2	Y	1168	GLN
2	Y	1184	ASN
2	Y	1230	ASN
2	Y	1235	GLN
2	Y	1350	HIS
2	Y	1363	GLN
2	Y	1364	GLN
2	Y	1369	ASN
2	Z	59	ASN
2	Z	76	HIS
2	Z	181	GLN
2	Z	194	GLN
2	Z	199	ASN
2	Z	257	ASN
2	Z	388	ASN
2	Z	432	ASN
2	Z	534	HIS
2	Z	637	ASN

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Mol	Chain	Res	Type
2	Z	660	HIS
2	Z	676	ASN
2	Z	803	ASN
2	Z	851	GLN
2	Z	901	HIS
2	Z	903	GLN
2	Z	985	ASN
2	Z	1027	HIS
2	Z	1082	ASN
2	Z	1100	ASN
2	Z	1166	HIS
2	Z	1168	GLN
2	Z	1191	ASN
2	Z	1235	GLN
2	Z	1248	HIS
2	Z	1313	ASN
2	Z	1363	GLN
3	h	7	ASN
3	h	209	ASN
3	h	258	HIS
3	I	39	HIS
3	I	79	ASN
3	I	96	ASN
3	I	148	GLN
3	I	171	GLN
3	I	173	GLN
3	I	191	GLN
3	I	257	GLN
3	n	14	HIS
3	n	39	HIS
3	n	67	ASN
3	n	79	ASN
3	n	80	GLN
3	n	116	HIS
3	n	171	GLN
3	n	277	GLN
3	o	7	ASN
3	o	191	GLN
3	o	297	ASN
4	g	183	GLN
4	g	278	ASN
4	m	183	GLN

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Mol	Chain	Res	Type
4	m	240	GLN
4	m	249	GLN
1	S	37	HIS
2	A	194	GLN
2	A	199	ASN
2	A	371	ASN
2	A	455	HIS
2	A	534	HIS
2	A	618	HIS
2	A	643	GLN
2	A	781	GLN
2	A	849	GLN
2	A	874	GLN
2	A	981	HIS
2	A	1000	ASN
2	A	1023	GLN
2	A	1080	ASN
2	A	1111	GLN
2	A	1133	HIS
2	A	1229	HIS
2	B	153	ASN
2	B	158	HIS
2	B	455	HIS
2	B	543	GLN
2	B	640	HIS
2	B	660	HIS
2	B	711	HIS
2	B	713	HIS
2	B	749	HIS
2	B	803	ASN
2	B	914	GLN
2	B	969	HIS
2	B	1080	ASN
2	B	1100	ASN
2	B	1111	GLN
2	B	1166	HIS
2	B	1168	GLN
2	B	1363	GLN
2	C	158	HIS
2	C	211	GLN
2	C	290	HIS
2	C	338	HIS

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Mol	Chain	Res	Type
2	C	432	ASN
2	C	534	HIS
2	C	618	HIS
2	C	620	ASN
2	C	660	HIS
2	C	697	GLN
2	C	743	ASN
2	C	794	ASN
2	C	849	GLN
2	C	914	GLN
2	C	965	HIS
2	C	981	HIS
2	C	985	ASN
2	C	1000	ASN
2	C	1060	ASN
2	C	1093	ASN
2	C	1120	ASN
2	C	1133	HIS
2	C	1223	GLN
5	M	34	ASN
5	M	90	GLN
5	M	109	GLN
5	M	120	GLN
5	M	321	GLN
5	M	322	HIS
5	M	517	GLN
5	M	571	HIS
5	M	577	GLN
6	N	63	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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.

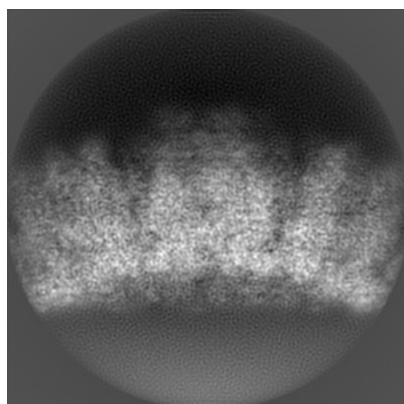
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34704. These allow visual inspection of the internal detail of the map and identification of artifacts.

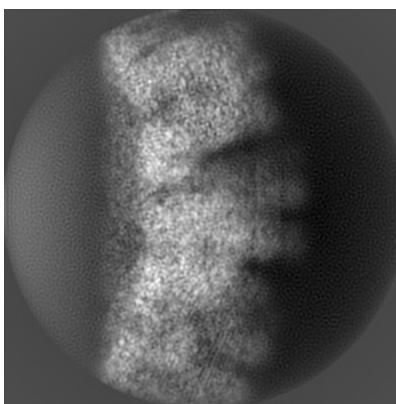
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

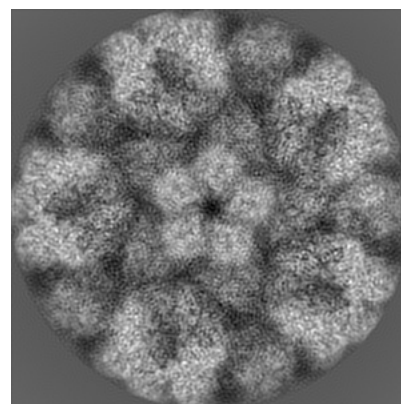
6.1.1 Primary map



X

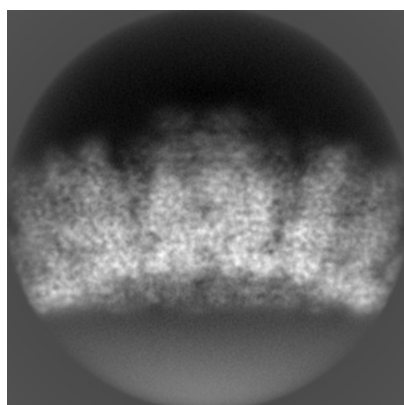


Y

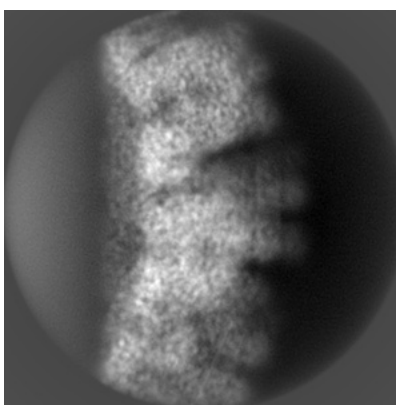


Z

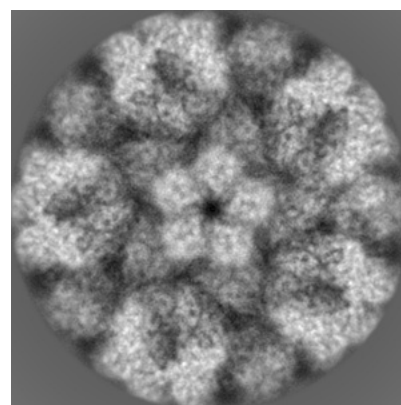
6.1.2 Raw map



X



Y

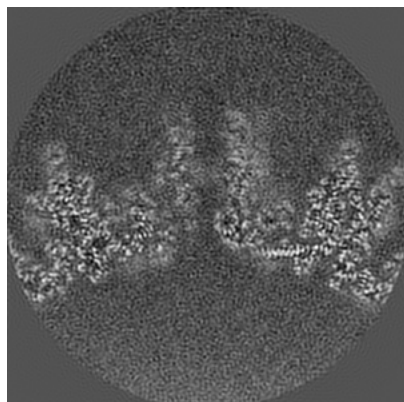


Z

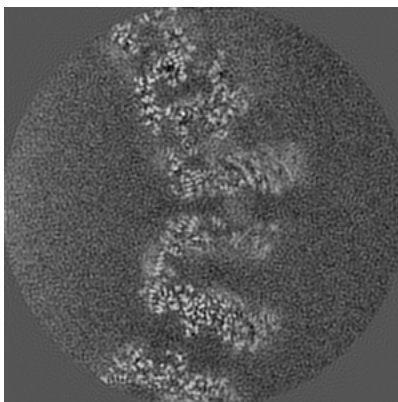
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

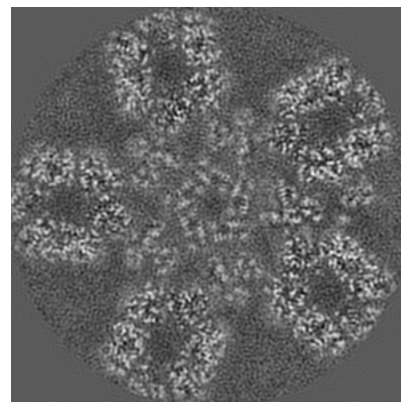
6.2.1 Primary map



X Index: 128

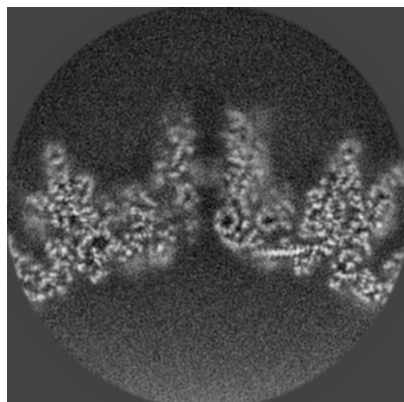


Y Index: 128

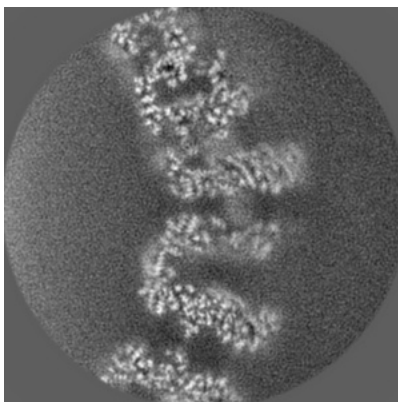


Z Index: 128

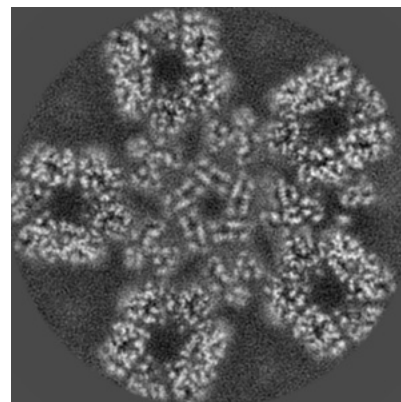
6.2.2 Raw map



X Index: 128



Y Index: 128

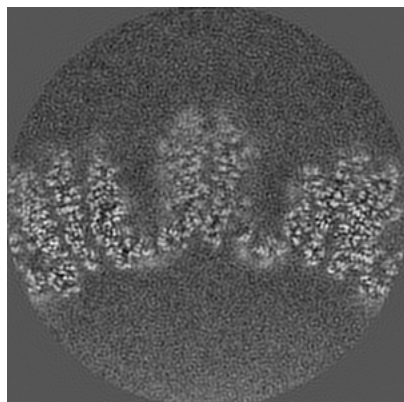


Z Index: 128

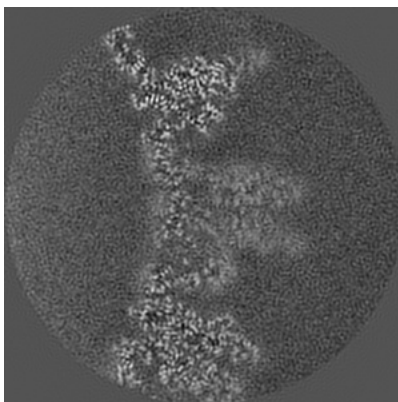
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

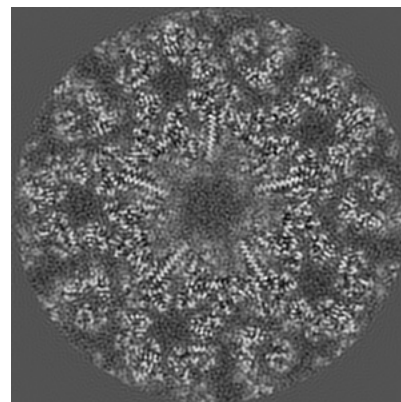
6.3.1 Primary map



X Index: 116

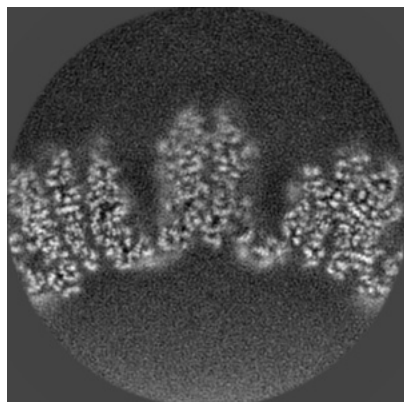


Y Index: 104

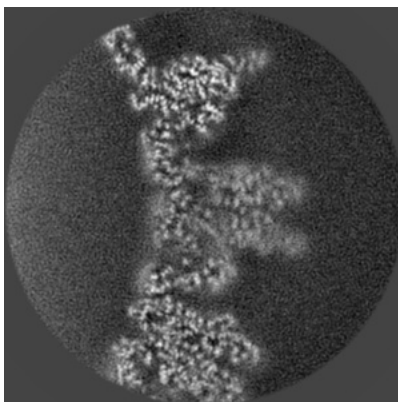


Z Index: 98

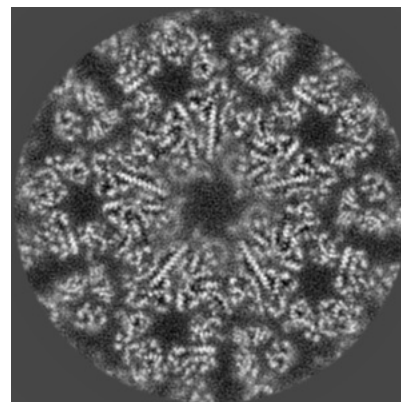
6.3.2 Raw map



X Index: 116



Y Index: 104

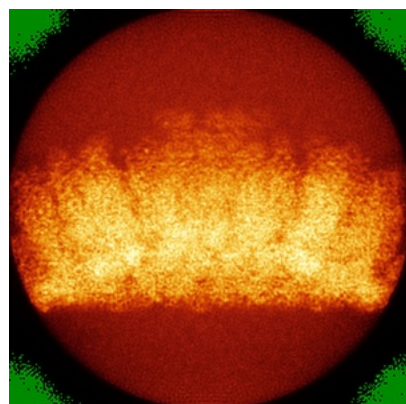


Z Index: 99

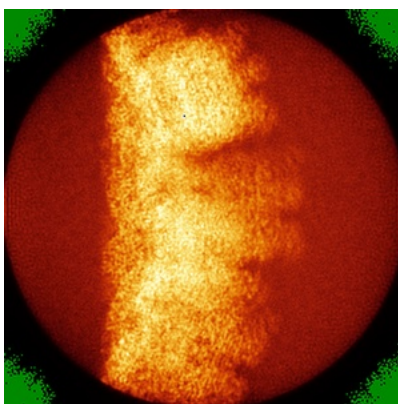
The images above show the largest variance slices of the map in three orthogonal directions.

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

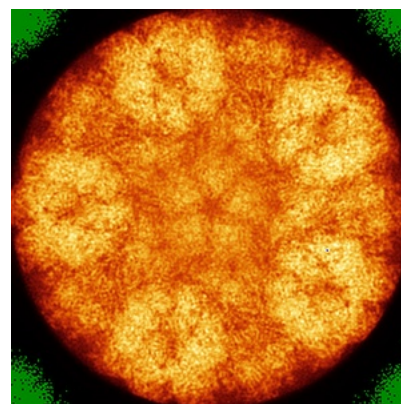
6.4.1 Primary map



X

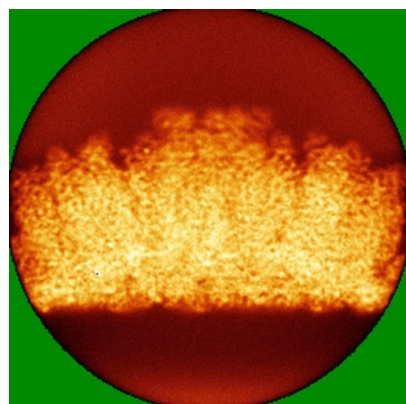


Y

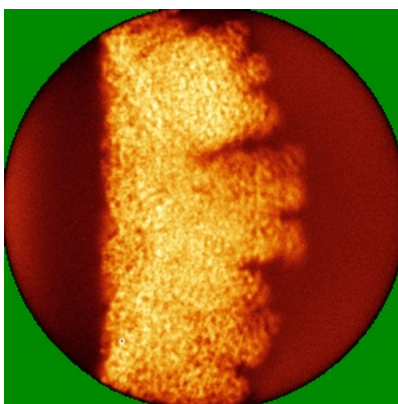


Z

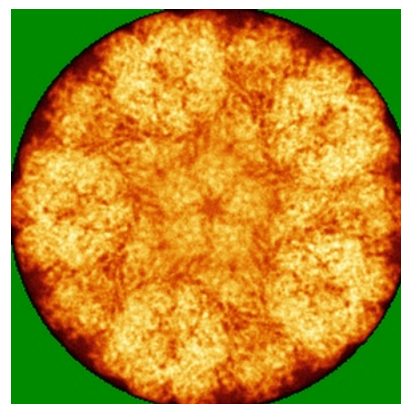
6.4.2 Raw map



X



Y

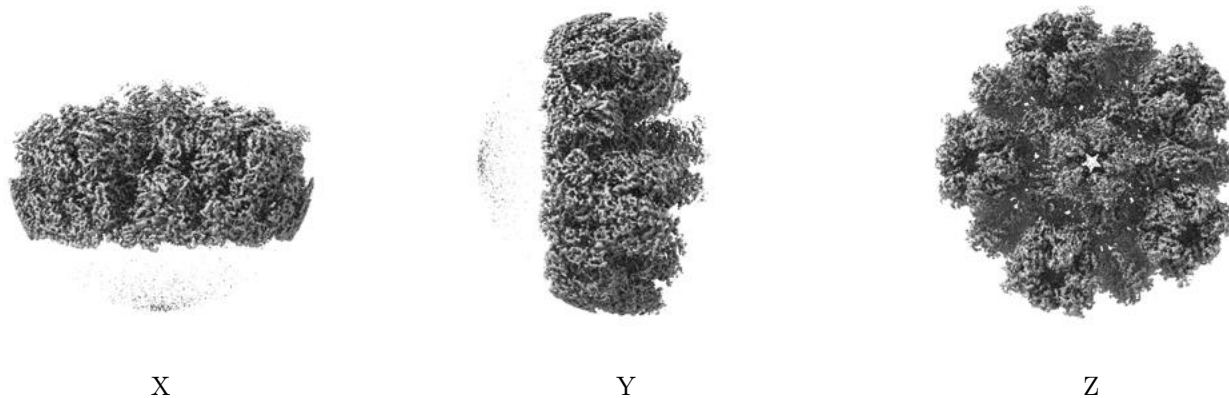


Z

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.

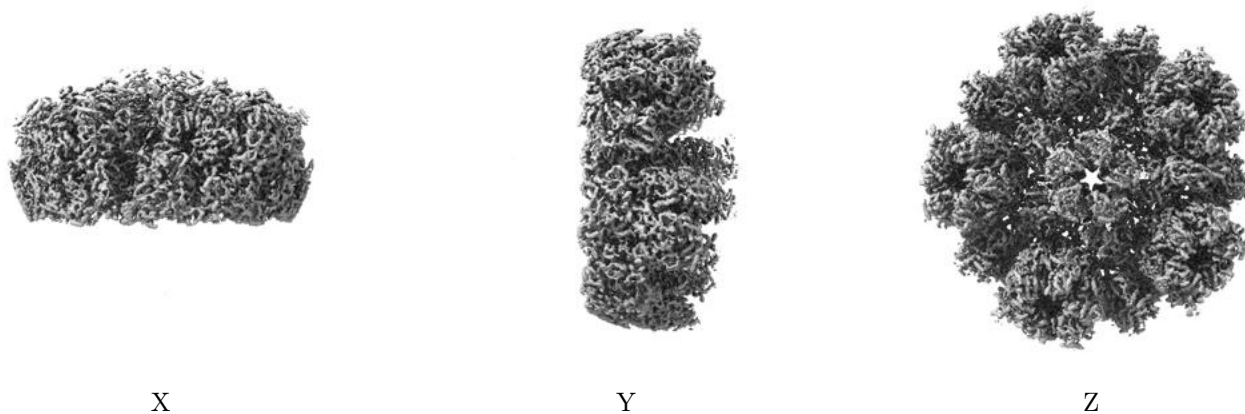
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

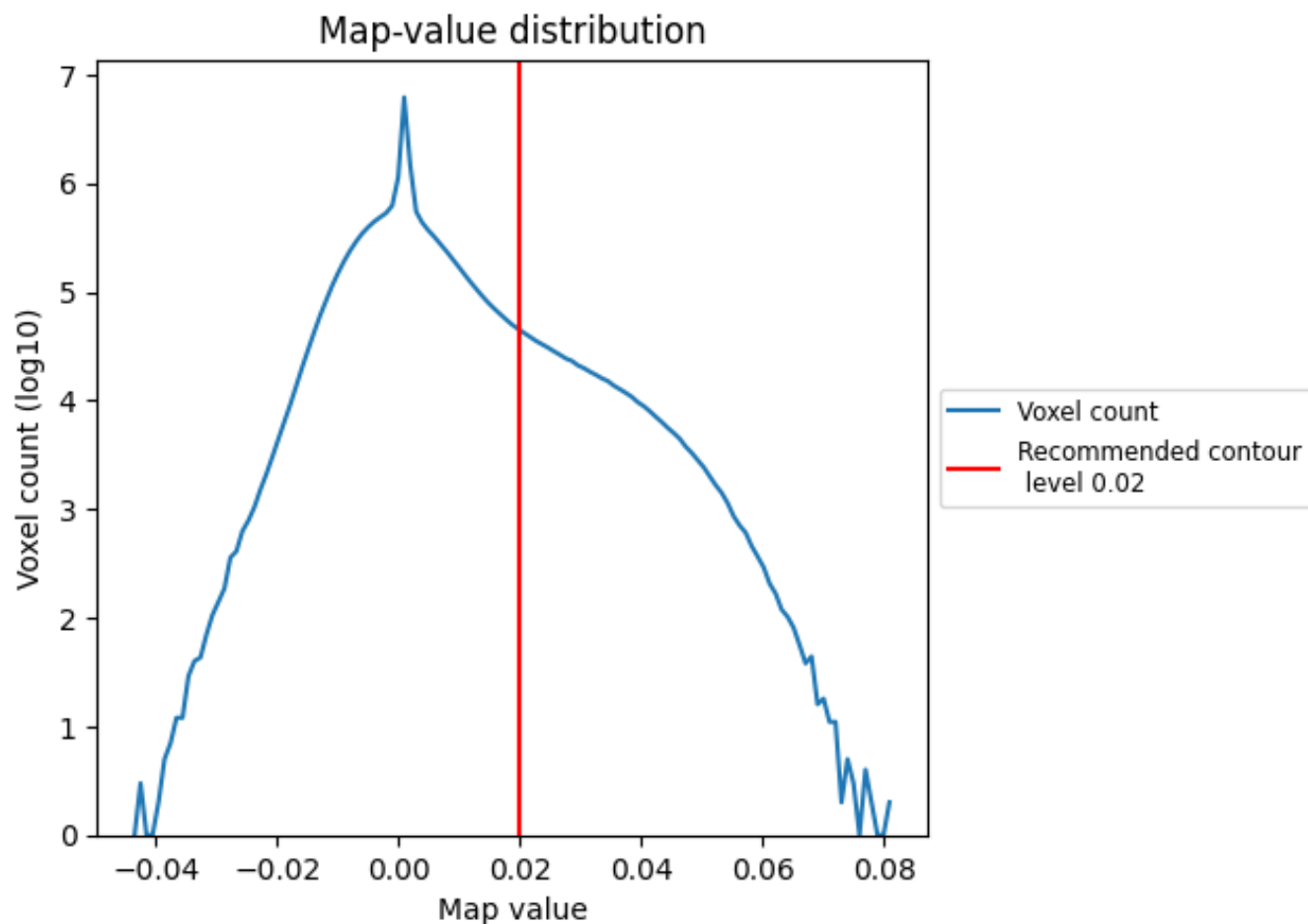
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

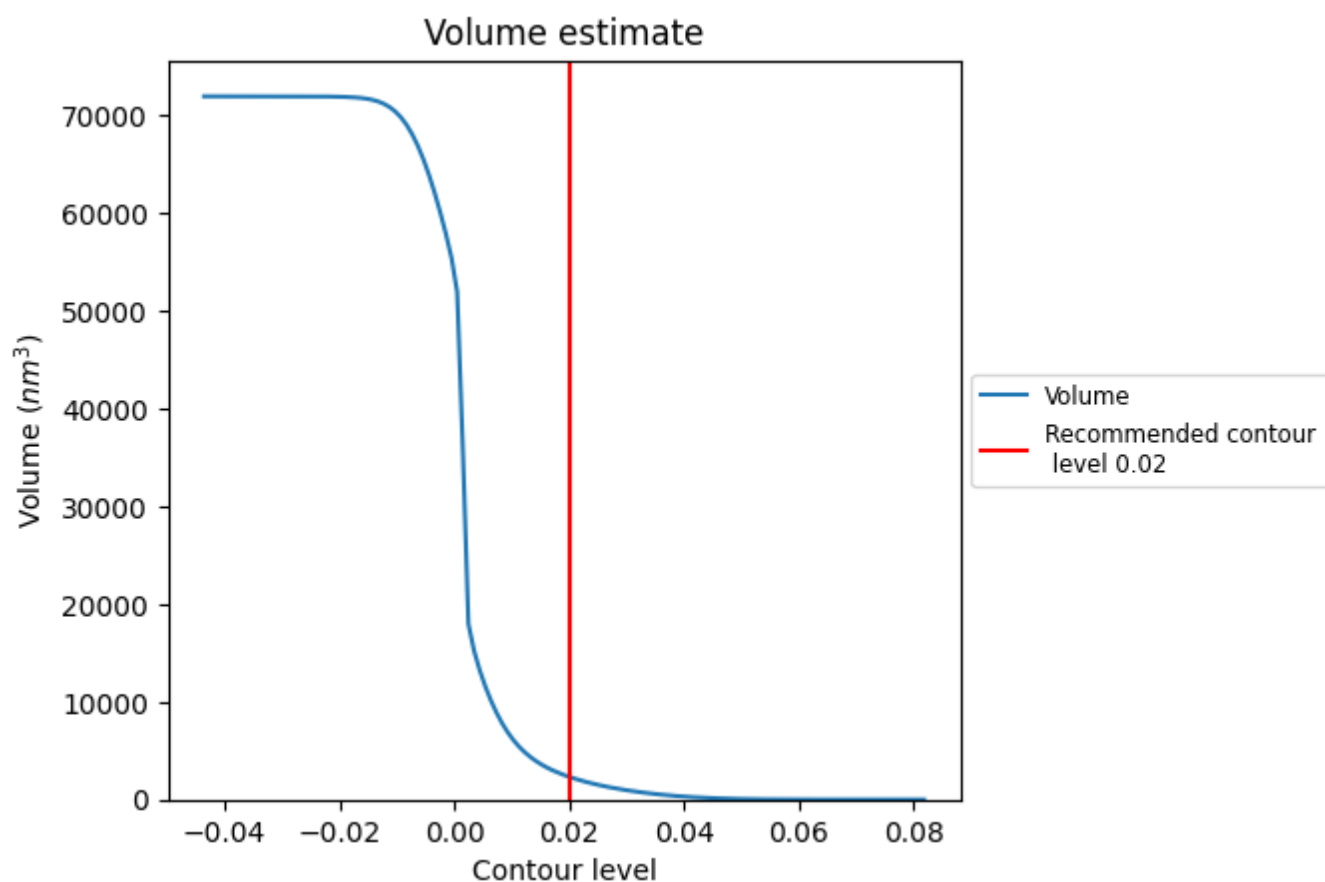
This section contains the results of statistical analysis of the map.

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.

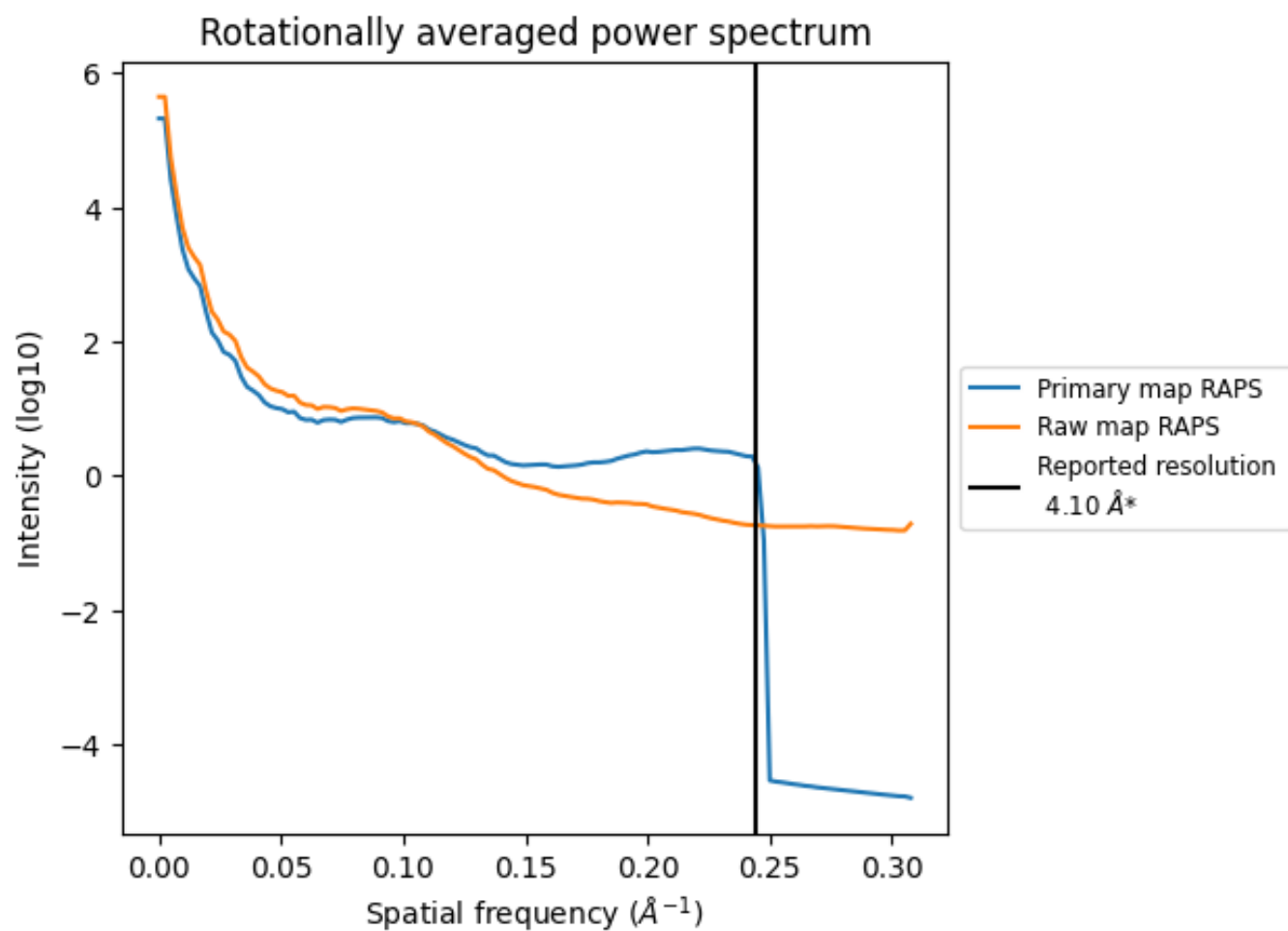
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2336 nm³; this corresponds to an approximate mass of 2110 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 ⓘ

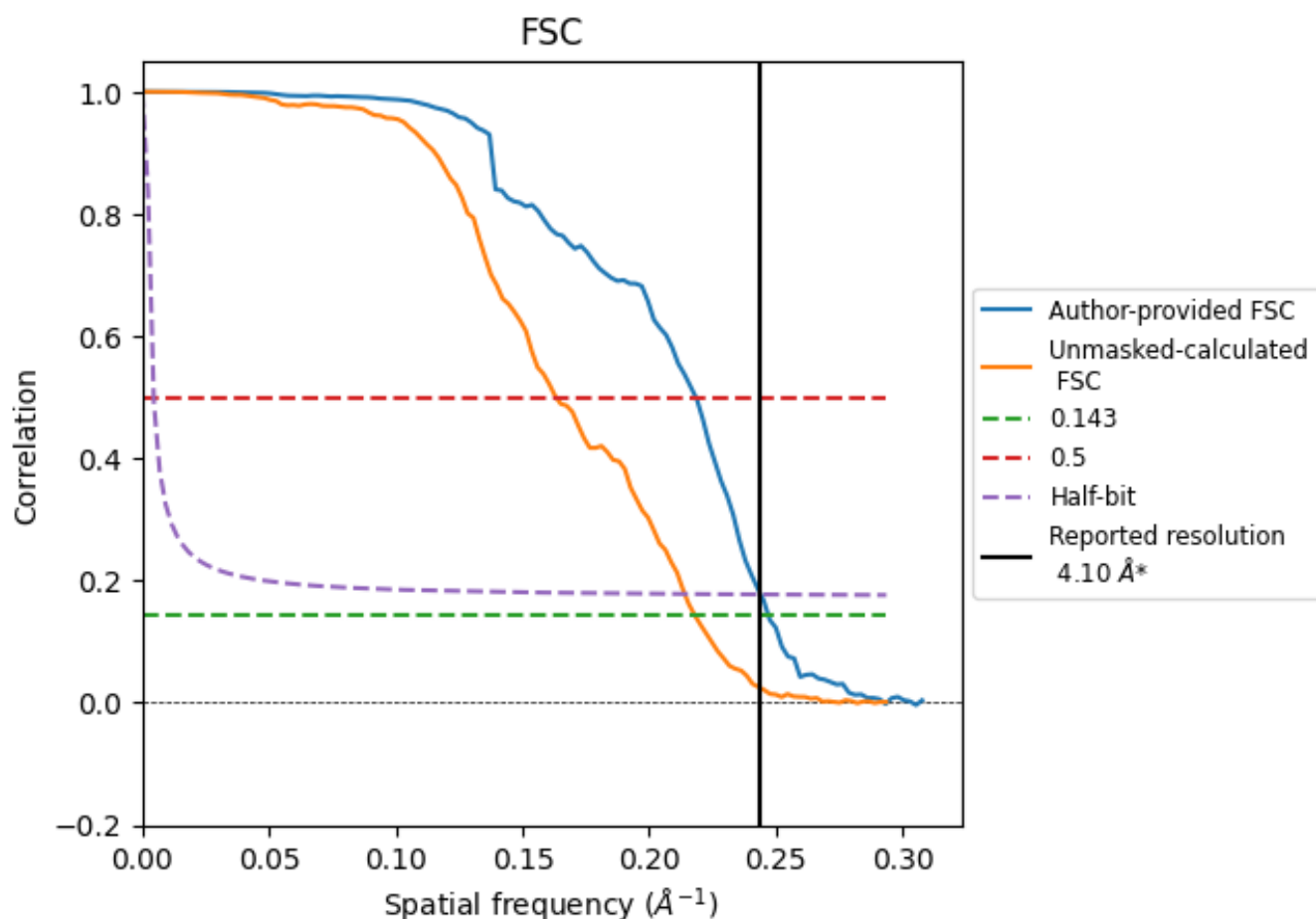


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 $0.244 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.05	4.58	4.10
Unmasked-calculated*	4.59	6.13	4.67

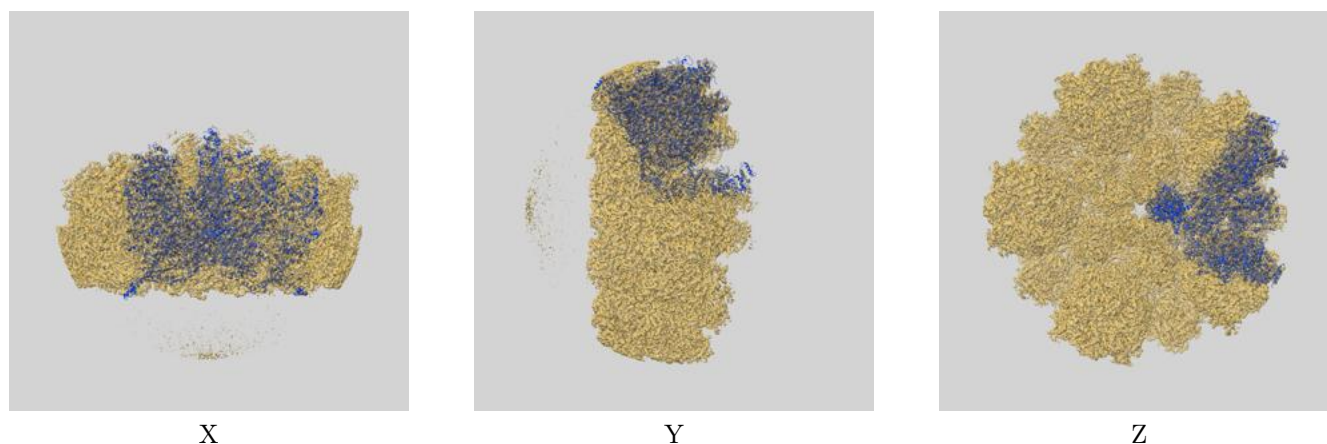
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.59 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

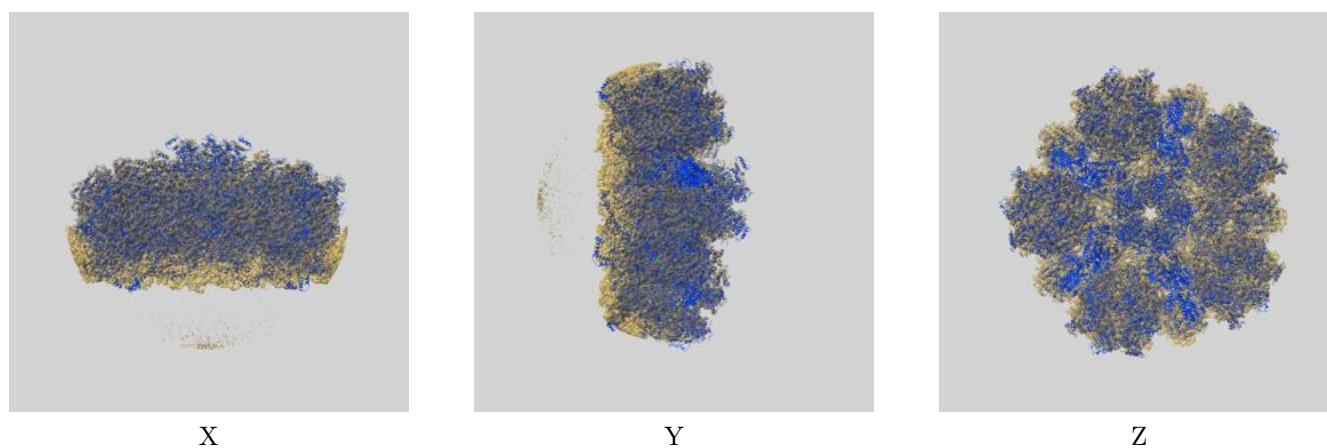
This section contains information regarding the fit between EMDB map EMD-34704 and PDB model 8HEY. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

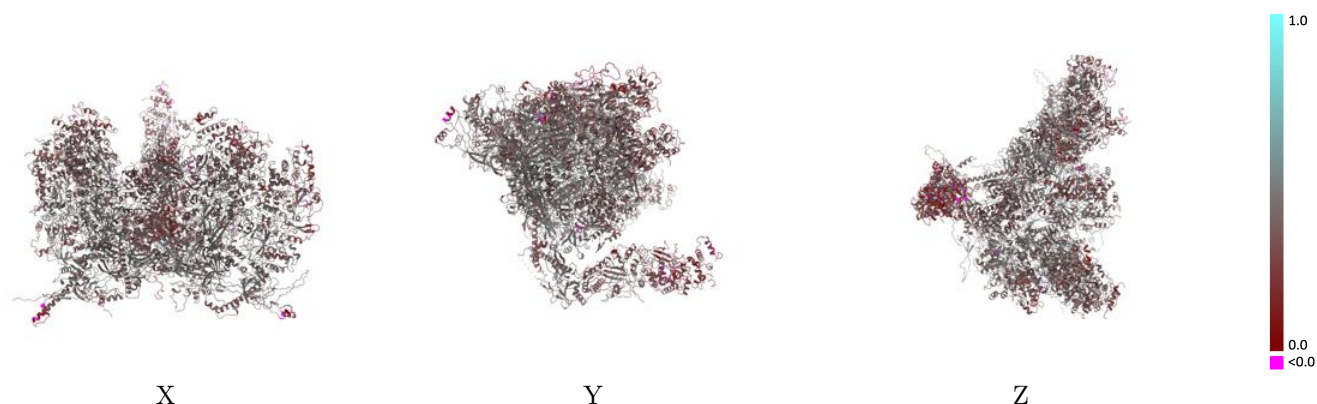


9.1.2 Map-model assembly overlay [i](#)



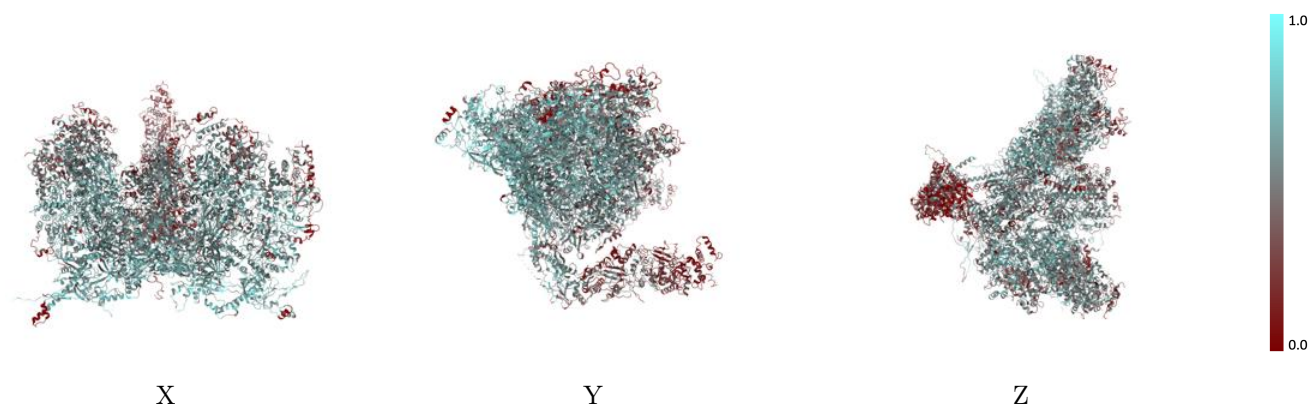
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



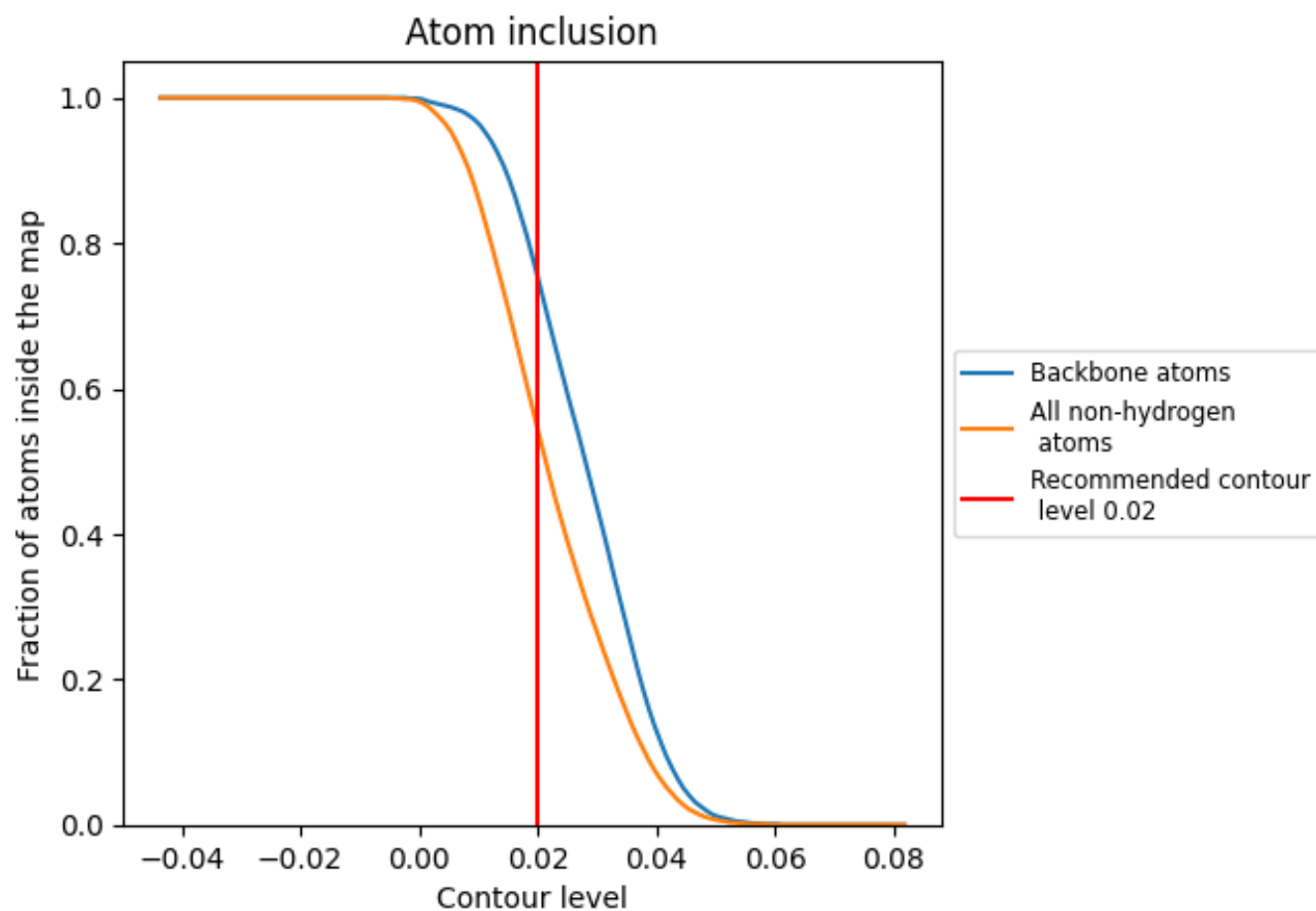
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 54% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5440	 0.3920
A	 0.3210	 0.3210
B	 0.5870	 0.4150
C	 0.6310	 0.4190
D	 0.5820	 0.4070
I	 0.4820	 0.3780
M	 0.5010	 0.3930
N	 0.3320	 0.2850
O	 0.2730	 0.2800
Q	 0.0650	 0.2280
R	 0.2470	 0.3080
S	 0.2940	 0.2930
T	 0.3210	 0.2940
Y	 0.5720	 0.3890
Z	 0.6060	 0.4140
a	 0.6090	 0.4140
g	 0.4890	 0.3740
h	 0.5410	 0.3830
i	 0.2320	 0.2540
j	 0.2910	 0.3010
m	 0.5800	 0.3990
n	 0.5060	 0.3780
o	 0.5390	 0.3770

