



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:02 PM UTC

PDB ID : 7BR7 / pdb_00007br7
EMDB ID : EMD-30158
Title : Epstein-Barr virus, C1 portal-proximal penton vertex, CATC binding
Authors : Li, Z.; Yu, X.
Deposited on : 2020-03-26
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

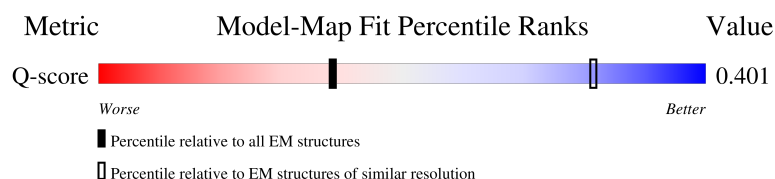
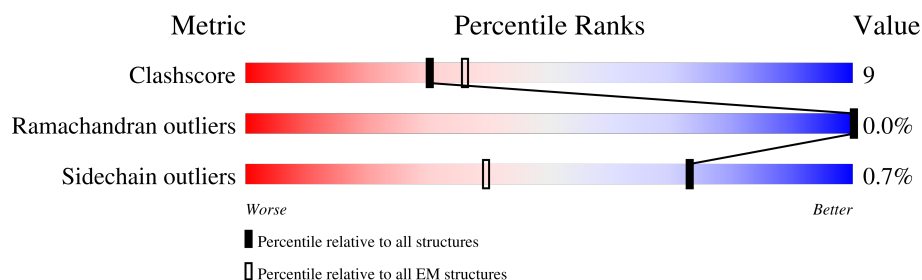
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.30 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.



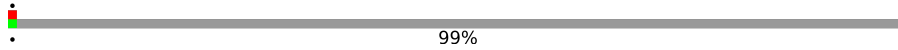
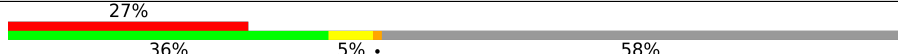
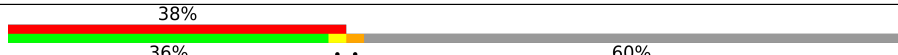
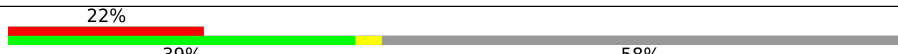
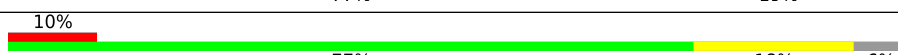
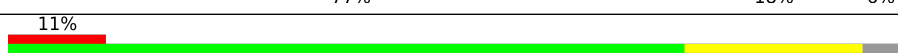
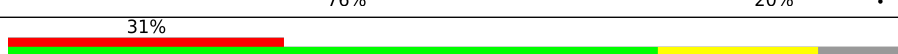
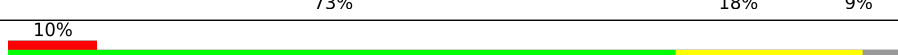
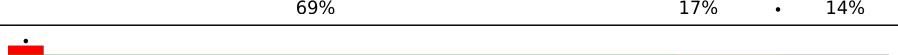
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	G	570	9% 10% 85%
1	K	570	7% 9% 88%
2	C	507	33% 43% 24% 32%
3	B	3149	99%

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Mol	Chain	Length	Quality of chain
3	O	3149	
4	2	176	
4	Y	176	
4	Z	176	
4	m	176	
4	y	176	
5	S	1381	
5	T	1381	
5	W	1381	
5	l	1381	
5	x	1381	
6	5	364	
6	e	364	
7	6	301	
7	7	301	
7	f	301	
7	g	301	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 73138 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 Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	68	Total	C	N	O	S	0	0
			563	343	113	104	3		
1	G	84	Total	C	N	O	S	0	0
			675	412	135	125	3		

- Molecule 2 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	346	Total	C	N	O	S	0	0
			2705	1733	482	478	12		

- Molecule 3 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	35	Total	C	N	O	0	0
			301	192	61	48		
3	O	29	Total	C	N	O	0	0
			252	163	49	40		

- Molecule 4 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	m	71	Total	C	N	O	S	0	0
			600	381	111	107	1		
4	Y	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
4	Z	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
4	2	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
4	y	74	Total	C	N	O	S	0	0
			621	394	114	112	1		

- Molecule 5 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	1327	Total	C	N	O	S	0	0
			10455	6644	1812	1940	59		
5	T	1305	Total	C	N	O	S	0	0
			10257	6513	1780	1905	59		
5	W	1331	Total	C	N	O	S	0	0
			10463	6650	1810	1944	59		
5	x	1325	Total	C	N	O	S	0	0
			10404	6607	1803	1935	59		
5	l	1250	Total	C	N	O	S	0	0
			9872	6274	1716	1823	59		

- Molecule 6 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	319	Total	C	N	O	S	0	0
			2505	1608	444	446	7		
6	5	313	Total	C	N	O	S	0	0
			2460	1576	438	440	6		

- Molecule 7 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	290	Total	C	N	O	S	0	0
			2279	1466	378	419	16		
7	g	290	Total	C	N	O	S	0	0
			2272	1464	376	414	18		
7	6	297	Total	C	N	O	S	0	0
			2329	1496	385	430	18		
7	7	287	Total	C	N	O	S	0	0
			2262	1452	375	417	18		





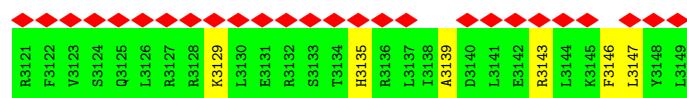
R3121
F3122
V3123
S3124
C3125
L3126
R3127
K3128
X3129
L3130
E3131
R3132
S3133
T3134
H3135
R3136
L3137
T3138
A3139
D3140
L3141
C3142
R3143
L3144
K3145
F3146
L3147
V3148
L3149

Chain 0:

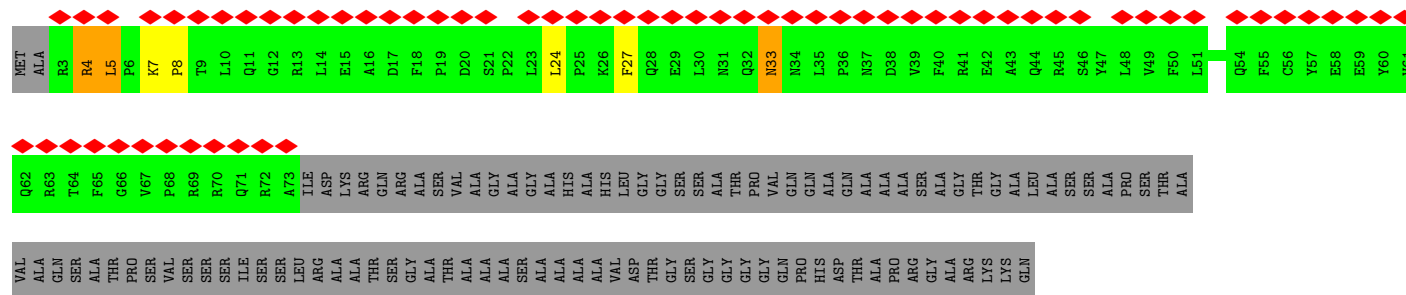
CYS	VAL	SER	ASN	CYS	VAL	LEU	TYR	LEU	VAL	LYS	SER	PHE	LEU	ALA	GLY	ARG	PRO	LEU	THR	SER	ARG	PRO	GLU	LEU	ASP	GLY	GLY	ALA	ARG	LEU	ASP	ALA	LEU	LEU	MET	GLY	GLN	SER	GLY	ILE	LEU	LYS	GLY	HIS	GLU	ASP	VAL	PRO	PRO	SER	SER	VAL	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



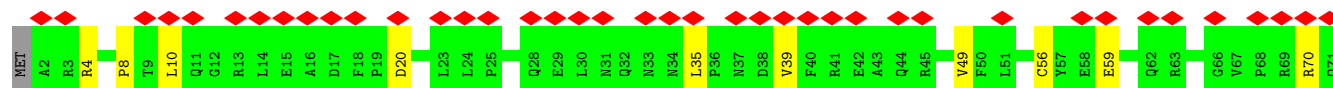
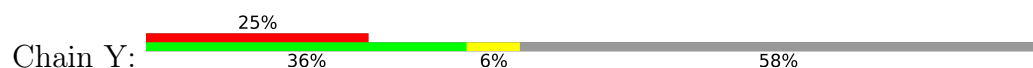


[illegible]

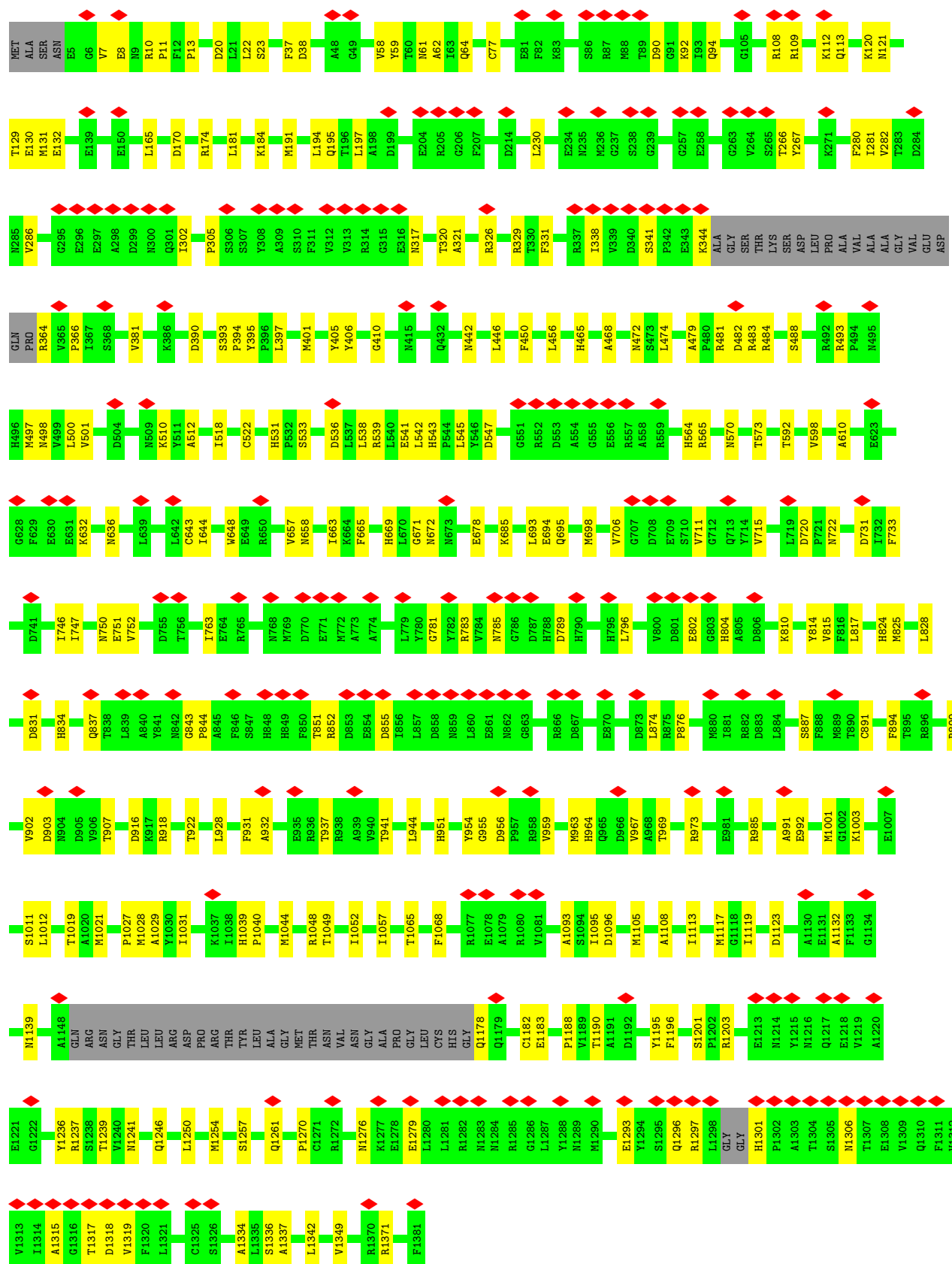
- Molecule 4: Small capsomere-interacting protein



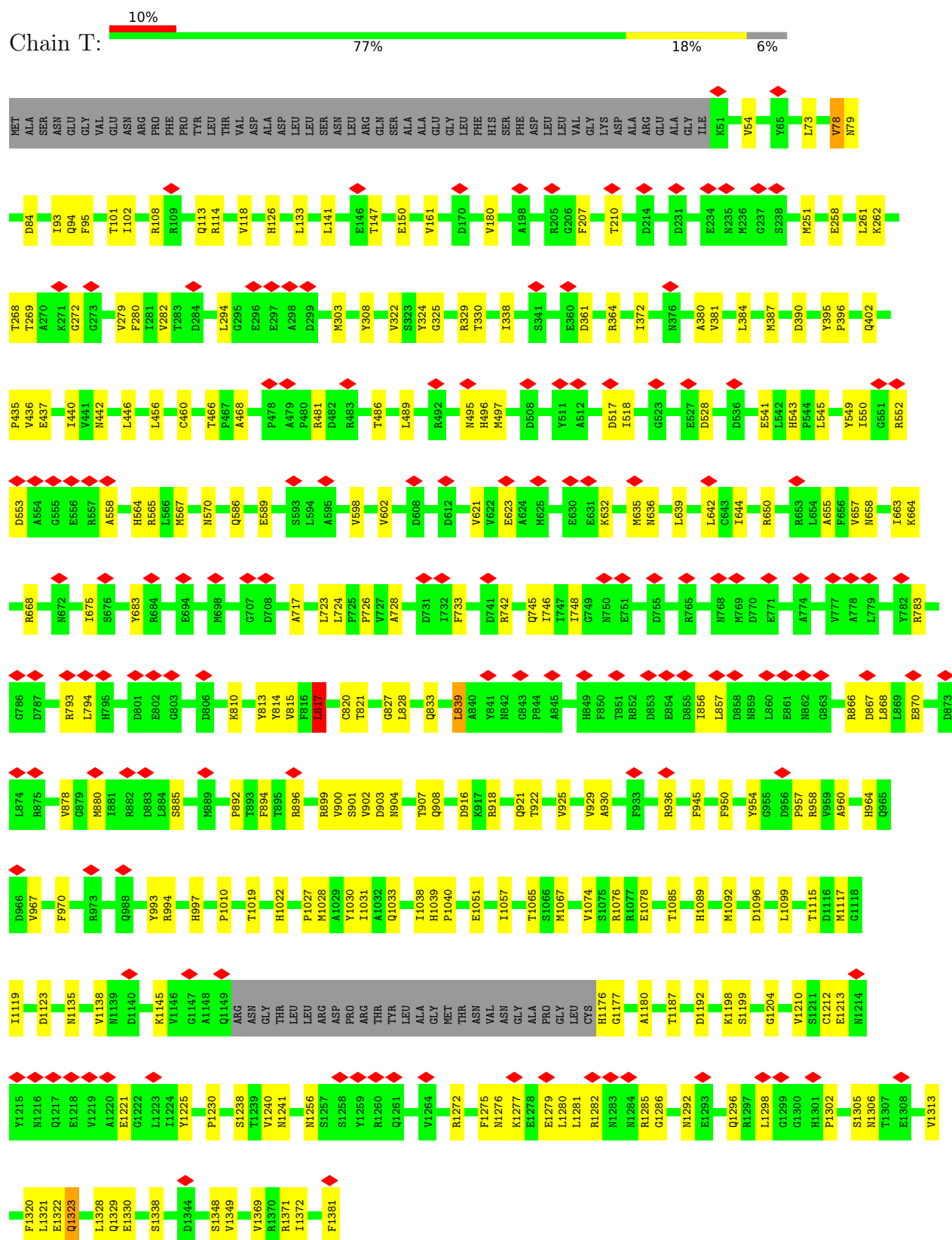
- Molecule 4: Small capsomere-interacting protein



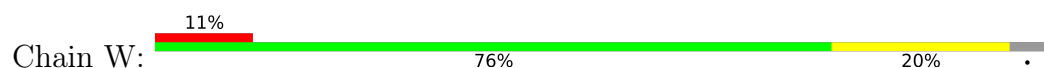




• Molecule 5: Major capsid protein

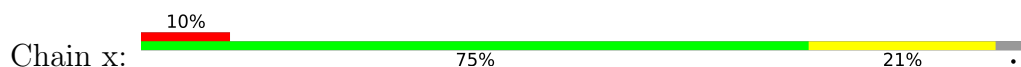


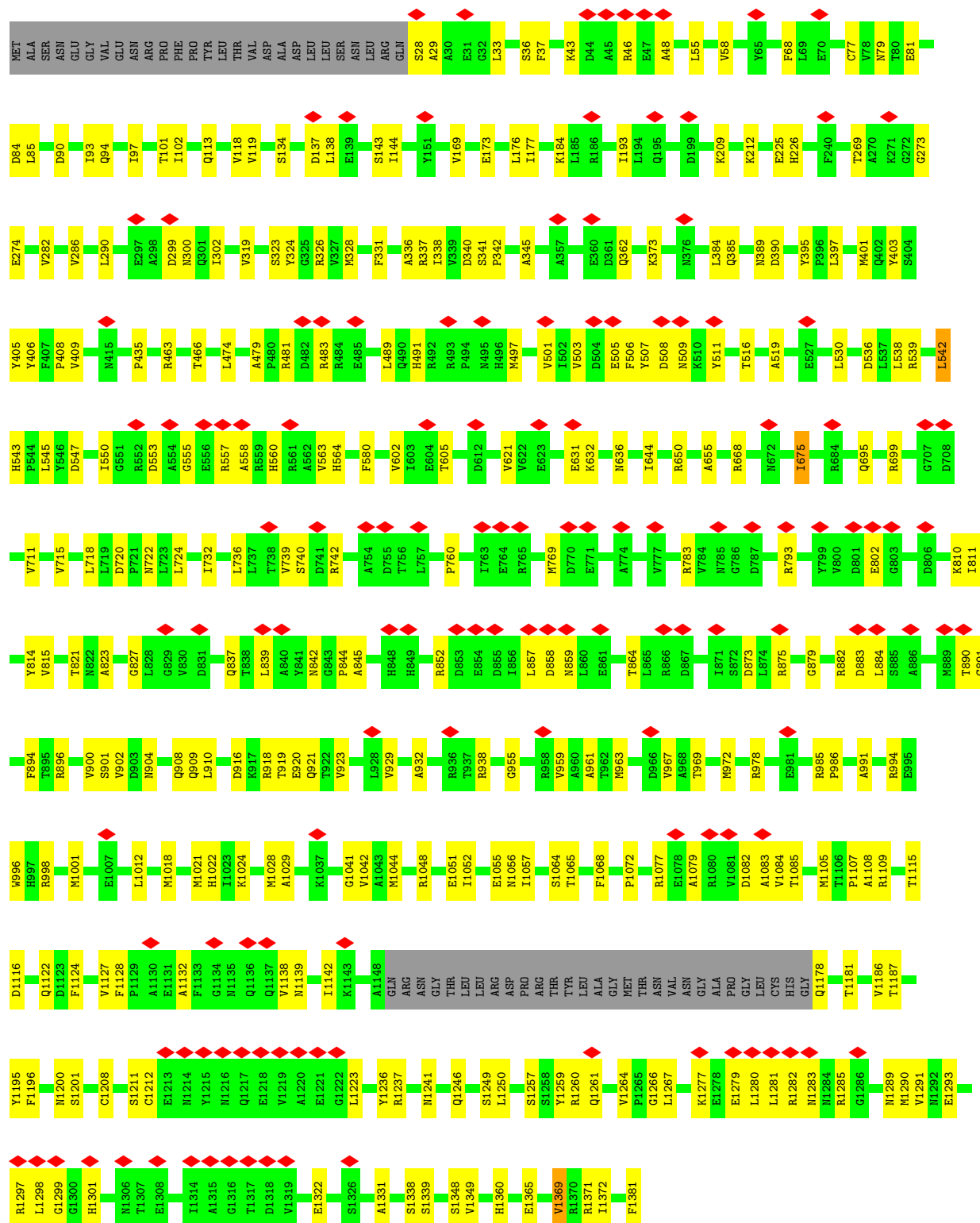
• Molecule 5: Major capsid protein





• Molecule 5: Major capsid protein

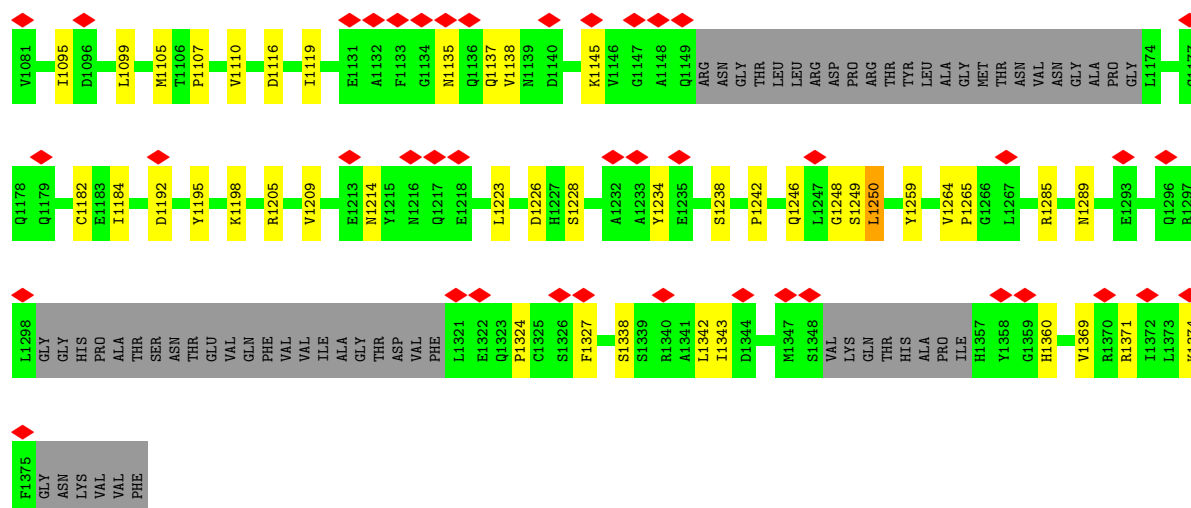




• Molecule 5: Major capsid protein

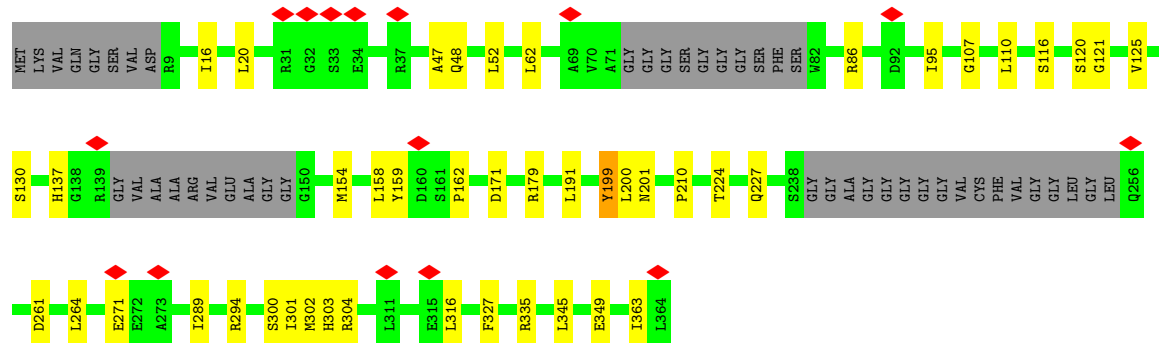






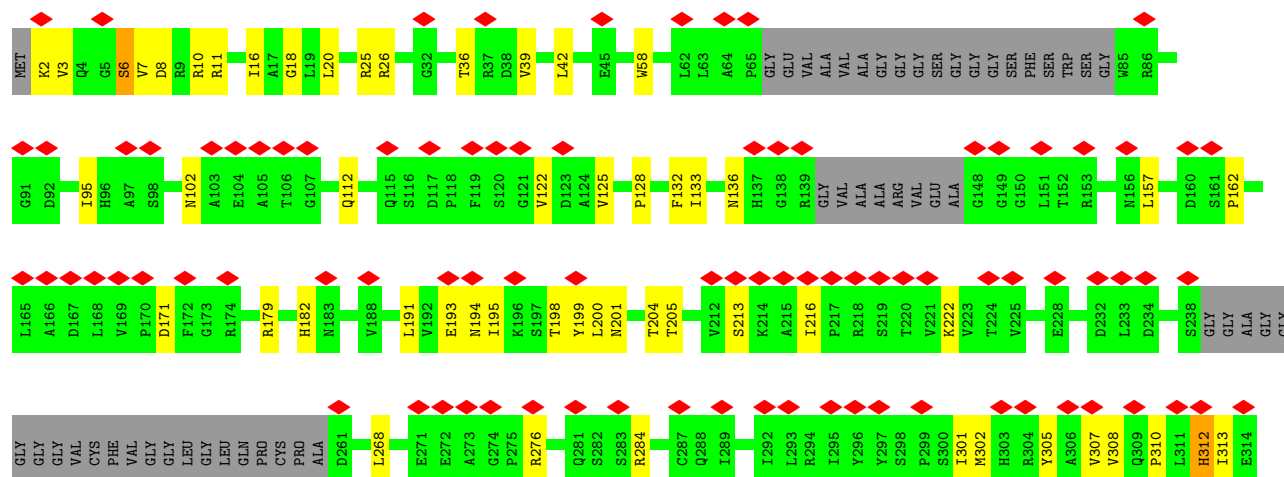
• Molecule 6: Triplex capsid protein 1

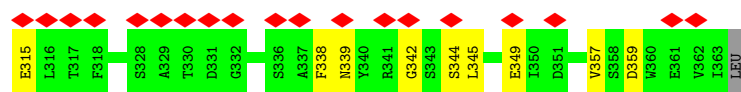
Chain e: 75% 12% 12%



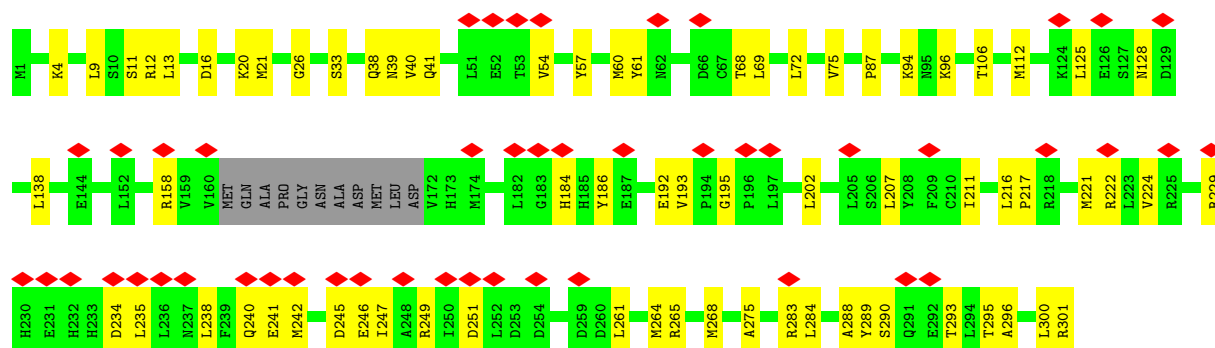
• Molecule 6: Triplex capsid protein 1

Chain 5: 30% 69% 17% 14%

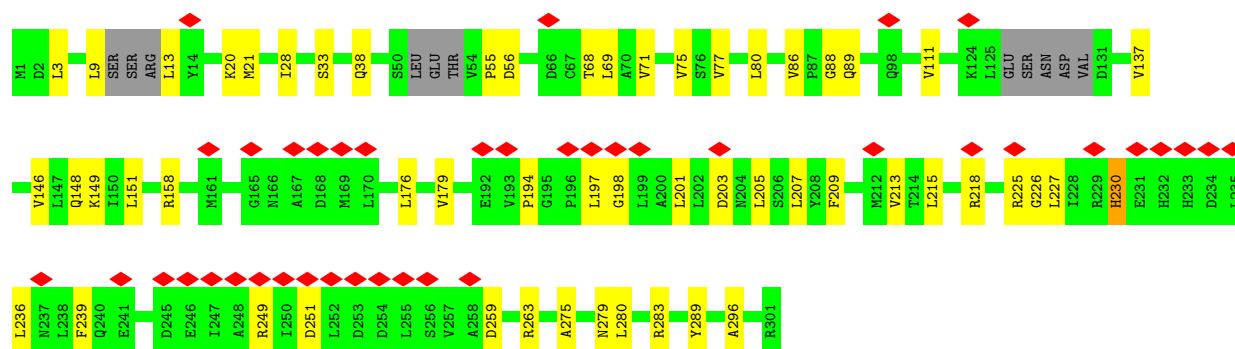
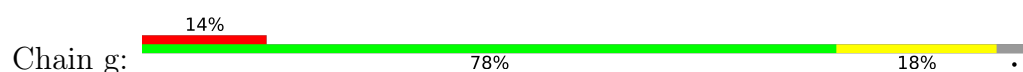




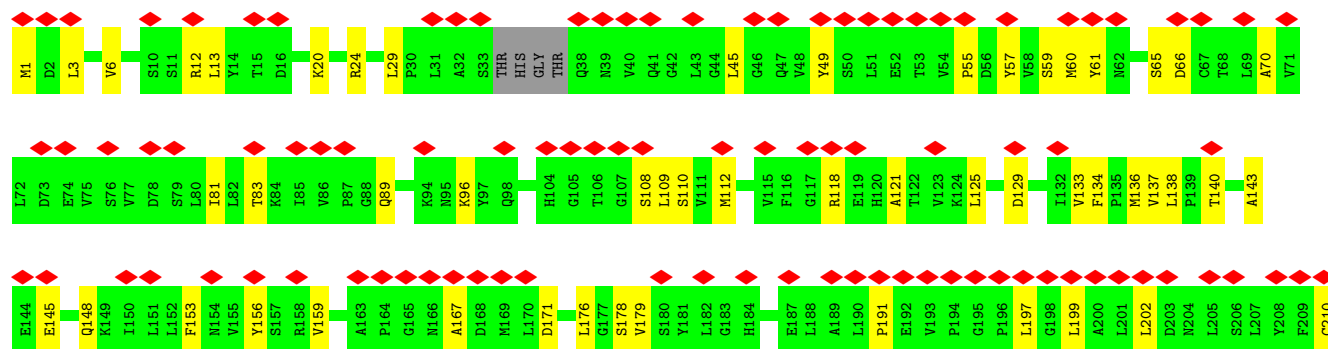
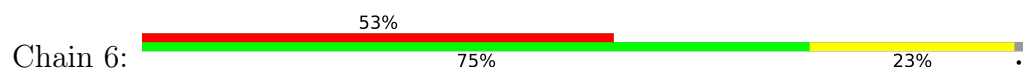
• Molecule 7: Triplex capsid protein 2



• Molecule 7: Triplex capsid protein 2



• Molecule 7: Triplex capsid protein 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93334	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	392.99997, 392.99997, 392.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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	G	0.46	0/684	0.83	0/924
1	K	0.22	0/570	0.63	0/765
2	C	0.53	2/2770 (0.1%)	0.83	4/3763 (0.1%)
3	B	0.18	0/304	0.56	0/404
3	O	0.24	0/255	0.65	0/339
4	2	0.26	0/636	0.65	1/861 (0.1%)
4	Y	0.23	0/636	0.62	0/861
4	Z	0.24	0/636	0.54	0/861
4	m	0.36	0/615	0.63	0/832
4	y	0.25	0/636	0.57	0/861
5	S	0.30	0/10699	0.52	0/14537
5	T	0.36	1/10499 (0.0%)	0.56	6/14270 (0.0%)
5	W	0.30	0/10706	0.52	0/14549
5	l	0.27	0/10102	0.52	0/13718
5	x	0.36	1/10648 (0.0%)	0.57	4/14471 (0.0%)
6	5	0.24	0/2523	0.51	0/3431
6	e	0.29	0/2572	0.51	0/3503
7	6	0.23	0/2377	0.53	1/3236 (0.0%)
7	7	0.27	0/2306	0.63	0/3135
7	f	0.26	0/2327	0.51	0/3169
7	g	0.28	0/2319	0.58	2/3155 (0.1%)
All	All	0.32	4/74820 (0.0%)	0.56	18/101645 (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
4	2	0	1
5	T	0	1
6	5	0	1
7	g	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	425	PRO	N-CA	18.45	1.70	1.47
5	T	1323	GLN	C-N	15.84	1.51	1.34
5	x	362	GLN	C-N	13.18	1.51	1.33
2	C	424	HIS	C-N	8.84	1.45	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	424	HIS	CA-C-N	18.55	138.88	119.78
2	C	424	HIS	C-N-CA	18.55	138.88	119.78
5	x	362	GLN	CA-C-N	12.81	132.98	119.78
5	x	362	GLN	C-N-CA	12.81	132.98	119.78
5	T	1323	GLN	CA-C-N	11.14	130.74	119.82
5	T	1323	GLN	C-N-CA	11.14	130.74	119.82
2	C	425	PRO	CA-N-CD	-8.35	100.32	112.00
7	g	230	HIS	CA-C-N	5.83	128.89	120.79
7	g	230	HIS	C-N-CA	5.83	128.89	120.79
5	T	1322	GLU	CA-C-N	-5.52	115.16	122.56
5	T	1322	GLU	C-N-CA	-5.52	115.16	122.56
5	T	1323	GLN	CA-C-O	-5.43	115.35	119.59
4	2	67	VAL	N-CA-C	5.40	120.55	108.88
5	x	362	GLN	CA-C-O	-5.31	115.25	120.19
5	x	711	VAL	N-CA-C	-5.31	106.69	113.22
7	6	257	VAL	N-CA-C	-5.16	108.26	113.47
2	C	425	PRO	N-CA-C	-5.12	103.07	111.21
5	T	817	LEU	CA-CB-CG	5.07	134.05	116.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	2	66	GLY	Peptide
6	5	312	HIS	Peptide
5	T	817	LEU	Peptide
7	g	230	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	675	0	678	26	0
1	K	563	0	566	24	0
2	C	2705	0	2712	114	0
3	B	301	0	328	5	0
3	O	252	0	269	8	0
4	2	621	0	611	8	0
4	Y	621	0	611	7	0
4	Z	621	0	611	7	0
4	m	600	0	591	12	0
4	y	621	0	611	6	0
5	S	10455	0	10285	174	0
5	T	10257	0	10089	183	0
5	W	10463	0	10288	193	0
5	l	9872	0	9701	153	0
5	x	10404	0	10234	211	0
6	5	2460	0	2439	42	0
6	e	2505	0	2480	38	0
7	6	2329	0	2363	46	0
7	7	2262	0	2293	92	0
7	f	2279	0	2316	54	0
7	g	2272	0	2308	41	0
All	All	73138	0	72384	1306	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 9.

All (1306) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:425:PRO:N	2:C:425:PRO:CA	1.69	1.42
5:x:507:TYR:CE2	5:x:967:VAL:HG12	1.63	1.32
7:7:204:ASN:O	7:7:208:TYR:CD1	1.85	1.27
5:x:507:TYR:CE2	5:x:967:VAL:CG1	2.19	1.25
2:C:124:LYS:HE2	2:C:312:HIS:O	1.45	1.14
5:x:507:TYR:CD2	5:x:967:VAL:HG12	1.84	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:LEU:HD13	2:C:499:ALA:CB	1.81	1.10
5:W:1132:ALA:HB1	5:W:1139:ASN:ND2	1.69	1.08
7:7:57:TYR:CB	7:7:205:LEU:HD11	1.84	1.07
5:T:395:TYR:HD1	5:T:396:PRO:HD2	1.19	1.06
7:7:57:TYR:CG	7:7:205:LEU:HD11	1.92	1.04
2:C:54:LEU:HD13	2:C:499:ALA:HB3	1.35	1.04
7:7:151:LEU:HD21	7:7:209:PHE:CD2	1.94	1.01
5:W:518:ILE:HD11	5:W:547:ASP:OD2	1.64	0.96
5:x:507:TYR:CD2	5:x:967:VAL:CG1	2.44	0.96
5:W:1132:ALA:HB1	5:W:1139:ASN:HD22	1.29	0.95
5:W:518:ILE:HD12	5:W:993:TYR:CE1	2.02	0.94
5:W:393:SER:OG	5:W:394:PRO:HD2	1.67	0.94
7:7:204:ASN:O	7:7:208:TYR:CE1	2.22	0.92
5:T:395:TYR:CD1	5:T:396:PRO:HD2	2.04	0.92
1:G:44:ARG:HH21	1:G:44:ARG:HG3	1.35	0.91
7:7:204:ASN:O	7:7:208:TYR:HD1	1.28	0.90
7:7:224:VAL:O	7:7:228:ILE:HB	1.72	0.90
5:T:395:TYR:HD1	5:T:396:PRO:CD	1.84	0.89
7:7:203:ASP:O	7:7:207:LEU:HG	1.72	0.89
5:T:1313:VAL:HG23	6:e:199:TYR:HE2	1.36	0.89
5:T:282:VAL:HG12	5:T:1057:ILE:HD12	1.51	0.89
5:l:772:MET:HE3	5:l:775:GLN:HB2	1.55	0.88
7:7:57:TYR:HB3	7:7:205:LEU:HD11	1.54	0.88
1:K:38:ALA:CB	2:C:385:LEU:HD12	2.04	0.87
5:S:665:PHE:O	5:S:669:HIS:HB2	1.75	0.86
7:7:58:VAL:HG13	7:7:205:LEU:CD2	2.06	0.85
5:S:393:SER:OG	5:S:394:PRO:HD2	1.77	0.84
5:W:518:ILE:HD12	5:W:993:TYR:HE1	1.39	0.84
5:T:1298:LEU:HD12	5:T:1298:LEU:O	1.79	0.83
7:7:204:ASN:HA	7:7:207:LEU:HD12	1.59	0.83
1:K:38:ALA:HB1	2:C:385:LEU:HD12	1.60	0.81
5:x:507:TYR:HE2	5:x:967:VAL:HG12	1.41	0.81
2:C:426:LEU:HD23	2:C:461:HIS:HA	1.63	0.80
7:f:264:MET:SD	7:g:209:PHE:CZ	2.74	0.80
5:S:518:ILE:HD13	5:S:547:ASP:OD2	1.81	0.80
2:C:54:LEU:CD1	2:C:499:ALA:HB3	2.13	0.79
5:W:518:ILE:CD1	5:W:993:TYR:HE1	1.95	0.79
2:C:9:VAL:HG21	7:7:249:ARG:HE	1.47	0.78
2:C:264:LEU:N	7:6:262:SER:HG	1.83	0.77
5:T:1321:LEU:O	5:T:1321:LEU:HD12	1.84	0.76
2:C:45:GLN:OE1	2:C:55:THR:OG1	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:301:ILE:O	6:5:305:TYR:HB2	1.86	0.76
7:f:264:MET:SD	7:g:209:PHE:HZ	2.09	0.75
7:7:151:LEU:CD2	7:7:209:PHE:CD2	2.70	0.74
5:T:402:GLN:HG2	5:T:1323:GLN:HB3	1.69	0.74
7:7:151:LEU:CD2	7:7:209:PHE:CE2	2.71	0.73
7:7:151:LEU:HD22	7:7:209:PHE:CE2	2.23	0.73
5:S:1048:ARG:HB3	5:S:1182:CYS:HB3	1.71	0.72
7:7:151:LEU:HD21	7:7:209:PHE:HD2	1.51	0.72
5:T:518:ILE:HD11	5:T:993:TYR:CE1	2.23	0.72
7:f:207:LEU:HD21	7:g:236:LEU:HB3	1.71	0.71
5:T:1313:VAL:HG23	6:e:199:TYR:CE2	2.24	0.71
5:W:518:ILE:CD1	5:W:993:TYR:CE1	2.72	0.71
7:7:201:LEU:O	7:7:205:LEU:HG	1.91	0.69
5:S:518:ILE:CD1	5:S:547:ASP:OD2	2.40	0.69
5:W:282:VAL:HG12	5:W:1057:ILE:HG12	1.75	0.69
5:W:495:ASN:HA	5:W:750:ASN:HD21	1.57	0.69
2:C:5:ILE:HD12	2:C:273:LYS:HE2	1.74	0.69
5:l:127:ILE:HD13	5:l:175:GLY:C	2.17	0.69
5:x:507:TYR:CE2	5:x:967:VAL:HG11	2.24	0.69
2:C:43:TRP:HB2	2:C:101:ARG:HB2	1.76	0.68
1:K:38:ALA:HB3	2:C:385:LEU:HD12	1.76	0.68
4:m:5:LEU:H	4:m:5:LEU:CD1	2.07	0.68
4:m:5:LEU:HD13	4:m:5:LEU:O	1.94	0.68
5:x:506:PHE:CE1	5:x:986:PRO:HA	2.29	0.68
5:T:101:THR:HG22	5:T:114:ARG:HH11	1.59	0.68
2:C:466:ALA:HB3	2:C:474:PHE:HB2	1.76	0.67
4:m:5:LEU:O	4:m:5:LEU:HD22	1.94	0.67
5:T:1302:PRO:HG2	5:T:1313:VAL:CG2	2.25	0.67
5:S:810:LYS:O	5:S:814:TYR:HB2	1.94	0.67
5:S:955:GLY:HA3	5:S:985:ARG:HE	1.60	0.66
5:x:395:TYR:CE2	5:x:397:LEU:HB2	2.30	0.66
5:x:1132:ALA:HB1	5:x:1139:ASN:ND2	2.10	0.66
5:x:507:TYR:CD2	5:x:967:VAL:HG13	2.28	0.66
7:7:58:VAL:HG13	7:7:205:LEU:HD21	1.78	0.65
2:C:426:LEU:HD23	2:C:461:HIS:CA	2.27	0.65
5:S:672:ASN:HA	5:T:650:ARG:HH11	1.62	0.65
5:T:639:LEU:HA	5:T:880:MET:HE3	1.78	0.65
5:W:1132:ALA:CB	5:W:1139:ASN:ND2	2.53	0.65
5:T:1285:ARG:HH11	5:T:1286:GLY:H	1.45	0.65
2:C:425:PRO:N	2:C:425:PRO:C	2.53	0.65
5:W:518:ILE:HD12	5:W:993:TYR:CD1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:90:THR:HG22	7:7:299:TRP:HB3	1.78	0.64
5:T:1204:GLY:HA2	5:T:1240:VAL:HG12	1.79	0.64
6:e:154:MET:HG2	6:e:345:LEU:HD22	1.79	0.64
5:x:176:LEU:O	5:x:176:LEU:HD23	1.98	0.64
5:T:402:GLN:HG3	5:T:1323:GLN:OE1	1.98	0.64
5:x:720:ASP:O	5:x:810:LYS:NZ	2.31	0.64
5:W:435:PRO:HB3	5:W:1338:SER:HB3	1.80	0.63
1:G:35:SER:O	1:G:39:LEU:HD23	1.98	0.63
5:S:1183:GLU:HG2	5:S:1270:PRO:HD2	1.80	0.63
1:K:73:ILE:HG22	3:B:3141:LEU:HD23	1.81	0.63
2:C:124:LYS:HE2	2:C:312:HIS:C	2.24	0.63
7:7:151:LEU:HD22	7:7:209:PHE:HE2	1.63	0.63
1:G:44:ARG:HH21	1:G:44:ARG:CG	2.10	0.62
2:C:279:ARG:NH2	2:C:303:PRO:O	2.32	0.62
5:T:724:LEU:HD12	5:T:900:VAL:HG11	1.81	0.62
4:Y:8:PRO:HB2	4:Y:10:LEU:HD23	1.81	0.62
5:l:742:ARG:NH2	5:l:905:ASP:OD1	2.32	0.62
5:S:1188:PRO:HD2	5:S:1241:ASN:HB2	1.80	0.62
5:x:176:LEU:HD23	5:x:176:LEU:C	2.24	0.62
5:S:1178:GLN:N	5:T:210:THR:HG1	1.97	0.62
7:7:114:PRO:HD3	7:7:135:PRO:HA	1.82	0.62
2:C:387:ARG:O	2:C:387:ARG:HD3	2.00	0.62
5:S:1117:MET:SD	5:S:1371:ARG:NH1	2.72	0.62
7:g:151:LEU:HD21	7:g:205:LEU:HD23	1.82	0.62
5:W:1077:ARG:HH12	7:f:4:LYS:H	1.48	0.61
5:x:543:HIS:HD2	5:x:545:LEU:H	1.47	0.61
5:x:722:ASN:HB3	5:x:902:VAL:HG21	1.82	0.61
5:W:79:ASN:HB3	5:W:308:TYR:CD1	2.36	0.61
5:W:715:VAL:HG23	5:W:1029:ALA:HA	1.83	0.61
7:6:45:LEU:HB3	7:6:133:VAL:HG23	1.82	0.61
7:g:149:LYS:HD2	7:g:179:VAL:HG12	1.83	0.60
7:7:94:LYS:NZ	7:7:293:THR:O	2.34	0.60
3:B:3123:VAL:HA	3:B:3126:LEU:HD12	1.82	0.60
5:W:270:ALA:HA	5:W:303:MET:HG2	1.84	0.60
1:G:27:SER:OG	1:G:28:LEU:N	2.34	0.60
5:T:621:VAL:HG21	5:T:868:LEU:HD21	1.83	0.60
5:T:1298:LEU:HD12	5:T:1298:LEU:C	2.26	0.60
5:W:132:GLU:H	5:x:113:GLN:HE21	1.50	0.60
5:W:279:VAL:HG12	5:W:380:ALA:HB3	1.83	0.60
5:x:81:GLU:HG3	5:x:81:GLU:O	2.00	0.60
5:l:1198:LYS:NZ	5:l:1234:TYR:OH	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:1001:MET:HE2	5:W:1021:MET:HG3	1.84	0.60
5:x:77:CYS:SG	5:x:184:LYS:NZ	2.73	0.60
5:l:442:ASN:O	5:l:1371:ARG:NH2	2.34	0.60
4:2:67:VAL:HG23	4:2:68:PRO:HD3	1.82	0.60
5:S:657:VAL:HA	5:S:663:ILE:HD11	1.83	0.60
7:f:261:LEU:HD21	7:g:176:LEU:HD21	1.82	0.60
5:x:827:GLY:HA2	5:x:929:VAL:HA	1.84	0.60
5:W:1372:ILE:CG2	5:W:1381:PHE:HD2	2.15	0.60
5:l:523:GLY:HA2	5:l:1003:LYS:HE2	1.82	0.60
6:5:102:ASN:HD22	6:5:194:ASN:HD21	1.50	0.60
5:W:760:PRO:O	5:W:793:ARG:NH2	2.35	0.60
7:7:58:VAL:HG13	7:7:205:LEU:HD23	1.82	0.60
4:2:10:LEU:HD21	5:W:838:THR:HA	1.83	0.59
5:W:308:TYR:CE1	5:W:1069:ILE:HG13	2.37	0.59
5:W:567:MET:SD	5:W:1022:HIS:ND1	2.73	0.59
5:W:955:GLY:HA3	5:W:985:ARG:HE	1.66	0.59
5:x:435:PRO:HB3	5:x:1338:SER:HB2	1.84	0.59
5:x:497:MET:HG3	5:x:896:ARG:HD2	1.83	0.59
5:l:724:LEU:HD11	5:l:736:LEU:HD22	1.84	0.59
5:l:820:CYS:HA	5:l:1010:PRO:HB3	1.83	0.59
7:7:57:TYR:HB3	7:7:205:LEU:HD21	1.83	0.59
5:l:180:VAL:HG22	5:l:1067:MET:HE3	1.84	0.59
2:C:49:SER:O	2:C:337:ARG:NH1	2.35	0.59
5:W:1254:MET:O	5:W:1260:ARG:NH2	2.35	0.59
6:5:213:SER:HB3	6:5:216:ILE:HG23	1.84	0.59
5:W:835:VAL:HG12	5:W:944:LEU:HD12	1.83	0.59
6:5:157:LEU:HD21	6:5:342:GLY:HA3	1.84	0.59
5:T:1117:MET:SD	5:T:1371:ARG:NH1	2.75	0.59
5:T:1123:ASP:OD1	5:T:1123:ASP:N	2.35	0.59
5:x:328:MET:CE	5:x:331:PHE:CE2	2.86	0.59
2:C:432:SER:HB2	5:x:555:GLY:HA2	1.84	0.59
5:W:79:ASN:HB3	5:W:308:TYR:HD1	1.67	0.59
5:W:79:ASN:CB	5:W:308:TYR:HD1	2.15	0.59
5:l:899:ARG:NH1	5:l:922:THR:OG1	2.35	0.59
2:C:464:HIS:HB2	2:C:476:VAL:HB	1.85	0.59
5:S:720:ASP:O	5:S:810:LYS:NZ	2.36	0.59
5:T:567:MET:HE3	5:T:570:ASN:HD21	1.67	0.59
7:f:202:LEU:HB3	7:g:227:LEU:HD21	1.85	0.59
7:7:151:LEU:HD12	7:7:206:SER:OG	2.03	0.59
1:G:43:GLU:HA	2:C:427:TYR:HD2	1.68	0.59
5:W:84:ASP:OD1	5:W:84:ASP:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:x:564:HIS:NE2	5:x:908:GLN:OE1	2.36	0.59
5:x:1372:ILE:HD12	5:x:1381:PHE:HD1	1.67	0.59
4:m:7:LYS:HG3	4:m:7:LYS:O	2.03	0.58
7:7:57:TYR:CD1	7:7:205:LEU:HD11	2.38	0.58
7:7:204:ASN:C	7:7:208:TYR:CE1	2.81	0.58
4:m:5:LEU:H	4:m:5:LEU:HD12	1.69	0.58
5:x:718:LEU:HD13	5:x:811:ILE:HG12	1.85	0.58
2:C:22:PHE:HB2	2:C:298:TYR:HB2	1.85	0.58
5:W:1302:PRO:HB2	5:W:1321:LEU:HD11	1.85	0.58
7:g:33:SER:O	7:g:38:GLN:NE2	2.36	0.58
5:S:497:MET:HE2	5:S:789:ASP:H	1.67	0.58
5:l:193:ILE:HG22	5:l:197:LEU:HD12	1.86	0.58
5:l:772:MET:HE3	5:l:775:GLN:CB	2.29	0.58
5:l:904:ASN:O	5:l:909:GLN:NE2	2.36	0.58
5:S:174:ARG:HB3	5:T:102:ILE:HG22	1.85	0.58
5:S:1132:ALA:HB1	5:S:1139:ASN:ND2	2.18	0.58
5:T:280:PHE:HB2	5:T:381:VAL:HG12	1.86	0.58
5:x:837:GLN:HB3	4:y:10:LEU:HD21	1.84	0.58
1:G:24:TRP:HB2	6:e:303:HIS:HD2	1.68	0.58
7:g:218:ARG:HG3	7:g:263:ARG:HH21	1.69	0.58
5:l:769:MET:HE1	5:l:889:MET:HB2	1.85	0.58
7:6:1:MET:SD	7:6:89:GLN:NE2	2.77	0.58
1:K:34:VAL:HG13	2:C:362:TRP:HB2	1.86	0.58
1:G:80:ARG:HH11	1:G:84:ILE:HD12	1.68	0.58
5:l:93:ILE:HD12	5:l:1095:ILE:HG21	1.86	0.58
5:S:479:ALA:O	5:S:539:ARG:NH2	2.37	0.58
5:W:137:ASP:HA	5:W:140:ILE:HG22	1.85	0.58
5:W:657:VAL:HA	5:W:663:ILE:HD11	1.86	0.58
7:f:268:MET:HB2	7:g:148:GLN:HE21	1.69	0.58
7:7:57:TYR:HB3	7:7:205:LEU:CD1	2.32	0.58
5:W:1266:GLY:HA2	5:W:1312:VAL:HG12	1.85	0.58
5:T:867:ASP:HA	5:T:870:GLU:HB2	1.85	0.57
7:7:221:MET:HE2	7:7:252:LEU:HB2	1.86	0.57
5:S:390:ASP:N	5:S:390:ASP:OD1	2.37	0.57
5:S:498:ASN:HD22	5:S:501:VAL:HG12	1.67	0.57
5:W:639:LEU:HB2	5:W:880:MET:HB2	1.86	0.57
4:Z:67:VAL:HG23	4:Z:68:PRO:HD3	1.87	0.57
5:T:495:ASN:OD1	5:T:496:HIS:ND1	2.37	0.57
5:W:421:SER:HB2	5:W:1354:ALA:HB2	1.85	0.57
2:C:5:ILE:HD12	2:C:273:LYS:HG3	1.85	0.57
5:S:338:ILE:HD12	6:5:18:GLY:HA2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:410:GLY:O	5:S:1039:HIS:NE2	2.38	0.57
5:S:648:TRP:NE1	5:S:678:GLU:OE2	2.36	0.57
5:T:728:ALA:HB3	5:T:925:VAL:HA	1.86	0.57
5:l:901:SER:HB2	5:l:920:GLU:HG2	1.86	0.57
6:5:359:ASP:OD2	7:7:283:ARG:NH2	2.38	0.57
5:T:916:ASP:OD1	5:T:994:ARG:NH2	2.38	0.57
7:g:236:LEU:HA	7:g:239:PHE:HB3	1.86	0.57
5:S:632:LYS:O	5:S:636:ASN:ND2	2.37	0.57
5:S:1123:ASP:OD1	5:S:1123:ASP:N	2.38	0.57
5:W:393:SER:OG	5:W:394:PRO:CD	2.47	0.57
5:l:227:SER:O	5:l:232:ARG:NH1	2.38	0.57
7:7:222:ARG:HD2	7:7:252:LEU:HD21	1.86	0.57
7:f:222:ARG:O	7:f:222:ARG:NH1	2.38	0.57
5:x:489:LEU:O	5:x:994:ARG:NH1	2.38	0.57
5:W:132:GLU:HG3	5:W:1085:THR:HG22	1.87	0.56
5:W:347:SER:OG	5:W:348:THR:N	2.37	0.56
5:W:671:GLY:O	5:x:650:ARG:NH1	2.39	0.56
5:l:609:THR:HG22	5:l:653:ARG:HB3	1.87	0.56
5:T:258:GLU:HG3	5:W:20:ASP:HB2	1.87	0.56
2:C:421:ILE:O	2:C:436:LYS:NZ	2.37	0.56
5:T:867:ASP:N	5:T:867:ASP:OD1	2.36	0.56
5:T:899:ARG:NH2	5:T:922:THR:OG1	2.38	0.56
5:x:632:LYS:O	5:x:636:ASN:ND2	2.38	0.56
6:e:224:THR:HG22	6:e:349:GLU:HG2	1.86	0.56
6:5:357:VAL:O	7:7:301:ARG:NH1	2.38	0.56
1:K:74:MET:HE1	3:O:3139:ALA:HA	1.87	0.56
5:T:456:LEU:HD13	5:T:1031:ILE:HD13	1.86	0.56
5:W:724:LEU:O	5:W:921:GLN:NE2	2.38	0.56
5:x:1372:ILE:HD12	5:x:1381:PHE:CD1	2.40	0.56
7:7:151:LEU:HD11	7:7:206:SER:HA	1.86	0.56
5:S:282:VAL:HG12	5:S:1057:ILE:HG12	1.86	0.56
5:x:509:ASN:C	5:x:509:ASN:HD22	2.13	0.56
5:S:518:ILE:O	5:S:518:ILE:HG22	2.05	0.56
5:T:1305:SER:OG	5:T:1306:ASN:N	2.38	0.56
5:W:722:ASN:OD1	5:W:742:ARG:NH2	2.38	0.56
5:W:361:ASP:OD1	5:W:362:GLN:NE2	2.39	0.56
5:l:1242:PRO:O	5:l:1246:GLN:NE2	2.39	0.56
7:7:268:MET:HA	7:7:271:LEU:HG	1.88	0.56
5:x:509:ASN:O	5:x:509:ASN:ND2	2.39	0.56
5:T:79:ASN:HB3	5:T:308:TYR:HD1	1.71	0.56
5:W:170:ASP:OD1	5:W:174:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:566:LEU:HD21	5:W:919:THR:HG21	1.87	0.56
5:l:720:ASP:O	5:l:810:LYS:NZ	2.38	0.56
5:S:671:GLY:O	5:T:650:ARG:NH1	2.39	0.55
5:x:1257:SER:O	5:x:1261:GLN:NE2	2.39	0.55
7:g:279:ASN:OD1	7:g:283:ARG:NH1	2.39	0.55
5:S:1257:SER:O	5:S:1261:GLN:NE2	2.38	0.55
5:T:329:ARG:HG2	5:T:330:THR:HG23	1.88	0.55
5:x:1277:LYS:HG2	5:x:1281:LEU:HD12	1.87	0.55
5:x:1298:LEU:HD21	5:x:1322:GLU:HA	1.88	0.55
6:e:294:ARG:NH1	6:e:363:ILE:O	2.39	0.55
5:l:518:ILE:HA	5:l:521:LYS:HB2	1.87	0.55
5:l:710:SER:OG	5:l:711:VAL:N	2.40	0.55
5:S:964:HIS:HB3	5:S:967:VAL:HG22	1.87	0.55
5:W:437:GLU:OE2	5:W:439:TRP:NE1	2.40	0.55
5:W:901:SER:O	5:W:918:ARG:NH2	2.38	0.55
5:x:695:GLN:OE1	5:x:699:ARG:NH2	2.39	0.55
5:x:724:LEU:HD22	5:x:732:ILE:HD12	1.88	0.55
5:x:1055:GLU:OE2	5:x:1109:ARG:NH1	2.40	0.55
6:5:8:ASP:OD1	6:5:10:ARG:NH2	2.39	0.55
5:x:328:MET:HE3	5:x:331:PHE:CE2	2.41	0.55
7:f:61:TYR:OH	7:f:112:MET:SD	2.57	0.55
5:S:10:ARG:HH11	5:T:325:GLY:HA3	1.71	0.55
5:T:481:ARG:NH1	5:T:517:ASP:OD2	2.39	0.55
5:x:1072:PRO:O	6:5:11:ARG:NH2	2.38	0.55
5:x:1279:GLU:OE2	5:x:1301:HIS:ND1	2.38	0.55
7:7:200:ALA:O	7:7:204:ASN:ND2	2.40	0.55
5:S:497:MET:HB3	5:S:789:ASP:HA	1.88	0.55
7:f:13:LEU:HD11	7:f:125:LEU:HD22	1.89	0.55
7:f:192:GLU:HG2	7:f:193:VAL:HG12	1.89	0.55
7:g:251:ASP:OD1	7:g:251:ASP:N	2.39	0.55
5:l:511:TYR:HA	5:l:973:ARG:HH12	1.71	0.55
7:6:65:SER:HA	7:6:282:PRO:HD3	1.89	0.55
5:W:481:ARG:HD2	5:W:536:ASP:HB2	1.88	0.55
2:C:7:ASN:C	2:C:7:ASN:HD22	2.14	0.55
2:C:387:ARG:HH21	2:C:427:TYR:HA	1.72	0.55
5:T:489:LEU:O	5:T:994:ARG:NH1	2.40	0.55
5:T:742:ARG:NH1	5:T:904:ASN:O	2.39	0.55
5:W:697:LEU:HB3	5:W:719:LEU:HD11	1.88	0.55
5:x:1001:MET:HE1	5:x:1021:MET:HG3	1.88	0.55
5:l:632:LYS:O	5:l:636:ASN:ND2	2.39	0.55
5:S:694:GLU:OE1	5:T:958:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:1230:PRO:HA	5:T:1238:SER:HA	1.87	0.55
5:W:783:ARG:NH1	5:W:891:CYS:O	2.34	0.55
7:6:178:SER:OG	7:6:179:VAL:N	2.39	0.55
2:C:28:MET:SD	2:C:64:ARG:NH2	2.77	0.54
5:x:506:PHE:CZ	5:x:986:PRO:HA	2.41	0.54
7:g:21:MET:HB3	7:g:75:VAL:HG21	1.87	0.54
6:5:284:ARG:HH11	7:6:66:ASP:HB3	1.72	0.54
7:7:144:GLU:OE1	7:7:148:GLN:NE2	2.41	0.54
5:S:281:ILE:HG22	5:S:397:LEU:HD11	1.88	0.54
5:S:317:ASN:HA	5:S:320:THR:HG22	1.90	0.54
5:S:541:GLU:OE1	5:S:565:ARG:NH2	2.40	0.54
5:S:747:ILE:HG12	5:S:752:VAL:HG12	1.88	0.54
5:S:941:THR:HG22	5:S:944:LEU:HD12	1.89	0.54
5:T:1272:ARG:O	5:T:1276:ASN:ND2	2.41	0.54
5:W:720:ASP:O	5:W:810:LYS:NZ	2.39	0.54
5:W:804:HIS:HB3	5:W:807:VAL:HG12	1.89	0.54
5:W:851:THR:OG1	5:W:852:ARG:N	2.40	0.54
5:S:903:ASP:HA	5:S:918:ARG:HG2	1.88	0.54
5:T:435:PRO:HB3	5:T:1338:SER:HB3	1.88	0.54
5:S:802:GLU:HG2	5:S:804:HIS:H	1.73	0.54
5:T:724:LEU:O	5:T:921:GLN:NE2	2.36	0.54
7:6:109:LEU:HD12	7:6:137:VAL:HG12	1.88	0.54
1:K:56:ARG:NH1	1:K:59:GLN:OE1	2.41	0.54
5:x:269:THR:HA	5:x:302:ILE:HG22	1.88	0.54
5:l:983:PHE:O	5:l:985:ARG:NH2	2.40	0.54
5:x:564:HIS:O	5:x:998:ARG:NH2	2.40	0.54
5:l:536:ASP:OD1	5:l:536:ASP:N	2.39	0.54
7:6:24:ARG:NH2	7:6:96:LYS:O	2.40	0.54
7:7:20:LYS:HD3	7:7:123:VAL:HB	1.90	0.54
7:7:228:ILE:HG23	7:7:229:ARG:HG2	1.90	0.54
5:W:1252:ASP:N	5:W:1252:ASP:OD1	2.36	0.54
5:l:584:ARG:NH1	5:l:1039:HIS:O	2.41	0.54
5:l:772:MET:CE	5:l:775:GLN:HB2	2.32	0.54
5:l:814:TYR:OH	5:l:921:GLN:NE2	2.41	0.54
5:S:783:ARG:NH2	5:S:891:CYS:O	2.40	0.54
5:T:1076:ARG:NH2	6:e:62:LEU:O	2.40	0.54
5:l:705:VAL:HG12	5:l:710:SER:HA	1.89	0.54
7:7:179:VAL:HG23	7:7:186:TYR:HB2	1.89	0.54
5:T:395:TYR:CD1	5:T:396:PRO:CD	2.76	0.54
5:l:587:GLN:NE2	5:l:1037:LYS:O	2.39	0.54
2:C:37:PRO:O	2:C:38:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:361:ASP:OD1	5:T:361:ASP:N	2.41	0.54
7:f:33:SER:OG	7:f:38:GLN:NE2	2.40	0.54
7:f:87:PRO:HG3	7:f:300:LEU:HD22	1.89	0.54
1:G:59:GLN:O	1:G:63:ASN:ND2	2.41	0.53
1:G:89:ASP:OD1	1:G:89:ASP:N	2.41	0.53
5:T:815:VAL:HG21	5:T:1019:THR:HB	1.90	0.53
5:l:202:PHE:HA	5:l:205:ARG:HH11	1.72	0.53
6:5:182:HIS:HB3	6:5:268:LEU:HD23	1.90	0.53
7:7:229:ARG:NH1	7:7:232:HIS:O	2.42	0.53
5:W:132:GLU:O	5:x:113:GLN:NE2	2.41	0.53
5:W:245:ARG:NH2	5:W:373:LYS:O	2.41	0.53
6:e:95:ILE:HG21	6:e:125:VAL:HG22	1.90	0.53
7:7:204:ASN:HB2	7:7:208:TYR:HE1	1.72	0.53
5:W:824:HIS:HE1	5:W:958:ARG:HD2	1.73	0.53
5:W:1285:ARG:NH2	5:W:1293:GLU:OE1	2.41	0.53
5:x:536:ASP:OD1	5:x:536:ASP:N	2.40	0.53
5:x:1122:GLN:HE22	5:x:1267:LEU:HD12	1.73	0.53
5:x:1283:ASN:HB3	5:x:1290:MET:HE3	1.88	0.53
5:l:748:ILE:HG12	5:l:794:LEU:HD21	1.90	0.53
6:5:313:ILE:HG21	7:6:215:LEU:HD21	1.90	0.53
7:7:86:VAL:HG22	7:7:88:GLY:H	1.74	0.53
2:C:380:TYR:OH	2:C:460:GLY:O	2.27	0.53
5:T:642:LEU:HD23	5:T:880:MET:HE1	1.89	0.53
2:C:305:LEU:HG	2:C:307:ALA:H	1.73	0.53
4:Y:70:ARG:NH1	4:Z:11:GLN:O	2.42	0.53
5:S:722:ASN:HB3	5:S:902:VAL:HG21	1.91	0.53
5:S:1011:SER:OG	5:S:1012:LEU:N	2.42	0.53
5:T:644:ILE:HG22	5:T:655:ALA:HB3	1.90	0.53
5:T:857:LEU:O	5:T:866:ARG:NH1	2.41	0.53
5:l:193:ILE:HG23	5:l:219:PHE:CZ	2.44	0.53
5:S:1236:TYR:OH	5:S:1237:ARG:NH2	2.41	0.53
5:T:269:THR:OG1	5:T:272:GLY:O	2.27	0.53
5:S:1048:ARG:HH12	5:S:1117:MET:HG3	1.74	0.53
5:T:497:MET:HG2	5:T:896:ARG:HG2	1.91	0.53
5:l:877:THR:HG22	5:l:880:MET:HE2	1.90	0.53
1:K:61:LEU:HD23	2:C:291:ILE:HG22	1.91	0.53
2:C:5:ILE:CD1	2:C:273:LYS:HG3	2.38	0.53
5:S:120:LYS:HB3	5:S:1095:ILE:HD11	1.90	0.53
7:f:158:ARG:HD3	7:g:226:GLY:HA2	1.90	0.53
7:f:193:VAL:HG22	7:f:195:GLY:H	1.72	0.53
7:g:56:ASP:OD1	7:g:56:ASP:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:l:1073:ASN:OD1	6:5:26:ARG:NH1	2.42	0.53
7:6:61:TYR:OH	7:6:280:LEU:O	2.21	0.53
1:G:45:GLU:OE2	1:G:45:GLU:HA	2.09	0.53
5:S:393:SER:OG	5:S:394:PRO:CD	2.55	0.53
5:W:609:THR:HA	5:W:653:ARG:HD3	1.90	0.53
5:x:269:THR:HG23	5:x:273:GLY:H	1.74	0.53
1:G:44:ARG:HG3	1:G:44:ARG:NH2	2.13	0.53
2:C:2:ASP:OD1	2:C:2:ASP:N	2.41	0.53
2:C:48:PHE:HE2	2:C:55:THR:CG2	2.22	0.53
2:C:90:GLU:HA	2:C:314:MET:HG2	1.91	0.53
5:S:1318:ASP:OD1	5:T:108:ARG:NH2	2.42	0.53
5:l:481:ARG:HE	5:l:536:ASP:HB2	1.74	0.53
7:f:290:SER:HG	7:f:293:THR:HG1	1.52	0.52
5:l:451:ASN:OD1	5:l:454:ASN:ND2	2.42	0.52
5:l:1342:LEU:HD11	5:l:1360:HIS:HB3	1.90	0.52
2:C:124:LYS:NZ	2:C:315:THR:HG23	2.24	0.52
5:S:543:HIS:HD2	5:S:545:LEU:H	1.56	0.52
5:W:959:VAL:HA	5:W:962:THR:HG22	1.91	0.52
5:W:1372:ILE:HG23	5:W:1381:PHE:HD2	1.73	0.52
5:l:993:TYR:O	5:l:998:ARG:NH1	2.40	0.52
7:6:145:GLU:HA	7:6:148:GLN:HG2	1.91	0.52
7:7:95:ASN:HB2	7:7:103:TRP:HE1	1.74	0.52
1:G:20:PRO:HD3	1:G:27:SER:HB2	1.90	0.52
5:x:68:PHE:HD1	5:x:177:ILE:HG12	1.75	0.52
5:x:94:GLN:HG2	5:x:119:VAL:HG12	1.90	0.52
5:x:336:ALA:HA	5:x:340:ASP:HB2	1.91	0.52
5:l:33:LEU:HB2	5:l:37:PHE:HZ	1.73	0.52
6:5:359:ASP:OD1	7:7:301:ARG:NH2	2.43	0.52
7:7:138:LEU:HD12	7:7:142:ILE:HG22	1.90	0.52
1:K:24:TRP:HB2	2:C:372:ILE:HG13	1.92	0.52
5:S:474:LEU:HD11	5:S:542:LEU:HD21	1.90	0.52
5:T:84:ASP:OD1	5:T:84:ASP:N	2.39	0.52
5:W:665:PHE:O	5:W:669:HIS:N	2.40	0.52
5:x:479:ALA:O	5:x:539:ARG:NH2	2.43	0.52
6:e:271:GLU:OE2	6:e:300:SER:OG	2.27	0.52
7:g:146:VAL:HG12	7:g:179:VAL:HG11	1.90	0.52
5:l:84:ASP:N	5:l:84:ASP:OD1	2.43	0.52
6:5:193:GLU:HB2	6:5:204:THR:HB	1.91	0.52
2:C:423:SER:O	2:C:432:SER:OG	2.27	0.52
2:C:425:PRO:HB3	2:C:429:GLU:HB2	1.92	0.52
5:S:899:ARG:NH1	5:S:922:THR:OG1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:x:842:ASN:HD21	5:x:845:ALA:H	1.55	0.52
5:l:844:PRO:HB2	5:l:878:VAL:HG11	1.92	0.52
5:T:1187:THR:HG22	5:T:1241:ASN:HD22	1.75	0.52
5:T:1272:ARG:HG2	5:T:1276:ASN:HD21	1.74	0.52
5:W:497:MET:HE1	5:W:896:ARG:HH21	1.74	0.52
5:W:1288:TYR:O	5:W:1292:ASN:ND2	2.42	0.52
5:x:844:PRO:O	5:x:882:ARG:NH1	2.43	0.52
7:7:111:VAL:HG22	7:7:137:VAL:HG22	1.92	0.52
7:7:150:ILE:HG12	7:7:202:LEU:HG	1.92	0.52
1:G:41:LEU:HD11	5:x:511:TYR:CE1	2.45	0.52
5:S:874:LEU:HG	5:S:876:PRO:HD3	1.91	0.52
5:W:79:ASN:CB	5:W:308:TYR:CD1	2.92	0.52
5:W:1120:HIS:CD2	5:W:1179:GLN:OE1	2.63	0.52
5:l:907:THR:OG1	5:l:908:GLN:OE1	2.28	0.52
5:T:114:ARG:HG2	5:W:41:VAL:HG12	1.92	0.52
5:T:664:LYS:HZ2	5:T:668:ARG:HH12	1.57	0.52
5:W:216:ILE:O	5:W:220:LYS:NZ	2.43	0.52
5:W:567:MET:H	5:W:570:ASN:HD22	1.57	0.52
5:W:1348:SER:OG	5:W:1349:VAL:N	2.43	0.52
6:e:86:ARG:NH1	7:g:88:GLY:O	2.42	0.52
5:l:465:HIS:O	5:l:546:TYR:OH	2.28	0.52
5:l:883:ASP:OD1	5:l:883:ASP:N	2.39	0.52
2:C:9:VAL:CG2	7:7:249:ARG:HE	2.21	0.52
5:S:395:TYR:HE2	5:S:397:LEU:HD12	1.75	0.52
5:S:715:VAL:HG23	5:S:1029:ALA:HA	1.90	0.52
5:T:828:LEU:HD22	5:T:930:ALA:HB2	1.91	0.52
5:T:903:ASP:HA	5:T:918:ARG:HA	1.92	0.52
5:T:1212:CYS:SG	5:T:1213:GLU:N	2.83	0.52
5:W:518:ILE:HD11	5:W:547:ASP:CG	2.34	0.52
5:x:557:ARG:NH2	5:x:558:ALA:O	2.43	0.52
6:5:301:ILE:O	6:5:305:TYR:CB	2.56	0.52
7:7:57:TYR:CG	7:7:205:LEU:CD1	2.81	0.52
5:S:267:TYR:HA	5:S:305:PRO:HB3	1.91	0.51
5:W:941:THR:HA	5:W:944:LEU:HD23	1.91	0.51
5:x:901:SER:O	5:x:918:ARG:NH2	2.42	0.51
5:x:904:ASN:O	5:x:909:GLN:NE2	2.43	0.51
5:x:1283:ASN:ND2	5:x:1293:GLU:OE1	2.43	0.51
6:5:136:ASN:OD1	6:5:276:ARG:NH2	2.38	0.51
2:C:9:VAL:HG21	7:7:249:ARG:NE	2.23	0.51
2:C:96:HIS:HB3	2:C:116:TYR:HD2	1.74	0.51
2:C:385:LEU:HB3	2:C:388:GLU:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:851:THR:OG1	5:S:852:ARG:N	2.41	0.51
5:T:402:GLN:CG	5:T:1323:GLN:HB3	2.39	0.51
5:W:747:ILE:HG13	5:W:752:VAL:HG12	1.91	0.51
5:l:788:HIS:HA	5:l:791:ASP:HB3	1.91	0.51
2:C:3:VAL:HA	2:C:6:ASP:HB2	1.92	0.51
2:C:3:VAL:HG21	2:C:77:PHE:HB3	1.90	0.51
2:C:4:HIS:HB3	2:C:20:HIS:CD2	2.46	0.51
3:O:3147:LEU:HA	5:x:793:ARG:HH12	1.74	0.51
5:T:282:VAL:HG12	5:T:1057:ILE:HG23	1.92	0.51
5:W:651:SER:OG	5:W:652:GLY:N	2.44	0.51
6:5:171:ASP:OD1	6:5:171:ASP:N	2.43	0.51
5:T:543:HIS:HD2	5:T:545:LEU:H	1.57	0.51
5:W:553:ASP:HA	5:W:558:ALA:HB2	1.93	0.51
5:x:1124:PHE:HA	5:x:1127:VAL:HG12	1.92	0.51
7:g:13:LEU:N	7:g:77:VAL:O	2.43	0.51
7:6:284:LEU:HD12	7:6:298:CYS:HB3	1.93	0.51
2:C:1:MET:HG3	2:C:4:HIS:CE1	2.46	0.51
5:S:442:ASN:HD22	5:S:446:LEU:HD12	1.74	0.51
5:T:1039:HIS:ND1	5:T:1040:PRO:O	2.38	0.51
5:W:1044:MET:SD	5:W:1044:MET:N	2.83	0.51
5:W:1113:ILE:HG21	5:W:1117:MET:HE3	1.92	0.51
5:x:644:ILE:HG22	5:x:655:ALA:HB3	1.92	0.51
5:x:715:VAL:HG23	5:x:1029:ALA:HA	1.92	0.51
5:x:938:ARG:HG3	5:x:963:MET:HA	1.92	0.51
6:5:195:ILE:O	6:5:201:ASN:ND2	2.44	0.51
5:x:1079:ALA:HB1	5:x:1084:VAL:HG12	1.93	0.51
6:e:264:LEU:HB2	6:e:327:PHE:HE1	1.76	0.51
1:K:67:ARG:HG2	3:O:3146:PHE:HE1	1.76	0.51
5:S:483:ARG:NH2	5:S:484:ARG:O	2.43	0.51
5:S:855:ASP:N	5:S:855:ASP:OD1	2.42	0.51
5:W:940:VAL:HG23	5:W:941:THR:HG23	1.92	0.51
5:x:85:LEU:HD11	5:x:1068:PHE:HB3	1.93	0.51
5:x:857:LEU:HD12	5:x:875:ARG:HE	1.75	0.51
5:l:479:ALA:O	5:l:539:ARG:NH1	2.43	0.51
5:l:737:LEU:HD23	5:l:744:PRO:HG2	1.93	0.51
5:S:305:PRO:O	5:S:364:ARG:N	2.44	0.51
5:T:282:VAL:CG1	5:T:1057:ILE:HD12	2.34	0.51
5:T:466:THR:HG22	5:T:468:ALA:H	1.75	0.51
5:x:328:MET:CE	5:x:331:PHE:HE2	2.24	0.51
5:x:328:MET:HE1	5:x:331:PHE:CE2	2.46	0.51
5:l:1078:GLU:HG3	5:l:1080:ARG:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:m:33:ASN:OD1	4:m:33:ASN:N	2.43	0.51
5:S:191:MET:HE3	5:S:195:GLN:HG3	1.92	0.51
5:T:632:LYS:O	5:T:636:ASN:ND2	2.38	0.51
5:x:883:ASP:OD1	5:x:883:ASP:N	2.44	0.51
6:e:110:LEU:HD11	6:e:191:LEU:HB2	1.91	0.51
5:l:1285:ARG:O	5:l:1289:ASN:ND2	2.44	0.51
5:S:498:ASN:HD21	5:S:500:LEU:HB2	1.76	0.50
7:g:111:VAL:HG12	7:g:137:VAL:HG22	1.92	0.50
7:g:289:TYR:HD1	7:g:296:ALA:HB2	1.76	0.50
5:l:594:LEU:HA	5:l:699:ARG:HH22	1.76	0.50
7:6:287:ALA:O	7:6:297:THR:OG1	2.29	0.50
4:m:8:PRO:HB3	5:l:834:HIS:CE1	2.47	0.50
5:W:658:ASN:OD1	5:W:658:ASN:N	2.42	0.50
5:W:1250:LEU:HG	5:W:1254:MET:HE2	1.93	0.50
7:f:217:PRO:HG3	7:f:264:MET:HE1	1.92	0.50
5:S:824:HIS:ND1	5:S:956:ASP:OD2	2.42	0.50
5:S:1044:MET:SD	5:S:1044:MET:N	2.85	0.50
5:T:1302:PRO:HG2	5:T:1313:VAL:HG21	1.91	0.50
5:x:282:VAL:HG12	5:x:1057:ILE:HG12	1.94	0.50
5:l:323:SER:OG	5:l:324:TYR:N	2.44	0.50
5:l:858:ASP:OD1	5:l:858:ASP:N	2.41	0.50
5:S:129:THR:OG1	5:S:130:GLU:N	2.44	0.50
5:S:1297:ARG:NH1	5:S:1319:VAL:O	2.44	0.50
5:T:268:THR:OG1	5:T:364:ARG:NH1	2.42	0.50
5:T:1323:GLN:HG3	5:T:1323:GLN:O	2.12	0.50
5:W:468:ALA:O	5:W:472:ASN:ND2	2.45	0.50
5:x:547:ASP:OD1	5:x:547:ASP:N	2.41	0.50
5:x:1077:ARG:HB2	5:x:1085:THR:HG23	1.93	0.50
5:x:1208:CYS:HB2	5:x:1211:SER:HB3	1.94	0.50
5:l:532:PRO:HG3	5:l:1238:SER:HB2	1.92	0.50
5:S:94:GLN:NE2	5:l:53:GLU:OE1	2.44	0.50
5:T:541:GLU:OE1	5:T:565:ARG:NH2	2.39	0.50
7:g:86:VAL:HG13	7:g:88:GLY:H	1.76	0.50
1:K:22:LEU:HG	1:G:13:ARG:HD3	1.92	0.50
2:C:390:PHE:O	2:C:393:VAL:HG12	2.12	0.50
5:T:1313:VAL:CG2	6:e:199:TYR:CE2	2.94	0.50
5:W:1315:ALA:HA	7:f:41:GLN:HE22	1.76	0.50
5:x:390:ASP:OD1	5:x:390:ASP:N	2.43	0.50
5:l:547:ASP:N	5:l:547:ASP:OD1	2.45	0.50
6:5:2:LYS:HG3	6:5:3:VAL:HG13	1.93	0.50
5:T:827:GLY:HA2	5:T:929:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:208:SER:OG	5:W:209:LYS:N	2.45	0.50
5:x:101:THR:OG1	5:x:102:ILE:N	2.45	0.50
5:x:269:THR:CG2	5:x:274:GLU:HG2	2.42	0.50
7:7:234:ASP:HB3	7:7:237:ASN:HB2	1.93	0.50
1:K:22:LEU:O	2:C:374:THR:OG1	2.30	0.50
5:S:632:LYS:NZ	5:S:887:SER:OG	2.41	0.50
7:f:229:ARG:NH2	7:f:241:GLU:OE2	2.45	0.50
5:l:1135:ASN:OD1	5:l:1138:VAL:N	2.44	0.50
5:l:1205:ARG:NH1	5:l:1226:ASP:O	2.45	0.50
6:5:307:VAL:HG23	6:5:308:VAL:HG13	1.93	0.50
5:S:1065:THR:HG22	5:S:1096:ASP:HA	1.93	0.50
5:T:586:GLN:NE2	5:T:589:GLU:OE1	2.44	0.50
5:T:1256:ASN:HB2	5:T:1275:PHE:HB3	1.94	0.50
5:x:134:SER:OG	5:x:137:ASP:OD1	2.27	0.50
7:6:3:LEU:HB3	7:6:83:THR:HG23	1.94	0.50
7:7:246:GLU:HG3	7:7:249:ARG:HH21	1.76	0.50
5:S:11:PRO:HG2	5:T:322:VAL:HG13	1.93	0.49
5:W:742:ARG:NH1	5:W:904:ASN:O	2.45	0.49
5:x:176:LEU:C	5:x:176:LEU:CD2	2.85	0.49
5:x:901:SER:HB2	5:x:920:GLU:HG2	1.93	0.49
5:l:251:MET:HE2	5:l:1059:PHE:HB2	1.93	0.49
2:C:48:PHE:CE2	2:C:55:THR:CG2	2.95	0.49
5:S:510:LYS:NZ	5:S:512:ALA:O	2.45	0.49
5:T:1221:GLU:HG3	5:T:1225:TYR:HD2	1.77	0.49
5:T:1302:PRO:HG2	5:T:1313:VAL:HG22	1.94	0.49
5:x:474:LEU:HD11	5:x:542:LEU:HD21	1.94	0.49
5:T:442:ASN:HD22	5:T:446:LEU:HD12	1.77	0.49
5:W:855:ASP:O	5:W:859:ASN:ND2	2.45	0.49
5:W:1209:VAL:HG21	5:W:1283:ASN:HB3	1.94	0.49
5:x:506:PHE:CD2	5:x:986:PRO:HG3	2.47	0.49
5:x:736:LEU:HA	5:x:739:VAL:HG22	1.94	0.49
7:g:158:ARG:HH22	7:g:194:PRO:HB2	1.76	0.49
5:l:90:ASP:N	5:l:90:ASP:OD1	2.43	0.49
5:l:193:ILE:CG2	5:l:197:LEU:HD12	2.41	0.49
7:7:211:ILE:HA	7:7:214:THR:HG22	1.93	0.49
2:C:15:THR:HG23	2:C:83:TYR:HB3	1.95	0.49
5:S:815:VAL:HG21	5:S:1019:THR:HG23	1.94	0.49
5:T:810:LYS:O	5:T:814:TYR:HB2	2.12	0.49
5:x:143:SER:OG	5:x:144:ILE:N	2.46	0.49
5:x:1282:ARG:NH1	5:x:1299:GLY:O	2.45	0.49
5:x:395:TYR:CD2	5:x:397:LEU:HB2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:331:PHE:HE1	6:5:58:TRP:HB2	1.78	0.49
5:S:817:LEU:HB3	5:S:825:MET:HE1	1.94	0.49
5:S:1195:TYR:OH	5:S:1201:SER:O	2.30	0.49
5:T:390:ASP:OD1	5:T:390:ASP:N	2.40	0.49
5:T:460:CYS:HB2	5:T:1027:PRO:HB3	1.94	0.49
5:T:745:GLN:HG3	5:T:901:SER:HB2	1.94	0.49
5:x:1338:SER:OG	5:x:1360:HIS:ND1	2.38	0.49
1:G:47:GLU:OE1	1:G:47:GLU:HA	2.13	0.49
5:S:969:THR:O	5:S:973:ARG:NH1	2.46	0.49
5:S:1057:ILE:HG13	5:S:1108:ALA:HB2	1.94	0.49
5:W:511:TYR:HA	5:W:973:ARG:HE	1.78	0.49
5:x:919:THR:OG1	5:x:996:TRP:NE1	2.46	0.49
7:f:21:MET:HG2	7:f:75:VAL:HG21	1.94	0.49
5:l:266:THR:O	5:l:364:ARG:NH1	2.45	0.49
5:l:632:LYS:NZ	5:l:890:THR:OG1	2.37	0.49
5:l:722:ASN:HB3	5:l:902:VAL:HG21	1.95	0.49
7:7:70:ALA:HA	7:7:84:LYS:HA	1.94	0.49
5:S:170:ASP:OD1	5:S:174:ARG:NH1	2.45	0.49
5:W:323:SER:OG	5:W:324:TYR:N	2.45	0.49
5:W:766:VAL:HG22	5:W:797:GLY:HA2	1.94	0.49
1:G:31:SER:HA	2:C:371:VAL:HG12	1.94	0.49
5:T:78:VAL:HG11	5:T:261:LEU:HD13	1.93	0.49
5:W:78:VAL:HG11	5:W:261:LEU:HD13	1.94	0.49
5:W:190:PRO:HD2	5:W:193:ILE:HD12	1.95	0.49
5:W:448:LEU:HD13	5:W:1119:ILE:HG12	1.94	0.49
5:x:580:PHE:HZ	5:x:1041:GLY:HA2	1.77	0.49
5:x:1200:ASN:O	5:x:1331:ALA:N	2.46	0.49
5:x:1236:TYR:OH	5:x:1237:ARG:NH1	2.45	0.49
5:x:1249:SER:OG	5:x:1250:LEU:N	2.45	0.49
5:l:1064:SER:OG	5:l:1065:THR:N	2.46	0.49
6:5:122:VAL:HG11	6:5:200:LEU:HD22	1.95	0.49
6:5:191:LEU:HA	6:5:205:THR:HG22	1.95	0.49
5:T:717:ALA:HB1	5:T:723:LEU:HD22	1.94	0.49
5:T:1078:GLU:HB3	5:T:1085:THR:HB	1.95	0.49
5:x:1028:MET:HE1	5:x:1138:VAL:HG13	1.94	0.49
2:C:21:LEU:HG	2:C:299:VAL:HG23	1.95	0.48
5:W:553:ASP:OD1	5:W:553:ASP:N	2.46	0.48
5:l:694:GLU:HG2	5:l:808:LEU:HD11	1.94	0.48
5:l:955:GLY:HA3	5:l:985:ARG:HE	1.78	0.48
5:T:486:THR:HG21	5:T:552:ARG:HD2	1.95	0.48
5:W:518:ILE:CG1	5:W:993:TYR:HE1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:l:97:ILE:HG13	5:l:1099:LEU:HD22	1.95	0.48
4:2:23:LEU:HD13	4:2:51:LEU:HD23	1.94	0.48
5:x:1064:SER:OG	5:x:1065:THR:N	2.46	0.48
2:C:20:HIS:HD2	2:C:302:TYR:HE1	1.60	0.48
2:C:368:ILE:HD12	2:C:369:PRO:HD2	1.95	0.48
5:S:59:TYR:HE2	5:T:93:ILE:HD11	1.78	0.48
5:S:538:LEU:O	5:S:1246:GLN:NE2	2.46	0.48
5:S:1239:THR:OG1	5:S:1241:ASN:O	2.31	0.48
5:S:1250:LEU:HG	5:S:1254:MET:HE2	1.96	0.48
5:T:456:LEU:HD21	5:T:1030:TYR:HB3	1.93	0.48
7:7:129:ASP:OD1	7:7:129:ASP:N	2.44	0.48
5:W:131:MET:HG2	5:W:1086:PHE:HB2	1.95	0.48
5:W:319:VAL:O	5:W:323:SER:HB3	2.14	0.48
5:W:1135:ASN:HB3	5:W:1138:VAL:HG12	1.94	0.48
5:x:46:ARG:HG3	5:x:48:ALA:H	1.78	0.48
7:f:247:ILE:O	7:f:251:ASP:HB2	2.14	0.48
2:C:4:HIS:CE1	2:C:300:VAL:HG11	2.48	0.48
5:x:530:LEU:HA	5:x:538:LEU:HD11	1.94	0.48
7:6:156:TYR:HA	7:6:159:VAL:HG22	1.95	0.48
7:6:171:ASP:OD1	7:6:171:ASP:N	2.45	0.48
7:6:256:SER:O	7:7:156:TYR:OH	2.29	0.48
1:G:82:GLU:OE2	1:G:86:GLN:NE2	2.47	0.48
2:C:309:GLY:O	2:C:313:ARG:NE	2.47	0.48
5:S:932:ALA:HA	5:S:959:VAL:HG23	1.96	0.48
5:S:951:HIS:HB3	5:S:954:TYR:HB2	1.96	0.48
5:T:745:GLN:HG2	5:T:918:ARG:HH22	1.78	0.48
5:T:820:CYS:HA	5:T:1010:PRO:HB3	1.94	0.48
5:W:155:VAL:HG11	5:x:342:PRO:HB2	1.96	0.48
5:W:783:ARG:HG2	5:W:833:GLN:HE21	1.79	0.48
5:x:134:SER:HA	5:x:1083:ALA:HA	1.94	0.48
5:x:405:TYR:O	5:x:1048:ARG:N	2.47	0.48
5:x:932:ALA:HA	5:x:959:VAL:HG23	1.96	0.48
6:e:261:ASP:OD1	6:e:261:ASP:N	2.43	0.48
5:l:495:ASN:HA	5:l:750:ASN:HD21	1.78	0.48
5:l:659:SER:OG	5:l:661:SER:OG	2.32	0.48
5:S:831:ASP:OD1	5:S:834:HIS:ND1	2.47	0.48
5:x:269:THR:OG1	5:x:299:ASP:OD2	2.31	0.48
5:l:1209:VAL:HG21	5:l:1223:LEU:HB3	1.96	0.48
6:5:302:MET:HA	6:5:305:TYR:HB3	1.96	0.48
1:K:64:ARG:HB2	2:C:291:ILE:HG23	1.96	0.48
5:T:567:MET:HE3	5:T:567:MET:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:371:VAL:HA	5:W:380:ALA:HA	1.96	0.48
5:W:655:ALA:O	5:W:683:TYR:OH	2.30	0.48
6:e:16:ILE:HG12	6:e:20:LEU:HG	1.96	0.48
5:l:644:ILE:HG22	5:l:655:ALA:HB3	1.96	0.48
7:6:264:MET:HE3	7:7:152:LEU:HD21	1.95	0.48
2:C:463:VAL:HA	2:C:478:PRO:HD3	1.95	0.47
5:S:131:MET:HE1	5:S:165:LEU:HD23	1.95	0.47
5:S:326:ARG:HA	5:S:329:ARG:HB2	1.96	0.47
5:T:828:LEU:HD12	5:T:945:PHE:HB3	1.96	0.47
5:W:977:GLN:NE2	5:W:982:ALA:O	2.42	0.47
5:l:373:LYS:HA	5:l:378:ALA:HA	1.95	0.47
5:l:1246:GLN:HB2	5:l:1249:SER:HB2	1.95	0.47
7:6:112:MET:HE3	7:6:143:ALA:HB1	1.95	0.47
7:7:116:PHE:HE2	7:7:136:MET:HG2	1.79	0.47
4:Y:20:ASP:OD1	4:Y:20:ASP:N	2.46	0.47
4:Y:56:CYS:HA	4:Y:59:GLU:HG2	1.97	0.47
5:S:406:TYR:HE2	5:S:1196:PHE:HD1	1.60	0.47
5:l:1024:LYS:HE2	5:l:1024:LYS:HB3	1.74	0.47
1:G:60:VAL:HA	1:G:63:ASN:HD22	1.78	0.47
3:O:3143:ARG:NH2	5:x:760:PRO:O	2.48	0.47
5:W:452:LEU:HD22	5:W:1040:PRO:HD3	1.96	0.47
5:x:28:SER:OG	5:x:29:ALA:N	2.46	0.47
5:x:463:ARG:NH1	5:x:1259:TYR:O	2.48	0.47
5:x:783:ARG:NH2	5:x:891:CYS:O	2.42	0.47
4:2:35:LEU:HD22	4:2:39:VAL:HG11	1.96	0.47
5:x:84:ASP:OD1	5:x:84:ASP:N	2.46	0.47
5:x:668:ARG:NH2	5:x:802:GLU:OE2	2.47	0.47
5:x:969:THR:HA	5:x:972:MET:HE3	1.96	0.47
6:e:179:ARG:HH22	6:e:304:ARG:HH11	1.61	0.47
5:l:435:PRO:HB3	5:l:1338:SER:HB2	1.96	0.47
2:C:266:ARG:HD3	6:5:312:HIS:H	1.79	0.47
7:f:235:LEU:HD22	7:g:207:LEU:HG	1.95	0.47
5:l:844:PRO:O	5:l:882:ARG:NH1	2.44	0.47
5:S:1049:THR:HG23	5:S:1270:PRO:HB3	1.96	0.47
5:W:463:ARG:NH2	5:W:1253:ILE:O	2.43	0.47
5:l:860:LEU:O	5:l:866:ARG:NH2	2.48	0.47
5:l:899:ARG:HH22	5:l:991:ALA:H	1.63	0.47
6:5:112:GLN:HA	6:5:125:VAL:HA	1.95	0.47
2:C:423:SER:OG	2:C:464:HIS:ND1	2.45	0.47
4:2:13:ARG:HD2	4:2:13:ARG:HA	1.73	0.47
5:S:321:ALA:HA	5:S:326:ARG:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:493:ARG:HB3	5:S:750:ASN:HB3	1.97	0.47
5:S:1293:GLU:HA	5:S:1296:GLN:HB2	1.96	0.47
5:T:794:LEU:HD13	5:T:896:ARG:HH11	1.80	0.47
5:W:129:THR:OG1	5:W:130:GLU:N	2.48	0.47
5:x:644:ILE:HD11	5:x:675:ILE:HG12	1.97	0.47
5:x:1187:THR:HG22	5:x:1241:ASN:HD22	1.79	0.47
7:f:106:THR:HG22	7:f:288:ALA:H	1.80	0.47
5:l:189:PRO:HG2	5:l:194:LEU:HD22	1.95	0.47
5:l:821:THR:HG22	5:l:824:HIS:H	1.79	0.47
6:5:310:PRO:HB3	6:5:315:GLU:HB2	1.96	0.47
1:K:53:ARG:NH2	2:C:393:VAL:O	2.48	0.47
5:S:108:ARG:O	5:S:109:ARG:NE	2.47	0.47
5:T:623:GLU:OE2	5:T:658:ASN:ND2	2.48	0.47
7:6:13:LEU:HD11	7:6:125:LEU:HD22	1.95	0.47
5:S:181:LEU:HD11	5:S:281:ILE:HG21	1.97	0.47
5:S:518:ILE:O	5:S:518:ILE:CG2	2.63	0.47
5:T:907:THR:HG21	5:T:1028:MET:HE1	1.96	0.47
5:x:409:VAL:HG21	5:x:1044:MET:HE3	1.97	0.47
5:l:655:ALA:O	5:l:683:TYR:OH	2.30	0.47
5:l:1056:ASN:HD22	5:l:1107:PRO:HA	1.80	0.47
4:m:4:ARG:H	4:m:4:ARG:HD3	1.80	0.47
5:S:907:THR:HG21	5:S:1028:MET:HE1	1.98	0.47
5:W:1051:GLU:OE1	5:W:1114:THR:OG1	2.33	0.47
5:W:1132:ALA:CB	5:W:1139:ASN:HD21	2.23	0.47
5:x:169:VAL:HG13	6:5:7:VAL:HB	1.95	0.47
5:x:509:ASN:C	5:x:509:ASN:ND2	2.73	0.47
5:l:822:ASN:HD21	5:l:1010:PRO:HG3	1.80	0.47
1:G:75:ARG:NE	3:B:3142:GLU:OE2	2.44	0.46
5:S:804:HIS:HE1	5:T:958:ARG:HH22	1.62	0.46
5:T:180:VAL:HG13	5:T:1067:MET:HE1	1.96	0.46
5:T:636:ASN:HB3	5:T:639:LEU:HD23	1.98	0.46
5:x:269:THR:HG22	5:x:274:GLU:O	2.14	0.46
5:x:501:VAL:O	5:x:505:GLU:CB	2.63	0.46
5:x:1186:VAL:HB	5:x:1250:LEU:HD22	1.97	0.46
5:l:447:LEU:HD11	5:l:1343:ILE:HG21	1.97	0.46
2:C:38:ASN:HD22	2:C:64:ARG:HD3	1.80	0.46
2:C:412:PRO:HD3	7:6:167:ALA:HA	1.97	0.46
5:T:726:PRO:HB3	5:T:950:PHE:HE2	1.80	0.46
5:T:1348:SER:OG	5:T:1349:VAL:N	2.48	0.46
5:x:563:VAL:HG22	5:x:998:ARG:HH22	1.79	0.46
5:x:814:TYR:HB3	5:x:1022:HIS:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:158:ARG:NH2	7:g:225:ARG:O	2.48	0.46
7:7:28:ILE:HG22	7:7:71:VAL:HA	1.95	0.46
4:m:24:LEU:HA	4:m:27:PHE:HB3	1.97	0.46
5:S:1039:HIS:ND1	5:S:1040:PRO:O	2.36	0.46
5:T:783:ARG:NH1	5:T:892:PRO:O	2.48	0.46
5:x:1105:MET:HE3	5:x:1105:MET:HB3	1.80	0.46
7:f:275:ALA:HB2	7:g:275:ALA:HB1	1.95	0.46
5:l:230:LEU:HD22	5:l:286:VAL:HG13	1.97	0.46
5:l:948:ILE:HG22	5:l:950:PHE:HB3	1.96	0.46
6:5:222:LYS:HD3	6:5:349:GLU:HB3	1.98	0.46
7:7:204:ASN:C	7:7:208:TYR:HE1	2.22	0.46
2:C:14:GLY:O	2:C:56:ARG:NH2	2.39	0.46
5:T:814:TYR:HB3	5:T:1022:HIS:HE1	1.81	0.46
5:T:1192:ASP:N	5:T:1192:ASP:OD1	2.42	0.46
5:T:1277:LYS:HZ3	5:T:1281:LEU:HD22	1.80	0.46
5:x:501:VAL:O	5:x:505:GLU:HB3	2.15	0.46
5:l:450:PHE:HZ	5:l:1184:ILE:HD11	1.80	0.46
5:S:174:ARG:NH2	5:S:390:ASP:OD2	2.49	0.46
5:T:902:VAL:HA	5:T:918:ARG:HH21	1.81	0.46
5:T:1199:SER:O	5:T:1199:SER:OG	2.33	0.46
5:W:477:ALA:O	5:W:557:ARG:NH1	2.42	0.46
5:x:385:GLN:HE21	5:x:389:ASN:HD21	1.64	0.46
5:l:195:GLN:OE1	5:l:222:HIS:ND1	2.49	0.46
5:l:517:ASP:OD1	5:l:993:TYR:OH	2.32	0.46
5:S:37:PHE:HB2	5:x:118:VAL:HG12	1.97	0.46
5:S:916:ASP:N	5:S:916:ASP:OD1	2.43	0.46
5:S:1297:ARG:NH1	5:S:1317:THR:O	2.49	0.46
5:T:133:LEU:HD23	5:T:133:LEU:HA	1.83	0.46
5:T:279:VAL:HG12	5:T:380:ALA:HB3	1.97	0.46
5:T:1328:LEU:HD12	5:T:1330:GLU:H	1.81	0.46
5:W:748:ILE:HB	5:W:898:VAL:HG12	1.97	0.46
5:x:852:ARG:HE	5:x:879:GLY:HA3	1.80	0.46
5:x:961:ALA:HA	5:x:967:VAL:HG23	1.98	0.46
6:e:171:ASP:OD1	6:e:171:ASP:N	2.43	0.46
4:m:5:LEU:CD1	4:m:5:LEU:N	2.73	0.46
5:S:693:LEU:HD22	5:S:1019:THR:HG21	1.98	0.46
5:T:338:ILE:HD11	5:x:319:VAL:HA	1.98	0.46
5:W:194:LEU:HD12	5:W:1104:THR:HG22	1.97	0.46
5:x:842:ASN:ND2	5:x:845:ALA:H	2.13	0.46
7:f:240:GLN:NE2	7:g:259:ASP:OD2	2.49	0.46
5:T:141:LEU:HD22	5:T:161:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:1074:VAL:HG22	5:W:1088:VAL:HG12	1.97	0.46
5:x:481:ARG:HB2	5:x:539:ARG:HD3	1.98	0.46
5:l:712:GLY:HA2	5:l:715:VAL:HG22	1.97	0.46
7:7:204:ASN:C	7:7:208:TYR:CD1	2.84	0.46
5:S:280:PHE:HB2	5:S:381:VAL:HG22	1.98	0.46
5:S:565:ARG:HB3	5:S:570:ASN:HB2	1.98	0.46
5:S:573:THR:HG21	5:S:1003:LYS:HD3	1.98	0.46
5:W:172:LEU:HD23	5:W:172:LEU:HA	1.78	0.46
5:W:612:ASP:OD2	5:W:647:TYR:OH	2.34	0.46
5:W:901:SER:HA	5:W:920:GLU:HA	1.97	0.46
5:W:1239:THR:OG1	5:W:1240:VAL:N	2.48	0.46
5:x:722:ASN:ND2	5:x:742:ARG:HH11	2.14	0.46
7:f:68:THR:OG1	7:f:69:LEU:N	2.49	0.46
5:S:598:VAL:HG12	5:S:685:LYS:HB3	1.98	0.45
5:S:1306:ASN:OD1	5:S:1306:ASN:N	2.49	0.45
5:T:436:VAL:HG13	5:T:437:GLU:HG3	1.97	0.45
5:T:1298:LEU:HD21	6:e:199:TYR:CE1	2.51	0.45
5:x:516:THR:HG23	5:x:519:ALA:H	1.81	0.45
7:f:11:SER:OG	7:f:128:ASN:ND2	2.48	0.45
5:l:76:SER:OG	5:l:184:LYS:NZ	2.49	0.45
6:5:339:ASN:HA	6:5:344:SER:HA	1.98	0.45
7:7:204:ASN:HA	7:7:207:LEU:CD1	2.39	0.45
7:7:204:ASN:HB2	7:7:208:TYR:CE1	2.50	0.45
5:W:389:ASN:O	5:W:392:GLN:NE2	2.50	0.45
2:C:425:PRO:HB2	2:C:429:GLU:H	1.82	0.45
2:C:436:LYS:HB3	2:C:436:LYS:HE3	1.79	0.45
5:T:1074:VAL:HB	6:e:52:LEU:HD13	1.97	0.45
5:T:1298:LEU:HD11	6:e:199:TYR:CE1	2.51	0.45
5:W:1033:GLN:HG2	5:W:1038:ILE:HD11	1.99	0.45
5:x:323:SER:OG	5:x:324:TYR:N	2.48	0.45
5:x:1195:TYR:OH	5:x:1201:SER:O	2.32	0.45
6:e:302:MET:HE2	6:e:302:MET:HB3	1.78	0.45
5:l:284:ASP:HB2	5:l:385:GLN:HB3	1.98	0.45
7:6:199:LEU:HD23	7:6:202:LEU:HD12	1.97	0.45
1:K:34:VAL:HG12	1:K:36:PRO:HD3	1.97	0.45
2:C:66:MET:HE2	7:7:233:HIS:CD2	2.51	0.45
2:C:493:GLU:HA	2:C:496:TYR:HB3	1.99	0.45
5:S:450:PHE:HB2	5:S:1119:ILE:HD11	1.98	0.45
5:S:899:ARG:NH2	5:S:991:ALA:H	2.14	0.45
5:x:225:GLU:OE2	5:x:226:HIS:NE2	2.50	0.45
5:l:1226:ASP:OD2	5:l:1228:SER:OG	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:151:LEU:CD1	7:7:206:SER:OG	2.64	0.45
2:C:18:LEU:HD13	2:C:81:PRO:HA	1.99	0.45
3:O:3143:ARG:HH22	5:x:793:ARG:NH1	2.14	0.45
5:T:1176:HIS:HB3	5:T:1177:GLY:H	1.53	0.45
5:W:803:GLY:O	5:x:978:ARG:NH2	2.49	0.45
5:x:1057:ILE:HG13	5:x:1108:ALA:HB2	1.99	0.45
6:e:316:LEU:HB3	7:f:211:ILE:HD11	1.98	0.45
7:6:210:CYS:SG	7:7:240:GLN:HB2	2.57	0.45
7:6:256:SER:OG	7:6:257:VAL:N	2.49	0.45
7:7:114:PRO:O	7:7:118:ARG:NH1	2.50	0.45
3:O:3129:LYS:HA	3:O:3129:LYS:HD3	1.83	0.45
5:S:522:CYS:O	5:S:573:THR:OG1	2.33	0.45
5:S:903:ASP:OD1	5:S:918:ARG:NE	2.49	0.45
5:W:159:LYS:HE3	5:x:345:ALA:HB2	1.99	0.45
5:W:690:LEU:HD22	5:W:811:ILE:HG23	1.99	0.45
7:f:284:LEU:HD23	7:f:300:LEU:HA	1.99	0.45
5:l:1249:SER:OG	5:l:1250:LEU:N	2.49	0.45
2:C:122:GLY:HA2	2:C:125:ARG:HB3	1.97	0.45
2:C:368:ILE:HD13	2:C:453:LEU:HD22	1.98	0.45
5:S:1001:MET:HG2	5:S:1021:MET:HE2	1.98	0.45
5:T:657:VAL:HA	5:T:663:ILE:HD11	1.98	0.45
5:T:1135:ASN:HB3	5:T:1138:VAL:HG12	1.99	0.45
7:6:176:LEU:HD12	7:7:265:ARG:HH11	1.81	0.45
7:6:264:MET:HG3	7:7:148:GLN:HG2	1.99	0.45
5:S:828:LEU:HB3	5:S:928:LEU:HB2	1.99	0.45
5:T:528:ASP:OD1	5:T:528:ASP:N	2.49	0.45
7:f:57:TYR:HA	7:f:60:MET:HE3	1.97	0.45
5:l:629:PHE:HB2	5:l:632:LYS:HB2	1.99	0.45
7:6:6:VAL:HA	7:6:81:ILE:HA	1.98	0.45
5:S:643:CYS:SG	5:S:644:ILE:N	2.90	0.45
5:T:1099:LEU:HD23	5:T:1099:LEU:HA	1.81	0.45
5:T:1115:THR:HB	5:T:1180:ALA:HB2	1.98	0.45
5:T:1145:LYS:HD3	5:T:1145:LYS:HA	1.77	0.45
5:T:1302:PRO:CG	5:T:1313:VAL:HG21	2.46	0.45
5:W:53:GLU:HG2	5:x:90:ASP:HB3	1.98	0.45
5:W:426:MET:HE1	5:W:1360:HIS:HD2	1.82	0.45
5:x:286:VAL:HG22	5:x:290:LEU:HD23	1.97	0.45
5:l:588:PHE:O	5:l:592:THR:OG1	2.33	0.45
7:6:218:ARG:HH21	7:6:250:ILE:HD12	1.80	0.45
2:C:20:HIS:HD2	2:C:302:TYR:CE1	2.35	0.45
5:S:1195:TYR:OH	5:S:1203:ARG:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:598:VAL:HG13	5:T:602:VAL:HB	1.99	0.45
5:W:498:ASN:HD21	5:W:500:LEU:HB3	1.82	0.45
5:x:1246:GLN:HB2	5:x:1249:SER:HB2	1.98	0.45
2:C:5:ILE:CD1	2:C:273:LYS:HE2	2.44	0.44
2:C:498:LEU:HG	2:C:504:ARG:HA	1.99	0.44
4:m:8:PRO:HB3	5:l:834:HIS:NE2	2.32	0.44
4:Z:4:ARG:HG2	5:T:894:PHE:HZ	1.82	0.44
5:T:73:LEU:HD22	5:T:384:LEU:HD11	1.98	0.44
5:T:481:ARG:HH21	5:T:550:ILE:HG22	1.82	0.44
5:T:1381:PHE:O	5:T:1381:PHE:CD1	2.70	0.44
5:x:401:MET:SD	5:x:403:TYR:OH	2.71	0.44
7:g:55:PRO:HB2	7:g:201:LEU:HD13	1.98	0.44
5:l:190:PRO:HG3	5:l:1324:PRO:HB3	1.99	0.44
5:l:1048:ARG:HB3	5:l:1182:CYS:HB3	2.00	0.44
2:C:53:GLY:O	2:C:54:LEU:HG	2.17	0.44
4:Z:22:PRO:O	4:Z:26:LYS:NZ	2.50	0.44
6:e:47:ALA:O	6:e:48:GLN:NE2	2.50	0.44
5:l:94:GLN:HE21	5:l:117:ILE:HG21	1.83	0.44
5:l:434:LEU:HD12	5:l:435:PRO:HD2	1.99	0.44
5:l:463:ARG:NH2	5:l:1259:TYR:O	2.50	0.44
5:l:1223:LEU:HD23	5:l:1223:LEU:HA	1.87	0.44
7:6:275:ALA:O	7:6:279:ASN:N	2.42	0.44
7:7:118:ARG:HH21	7:7:201:LEU:HD21	1.83	0.44
1:K:54:TRP:HZ2	2:C:336:GLU:HG3	1.82	0.44
5:S:401:MET:HE3	5:S:401:MET:HB3	1.86	0.44
5:T:1292:ASN:O	5:T:1296:GLN:HB2	2.17	0.44
5:W:724:LEU:H	5:W:921:GLN:HE22	1.65	0.44
5:x:894:PHE:HB2	5:x:896:ARG:HE	1.82	0.44
5:x:1285:ARG:HH22	5:x:1289:ASN:HD22	1.64	0.44
5:l:404:SER:HA	5:l:1049:THR:HA	1.98	0.44
5:l:626:ILE:HG23	5:l:632:LYS:HB3	1.99	0.44
5:l:691:ILE:HA	5:l:694:GLU:HG3	2.00	0.44
5:l:828:LEU:HD22	5:l:930:ALA:HB2	2.00	0.44
7:7:39:ASN:OD1	7:7:39:ASN:N	2.48	0.44
7:7:117:GLY:HA3	7:7:120:HIS:CD2	2.53	0.44
2:C:28:MET:HE2	2:C:28:MET:HB2	1.74	0.44
5:S:405:TYR:HD2	5:S:1334:ALA:HB2	1.83	0.44
5:W:1183:GLU:HG2	5:W:1270:PRO:HD2	1.99	0.44
6:e:95:ILE:HG13	6:e:201:ASN:HB3	1.99	0.44
7:f:283:ARG:HG2	7:f:301:ARG:HH11	1.80	0.44
5:l:724:LEU:O	5:l:921:GLN:NE2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:l:724:LEU:HD21	5:l:736:LEU:HD13	2.00	0.44
5:T:553:ASP:HA	5:T:558:ALA:HB2	1.99	0.44
5:W:347:SER:N	5:W:350:SER:OG	2.49	0.44
5:x:1082:ASP:OD1	5:x:1082:ASP:N	2.46	0.44
5:x:1116:ASP:OD1	5:x:1116:ASP:N	2.50	0.44
7:f:9:LEU:HG	7:f:40:VAL:HG11	1.98	0.44
5:l:565:ARG:HB3	5:l:570:ASN:HB2	2.00	0.44
5:l:772:MET:CE	5:l:775:GLN:CB	2.95	0.44
4:Y:35:LEU:HG	4:Y:39:VAL:HG13	1.98	0.44
5:S:7:VAL:HG11	5:S:38:ASP:HB2	2.00	0.44
5:S:20:ASP:OD1	5:S:20:ASP:N	2.43	0.44
5:S:1279:GLU:HG2	5:S:1301:HIS:HE1	1.82	0.44
5:S:1336:SER:OG	5:S:1337:ALA:N	2.51	0.44
5:T:294:LEU:HD13	5:T:372:ILE:HG21	1.99	0.44
5:W:180:VAL:HG22	5:W:1067:MET:HE1	2.00	0.44
5:W:471:LEU:HD21	5:W:562:ALA:HB2	1.99	0.44
5:W:973:ARG:HG3	5:W:974:ASN:HD22	1.82	0.44
5:W:1081:VAL:HB	6:e:210:PRO:HB3	1.99	0.44
5:x:1052:ILE:HG12	5:x:1369:VAL:HG11	2.00	0.44
5:x:1338:SER:OG	5:x:1339:SER:N	2.50	0.44
7:g:9:LEU:HD11	7:g:80:LEU:HD21	2.00	0.44
2:C:345:VAL:HA	2:C:348:ARG:HG2	1.99	0.44
5:S:545:LEU:HD23	5:S:564:HIS:HE1	1.81	0.44
5:S:763:ILE:HD11	5:S:796:LEU:HB2	2.00	0.44
5:T:207:PHE:HE1	5:W:27:GLN:HB3	1.83	0.44
5:x:138:LEU:HD11	6:5:20:LEU:HD11	1.99	0.44
5:x:1142:ILE:HD13	5:x:1142:ILE:HA	1.86	0.44
6:e:227:GLN:HE22	6:e:335:ARG:HE	1.66	0.44
7:f:268:MET:HE2	7:f:268:MET:HB3	1.94	0.44
6:5:25:ARG:HH22	6:5:42:LEU:HA	1.83	0.44
7:6:112:MET:O	7:6:136:MET:N	2.43	0.44
7:6:266:VAL:HA	7:6:269:THR:HG22	2.00	0.44
7:7:103:TRP:HZ3	7:7:109:LEU:HD11	1.82	0.44
2:C:21:LEU:HB2	2:C:78:THR:HG23	2.00	0.44
4:m:5:LEU:H	4:m:5:LEU:HD13	1.83	0.44
5:S:62:ALA:O	5:S:64:GLN:NE2	2.51	0.44
5:W:813:TYR:O	5:W:954:TYR:OH	2.30	0.44
5:x:1277:LYS:HA	5:x:1280:LEU:HG	1.99	0.44
7:f:246:GLU:HA	7:f:249:ARG:HG2	1.99	0.44
5:l:566:LEU:HD12	5:l:996:TRP:HA	2.00	0.44
5:l:1214:ASN:OD1	5:l:1214:ASN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:95:ILE:HG21	6:5:125:VAL:HG22	1.99	0.44
7:6:153:PHE:HB2	7:6:176:LEU:HD22	1.99	0.44
2:C:273:LYS:HB2	2:C:273:LYS:HE3	1.76	0.44
5:S:488:SER:OG	5:S:992:GLU:N	2.39	0.44
5:x:385:GLN:HG2	5:x:389:ASN:HD21	1.83	0.44
5:x:1056:ASN:HD22	5:x:1107:PRO:HA	1.83	0.44
6:e:107:GLY:O	6:e:224:THR:N	2.43	0.44
7:f:245:ASP:OD1	7:g:218:ARG:NH1	2.51	0.44
5:l:997:HIS:HB3	5:l:1001:MET:HG2	1.98	0.44
7:7:151:LEU:HD21	7:7:209:PHE:CE2	2.36	0.44
7:7:209:PHE:O	7:7:213:VAL:HG22	2.17	0.44
1:K:69:GLU:HB3	3:B:3145:LYS:HE3	2.00	0.43
2:C:91:LEU:HA	2:C:316:ALA:HB2	1.99	0.43
5:S:112:LYS:NZ	5:S:113:GLN:O	2.42	0.43
5:W:844:PRO:O	5:W:882:ARG:NH1	2.51	0.43
5:W:1080:ARG:HA	5:W:1080:ARG:HD3	1.79	0.43
5:x:908:GLN:HE22	5:x:1024:LYS:HD3	1.81	0.43
5:x:1212:CYS:HA	5:x:1223:LEU:HD12	2.01	0.43
6:e:363:ILE:HD13	6:e:363:ILE:HA	1.88	0.43
6:5:198:THR:OG1	6:5:199:TYR:N	2.51	0.43
1:G:67:ARG:HH22	3:B:3149:LEU:HB3	1.83	0.43
4:2:70:ARG:HH12	4:y:14:LEU:HA	1.83	0.43
5:S:610:ALA:HA	5:S:931:PHE:HB3	2.01	0.43
5:T:964:HIS:HB3	5:T:967:VAL:HG22	2.00	0.43
5:W:124:LYS:NZ	5:W:1091:GLU:OE1	2.44	0.43
5:W:376:ASN:OD1	5:W:376:ASN:N	2.49	0.43
5:W:706:VAL:HG12	5:W:711:VAL:HG12	2.00	0.43
5:W:724:LEU:HD12	5:W:900:VAL:HG21	1.99	0.43
5:W:986:PRO:HB2	5:W:989:LEU:HB3	2.01	0.43
5:W:1067:MET:HE2	5:W:1094:SER:HB3	2.00	0.43
5:x:337:ARG:NH1	5:x:341:SER:OG	2.51	0.43
5:l:148:PRO:HA	5:l:151:TYR:HB3	1.99	0.43
5:S:13:PRO:HG3	5:x:338:ILE:HG13	1.99	0.43
5:S:843:GLY:HA3	5:S:844:PRO:HD3	1.87	0.43
5:T:402:GLN:NE2	5:T:1051:GLU:OE1	2.47	0.43
5:T:839:LEU:HD21	5:T:885:SER:HA	2.00	0.43
5:W:731:ASP:HB2	5:W:799:TYR:HB2	2.01	0.43
5:x:724:LEU:HD12	5:x:900:VAL:HG11	2.01	0.43
5:x:1348:SER:OG	5:x:1349:VAL:N	2.49	0.43
7:f:242:MET:HE3	7:f:242:MET:HB3	1.85	0.43
5:l:817:LEU:HD23	5:l:818:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:l:904:ASN:ND2	5:l:917:LYS:O	2.51	0.43
7:7:7:VAL:HB	7:7:80:LEU:HB3	2.00	0.43
2:C:78:THR:OG1	2:C:79:SER:N	2.51	0.43
2:C:402:CYS:H	2:C:422:ASP:CG	2.27	0.43
2:C:425:PRO:HD3	2:C:432:SER:HB3	2.00	0.43
4:2:26:LYS:HB3	4:2:26:LYS:HE2	1.78	0.43
5:T:324:TYR:CZ	5:x:326:ARG:HB3	2.53	0.43
5:x:90:ASP:OD2	7:6:12:ARG:NH2	2.52	0.43
6:e:95:ILE:O	6:e:201:ASN:N	2.50	0.43
7:f:12:ARG:HD2	7:f:12:ARG:HA	1.84	0.43
7:g:28:ILE:HA	7:g:71:VAL:HA	2.01	0.43
6:5:133:ILE:HG12	6:5:162:PRO:HB3	2.00	0.43
7:6:110:SER:OG	7:6:138:LEU:O	2.30	0.43
1:K:50:ARG:HH12	2:C:340:ARG:HE	1.66	0.43
2:C:385:LEU:O	2:C:389:ALA:N	2.46	0.43
5:S:22:LEU:HB3	5:x:97:ILE:HG21	2.00	0.43
5:T:1280:LEU:HD23	5:T:1329:GLN:HE21	1.84	0.43
5:W:184:LYS:HD3	5:W:184:LYS:HA	1.71	0.43
5:x:1115:THR:HG22	5:x:1178:GLN:HG2	2.00	0.43
7:f:238:LEU:HD11	7:g:215:LEU:HD11	2.01	0.43
7:f:265:ARG:HA	7:g:148:GLN:HE22	1.82	0.43
5:l:218:MET:HE3	5:l:218:MET:HB2	1.88	0.43
7:7:57:TYR:CD1	7:7:205:LEU:CD1	3.02	0.43
2:C:5:ILE:HD12	2:C:273:LYS:CG	2.49	0.43
5:x:406:TYR:HE2	5:x:1196:PHE:HD1	1.65	0.43
5:x:839:LEU:HD13	5:x:884:LEU:HG	2.00	0.43
4:Z:24:LEU:HA	4:Z:27:PHE:HB3	2.00	0.43
5:S:77:CYS:HG	5:S:1065:THR:HG1	1.58	0.43
5:W:133:LEU:HD12	5:W:1086:PHE:HE2	1.84	0.43
5:W:808:LEU:HA	5:W:811:ILE:HG22	2.00	0.43
5:x:36:SER:OG	5:x:37:PHE:N	2.52	0.43
5:x:481:ARG:HH11	5:x:483:ARG:HD3	1.83	0.43
5:x:815:VAL:HG12	5:x:1018:MET:HG3	2.00	0.43
7:f:112:MET:HE3	7:f:138:LEU:HD21	2.00	0.43
1:K:56:ARG:HH12	1:G:60:VAL:HG21	1.83	0.43
5:S:395:TYR:CE2	5:S:397:LEU:HD12	2.53	0.43
5:S:781:GLY:O	5:S:785:ASN:HB2	2.18	0.43
5:T:793:ARG:HE	5:T:793:ARG:HB3	1.62	0.43
5:W:694:GLU:OE2	5:x:978:ARG:NH1	2.52	0.43
7:f:26:GLY:N	7:f:72:LEU:O	2.45	0.43
5:l:879:GLY:H	5:l:882:ARG:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:VAL:HG23	7:7:249:ARG:HD2	1.99	0.43
5:x:631:GLU:OE2	5:x:769:MET:N	2.47	0.43
7:7:274:LEU:HD13	7:7:277:LEU:HD23	2.00	0.43
1:G:40:GLU:O	1:G:44:ARG:HG2	2.19	0.43
2:C:410:ASN:ND2	2:C:469:SER:O	2.52	0.43
5:S:446:LEU:HD23	5:T:1198:LYS:HG3	2.01	0.43
5:S:531:HIS:HD2	5:S:533:SER:H	1.67	0.43
5:S:963:MET:HB3	5:S:963:MET:HE2	1.70	0.43
5:x:43:LYS:HD2	5:x:46:ARG:HB3	2.01	0.43
5:l:1135:ASN:HD21	5:l:1137:GLN:HG3	1.84	0.43
5:l:1145:LYS:HD2	5:l:1145:LYS:HA	1.84	0.43
1:K:32:LEU:HD23	2:C:364:ALA:HB2	2.01	0.42
2:C:461:HIS:NE2	5:x:553:ASP:O	2.35	0.42
5:S:341:SER:O	5:S:344:LYS:NZ	2.40	0.42
5:S:1188:PRO:HB2	5:S:1190:THR:HG22	2.01	0.42
5:T:126:HIS:CE1	5:T:1089:HIS:HD2	2.37	0.42
5:T:783:ARG:O	5:T:833:GLN:NE2	2.52	0.42
5:T:1065:THR:HG22	5:T:1096:ASP:HA	2.01	0.42
5:W:992:GLU:OE1	5:W:999:SER:N	2.52	0.42
5:W:1352:THR:O	5:W:1352:THR:OG1	2.35	0.42
5:x:864:THR:HB	4:y:9:THR:HG23	2.01	0.42
5:l:1264:VAL:HA	5:l:1265:PRO:HD3	1.87	0.42
6:5:179:ARG:HG3	6:5:315:GLU:HA	2.00	0.42
2:C:98:ALA:N	2:C:114:ILE:O	2.46	0.42
2:C:342:LEU:HD22	2:C:398:SER:HB3	2.01	0.42
4:Z:15:GLU:HB2	4:Z:24:LEU:HD11	2.01	0.42
5:T:545:LEU:HD23	5:T:564:HIS:HE1	1.84	0.42
5:T:856:ILE:HD12	5:T:878:VAL:HA	2.00	0.42
5:W:607:GLN:HE21	5:W:1010:PRO:HG2	1.83	0.42
5:W:630:GLU:HB2	5:W:669:HIS:HE1	1.84	0.42
5:x:373:LYS:HE3	5:x:373:LYS:HB3	1.78	0.42
7:f:96:LYS:HD2	7:f:96:LYS:HA	1.83	0.42
5:l:748:ILE:HB	5:l:898:VAL:HG23	2.01	0.42
2:C:432:SER:OG	2:C:433:ALA:N	2.53	0.42
5:W:71:THR:OG1	5:W:382:GLU:OE1	2.37	0.42
5:W:393:SER:HG	5:W:394:PRO:HD2	1.75	0.42
5:W:919:THR:O	5:W:919:THR:OG1	2.37	0.42
5:W:963:MET:HE3	5:W:963:MET:HB2	1.96	0.42
7:f:39:ASN:OD1	7:f:39:ASN:N	2.53	0.42
5:l:670:LEU:HD23	5:l:675:ILE:HD11	2.00	0.42
7:6:129:ASP:N	7:6:129:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:101:ARG:NE	2:C:111:GLU:OE1	2.52	0.42
5:S:8:GLU:HB2	5:x:94:GLN:HE22	1.84	0.42
5:S:644:ILE:HD12	5:S:644:ILE:HA	1.84	0.42
5:T:748:ILE:HD13	5:T:794:LEU:HD23	2.02	0.42
5:x:328:MET:HE3	5:x:331:PHE:CD2	2.54	0.42
5:x:491:HIS:HB2	5:x:991:ALA:HB2	2.02	0.42
5:x:955:GLY:HA3	5:x:985:ARG:HE	1.84	0.42
7:f:216:LEU:HD12	7:g:213:VAL:HG13	2.00	0.42
7:f:221:MET:HA	7:f:224:VAL:HG12	2.02	0.42
7:6:29:LEU:O	7:6:70:ALA:N	2.52	0.42
7:6:59:SER:HA	7:6:197:LEU:HD23	2.01	0.42
5:S:1068:PHE:HD2	5:S:1093:ALA:HB3	1.84	0.42
5:T:813:TYR:O	5:T:954:TYR:OH	2.37	0.42
5:W:134:SER:HA	5:W:1083:ALA:HA	2.00	0.42
5:W:458:VAL:HG11	5:W:1184:ILE:HB	2.01	0.42
5:W:704:ASP:OD2	5:W:1141:TYR:OH	2.36	0.42
4:y:9:THR:OG1	4:y:10:LEU:N	2.53	0.42
5:l:1105:MET:HE2	5:l:1105:MET:HB3	1.89	0.42
4:Y:4:ARG:HH21	5:S:834:HIS:CE1	2.37	0.42
5:T:726:PRO:HG2	5:T:954:TYR:HE2	1.84	0.42
5:W:178:ASN:HA	5:W:388:TYR:OH	2.19	0.42
5:W:1342:LEU:HD23	5:W:1342:LEU:HA	1.84	0.42
7:7:21:MET:HG2	7:7:75:VAL:HB	2.02	0.42
1:G:36:PRO:HA	1:G:39:LEU:HD21	2.01	0.42
2:C:3:VAL:HG11	2:C:63:ALA:H	1.84	0.42
5:S:497:MET:HE3	5:S:894:PHE:HD2	1.85	0.42
5:T:549:TYR:OH	5:T:994:ARG:NH1	2.46	0.42
5:T:817:LEU:HB2	5:T:821:THR:HG23	2.02	0.42
5:W:895:THR:OG1	5:W:926:ASN:O	2.30	0.42
5:W:942:GLN:H	5:W:942:GLN:HG3	1.71	0.42
5:x:1128:PHE:HZ	5:x:1260:ARG:HG2	1.84	0.42
7:g:75:VAL:HG22	7:g:80:LEU:HD22	2.02	0.42
1:K:81:ALA:HB2	3:O:3135:HIS:CE1	2.55	0.42
2:C:66:MET:HE2	7:7:233:HIS:NE2	2.35	0.42
5:S:92:LYS:HA	5:S:121:ASN:HA	2.01	0.42
5:S:132:GLU:O	5:T:113:GLN:NE2	2.52	0.42
5:S:194:LEU:HD23	5:S:194:LEU:HA	1.89	0.42
5:S:658:ASN:OD1	5:S:658:ASN:N	2.49	0.42
5:T:1028:MET:HE2	5:T:1028:MET:HB2	1.94	0.42
5:T:1092:MET:HE2	5:T:1092:MET:HB2	1.91	0.42
5:W:413:MET:SD	5:W:413:MET:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:1028:MET:HB2	5:W:1028:MET:HE3	1.81	0.42
5:l:470:THR:OG1	5:l:1248:GLY:O	2.37	0.42
2:C:264:LEU:HD12	7:6:258:ALA:HB1	2.01	0.42
5:S:302:ILE:HG23	5:S:366:PRO:HB3	2.01	0.42
5:S:695:GLN:HG2	5:S:698:MET:HE2	2.01	0.42
5:W:256:SER:OG	5:W:1100:SER:OG	2.30	0.42
5:W:526:THR:OG1	5:W:574:PRO:O	2.32	0.42
5:W:839:LEU:O	5:W:842:ASN:ND2	2.47	0.42
5:x:1028:MET:HE2	5:x:1028:MET:HB3	1.89	0.42
5:x:1122:GLN:HB2	5:x:1181:THR:HG23	2.02	0.42
6:e:137:HIS:CD2	6:e:162:PRO:HG3	2.55	0.42
7:f:222:ARG:HA	7:f:222:ARG:HD2	1.87	0.42
7:f:245:ASP:OD1	7:f:245:ASP:N	2.42	0.42
7:g:3:LEU:HD22	7:g:89:GLN:HE21	1.85	0.42
5:l:376:ASN:OD1	5:l:376:ASN:N	2.52	0.42
7:6:121:ALA:HB1	7:6:134:PHE:HB2	2.01	0.42
7:7:21:MET:HE3	7:7:75:VAL:H	1.85	0.42
1:K:22:LEU:HB3	1:G:13:ARG:HB2	2.01	0.42
5:S:401:MET:O	5:S:1052:ILE:N	2.46	0.42
5:S:465:HIS:CE1	5:S:1027:PRO:HD3	2.55	0.42
5:T:251:MET:HE3	5:T:251:MET:HB2	1.86	0.42
5:T:1321:LEU:HD12	5:T:1321:LEU:C	2.43	0.42
5:x:173:GLU:OE2	6:5:6:SER:N	2.45	0.42
6:e:200:LEU:HD12	6:e:200:LEU:HA	1.91	0.42
7:f:16:ASP:OD1	7:f:16:ASP:N	2.51	0.42
5:l:129:THR:OG1	5:l:130:GLU:N	2.52	0.42
5:l:193:ILE:HD11	5:l:1327:PHE:CD2	2.55	0.42
7:7:140:THR:HG21	7:7:283:ARG:HH22	1.85	0.42
1:G:44:ARG:CG	1:G:44:ARG:NH2	2.73	0.41
5:S:731:ASP:HA	5:S:796:LEU:HD13	2.01	0.41
5:T:147:THR:HB	5:T:150:GLU:HB2	2.02	0.41
5:T:967:VAL:HA	5:T:970:PHE:HB3	2.02	0.41
5:x:724:LEU:O	5:x:921:GLN:NE2	2.34	0.41
6:5:36:THR:HA	6:5:39:VAL:HG12	2.02	0.41
2:C:115:TYR:HD2	2:C:291:ILE:HD13	1.85	0.41
5:S:518:ILE:HD11	5:S:547:ASP:CG	2.45	0.41
5:S:937:THR:O	5:S:941:THR:OG1	2.34	0.41
5:S:1105:MET:HE2	5:S:1105:MET:HB3	1.95	0.41
5:T:866:ARG:NH2	5:T:870:GLU:OE2	2.43	0.41
5:T:1033:GLN:HG2	5:T:1038:ILE:HD11	2.02	0.41
5:W:399:ARG:HG2	5:W:1320:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:1246:GLN:HB2	5:W:1249:SER:HB3	2.01	0.41
5:x:810:LYS:O	5:x:814:TYR:HB2	2.20	0.41
5:x:1365:GLU:OE1	5:x:1371:ARG:NH2	2.52	0.41
7:6:57:TYR:HE2	7:6:191:PRO:HD3	1.84	0.41
7:7:10:SER:OG	7:7:11:SER:N	2.51	0.41
1:G:46:ALA:HB3	2:C:427:TYR:CD2	2.55	0.41
2:C:35:ARG:HH11	2:C:76:THR:HB	1.85	0.41
5:T:262:LYS:HB2	5:T:262:LYS:HE2	1.86	0.41
5:T:303:MET:O	5:T:364:ARG:NH1	2.49	0.41
5:T:1298:LEU:HD21	6:e:199:TYR:CD1	2.55	0.41
5:W:712:GLY:HA2	5:W:715:VAL:HG12	2.01	0.41
5:W:919:THR:OG1	5:W:996:TRP:NE1	2.54	0.41
5:x:550:ILE:HD13	5:x:560:HIS:CE1	2.55	0.41
7:g:225:ARG:HH22	7:g:249:ARG:HD2	1.86	0.41
7:6:49:TYR:O	7:6:118:ARG:NH1	2.52	0.41
2:C:10:LEU:HD13	2:C:61:PHE:CE2	2.56	0.41
5:S:61:ASN:HD22	5:W:22:LEU:HG	1.85	0.41
5:W:856:ILE:HG22	5:W:860:LEU:HB2	2.01	0.41
5:x:858:ASP:OD1	5:x:858:ASP:N	2.49	0.41
7:g:20:LYS:HE2	7:g:20:LYS:HB3	1.91	0.41
5:l:135:MET:HE3	5:l:135:MET:HB3	1.95	0.41
5:l:1001:MET:HE2	5:l:1001:MET:HB2	1.95	0.41
6:5:338:PHE:N	6:5:345:LEU:O	2.45	0.41
5:S:58:VAL:HG23	5:T:94:GLN:HB3	2.03	0.41
5:S:468:ALA:O	5:S:472:ASN:HB2	2.20	0.41
5:T:567:MET:H	5:T:570:ASN:HD22	1.67	0.41
5:x:1264:VAL:HG12	5:x:1266:GLY:H	1.86	0.41
5:l:1035:LYS:HD2	5:l:1035:LYS:HA	1.86	0.41
5:l:1374:LYS:HA	5:l:1374:LYS:HD2	1.86	0.41
5:T:387:MET:HE3	5:T:387:MET:HB3	1.73	0.41
5:W:487:TYR:OH	5:W:985:ARG:O	2.32	0.41
5:W:685:LYS:HA	5:W:685:LYS:HD3	1.81	0.41
5:W:1145:LYS:HA	5:W:1145:LYS:HD3	1.91	0.41
5:x:1042:VAL:HG11	5:x:1186:VAL:HG13	2.02	0.41
5:x:1051:GLU:HB3	5:x:1115:THR:HG23	2.02	0.41
7:6:108:SER:O	7:6:140:THR:OG1	2.30	0.41
7:7:30:PRO:HA	7:7:69:LEU:HA	2.02	0.41
7:7:287:ALA:HB2	7:7:299:TRP:HZ3	1.86	0.41
2:C:20:HIS:HB2	2:C:300:VAL:O	2.21	0.41
5:S:184:LYS:HD3	5:S:184:LYS:HA	1.93	0.41
5:x:506:PHE:CG	5:x:986:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:x:821:THR:O	5:x:823:ALA:N	2.51	0.41
5:x:1297:ARG:NH1	5:x:1299:GLY:H	2.19	0.41
6:e:158:LEU:HD23	6:e:158:LEU:HA	1.93	0.41
7:6:55:PRO:HB2	7:6:57:TYR:CZ	2.56	0.41
2:C:24:PRO:HB3	2:C:73:HIS:CE1	2.56	0.41
4:Z:60:TYR:CZ	5:T:635:MET:HG2	2.56	0.41
5:S:197:LEU:HD23	5:S:197:LEU:HA	1.89	0.41
5:S:1315:ALA:HB2	7:7:41:GLN:HB2	2.03	0.41
5:T:564:HIS:CD2	5:T:908:GLN:HG2	2.55	0.41
5:W:200:PRO:HA	5:W:203:THR:HG22	2.02	0.41
5:W:230:LEU:HB3	5:W:1109:ARG:HG3	2.03	0.41
5:W:465:HIS:O	5:W:546:TYR:OH	2.29	0.41
5:x:916:ASP:OD2	5:x:994:ARG:NH2	2.49	0.41
7:g:68:THR:OG1	7:g:69:LEU:N	2.54	0.41
5:l:91:GLY:O	5:l:122:CYS:N	2.48	0.41
5:l:385:GLN:NE2	5:l:389:ASN:OD1	2.44	0.41
5:l:386:LYS:HA	5:l:386:LYS:HD3	1.78	0.41
5:l:916:ASP:OD1	5:l:994:ARG:NH2	2.54	0.41
7:6:57:TYR:H	7:6:60:MET:HE3	1.85	0.41
2:C:338:GLU:HB3	2:C:399:TRP:HH2	1.86	0.41
4:2:57:TYR:OH	5:W:770:ASP:OD1	2.39	0.41
5:S:230:LEU:HD11	5:S:286:VAL:HG23	2.03	0.41
5:S:482:ASP:OD1	5:S:483:ARG:N	2.54	0.41
5:S:1276:ASN:HB3	5:S:1279:GLU:HG3	2.03	0.41
5:T:567:MET:HE1	5:T:997:HIS:HD2	1.85	0.41
5:W:215:LEU:HD23	5:W:215:LEU:HA	1.90	0.41
5:W:395:TYR:HE2	5:W:397:LEU:HD12	1.86	0.41
5:W:395:TYR:CE2	5:W:397:LEU:HD12	2.56	0.41
5:W:415:ASN:OD1	5:W:415:ASN:N	2.37	0.41
5:W:497:MET:HB3	5:W:497:MET:HE3	1.85	0.41
5:W:1327:PHE:HD2	5:W:1328:LEU:HG	1.86	0.41
5:x:193:ILE:HD13	5:x:1291:VAL:HG22	2.03	0.41
5:x:212:LYS:HE3	5:x:212:LYS:HB2	1.88	0.41
5:x:299:ASP:OD1	5:x:300:ASN:N	2.53	0.41
5:x:864:THR:HG21	4:y:8:PRO:HB3	2.02	0.41
6:e:116:SER:O	6:e:116:SER:OG	2.38	0.41
6:e:301:ILE:HD12	7:g:236:LEU:HD21	2.03	0.41
7:f:94:LYS:HA	7:f:295:THR:HA	2.02	0.41
5:l:408:PRO:HB3	5:l:1045:THR:HG22	2.03	0.41
5:l:443:LYS:HG2	5:l:1116:ASP:HA	2.02	0.41
5:l:1192:ASP:OD1	5:l:1195:TYR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:128:PRO:O	6:5:132:PHE:HB2	2.20	0.41
7:7:221:MET:HA	7:7:224:VAL:HG22	2.03	0.41
2:C:333:GLY:HA2	2:C:336:GLU:HB2	2.03	0.41
5:T:655:ALA:O	5:T:683:TYR:OH	2.29	0.41
5:W:825:MET:HB2	5:W:825:MET:HE3	1.79	0.41
5:x:503:VAL:O	5:x:507:TYR:HD1	2.04	0.41
5:x:890:THR:O	5:x:890:THR:OG1	2.33	0.41
5:x:1012:LEU:HA	5:x:1012:LEU:HD23	1.87	0.41
6:e:120:SER:OG	6:e:121:GLY:N	2.54	0.41
5:l:733:PHE:HD2	5:l:746:ILE:HD13	1.86	0.41
5:l:986:PRO:HG2	5:l:989:LEU:HB3	2.03	0.41
7:6:20:LYS:HB3	7:6:20:LYS:HE2	1.89	0.41
2:C:302:TYR:O	2:C:304:GLU:N	2.54	0.40
5:S:90:ASP:OD1	5:S:90:ASP:N	2.42	0.40
5:S:456:LEU:HD13	5:S:1031:ILE:HG12	2.02	0.40
5:T:733:PHE:HB3	5:T:746:ILE:HD13	2.02	0.40
5:T:1372:ILE:HD13	5:T:1372:ILE:HA	1.99	0.40
5:W:79:ASN:HB2	5:W:308:TYR:HD1	1.84	0.40
5:W:441:VAL:HG21	5:W:1335:LEU:HD23	2.02	0.40
5:x:466:THR:HG22	5:x:910:LEU:HB3	2.03	0.40
5:x:602:VAL:HA	5:x:605:THR:HG22	2.02	0.40
7:7:200:ALA:N	7:7:203:ASP:OD2	2.54	0.40
5:S:23:SER:OG	5:S:23:SER:O	2.39	0.40
5:S:481:ARG:NH1	5:S:536:ASP:O	2.53	0.40
5:T:95:PHE:HD2	5:T:118:VAL:HG13	1.86	0.40
5:T:294:LEU:HA	5:T:294:LEU:HD23	1.84	0.40
5:T:440:ILE:HD11	5:T:1119:ILE:HG23	2.03	0.40
5:T:1279:GLU:HA	5:T:1282:ARG:HB2	2.03	0.40
5:l:372:ILE:HD12	5:l:374:LEU:HD21	2.03	0.40
5:l:937:THR:O	5:l:941:THR:OG1	2.31	0.40
7:7:17:GLU:HA	7:7:20:LYS:HG2	2.03	0.40
2:C:290:HIS:HB2	2:C:297:LEU:HD23	2.03	0.40
5:S:733:PHE:HD2	5:S:746:ILE:HD13	1.85	0.40
5:W:510:LYS:O	5:W:973:ARG:NH2	2.38	0.40
5:W:1105:MET:HE2	5:W:1105:MET:HB3	1.95	0.40
5:x:408:PRO:HG3	5:x:1196:PHE:CG	2.56	0.40
5:x:837:GLN:HA	4:y:49:VAL:HG11	2.02	0.40
5:x:859:ASN:OD1	5:x:859:ASN:N	2.53	0.40
6:e:289:ILE:HD12	6:e:289:ILE:HA	1.81	0.40
7:f:184:HIS:HB3	7:f:186:TYR:CZ	2.56	0.40
7:f:234:ASP:OD1	7:f:234:ASP:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:16:ILE:HD13	6:5:16:ILE:HA	1.94	0.40
7:6:112:MET:N	7:6:136:MET:O	2.54	0.40
5:S:1113:ILE:HG21	5:S:1117:MET:HE3	2.04	0.40
5:S:1342:LEU:HA	5:S:1342:LEU:HD23	1.90	0.40
5:T:794:LEU:HD13	5:T:794:LEU:HA	1.96	0.40
5:T:936:ARG:HD2	5:T:936:ARG:HA	1.90	0.40
5:W:672:ASN:HB2	5:x:873:ASP:HB2	2.04	0.40
7:f:20:LYS:HE3	7:f:20:LYS:HB2	1.80	0.40
7:f:289:TYR:HD1	7:f:296:ALA:HB2	1.86	0.40
5:l:127:ILE:CD1	5:l:175:GLY:C	2.89	0.40
5:l:844:PRO:HB3	5:l:850:PHE:HB2	2.04	0.40
7:7:293:THR:HB	7:7:295:THR:HG22	2.04	0.40
1:K:81:ALA:HB2	3:O:3135:HIS:HE1	1.86	0.40
1:K:84:ILE:HD13	1:K:84:ILE:HA	1.94	0.40
2:C:88:LEU:HA	2:C:89:PRO:HD3	1.93	0.40
4:Y:49:VAL:HG11	5:S:837:GLN:HA	2.04	0.40
5:S:706:VAL:HG23	5:S:711:VAL:HG12	2.04	0.40
5:T:957:PRO:HA	5:T:960:ALA:HB3	2.03	0.40
5:W:643:CYS:HA	5:W:646:THR:HG22	2.04	0.40
5:x:33:LEU:HB2	5:x:55:LEU:HD22	2.03	0.40
5:x:209:LYS:NZ	5:x:1211:SER:O	2.46	0.40
5:x:740:SER:OG	5:x:742:ARG:O	2.34	0.40
6:e:130:SER:HB3	6:e:159:TYR:CZ	2.56	0.40
7:g:198:GLY:HA2	7:g:203:ASP:HB2	2.03	0.40
5:l:565:ARG:HH11	5:l:571:LEU:HD23	1.86	0.40
5:l:693:LEU:HD13	5:l:693:LEU:HA	1.94	0.40
5:l:898:VAL:HG13	5:l:923:VAL:HG13	2.03	0.40
5:l:940:VAL:HG13	5:l:941:THR:HG23	2.03	0.40
7:7:150:ILE:HG23	7:7:202:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	82/570 (14%)	74 (90%)	8 (10%)	0	100	100
1	K	66/570 (12%)	65 (98%)	1 (2%)	0	100	100
2	C	334/507 (66%)	318 (95%)	16 (5%)	0	100	100
3	B	33/3149 (1%)	33 (100%)	0	0	100	100
3	O	27/3149 (1%)	26 (96%)	1 (4%)	0	100	100
4	2	72/176 (41%)	61 (85%)	11 (15%)	0	100	100
4	Y	72/176 (41%)	66 (92%)	6 (8%)	0	100	100
4	Z	72/176 (41%)	67 (93%)	5 (7%)	0	100	100
4	m	69/176 (39%)	66 (96%)	3 (4%)	0	100	100
4	y	72/176 (41%)	62 (86%)	10 (14%)	0	100	100
5	S	1319/1381 (96%)	1236 (94%)	83 (6%)	0	100	100
5	T	1301/1381 (94%)	1201 (92%)	100 (8%)	0	100	100
5	W	1321/1381 (96%)	1226 (93%)	95 (7%)	0	100	100
5	l	1236/1381 (90%)	1162 (94%)	74 (6%)	0	100	100
5	x	1321/1381 (96%)	1227 (93%)	94 (7%)	0	100	100
6	5	305/364 (84%)	288 (94%)	17 (6%)	0	100	100
6	e	311/364 (85%)	291 (94%)	20 (6%)	0	100	100
7	6	293/301 (97%)	280 (96%)	13 (4%)	0	100	100
7	7	281/301 (93%)	254 (90%)	26 (9%)	1 (0%)	30	66
7	f	286/301 (95%)	272 (95%)	14 (5%)	0	100	100
7	g	282/301 (94%)	259 (92%)	23 (8%)	0	100	100
All	All	9155/17662 (52%)	8534 (93%)	620 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	7	101	PHE

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	G	70/465 (15%)	68 (97%)	2 (3%)	37	58
1	K	59/465 (13%)	59 (100%)	0	100	100
2	C	288/400 (72%)	281 (98%)	7 (2%)	43	63
3	B	33/2539 (1%)	33 (100%)	0	100	100
3	O	27/2539 (1%)	27 (100%)	0	100	100
4	2	68/128 (53%)	67 (98%)	1 (2%)	57	70
4	Y	68/128 (53%)	68 (100%)	0	100	100
4	Z	68/128 (53%)	67 (98%)	1 (2%)	57	70
4	m	66/128 (52%)	63 (96%)	3 (4%)	24	47
4	y	68/128 (53%)	67 (98%)	1 (2%)	57	70
5	S	1133/1171 (97%)	1129 (100%)	4 (0%)	84	82
5	T	1111/1171 (95%)	1104 (99%)	7 (1%)	78	80
5	W	1132/1171 (97%)	1125 (99%)	7 (1%)	78	80
5	l	1069/1171 (91%)	1062 (99%)	7 (1%)	76	79
5	x	1125/1171 (96%)	1115 (99%)	10 (1%)	70	76
6	5	264/289 (91%)	263 (100%)	1 (0%)	84	82
6	e	268/289 (93%)	267 (100%)	1 (0%)	84	82
7	6	264/267 (99%)	264 (100%)	0	100	100
7	7	256/267 (96%)	255 (100%)	1 (0%)	84	82
7	f	259/267 (97%)	258 (100%)	1 (0%)	84	82
7	g	256/267 (96%)	254 (99%)	2 (1%)	73	77
All	All	7952/14549 (55%)	7896 (99%)	56 (1%)	73	79

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	41	LEU
1	G	44	ARG
2	C	7	ASN
2	C	82	VAL
2	C	109	VAL
2	C	315	THR
2	C	426	LEU
2	C	427	TYR
2	C	453	LEU
4	m	4	ARG

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Mol	Chain	Res	Type
4	m	5	LEU
4	m	33	ASN
4	Z	67	VAL
4	2	67	VAL
5	S	266	THR
5	S	592	THR
5	S	751	GLU
5	S	1349	VAL
5	T	54	VAL
5	T	78	VAL
5	T	675	ILE
5	T	839	LEU
5	T	1210	VAL
5	T	1320	PHE
5	T	1369	VAL
5	W	7	VAL
5	W	371	VAL
5	W	415	ASN
5	W	705	VAL
5	W	948	ILE
5	W	1088	VAL
5	W	1380	VAL
5	x	58	VAL
5	x	79	ASN
5	x	93	ILE
5	x	384	LEU
5	x	508	ASP
5	x	542	LEU
5	x	621	VAL
5	x	675	ILE
5	x	923	VAL
5	x	1369	VAL
4	y	67	VAL
6	e	199	TYR
7	f	54	VAL
7	g	197	LEU
7	g	280	LEU
5	l	99	VAL
5	l	279	VAL
5	l	675	ILE
5	l	1110	VAL
5	l	1119	ILE

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Mol	Chain	Res	Type
5	1	1250	LEU
5	1	1369	VAL
6	5	6	SER
7	7	251	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (176) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	63	ASN
1	G	30	ASN
1	G	63	ASN
2	C	7	ASN
2	C	20	HIS
2	C	38	ASN
2	C	73	HIS
2	C	410	ASN
2	C	486	GLN
3	B	3135	HIS
4	m	54	GLN
4	Y	28	GLN
4	Y	37	ASN
4	Z	33	ASN
4	2	11	GLN
4	2	44	GLN
4	2	54	GLN
4	2	71	GLN
5	S	24	ASN
5	S	64	GLN
5	S	113	GLN
5	S	442	ASN
5	S	445	ASN
5	S	498	ASN
5	S	531	HIS
5	S	534	ASN
5	S	543	HIS
5	S	560	HIS
5	S	564	HIS
5	S	581	GLN
5	S	596	HIS
5	S	600	GLN
5	S	627	HIS
5	S	636	ASN

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Mol	Chain	Res	Type
5	S	672	ASN
5	S	750	ASN
5	S	822	ASN
5	S	921	GLN
5	S	951	HIS
5	S	988	GLN
5	S	1089	HIS
5	S	1137	GLN
5	S	1241	ASN
5	S	1289	ASN
5	S	1353	HIS
5	T	226	HIS
5	T	317	ASN
5	T	398	ASN
5	T	429	ASN
5	T	432	GLN
5	T	465	HIS
5	T	469	HIS
5	T	475	ASN
5	T	531	HIS
5	T	534	ASN
5	T	543	HIS
5	T	570	ASN
5	T	750	ASN
5	T	785	ASN
5	T	837	GLN
5	T	842	ASN
5	T	859	ASN
5	T	904	ASN
5	T	965	GLN
5	T	997	HIS
5	T	1033	GLN
5	T	1089	HIS
5	T	1136	GLN
5	T	1139	ASN
5	T	1214	ASN
5	T	1246	GLN
5	T	1261	GLN
5	T	1276	ASN
5	T	1283	ASN
5	T	1329	GLN
5	T	1360	HIS

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Mol	Chain	Res	Type
5	W	142	HIS
5	W	432	GLN
5	W	472	ASN
5	W	498	ASN
5	W	534	ASN
5	W	596	HIS
5	W	607	GLN
5	W	669	HIS
5	W	750	ASN
5	W	761	GLN
5	W	790	HIS
5	W	824	HIS
5	W	926	ASN
5	W	964	HIS
5	W	965	GLN
5	W	984	ASN
5	W	1136	GLN
5	W	1139	ASN
5	W	1197	GLN
5	W	1246	GLN
5	W	1329	GLN
5	W	1360	HIS
5	x	113	GLN
5	x	126	HIS
5	x	285	ASN
5	x	389	ASN
5	x	415	ASN
5	x	509	ASN
5	x	534	ASN
5	x	543	HIS
5	x	581	GLN
5	x	722	ASN
5	x	750	ASN
5	x	804	HIS
5	x	824	HIS
5	x	842	ASN
5	x	974	ASN
5	x	997	HIS
5	x	1022	HIS
5	x	1056	ASN
5	x	1089	HIS
5	x	1122	GLN

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Mol	Chain	Res	Type
5	x	1139	ASN
5	x	1283	ASN
5	x	1284	ASN
5	x	1289	ASN
5	x	1306	ASN
5	x	1310	GLN
5	x	1351	GLN
4	y	54	GLN
6	e	46	HIS
6	e	136	ASN
6	e	137	HIS
6	e	227	GLN
6	e	286	HIS
6	e	291	ASN
7	f	35	HIS
7	f	41	GLN
7	f	89	GLN
7	f	120	HIS
7	f	128	ASN
7	f	175	HIS
7	f	240	GLN
7	g	23	GLN
7	g	35	HIS
7	g	41	GLN
7	g	62	ASN
7	g	89	GLN
7	g	148	GLN
7	g	154	ASN
7	g	173	HIS
5	l	195	GLN
5	l	226	HIS
5	l	402	GLN
5	l	472	ASN
5	l	490	GLN
5	l	509	ASN
5	l	586	GLN
5	l	636	ASN
5	l	673	ASN
5	l	750	ASN
5	l	768	ASN
5	l	904	ASN
5	l	926	ASN

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Mol	Chain	Res	Type
5	1	977	GLN
5	1	997	HIS
5	1	1039	HIS
5	1	1056	ASN
5	1	1289	ASN
6	5	28	ASN
6	5	102	ASN
6	5	194	ASN
6	5	208	HIS
6	5	309	GLN
6	5	356	ASN
7	6	148	GLN
7	6	166	ASN
7	7	62	ASN
7	7	204	ASN
7	7	230	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

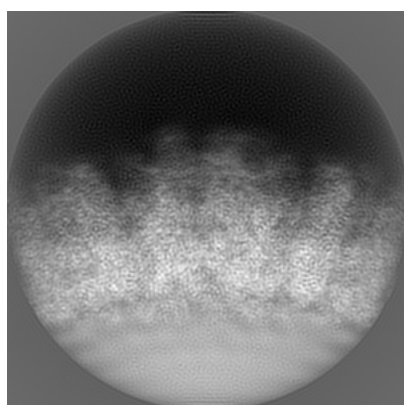
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30158. These allow visual inspection of the internal detail of the map and identification of artifacts.

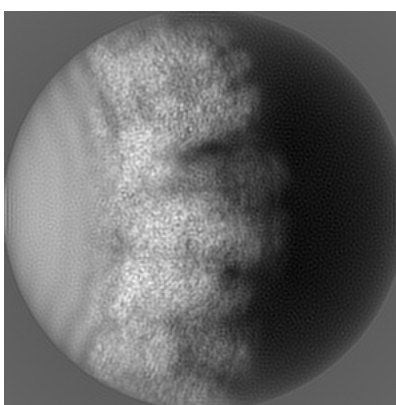
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

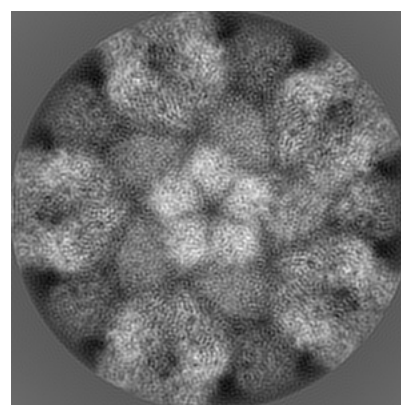
6.1.1 Primary map



X



Y

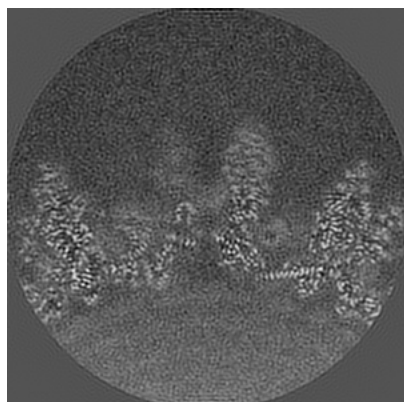


Z

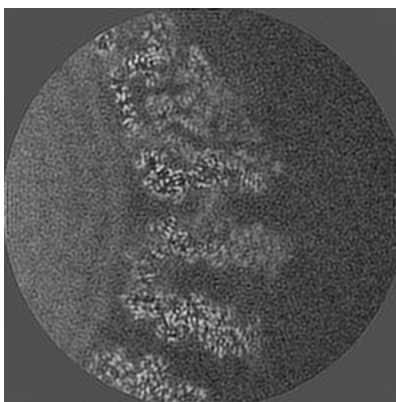
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

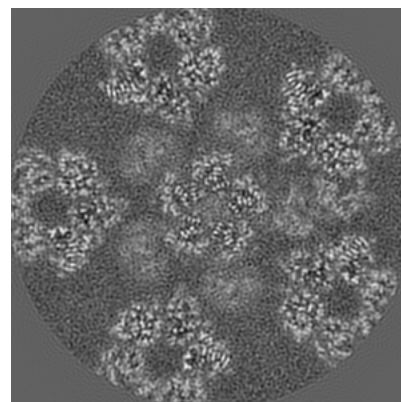
6.2.1 Primary map



X Index: 150



Y Index: 150

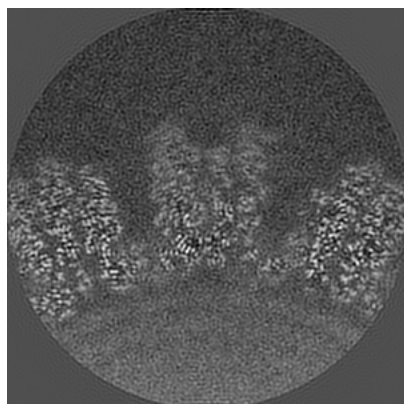


Z Index: 150

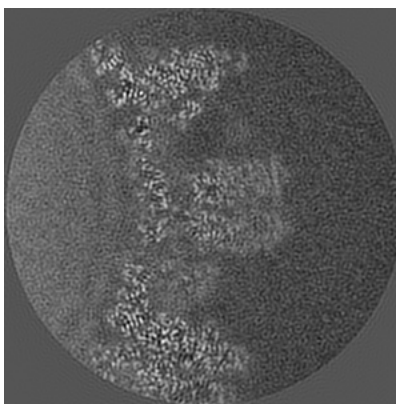
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

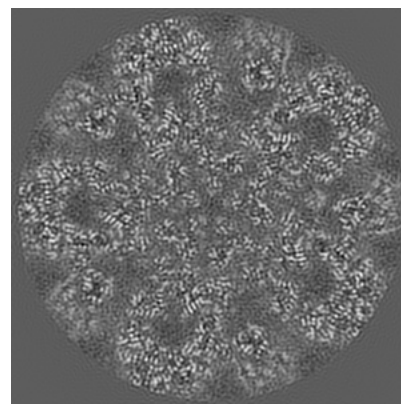
6.3.1 Primary map



X Index: 137



Y Index: 122

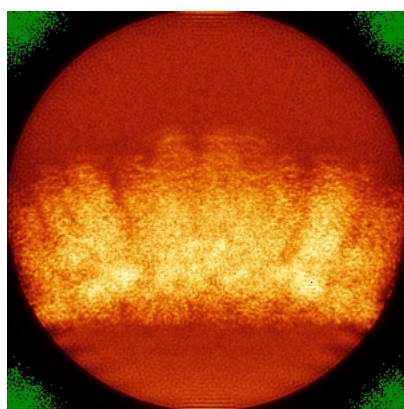


Z Index: 107

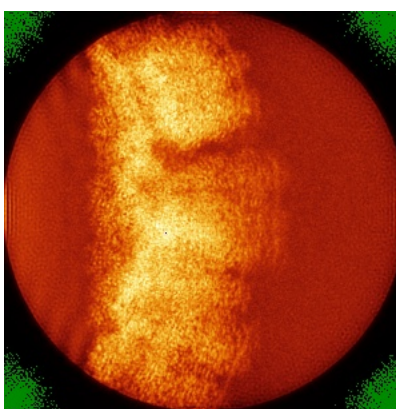
The images above show the largest variance slices of the map in three orthogonal directions.

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

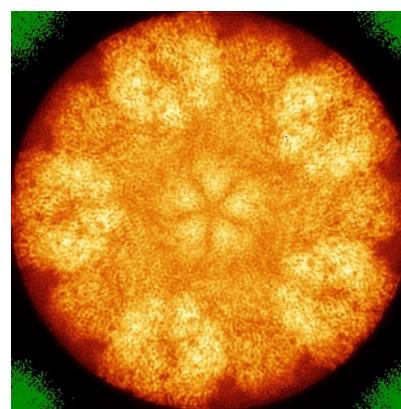
6.4.1 Primary map



X



Y

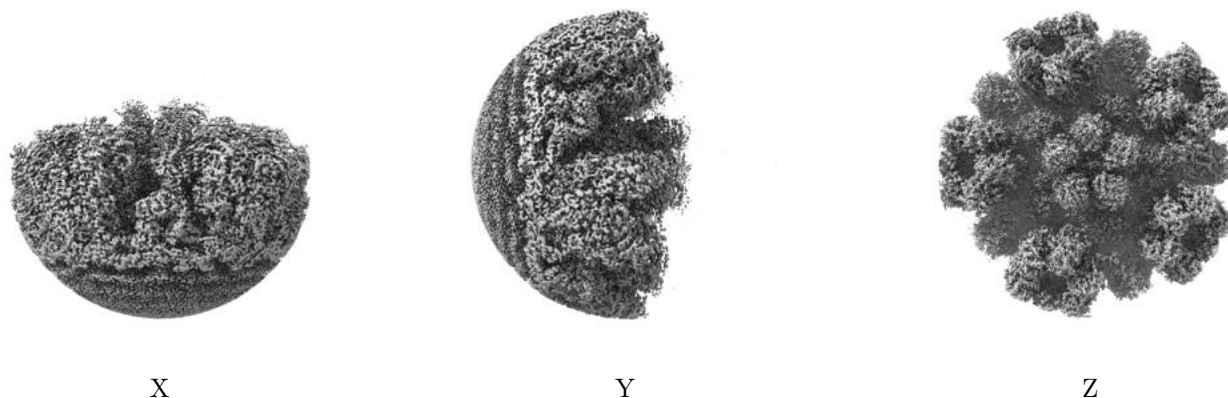


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

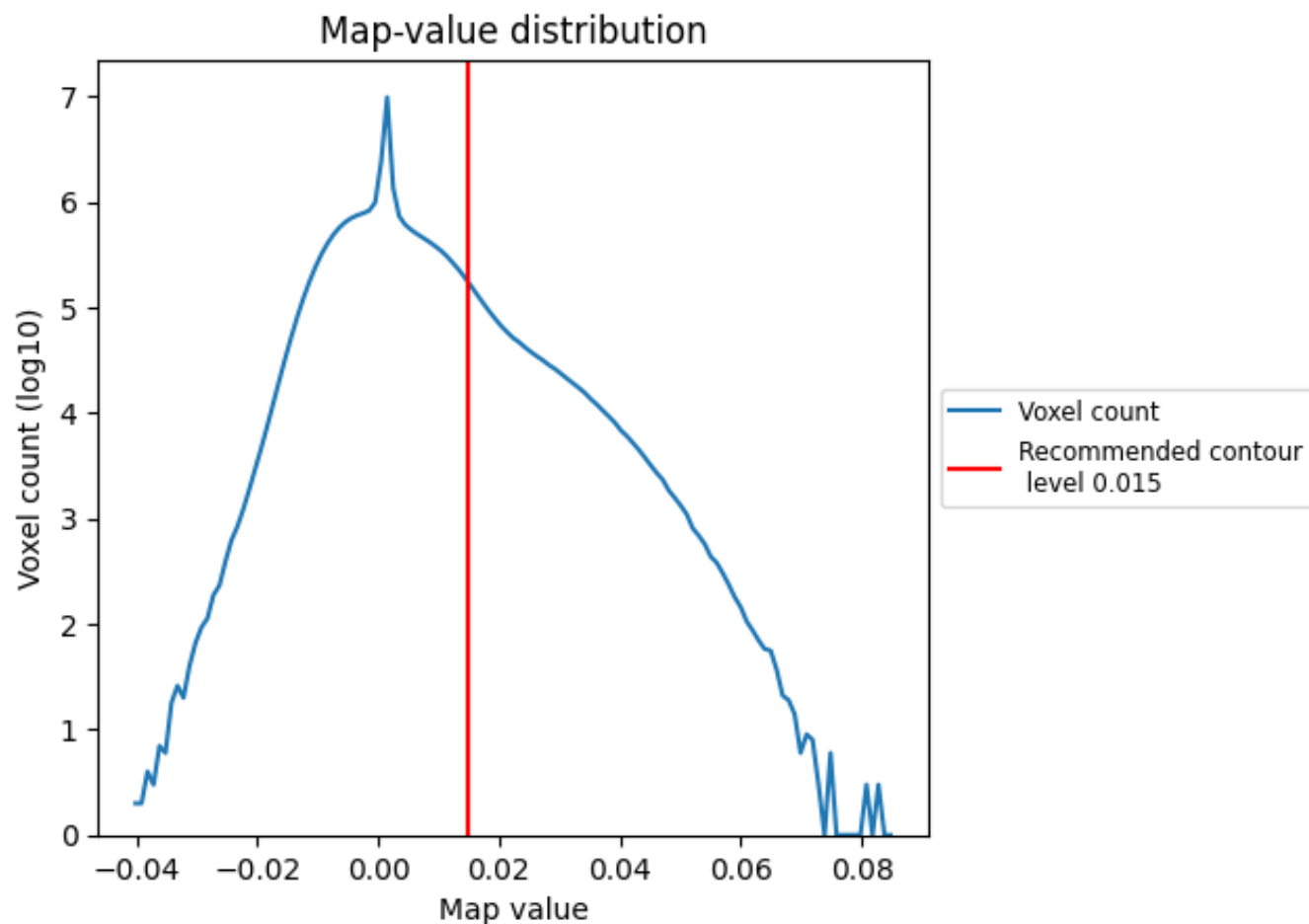
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

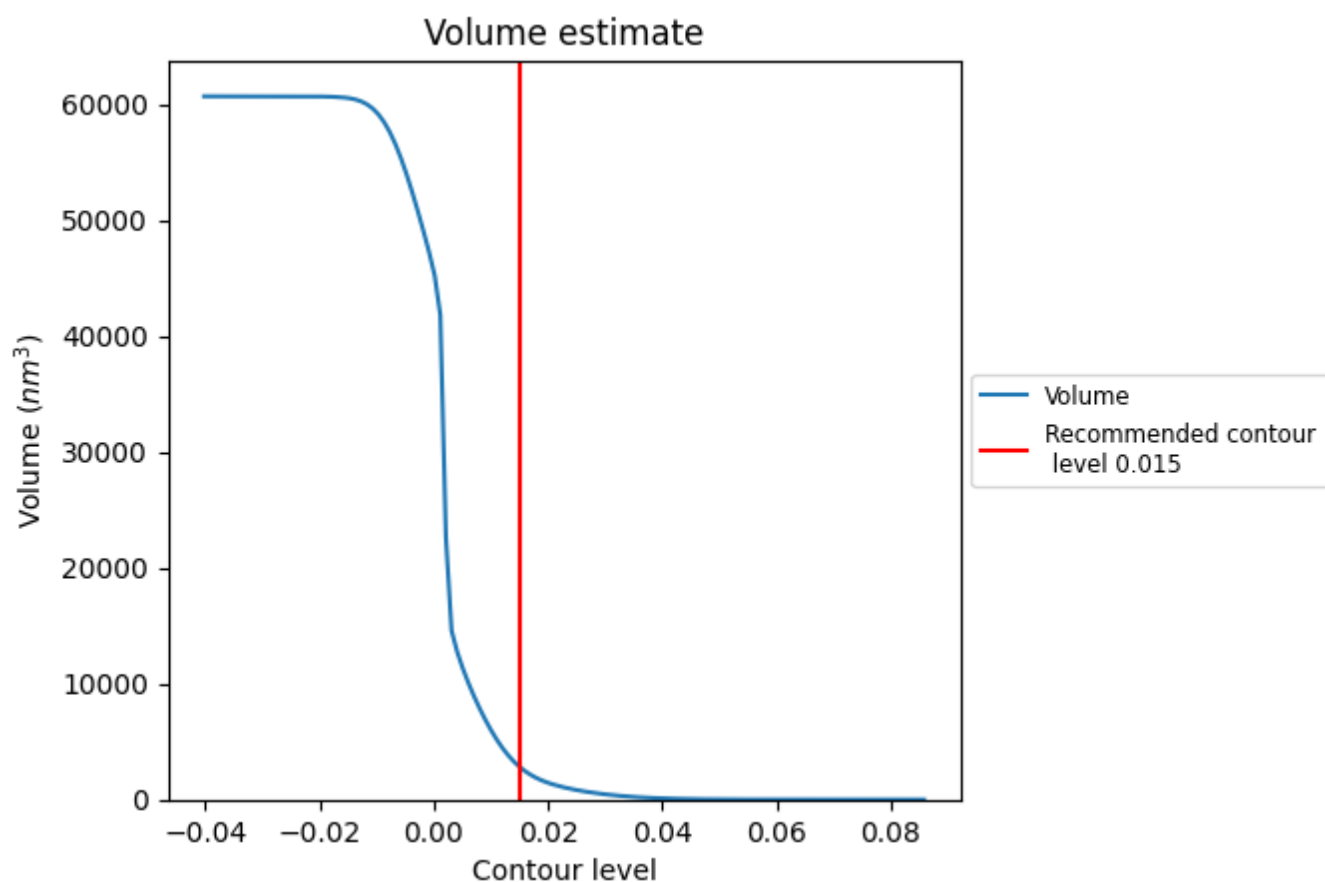
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

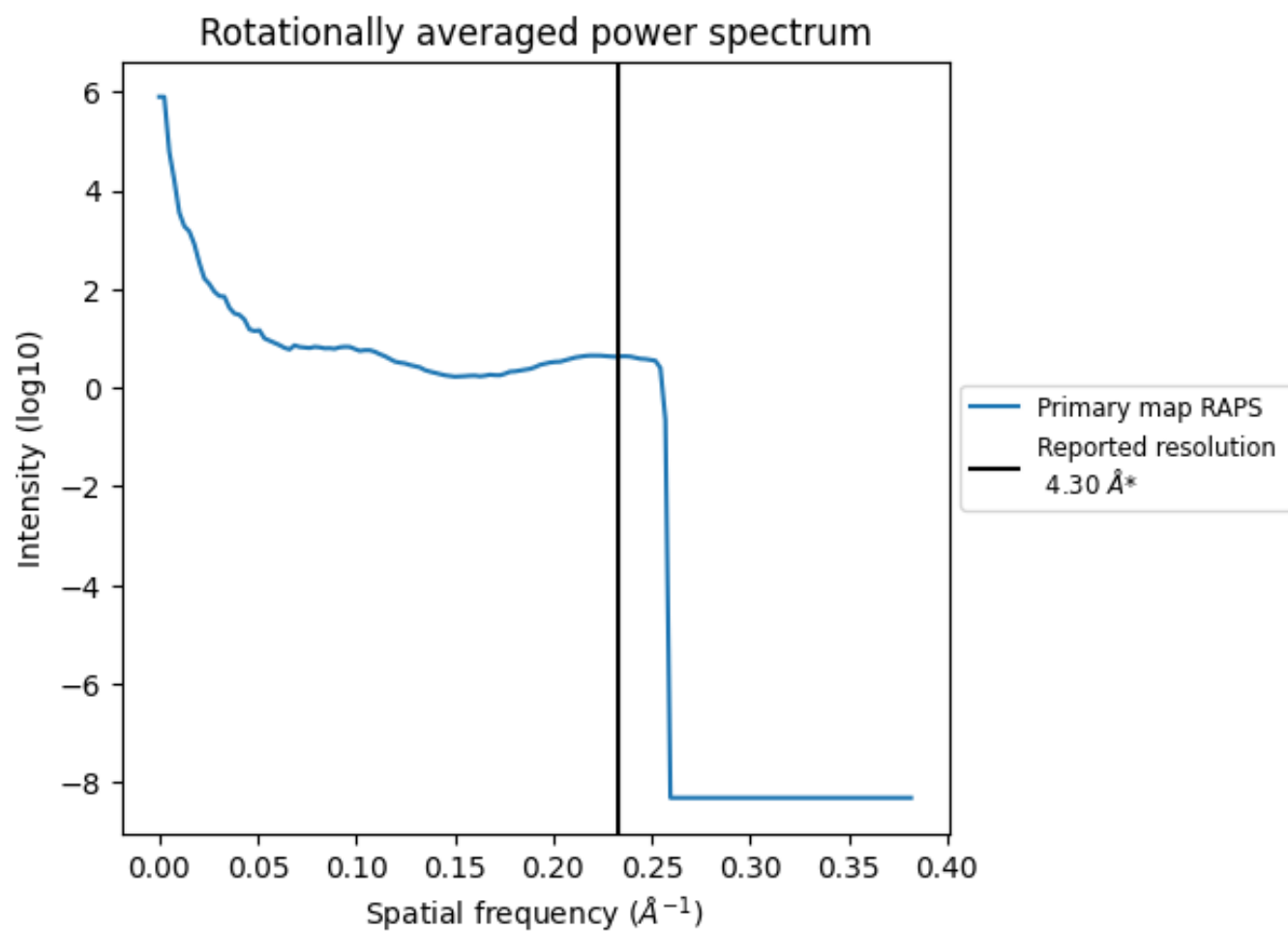
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2834 nm³; this corresponds to an approximate mass of 2560 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 0.233 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

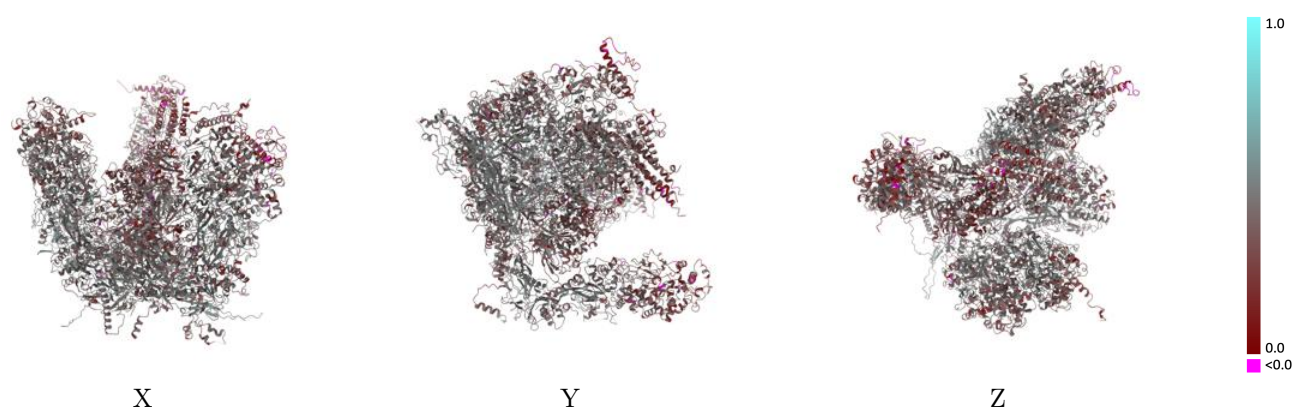
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30158 and PDB model 7BR7. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

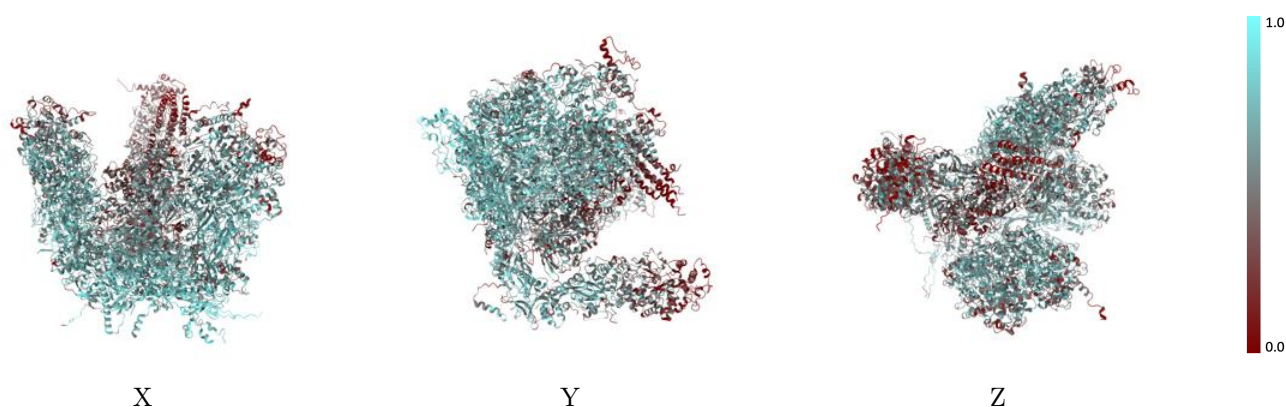
This section was not generated.

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



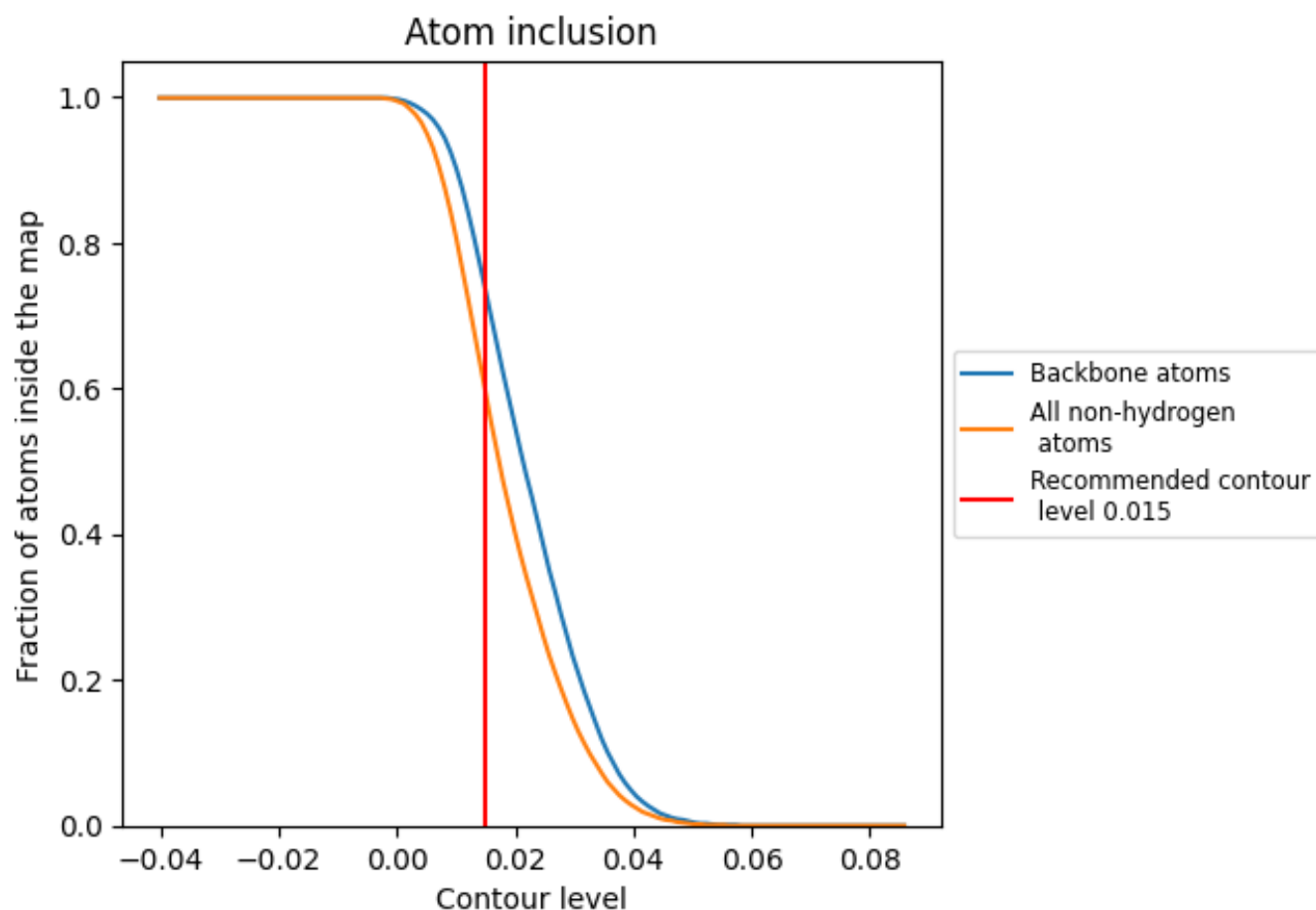
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 59% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5910	 0.4010
2	 0.2020	 0.1920
5	 0.5120	 0.3760
6	 0.3890	 0.3170
7	 0.3490	 0.2900
B	 0.1190	 0.2240
C	 0.4190	 0.3250
G	 0.3320	 0.3020
K	 0.3780	 0.3370
O	 0.1660	 0.2240
S	 0.6400	 0.4260
T	 0.6870	 0.4350
W	 0.6850	 0.4260
Y	 0.3530	 0.3450
Z	 0.3430	 0.3240
e	 0.7250	 0.4360
f	 0.6330	 0.3990
g	 0.6470	 0.4090
l	 0.5110	 0.3890
m	 0.1140	 0.2250
x	 0.6800	 0.4410
y	 0.4080	 0.3350

