



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:49 AM UTC

PDB ID : 8TEP / pdb_00008tep
EMDB ID : EMD-41194
Title : Human cytomegalovirus portal vertex, virion configuration 1 (VC1)
Authors : Jih, J.; Liu, Y.T.; Liu, W.; Zhou, H.
Deposited on : 2023-07-06
Resolution : 3.50 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

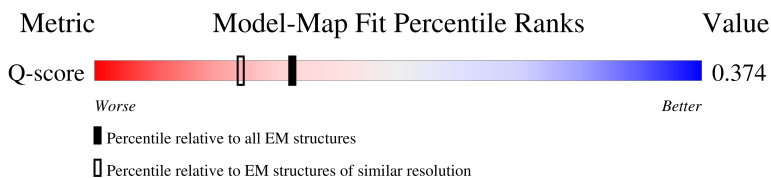
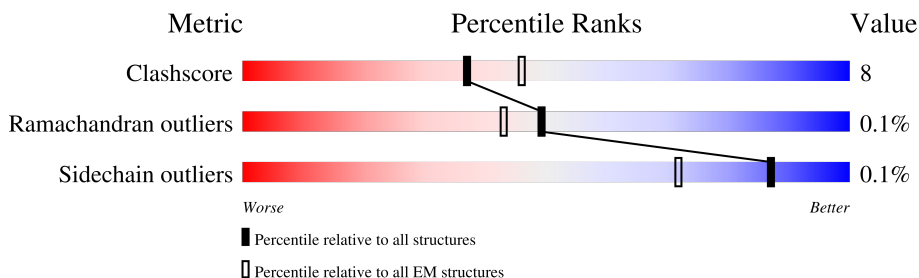
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	2241	 19% 23% 10% 68%
1	C	2241	 28% 23% 8% 69%
2	B	983	 26% 33% 17% 50%
2	D	983	 43% 32% 14% 54%

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Mol	Chain	Length	Quality of chain
3	E	642	
3	F	642	
4	G	594	
5	H	1370	
5	I	1370	
5	J	1370	
5	K	1370	
5	L	1370	
5	M	1370	
6	N	75	
6	O	75	
6	P	75	
6	Q	75	
6	R	75	
6	S	75	
7	T	290	
7	W	290	
8	U	306	
8	V	306	
8	X	306	
8	Y	306	
9	Z	1048	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 112987 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 Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	723	Total	C	N	O	S	0	0
			5833	3733	1026	1052	22		
1	C	699	Total	C	N	O	S	0	0
			5651	3626	997	1006	22		

- Molecule 2 is a protein called Inner tegument protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	492	Total	C	N	O	S	0	0
			3993	2535	709	734	15		
2	D	453	Total	C	N	O	S	0	0
			3685	2349	645	676	15		

- Molecule 3 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	482	Total	C	N	O	S	0	0
			3915	2516	688	699	12		
3	F	492	Total	C	N	O	S	0	0
			3986	2562	705	708	11		

- Molecule 4 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	472	Total	C	N	O	S	0	0
			3873	2422	744	693	14		

- Molecule 5 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	1311	Total	C	N	O	S	0	0
			10406	6630	1802	1913	61		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
5	J	1317	Total	C	N	O	S	0	0
			10433	6641	1814	1919	59		
5	K	1298	Total	C	N	O	S	0	0
			10282	6544	1792	1887	59		
5	L	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
5	M	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

- Molecule 6 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
6	O	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
6	P	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
6	Q	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
6	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
6	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 7 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	240	Total	C	N	O	S	0	0
			1919	1235	335	338	11		
7	W	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 8 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	292	Total	C	N	O	S	0	0
			2317	1489	399	411	18		
8	V	288	Total	C	N	O	S	0	0
			2292	1471	397	407	17		

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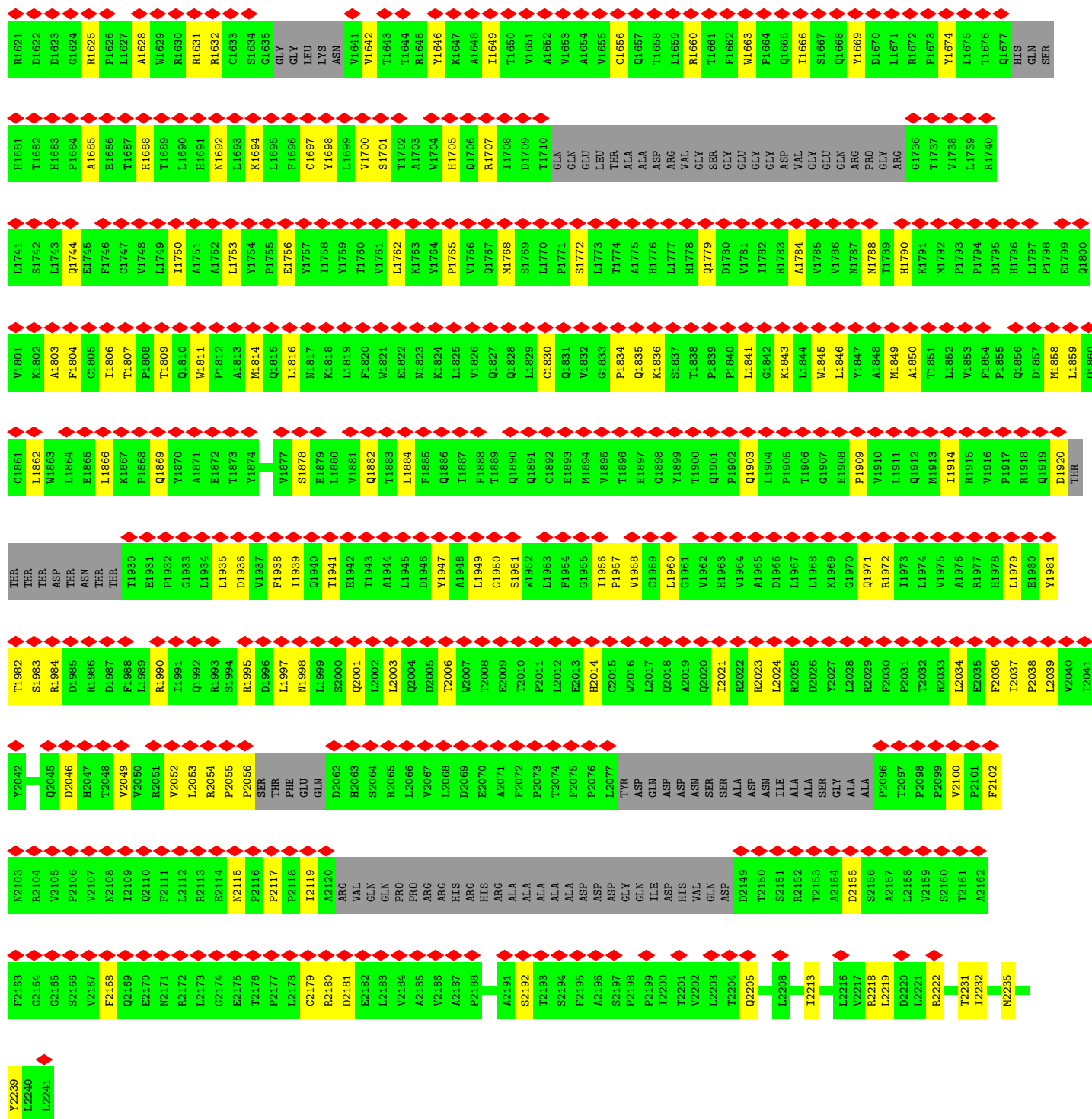
Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
8	Y	285	Total	C	N	O	S	0	0
			2266	1456	387	405	18		

- Molecule 9 is a protein called Large structural phosphoprotein.

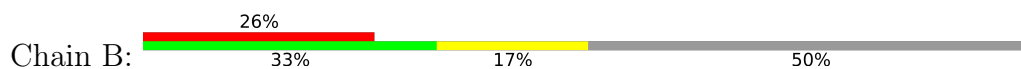
Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	284	Total	C	N	O	S	0	0
			2320	1463	425	420	12		







• Molecule 2: Inner tegument protein



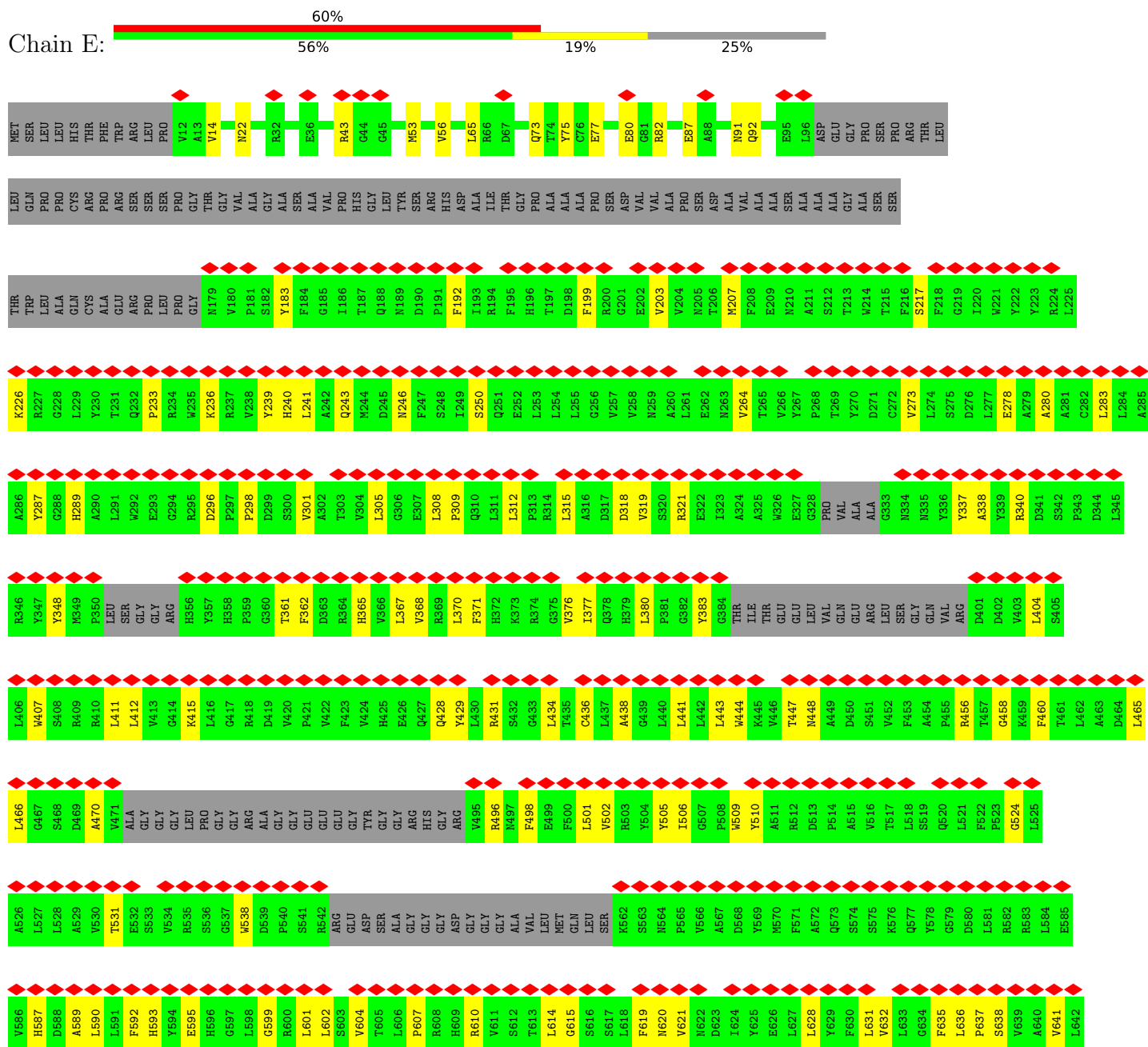




LEU
SER
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THR
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VAL
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PRO
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SER
PRO

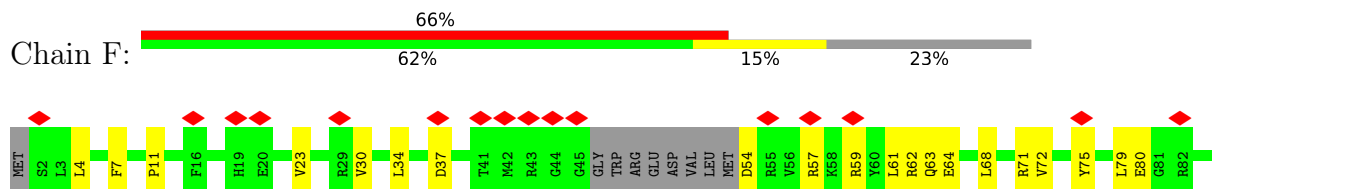
• Molecule 3: Capsid vertex component 2

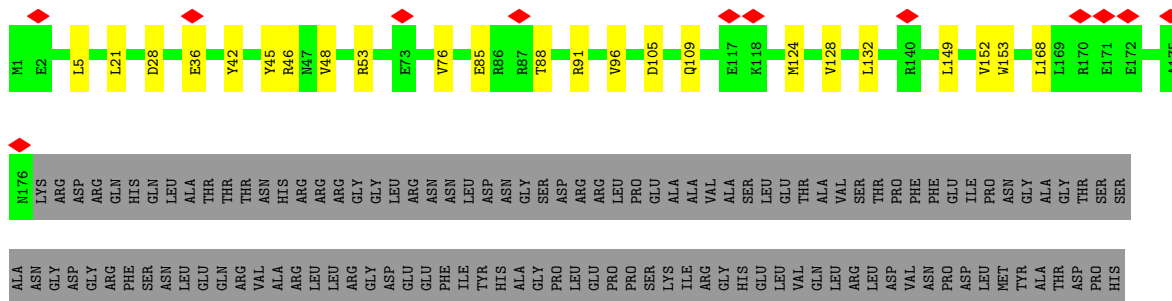
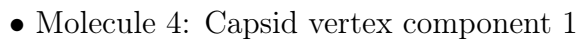
Chain E:

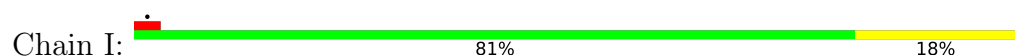


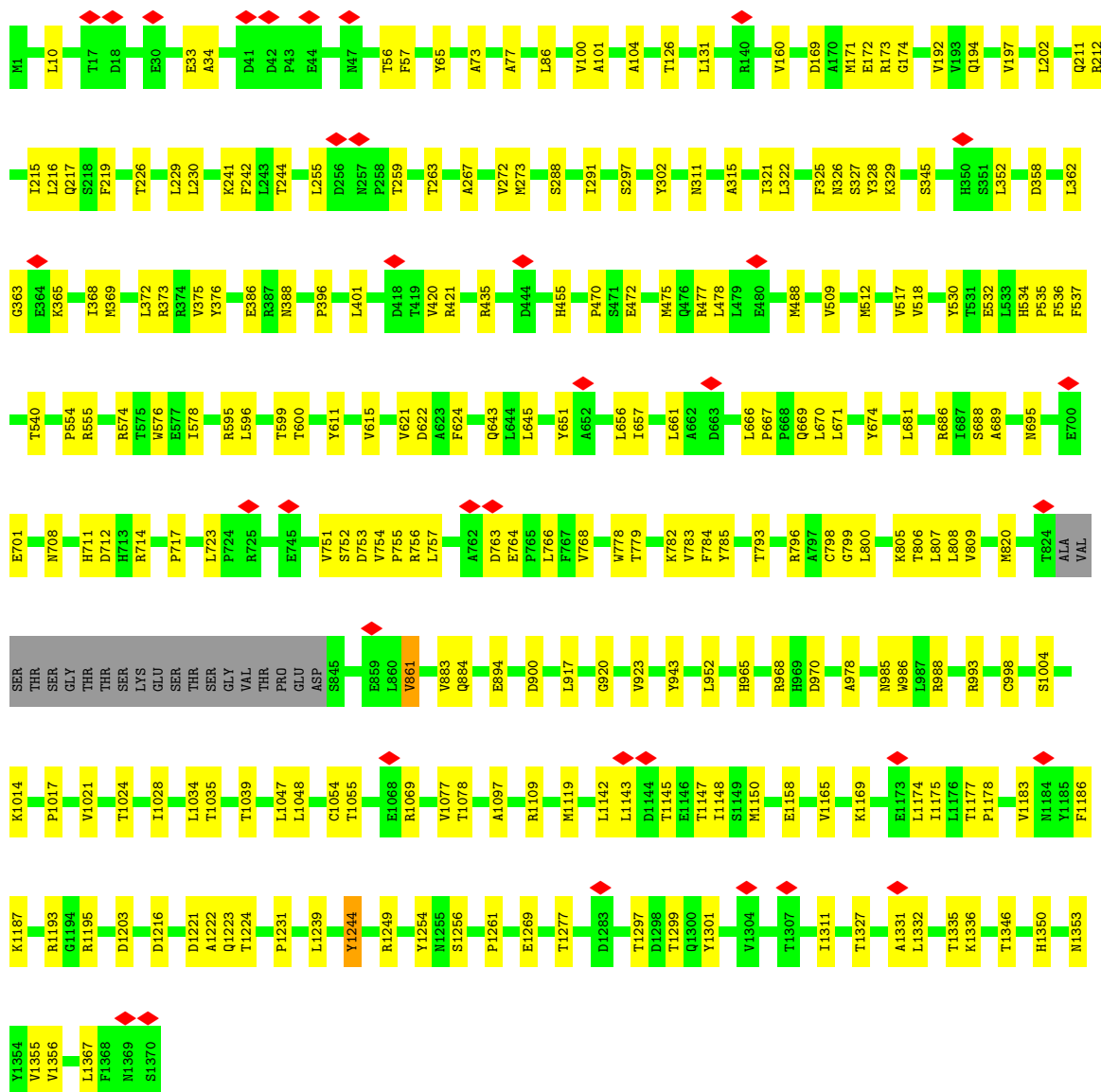
• Molecule 3: Capsid vertex component 2

Chain F:

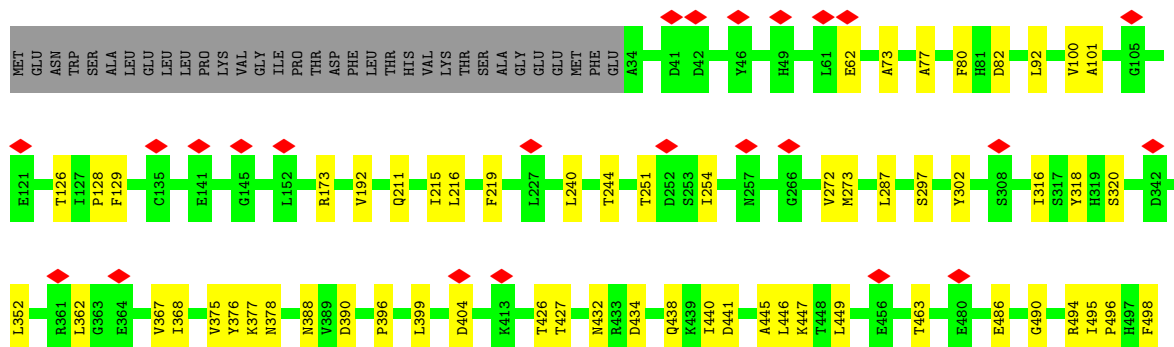
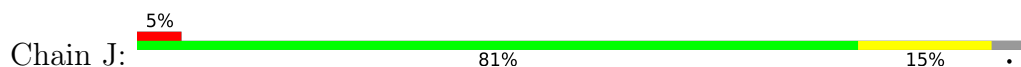


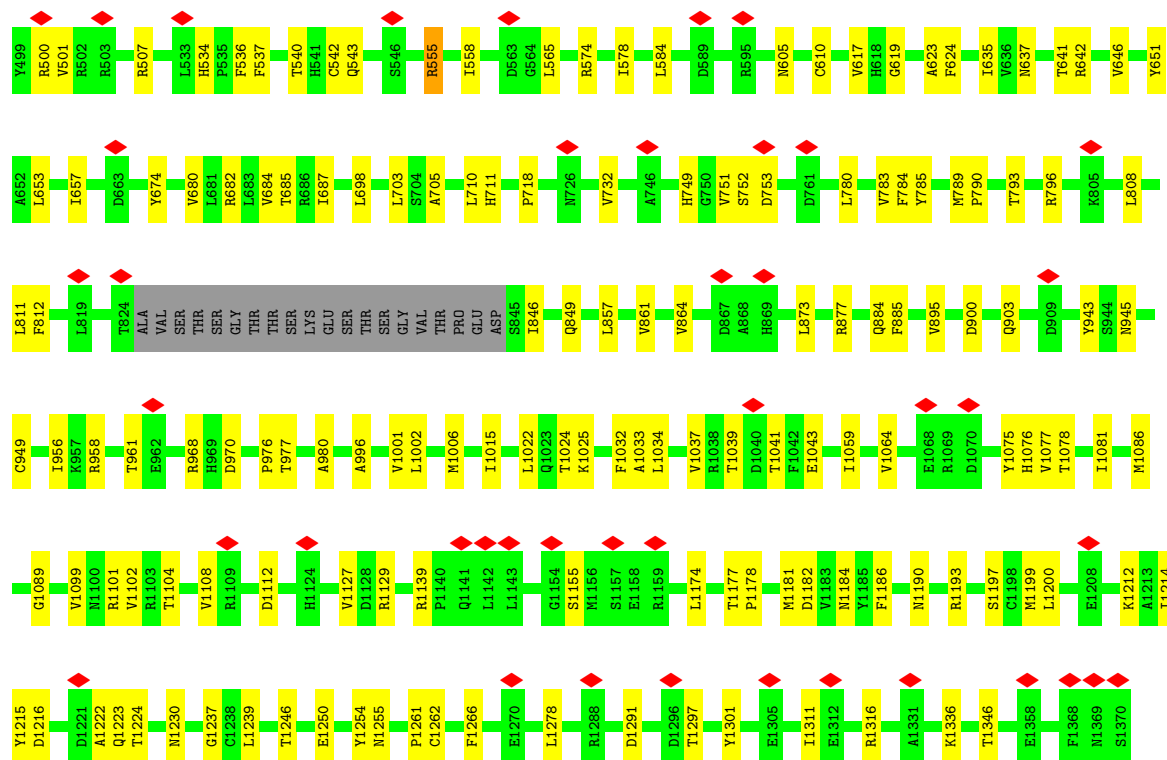






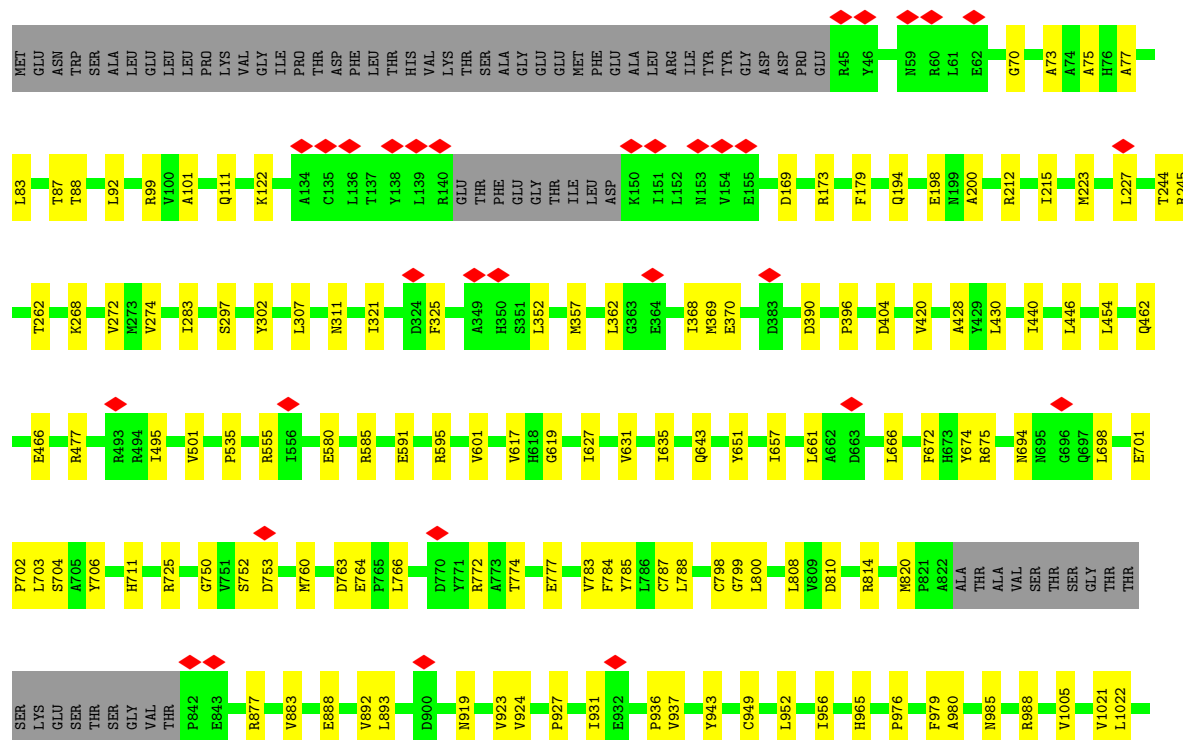
• Molecule 5: Major capsid protein

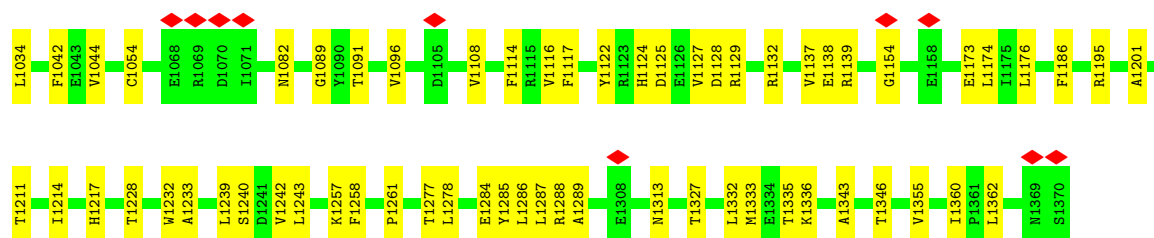




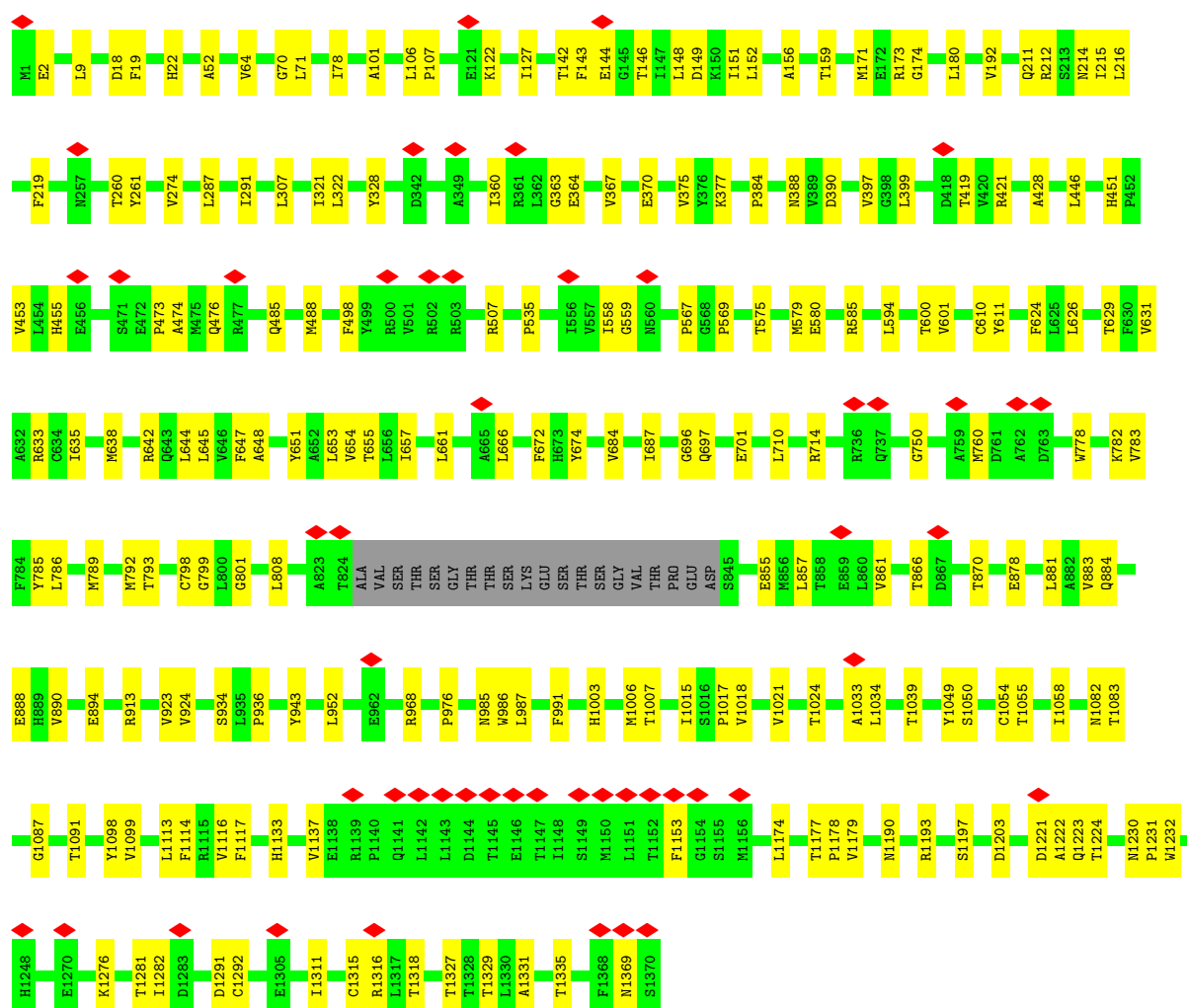
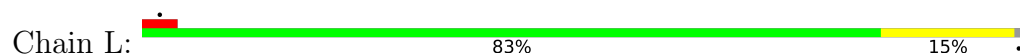
• Molecule 5: Major capsid protein

Chain K: 81% 14% 5%

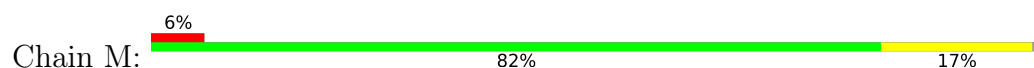


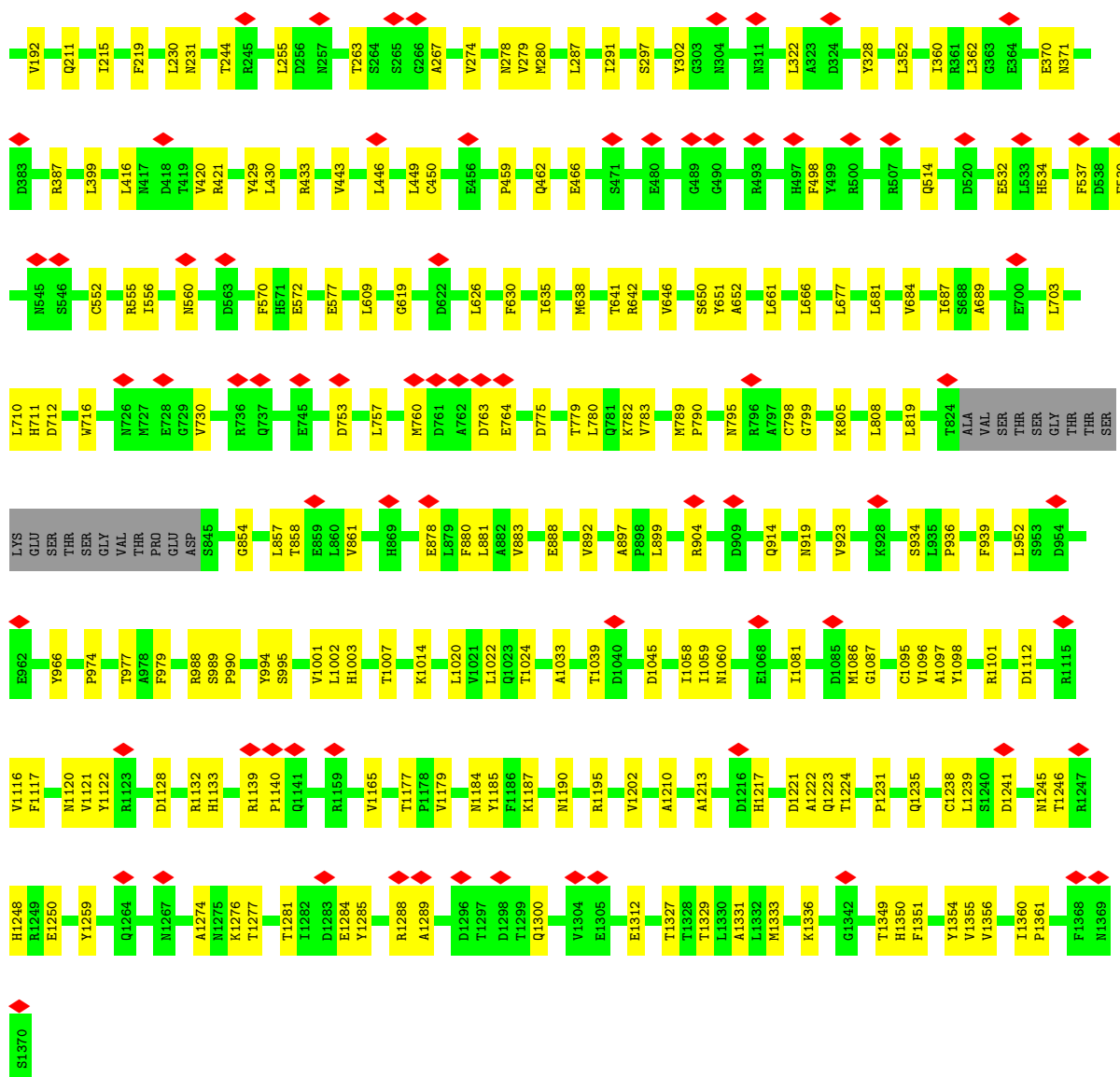


• Molecule 5: Major capsid protein



• Molecule 5: Major capsid protein

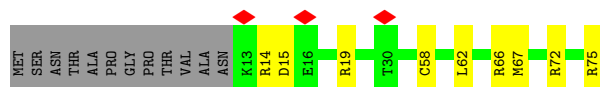




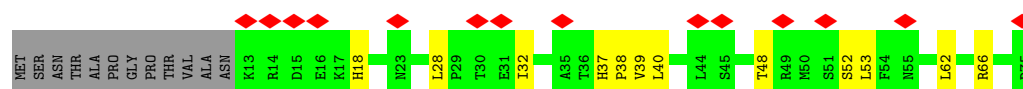
- Molecule 6: Small capsomere-interacting protein



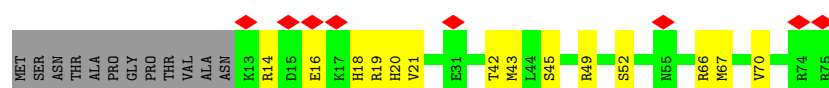
- Molecule 6: Small capsomere-interacting protein



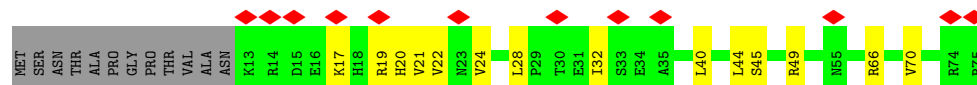
- Molecule 6: Small capsomere-interacting protein



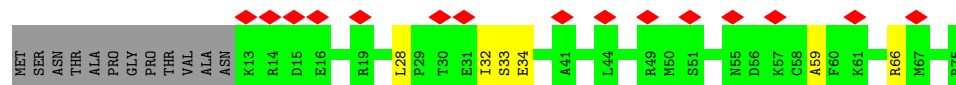
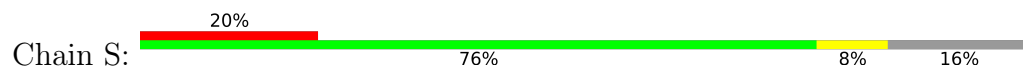
- Molecule 6: Small capsomere-interacting protein



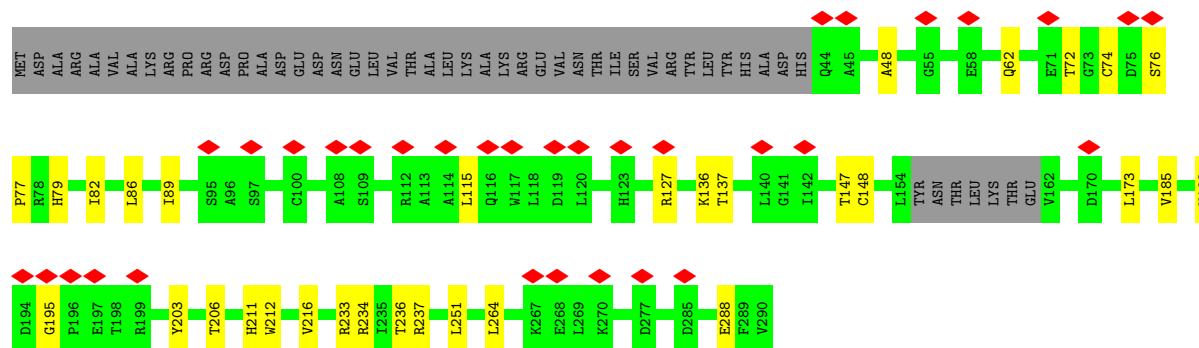
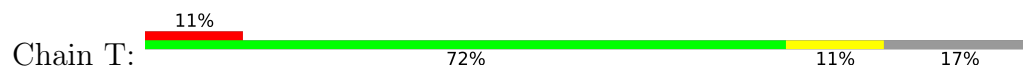
- Molecule 6: Small capsomere-interacting protein



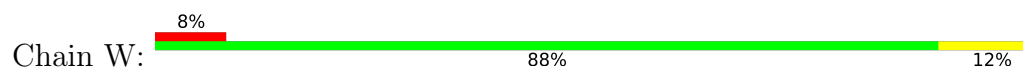
- Molecule 6: Small capsomere-interacting protein



- Molecule 7: Triplex capsid protein 1

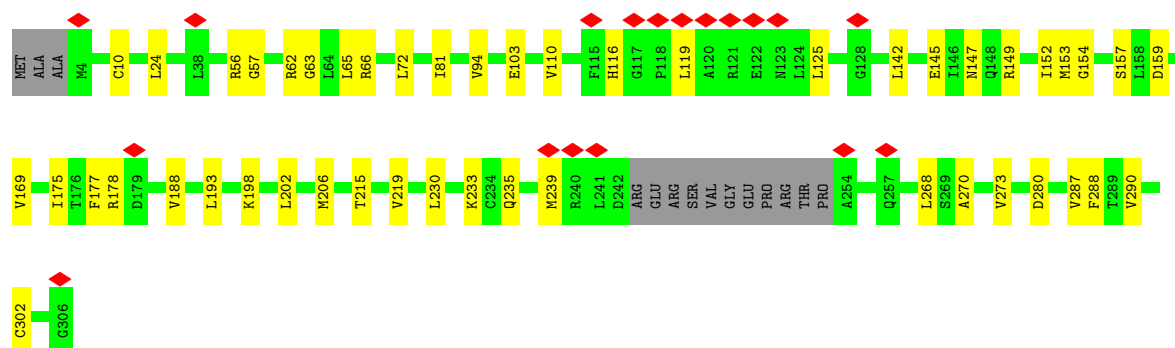
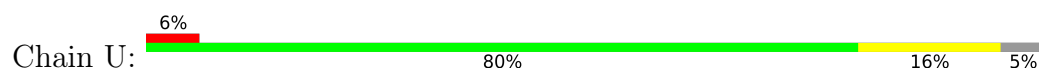


- Molecule 7: Triplex capsid protein 1

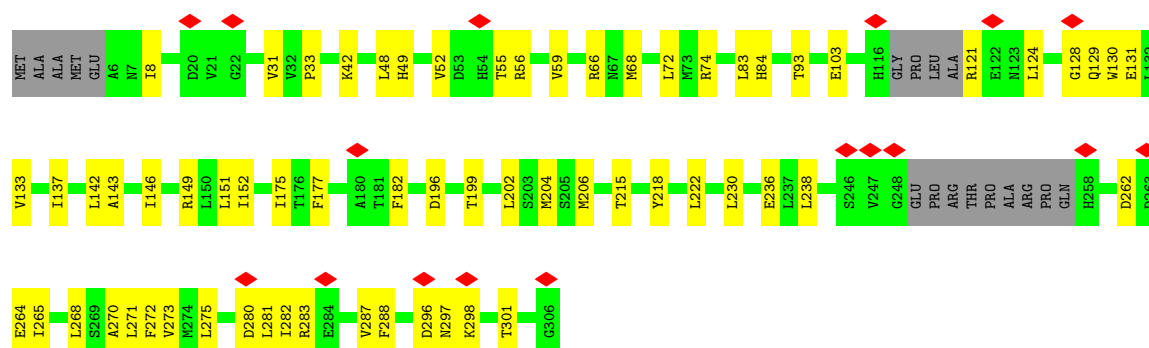
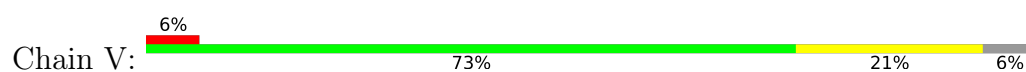




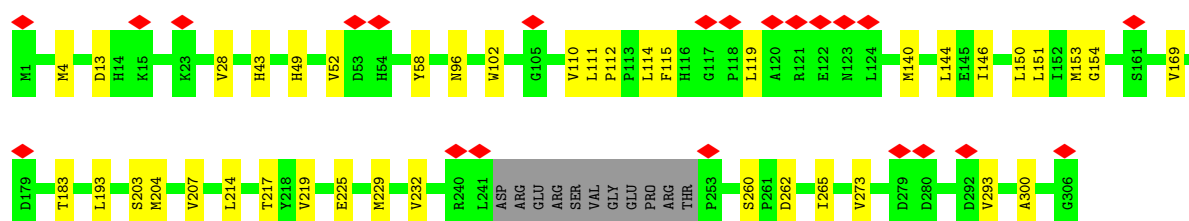
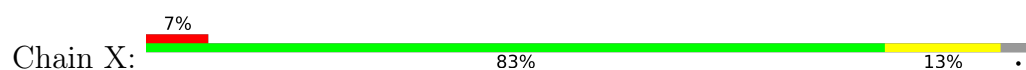
• Molecule 8: Triplex capsid protein 2



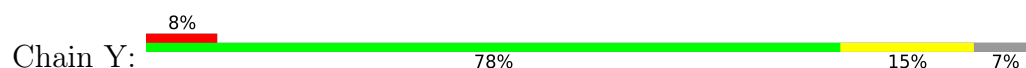
• Molecule 8: Triplex capsid protein 2



• Molecule 8: Triplex capsid protein 2



• Molecule 8: Triplex capsid protein 2



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	35055	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 ($e^-/\text{\AA}^2$)	47.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.035	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	489.6, 489.6, 489.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.14	0/5975	0.41	0/8149
1	C	0.18	0/5787	0.48	1/7885 (0.0%)
2	B	0.15	0/4082	0.45	1/5535 (0.0%)
2	D	0.19	0/3768	0.46	0/5111
3	E	0.14	0/4015	0.42	0/5453
3	F	0.13	0/4090	0.42	0/5557
4	G	0.17	0/3962	0.55	0/5371
5	H	0.30	0/10653	0.65	8/14508 (0.1%)
5	I	0.27	0/10949	0.61	6/14916 (0.0%)
5	J	0.23	0/10682	0.54	1/14553 (0.0%)
5	K	0.25	0/10527	0.58	7/14339 (0.0%)
5	L	0.21	0/10949	0.54	4/14916 (0.0%)
5	M	0.15	0/10949	0.46	2/14916 (0.0%)
6	N	0.14	0/520	0.46	0/697
6	O	0.12	0/520	0.45	0/697
6	P	0.15	0/520	0.48	0/697
6	Q	0.16	0/520	0.50	0/697
6	R	0.16	0/520	0.51	0/697
6	S	0.15	0/520	0.49	0/697
7	T	0.15	0/1960	0.50	0/2658
7	W	0.31	0/2374	0.66	0/3221
8	U	0.16	0/2361	0.45	0/3206
8	V	0.18	0/2333	0.52	0/3164
8	X	0.18	0/2379	0.48	0/3230
8	Y	0.20	0/2305	0.55	0/3126
9	Z	0.16	0/2358	0.49	0/3182
All	All	0.21	0/115578	0.53	30/157178 (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
5	H	0	1
5	J	0	1
All	All	0	2

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	555	ARG	NE-CZ-NH2	7.03	125.53	119.20
5	H	1195	ARG	NE-CZ-NH2	6.81	125.33	119.20
5	H	1215	TYR	N-CA-C	6.50	121.41	112.90
5	I	1244	TYR	N-CA-C	6.15	119.98	112.23
5	L	18	ASP	CA-CB-CG	5.80	118.40	112.60
5	K	988	ARG	NE-CZ-NH2	5.79	124.41	119.20
5	H	1288	ARG	N-CA-C	5.72	120.39	112.90
5	I	1109	ARG	CA-C-N	5.71	128.37	120.49
5	I	1109	ARG	C-N-CA	5.71	128.37	120.49
5	H	663	ASP	CA-CB-CG	5.64	118.24	112.60
5	L	1153	PHE	N-CA-C	5.49	118.44	111.69
5	K	555	ARG	NE-CZ-NH2	5.47	124.12	119.20
5	K	1217	HIS	CB-CG-CD2	-5.45	124.12	131.20
5	H	219	PHE	CA-CB-CG	5.42	119.22	113.80
5	L	19	PHE	CA-CB-CG	5.35	119.15	113.80
5	H	649	HIS	CB-CG-CD2	-5.30	124.31	131.20
5	K	985	ASN	CA-CB-CG	5.29	117.89	112.60
5	K	753	ASP	CA-C-N	5.28	123.57	120.24
5	K	753	ASP	C-N-CA	5.28	123.57	120.24
5	K	1195	ARG	NE-CZ-NH2	5.26	123.94	119.20
5	I	861	VAL	N-CA-C	5.26	118.49	111.44
2	B	196	VAL	N-CA-C	-5.23	108.74	113.71
5	H	185	ARG	NE-CZ-NH2	5.17	123.85	119.20
5	L	22	HIS	CB-CG-CD2	-5.17	124.48	131.20
5	J	555	ARG	NE-CZ-NH2	5.12	123.80	119.20
1	C	2181	ASP	CA-CB-CG	5.08	117.68	112.60
5	M	753	ASP	CA-C-N	5.08	123.44	120.24
5	M	753	ASP	C-N-CA	5.08	123.44	120.24
5	I	1277	THR	CA-C-N	5.05	127.00	120.44
5	I	1277	THR	C-N-CA	5.05	127.00	120.44

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	H	611	TYR	Sidechain
5	J	555	ARG	Sidechain

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	5833	0	5848	155	0
1	C	5651	0	5691	131	0
2	B	3993	0	3925	124	0
2	D	3685	0	3611	101	0
3	E	3915	0	3838	85	0
3	F	3986	0	3912	70	0
4	G	3873	0	3792	49	0
5	H	10406	0	10362	139	0
5	I	10693	0	10635	168	0
5	J	10433	0	10379	139	0
5	K	10282	0	10238	124	0
5	L	10693	0	10635	140	0
5	M	10693	0	10635	151	0
6	N	513	0	539	9	0
6	O	513	0	539	9	0
6	P	513	0	539	11	0
6	Q	513	0	539	11	0
6	R	513	0	539	9	0
6	S	513	0	539	5	0
7	T	1919	0	1957	21	0
7	W	2325	0	2363	25	0
8	U	2317	0	2405	37	0
8	V	2292	0	2379	44	0
8	X	2334	0	2431	28	0
8	Y	2266	0	2355	28	0
9	Z	2320	0	2351	26	0
All	All	112987	0	112976	1709	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 (1709) 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)
5:K:1327:THR:HG21	5:K:1333:MET:HB2	1.58	0.83
5:M:446:LEU:HD21	5:M:1024:THR:HG21	1.61	0.83
1:A:1553:PRO:HB3	2:B:402:ILE:HA	1.62	0.80
5:H:446:LEU:HD11	5:H:1021:VAL:HG23	1.64	0.80
9:Z:57:MET:HE1	9:Z:272:ILE:HD11	1.64	0.80
1:A:1792:MET:HE2	1:A:2039:LEU:HB2	1.65	0.79
1:C:1700:VAL:HG11	1:C:1750:ILE:HG21	1.66	0.78
1:C:2232:ILE:HB	3:E:65:LEU:HD21	1.66	0.77
5:M:255:LEU:HD23	5:M:1086:MET:HE2	1.65	0.77
4:G:514:TRP:CD1	4:G:522:VAL:HG11	2.21	0.76
7:T:137:THR:HB	7:T:147:THR:HG22	1.68	0.75
5:M:760:MET:HG2	5:M:805:LYS:HB2	1.67	0.75
1:C:1697:CYS:HA	1:C:1700:VAL:HG12	1.69	0.75
5:L:212:ARG:HH22	5:L:1203:ASP:HA	1.52	0.75
3:E:505:TYR:HA	3:E:509:TRP:HD1	1.52	0.74
3:F:606:LEU:HD13	3:F:609:HIS:HB2	1.69	0.74
5:I:470:PRO:HB2	5:I:475:MET:HG2	1.68	0.74
7:W:61:ALA:HA	7:W:138:VAL:HG11	1.68	0.74
5:L:594:LEU:HD12	5:L:792:MET:HE3	1.70	0.74
5:H:672:PHE:HE2	5:I:643:GLN:HB2	1.52	0.73
5:H:716:TRP:O	5:H:914:GLN:NE2	2.21	0.73
2:D:220:MET:HE1	2:D:384:VAL:HB	1.71	0.72
5:I:701:GLU:OE2	5:I:714:ARG:NH2	2.22	0.72
5:L:760:MET:HG3	5:L:888:GLU:HB2	1.70	0.72
5:J:1039:THR:HG23	5:J:1261:PRO:HB3	1.70	0.72
5:H:575:THR:HG21	5:H:1007:THR:HA	1.70	0.72
3:E:604:VAL:HB	3:E:607:PRO:HG3	1.70	0.72
2:D:210:GLN:NE2	2:D:435:TYR:O	2.22	0.72
5:I:1047:LEU:HD22	5:I:1097:ALA:HB2	1.72	0.72
5:K:783:VAL:O	5:K:787:CYS:HB3	1.89	0.72
1:A:1618:LEU:HA	1:A:1621:ARG:HD3	1.72	0.71
8:U:72:LEU:HD11	8:U:94:VAL:HG12	1.73	0.71
9:Z:129:LEU:HD11	9:Z:204:VAL:HA	1.71	0.71
2:B:55:LEU:HD12	2:B:66:ARG:HH22	1.54	0.70
5:M:99:ARG:NH2	5:M:109:SER:O	2.24	0.70
5:H:432:ASN:OD1	5:H:438:GLN:NE2	2.25	0.70
1:A:1586:GLU:HB3	1:A:1596:ILE:HG12	1.73	0.70
2:B:223:VAL:HA	2:B:226:ARG:HH11	1.57	0.70
5:H:1101:ARG:HH22	5:I:202:LEU:HG	1.57	0.70
5:J:446:LEU:HD11	5:J:1024:THR:HG21	1.72	0.70
5:I:681:LEU:HD21	5:I:784:PHE:HB2	1.72	0.70
1:A:1579:ARG:NH2	1:A:1831:GLN:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1797:LEU:O	1:A:1800:GLN:NE2	2.25	0.69
1:A:1859:LEU:HD12	1:A:1877:VAL:HG11	1.74	0.69
5:L:474:ALA:HA	5:M:1133:HIS:CE1	2.28	0.69
5:K:70:GLY:N	5:K:370:GLU:OE2	2.25	0.69
6:Q:43:MET:HE3	6:Q:67:MET:HG2	1.74	0.69
2:B:74:LEU:HD21	2:B:96:LEU:HD11	1.75	0.68
5:J:272:VAL:HG12	5:J:368:ILE:HB	1.74	0.68
4:G:132:LEU:HD11	4:G:149:LEU:HD13	1.75	0.68
5:I:1142:LEU:HD13	5:I:1147:THR:HB	1.76	0.68
5:K:194:GLN:HE22	5:K:245:ARG:HG2	1.58	0.68
5:K:820:MET:HE2	5:K:877:ARG:HD3	1.74	0.68
2:B:48:VAL:HB	2:B:99:PHE:CZ	2.28	0.68
5:H:139:LEU:HD22	5:H:160:VAL:HG21	1.76	0.68
3:F:293:GLU:O	4:G:313:ARG:NH1	2.26	0.68
7:W:258:ASP:OD2	7:W:277:ASP:N	2.27	0.68
2:D:447:ARG:HH11	2:D:476:VAL:HG11	1.58	0.68
5:K:274:VAL:HG12	5:K:370:GLU:HB2	1.76	0.68
5:J:617:VAL:HG13	5:J:619:GLY:H	1.57	0.67
7:W:167:ILE:HD13	7:W:204:VAL:HG11	1.74	0.67
1:A:1548:ARG:HE	1:A:1549:LEU:H	1.43	0.67
5:I:173:ARG:HB3	5:J:100:VAL:HG12	1.75	0.67
5:K:694:ASN:ND2	5:K:704:SER:OG	2.28	0.67
5:L:750:GLY:HA2	6:R:70:VAL:HG11	1.77	0.67
5:J:710:LEU:HD21	5:J:783:VAL:HG22	1.76	0.67
5:H:36:ARG:NH2	5:H:44:GLU:OE2	2.27	0.67
5:L:600:THR:HG23	5:L:644:LEU:HD12	1.77	0.67
1:C:1519:THR:HA	1:C:1522:LEU:HD12	1.77	0.67
5:J:732:VAL:HG12	5:J:895:VAL:HG12	1.77	0.67
5:J:703:LEU:HD22	5:J:1022:LEU:HD11	1.77	0.66
5:I:1195:ARG:NH1	5:I:1216:ASP:O	2.28	0.66
5:I:666:LEU:HD12	5:I:667:PRO:HD2	1.76	0.66
5:I:1332:LEU:HD23	5:I:1355:VAL:HG23	1.77	0.66
5:K:1124:HIS:HB3	5:K:1127:VAL:HG12	1.77	0.66
1:A:1957:PRO:HG3	1:A:2036:PHE:HD1	1.61	0.66
1:C:1753:LEU:HD23	1:C:1803:ALA:HB3	1.78	0.66
5:M:1235:GLN:HB2	5:M:1238:CYS:HB3	1.77	0.66
5:L:610:CYS:HA	5:L:647:PHE:HE1	1.61	0.66
5:H:440:ILE:HB	5:H:1108:VAL:HG21	1.77	0.66
5:K:1154:GLY:HA3	5:K:1257:LYS:HE3	1.77	0.66
1:C:1843:LYS:NZ	1:C:1938:PHE:O	2.29	0.65
5:M:462:GLN:O	5:M:466:GLU:HG2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:202:LEU:HD22	8:V:230:LEU:HD11	1.79	0.65
2:D:222:TYR:O	2:D:226:ARG:NH2	2.29	0.65
3:E:377:ILE:HD12	3:E:380:LEU:HD11	1.78	0.65
1:A:1596:ILE:HB	1:A:1604:ILE:HD11	1.79	0.65
2:D:239:MET:HE3	2:D:257:PHE:HD1	1.61	0.65
4:G:571:HIS:HA	8:U:188:VAL:HG23	1.79	0.65
5:J:1214:ILE:HG22	5:J:1215:TYR:HD1	1.62	0.65
2:D:399:MET:HA	2:D:402:ILE:HB	1.79	0.64
5:J:1037:VAL:HG21	5:J:1262:CYS:HB3	1.79	0.64
2:B:32:GLN:HA	2:B:35:ILE:HG12	1.79	0.64
1:A:1862:LEU:HD11	1:A:1952:TRP:HH2	1.60	0.64
8:X:154:GLY:HA3	8:X:193:LEU:HD21	1.79	0.64
5:J:641:THR:HG23	5:J:642:ARG:HG3	1.77	0.64
1:C:1983:SER:OG	1:C:1984:ARG:NH2	2.30	0.64
5:K:766:LEU:HD11	5:K:893:LEU:HD21	1.80	0.64
5:K:1336:LYS:NZ	5:K:1343:ALA:O	2.29	0.64
2:B:492:HIS:HD2	2:B:493:THR:HG23	1.63	0.64
1:A:1952:TRP:O	1:A:1995:ARG:NH1	2.28	0.64
1:A:2228:VAL:HG11	3:F:72:VAL:HG11	1.80	0.64
2:B:447:ARG:NH2	2:B:480:PHE:O	2.30	0.64
5:M:716:TRP:O	5:M:914:GLN:NE2	2.31	0.64
2:B:331:HIS:CD2	2:B:334:LEU:H	2.15	0.64
4:G:42:TYR:HB2	4:G:152:VAL:HB	1.79	0.64
8:U:24:LEU:HD21	8:U:81:ILE:HD12	1.80	0.64
8:U:62:ARG:NH2	8:U:147:ASN:OD1	2.31	0.64
5:L:778:TRP:CD1	5:L:782:LYS:HZ1	2.16	0.63
6:S:28:LEU:HD12	6:S:32:ILE:HD11	1.79	0.63
1:C:1765:PRO:HB3	1:C:2119:ILE:HA	1.79	0.63
8:U:149:ARG:HD2	8:U:175:ILE:HD11	1.80	0.63
1:C:1566:LEU:HA	1:C:1569:ARG:HG2	1.80	0.63
1:A:1627:LEU:HD23	1:A:1630:ARG:HG3	1.80	0.63
1:A:1607:VAL:HG13	1:A:1608:THR:HG23	1.80	0.63
5:M:278:ASN:ND2	5:M:1098:TYR:OH	2.31	0.63
1:A:1602:GLU:HG2	1:A:1607:VAL:HB	1.81	0.63
8:Y:74:ARG:HG3	8:Y:75:ARG:H	1.63	0.63
1:A:1548:ARG:HG3	1:A:1550:GLU:H	1.64	0.63
4:G:316:GLU:OE1	4:G:325:ARG:NH2	2.32	0.63
5:K:1239:LEU:HA	5:K:1242:VAL:HG12	1.81	0.63
5:I:104:ALA:HB3	8:V:42:LYS:HE2	1.80	0.63
5:J:1177:THR:OG1	5:J:1230:ASN:ND2	2.32	0.62
5:H:1168:GLN:NE2	5:H:1297:THR:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1224:THR:HG23	5:H:1226:ALA:H	1.63	0.62
5:I:315:ALA:HB2	5:I:321:ILE:HD11	1.79	0.62
8:V:72:LEU:O	8:V:84:HIS:N	2.31	0.62
1:C:1604:ILE:HA	1:C:1607:VAL:HG12	1.80	0.62
3:F:23:VAL:HG12	4:G:393:HIS:HB2	1.81	0.62
5:J:682:ARG:HH11	5:J:780:LEU:HD11	1.64	0.62
2:B:300:GLN:O	2:B:302:ARG:NH2	2.31	0.62
8:U:65:LEU:HD21	8:U:110:VAL:HG22	1.80	0.62
2:B:505:TYR:OH	2:B:515:HIS:ND1	2.31	0.62
1:A:1789:THR:O	1:A:1790:HIS:ND1	2.33	0.62
1:C:1835:GLN:HG3	1:C:1836:LYS:H	1.63	0.62
3:E:411:LEU:HD12	3:E:412:LEU:HG	1.79	0.62
9:Z:174:VAL:HG13	9:Z:181:VAL:HG11	1.82	0.62
5:L:446:LEU:HD11	5:L:1021:VAL:HG23	1.82	0.62
1:C:1486:PHE:HD2	1:C:1522:LEU:HD11	1.63	0.62
1:C:1501:GLY:O	1:C:1520:ARG:NH2	2.33	0.62
2:D:293:LYS:HA	2:D:296:VAL:HG12	1.82	0.62
5:H:730:VAL:HG23	5:H:897:ALA:HB2	1.82	0.62
5:L:701:GLU:OE1	5:L:714:ARG:NH1	2.29	0.62
5:M:798:CYS:SG	5:M:799:GLY:N	2.73	0.61
3:E:278:GLU:OE2	3:E:415:LYS:NZ	2.33	0.61
4:G:312:SER:O	4:G:313:ARG:HG3	2.00	0.61
5:J:534:HIS:CE1	5:J:1239:LEU:HD12	2.36	0.61
5:K:657:ILE:HA	5:K:661:LEU:HD13	1.82	0.61
2:B:399:MET:HA	2:B:402:ILE:HB	1.82	0.61
4:G:476:ASP:HB2	4:G:523:LEU:HD23	1.81	0.61
5:H:40:GLY:HA2	5:K:111:GLN:HB2	1.82	0.61
5:I:1336:LYS:HE3	5:I:1355:VAL:HG11	1.81	0.61
5:J:624:PHE:HZ	5:J:657:ILE:HD13	1.65	0.61
5:K:169:ASP:OD1	5:K:173:ARG:NH2	2.31	0.61
5:K:244:THR:HA	5:K:362:LEU:HD23	1.82	0.61
5:L:558:ILE:HD13	5:L:1015:ILE:HD13	1.82	0.61
2:D:378:GLN:HA	2:D:381:MET:SD	2.40	0.61
5:I:820:MET:O	6:O:72:ARG:NH2	2.34	0.61
8:Y:32:VAL:O	8:Y:71:THR:OG1	2.17	0.61
2:B:5:ARG:HH11	2:B:199:ARG:HE	1.48	0.61
5:L:535:PRO:HG3	5:L:1232:TRP:CD2	2.35	0.61
1:A:1586:GLU:HA	1:A:1596:ILE:HA	1.82	0.61
1:C:1584:PHE:HZ	1:C:1596:ILE:HB	1.64	0.61
5:H:617:VAL:HG13	5:H:619:GLY:H	1.64	0.61
5:M:710:LEU:HD21	5:M:783:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:970:ASP:OD2	5:I:993:ARG:NH2	2.32	0.61
5:L:473:PRO:HA	5:L:476:GLN:HB2	1.82	0.61
2:B:70:VAL:HG22	2:B:96:LEU:HD22	1.82	0.60
1:C:1990:ARG:NH2	1:C:2168:PHE:O	2.34	0.60
2:D:422:GLN:O	2:D:426:ASN:ND2	2.29	0.60
5:J:1193:ARG:NH1	5:J:1197:SER:OG	2.25	0.60
1:A:1567:ILE:O	1:A:1571:ARG:HG2	2.00	0.60
5:K:965:HIS:CE1	5:L:696:GLY:H	2.19	0.60
1:C:1846:LEU:HD11	1:C:1950:GLY:HA2	1.83	0.60
5:J:1155:SER:HA	5:J:1255:ASN:HD21	1.66	0.60
5:M:1327:THR:HG21	5:M:1333:MET:HB2	1.83	0.60
5:H:578:ILE:HD13	5:H:1028:ILE:HD12	1.83	0.60
5:L:631:VAL:HG23	5:L:647:PHE:CD2	2.37	0.60
5:M:1139:ARG:HD3	5:M:1140:PRO:HD2	1.83	0.60
1:A:1659:LEU:HD21	1:A:1693:LEU:HD22	1.84	0.60
2:D:75:SER:HA	2:D:198:CYS:HA	1.84	0.60
3:E:308:LEU:HG	3:E:309:PRO:HD3	1.83	0.60
3:F:284:LEU:HD13	3:F:315:LEU:HD22	1.82	0.60
8:Y:33:PRO:HB2	8:Y:68:MET:HG2	1.84	0.60
2:D:485:THR:HG22	2:D:487:GLU:H	1.67	0.60
3:F:227:ARG:HG3	3:F:244:MET:HE3	1.83	0.60
5:L:631:VAL:HG23	5:L:647:PHE:HD2	1.67	0.60
1:A:1867:LYS:HD2	1:A:1872:GLU:HA	1.82	0.60
1:C:1656:CYS:HB3	1:C:1660:ARG:HH22	1.65	0.60
4:G:316:GLU:HB3	4:G:325:ARG:HD3	1.84	0.60
1:A:1875:ALA:HB3	1:A:1879:GLU:HG2	1.83	0.59
1:A:1992:GLN:OE1	1:A:1995:ARG:NH1	2.35	0.59
5:I:624:PHE:HZ	5:I:657:ILE:HD13	1.67	0.59
5:I:985:ASN:O	5:I:988:ARG:NH2	2.35	0.59
5:L:1222:ALA:O	5:L:1223:GLN:HG3	2.01	0.59
5:M:1329:THR:HG22	5:M:1331:ALA:H	1.67	0.59
8:U:268:LEU:HD22	8:V:152:ILE:HG23	1.84	0.59
5:K:99:ARG:NH1	5:K:111:GLN:OE1	2.35	0.59
1:A:2016:TRP:O	1:A:2020:GLN:NE2	2.35	0.59
3:E:278:GLU:HG2	3:E:412:LEU:HD21	1.84	0.59
5:H:433:ARG:HH22	5:I:217:GLN:HB2	1.67	0.59
5:I:373:ARG:NH2	5:I:376:TYR:O	2.35	0.59
5:K:446:LEU:HD11	5:K:1021:VAL:HG22	1.83	0.59
1:C:1814:MET:HG3	1:C:2054:ARG:HB2	1.84	0.59
3:E:538:TRP:HZ3	3:E:593:HIS:HA	1.68	0.59
5:I:1193:ARG:HH21	5:I:1195:ARG:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:763:ASP:OD1	5:K:764:GLU:N	2.35	0.59
5:M:514:GLN:NE2	5:M:989:SER:OG	2.35	0.59
1:A:1585:LEU:N	1:A:1597:VAL:O	2.27	0.59
5:K:643:GLN:HB2	5:L:672:PHE:CE2	2.38	0.59
2:D:198:CYS:HB2	2:D:201:VAL:HG22	1.84	0.59
2:B:113:LEU:HD12	2:B:116:TYR:H	1.67	0.59
1:C:1790:HIS:HA	1:C:2056:PRO:HD2	1.84	0.59
3:E:460:PHE:HE1	3:E:465:LEU:HD11	1.68	0.59
5:H:112:THR:HG22	5:H:113:THR:HG23	1.85	0.59
1:C:1452:LEU:HB3	1:C:1486:PHE:HE1	1.68	0.59
1:C:1620:LEU:HD11	1:C:2006:THR:HG22	1.84	0.59
3:E:444:TRP:O	3:E:448:ASN:ND2	2.35	0.59
2:B:368:ARG:HA	2:B:478:THR:HG23	1.84	0.58
1:C:1536:LEU:HA	1:C:1539:LYS:HE3	1.85	0.58
1:C:1566:LEU:HD23	1:C:1569:ARG:HD3	1.84	0.58
5:M:888:GLU:H	5:M:919:ASN:ND2	2.01	0.58
5:M:899:LEU:O	5:M:904:ARG:NH2	2.32	0.58
5:J:574:ARG:O	5:J:578:ILE:HG12	2.03	0.58
1:A:1903:GLN:HA	1:A:1909:PRO:HA	1.85	0.58
2:B:196:VAL:HG13	2:B:440:THR:HG22	1.85	0.58
1:C:1859:LEU:HD23	1:C:1862:LEU:HD21	1.85	0.58
5:H:757:LEU:HD11	6:N:62:LEU:HD22	1.85	0.58
5:K:1332:LEU:HD23	5:K:1355:VAL:HG23	1.83	0.58
7:W:182:LEU:HB2	8:X:4:MET:HE3	1.85	0.58
2:D:199:ARG:HG3	2:D:511:LYS:HE3	1.85	0.58
5:L:106:LEU:HD12	5:L:107:PRO:HD2	1.85	0.58
7:T:86:LEU:HD11	7:T:115:LEU:HD21	1.84	0.58
1:A:2014:HIS:O	1:A:2018:GLN:HG2	2.03	0.58
5:H:934:SER:OG	5:H:952:LEU:HD11	2.03	0.58
7:W:76:SER:HB3	7:W:77:PRO:HD2	1.85	0.58
9:Z:239:LEU:HD22	9:Z:251:ARG:HG3	1.85	0.58
5:K:101:ALA:HB3	5:L:174:GLY:HA3	1.86	0.58
5:L:798:CYS:SG	5:L:799:GLY:N	2.77	0.58
5:M:1327:THR:HB	5:M:1355:VAL:HG12	1.85	0.58
5:K:1176:LEU:HB2	5:K:1239:LEU:HD21	1.86	0.58
5:K:1284:GLU:OE1	5:K:1288:ARG:NH2	2.36	0.58
5:K:1336:LYS:NZ	5:K:1346:THR:O	2.35	0.58
2:D:206:ASP:O	2:D:210:GLN:HG2	2.04	0.58
4:G:5:LEU:HD13	4:G:306:TRP:CD1	2.39	0.58
3:E:289:HIS:HB2	3:E:407:TRP:HE1	1.69	0.57
1:C:1613:VAL:HG11	1:C:2021:ILE:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:226:LYS:HG3	3:E:241:LEU:HD22	1.85	0.57
5:K:70:GLY:HA3	5:K:357:MET:HE1	1.85	0.57
6:R:28:LEU:HD12	6:R:32:ILE:HG21	1.85	0.57
9:Z:197:VAL:HA	9:Z:200:VAL:HG12	1.85	0.57
1:A:1785:VAL:HG13	1:A:1804:PHE:HA	1.86	0.57
5:I:230:LEU:HD23	5:I:1097:ALA:HB1	1.85	0.57
5:L:661:LEU:HD23	5:L:666:LEU:HD11	1.85	0.57
6:Q:42:THR:O	6:Q:45:SER:OG	2.22	0.57
3:E:243:GLN:HE21	3:E:246:ASN:HB3	1.70	0.57
5:H:689:ALA:HB2	5:H:711:HIS:CE1	2.39	0.57
5:L:192:VAL:HG11	5:L:1282:ILE:HD12	1.86	0.57
2:D:241:PHE:HA	2:D:244:THR:HG22	1.86	0.57
3:F:291:LEU:HD11	3:F:314:ARG:HG3	1.86	0.57
5:H:704:SER:HA	5:H:707:VAL:HG12	1.86	0.57
5:K:1125:ASP:OD2	5:K:1129:ARG:NH1	2.37	0.57
5:K:1128:ASP:O	5:K:1132:ARG:HG2	2.05	0.57
5:I:596:LEU:O	5:I:600:THR:HG23	2.04	0.57
5:M:626:LEU:HD21	5:M:881:LEU:HB2	1.86	0.57
5:H:1124:HIS:HB3	5:H:1127:VAL:HG12	1.87	0.57
5:I:534:HIS:CE1	5:I:1239:LEU:HD12	2.40	0.57
5:I:1169:LYS:HE2	5:I:1299:THR:HG22	1.87	0.57
5:J:1297:THR:HG21	5:J:1301:TYR:HD2	1.70	0.57
2:B:501:ARG:HD2	2:B:519:LEU:HD23	1.86	0.57
1:C:2231:THR:HG22	1:C:2235:MET:HE2	1.86	0.57
5:I:600:THR:HG21	5:I:645:LEU:HG	1.86	0.57
5:K:272:VAL:HG12	5:K:368:ILE:HB	1.87	0.57
5:M:1285:TYR:HA	5:M:1289:ALA:HB3	1.86	0.57
1:A:1755:PRO:HB2	1:A:2105:VAL:HG23	1.87	0.57
2:B:113:LEU:HD13	2:B:115:PHE:HB3	1.87	0.57
1:C:1707:ARG:NH1	1:C:1779:GLN:OE1	2.37	0.57
1:C:2205:GLN:HG2	3:F:90:LEU:HA	1.86	0.57
3:F:330:VAL:HG21	3:F:364:ARG:HA	1.87	0.57
5:H:390:ASP:HB2	5:H:1311:ILE:HG21	1.87	0.57
5:L:1193:ARG:HH12	5:L:1197:SER:HB3	1.69	0.57
5:M:416:LEU:HD21	5:M:1329:THR:HG21	1.86	0.57
8:Y:296:ASP:O	8:Y:298:LYS:N	2.38	0.57
1:A:1754:TYR:HB2	1:A:1757:TYR:CE2	2.40	0.57
2:B:293:LYS:HB3	2:B:299:LEU:HD13	1.87	0.57
5:H:1122:TYR:HB2	5:H:1128:ASP:HB2	1.87	0.57
8:X:265:ILE:HD11	8:Y:148:GLN:HB3	1.87	0.57
5:K:454:LEU:HD21	5:K:1243:LEU:HD11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:173:ARG:NH2	5:L:375:VAL:O	2.37	0.56
5:L:866:THR:OG1	5:L:870:THR:O	2.22	0.56
5:L:1291:ASP:OD1	5:L:1316:ARG:NH1	2.33	0.56
7:T:136:LYS:HD2	7:T:136:LYS:O	2.05	0.56
2:B:65:VAL:O	2:B:69:VAL:HB	2.05	0.56
2:B:497:THR:HG23	2:B:499:ALA:H	1.69	0.56
5:H:155:GLU:HG3	5:L:9:LEU:HD13	1.87	0.56
5:J:432:ASN:HB2	5:J:434:ASP:O	2.06	0.56
8:V:264:GLU:O	8:V:268:LEU:HD12	2.06	0.56
4:G:91:ARG:NH2	8:U:159:ASP:OD1	2.37	0.56
5:H:433:ARG:HD2	5:H:1105:ASP:HA	1.88	0.56
5:H:449:LEU:HD21	5:H:1034:LEU:HD21	1.88	0.56
5:L:633:ARG:NH1	5:L:878:GLU:OE2	2.26	0.56
8:U:202:LEU:HB2	8:V:230:LEU:HD21	1.86	0.56
1:A:1815:GLN:HB2	1:A:1818:LYS:HE2	1.88	0.56
1:A:2236:ARG:HA	1:A:2240:LEU:HD23	1.87	0.56
5:H:216:LEU:HD13	5:H:1200:LEU:HD12	1.86	0.56
5:I:311:ASN:HD21	5:I:325:PHE:HB2	1.70	0.56
5:J:440:ILE:HD12	5:J:1108:VAL:HB	1.86	0.56
3:E:264:VAL:HG21	3:E:590:LEU:HD22	1.86	0.56
5:H:83:LEU:HA	5:H:86:LEU:HD23	1.87	0.56
5:H:1105:ASP:HB3	5:H:1166:HIS:O	2.05	0.56
1:A:1814:MET:HB2	1:C:1631:ARG:HH22	1.70	0.56
2:B:112:ARG:NH2	2:B:500:GLU:OE2	2.38	0.56
5:I:1034:LEU:HD12	5:I:1174:LEU:HB3	1.87	0.56
5:J:1250:GLU:OE2	5:J:1254:TYR:OH	2.22	0.56
8:U:280:ASP:OD1	8:V:283:ARG:NH1	2.36	0.56
5:M:291:ILE:HG22	5:M:360:ILE:HG22	1.86	0.56
1:C:2218:ARG:NH1	3:E:87:GLU:OE1	2.39	0.56
5:I:965:HIS:O	5:I:968:ARG:NH2	2.38	0.56
5:K:949:CYS:HB3	5:K:956:ILE:HD13	1.88	0.56
8:V:215:THR:HG22	8:V:238:LEU:HD22	1.88	0.56
2:B:315:ARG:HH12	2:B:347:ALA:HB2	1.70	0.56
2:D:337:ARG:HH12	2:D:343:VAL:HG13	1.71	0.56
5:H:886:VAL:HG21	6:N:62:LEU:HD21	1.87	0.56
8:V:218:TYR:OH	8:V:268:LEU:HD11	2.06	0.56
1:C:1688:HIS:NE2	1:C:2115:ASN:OD1	2.37	0.56
5:H:424:LEU:HD13	5:H:573:LEU:HD23	1.88	0.56
8:Y:49:HIS:O	8:Y:52:VAL:HG12	2.06	0.56
2:D:453:GLN:O	2:D:457:THR:HG22	2.06	0.55
5:H:1027:HIS:CD2	5:I:517:VAL:HG11	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1350:HIS:CG	5:M:1351:PHE:H	2.24	0.55
1:A:2179:CYS:SG	1:A:2180:ARG:N	2.79	0.55
1:A:1799:GLU:HG3	1:A:2164:GLY:HA3	1.86	0.55
5:H:1329:THR:HG22	5:H:1331:ALA:H	1.70	0.55
8:V:151:LEU:HD11	8:V:281:LEU:HD13	1.88	0.55
1:A:1800:GLN:HE21	1:A:1801:VAL:HG12	1.70	0.55
1:C:1586:GLU:HG3	1:C:1596:ILE:HG22	1.88	0.55
1:C:1597:VAL:HG12	1:C:1603:PRO:HA	1.88	0.55
2:D:34:GLU:OE2	2:D:72:TYR:OH	2.25	0.55
2:D:278:GLY:HA2	2:D:281:LYS:HE2	1.89	0.55
5:H:571:HIS:O	5:H:575:THR:HG23	2.06	0.55
6:N:28:LEU:HD12	6:N:29:PRO:HD2	1.88	0.55
8:U:10:CYS:HB3	8:U:81:ILE:HG23	1.88	0.55
2:D:127:LYS:O	2:D:131:THR:HG23	2.06	0.55
5:M:572:GLU:OE2	5:M:994:TYR:OH	2.16	0.55
7:T:236:THR:HG23	7:T:237:ARG:HG3	1.89	0.55
8:X:293:VAL:HG23	8:X:300:ALA:HB2	1.88	0.55
2:B:328:MET:HE2	2:B:334:LEU:HD13	1.89	0.55
1:C:1806:ILE:HD11	1:C:1811:TRP:CE2	2.41	0.55
3:E:592:PHE:HA	3:E:595:GLU:OE1	2.07	0.55
5:H:574:ARG:O	5:H:578:ILE:HG12	2.07	0.55
8:Y:70:LEU:HD21	8:Y:110:VAL:HG21	1.89	0.55
3:E:456:ARG:NH2	3:E:458:GLY:O	2.35	0.55
5:I:712:ASP:O	5:I:782:LYS:NZ	2.40	0.55
5:I:800:LEU:HD23	5:I:923:VAL:HG11	1.88	0.55
5:M:84:ASN:OD1	5:M:1060:ASN:ND2	2.39	0.55
3:F:315:LEU:HD23	3:F:441:LEU:HD13	1.89	0.55
5:I:211:GLN:O	5:I:215:ILE:HG12	2.07	0.55
5:K:390:ASP:OD1	5:K:1313:ASN:ND2	2.40	0.55
5:L:1018:VAL:HA	5:L:1021:VAL:HG12	1.89	0.55
5:M:619:GLY:HA3	5:M:652:ALA:HB1	1.87	0.55
5:M:795:ASN:ND2	5:M:995:SER:OG	2.39	0.55
1:A:1796:HIS:HB2	1:A:1800:GLN:NE2	2.22	0.55
5:J:486:GLU:OE2	5:J:977:THR:OG1	2.23	0.55
5:K:198:GLU:OE2	5:K:245:ARG:NH2	2.40	0.55
7:T:234:ARG:HG2	8:U:206:MET:HE1	1.89	0.55
1:A:2001:GLN:HG2	1:A:2002:LEU:HD12	1.89	0.54
5:I:272:VAL:HG22	5:I:368:ILE:HB	1.89	0.54
5:M:274:VAL:HG12	5:M:370:GLU:HB2	1.89	0.54
8:U:56:ARG:HG2	8:U:57:GLY:H	1.72	0.54
1:A:1749:LEU:HD11	1:A:1974:LEU:HG	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1772:SER:O	1:A:1776:HIS:ND1	2.29	0.54
1:A:2221:LEU:HD23	3:F:80:GLU:HB2	1.88	0.54
3:E:438:ALA:HB1	3:E:602:LEU:HD11	1.89	0.54
5:K:297:SER:HB3	5:K:352:LEU:HD12	1.89	0.54
1:A:1468:TYR:HB3	1:A:1475:GLN:NE2	2.22	0.54
5:H:174:GLY:HA3	5:I:101:ALA:HB3	1.88	0.54
5:I:1178:PRO:HG3	5:I:1231:PRO:HD2	1.90	0.54
5:M:936:PRO:HB3	5:M:952:LEU:HD23	1.89	0.54
8:U:103:GLU:OE1	8:U:178:ARG:NH2	2.39	0.54
9:Z:172:GLU:OE2	9:Z:176:ARG:NH1	2.40	0.54
2:B:319:VAL:HG11	2:B:334:LEU:HD11	1.88	0.54
3:F:37:ASP:HB3	5:K:501:VAL:HG23	1.89	0.54
5:H:672:PHE:CE2	5:I:643:GLN:HB2	2.39	0.54
5:M:560:ASN:CG	5:M:988:ARG:HG3	2.32	0.54
1:A:1987:ASP:HB3	1:A:2168:PHE:HD2	1.72	0.54
2:B:79:VAL:HG13	2:B:88:ALA:HB3	1.90	0.54
2:D:284:ALA:HA	2:D:287:MET:HG2	1.89	0.54
5:J:646:VAL:O	5:J:674:TYR:OH	2.25	0.54
9:Z:121:ASP:OD1	9:Z:122:ALA:N	2.40	0.54
1:A:1545:LEU:HD13	1:A:1825:LEU:HD21	1.89	0.54
2:B:379:MET:O	2:B:383:LEU:HG	2.08	0.54
1:C:1476:LEU:HD23	1:C:1479:ILE:HD11	1.90	0.54
1:C:1756:GLU:HB2	1:C:2102:PHE:CE1	2.42	0.54
5:H:211:GLN:O	5:H:215:ILE:HG12	2.08	0.54
5:I:688:SER:OG	5:I:708:ASN:ND2	2.41	0.54
8:Y:74:ARG:HG3	8:Y:75:ARG:HD3	1.90	0.54
2:B:85:PRO:HG2	2:B:86:LEU:HD12	1.89	0.54
1:C:1663:TRP:HA	1:C:1666:ILE:HG22	1.89	0.54
3:E:264:VAL:O	3:E:587:HIS:NE2	2.40	0.54
5:I:1165:VAL:HG22	5:J:1222:ALA:HB1	1.89	0.54
7:W:126:HIS:HE1	7:W:286:PHE:HB3	1.73	0.54
8:U:215:THR:HG22	8:V:204:MET:HE1	1.90	0.54
2:B:135:ILE:HG12	2:B:185:LEU:HD11	1.90	0.54
2:D:327:ARG:HH22	2:D:386:LEU:HD23	1.73	0.54
5:I:1165:VAL:HG21	5:J:1223:GLN:HB3	1.90	0.54
5:L:801:GLY:HA3	5:L:890:VAL:HG11	1.88	0.54
1:C:2003:LEU:HD23	1:C:2014:HIS:CD2	2.43	0.53
5:J:495:ILE:HD12	5:J:976:PRO:HG2	1.89	0.53
5:M:1360:ILE:HD12	5:M:1361:PRO:HD2	1.90	0.53
8:V:296:ASP:O	8:V:298:LYS:N	2.41	0.53
5:J:463:THR:HG21	5:J:1237:GLY:HA3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1802:LYS:HZ2	1:A:2163:PHE:HE2	1.55	0.53
1:C:1520:ARG:HA	1:C:1523:ASN:ND2	2.22	0.53
2:D:174:GLN:HA	2:D:177:LEU:HD12	1.91	0.53
5:H:382:LYS:HD3	5:H:1309:GLN:HE22	1.72	0.53
5:I:241:LYS:HA	5:I:244:THR:HG22	1.90	0.53
5:K:635:ILE:HD11	5:K:674:TYR:HE2	1.73	0.53
5:M:399:LEU:HD22	5:M:1033:ALA:HB1	1.90	0.53
5:M:539:PHE:HE1	5:M:552:CYS:HG	1.54	0.53
5:M:857:LEU:O	5:M:861:VAL:HG22	2.08	0.53
1:A:1585:LEU:HD23	1:A:1913:MET:HG3	1.89	0.53
1:A:1818:LYS:HA	1:A:1822:GLU:HB3	1.89	0.53
1:C:1936:ASP:O	1:C:1939:ILE:N	2.42	0.53
3:E:203:VAL:HG22	3:E:207:MET:HE3	1.90	0.53
1:A:1575:LEU:HD13	1:A:1914:ILE:HG21	1.91	0.53
1:A:1579:ARG:NH1	1:A:1835:GLN:O	2.41	0.53
1:A:1772:SER:HB2	1:A:2100:VAL:H	1.73	0.53
1:C:1573:ARG:HH12	1:C:1620:LEU:HB3	1.74	0.53
1:C:1584:PHE:CZ	1:C:1596:ILE:HB	2.43	0.53
5:J:297:SER:HB3	5:J:352:LEU:HD12	1.89	0.53
5:K:651:TYR:HB2	5:K:784:PHE:CD1	2.43	0.53
5:M:1122:TYR:HB2	5:M:1128:ASP:HB2	1.89	0.53
7:T:86:LEU:O	7:T:89:ILE:HG22	2.08	0.53
1:A:2215:ARG:HE	1:A:2218:ARG:HD3	1.73	0.53
5:H:936:PRO:HB3	5:H:952:LEU:HD23	1.91	0.53
2:D:314:THR:HG23	2:D:331:HIS:HE1	1.73	0.53
3:E:296:ASP:O	3:E:298:PRO:HD3	2.09	0.53
5:H:21:THR:HA	5:K:200:ALA:HB1	1.89	0.53
5:H:83:LEU:HB2	5:H:1060:ASN:HD21	1.73	0.53
5:J:610:CYS:SG	5:J:646:VAL:HG22	2.49	0.53
5:J:653:LEU:O	5:J:657:ILE:HG12	2.08	0.53
5:M:42:ASP:N	5:M:42:ASP:OD1	2.42	0.53
5:M:703:LEU:HD21	5:M:1022:LEU:HG	1.91	0.53
2:D:327:ARG:NH1	2:D:385:GLU:O	2.42	0.53
5:M:146:THR:OG1	5:M:149:ASP:OD2	2.24	0.53
3:E:287:TYR:OH	3:E:318:ASP:OD2	2.24	0.53
3:F:323:ILE:HA	3:F:326:TRP:CD1	2.44	0.53
8:X:144:LEU:HD13	8:Y:276:ARG:HD2	1.91	0.53
1:A:1618:LEU:HA	1:A:1621:ARG:CD	2.37	0.53
1:C:1569:ARG:HA	1:C:1572:LEU:HG	1.91	0.53
1:C:1701:SER:O	1:C:1705:HIS:ND1	2.40	0.53
2:D:65:VAL:O	2:D:69:VAL:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1239:LEU:C	5:H:1239:LEU:HD12	2.33	0.53
5:I:73:ALA:HB3	5:I:272:VAL:HG21	1.91	0.53
5:J:445:ALA:HB1	5:J:449:LEU:HD23	1.90	0.53
5:M:1185:TYR:O	5:M:1190:ASN:ND2	2.40	0.53
1:C:1674:TYR:OH	1:C:2117:PRO:O	2.26	0.52
5:H:392:THR:HG21	5:H:1264:GLN:HE22	1.73	0.52
5:K:725:ARG:HH11	5:K:772:ARG:HB2	1.74	0.52
5:L:143:PHE:HD2	5:L:144:GLU:HG2	1.74	0.52
5:L:211:GLN:O	5:L:215:ILE:HG12	2.09	0.52
4:G:399:SER:O	4:G:402:VAL:HG22	2.10	0.52
5:M:387:ARG:NH2	5:M:1312:GLU:OE2	2.42	0.52
1:A:1587:VAL:HB	1:A:1908:GLU:HB3	1.92	0.52
1:C:1581:HIS:CE1	1:C:1600:ALA:HB2	2.44	0.52
3:F:365:HIS:HD2	3:F:368:VAL:HG13	1.73	0.52
5:I:65:TYR:HA	5:I:172:GLU:HG2	1.90	0.52
5:K:888:GLU:O	5:K:919:ASN:ND2	2.43	0.52
9:Z:111:ARG:HD2	9:Z:111:ARG:O	2.10	0.52
9:Z:201:ASN:HA	9:Z:204:VAL:HG12	1.91	0.52
9:Z:239:LEU:HD21	9:Z:247:SER:HB3	1.91	0.52
1:A:1952:TRP:HA	1:A:1992:GLN:HE22	1.74	0.52
2:B:52:VAL:HG22	2:B:66:ARG:HH11	1.74	0.52
3:E:589:ALA:O	3:E:593:HIS:ND1	2.43	0.52
5:H:665:ALA:C	5:H:666:LEU:HD12	2.34	0.52
5:K:635:ILE:HD11	5:K:674:TYR:CE2	2.44	0.52
5:K:1360:ILE:O	5:K:1362:LEU:N	2.42	0.52
5:L:1327:THR:HG22	5:L:1329:THR:H	1.73	0.52
5:L:1331:ALA:O	5:L:1335:THR:HG23	2.10	0.52
5:M:1231:PRO:O	5:M:1235:GLN:HG2	2.09	0.52
1:C:1486:PHE:CD2	1:C:1522:LEU:HD11	2.43	0.52
1:C:1998:ASN:O	1:C:2001:GLN:NE2	2.36	0.52
4:G:366:VAL:HG13	4:G:550:LEU:HD21	1.90	0.52
5:H:50:PHE:CE1	5:I:86:LEU:HB3	2.44	0.52
5:J:244:THR:HA	5:J:362:LEU:HD12	1.91	0.52
5:J:1190:ASN:OD1	5:J:1223:GLN:NE2	2.42	0.52
5:K:703:LEU:HD21	5:K:1022:LEU:HD11	1.92	0.52
1:A:1957:PRO:HG3	1:A:2036:PHE:CD1	2.41	0.52
2:B:356:CYS:HA	2:B:359:VAL:HG22	1.91	0.52
2:B:356:CYS:HB3	2:B:419:LYS:HZ2	1.74	0.52
5:I:753:ASP:O	5:I:756:ARG:HG2	2.09	0.52
6:Q:18:HIS:HA	6:Q:21:VAL:HG12	1.91	0.52
1:A:1828:GLN:NE2	1:A:1831:GLN:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1694:LYS:O	1:C:1698:TYR:HB2	2.10	0.52
3:E:280:ALA:HB2	3:E:436:CYS:HB3	1.91	0.52
4:G:455:GLN:HE21	5:I:1119:MET:HG3	1.74	0.52
5:H:985:ASN:O	5:H:988:ARG:NH2	2.42	0.52
5:L:1113:LEU:HA	5:L:1116:VAL:HG12	1.91	0.52
1:A:1572:LEU:HA	1:A:1575:LEU:HG	1.91	0.52
1:A:1745:GLU:HG2	1:A:1967:LEU:HD22	1.90	0.52
2:B:316:ILE:HA	2:B:319:VAL:HB	1.91	0.52
2:B:459:ILE:HA	2:B:465:LEU:HD22	1.91	0.52
3:F:407:TRP:O	3:F:410:ARG:HG2	2.10	0.52
5:M:638:MET:HE1	5:M:642:ARG:HD2	1.91	0.52
2:B:138:VAL:HA	2:B:141:GLU:HG2	1.90	0.52
1:C:1957:PRO:HG3	1:C:2036:PHE:CD2	2.45	0.52
5:H:1143:LEU:HD21	8:U:233:LYS:HB3	1.92	0.52
7:T:72:THR:HG22	7:T:74:CYS:H	1.74	0.52
1:C:1607:VAL:HG13	1:C:1608:THR:HG23	1.91	0.52
2:D:40:ALA:HB1	2:D:92:LEU:HB2	1.92	0.52
2:D:210:GLN:HE22	2:D:436:VAL:HA	1.75	0.52
5:H:725:ARG:HD2	5:H:726:ASN:HB3	1.91	0.52
7:T:48:ALA:N	7:T:148:CYS:O	2.42	0.52
3:F:630:PHE:HB2	3:F:636:LEU:HB2	1.91	0.51
5:H:276:THR:HG1	5:H:373:ARG:HH11	1.58	0.51
5:I:917:LEU:HD21	5:I:920:GLY:HA3	1.92	0.51
5:J:1222:ALA:O	5:J:1223:GLN:HG2	2.10	0.51
7:T:76:SER:OG	7:T:77:PRO:HD3	2.10	0.51
1:A:1586:GLU:CB	1:A:1596:ILE:HG12	2.39	0.51
1:A:1770:LEU:HD12	1:A:1773:LEU:HD11	1.92	0.51
2:D:100:LEU:HD21	2:D:118:ASN:HB3	1.91	0.51
3:E:91:ASN:OD1	3:E:92:GLN:N	2.43	0.51
6:P:37:HIS:ND1	6:P:40:LEU:HD23	2.26	0.51
1:C:1555:VAL:HG21	1:C:2014:HIS:CE1	2.45	0.51
1:C:2034:LEU:HD13	1:C:2054:ARG:HH22	1.75	0.51
3:E:217:SER:N	3:E:638:SER:O	2.37	0.51
4:G:573:GLU:OE1	4:G:576:ARG:NH2	2.42	0.51
5:J:584:LEU:HD12	5:J:687:ILE:HD11	1.91	0.51
5:L:610:CYS:HA	5:L:647:PHE:CE1	2.43	0.51
2:B:399:MET:HB2	2:B:403:GLN:HE21	1.76	0.51
2:D:516:LEU:HD12	2:D:517:PHE:HB2	1.90	0.51
5:I:244:THR:HA	5:I:362:LEU:HD23	1.91	0.51
5:J:192:VAL:HG23	5:J:219:PHE:CZ	2.45	0.51
5:J:753:ASP:OD1	6:P:66:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:532:GLU:CD	5:M:555:ARG:HH12	2.18	0.51
3:F:365:HIS:HB3	3:F:368:VAL:HG22	1.92	0.51
5:J:399:LEU:HD22	5:J:1033:ALA:HB1	1.91	0.51
5:J:884:GLN:O	6:P:66:ARG:NH1	2.37	0.51
2:D:328:MET:HG3	2:D:334:LEU:HD23	1.91	0.51
5:M:231:ASN:OD1	5:M:1098:TYR:HB2	2.09	0.51
5:M:808:LEU:HD21	5:M:883:VAL:HG23	1.92	0.51
2:B:93:HIS:CE1	2:B:126:GLN:HB3	2.46	0.51
2:B:379:MET:HA	2:B:382:ARG:HG2	1.93	0.51
1:C:1556:LEU:HD12	1:C:1557:PRO:HD2	1.93	0.51
1:C:1903:GLN:HG2	1:C:1909:PRO:HA	1.92	0.51
3:F:59:ARG:O	3:F:62:ARG:HG2	2.11	0.51
3:F:186:ILE:HG22	3:F:501:LEU:HA	1.91	0.51
5:I:174:GLY:HA3	5:J:101:ALA:HB3	1.93	0.51
1:A:2149:ASP:HB3	1:A:2152:ARG:HG3	1.92	0.51
5:H:276:THR:OG1	5:H:373:ARG:NH1	2.42	0.51
5:I:1331:ALA:O	5:I:1335:THR:HG23	2.11	0.51
5:M:1003:HIS:O	5:M:1007:THR:HG23	2.11	0.51
8:Y:31:VAL:HG21	8:Y:137:ILE:HD11	1.92	0.51
1:A:1988:PHE:O	1:A:1992:GLN:HG2	2.11	0.51
1:C:1574:ARG:HE	1:C:1605:HIS:HA	1.75	0.51
5:H:808:LEU:HD21	5:H:883:VAL:HG13	1.93	0.51
5:K:477:ARG:HD3	5:L:1133:HIS:CE1	2.46	0.51
1:A:1968:LEU:O	1:A:1969:LYS:HG3	2.11	0.51
5:K:404:ASP:HB3	5:L:421:ARG:HG2	1.92	0.51
5:M:78:ILE:HB	5:M:1058:ILE:HG22	1.93	0.51
7:W:165:LEU:HD13	7:W:279:PHE:CE2	2.46	0.51
8:Y:41:ILE:HD11	8:Y:45:GLN:HG3	1.92	0.51
9:Z:86:ALA:O	9:Z:90:ARG:HG2	2.10	0.51
1:C:1663:TRP:CE2	1:C:1744:GLN:HB3	2.47	0.50
5:I:751:VAL:O	6:O:66:ARG:NH2	2.41	0.50
5:L:148:LEU:HA	5:L:151:ILE:HG22	1.92	0.50
1:A:1688:HIS:CD2	1:A:2116:PRO:HD3	2.46	0.50
1:C:1584:PHE:HD2	1:C:1914:ILE:HB	1.76	0.50
5:I:764:GLU:O	5:I:766:LEU:N	2.45	0.50
5:K:1034:LEU:HD13	5:K:1174:LEU:HD13	1.93	0.50
5:M:681:LEU:HB3	5:M:780:LEU:HD11	1.93	0.50
8:Y:144:LEU:O	8:Y:148:GLN:HG2	2.12	0.50
1:A:1851:THR:HG22	1:A:1877:VAL:HB	1.94	0.50
1:C:1617:TYR:HA	1:C:2006:THR:HG21	1.93	0.50
5:K:617:VAL:HG23	5:K:619:GLY:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:798:CYS:SG	5:I:799:GLY:N	2.84	0.50
5:J:1199:MET:HE3	5:J:1214:ILE:HD11	1.94	0.50
8:Y:100:VAL:HG21	8:Y:142:LEU:HD13	1.94	0.50
9:Z:5:PHE:CZ	9:Z:13:VAL:HG22	2.47	0.50
2:D:342:GLU:OE2	2:D:407:GLN:NE2	2.44	0.50
3:E:338:ALA:HB1	3:E:340:ARG:HE	1.77	0.50
4:G:302:ARG:N	8:V:236:GLU:OE2	2.27	0.50
5:H:29:GLU:OE1	5:K:1277:THR:OG1	2.21	0.50
5:J:496:PRO:O	5:J:500:ARG:HG3	2.12	0.50
5:L:101:ALA:HB3	5:M:174:GLY:HA3	1.93	0.50
5:L:156:ALA:O	5:L:159:THR:HG22	2.12	0.50
5:L:785:TYR:O	5:L:943:TYR:OH	2.26	0.50
5:L:1292:CYS:HA	5:L:1311:ILE:HG12	1.92	0.50
1:A:1621:ARG:NH1	1:A:1627:LEU:HD11	2.27	0.50
2:B:360:LEU:HB2	2:B:423:ILE:HD11	1.93	0.50
2:B:396:TYR:HD1	2:B:399:MET:HE3	1.77	0.50
1:C:1971:GLN:HB3	1:C:1972:ARG:HH21	1.76	0.50
2:D:296:VAL:HG13	2:D:298:ASN:H	1.77	0.50
3:E:318:ASP:HA	3:E:321:ARG:HD2	1.93	0.50
4:G:76:VAL:HG23	4:G:556:ARG:HH21	1.75	0.50
4:G:498:ARG:HH12	7:W:225:ARG:HG2	1.77	0.50
5:I:1249:ARG:HD2	5:I:1254:TYR:CD1	2.46	0.50
5:J:1291:ASP:OD1	5:J:1316:ARG:NH1	2.45	0.50
5:L:71:LEU:HD13	5:L:274:VAL:HG11	1.92	0.50
5:L:122:LYS:HD2	5:L:1082:ASN:ND2	2.27	0.50
1:A:2037:ILE:N	1:A:2038:PRO:HD3	2.26	0.50
1:C:1663:TRP:CD2	1:C:1744:GLN:HB3	2.46	0.50
1:C:2039:LEU:HD23	1:C:2053:LEU:HB2	1.93	0.50
1:C:2239:TYR:HB3	3:F:61:LEU:HD12	1.94	0.50
3:F:624:ILE:HA	3:F:627:LEU:HB3	1.94	0.50
5:I:478:LEU:HD12	5:I:512:MET:HE2	1.94	0.50
5:J:73:ALA:HB3	5:J:272:VAL:HG11	1.93	0.50
5:M:297:SER:HB3	5:M:352:LEU:HD23	1.93	0.50
7:W:80:LEU:HD23	7:W:114:ALA:HB2	1.93	0.50
2:B:116:TYR:HE2	2:B:492:HIS:CE1	2.30	0.50
3:F:305:LEU:HD13	3:F:506:ILE:HG22	1.92	0.50
5:H:726:ASN:O	5:H:727:MET:HE2	2.12	0.50
5:I:488:MET:HG3	5:I:894:GLU:HG3	1.93	0.50
5:J:173:ARG:NH2	5:J:375:VAL:O	2.45	0.50
5:J:900:ASP:HB2	5:J:903:GLN:HE22	1.76	0.50
1:A:1958:VAL:H	1:A:1981:TYR:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2034:LEU:HD22	1:C:1632:ARG:HA	1.94	0.50
3:F:362:PHE:HZ	3:F:380:LEU:HB3	1.77	0.50
5:H:7:LEU:HD22	5:K:92:LEU:HD12	1.92	0.50
5:H:225:ALA:O	5:H:232:ARG:NH2	2.39	0.50
5:H:724:PRO:HA	5:H:773:ALA:HB3	1.93	0.50
1:A:2224:LEU:HD21	3:E:75:TYR:HB3	1.94	0.49
5:K:1211:THR:HA	5:K:1214:ILE:HG12	1.94	0.49
5:M:443:VAL:HA	5:M:446:LEU:HD23	1.93	0.49
9:Z:121:ASP:OD2	9:Z:214:ARG:NH2	2.41	0.49
3:E:239:TYR:O	3:E:250:SER:OG	2.22	0.49
5:K:311:ASN:HD21	5:K:325:PHE:HB2	1.76	0.49
5:K:1116:VAL:HG23	5:K:1117:PHE:HD1	1.77	0.49
1:A:1490:ALA:HA	1:A:1493:ARG:HG2	1.94	0.49
1:A:1674:TYR:OH	1:A:2117:PRO:O	2.31	0.49
2:D:355:VAL:HG22	2:D:358:ARG:HH11	1.76	0.49
5:H:83:LEU:HD11	5:H:1058:ILE:HG22	1.94	0.49
5:H:883:VAL:O	5:H:886:VAL:HG13	2.12	0.49
2:D:448:ARG:O	2:D:451:LEU:HG	2.12	0.49
5:J:216:LEU:HD12	5:J:1200:LEU:HB2	1.94	0.49
5:J:396:PRO:HB3	5:J:1186:PHE:CZ	2.47	0.49
5:J:1336:LYS:NZ	5:J:1346:THR:OG1	2.45	0.49
5:L:1055:THR:HG1	5:L:1083:THR:HG1	1.59	0.49
5:M:1222:ALA:C	5:M:1224:THR:H	2.20	0.49
2:B:176:PRO:O	2:B:180:ARG:HG2	2.12	0.49
2:B:423:ILE:HA	2:B:426:ASN:HD21	1.78	0.49
1:C:1947:TYR:HE2	1:C:2049:VAL:HG11	1.78	0.49
3:F:226:LYS:HG3	3:F:241:LEU:HD13	1.95	0.49
5:J:751:VAL:HG22	5:J:752:SER:H	1.78	0.49
5:M:1223:GLN:O	5:M:1224:THR:HG23	2.11	0.49
8:U:290:VAL:HG12	8:U:302:CYS:SG	2.52	0.49
1:A:1549:LEU:HD23	1:A:1552:ILE:HD12	1.93	0.49
2:B:236:VAL:HG12	2:B:240:HIS:NE2	2.28	0.49
2:D:423:ILE:HG23	2:D:427:PHE:CE2	2.48	0.49
5:I:666:LEU:HD11	5:I:670:LEU:HB2	1.95	0.49
5:K:750:GLY:HA2	6:Q:70:VAL:HG21	1.95	0.49
5:K:752:SER:O	6:Q:66:ARG:NH2	2.45	0.49
5:L:808:LEU:HD21	5:L:883:VAL:HG13	1.94	0.49
1:A:1456:TYR:HB2	1:A:1482:LEU:HD21	1.95	0.49
5:I:171:MET:HE3	5:I:1077:VAL:HG12	1.95	0.49
5:J:949:CYS:SG	5:J:956:ILE:HG21	2.53	0.49
5:M:883:VAL:HG13	6:S:66:ARG:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:13:ASP:OD1	8:X:43:HIS:NE2	2.35	0.49
2:D:316:ILE:HD13	2:D:347:ALA:HB1	1.93	0.49
3:E:524:GLY:HA3	3:E:631:LEU:HA	1.94	0.49
5:I:532:GLU:OE2	5:I:555:ARG:NH1	2.46	0.49
5:L:291:ILE:HA	5:L:360:ILE:HG22	1.94	0.49
1:A:2240:LEU:HD11	3:F:61:LEU:HD22	1.93	0.49
2:B:103:GLN:O	2:B:107:GLY:N	2.42	0.49
1:C:1692:ASN:HB3	1:C:1762:LEU:HD13	1.94	0.49
1:C:2222:ARG:NH1	3:E:80:GLU:OE2	2.46	0.49
3:F:249:ILE:HG23	3:F:253:LEU:HD23	1.94	0.49
5:J:215:ILE:HG21	5:J:1278:LEU:HD11	1.93	0.49
5:K:430:LEU:HD12	5:K:1108:VAL:HG12	1.95	0.49
5:L:399:LEU:HD22	5:L:1033:ALA:HB1	1.94	0.49
2:D:124:ALA:HB1	2:D:195:TYR:CE2	2.48	0.49
4:G:414:TRP:HB2	4:G:478:VAL:HG11	1.94	0.49
5:K:73:ALA:HB3	5:K:272:VAL:HG11	1.95	0.49
5:L:626:LEU:HD21	5:L:881:LEU:HB2	1.93	0.49
1:A:1649:ILE:HD13	1:A:1978:HIS:ND1	2.28	0.48
1:A:1792:MET:HB3	1:A:2055:PRO:HG3	1.95	0.48
1:C:1772:SER:HB2	1:C:2100:VAL:H	1.77	0.48
5:I:805:LYS:HE2	6:O:58:CYS:HB2	1.94	0.48
5:L:455:HIS:CD2	5:L:1017:PRO:HG3	2.48	0.48
5:L:710:LEU:HD21	5:L:783:VAL:HG22	1.94	0.48
5:M:1277:THR:O	5:M:1281:THR:N	2.41	0.48
9:Z:14:VAL:HA	9:Z:17:VAL:HG12	1.95	0.48
1:A:1839:PRO:HG2	1:A:1939:ILE:HD13	1.95	0.48
1:A:2238:LEU:HD13	4:G:350:LEU:HD22	1.94	0.48
1:C:1459:LEU:HD13	1:C:1478:LYS:HD3	1.96	0.48
3:F:274:LEU:H	3:F:429:TYR:HE2	1.61	0.48
3:F:301:VAL:O	3:F:305:LEU:HG	2.13	0.48
5:J:432:ASN:ND2	5:J:438:GLN:HE21	2.11	0.48
1:A:1760:THR:HG21	1:A:2102:PHE:HE1	1.76	0.48
2:B:338:LEU:HD11	2:B:349:LEU:HD13	1.94	0.48
2:D:64:PHE:HB2	2:D:500:GLU:OE1	2.13	0.48
5:I:534:HIS:CD2	5:I:537:PHE:HD2	2.31	0.48
5:I:578:ILE:HD13	5:I:1028:ILE:HD12	1.94	0.48
7:T:195:GLY:O	7:T:233:ARG:NH1	2.46	0.48
8:X:260:SER:HG	9:Z:93:THR:HG1	1.58	0.48
2:B:70:VAL:HG13	2:B:96:LEU:HD13	1.95	0.48
3:F:462:LEU:HD12	3:F:465:LEU:HD12	1.94	0.48
4:G:367:LEU:O	4:G:371:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1127:VAL:O	5:H:1131:ILE:HG12	2.13	0.48
5:I:212:ARG:NH1	5:I:1203:ASP:OD1	2.40	0.48
5:I:1021:VAL:HA	5:I:1024:THR:HG22	1.95	0.48
5:J:565:LEU:HB3	5:J:1178:PRO:HB3	1.96	0.48
5:J:1246:THR:O	5:J:1250:GLU:HG2	2.13	0.48
8:V:199:THR:HA	8:V:202:LEU:HG	1.96	0.48
1:C:1700:VAL:HG21	1:C:1750:ILE:HG12	1.96	0.48
3:E:599:GLY:HA2	3:E:602:LEU:HD12	1.95	0.48
4:G:105:ASP:O	4:G:109:GLN:HG2	2.13	0.48
4:G:318:TRP:CE3	4:G:325:ARG:HB2	2.49	0.48
5:H:892:VAL:HG11	5:H:979:PHE:CE1	2.49	0.48
5:I:226:THR:HG22	5:I:226:THR:O	2.13	0.48
5:K:1122:TYR:N	5:K:1128:ASP:OD2	2.44	0.48
5:L:1033:ALA:HB2	5:L:1179:VAL:HA	1.95	0.48
8:X:225:GLU:OE1	8:X:225:GLU:N	2.47	0.48
1:A:1698:TYR:CE2	1:A:2074:THR:HB	2.49	0.48
1:A:1830:CYS:HB2	1:A:1841:LEU:HB2	1.95	0.48
5:H:600:THR:HG21	5:H:645:LEU:CD1	2.44	0.48
5:J:388:ASN:HB2	5:J:1311:ILE:HD12	1.94	0.48
5:J:1214:ILE:HG22	5:J:1215:TYR:CD1	2.46	0.48
5:L:390:ASP:OD1	5:L:1039:THR:OG1	2.31	0.48
5:M:1350:HIS:CD2	5:M:1351:PHE:H	2.32	0.48
1:A:1830:CYS:SG	1:A:1842:GLY:N	2.86	0.48
2:B:291:SER:O	2:B:294:LEU:HG	2.13	0.48
1:C:1620:LEU:HD21	1:C:2006:THR:HB	1.96	0.48
1:C:1830:CYS:O	1:C:1834:PRO:HD2	2.14	0.48
2:D:227:ARG:HH11	2:D:327:ARG:HG2	1.79	0.48
3:E:365:HIS:CE1	3:E:434:LEU:HD21	2.49	0.48
5:J:390:ASP:CG	5:J:1311:ILE:HG21	2.39	0.48
5:J:427:THR:HG22	5:J:441:ASP:HB3	1.96	0.48
5:J:438:GLN:OE1	5:J:1108:VAL:HG22	2.13	0.48
5:K:477:ARG:HD3	5:L:1133:HIS:NE2	2.29	0.48
5:K:810:ASP:O	5:K:814:ARG:NH2	2.46	0.48
5:M:244:THR:HA	5:M:362:LEU:HD23	1.96	0.48
8:V:262:ASP:OD1	8:V:262:ASP:N	2.46	0.48
2:B:459:ILE:HG23	2:B:465:LEU:HB2	1.96	0.48
5:H:719:PHE:CZ	5:H:922:CYS:HB3	2.49	0.48
5:J:861:VAL:HA	5:J:864:VAL:HG12	1.95	0.48
5:M:1045:ASP:HB2	5:M:1097:ALA:HB3	1.96	0.48
8:U:57:GLY:HA2	8:U:188:VAL:HG12	1.96	0.48
1:A:1614:ALA:HB3	1:A:1845:TRP:CZ3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1874:TYR:HB3	1:A:1879:GLU:OE2	2.14	0.48
2:B:181:VAL:O	2:B:185:LEU:HD23	2.14	0.48
2:D:132:LEU:HA	2:D:135:ILE:HG12	1.96	0.48
2:D:379:MET:O	2:D:383:LEU:HG	2.14	0.48
3:F:71:ARG:NH1	3:F:75:TYR:OH	2.46	0.48
4:G:45:TYR:HB3	4:G:132:LEU:HD22	1.96	0.48
5:J:254:ILE:HG12	5:J:1086:MET:O	2.14	0.48
5:L:638:MET:SD	5:L:642:ARG:HD2	2.54	0.48
5:L:1190:ASN:OD1	5:L:1223:GLN:NE2	2.46	0.48
5:L:1276:LYS:O	5:L:1281:THR:OG1	2.32	0.48
5:M:421:ARG:NH2	5:M:577:GLU:OE2	2.40	0.48
6:R:20:HIS:O	6:R:24:VAL:HG22	2.13	0.48
7:W:54:GLU:O	7:W:57:VAL:HG12	2.13	0.48
1:A:1982:THR:HG22	1:A:1984:ARG:H	1.79	0.48
3:F:285:ALA:HB3	3:F:407:TRP:HH2	1.78	0.48
5:L:629:THR:OG1	5:L:878:GLU:OE1	2.31	0.48
7:T:185:VAL:HB	7:T:206:THR:HG22	1.96	0.48
8:V:33:PRO:HB2	8:V:68:MET:SD	2.54	0.48
2:D:70:VAL:HG13	2:D:96:LEU:HD13	1.94	0.47
2:D:135:ILE:HG13	2:D:136:GLN:N	2.29	0.47
2:D:447:ARG:HA	2:D:450:ILE:HB	1.96	0.47
4:G:514:TRP:HE1	4:G:522:VAL:HG21	1.79	0.47
5:J:605:ASN:ND2	5:J:642:ARG:HD3	2.29	0.47
5:K:800:LEU:HD22	5:K:952:LEU:HD21	1.96	0.47
5:L:142:THR:O	7:W:36:ARG:NH1	2.47	0.47
5:L:1193:ARG:NH1	5:L:1197:SER:HB3	2.29	0.47
5:M:446:LEU:HD21	5:M:1024:THR:CG2	2.40	0.47
5:M:730:VAL:HG13	5:M:897:ALA:HB2	1.95	0.47
9:Z:63:TYR:HB2	9:Z:224:CYS:SG	2.53	0.47
1:A:1456:TYR:CZ	1:A:1460:LEU:HD11	2.50	0.47
1:A:1602:GLU:CG	1:A:1607:VAL:HB	2.42	0.47
1:A:1868:PRO:HD2	1:A:1871:ALA:HB3	1.95	0.47
1:C:1869:GLN:HB2	1:C:2046:ASP:HA	1.96	0.47
2:D:319:VAL:HA	2:D:323:LEU:HD13	1.96	0.47
5:K:283:ILE:HG21	5:K:369:MET:HE1	1.96	0.47
5:K:785:TYR:O	5:K:943:TYR:OH	2.32	0.47
5:K:1116:VAL:HG12	5:K:1258:PHE:CD1	2.50	0.47
5:M:1039:THR:HG21	5:M:1259:TYR:HE2	1.79	0.47
8:X:203:SER:O	8:X:207:VAL:HG13	2.14	0.47
1:C:1957:PRO:HG3	1:C:2036:PHE:HD2	1.79	0.47
5:H:857:LEU:HD21	5:H:876:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:786:LEU:HD11	5:L:987:LEU:HD22	1.96	0.47
5:L:1114:PHE:HB2	5:L:1137:VAL:HG11	1.96	0.47
5:M:684:VAL:HA	5:M:687:ILE:HG22	1.96	0.47
5:M:854:GLY:O	5:M:858:THR:HG23	2.14	0.47
6:N:27:GLU:OE2	6:N:61:LYS:NZ	2.45	0.47
8:V:142:LEU:HD12	8:V:177:PHE:CG	2.49	0.47
2:B:30:VAL:HG22	2:B:72:TYR:OH	2.13	0.47
2:B:257:PHE:O	2:B:261:VAL:HG23	2.13	0.47
1:C:1807:THR:HG22	1:C:1809:THR:HG22	1.96	0.47
2:D:383:LEU:HD13	2:D:427:PHE:HE1	1.78	0.47
3:F:469:ASP:OD1	3:F:469:ASP:N	2.45	0.47
5:H:1144:ASP:OD1	5:H:1145:THR:N	2.48	0.47
5:H:1249:ARG:HG2	5:H:1254:TYR:CD1	2.50	0.47
5:I:1195:ARG:HD2	5:I:1221:ASP:CG	2.40	0.47
5:K:698:LEU:HD21	5:K:1127:VAL:HB	1.97	0.47
5:L:1116:VAL:HG13	5:L:1117:PHE:HD1	1.80	0.47
2:B:9:PHE:O	2:B:13:ILE:HG12	2.15	0.47
2:B:238:LEU:HD21	2:B:327:ARG:HD2	1.97	0.47
1:C:2003:LEU:HD23	1:C:2014:HIS:NE2	2.29	0.47
3:E:641:VAL:O	3:E:641:VAL:HG12	2.14	0.47
3:F:68:LEU:HA	3:F:71:ARG:HG2	1.97	0.47
5:I:785:TYR:O	5:I:943:TYR:OH	2.32	0.47
5:K:1044:VAL:HG11	5:K:1096:VAL:HG13	1.95	0.47
5:L:579:MET:HE1	5:L:1003:HIS:CD2	2.49	0.47
5:M:420:VAL:HG11	5:M:577:GLU:HA	1.97	0.47
5:M:1001:VAL:HG12	5:M:1002:LEU:HD23	1.97	0.47
5:M:1039:THR:HG23	5:M:1300:GLN:HE22	1.79	0.47
7:W:18:ASN:O	7:W:22:THR:HG23	2.15	0.47
1:A:1969:LYS:HG2	1:C:2155:ASP:HB3	1.96	0.47
3:E:183:TYR:HB2	3:E:192:PHE:HB3	1.96	0.47
3:E:338:ALA:HB1	3:E:340:ARG:NE	2.30	0.47
3:E:506:ILE:HG23	3:E:510:TYR:CE2	2.50	0.47
3:F:340:ARG:HB3	3:F:361:THR:HA	1.96	0.47
5:H:229:LEU:HD12	5:H:230:LEU:HD22	1.96	0.47
5:I:595:ARG:O	5:I:599:THR:HG23	2.15	0.47
5:I:1039:THR:HG23	5:I:1261:PRO:HB3	1.97	0.47
5:J:273:MET:HE3	5:J:367:VAL:HG11	1.94	0.47
5:J:498:PHE:O	5:J:501:VAL:HG12	2.14	0.47
5:K:643:GLN:HB2	5:L:672:PHE:HE2	1.78	0.47
5:M:534:HIS:HB3	5:M:537:PHE:O	2.14	0.47
8:Y:218:TYR:OH	8:Y:264:GLU:OE2	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:161:ASP:HA	9:Z:164:VAL:HG12	1.96	0.47
1:A:1493:ARG:HG3	1:A:1495:THR:H	1.80	0.47
2:B:227:ARG:HH12	2:B:326:GLU:HB2	1.79	0.47
2:B:245:HIS:ND1	2:B:389:ASN:OD1	2.48	0.47
2:B:296:VAL:HG13	2:B:298:ASN:H	1.79	0.47
1:C:1951:SER:HA	1:C:1956:ILE:HG22	1.97	0.47
3:E:305:LEU:HD11	3:E:510:TYR:HD2	1.79	0.47
3:E:531:THR:HG21	3:E:619:PHE:HZ	1.80	0.47
5:J:884:GLN:HA	6:P:66:ARG:HB2	1.97	0.47
5:K:212:ARG:NH2	5:K:1201:ALA:O	2.42	0.47
5:K:672:PHE:HE1	5:K:675:ARG:HH12	1.61	0.47
5:L:1221:ASP:OD1	5:L:1222:ALA:N	2.46	0.47
5:M:689:ALA:HB2	5:M:711:HIS:NE2	2.29	0.47
5:M:712:ASP:O	5:M:782:LYS:NZ	2.47	0.47
5:M:760:MET:SD	5:M:888:GLU:HA	2.55	0.47
6:S:33:SER:OG	6:S:34:GLU:OE1	2.31	0.47
7:T:251:LEU:HD12	7:T:251:LEU:O	2.14	0.47
3:E:365:HIS:CD2	3:E:368:VAL:HG23	2.49	0.47
5:H:263:THR:HG1	5:H:267:ALA:H	1.61	0.47
5:I:421:ARG:NH2	5:J:404:ASP:OD2	2.46	0.47
5:L:1116:VAL:HG13	5:L:1117:PHE:CD1	2.50	0.47
1:A:1645:ARG:HA	1:A:2163:PHE:CE1	2.50	0.47
2:D:439:PRO:HA	2:D:482:VAL:HG22	1.97	0.47
2:D:441:PHE:HB3	2:D:512:TRP:CE2	2.50	0.47
5:H:698:LEU:HD21	5:H:1127:VAL:HG23	1.97	0.47
5:K:99:ARG:NH2	5:K:111:GLN:OE1	2.48	0.47
5:L:651:TYR:CZ	5:L:655:THR:HG21	2.50	0.47
5:M:287:LEU:O	5:M:291:ILE:HG23	2.15	0.47
5:M:641:THR:HG23	5:M:642:ARG:HG3	1.96	0.47
8:U:116:HIS:O	8:U:119:LEU:HD22	2.15	0.47
1:A:1461:HIS:HA	1:A:1464:GLN:HG2	1.97	0.47
1:A:2027:TYR:HD1	1:A:2028:LEU:HD22	1.80	0.47
2:B:117:HIS:O	2:B:121:THR:N	2.33	0.47
2:B:292:TYR:CE1	2:B:307:LEU:HD11	2.50	0.47
2:B:422:GLN:HG2	2:B:468:VAL:HG23	1.96	0.47
5:H:1297:THR:HG22	5:H:1299:THR:H	1.79	0.47
8:X:229:MET:HA	8:X:232:VAL:HG12	1.96	0.47
1:C:1545:LEU:HB3	1:C:2023:ARG:HG2	1.97	0.46
1:C:1642:VAL:O	1:C:2192:SER:N	2.35	0.46
3:E:447:THR:HG22	3:E:628:LEU:HD21	1.97	0.46
5:H:575:THR:HG22	5:H:1010:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:229:LEU:HD22	5:I:242:PHE:CD2	2.49	0.46
5:I:358:ASP:HB2	5:I:369:MET:HB2	1.97	0.46
5:J:440:ILE:HB	5:J:1108:VAL:HG21	1.97	0.46
5:J:846:ILE:HD12	5:J:849:GLN:HE21	1.81	0.46
5:L:559:GLY:HA3	5:L:991:PHE:HE1	1.80	0.46
5:L:684:VAL:HG23	5:L:1006:MET:HG2	1.97	0.46
5:M:757:LEU:HB3	6:S:59:ALA:HB1	1.98	0.46
9:Z:105:HIS:HA	9:Z:108:VAL:HG22	1.96	0.46
1:A:1573:ARG:NH2	1:A:1619:ALA:O	2.48	0.46
1:A:1862:LEU:HD11	1:A:1952:TRP:CH2	2.45	0.46
2:B:326:GLU:HA	2:B:355:VAL:HG11	1.97	0.46
4:G:96:VAL:HA	4:G:128:VAL:HA	1.97	0.46
5:L:214:ASN:HB3	5:M:1101:ARG:HD2	1.98	0.46
5:L:388:ASN:HB2	5:L:1311:ILE:HD12	1.97	0.46
5:L:567:PRO:HB2	5:L:569:PRO:HD2	1.97	0.46
1:A:1792:MET:HB2	1:A:1811:TRP:HH2	1.81	0.46
2:B:412:PHE:O	2:B:416:ILE:HG12	2.16	0.46
1:C:1859:LEU:O	1:C:1862:LEU:HG	2.15	0.46
4:G:85:GLU:O	4:G:88:THR:HG22	2.15	0.46
4:G:449:ARG:NH2	4:G:464:GLU:OE1	2.44	0.46
5:I:326:ASN:O	5:I:329:LYS:HG2	2.15	0.46
5:I:488:MET:HE1	5:I:978:ALA:HB1	1.97	0.46
5:J:749:HIS:NE2	5:J:885:PHE:HA	2.30	0.46
5:J:1193:ARG:HD3	5:J:1266:PHE:CE2	2.50	0.46
5:M:635:ILE:HG22	5:M:646:VAL:HG23	1.96	0.46
1:A:1531:LEU:O	1:A:1534:GLN:HG3	2.15	0.46
1:A:2234:HIS:CE1	1:A:2238:LEU:HD12	2.50	0.46
3:E:22:ASN:HB3	3:F:7:PHE:H	1.80	0.46
3:E:615:GLY:HA3	3:E:621:VAL:HB	1.98	0.46
5:H:785:TYR:O	5:H:790:PRO:HD3	2.16	0.46
5:I:534:HIS:CD2	5:I:536:PHE:H	2.33	0.46
5:K:1173:GLU:HG3	5:K:1261:PRO:HD2	1.98	0.46
5:L:789:MET:O	5:L:793:THR:HG22	2.15	0.46
5:L:884:GLN:HA	6:R:66:ARG:HB2	1.98	0.46
5:M:1184:ASN:O	5:M:1184:ASN:ND2	2.48	0.46
6:Q:16:GLU:O	6:Q:20:HIS:ND1	2.48	0.46
2:D:233:LEU:HD13	2:D:323:LEU:HD11	1.97	0.46
3:E:348:TYR:O	3:E:431:ARG:NH1	2.48	0.46
4:G:566:LEU:HD12	8:U:157:SER:HB2	1.97	0.46
5:H:860:LEU:HD11	5:H:930:LEU:HD21	1.97	0.46
5:J:1064:VAL:HG22	5:J:1077:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:215:ILE:HG21	5:K:1278:LEU:HD11	1.97	0.46
5:L:488:MET:HE3	5:L:894:GLU:HB2	1.97	0.46
5:M:192:VAL:HG23	5:M:219:PHE:CZ	2.51	0.46
5:M:280:MET:HG3	5:M:371:ASN:HB3	1.97	0.46
8:U:154:GLY:HA3	8:U:193:LEU:HD21	1.98	0.46
1:C:1982:THR:HG22	1:C:1983:SER:H	1.81	0.46
2:D:131:THR:HA	2:D:134:GLU:HG2	1.96	0.46
3:E:82:ARG:HD3	3:E:82:ARG:HA	1.73	0.46
3:F:59:ARG:O	3:F:63:GLN:OE1	2.32	0.46
5:H:935:LEU:HD12	5:H:936:PRO:HD2	1.98	0.46
5:J:240:LEU:HD12	5:J:287:LEU:HD11	1.98	0.46
5:J:376:TYR:O	5:J:378:ASN:N	2.48	0.46
5:K:307:LEU:HD23	5:K:307:LEU:H	1.80	0.46
5:K:798:CYS:SG	5:K:799:GLY:N	2.89	0.46
5:L:1034:LEU:HD12	5:L:1174:LEU:HB3	1.96	0.46
5:M:1121:VAL:HA	5:M:1132:ARG:HH11	1.81	0.46
8:X:58:TYR:CE1	8:X:112:PRO:HG2	2.51	0.46
1:A:1500:GLU:HA	1:A:1520:ARG:HH11	1.81	0.46
2:B:92:LEU:HD12	2:B:95:GLN:NE2	2.31	0.46
1:C:1570:ASP:OD1	1:C:1571:ARG:N	2.49	0.46
1:C:1784:ALA:O	1:C:1788:ASN:N	2.49	0.46
1:C:1843:LYS:NZ	1:C:1941:THR:O	2.42	0.46
2:D:182:ILE:O	2:D:186:GLU:HG3	2.15	0.46
2:D:334:LEU:HA	2:D:337:ARG:HG2	1.98	0.46
3:E:621:VAL:HG22	3:E:636:LEU:HD22	1.98	0.46
3:F:30:VAL:O	3:F:34:LEU:HD23	2.15	0.46
5:H:1057:VAL:HG12	5:H:1083:THR:HG22	1.97	0.46
5:K:698:LEU:HD22	5:K:706:TYR:HE2	1.80	0.46
5:M:556:ILE:HD11	5:M:1014:LYS:HE3	1.97	0.46
8:Y:195:ILE:O	8:Y:199:THR:HG23	2.16	0.46
1:A:1920:ASP:OD1	1:A:1921:THR:N	2.38	0.46
2:B:332:PRO:HB3	2:B:396:TYR:CZ	2.51	0.46
5:H:753:ASP:N	5:H:753:ASP:OD1	2.49	0.46
5:J:1034:LEU:HD13	5:J:1174:LEU:HG	1.97	0.46
5:L:192:VAL:HG13	5:L:219:PHE:CZ	2.51	0.46
5:M:459:PRO:O	5:M:462:GLN:HG3	2.16	0.46
8:X:153:MET:SD	8:X:169:VAL:HG22	2.56	0.46
8:X:262:ASP:O	8:X:265:ILE:HG22	2.16	0.46
1:C:2179:CYS:SG	1:C:2180:ARG:N	2.89	0.46
3:F:606:LEU:HD12	3:F:606:LEU:O	2.16	0.46
5:H:1332:LEU:HD13	5:H:1355:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1177:THR:OG1	5:L:1230:ASN:ND2	2.40	0.46
5:M:77:ALA:HB1	5:M:302:TYR:CD2	2.50	0.46
6:Q:14:ARG:HB2	6:Q:18:HIS:CE1	2.50	0.46
8:U:230:LEU:HD21	8:V:202:LEU:HD11	1.96	0.46
8:V:287:VAL:HG23	8:V:288:PHE:HD2	1.81	0.46
2:D:473:THR:HA	2:D:476:VAL:HG12	1.96	0.46
3:E:278:GLU:HB3	3:E:412:LEU:HD11	1.98	0.46
3:F:423:PHE:HB2	3:F:426:GLU:HB2	1.98	0.46
5:I:651:TYR:HB2	5:I:784:PHE:CD1	2.51	0.46
5:I:689:ALA:HB2	5:I:711:HIS:NE2	2.31	0.46
5:J:635:ILE:HG13	5:J:646:VAL:HG12	1.98	0.46
1:A:1899:TYR:HB2	1:A:1913:MET:SD	2.55	0.45
1:A:2043:ASN:ND2	1:A:2046:ASP:OD1	2.49	0.45
2:D:240:HIS:HE1	2:D:293:LYS:HG3	1.81	0.45
5:H:1133:HIS:CE1	5:I:477:ARG:HD3	2.51	0.45
5:I:1327:THR:HB	5:I:1355:VAL:HG22	1.97	0.45
8:U:63:GLY:HA2	8:U:66:ARG:HG2	1.98	0.45
1:A:1753:LEU:HD21	1:A:1785:VAL:HG11	1.98	0.45
1:A:2177:PRO:HB2	2:B:307:LEU:HD13	1.97	0.45
2:B:351:ALA:HA	2:B:354:ARG:NE	2.31	0.45
2:B:361:GLU:O	2:B:365:HIS:ND1	2.34	0.45
3:F:460:PHE:CZ	3:F:465:LEU:HD11	2.51	0.45
4:G:168:LEU:HD23	4:G:317:VAL:HG21	1.98	0.45
5:H:757:LEU:HB3	6:N:59:ALA:HB1	1.99	0.45
5:I:363:GLY:C	5:I:365:LYS:H	2.24	0.45
5:K:661:LEU:HD23	5:K:666:LEU:HD21	1.98	0.45
5:L:653:LEU:O	5:L:657:ILE:HG12	2.16	0.45
5:M:77:ALA:HB1	5:M:302:TYR:HD2	1.81	0.45
8:V:8:ILE:HB	8:V:83:LEU:HB2	1.98	0.45
7:W:244:CYS:SG	8:X:273:VAL:HG11	2.57	0.45
8:X:204:MET:O	8:X:207:VAL:HG22	2.16	0.45
1:A:1524:ALA:O	1:A:1527:ARG:HG2	2.17	0.45
2:B:96:LEU:HB3	2:B:122:LEU:HD21	1.98	0.45
2:D:271:PHE:HD1	2:D:312:ILE:HG23	1.80	0.45
3:E:318:ASP:HB3	3:E:370:LEU:HD21	1.98	0.45
5:I:754:VAL:N	5:I:755:PRO:HD2	2.31	0.45
5:J:1001:VAL:HG12	5:J:1002:LEU:HD23	1.98	0.45
5:J:1059:ILE:HG22	5:J:1081:ILE:HG22	1.97	0.45
5:L:214:ASN:OD1	5:M:433:ARG:NH1	2.49	0.45
5:M:118:LYS:NZ	5:M:1087:GLY:O	2.46	0.45
5:M:1033:ALA:HB2	5:M:1179:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:VAL:HG11	2:B:73:LEU:HD11	1.99	0.45
2:D:213:ILE:HG12	2:D:434:LEU:HG	1.97	0.45
2:D:325:PRO:HB2	2:D:355:VAL:HG21	1.99	0.45
3:E:301:VAL:HG23	3:E:411:LEU:HD13	1.99	0.45
4:G:441:GLN:OE1	4:G:444:ARG:NH1	2.50	0.45
5:H:753:ASP:OD1	6:N:66:ARG:NH2	2.37	0.45
5:I:455:HIS:CE1	5:I:1017:PRO:HD3	2.51	0.45
5:I:753:ASP:C	5:I:755:PRO:HD2	2.41	0.45
5:J:211:GLN:O	5:J:215:ILE:HG12	2.17	0.45
5:J:318:TYR:CD2	5:J:320:SER:HB2	2.51	0.45
5:K:580:GLU:OE1	5:K:585:ARG:NH2	2.49	0.45
5:L:624:PHE:HZ	5:L:657:ILE:HD13	1.81	0.45
5:M:1241:ASP:CG	5:M:1245:ASN:HD21	2.24	0.45
6:O:75:ARG:OXT	9:Z:251:ARG:NH1	2.38	0.45
7:T:79:HIS:CD2	8:V:103:GLU:HG2	2.51	0.45
8:V:270:ALA:HA	8:V:273:VAL:HG12	1.98	0.45
2:B:315:ARG:HD2	2:B:337:ARG:HH12	1.82	0.45
2:B:351:ALA:O	2:B:354:ARG:HG2	2.16	0.45
3:E:498:PHE:HE1	3:E:501:LEU:HD22	1.82	0.45
5:I:388:ASN:HB2	5:I:1311:ILE:HD12	1.98	0.45
5:I:1035:THR:HG22	5:I:1177:THR:OG1	2.17	0.45
5:L:1178:PRO:HG3	5:L:1231:PRO:HD2	1.99	0.45
6:P:18:HIS:HA	6:P:48:THR:HG21	1.98	0.45
8:U:152:ILE:HD12	8:V:268:LEU:HB3	1.99	0.45
8:V:59:VAL:HB	8:V:196:ASP:OD2	2.16	0.45
9:Z:74:SER:HA	9:Z:77:LEU:HD12	1.97	0.45
1:C:2037:ILE:N	1:C:2038:PRO:HD3	2.31	0.45
3:E:309:PRO:HA	3:E:312:LEU:HD12	1.98	0.45
3:F:526:ALA:HA	3:F:594:TYR:CD1	2.51	0.45
4:G:36:GLU:HB2	4:G:153:TRP:CE2	2.51	0.45
5:I:475:MET:SD	5:I:530:TYR:CE1	3.10	0.45
5:I:752:SER:HB3	6:O:67:MET:HE3	1.98	0.45
5:J:785:TYR:O	5:J:943:TYR:OH	2.28	0.45
5:J:1043:GLU:OE1	5:J:1101:ARG:NE	2.40	0.45
5:M:450:CYS:O	5:M:1122:TYR:OH	2.23	0.45
7:T:127:ARG:NH2	7:T:288:GLU:OE2	2.42	0.45
7:W:193:TYR:CD1	7:W:233:ARG:HD2	2.51	0.45
8:X:214:LEU:HA	8:X:217:THR:HG22	1.99	0.45
1:A:1527:ARG:O	1:A:1531:LEU:HB2	2.16	0.45
1:A:1685:ALA:O	1:A:1688:HIS:ND1	2.50	0.45
1:A:1857:ASP:O	1:A:1860:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1953:LEU:O	1:A:2028:LEU:HD12	2.17	0.45
1:A:2040:VAL:HG22	1:A:2052:VAL:HG12	1.98	0.45
2:B:271:PHE:HB3	2:B:322:TYR:CD2	2.52	0.45
2:D:239:MET:HB2	2:D:253:LEU:HD11	1.99	0.45
3:E:371:PHE:HB3	3:E:376:VAL:HB	1.98	0.45
3:E:635:PHE:HD2	3:E:637:PRO:HD3	1.80	0.45
4:G:5:LEU:HD13	4:G:306:TRP:CG	2.52	0.45
5:I:194:GLN:HA	5:I:197:VAL:HG12	1.98	0.45
5:I:326:ASN:OD1	5:I:327:SER:N	2.49	0.45
5:K:1286:LEU:HD12	5:K:1287:LEU:HG	1.98	0.45
5:M:449:LEU:HD13	5:M:1020:LEU:HD21	1.99	0.45
1:A:1703:ALA:HB2	1:A:1773:LEU:HD13	1.98	0.45
1:C:1449:GLN:OE1	1:C:1493:ARG:NH2	2.49	0.45
1:C:1574:ARG:NH1	1:C:1608:THR:O	2.49	0.45
2:D:209:TYR:HA	2:D:212:LEU:HG	1.99	0.45
2:D:279:ASP:N	2:D:279:ASP:OD1	2.50	0.45
2:D:399:MET:HB2	2:D:403:GLN:HE21	1.81	0.45
3:F:239:TYR:OH	3:F:570:MET:SD	2.69	0.45
3:F:362:PHE:CE1	3:F:380:LEU:HD13	2.51	0.45
3:F:427:GLN:HB3	3:F:429:TYR:HD1	1.82	0.45
5:H:754:VAL:N	5:H:755:PRO:HD2	2.32	0.45
5:H:917:LEU:HD21	5:H:920:GLY:HA3	1.99	0.45
5:I:33:GLU:HG2	5:I:34:ALA:N	2.32	0.45
5:I:1054:CYS:SG	5:I:1055:THR:HG23	2.57	0.45
5:L:70:GLY:N	5:L:370:GLU:OE1	2.49	0.45
5:L:507:ARG:NH1	5:L:968:ARG:HH12	2.15	0.45
8:X:115:PHE:HD2	8:X:183:THR:HB	1.82	0.45
2:D:508:LEU:HD23	2:D:516:LEU:HD21	1.99	0.45
3:F:339:TYR:HB3	3:F:364:ARG:HD2	1.98	0.45
5:J:534:HIS:CD2	5:J:537:PHE:HD2	2.35	0.45
5:K:223:MET:O	5:K:227:LEU:HG	2.17	0.45
5:K:760:MET:SD	5:K:888:GLU:HA	2.57	0.45
5:K:937:VAL:HG13	5:K:937:VAL:O	2.16	0.45
5:L:559:GLY:HA3	5:L:991:PHE:CE1	2.52	0.45
5:L:601:VAL:HG13	5:L:924:VAL:HG11	1.99	0.45
5:L:611:TYR:CZ	5:L:923:VAL:HG23	2.52	0.45
6:N:21:VAL:O	6:N:25:VAL:HB	2.16	0.45
7:T:211:HIS:CE1	8:U:66:ARG:HD3	2.52	0.45
8:V:66:ARG:NH1	8:V:280:ASP:O	2.50	0.45
8:V:93:THR:HG22	8:V:301:THR:HG22	1.98	0.45
2:B:92:LEU:O	2:B:95:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1575:LEU:O	1:C:1579:ARG:NH2	2.50	0.45
5:J:447:LYS:HB3	5:J:1112:ASP:HA	1.99	0.45
5:J:1212:LYS:HA	5:J:1216:ASP:OD1	2.17	0.45
5:K:698:LEU:HD11	5:K:1127:VAL:HA	1.99	0.45
5:M:75:ALA:HB2	5:M:179:PHE:CZ	2.52	0.45
9:Z:98:ASP:OD1	9:Z:98:ASP:N	2.50	0.45
2:B:454:HIS:O	2:B:458:LEU:HB2	2.17	0.44
1:C:1536:LEU:HA	1:C:1539:LYS:HG2	1.98	0.44
2:D:62:PHE:HA	2:D:65:VAL:HG12	1.99	0.44
2:D:383:LEU:HD13	2:D:427:PHE:CE1	2.52	0.44
5:I:126:THR:HG22	5:I:1078:THR:HG22	1.99	0.44
5:I:297:SER:HB3	5:I:352:LEU:HD12	1.98	0.44
5:J:718:PRO:HD2	5:J:785:TYR:HB3	1.99	0.44
5:K:122:LYS:HE3	5:K:1082:ASN:HD21	1.82	0.44
5:K:591:GLU:CD	5:K:595:ARG:HE	2.25	0.44
5:L:146:THR:HG23	5:L:149:ASP:H	1.82	0.44
5:L:610:CYS:SG	5:L:647:PHE:HD1	2.40	0.44
5:M:677:LEU:O	5:M:681:LEU:HG	2.17	0.44
5:M:888:GLU:H	5:M:919:ASN:HD21	1.64	0.44
6:N:67:MET:HA	6:N:67:MET:HE2	1.98	0.44
7:W:184:TYR:CE1	7:W:210:ALA:HB2	2.52	0.44
1:A:2046:ASP:OD1	1:A:2046:ASP:N	2.46	0.44
2:B:296:VAL:HG11	2:B:301:ALA:HB3	1.98	0.44
2:B:398:GLN:O	2:B:402:ILE:HG13	2.16	0.44
5:J:396:PRO:HB2	5:J:399:LEU:HD23	1.98	0.44
5:J:534:HIS:CD2	5:J:536:PHE:H	2.35	0.44
5:J:623:ALA:HB2	5:J:885:PHE:CD2	2.52	0.44
5:J:811:LEU:HD23	5:J:812:PHE:CE1	2.52	0.44
5:J:968:ARG:NH2	5:J:970:ASP:OD1	2.49	0.44
5:K:75:ALA:HB2	5:K:179:PHE:CZ	2.53	0.44
5:M:555:ARG:HA	5:M:560:ASN:HD22	1.82	0.44
8:V:55:THR:HG23	8:V:56:ARG:HG2	1.99	0.44
7:W:258:ASP:OD1	7:W:277:ASP:HB2	2.17	0.44
2:B:400:ALA:HB3	2:B:425:TYR:OH	2.17	0.44
2:D:316:ILE:HD11	2:D:337:ARG:NH2	2.33	0.44
3:E:73:GLN:NE2	3:E:77:GLU:HG3	2.32	0.44
5:J:426:THR:HG23	5:J:427:THR:HG23	1.99	0.44
5:J:796:ARG:O	5:J:945:ASN:ND2	2.50	0.44
5:J:1177:THR:HG21	5:J:1181:MET:HE2	1.99	0.44
5:K:800:LEU:HD23	5:K:923:VAL:HG21	2.00	0.44
5:K:808:LEU:HD23	5:K:883:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:857:LEU:O	5:L:861:VAL:HG22	2.17	0.44
5:M:880:PHE:O	5:M:883:VAL:HG12	2.17	0.44
7:T:193:TYR:HB3	7:T:233:ARG:HB2	2.00	0.44
2:B:262:LYS:HD2	2:B:262:LYS:HA	1.68	0.44
2:B:391:ASP:N	2:B:391:ASP:OD1	2.48	0.44
3:E:296:ASP:OD1	3:E:296:ASP:N	2.47	0.44
3:F:54:ASP:OD1	3:F:57:ARG:NH2	2.51	0.44
5:H:473:PRO:HA	5:H:476:GLN:HB2	2.00	0.44
5:I:57:PHE:HE2	5:J:254:ILE:HD12	1.82	0.44
5:I:517:VAL:HG22	5:I:518:VAL:H	1.81	0.44
5:K:1114:PHE:CD1	5:K:1137:VAL:HG11	2.51	0.44
5:L:180:LEU:HD23	5:L:384:PRO:HG2	2.00	0.44
5:M:1112:ASP:OD1	5:M:1112:ASP:N	2.50	0.44
2:D:74:LEU:HD13	2:D:125:PHE:CZ	2.53	0.44
5:H:147:ILE:O	5:H:151:ILE:HG12	2.17	0.44
5:H:726:ASN:HB2	5:H:728:GLU:OE1	2.17	0.44
5:I:1069:ARG:HD2	8:Y:301:THR:HG21	1.99	0.44
5:I:1187:LYS:HG2	5:I:1356:VAL:HG12	2.00	0.44
5:J:637:ASN:O	5:J:641:THR:HG22	2.17	0.44
5:J:749:HIS:CE1	5:J:885:PHE:HA	2.53	0.44
9:Z:57:MET:CE	9:Z:272:ILE:HD11	2.44	0.44
4:G:85:GLU:HB3	4:G:560:GLN:HE22	1.82	0.44
5:H:97:VAL:O	5:H:97:VAL:HG13	2.18	0.44
5:I:998:CYS:SG	5:I:1004:SER:HB3	2.58	0.44
5:K:495:ILE:HD12	5:K:976:PRO:HG2	2.00	0.44
5:K:1054:CYS:SG	5:K:1091:THR:HB	2.58	0.44
5:M:534:HIS:NE2	5:M:1239:LEU:HD12	2.32	0.44
2:B:34:GLU:HB2	2:B:72:TYR:OH	2.17	0.44
2:B:55:LEU:HD12	2:B:55:LEU:O	2.18	0.44
2:B:55:LEU:O	2:B:66:ARG:NH2	2.49	0.44
2:B:87:TYR:O	2:B:90:GLU:HG3	2.18	0.44
2:B:113:LEU:HB3	2:B:495:GLY:HA3	1.99	0.44
2:D:319:VAL:O	2:D:323:LEU:N	2.51	0.44
2:D:447:ARG:NH2	2:D:451:LEU:HB3	2.33	0.44
5:H:1348:GLU:H	5:H:1355:VAL:HG22	1.83	0.44
5:I:574:ARG:O	5:I:578:ILE:HG12	2.18	0.44
5:L:580:GLU:HG2	5:L:585:ARG:HD3	1.99	0.44
5:M:322:LEU:HD21	5:M:328:TYR:CD2	2.52	0.44
5:M:1033:ALA:O	5:M:1177:THR:HB	2.18	0.44
5:M:1246:THR:O	5:M:1250:GLU:HG2	2.17	0.44
6:P:37:HIS:HD1	6:P:40:LEU:HD23	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:149:ARG:HA	8:Y:152:ILE:HG22	2.00	0.44
1:A:2003:LEU:HD11	1:A:2017:LEU:HB3	1.99	0.44
5:I:793:THR:HG23	5:I:796:ARG:H	1.83	0.44
5:I:1143:LEU:O	5:I:1147:THR:OG1	2.34	0.44
5:L:446:LEU:HD12	5:L:1024:THR:HG21	2.00	0.44
5:M:789:MET:HB3	5:M:790:PRO:HD3	2.00	0.44
1:A:1762:LEU:HA	1:A:2117:PRO:HG3	2.00	0.44
1:A:2016:TRP:CG	1:A:2020:GLN:HE22	2.36	0.44
2:D:237:LEU:HD21	2:D:331:HIS:HB2	1.99	0.44
4:G:322:HIS:ND1	4:G:322:HIS:O	2.51	0.44
5:H:1350:HIS:HB3	5:H:1353:ASN:HB2	2.00	0.44
5:I:611:TYR:O	5:I:615:VAL:HG23	2.18	0.44
5:I:621:VAL:HG13	5:I:622:ASP:H	1.83	0.44
5:K:1332:LEU:O	5:K:1335:THR:HG22	2.17	0.44
5:M:966:TYR:CE2	5:M:974:PRO:HG2	2.53	0.44
7:T:82:ILE:HG23	7:T:86:LEU:HD23	2.00	0.44
1:A:1743:LEU:HA	1:A:2068:LEU:HD11	2.00	0.43
1:A:2221:LEU:HD12	1:A:2224:LEU:HD12	1.98	0.43
2:B:9:PHE:HA	2:B:12:LEU:HB2	2.00	0.43
2:B:200:ALA:O	2:B:203:GLU:HG3	2.17	0.43
1:C:1579:ARG:HG3	1:C:1581:HIS:O	2.18	0.43
1:C:1862:LEU:O	1:C:1866:LEU:HG	2.18	0.43
1:C:2213:ILE:HG21	3:F:86:ALA:HB1	2.00	0.43
2:D:240:HIS:CE1	2:D:290:VAL:HA	2.52	0.43
5:H:173:ARG:HB3	5:I:100:VAL:HG23	2.00	0.43
5:I:807:LEU:C	5:I:807:LEU:HD23	2.43	0.43
5:L:1222:ALA:C	5:L:1224:THR:H	2.25	0.43
8:U:268:LEU:HD22	8:V:152:ILE:CG2	2.47	0.43
2:B:423:ILE:HA	2:B:426:ASN:ND2	2.33	0.43
3:F:280:ALA:HB1	3:F:437:LEU:HB3	1.99	0.43
4:G:512:ARG:HA	4:G:512:ARG:HD3	1.77	0.43
5:H:278:ASN:O	5:H:282:ILE:HG12	2.18	0.43
5:H:888:GLU:H	5:H:919:ASN:ND2	2.15	0.43
5:H:1165:VAL:HG23	5:I:216:LEU:HD23	2.00	0.43
5:I:1158:GLU:HG3	5:I:1301:TYR:OH	2.19	0.43
5:L:78:ILE:HB	5:L:1058:ILE:HG22	1.99	0.43
5:L:419:THR:HG22	5:L:421:ARG:H	1.81	0.43
5:M:1185:TYR:CZ	5:M:1190:ASN:HB3	2.53	0.43
1:A:1612:ASN:HB3	1:A:1845:TRP:CH2	2.53	0.43
1:C:1685:ALA:HA	1:C:1688:HIS:NE2	2.34	0.43
1:C:2235:MET:HE1	3:F:68:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:21:LEU:HD22	4:G:341:LEU:HD21	2.00	0.43
5:I:169:ASP:OD2	5:I:173:ARG:NH2	2.47	0.43
5:J:796:ARG:C	5:J:945:ASN:HD21	2.26	0.43
5:K:927:PRO:O	5:K:931:ILE:HG13	2.17	0.43
5:M:4:TRP:CG	5:M:36:ARG:HD3	2.54	0.43
6:N:34:GLU:OE1	6:N:34:GLU:N	2.48	0.43
8:V:262:ASP:O	8:V:265:ILE:HG22	2.18	0.43
7:W:181:ARG:HG3	8:X:4:MET:HE1	2.00	0.43
2:B:516:LEU:HD12	2:B:517:PHE:HD1	1.82	0.43
1:C:1452:LEU:HD12	1:C:1489:LEU:HD11	2.00	0.43
5:I:1269:GLU:OE1	5:I:1269:GLU:N	2.49	0.43
5:K:704:SER:HB3	5:K:711:HIS:CD2	2.52	0.43
5:L:631:VAL:HG21	5:L:657:ILE:HD11	2.00	0.43
5:M:1284:GLU:CD	5:M:1288:ARG:HE	2.26	0.43
6:O:14:ARG:H	6:O:14:ARG:HD3	1.83	0.43
8:U:142:LEU:HB2	8:U:177:PHE:CD1	2.53	0.43
8:U:145:GLU:OE2	8:U:149:ARG:NH1	2.38	0.43
1:A:1488:GLU:HA	1:A:1491:LYS:HE3	2.00	0.43
1:A:1663:TRP:CD1	1:A:1744:GLN:HB3	2.54	0.43
1:A:1858:MET:HE3	1:A:1991:ILE:HD12	1.99	0.43
1:C:1858:MET:SD	1:C:1862:LEU:HD23	2.58	0.43
3:E:365:HIS:CD2	3:E:434:LEU:HD11	2.53	0.43
3:E:498:PHE:CE1	3:E:501:LEU:HD22	2.54	0.43
4:G:506:ASP:OD2	4:G:512:ARG:NH1	2.52	0.43
5:I:192:VAL:HG23	5:I:219:PHE:CZ	2.54	0.43
5:K:774:THR:HG23	5:K:777:GLU:H	1.83	0.43
5:L:645:LEU:HD23	5:L:645:LEU:H	1.84	0.43
5:M:1187:LYS:HG2	5:M:1356:VAL:HG12	2.01	0.43
6:P:28:LEU:HD12	6:P:32:ILE:HD11	2.00	0.43
7:W:76:SER:HB3	7:W:77:PRO:CD	2.49	0.43
8:Y:91:LEU:HD23	8:Y:91:LEU:H	1.84	0.43
1:A:1862:LEU:HD21	1:A:1952:TRP:CH2	2.54	0.43
2:B:325:PRO:HB2	2:B:355:VAL:HG21	2.01	0.43
1:C:1503:LEU:HD12	1:C:1590:VAL:HA	2.00	0.43
3:E:365:HIS:HD2	3:E:368:VAL:HG23	1.82	0.43
3:F:64:GLU:OE2	6:Q:52:SER:OG	2.36	0.43
4:G:48:VAL:HG13	4:G:53:ARG:O	2.19	0.43
5:H:396:PRO:HB3	5:H:1186:PHE:CZ	2.54	0.43
5:I:396:PRO:HB3	5:I:1186:PHE:CZ	2.54	0.43
5:I:808:LEU:HD21	5:I:883:VAL:HG13	2.01	0.43
5:J:705:ALA:HA	5:J:711:HIS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:535:PRO:HD2	5:K:1239:LEU:HD23	2.00	0.43
5:L:2:GLU:OE1	5:L:2:GLU:N	2.50	0.43
5:L:122:LYS:HD2	5:L:1082:ASN:HD21	1.83	0.43
5:L:451:HIS:CE1	5:L:453:VAL:HG13	2.53	0.43
6:R:45:SER:O	6:R:49:ARG:HG2	2.18	0.43
8:V:149:ARG:NH2	8:V:175:ILE:HD13	2.32	0.43
7:W:238:PRO:C	7:W:240:GLN:H	2.26	0.43
8:X:114:LEU:HD21	8:X:146:ILE:HD11	2.01	0.43
1:A:1758:ILE:HD12	1:A:2111:PHE:CE2	2.54	0.43
2:B:320:ASN:OD1	2:B:321:LEU:N	2.51	0.43
2:B:443:PHE:CE2	2:B:480:PHE:HB3	2.54	0.43
2:D:135:ILE:HG13	2:D:136:GLN:H	1.83	0.43
2:D:135:ILE:HD13	2:D:208:THR:HG23	2.01	0.43
3:E:283:LEU:HA	3:E:404:LEU:HD21	2.00	0.43
5:I:900:ASP:OD2	5:I:1014:LYS:NZ	2.33	0.43
5:I:985:ASN:OD1	5:I:986:TRP:N	2.51	0.43
5:M:230:LEU:HD22	5:M:279:VAL:HG23	2.01	0.43
8:U:219:VAL:HG11	8:V:206:MET:HE2	2.00	0.43
7:W:82:ILE:HD11	7:W:86:LEU:HD22	2.00	0.43
1:C:1646:TYR:HA	1:C:1649:ILE:HG22	2.00	0.43
1:C:1957:PRO:O	1:C:2038:PRO:HG2	2.18	0.43
3:E:340:ARG:HB2	3:E:361:THR:HA	2.01	0.43
3:F:410:ARG:NH1	4:G:332:VAL:HG11	2.33	0.43
3:F:635:PHE:CD2	3:F:637:PRO:HD3	2.54	0.43
5:I:77:ALA:HB1	5:I:302:TYR:HD1	1.84	0.43
5:J:1102:VAL:HG23	5:J:1102:VAL:O	2.19	0.43
5:M:779:THR:O	5:M:783:VAL:HG23	2.19	0.43
2:B:399:MET:O	2:B:403:GLN:HG2	2.19	0.43
1:C:1982:THR:HG22	1:C:1983:SER:N	2.34	0.43
2:D:175:GLN:HG2	2:D:221:PRO:HG3	2.01	0.43
3:E:14:VAL:HG22	3:F:11:PRO:HB2	2.00	0.43
5:H:74:ALA:HB2	5:H:272:VAL:HG21	2.00	0.43
5:H:420:VAL:HG11	5:H:577:GLU:HA	2.01	0.43
5:H:724:PRO:HG2	5:H:727:MET:HE1	2.00	0.43
5:I:322:LEU:HD21	5:I:328:TYR:CD2	2.53	0.43
5:I:401:LEU:HD23	5:I:1183:VAL:HG21	2.01	0.43
5:I:420:VAL:HG11	5:I:576:TRP:HB3	2.00	0.43
5:J:900:ASP:HB2	5:J:903:GLN:NE2	2.33	0.43
5:K:701:GLU:HG3	5:K:702:PRO:HD2	2.00	0.43
5:K:965:HIS:HD2	5:L:697:GLN:OE1	2.02	0.43
5:M:1336:LYS:HE2	5:M:1355:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1614:ALA:O	1:A:1618:LEU:HG	2.19	0.43
1:C:1920:ASP:N	1:C:1920:ASP:OD1	2.50	0.43
2:D:113:LEU:HD13	2:D:495:GLY:H	1.84	0.43
5:H:262:THR:O	5:H:296:VAL:HG23	2.19	0.43
5:H:763:ASP:O	5:H:765:PRO:HD2	2.19	0.43
5:K:99:ARG:HH12	5:K:111:GLN:CD	2.27	0.43
5:K:122:LYS:HG2	5:K:1082:ASN:ND2	2.33	0.43
5:L:148:LEU:O	5:L:152:LEU:HD23	2.19	0.43
6:P:52:SER:OG	6:P:53:LEU:N	2.51	0.43
2:B:331:HIS:HD2	2:B:334:LEU:H	1.63	0.42
2:B:383:LEU:HD22	2:B:427:PHE:CZ	2.54	0.42
1:C:1788:ASN:HB3	1:C:1804:PHE:HE1	1.82	0.42
1:C:1849:MET:HE2	1:C:1849:MET:N	2.34	0.42
2:D:72:TYR:O	2:D:75:SER:OG	2.28	0.42
3:F:210:ASN:HD22	3:F:466:LEU:HG	1.83	0.42
3:F:536:SER:OG	3:F:600:ARG:HD2	2.19	0.42
5:I:666:LEU:HD23	5:I:671:LEU:HB2	2.00	0.42
5:J:789:MET:HB3	5:J:790:PRO:HD3	2.01	0.42
5:J:1222:ALA:C	5:J:1224:THR:H	2.27	0.42
5:M:148:LEU:O	5:M:152:LEU:HG	2.19	0.42
5:M:989:SER:N	5:M:990:PRO:HD2	2.33	0.42
5:M:1202:VAL:HG21	5:M:1210:ALA:HA	2.01	0.42
8:V:271:LEU:HD23	8:V:275:LEU:HD23	2.01	0.42
8:Y:22:GLY:O	8:Y:25:THR:HG22	2.19	0.42
1:A:1778:HIS:CD2	1:A:1781:VAL:H	2.36	0.42
1:A:2221:LEU:HD22	3:F:79:LEU:HD22	2.01	0.42
2:D:394:ALA:O	2:D:398:GLN:HG2	2.19	0.42
3:E:53:MET:HA	3:E:56:VAL:HG12	2.01	0.42
4:G:168:LEU:HA	4:G:317:VAL:HG21	2.01	0.42
5:H:31:MET:HE1	5:K:1089:GLY:HA2	2.01	0.42
7:T:82:ILE:HG23	7:T:86:LEU:HB3	2.00	0.42
8:V:143:ALA:O	8:V:146:ILE:HG22	2.18	0.42
1:A:1448:LEU:HG	1:A:1489:LEU:HD11	2.01	0.42
1:A:1755:PRO:HD3	1:A:1802:LYS:HG3	2.01	0.42
1:A:1878:SER:O	1:A:1882:GLN:HG3	2.19	0.42
2:B:257:PHE:HZ	2:B:294:LEU:HA	1.84	0.42
2:B:346:ARG:HA	2:B:346:ARG:HD2	1.89	0.42
1:C:1577:PHE:O	1:C:1579:ARG:NH2	2.52	0.42
1:C:1845:TRP:O	1:C:1849:MET:HG2	2.19	0.42
2:D:177:LEU:HD23	2:D:180:ARG:HH21	1.85	0.42
5:H:271:GLY:C	5:H:367:VAL:HG23	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:588:PRO:HB2	5:H:590:TYR:CE2	2.54	0.42
5:H:760:MET:HE3	5:H:805:LYS:HB2	2.02	0.42
5:H:1350:HIS:N	5:H:1353:ASN:O	2.44	0.42
5:K:892:VAL:HG11	5:K:979:PHE:CE1	2.54	0.42
5:L:1087:GLY:HA3	5:L:1091:THR:HG21	2.02	0.42
6:O:15:ASP:O	6:O:19:ARG:HG2	2.18	0.42
8:X:96:ASN:HB3	8:X:102:TRP:CZ2	2.54	0.42
1:C:1460:LEU:HD21	1:C:1591:PHE:HA	2.00	0.42
2:D:375:ASP:O	2:D:379:MET:HG2	2.17	0.42
5:I:386:GLU:OE1	5:I:386:GLU:N	2.53	0.42
5:J:62:GLU:OE1	5:J:62:GLU:N	2.52	0.42
5:K:262:THR:HG22	5:K:268:LYS:HG2	2.01	0.42
5:K:462:GLN:O	5:K:466:GLU:HG2	2.19	0.42
5:K:1285:TYR:HA	5:K:1289:ALA:HB3	2.01	0.42
5:L:64:VAL:HG21	5:L:375:VAL:HG12	2.00	0.42
5:L:684:VAL:O	5:L:687:ILE:HG22	2.19	0.42
5:L:985:ASN:OD1	5:L:986:TRP:N	2.53	0.42
5:M:775:ASP:O	5:M:779:THR:HG23	2.19	0.42
8:Y:285:GLN:H	8:Y:285:GLN:CD	2.28	0.42
1:C:1448:LEU:N	2:D:35:ILE:HD13	2.34	0.42
2:D:135:ILE:HG22	2:D:185:LEU:HD22	2.01	0.42
3:E:315:LEU:O	3:E:319:VAL:HG23	2.19	0.42
3:E:443:LEU:HD23	3:E:443:LEU:HA	1.82	0.42
3:E:498:PHE:O	3:E:502:VAL:HG23	2.19	0.42
5:H:1087:GLY:HA3	5:H:1091:THR:HG21	2.01	0.42
5:H:1166:HIS:CD2	5:I:1223:GLN:HA	2.55	0.42
5:I:645:LEU:HD13	5:I:674:TYR:HE1	1.84	0.42
5:I:661:LEU:O	5:I:661:LEU:HD23	2.20	0.42
5:L:127:ILE:HD12	5:L:171:MET:SD	2.60	0.42
5:L:260:THR:HG22	5:L:261:TYR:CD2	2.55	0.42
5:L:1315:CYS:HA	5:L:1318:THR:HG22	2.02	0.42
5:M:43:PRO:HG2	8:X:28:VAL:HG11	2.01	0.42
5:M:1195:ARG:HG3	5:M:1221:ASP:CG	2.44	0.42
5:M:1245:ASN:HB2	5:M:1248:HIS:HB3	2.02	0.42
8:X:146:ILE:O	8:X:150:LEU:HD23	2.19	0.42
2:B:123:THR:O	2:B:126:GLN:HG3	2.19	0.42
2:B:126:GLN:O	2:B:130:GLN:HG2	2.20	0.42
2:B:464:GLU:HG2	2:B:465:LEU:HD12	2.01	0.42
1:C:1768:MET:N	1:C:1768:MET:SD	2.93	0.42
2:D:134:GLU:O	2:D:138:VAL:HG23	2.20	0.42
2:D:377:THR:HG22	2:D:381:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:505:TYR:OH	2:D:515:HIS:ND1	2.45	0.42
3:E:615:GLY:O	3:E:620:ASN:N	2.52	0.42
3:F:200:ARG:HG3	3:F:201:GLY:H	1.84	0.42
4:G:514:TRP:NE1	4:G:522:VAL:HG11	2.34	0.42
5:H:227:LEU:O	5:H:1096:VAL:HG13	2.19	0.42
5:I:723:LEU:HD23	5:I:768:VAL:HG23	2.01	0.42
5:J:558:ILE:HA	5:J:1015:ILE:HD11	2.02	0.42
5:K:454:LEU:CD2	5:K:1243:LEU:HD11	2.48	0.42
5:K:601:VAL:HG13	5:K:924:VAL:HG11	2.01	0.42
5:M:630:PHE:HB2	5:M:878:GLU:OE2	2.20	0.42
5:M:661:LEU:HD23	5:M:666:LEU:HD11	2.02	0.42
1:A:2194:SER:OG	1:A:2195:PHE:N	2.52	0.42
1:C:1816:LEU:HG	1:C:2052:VAL:HG11	2.01	0.42
2:D:284:ALA:HA	2:D:287:MET:HE2	2.01	0.42
3:E:438:ALA:O	3:E:441:LEU:HG	2.20	0.42
3:F:267:TYR:HE2	3:F:270:TYR:HB3	1.85	0.42
5:H:375:VAL:HG13	5:H:376:TYR:CD2	2.54	0.42
5:I:56:THR:HG22	5:J:92:LEU:HB3	2.01	0.42
5:K:83:LEU:HD23	5:K:83:LEU:HA	1.89	0.42
5:K:788:LEU:HA	5:K:1005:VAL:HG13	2.00	0.42
5:L:216:LEU:HD23	5:M:1165:VAL:HG13	2.01	0.42
8:V:272:PHE:HA	8:V:275:LEU:HG	2.01	0.42
1:A:1743:LEU:O	1:A:1747:CYS:HB2	2.19	0.42
2:B:257:PHE:CZ	2:B:294:LEU:HA	2.54	0.42
2:B:447:ARG:HA	2:B:450:ILE:HB	2.01	0.42
3:E:233:PRO:HA	3:E:236:LYS:HG2	2.02	0.42
3:E:601:LEU:O	3:E:607:PRO:HG2	2.19	0.42
3:F:410:ARG:HH11	4:G:332:VAL:HG11	1.82	0.42
3:F:619:PHE:HB2	3:F:621:VAL:HG23	2.02	0.42
5:H:675:ARG:HA	5:H:678:VAL:HG22	2.01	0.42
5:H:888:GLU:CD	5:H:919:ASN:HD22	2.28	0.42
5:H:1180:THR:HG22	5:H:1180:THR:O	2.20	0.42
5:I:288:SER:HA	5:I:291:ILE:HD12	2.02	0.42
5:J:682:ARG:HA	5:J:685:THR:HG22	2.02	0.42
5:L:936:PRO:HB3	5:L:952:LEU:HD23	2.00	0.42
5:M:808:LEU:HD12	5:M:808:LEU:HA	1.89	0.42
8:U:153:MET:SD	8:U:169:VAL:HG12	2.60	0.42
8:Y:110:VAL:HG23	8:Y:287:VAL:HG21	2.01	0.42
8:Y:262:ASP:O	8:Y:265:ILE:HG22	2.20	0.42
2:B:72:TYR:O	2:B:75:SER:OG	2.32	0.42
2:B:454:HIS:O	2:B:458:LEU:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1498:SER:HB3	1:C:1516:GLY:HA3	2.02	0.42
1:C:1878:SER:O	1:C:1882:GLN:OE1	2.38	0.42
1:C:1884:LEU:HD22	1:C:1935:LEU:HD13	2.02	0.42
1:C:1979:LEU:HD23	1:C:1979:LEU:HA	1.92	0.42
2:D:328:MET:CG	2:D:334:LEU:HD23	2.50	0.42
3:E:466:LEU:HB3	3:E:470:ALA:HB3	2.02	0.42
3:E:496:ARG:HD2	3:E:498:PHE:HB3	2.02	0.42
3:F:457:THR:OG1	3:F:622:ASN:O	2.37	0.42
4:G:415:MET:HE3	4:G:415:MET:HB2	1.96	0.42
5:I:263:THR:HG1	5:I:267:ALA:H	1.62	0.42
5:L:855:GLU:OE1	5:L:855:GLU:N	2.46	0.42
5:M:147:ILE:O	5:M:151:ILE:HG12	2.20	0.42
5:M:819:LEU:HD21	6:S:32:ILE:HG21	2.02	0.42
6:P:37:HIS:CE1	6:P:39:VAL:HG22	2.54	0.42
8:X:119:LEU:HD23	8:X:119:LEU:O	2.20	0.42
1:A:1589:ASP:HB3	1:A:1595:GLN:NE2	2.35	0.42
1:A:1672:ARG:O	1:A:1676:THR:OG1	2.29	0.42
1:A:1979:LEU:HD21	1:A:1981:TYR:CZ	2.55	0.42
1:A:2210:ALA:O	1:A:2214:LEU:HG	2.20	0.42
2:B:40:ALA:HB3	2:B:88:ALA:HB1	2.02	0.42
2:B:507:ASP:OD1	2:B:511:LYS:NZ	2.33	0.42
2:D:200:ALA:O	2:D:203:GLU:HG3	2.20	0.42
3:F:357:TYR:OH	3:F:427:GLN:O	2.35	0.42
5:H:989:SER:N	5:H:990:PRO:HD2	2.35	0.42
5:H:1224:THR:C	5:H:1226:ALA:H	2.28	0.42
5:I:717:PRO:HD2	5:I:778:TRP:CH2	2.55	0.42
5:J:542:CYS:SG	5:J:543:GLN:N	2.92	0.42
5:L:645:LEU:HD12	5:L:674:TYR:CZ	2.55	0.42
6:Q:14:ARG:HD2	6:Q:14:ARG:C	2.44	0.42
1:A:1621:ARG:HH11	1:A:1627:LEU:HD11	1.84	0.41
1:C:2034:LEU:HD13	1:C:2054:ARG:NH2	2.35	0.41
2:D:236:VAL:HA	2:D:239:MET:HE2	2.02	0.41
3:F:4:LEU:HD23	3:F:4:LEU:H	1.85	0.41
3:F:450:ASP:OD1	3:F:450:ASP:N	2.47	0.41
3:F:498:PHE:O	3:F:502:VAL:HG23	2.20	0.41
3:F:635:PHE:HD2	3:F:637:PRO:HD3	1.85	0.41
5:H:572:GLU:O	5:H:575:THR:OG1	2.26	0.41
5:I:669:GLN:OE1	5:I:669:GLN:N	2.48	0.41
5:I:1254:TYR:CZ	5:I:1256:SER:HA	2.55	0.41
5:K:428:ALA:O	5:K:440:ILE:HG22	2.20	0.41
5:L:600:THR:OG1	5:L:644:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:892:VAL:HG11	5:M:979:PHE:CZ	2.55	0.41
5:M:939:PHE:HA	5:M:979:PHE:CD2	2.55	0.41
7:T:173:LEU:HD23	7:T:203:TYR:CD1	2.55	0.41
8:U:57:GLY:HA2	8:U:188:VAL:CG1	2.50	0.41
8:U:270:ALA:O	8:U:273:VAL:HG12	2.20	0.41
1:A:1563:ASP:O	1:A:1567:ILE:HG12	2.20	0.41
1:A:1960:LEU:O	1:A:1978:HIS:HB3	2.20	0.41
2:B:62:PHE:O	2:B:66:ARG:HG2	2.20	0.41
2:B:100:LEU:HD22	2:B:122:LEU:HD12	2.02	0.41
2:B:484:TYR:CE1	2:B:516:LEU:HD22	2.56	0.41
3:E:628:LEU:O	3:E:632:VAL:HG22	2.20	0.41
4:G:490:GLU:OE2	4:G:492:ARG:NH1	2.54	0.41
5:H:75:ALA:HB2	5:H:179:PHE:CZ	2.54	0.41
5:J:251:THR:HG21	5:J:1089:GLY:H	1.84	0.41
5:J:536:PHE:HE1	5:J:1032:PHE:CE2	2.37	0.41
5:K:77:ALA:HB1	5:K:302:TYR:CD1	2.56	0.41
5:K:1116:VAL:HG12	5:K:1258:PHE:CG	2.56	0.41
5:K:1138:GLU:HG3	5:K:1139:ARG:H	1.85	0.41
5:K:1332:LEU:O	5:K:1336:LYS:HG2	2.20	0.41
5:L:307:LEU:HD22	5:L:321:ILE:CD1	2.50	0.41
5:L:322:LEU:HD21	5:L:328:TYR:CD2	2.55	0.41
5:M:651:TYR:OH	5:M:780:LEU:HD23	2.20	0.41
5:M:1120:ASN:O	5:M:1132:ARG:NH1	2.53	0.41
6:R:17:LYS:HA	6:R:17:LYS:HD3	1.75	0.41
8:V:175:ILE:HG22	8:V:182:PHE:HB2	2.01	0.41
8:Y:228:SER:O	8:Y:229:MET:HG3	2.19	0.41
1:C:2021:ILE:HA	1:C:2024:LEU:HG	2.02	0.41
3:F:620:ASN:C	3:F:620:ASN:HD22	2.28	0.41
5:H:1101:ARG:NH2	5:I:202:LEU:HG	2.31	0.41
5:I:255:LEU:HD21	5:I:345:SER:HB3	2.02	0.41
5:J:811:LEU:HG	5:J:857:LEU:HD21	2.00	0.41
5:K:1233:ALA:HB1	5:K:1240:SER:HB3	2.02	0.41
5:L:287:LEU:O	5:L:291:ILE:HG23	2.20	0.41
5:M:211:GLN:O	5:M:215:ILE:HG12	2.20	0.41
5:M:798:CYS:O	5:M:923:VAL:HG12	2.21	0.41
5:M:934:SER:OG	5:M:952:LEU:HD11	2.20	0.41
5:M:1349:THR:HA	5:M:1354:TYR:HA	2.01	0.41
8:U:198:LYS:HG2	8:V:222:LEU:HD21	2.02	0.41
8:X:151:LEU:HD22	8:Y:272:PHE:CZ	2.55	0.41
9:Z:47:HIS:O	9:Z:50:THR:OG1	2.33	0.41
1:A:1596:ILE:HB	1:A:1604:ILE:CD1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:236:VAL:HG12	2:D:239:MET:HE2	2.01	0.41
2:D:397:ALA:HB2	2:D:424:ILE:HB	2.02	0.41
3:E:199:PHE:O	3:E:203:VAL:HG12	2.20	0.41
5:H:230:LEU:HD23	5:H:1097:ALA:HB1	2.03	0.41
5:H:288:SER:HA	5:H:291:ILE:HG12	2.02	0.41
5:H:1165:VAL:HG11	5:I:1223:GLN:HB2	2.03	0.41
5:I:259:THR:O	5:I:259:THR:HG22	2.20	0.41
5:I:695:ASN:HD21	5:J:507:ARG:NE	2.19	0.41
5:J:128:PRO:HB3	5:J:1076:HIS:ND1	2.35	0.41
5:M:888:GLU:O	5:M:919:ASN:ND2	2.53	0.41
5:M:1095:CYS:SG	5:M:1096:VAL:N	2.94	0.41
8:U:24:LEU:HD13	8:U:125:LEU:HD11	2.01	0.41
8:V:49:HIS:O	8:V:52:VAL:HG12	2.20	0.41
2:B:319:VAL:HG13	2:B:323:LEU:HD21	2.03	0.41
3:E:506:ILE:HG23	3:E:510:TYR:HE2	1.85	0.41
5:H:433:ARG:HH22	5:I:217:GLN:CB	2.33	0.41
5:H:600:THR:HG21	5:H:645:LEU:HD11	2.01	0.41
5:I:472:GLU:O	5:I:475:MET:HB3	2.20	0.41
5:I:532:GLU:CD	5:I:555:ARG:HH12	2.29	0.41
5:I:534:HIS:ND1	5:I:535:PRO:HD2	2.36	0.41
5:I:537:PHE:HD1	5:I:554:PRO:HA	1.85	0.41
5:J:1041:THR:OG1	5:J:1104:THR:HG23	2.20	0.41
5:K:87:THR:HG23	5:K:88:THR:N	2.35	0.41
5:K:535:PRO:HB3	5:K:1232:TRP:CE2	2.56	0.41
5:L:498:PHE:CE2	5:L:976:PRO:HA	2.56	0.41
5:L:635:ILE:HD11	5:L:674:TYR:CE1	2.54	0.41
5:M:1116:VAL:HG13	5:M:1117:PHE:CD2	2.56	0.41
5:M:1195:ARG:NE	5:M:1213:ALA:O	2.40	0.41
7:T:212:TRP:O	7:T:216:VAL:HG23	2.20	0.41
8:V:48:LEU:HB2	8:V:133:VAL:HG13	2.02	0.41
7:W:188:ILE:HB	7:W:203:TYR:HB2	2.03	0.41
8:Y:51:PHE:CD1	8:Y:64:LEU:HD13	2.55	0.41
9:Z:70:ASN:O	9:Z:72:ASP:N	2.54	0.41
1:A:1640:ASN:HA	1:A:1864:LEU:HG	2.03	0.41
1:A:1699:LEU:HA	1:A:1702:THR:HG22	2.02	0.41
2:B:86:LEU:HD12	2:B:86:LEU:H	1.86	0.41
1:C:1841:LEU:HD23	1:C:1841:LEU:H	1.86	0.41
3:E:301:VAL:O	3:E:305:LEU:HB2	2.20	0.41
3:F:330:VAL:HB	3:F:364:ARG:HG2	2.03	0.41
4:G:462:ARG:HE	7:W:103:GLU:CD	2.25	0.41
5:H:697:GLN:HB3	5:I:965:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:779:THR:O	5:I:783:VAL:HG23	2.20	0.41
5:I:884:GLN:HA	6:O:66:ARG:HB2	2.02	0.41
5:J:388:ASN:HB2	5:J:1311:ILE:CD1	2.51	0.41
5:L:558:ILE:HD12	5:L:558:ILE:HA	1.94	0.41
5:L:575:THR:OG1	5:L:1007:THR:HA	2.20	0.41
5:M:681:LEU:CB	5:M:780:LEU:HD11	2.51	0.41
5:M:1350:HIS:CG	5:M:1351:PHE:N	2.88	0.41
6:R:19:ARG:HA	6:R:22:VAL:HG12	2.03	0.41
1:A:1492:ARG:HH12	1:A:1493:ARG:HB3	1.86	0.41
2:B:370:VAL:HG22	2:B:481:ALA:HB3	2.03	0.41
2:B:425:TYR:CD2	2:B:458:LEU:HG	2.56	0.41
5:I:131:LEU:HD21	5:I:160:VAL:HG23	2.02	0.41
5:J:495:ILE:HB	5:J:496:PRO:HD3	2.03	0.41
5:J:651:TYR:HB2	5:J:784:PHE:CD1	2.56	0.41
5:K:1042:PHE:CE2	5:K:1362:LEU:HD11	2.55	0.41
5:L:78:ILE:O	5:L:1058:ILE:HA	2.21	0.41
5:M:19:PHE:HE1	5:M:32:PHE:HZ	1.69	0.41
5:M:86:LEU:HG	5:M:87:THR:O	2.20	0.41
7:W:126:HIS:CE1	7:W:286:PHE:HB3	2.55	0.41
1:A:1709:ASP:OD1	1:A:1710:THR:N	2.54	0.41
1:A:1745:GLU:HB3	1:A:1967:LEU:HD13	2.01	0.41
1:A:1863:TRP:O	1:A:1867:LYS:HB3	2.20	0.41
2:B:477:ASN:O	2:B:481:ALA:HB2	2.20	0.41
1:C:1625:ARG:HE	1:C:1628:ALA:HA	1.85	0.41
2:D:70:VAL:HG22	2:D:96:LEU:HD22	2.03	0.41
3:E:240:HIS:O	3:E:240:HIS:ND1	2.51	0.41
5:H:236:ARG:HA	5:H:286:LEU:HD21	2.02	0.41
5:H:431:LEU:HD12	5:H:435:ARG:HA	2.03	0.41
5:H:638:MET:HE1	5:H:642:ARG:HD2	2.02	0.41
5:I:174:GLY:HA3	5:J:101:ALA:H	1.85	0.41
5:I:808:LEU:HD12	5:I:808:LEU:HA	1.95	0.41
5:I:1175:ILE:HG22	5:I:1244:TYR:CE2	2.56	0.41
5:L:1099:VAL:O	5:L:1369:ASN:ND2	2.54	0.41
5:M:1195:ARG:HA	5:M:1221:ASP:OD2	2.20	0.41
8:V:31:VAL:HG21	8:V:137:ILE:HD11	2.02	0.41
7:W:195:GLY:O	7:W:233:ARG:NH1	2.54	0.41
1:A:1492:ARG:NH1	1:A:1493:ARG:HB3	2.35	0.41
1:A:1956:ILE:HD12	1:A:1957:PRO:HD2	2.02	0.41
1:A:2159:VAL:HG12	1:A:2161:THR:H	1.86	0.41
2:B:342:GLU:OE2	2:B:407:GLN:NE2	2.52	0.41
1:C:1995:ARG:NH2	1:C:1997:LEU:HD21	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2219:LEU:HD23	1:C:2219:LEU:HA	1.89	0.41
2:D:143:SER:OG	2:D:215:TRP:NE1	2.53	0.41
2:D:195:TYR:O	2:D:201:VAL:HG21	2.20	0.41
2:D:268:MET:HA	2:D:271:PHE:CE2	2.56	0.41
3:E:43:ARG:NE	3:E:43:ARG:HA	2.35	0.41
3:E:337:TYR:HE2	3:E:367:LEU:HD23	1.85	0.41
3:F:600:ARG:HH12	3:F:610:ARG:HH22	1.67	0.41
4:G:28:ASP:HB3	4:G:124:MET:SD	2.60	0.41
5:H:850:ARG:HG3	5:H:858:THR:HG21	2.03	0.41
5:I:229:LEU:HD22	5:I:242:PHE:CE2	2.56	0.41
5:I:273:MET:HA	5:I:1048:LEU:O	2.21	0.41
5:I:435:ARG:HG3	5:I:1367:LEU:HD22	2.03	0.41
5:I:686:ARG:NH1	5:J:996:ALA:O	2.54	0.41
5:I:763:ASP:OD1	5:I:764:GLU:N	2.51	0.41
5:I:952:LEU:HD12	5:I:952:LEU:HA	1.87	0.41
5:I:1145:THR:O	5:I:1148:ILE:HG22	2.21	0.41
5:J:77:ALA:HB1	5:J:302:TYR:HD1	1.85	0.41
5:J:808:LEU:HD23	6:P:62:LEU:HD11	2.03	0.41
5:J:873:LEU:HD21	5:J:877:ARG:HH11	1.85	0.41
5:K:321:ILE:HB	5:L:52:ALA:HA	2.03	0.41
5:K:627:ILE:HG22	5:K:631:VAL:HG23	2.03	0.41
5:L:485:GLN:OE1	5:L:913:ARG:NH1	2.51	0.41
5:L:1050:SER:OG	5:L:1054:CYS:SG	2.63	0.41
5:L:1098:TYR:OH	5:L:1369:ASN:HB2	2.20	0.41
5:M:62:GLU:HG2	5:M:62:GLU:O	2.21	0.41
8:U:235:GLN:O	8:U:239:MET:N	2.54	0.41
8:U:287:VAL:HG23	8:U:288:PHE:HD2	1.85	0.41
8:V:74:ARG:HG2	8:V:74:ARG:O	2.21	0.41
8:V:121:ARG:HE	8:V:124:LEU:HD11	1.85	0.41
8:X:49:HIS:O	8:X:52:VAL:HG12	2.21	0.41
2:B:91:GLN:HA	2:B:94:GLU:OE1	2.20	0.41
2:B:390:HIS:HB2	2:B:432:MET:HE1	2.03	0.41
1:C:1589:ASP:HB3	1:C:1595:GLN:HB3	2.02	0.41
1:C:1603:PRO:HG2	1:C:1606:LEU:HD12	2.01	0.41
1:C:1850:ALA:HB1	1:C:1949:LEU:HD22	2.02	0.41
2:D:352:TYR:OH	2:D:420:LEU:HD13	2.21	0.41
3:E:610:ARG:CZ	3:E:614:LEU:HG	2.51	0.41
5:H:199:ASN:HD21	5:H:215:ILE:HD11	1.85	0.41
5:H:450:CYS:O	5:H:1122:TYR:OH	2.33	0.41
5:H:1184:ASN:O	5:H:1184:ASN:ND2	2.51	0.41
5:J:126:THR:HG22	5:J:1078:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:129:PHE:CE1	5:J:1075:TYR:HB2	2.56	0.41
5:J:680:VAL:O	5:J:684:VAL:HG13	2.21	0.41
5:K:420:VAL:HG22	5:K:580:GLU:CD	2.46	0.41
5:M:127:ILE:HD12	5:M:128:PRO:HD2	2.03	0.41
5:M:429:TYR:C	5:M:430:LEU:HD12	2.46	0.41
5:M:609:LEU:HD22	5:M:861:VAL:HG12	2.03	0.41
5:M:1217:HIS:HE1	5:M:1235:GLN:HA	1.86	0.41
5:M:1274:ALA:O	5:M:1276:LYS:N	2.54	0.41
6:Q:19:ARG:NE	6:Q:19:ARG:HA	2.36	0.41
6:Q:49:ARG:HA	6:Q:49:ARG:NE	2.36	0.41
9:Z:20:LEU:HD23	9:Z:20:LEU:HA	1.91	0.41
2:B:455:ARG:HB2	2:B:469:TRP:CZ2	2.56	0.40
1:C:1459:LEU:HD21	1:C:1479:ILE:HG22	2.03	0.40
1:C:1960:LEU:HD23	1:C:1960:LEU:H	1.85	0.40
1:C:2037:ILE:HB	1:C:2055:PRO:HG2	2.03	0.40
5:H:441:ASP:OD1	5:H:442:PHE:N	2.54	0.40
5:I:194:GLN:O	5:I:197:VAL:HG12	2.21	0.40
5:I:509:VAL:HG21	5:I:540:THR:HG23	2.03	0.40
5:I:624:PHE:CD2	5:I:656:LEU:HB3	2.55	0.40
5:I:757:LEU:HD12	6:O:62:LEU:HD23	2.02	0.40
5:I:806:THR:HA	5:I:809:VAL:HG12	2.03	0.40
5:I:1150:MET:HG2	7:W:76:SER:HB2	2.03	0.40
5:I:1297:THR:HG21	5:I:1301:TYR:CE2	2.56	0.40
5:J:684:VAL:CG2	5:J:783:VAL:HG11	2.51	0.40
5:J:789:MET:O	5:J:793:THR:HG22	2.22	0.40
5:J:1129:ARG:HE	5:J:1139:ARG:NH2	2.19	0.40
5:J:1182:ASP:OD2	5:J:1184:ASN:ND2	2.53	0.40
5:K:936:PRO:HB3	5:K:952:LEU:HD22	2.02	0.40
5:L:535:PRO:HG3	5:L:1232:TRP:CE3	2.56	0.40
5:L:600:THR:OG1	5:L:645:LEU:HD23	2.20	0.40
6:P:37:HIS:HA	6:P:38:PRO:HD3	1.92	0.40
8:X:219:VAL:HG23	8:Y:205:SER:OG	2.20	0.40
1:A:1570:ASP:OD2	1:A:2008:THR:HG21	2.21	0.40
1:A:1627:LEU:CD2	1:A:1630:ARG:HG3	2.48	0.40
1:A:1951:SER:HA	1:A:1956:ILE:HG22	2.03	0.40
1:A:1979:LEU:HD21	1:A:1981:TYR:OH	2.21	0.40
2:B:189:ALA:O	2:B:193:ARG:N	2.54	0.40
2:B:443:PHE:O	2:B:447:ARG:HB3	2.20	0.40
2:D:277:ASP:O	2:D:280:GLN:HG2	2.22	0.40
3:E:273:VAL:N	3:E:429:TYR:OH	2.43	0.40
3:F:336:TYR:CG	3:F:337:TYR:N	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:486:GLU:OE2	5:H:977:THR:OG1	2.33	0.40
5:H:763:ASP:C	5:H:765:PRO:HD2	2.46	0.40
5:H:777:GLU:HA	5:H:780:LEU:HB2	2.03	0.40
5:I:478:LEU:HD21	5:I:509:VAL:HG13	2.03	0.40
5:L:192:VAL:HG11	5:L:1282:ILE:CD1	2.51	0.40
5:L:397:VAL:HG23	5:L:428:ALA:HB2	2.03	0.40
6:R:17:LYS:O	6:R:21:VAL:HG22	2.20	0.40
7:T:62:GLN:HG3	7:T:264:LEU:HD11	2.02	0.40
8:V:128:GLY:C	8:V:130:TRP:H	2.29	0.40
8:Y:127:LEU:HB2	8:Y:130:TRP:HB3	2.02	0.40
8:Y:228:SER:C	8:Y:229:MET:HG3	2.46	0.40
9:Z:114:PHE:CD1	9:Z:124:ILE:HD11	2.57	0.40
2:B:48:VAL:HA	2:B:51:PHE:HB3	2.04	0.40
1:C:1553:PRO:HG3	2:D:402:ILE:HG12	2.03	0.40
3:E:501:LEU:HG	3:E:505:TYR:HD2	1.87	0.40
4:G:46:ARG:HH12	4:G:557:ASP:CG	2.25	0.40
5:H:392:THR:HG21	5:H:1264:GLN:NE2	2.35	0.40
5:H:451:HIS:CE1	5:H:1117:PHE:HB2	2.56	0.40
5:H:535:PRO:HD3	5:H:1232:TRP:CG	2.57	0.40
5:I:10:LEU:HD21	5:J:316:ILE:HG21	2.04	0.40
5:I:1336:LYS:NZ	5:I:1346:THR:O	2.53	0.40
5:J:80:PHE:HD1	5:J:82:ASP:H	1.69	0.40
5:J:687:ILE:HG13	5:J:1006:MET:SD	2.61	0.40
5:J:958:ARG:HA	5:J:961:THR:HG22	2.04	0.40
5:J:1043:GLU:O	5:J:1099:VAL:HG23	2.21	0.40
5:L:363:GLY:O	5:L:364:GLU:HG2	2.21	0.40
5:M:498:PHE:CE1	5:M:977:THR:HG23	2.57	0.40
8:X:110:VAL:C	8:X:111:LEU:HD12	2.46	0.40
1:A:1859:LEU:HB3	1:A:1877:VAL:HG21	2.03	0.40
1:C:1669:TYR:HB3	1:C:1694:LYS:HG2	2.03	0.40
2:D:79:VAL:HB	2:D:203:GLU:OE2	2.21	0.40
2:D:113:LEU:HG	2:D:116:TYR:H	1.87	0.40
2:D:210:GLN:NE2	2:D:436:VAL:HA	2.37	0.40
3:E:362:PHE:HE1	3:E:383:TYR:HD1	1.70	0.40
3:E:428:GLN:HG2	3:E:429:TYR:N	2.37	0.40
5:H:958:ARG:HA	5:H:961:THR:HG22	2.02	0.40
5:H:1325:LEU:HA	5:H:1356:VAL:O	2.21	0.40
5:I:372:LEU:O	5:I:375:VAL:HG12	2.21	0.40
5:I:1222:ALA:C	5:I:1224:THR:H	2.29	0.40
5:J:490:GLY:O	5:J:494:ARG:HG3	2.22	0.40
5:J:698:LEU:HD12	5:J:1127:VAL:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:1025:LYS:HE2	5:J:1025:LYS:HB2	1.94	0.40
5:K:396:PRO:HB3	5:K:1186:PHE:CZ	2.57	0.40
5:K:698:LEU:HD22	5:K:706:TYR:CE2	2.57	0.40
5:K:725:ARG:NH1	5:K:772:ARG:HB2	2.36	0.40
5:L:367:VAL:HG11	5:L:1049:TYR:HE2	1.86	0.40
5:L:934:SER:OG	5:L:952:LEU:HD11	2.22	0.40
5:M:263:THR:HG22	5:M:267:ALA:H	1.87	0.40
5:M:1059:ILE:HG22	5:M:1081:ILE:HG22	2.04	0.40
6:R:40:LEU:HD12	6:R:44:LEU:HD21	2.03	0.40
8:X:140:MET:HG3	8:X:144:LEU:HD12	2.02	0.40
2:B:37:ALA:HB1	2:B:78:THR:HB	2.03	0.40
2:B:125:PHE:O	2:B:129:LEU:HG	2.20	0.40
2:B:275:ASP:N	2:B:275:ASP:OD1	2.51	0.40
1:C:1958:VAL:H	1:C:1981:TYR:HB2	1.86	0.40
1:C:2213:ILE:HD12	1:C:2213:ILE:HA	1.99	0.40
2:D:441:PHE:HB3	2:D:512:TRP:CD2	2.57	0.40
5:H:952:LEU:HA	5:H:952:LEU:HD12	1.88	0.40
5:I:624:PHE:CZ	5:I:657:ILE:HD13	2.51	0.40
5:I:1350:HIS:N	5:I:1353:ASN:O	2.43	0.40
5:J:534:HIS:CD2	5:J:536:PHE:HB2	2.56	0.40
5:L:451:HIS:ND1	5:L:453:VAL:HG22	2.37	0.40
5:L:648:ALA:HA	5:L:654:VAL:HG12	2.03	0.40
5:M:555:ARG:HB3	5:M:560:ASN:HB3	2.03	0.40
5:M:570:PHE:CE1	5:M:1179:VAL:HG11	2.56	0.40
5:M:763:ASP:OD1	5:M:764:GLU:N	2.53	0.40
8:V:49:HIS:ND1	8:V:131:GLU:HG2	2.37	0.40
8:V:282:ILE:HG13	8:V:283:ARG:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	711/2241 (32%)	685 (96%)	26 (4%)	0	100	100
1	C	681/2241 (30%)	657 (96%)	24 (4%)	0	100	100
2	B	488/983 (50%)	476 (98%)	12 (2%)	0	100	100
2	D	445/983 (45%)	436 (98%)	9 (2%)	0	100	100
3	E	468/642 (73%)	461 (98%)	7 (2%)	0	100	100
3	F	478/642 (74%)	467 (98%)	11 (2%)	0	100	100
4	G	468/594 (79%)	446 (95%)	22 (5%)	0	100	100
5	H	1305/1370 (95%)	1255 (96%)	47 (4%)	3 (0%)	43	74
5	I	1346/1370 (98%)	1291 (96%)	55 (4%)	0	100	100
5	J	1313/1370 (96%)	1245 (95%)	66 (5%)	2 (0%)	43	74
5	K	1292/1370 (94%)	1238 (96%)	53 (4%)	1 (0%)	48	79
5	L	1346/1370 (98%)	1280 (95%)	65 (5%)	1 (0%)	48	79
5	M	1346/1370 (98%)	1284 (95%)	61 (4%)	1 (0%)	48	79
6	N	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
6	O	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
6	P	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
6	Q	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
6	R	61/75 (81%)	61 (100%)	0	0	100	100
6	S	61/75 (81%)	57 (93%)	4 (7%)	0	100	100
7	T	236/290 (81%)	228 (97%)	8 (3%)	0	100	100
7	W	288/290 (99%)	274 (95%)	14 (5%)	0	100	100
8	U	288/306 (94%)	281 (98%)	7 (2%)	0	100	100
8	V	282/306 (92%)	262 (93%)	18 (6%)	2 (1%)	18	51
8	X	291/306 (95%)	281 (97%)	10 (3%)	0	100	100
8	Y	279/306 (91%)	266 (95%)	11 (4%)	2 (1%)	18	51
9	Z	282/1048 (27%)	270 (96%)	12 (4%)	0	100	100
All	All	13999/19848 (70%)	13437 (96%)	550 (4%)	12 (0%)	49	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	764	GLU
8	Y	297	ASN
5	J	377	LYS

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Mol	Chain	Res	Type
5	L	377	LYS
8	V	297	ASN
5	J	980	ALA
8	V	129	GLN
5	M	650	SER
5	H	665	ALA
5	K	980	ALA
8	Y	179	ASP
5	H	378	ASN

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	647/1941 (33%)	647 (100%)	0	100	100
1	C	626/1941 (32%)	626 (100%)	0	100	100
2	B	431/837 (52%)	431 (100%)	0	100	100
2	D	400/837 (48%)	399 (100%)	1 (0%)	86	83
3	E	417/526 (79%)	417 (100%)	0	100	100
3	F	423/526 (80%)	423 (100%)	0	100	100
4	G	398/500 (80%)	398 (100%)	0	100	100
5	H	1144/1192 (96%)	1140 (100%)	4 (0%)	86	83
5	I	1175/1192 (99%)	1174 (100%)	1 (0%)	88	87
5	J	1146/1192 (96%)	1145 (100%)	1 (0%)	88	87
5	K	1131/1192 (95%)	1130 (100%)	1 (0%)	88	87
5	L	1175/1192 (99%)	1175 (100%)	0	100	100
5	M	1175/1192 (99%)	1175 (100%)	0	100	100
6	N	59/68 (87%)	59 (100%)	0	100	100
6	O	59/68 (87%)	59 (100%)	0	100	100
6	P	59/68 (87%)	59 (100%)	0	100	100
6	Q	59/68 (87%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	R	59/68 (87%)	59 (100%)	0	100	100
6	S	59/68 (87%)	59 (100%)	0	100	100
7	T	209/252 (83%)	209 (100%)	0	100	100
7	W	252/252 (100%)	251 (100%)	1 (0%)	84	81
8	U	262/273 (96%)	262 (100%)	0	100	100
8	V	260/273 (95%)	260 (100%)	0	100	100
8	X	263/273 (96%)	263 (100%)	0	100	100
8	Y	257/273 (94%)	257 (100%)	0	100	100
9	Z	255/883 (29%)	255 (100%)	0	100	100
All	All	12400/17147 (72%)	12391 (100%)	9 (0%)	87	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	273	SER
5	H	192	VAL
5	H	379	THR
5	H	1228	THR
5	H	1239	LEU
5	I	861	VAL
5	J	540	THR
5	K	1228	THR
7	W	40	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1475	GLN
1	A	1533	HIS
1	A	1706	GLN
1	A	1778	HIS
1	A	1796	HIS
1	A	1828	GLN
1	A	1835	GLN
1	A	2018	GLN
1	A	2110	GLN
2	B	15	GLN
2	B	286	HIS

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Mol	Chain	Res	Type
2	B	466	GLN
2	B	492	HIS
2	B	509	HIS
1	C	1475	GLN
1	C	1534	GLN
1	C	1912	GLN
1	C	2169	GLN
1	C	2229	GLN
2	D	258	GLN
2	D	286	HIS
2	D	331	HIS
2	D	363	HIS
2	D	378	GLN
2	D	403	GLN
2	D	467	HIS
3	E	259	ASN
3	E	365	HIS
3	E	427	GLN
3	E	448	ASN
3	F	289	HIS
3	F	358	HIS
3	F	379	HIS
3	F	427	GLN
3	F	620	ASN
4	G	333	ASN
4	G	409	HIS
4	G	455	GLN
4	G	560	GLN
5	H	199	ASN
5	H	581	HIS
5	H	694	ASN
5	H	713	HIS
5	H	731	GLN
5	H	740	ASN
5	H	889	HIS
5	H	903	GLN
5	H	1184	ASN
5	H	1264	GLN
5	H	1275	ASN
5	I	59	ASN
5	I	76	HIS
5	I	534	HIS

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Mol	Chain	Res	Type
5	I	637	ASN
5	I	708	ASN
5	I	713	HIS
5	I	731	GLN
5	I	849	GLN
5	I	915	HIS
5	I	965	HIS
5	I	1166	HIS
5	I	1229	HIS
5	I	1300	GLN
5	I	1353	ASN
5	J	59	ASN
5	J	199	ASN
5	J	319	HIS
5	J	432	ASN
5	J	510	ASN
5	J	534	HIS
5	J	660	HIS
5	J	731	GLN
5	J	849	GLN
5	J	1029	HIS
5	J	1223	GLN
5	J	1230	ASN
5	J	1255	ASN
5	J	1353	ASN
5	K	153	ASN
5	K	194	GLN
5	K	326	ASN
5	K	676	ASN
5	K	694	ASN
5	K	740	ASN
5	K	905	GLN
5	K	965	HIS
5	K	1079	GLN
5	K	1275	ASN
5	K	1353	ASN
5	K	1364	GLN
5	L	76	HIS
5	L	331	HIS
5	L	336	GLN
5	L	378	ASN
5	L	476	GLN

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Mol	Chain	Res	Type
5	L	649	HIS
5	L	694	ASN
5	L	697	GLN
5	L	781	GLN
5	L	1079	GLN
5	L	1082	ASN
5	L	1133	HIS
5	M	278	ASN
5	M	331	HIS
5	M	378	ASN
5	M	388	ASN
5	M	510	ASN
5	M	514	GLN
5	M	722	HIS
5	M	726	ASN
5	M	915	HIS
5	M	919	ASN
5	M	965	HIS
5	M	1079	GLN
5	M	1124	HIS
5	M	1133	HIS
5	M	1184	ASN
6	P	37	HIS
7	T	211	HIS
8	U	209	ASN
8	V	7	ASN
8	V	147	ASN
8	V	258	HIS
7	W	40	HIS
7	W	43	HIS
7	W	116	GLN
8	X	116	HIS
8	X	258	HIS
8	Y	49	HIS
8	Y	129	GLN

5.3.3 RNA ⓘ

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.

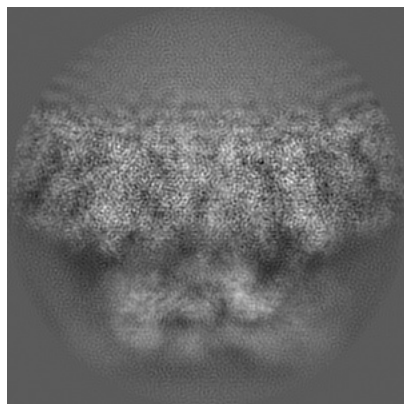
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41194. These allow visual inspection of the internal detail of the map and identification of artifacts.

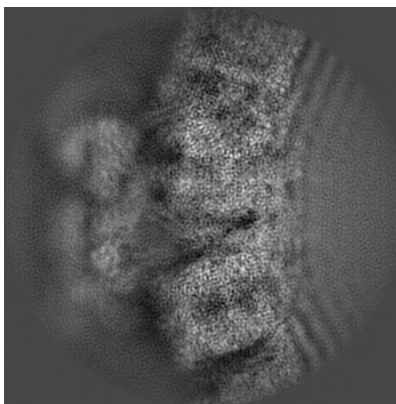
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

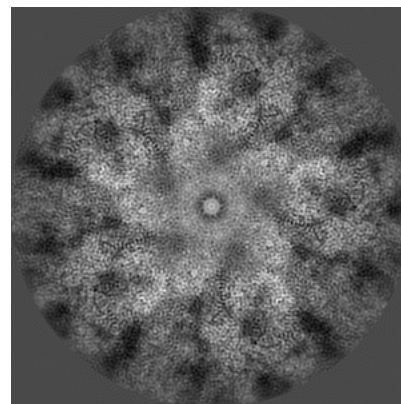
6.1.1 Primary map



X

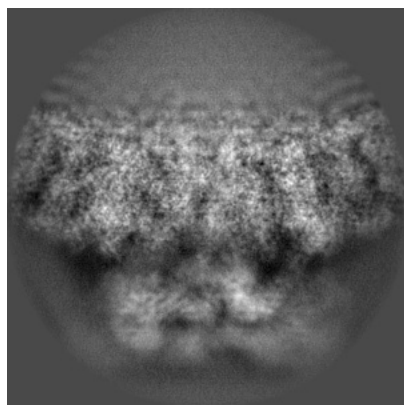


Y

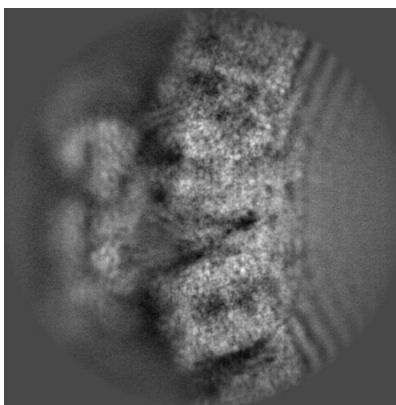


Z

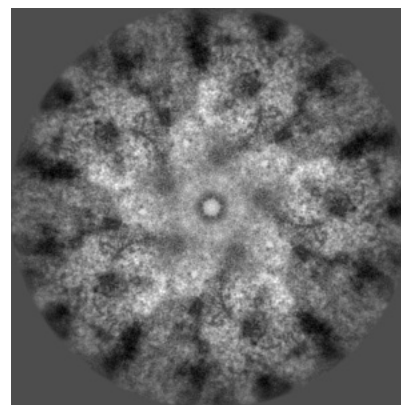
6.1.2 Raw map



X



Y

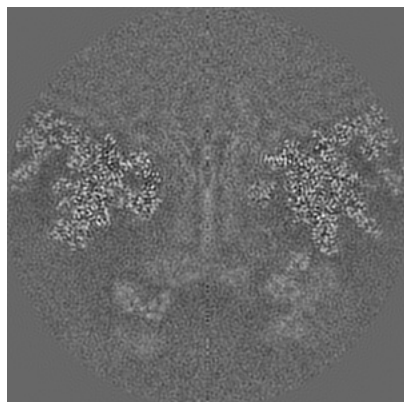


Z

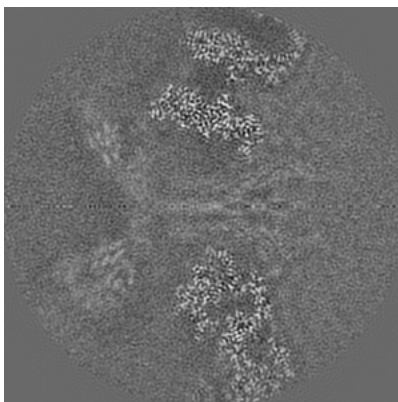
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

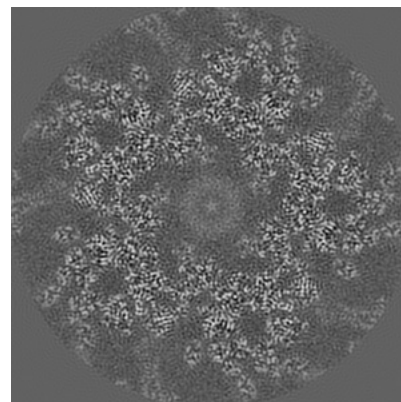
6.2.1 Primary map



X Index: 180

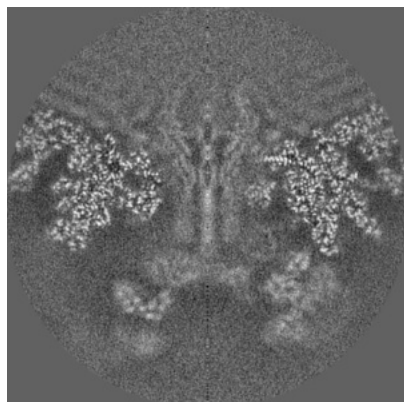


Y Index: 180

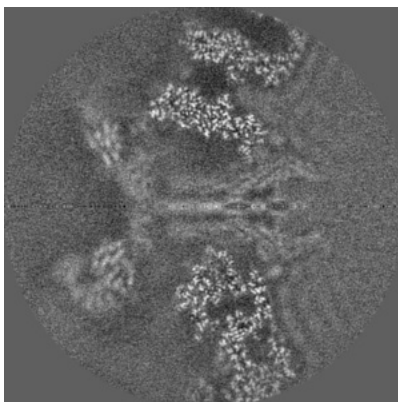


Z Index: 180

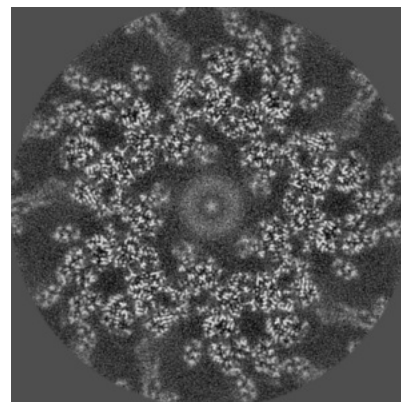
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

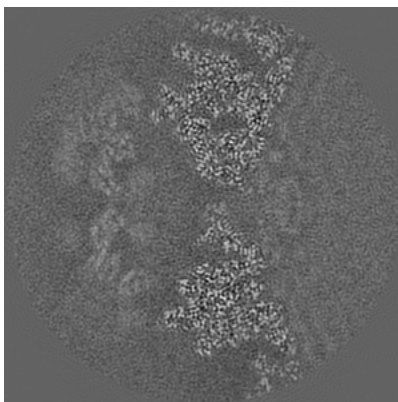
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

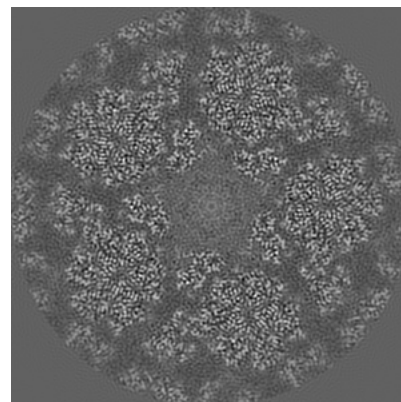
6.3.1 Primary map



X Index: 235

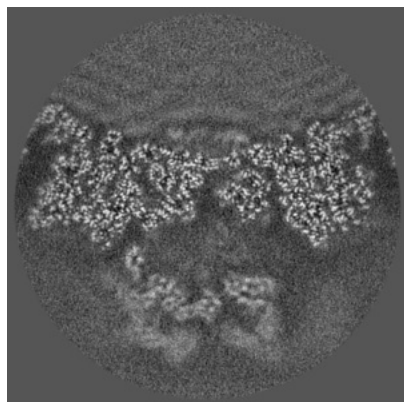


Y Index: 218

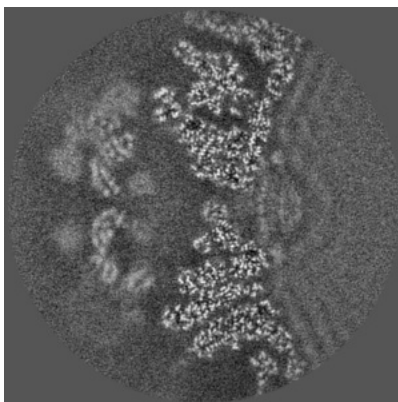


Z Index: 203

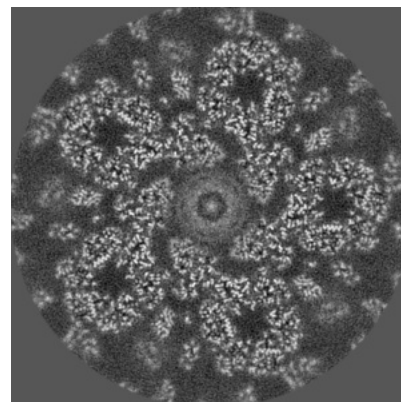
6.3.2 Raw map



X Index: 233



Y Index: 221

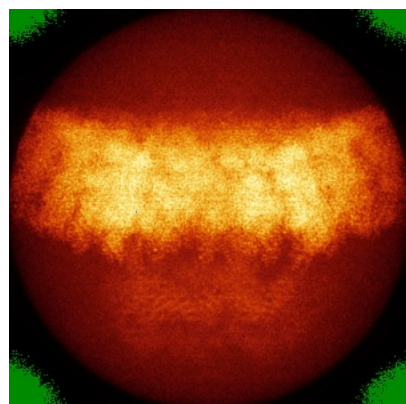


Z Index: 189

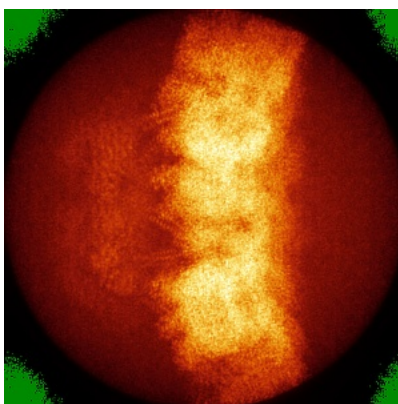
The images above show the largest variance slices of the map in three orthogonal directions.

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

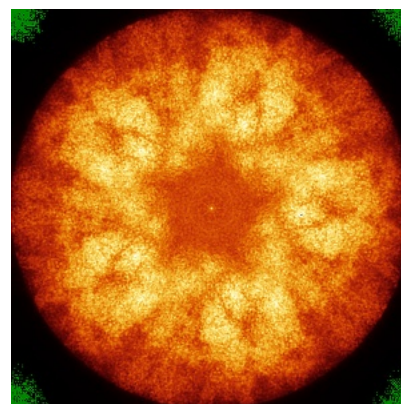
6.4.1 Primary map



X

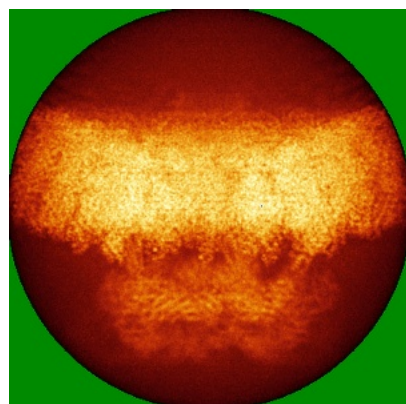


Y

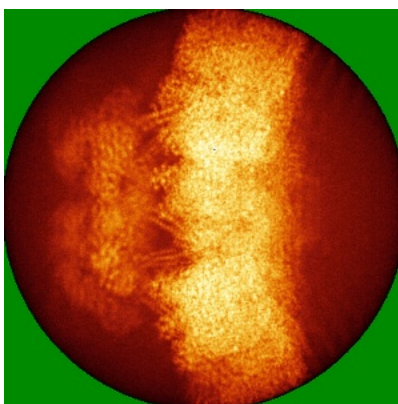


Z

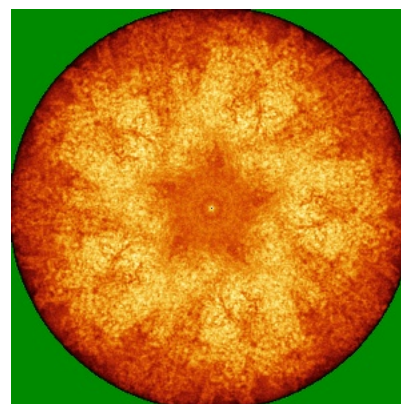
6.4.2 Raw map



X



Y

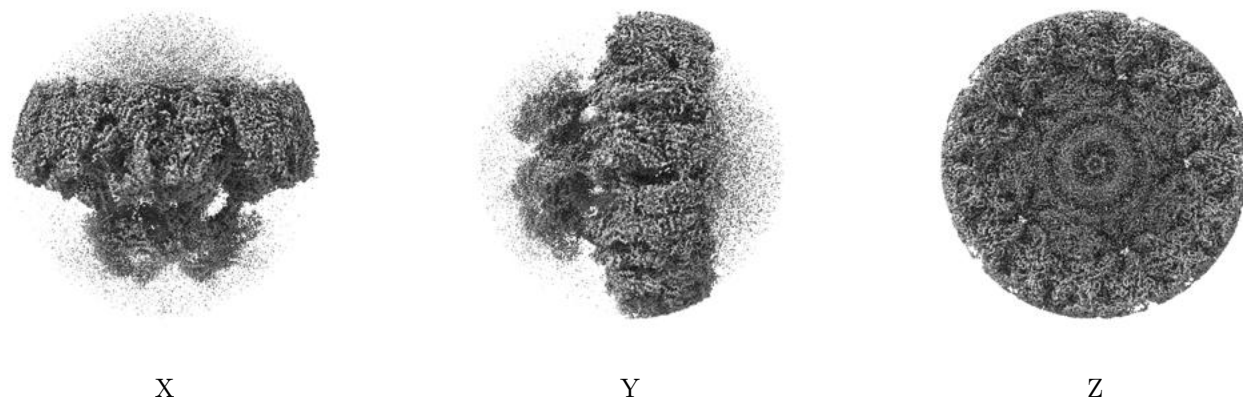


Z

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.

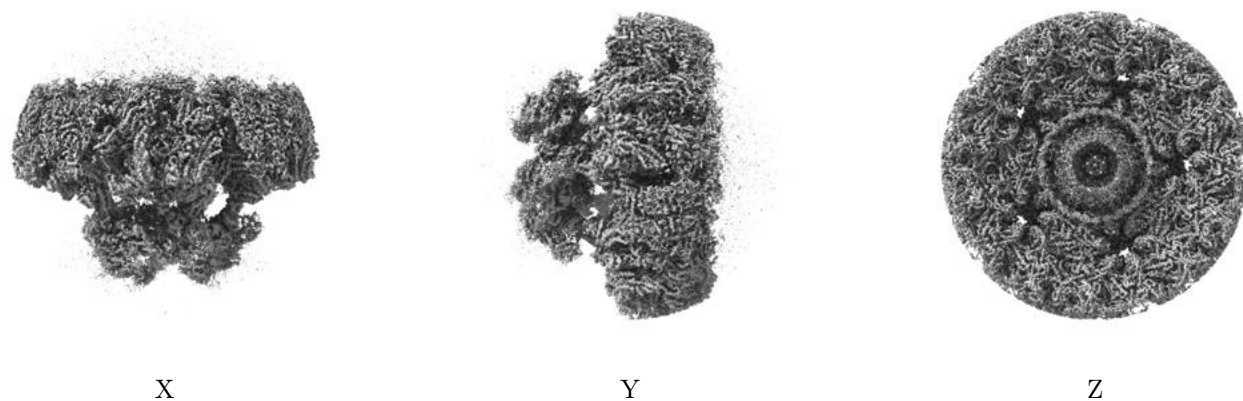
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

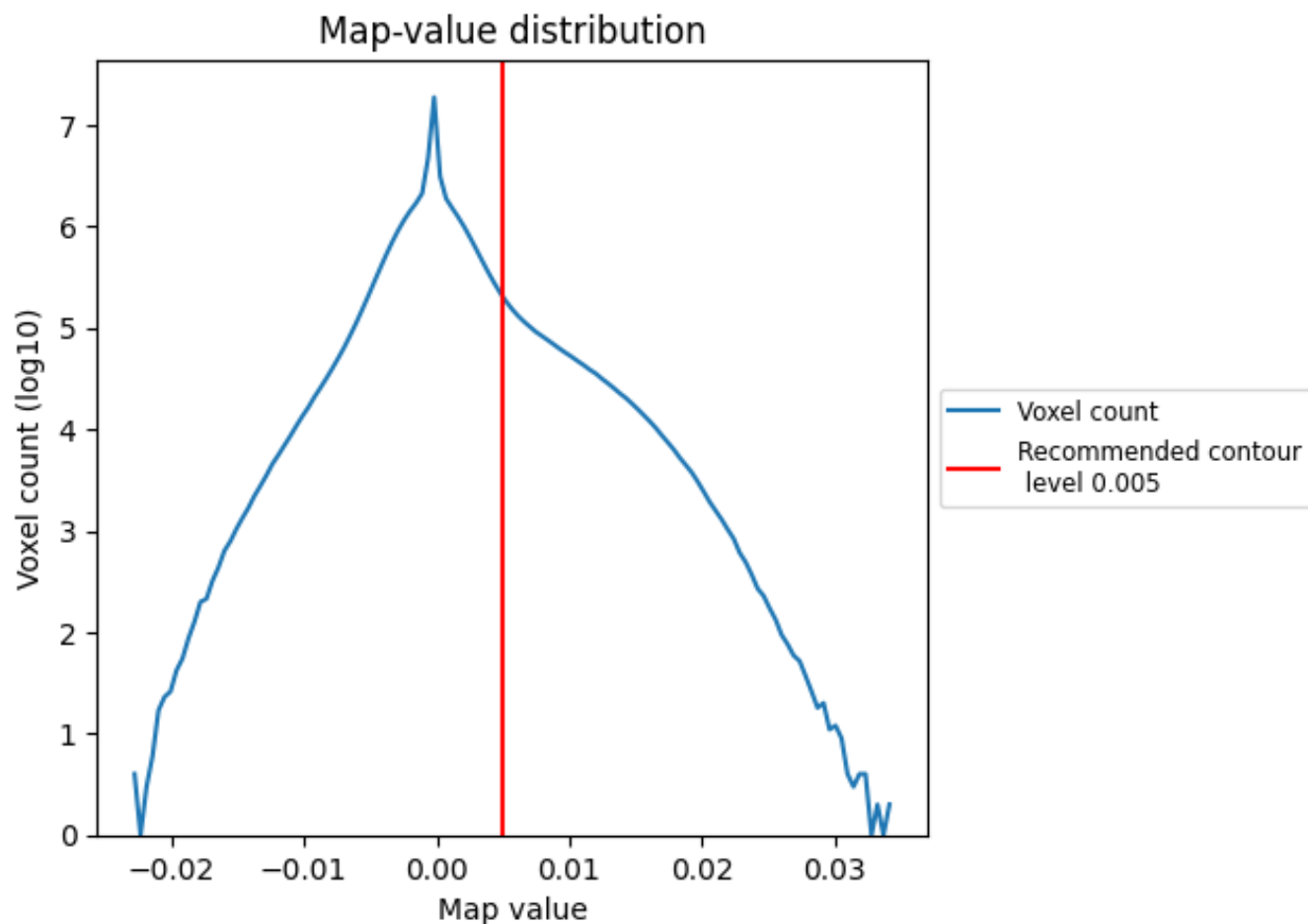
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

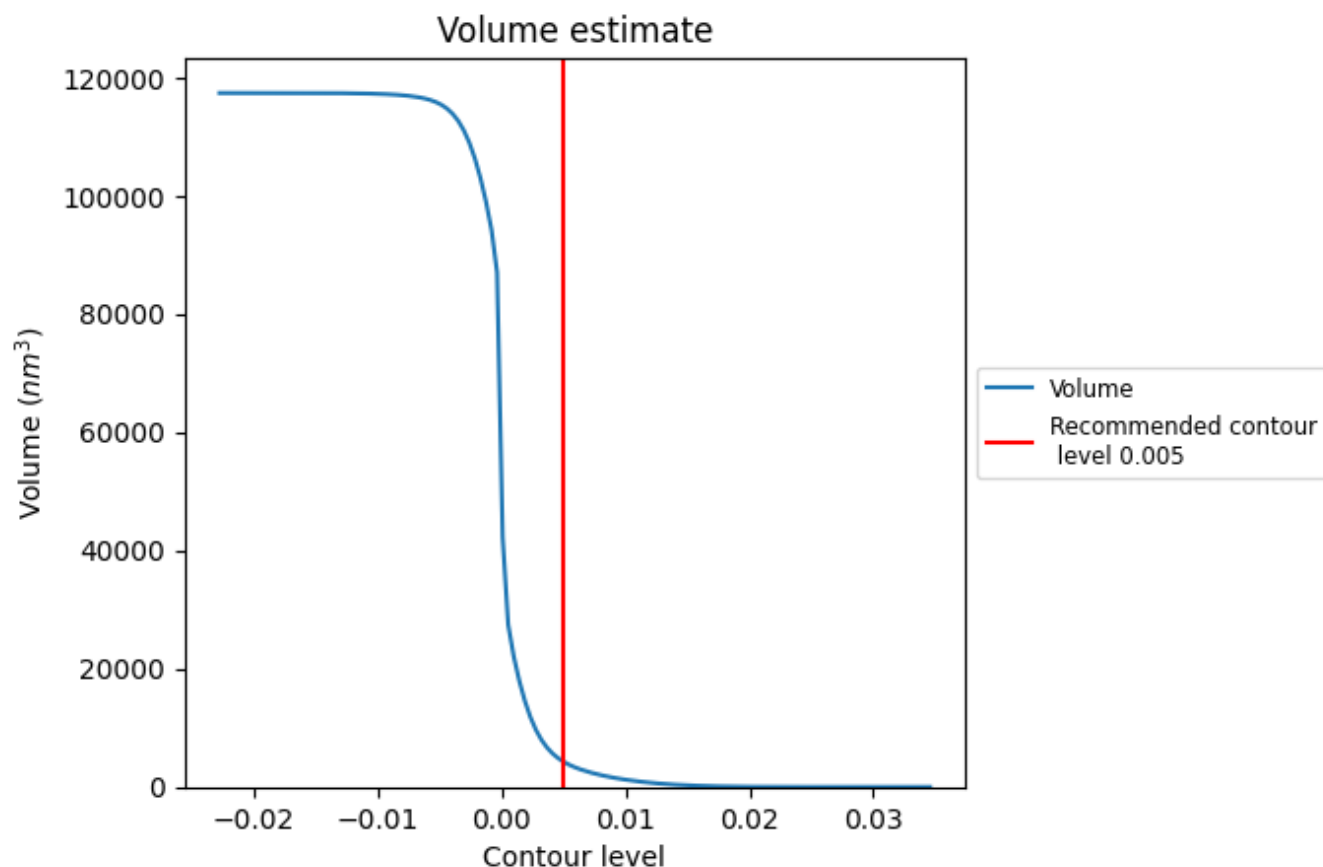
This section contains the results of statistical analysis of the map.

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.

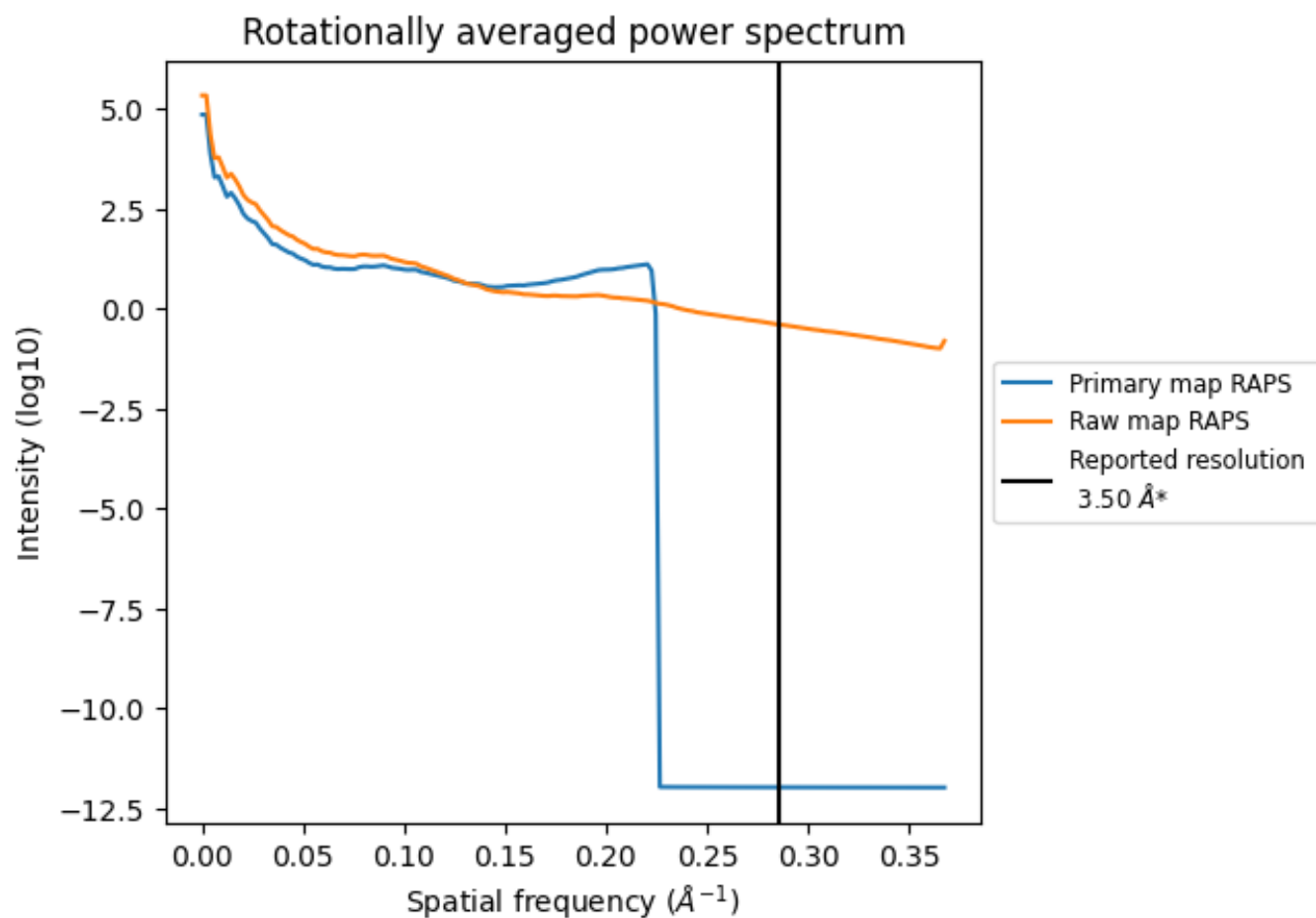
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4271 nm³; this corresponds to an approximate mass of 3858 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 ⓘ

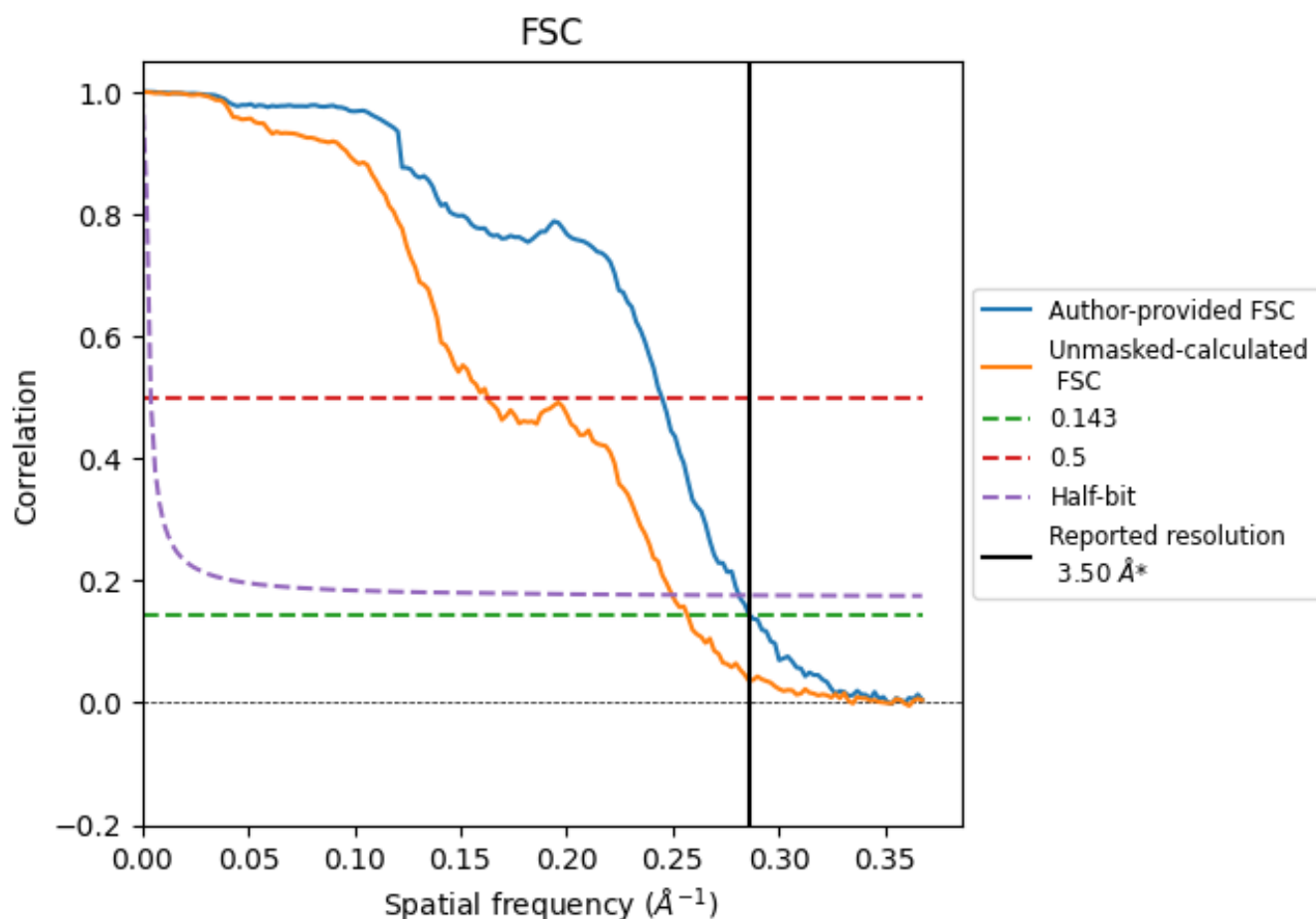


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

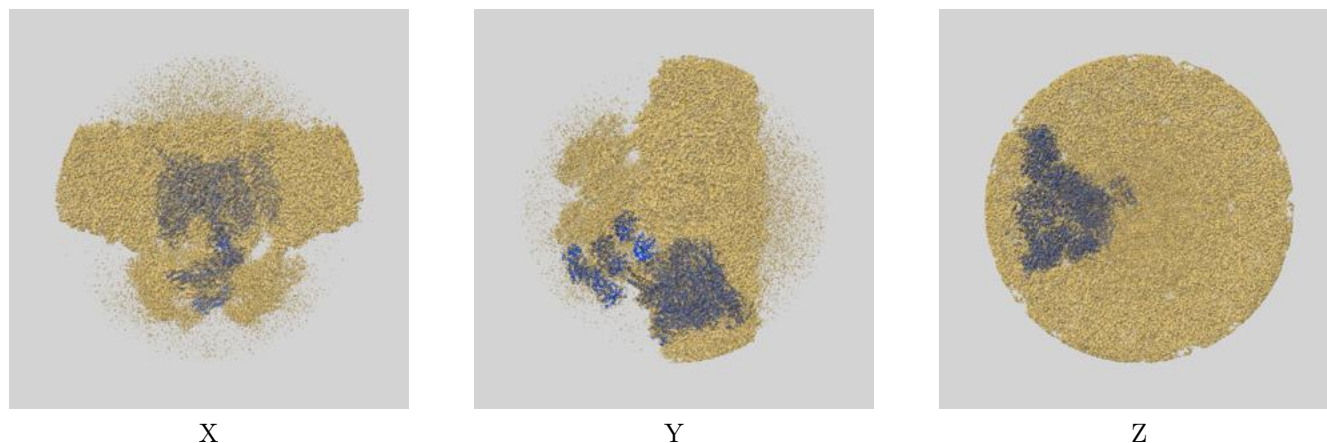
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.49	4.08	3.55
Unmasked-calculated*	3.89	6.15	4.00

*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 3.89 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

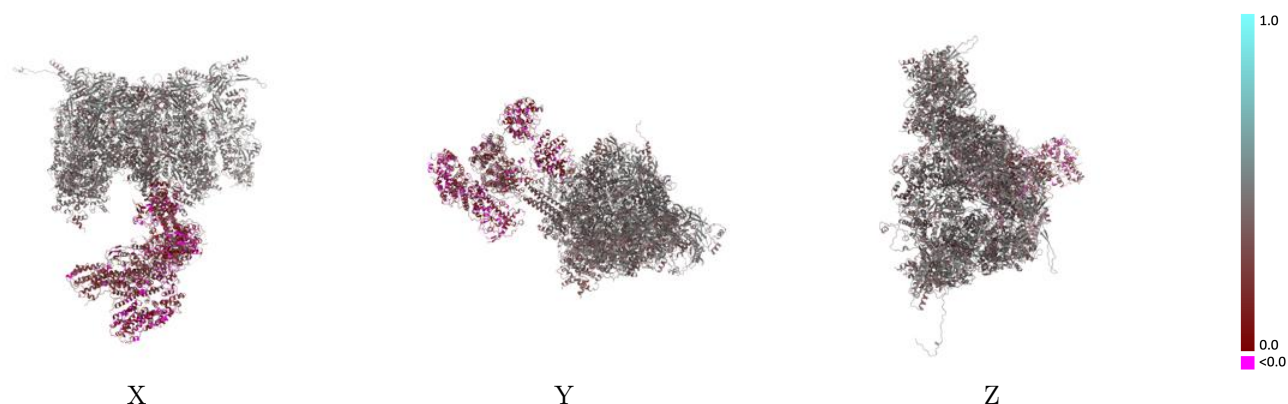
This section contains information regarding the fit between EMDB map EMD-41194 and PDB model 8TEP. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



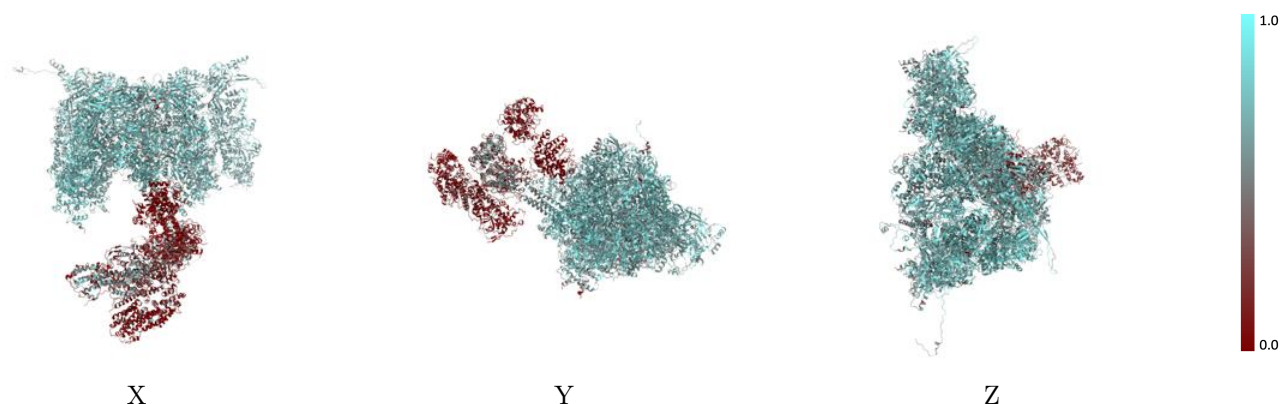
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



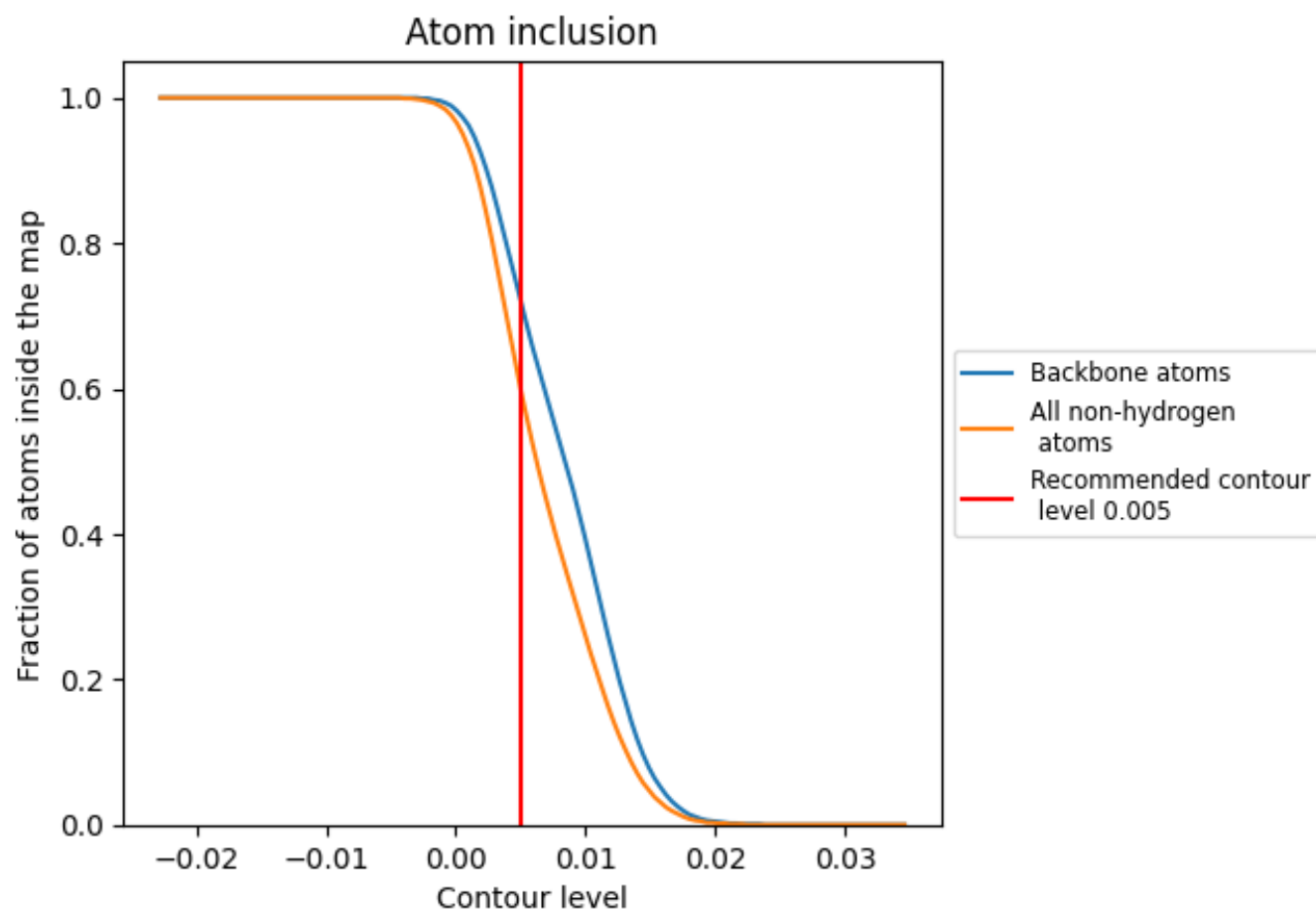
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 60% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5980	 0.3740
A	 0.3660	 0.2590
B	 0.3970	 0.2380
C	 0.1390	 0.1570
D	 0.1140	 0.1200
E	 0.2180	 0.2180
F	 0.1150	 0.1960
G	 0.7370	 0.4310
H	 0.7570	 0.4380
I	 0.7440	 0.4340
J	 0.6960	 0.4280
K	 0.7470	 0.4340
L	 0.7190	 0.4320
M	 0.6800	 0.4260
N	 0.6930	 0.3750
O	 0.7210	 0.4110
P	 0.5840	 0.3640
Q	 0.6730	 0.3730
R	 0.5940	 0.3800
S	 0.5120	 0.3750
T	 0.6480	 0.4150
U	 0.7190	 0.4300
V	 0.7250	 0.4310
W	 0.7210	 0.4410
X	 0.6620	 0.4320
Y	 0.6510	 0.4240
Z	 0.6320	 0.4060

