



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:00 PM UTC

PDB ID : 7ETO / pdb_00007eto
EMDB ID : EMD-31301
Title : C1 CVSC-binding penton vertex in the virion capsid of Human Cytomegalovirus
Authors : Li, Z.; Yu, X.
Deposited on : 2021-05-13
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

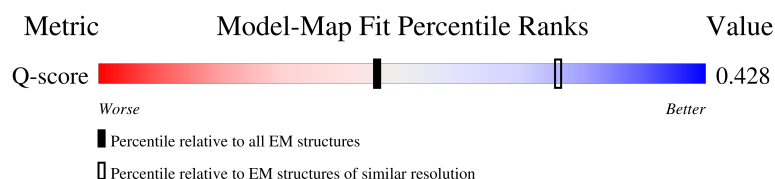
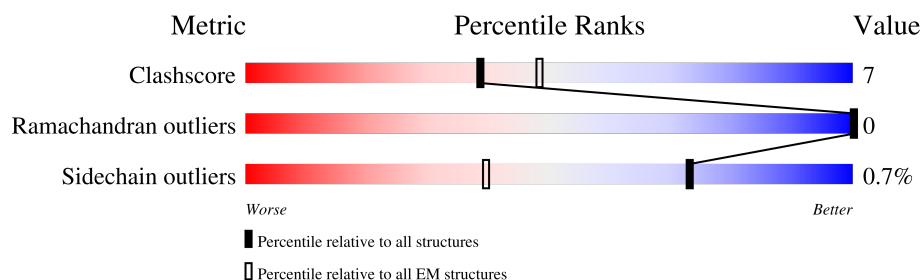
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	7587 (3.50 - 4.50)

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	1	1048	13% 22% 5% 73%
1	x	1048	11% 22% 5% 73%
2	I	306	18% 80% 17% .
2	h	306	8% 77% 21% .

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Mol	Chain	Length	Quality of chain
2	n	306	
2	o	306	
3	H	2241	
3	P	2241	
4	g	290	
4	m	290	
5	M	594	
6	N	642	
6	O	642	
7	Q	75	
7	R	75	
7	S	75	
7	T	75	
7	i	75	
7	j	75	
8	A	1370	
8	B	1370	
8	C	1370	
8	D	1370	
8	Y	1370	
8	Z	1370	
8	a	1370	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 98674 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 ORFL92C_UL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	x	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		
1	1	285	Total	C	N	O	S	0	0
			2328	1468	426	421	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	h	302	Total	C	N	O	S	0	0
			2398	1536	418	427	17		
2	I	296	Total	C	N	O	S	0	0
			2349	1506	409	417	17		
2	n	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
2	o	289	Total	C	N	O	S	0	0
			2291	1473	393	407	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	20	Total	C	N	O	S	0	0
			172	110	32	29	1		
3	P	20	Total	C	N	O	S	0	0
			172	110	32	29	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	468	Total	C	N	O	S	0	0
			3848	2408	740	686	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	66	Total	C	N	O	S	0	0
			558	346	111	97	4		
6	O	69	Total	C	N	O	S	0	0
			589	371	113	102	3		

- Molecule 7 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	T	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	i	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	j	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 8 is a protein called Major capsid protein.

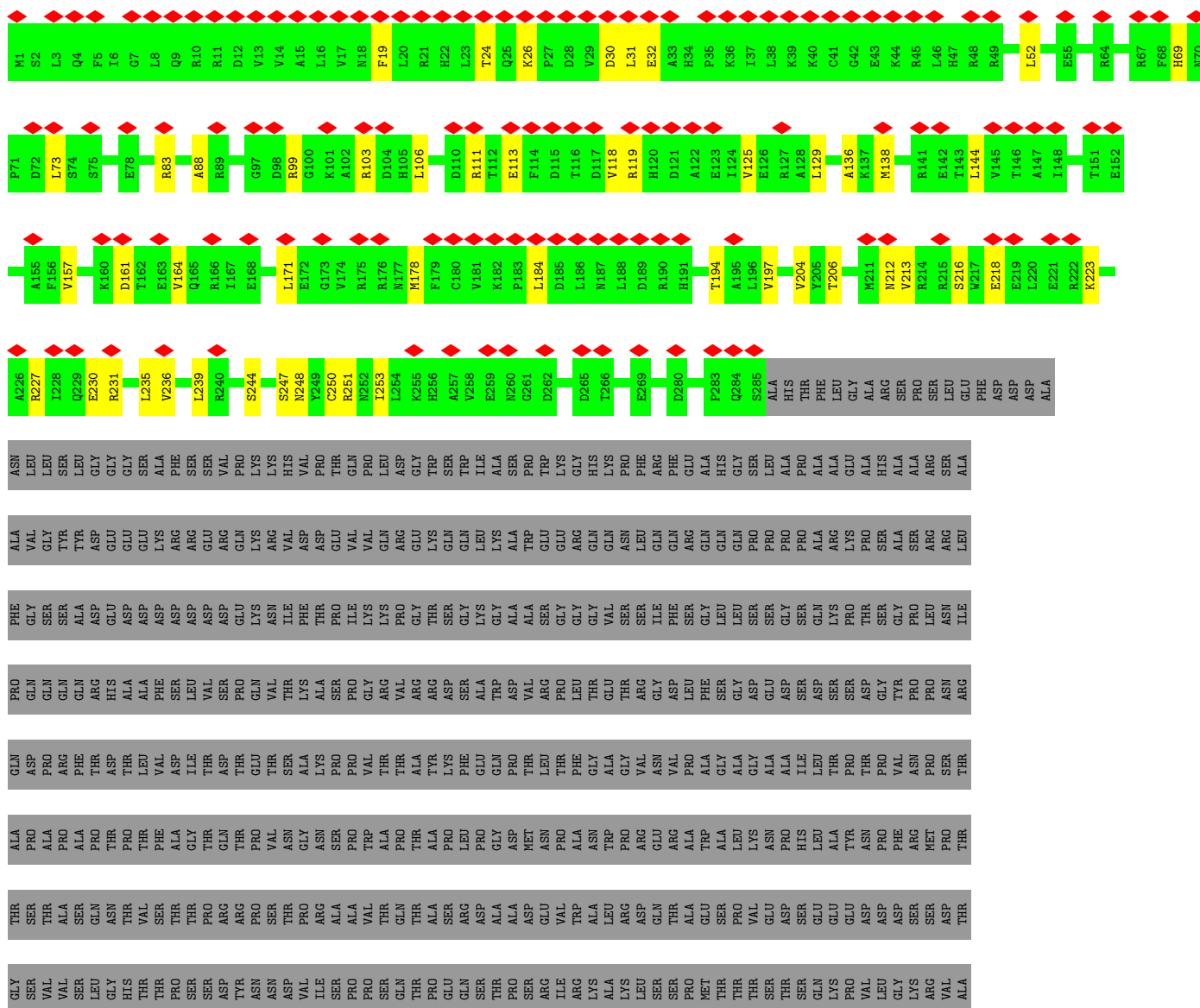
Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	1297	Total	C	N	O	S	0	0
			10260	6526	1785	1890	59		
8	A	1271	Total	C	N	O	S	0	0
			10096	6446	1746	1847	57		
8	B	1335	Total	C	N	O	S	0	0
			10574	6733	1830	1950	61		
8	C	1331	Total	C	N	O	S	0	0
			10549	6718	1831	1939	61		
8	D	1297	Total	C	N	O	S	0	0
			10269	6538	1785	1887	59		
8	Y	1347	Total	C	N	O	S	0	0
			10676	6799	1850	1966	61		

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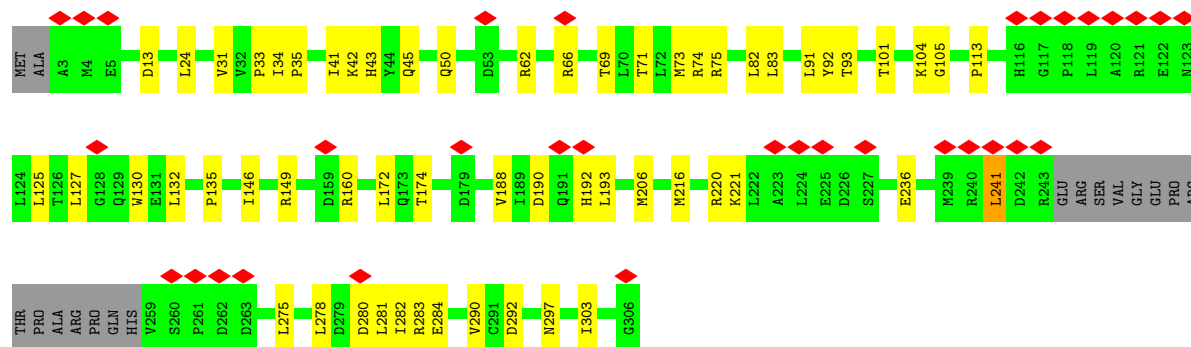
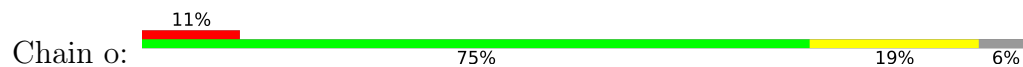
Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	1333	Total	C	N	O	S	0	0
			10551	6720	1827	1945	59		

- Molecule 1: ORFL92C UL32

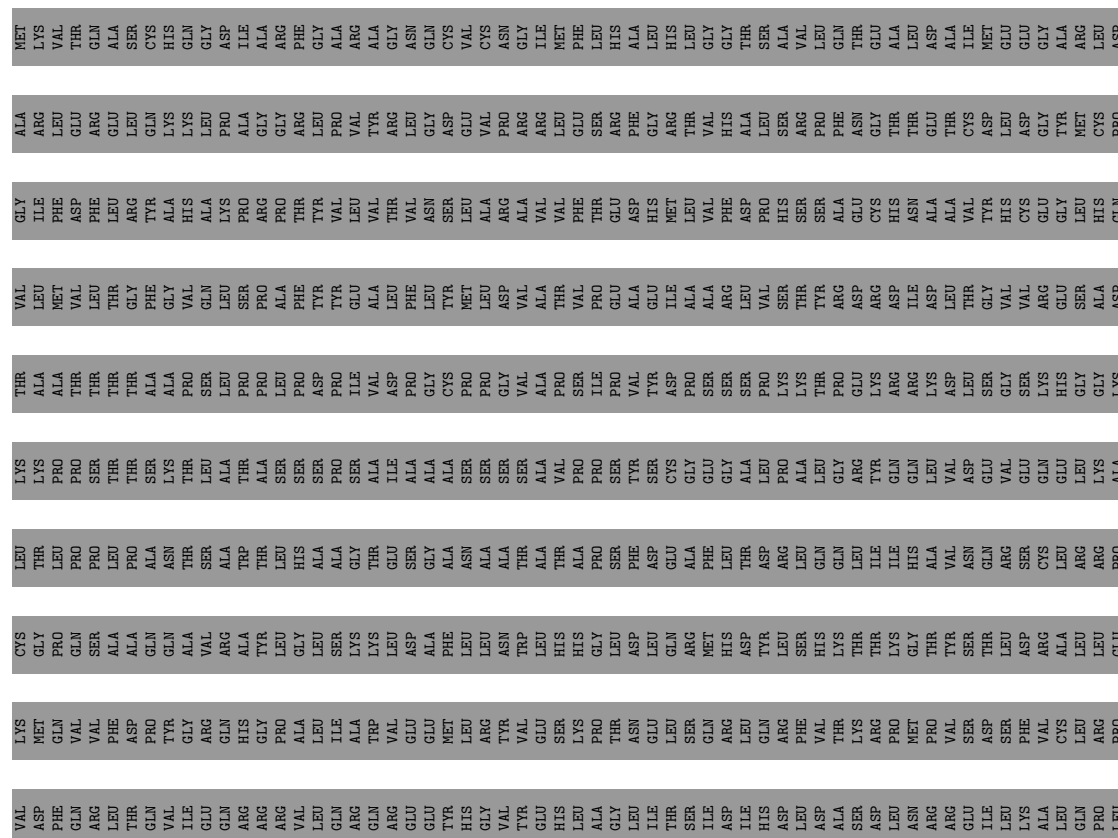




• Molecule 2: Triplex capsid protein 2



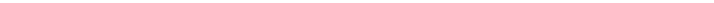
• Molecule 3: Large tegument protein deneddylase





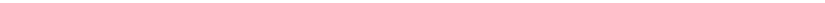


L2221	R2222	Q2223	L2224	A2225	Q2226	S2227	V2228	Q2229	D2230	T2231	I2232	Q2233	H2234	M2235	R2236	F2237	L2240	LEU
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----

Chain g: 

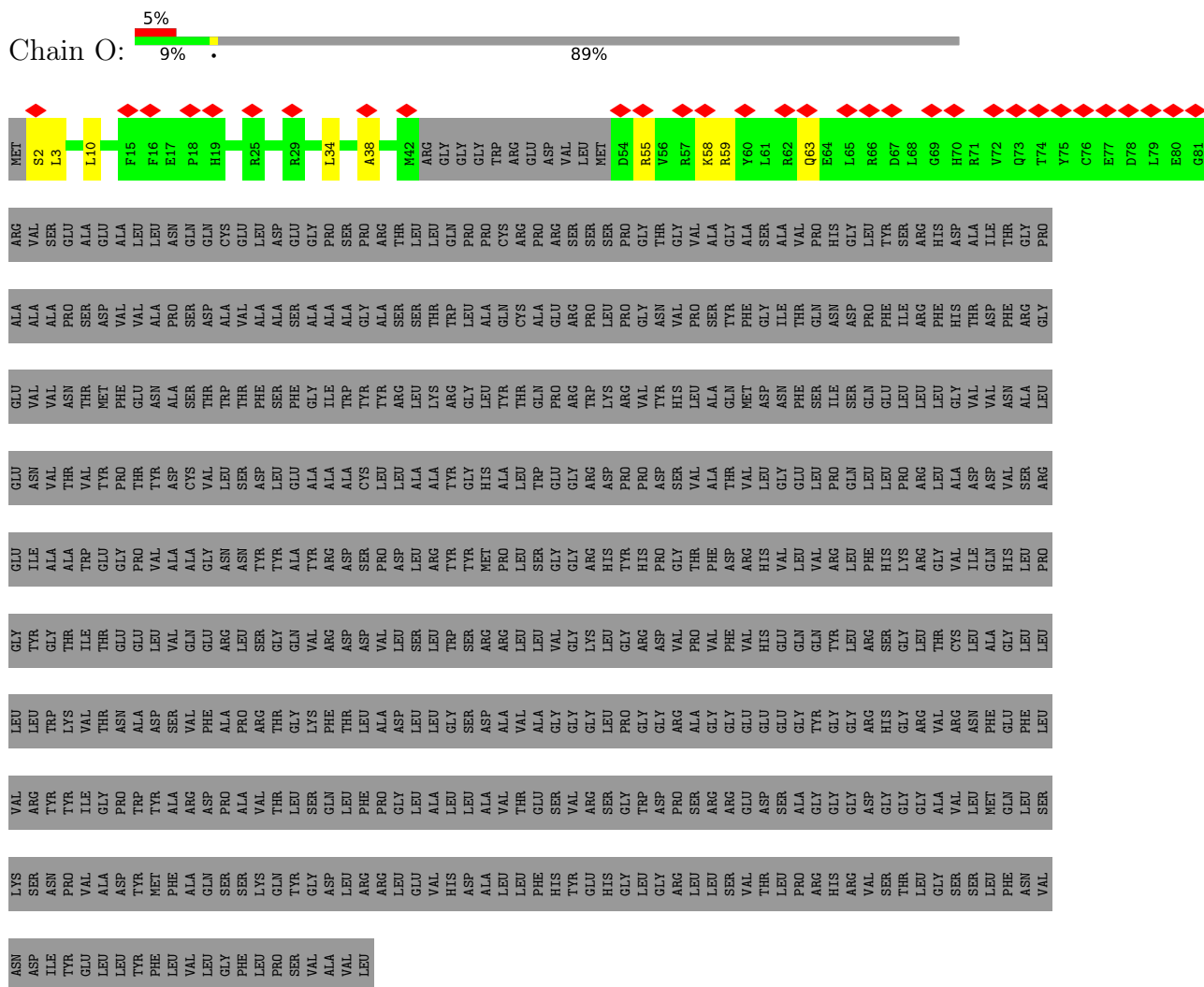
[illegible]

G195 P196 E197 L205 H211 H212 Q213 D217 R220 R227 R233 R234 T235 T236 R237 P238 R239 R240 T241 P242 T245 K250 L251 D257 D258 I259 H260 T261 SER PHE LEU VAL HIS LYS GLU LEU LYS LEU SER V273 D277 E282 L283 F286 I290

Chain m:  9% 82% 18%

M1	C134
R4	V135
K3	K136
R11	T137
D12	T147
P13	C148
A14	V149
D15	K159
E16	D170
D17	E176
A23	E177
V35	Q183
R36	Y184
L38	V185
Y39	I188
H40	D192
A41	Y193
D42	D194
R49	G195
E54	P196
A61	E197
R69	T198
M70	R199
E71	H211
D75	W212
S76	Q213
H79	R220
T89	R234
R90	R239
A91	Q240
S92	T241
N93	P242
R99	T245
G100	G246
L101	V247
S104	L248
L115	Q249
H126	K250
E130	L251
T131	A256
L132	S262
G133	F263
	L269
	D277

- Molecule 6: Capsid vertex component 2

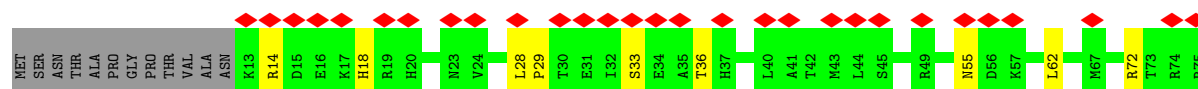
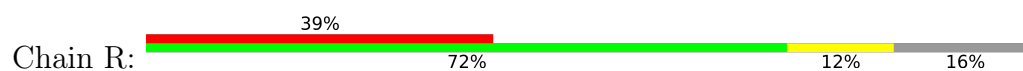


- Molecule 7: Small capsomere-interacting protein

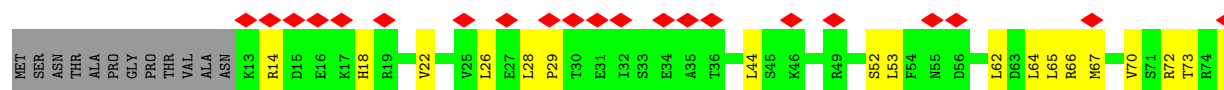




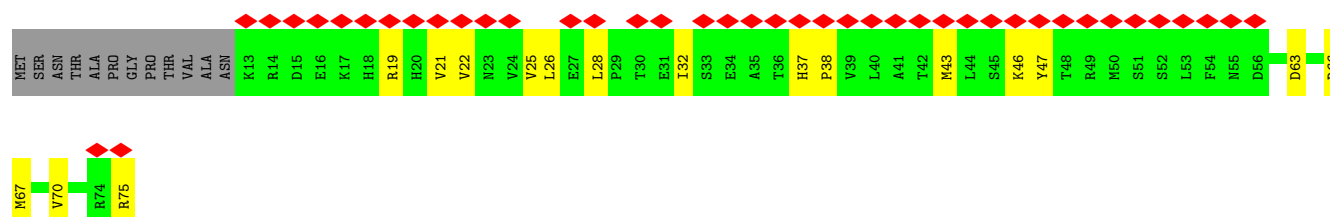
• Molecule 7: Small capsomere-interacting protein



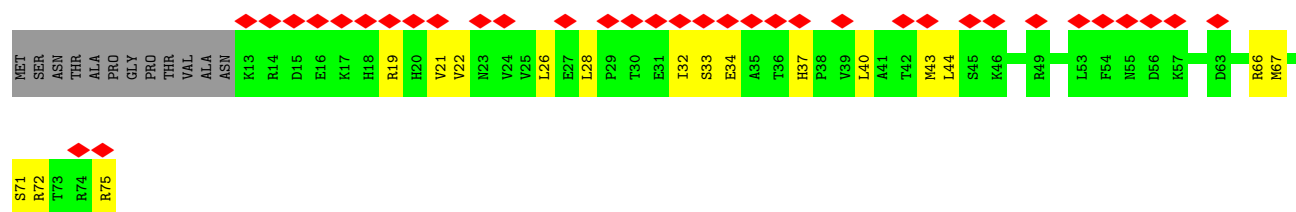
• Molecule 7: Small capsomere-interacting protein



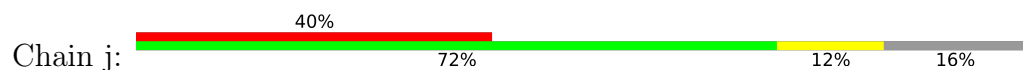
• Molecule 7: Small capsomere-interacting protein

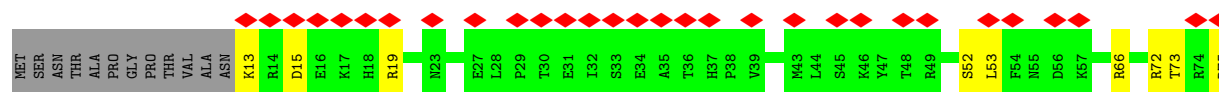


• Molecule 7: Small capsomere-interacting protein

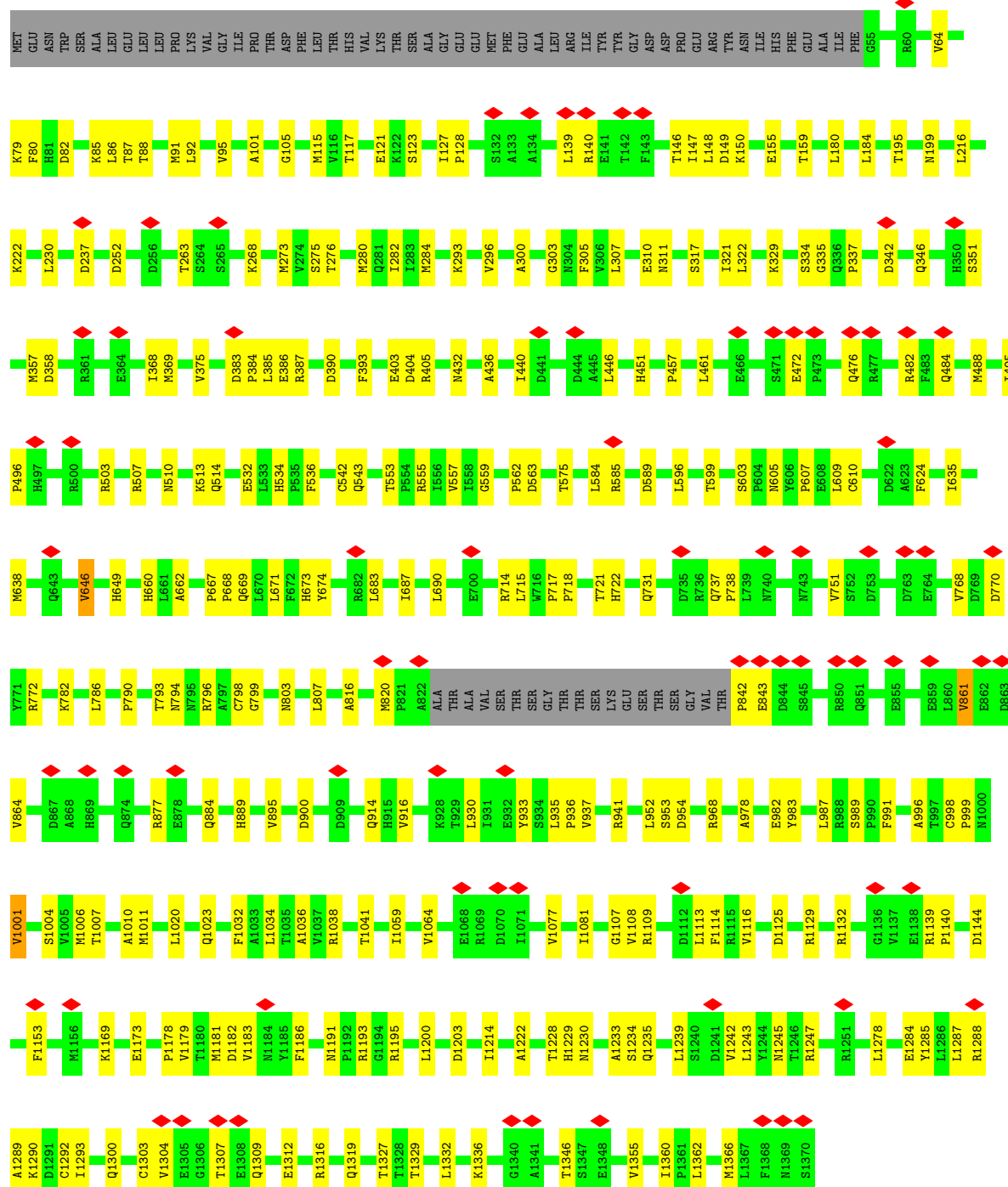
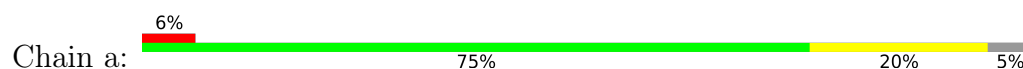


• Molecule 7: Small capsomere-interacting protein

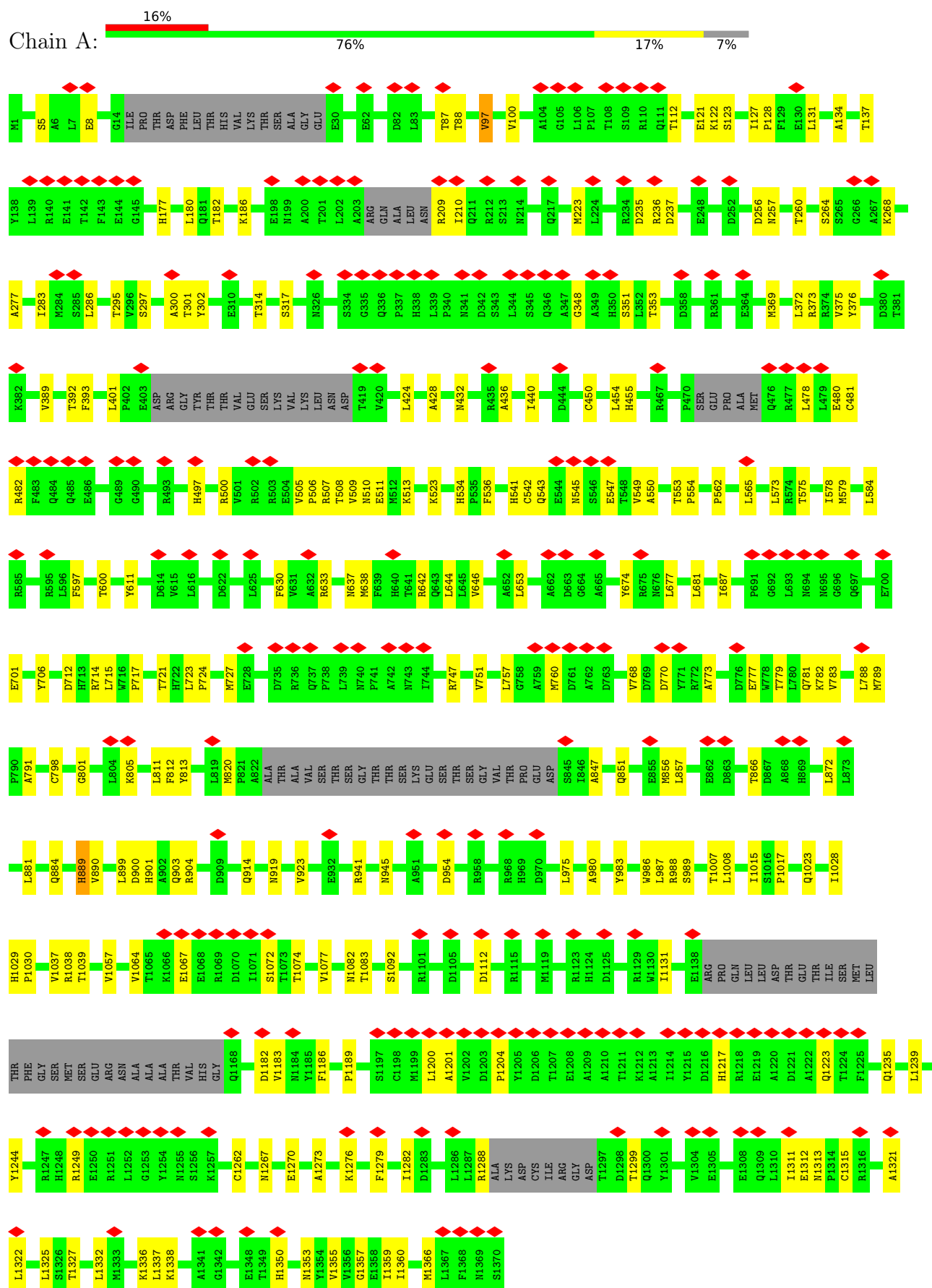




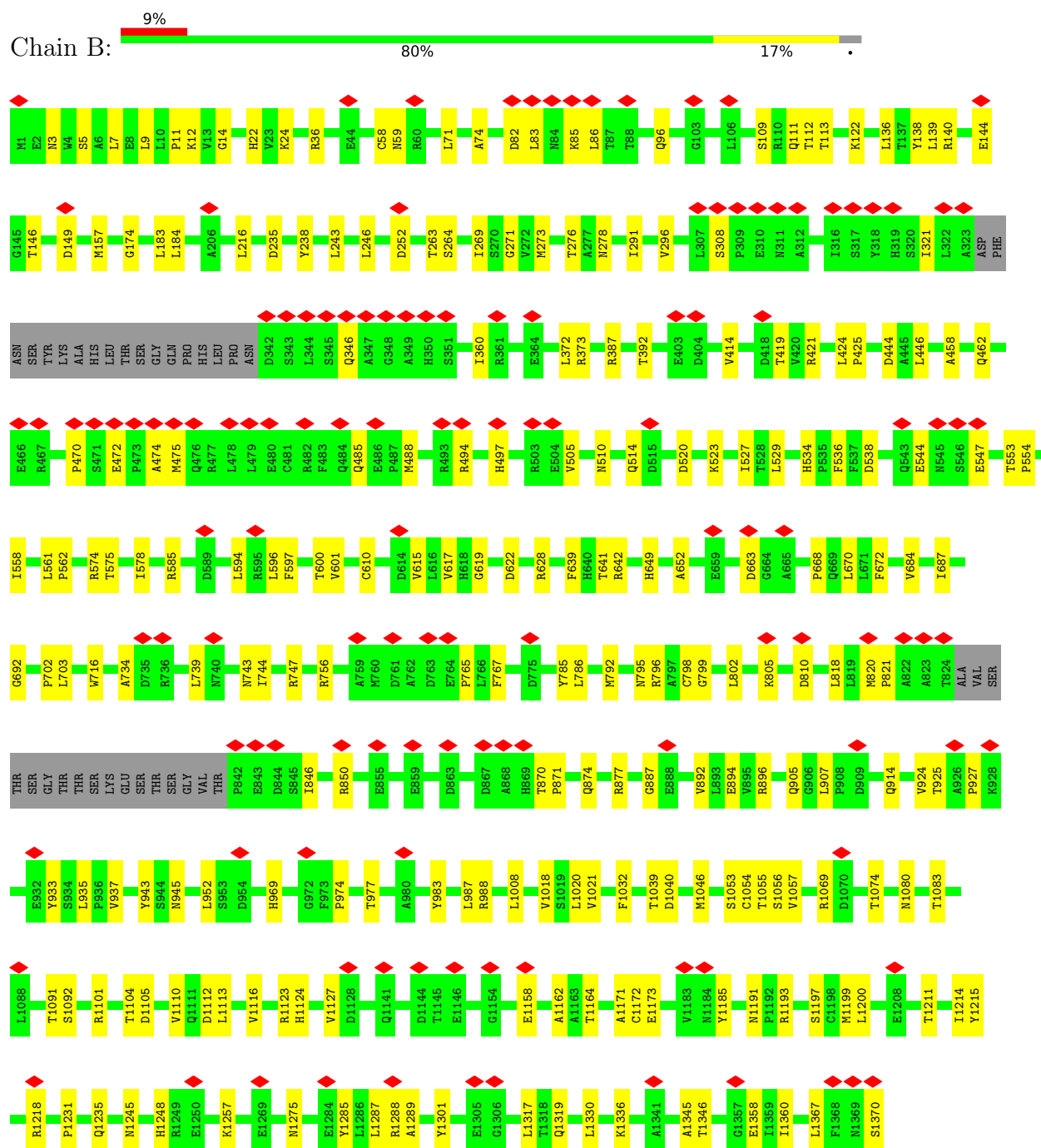
• Molecule 8: Major capsid protein



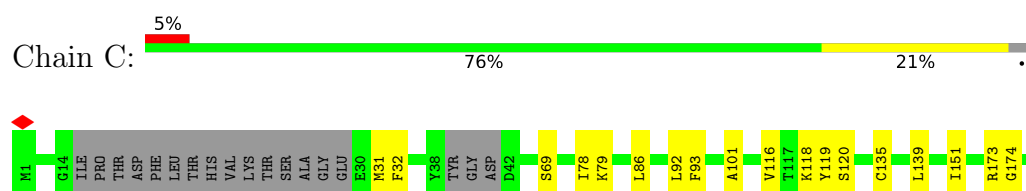
• Molecule 8: Major capsid protein

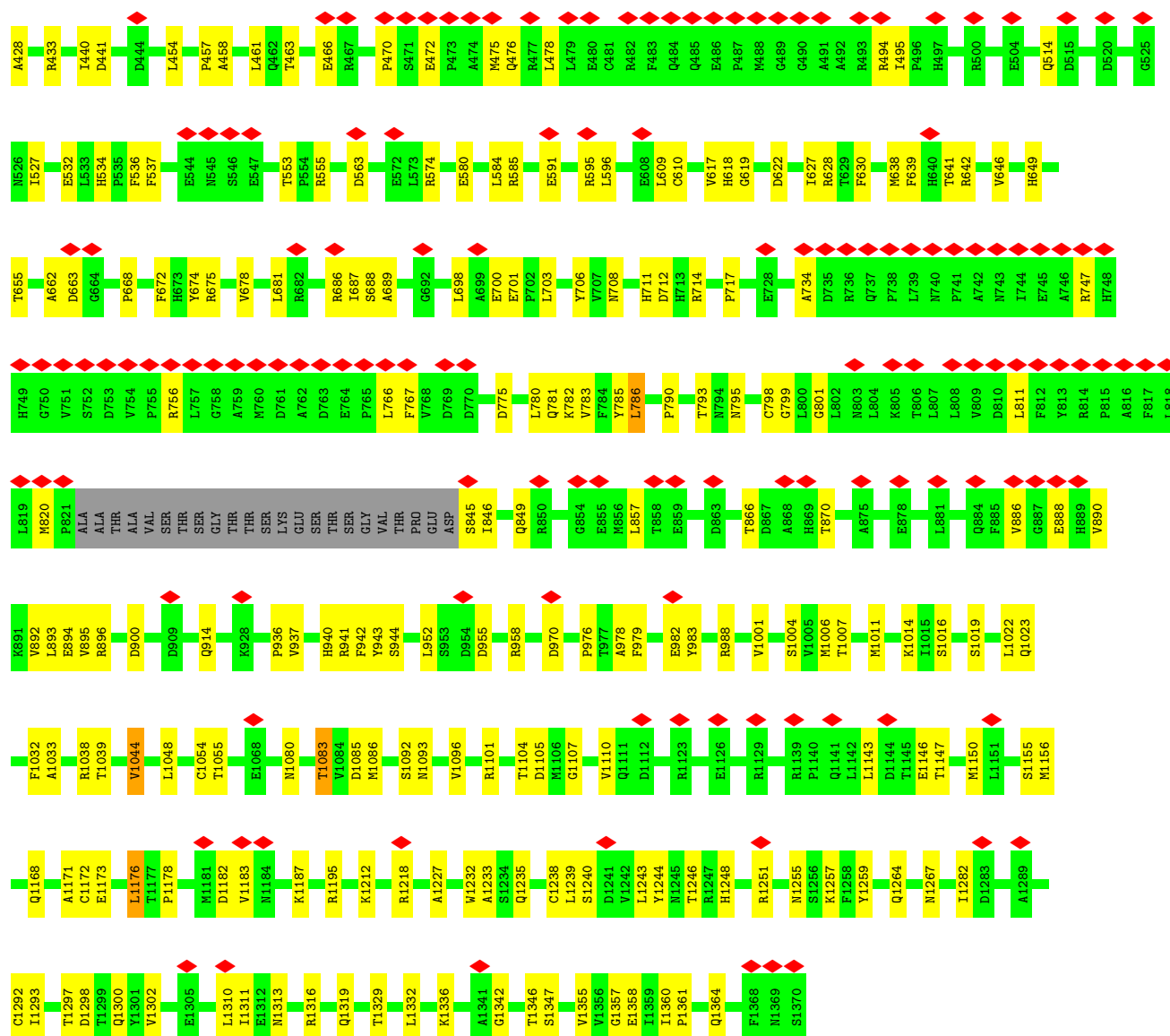


- Molecule 8: Major capsid protein

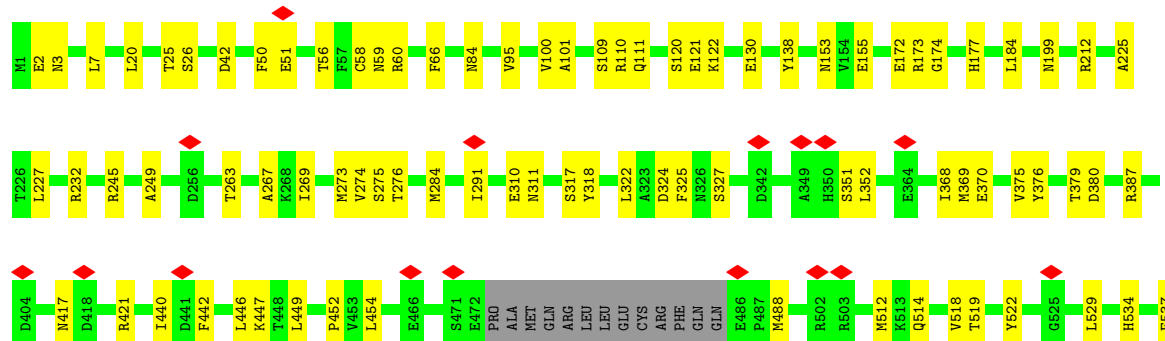
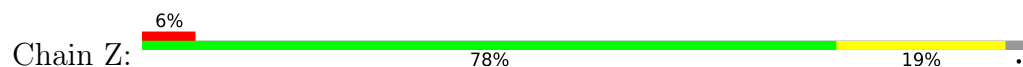


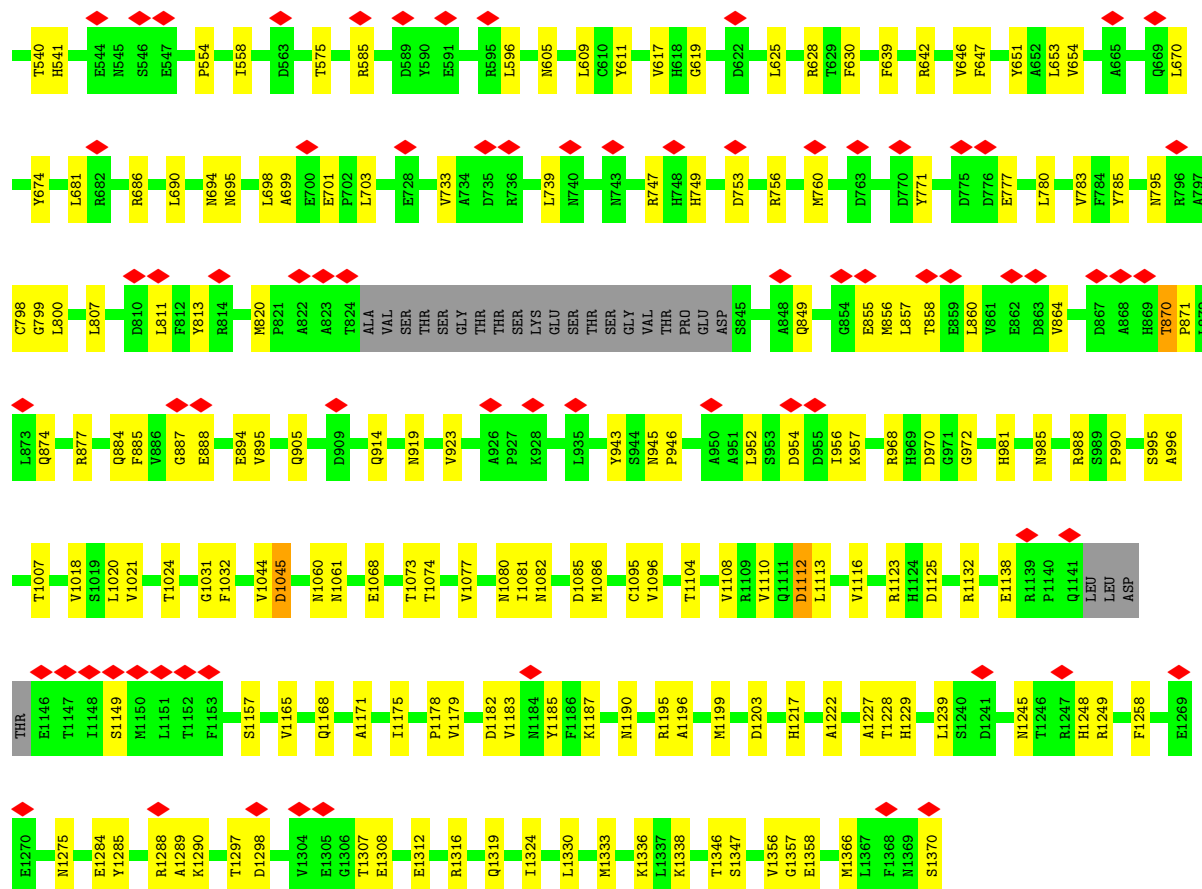
- Molecule 8: Major capsid protein





• Molecule 8: Major capsid protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131384	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.215	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.625, 1.625, 1.625	Depositor

5 Model quality

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	l	0.25	0/2366	0.56	1/3192 (0.0%)
1	x	0.26	0/2366	0.55	0/3192
2	I	0.29	0/2394	0.56	0/3251
2	h	0.31	0/2445	0.56	1/3322 (0.0%)
2	n	0.27	0/2379	0.52	0/3230
2	o	0.27	0/2333	0.47	0/3167
3	H	0.30	0/174	0.69	0/233
3	P	0.28	0/174	0.61	0/233
4	g	0.28	0/951	0.53	0/1288
4	m	0.31	0/2374	0.52	0/3221
5	M	0.33	0/3935	0.55	0/5331
6	N	0.29	0/567	0.65	0/761
6	O	0.26	0/600	0.58	0/808
7	Q	0.28	0/520	0.67	0/697
7	R	0.27	0/520	0.57	0/697
7	S	0.27	0/520	0.54	0/697
7	T	0.21	0/520	0.53	0/697
7	i	0.25	0/520	0.56	0/697
7	j	0.23	0/520	0.55	0/697
8	A	0.31	0/10338	0.55	0/14079
8	B	0.32	0/10824	0.54	0/14743
8	C	0.32	0/10799	0.51	0/14707
8	D	0.30	0/10513	0.51	0/14322
8	Y	0.29	0/10932	0.51	0/14892
8	Z	0.30	0/10803	0.49	0/14716
8	a	0.33	0/10503	0.53	0/14309
All	All	0.30	0/100890	0.53	2/137179 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	1
8	B	0	1
8	C	0	2
8	D	0	2
8	Z	0	1
8	a	0	2
All	All	0	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	247	VAL	N-CA-C	-5.77	106.87	112.29
1	1	184	LEU	CA-CB-CG	5.01	133.84	116.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	B	585	ARG	Peptide
8	C	585	ARG	Peptide
8	C	764	GLU	Peptide
8	D	765	PRO	Peptide
8	D	972	GLY	Peptide
2	I	250	PRO	Peptide
8	Z	585	ARG	Peptide
8	a	542	CYS	Peptide
8	a	585	ARG	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2328	0	2363	32	0
1	x	2328	0	2363	32	0
2	I	2349	0	2437	32	0
2	h	2398	0	2486	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	n	2334	0	2431	36	0
2	o	2291	0	2383	38	0
3	H	172	0	176	5	0
3	P	172	0	176	2	0
4	g	929	0	922	17	0
4	m	2325	0	2363	34	0
5	M	3848	0	3773	69	0
6	N	558	0	557	11	0
6	O	589	0	587	8	0
7	Q	513	0	539	23	0
7	R	513	0	539	9	0
7	S	513	0	539	12	0
7	T	513	0	539	12	0
7	i	513	0	539	12	0
7	j	513	0	539	7	0
8	A	10096	0	10042	147	0
8	B	10574	0	10522	151	0
8	C	10549	0	10499	184	0
8	D	10269	0	10229	159	0
8	Y	10676	0	10618	165	0
8	Z	10551	0	10487	171	0
8	a	10260	0	10215	169	0
All	All	98674	0	98863	1446	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 7.

All (1446) 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)
8:C:856:MET:O	8:C:860:LEU:HB2	1.82	0.79
8:a:1239:LEU:O	8:a:1243:LEU:HB2	1.84	0.78
2:o:62:ARG:HH22	2:o:284:GLU:HB3	1.57	0.68
8:C:92:LEU:HD23	8:Z:7:LEU:HB2	1.75	0.67
8:Z:1044:VAL:HG21	8:Z:1096:VAL:HG13	1.76	0.67
2:I:8:ILE:HB	2:I:83:LEU:HB2	1.77	0.67
8:B:291:ILE:HG12	8:B:360:ILE:HG22	1.77	0.67
8:C:760:MET:HE2	8:C:888:GLU:HA	1.78	0.66
8:Y:182:THR:HG21	8:Y:1083:THR:HG21	1.78	0.66
8:D:1327:THR:HG21	8:D:1333:MET:HB2	1.77	0.66
8:C:575:THR:HG21	8:C:1007:THR:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:534:HIS:HD2	8:B:536:PHE:H	1.45	0.65
8:B:112:THR:HG23	8:B:113:THR:HG23	1.79	0.65
8:C:798:CYS:SG	8:C:799:GLY:N	2.70	0.65
8:Y:617:VAL:HG13	8:Y:619:GLY:H	1.62	0.65
8:B:1172:CYS:SG	8:B:1173:GLU:N	2.68	0.64
8:Y:472:GLU:HB3	8:Y:475:MET:HG2	1.78	0.64
8:A:575:THR:HG21	8:A:1007:THR:HA	1.77	0.64
8:a:553:THR:HG21	8:a:983:TYR:HB3	1.79	0.64
8:Y:129:PHE:HB2	8:Z:111:GLN:HE21	1.63	0.64
8:Z:849:GLN:HE22	8:Z:871:PRO:HB2	1.62	0.64
2:h:209:ASN:HD22	2:h:210:LEU:HD22	1.62	0.63
8:B:58:CYS:SG	8:B:59:ASN:N	2.72	0.63
8:D:895:VAL:HB	8:D:914:GLN:HB3	1.80	0.63
8:Z:1095:CYS:SG	8:Z:1096:VAL:N	2.71	0.63
6:O:55:ARG:HH11	6:O:58:LYS:HB2	1.64	0.63
8:Y:174:GLY:HA3	8:Z:101:ALA:HB3	1.81	0.63
8:Y:494:ARG:HH22	8:Y:978:ALA:HB3	1.64	0.62
7:T:43:MET:HG2	7:T:46:LYS:HE3	1.80	0.62
8:D:1155:SER:OG	8:D:1156:MET:N	2.31	0.62
2:n:102:TRP:H	2:n:297:ASN:HD21	1.46	0.62
8:D:272:VAL:HG23	8:D:368:ILE:HB	1.81	0.62
8:D:798:CYS:SG	8:D:799:GLY:N	2.72	0.62
8:Y:1235:GLN:HB2	8:Y:1238:CYS:HB3	1.82	0.62
8:A:542:CYS:SG	8:A:543:GLN:N	2.71	0.62
6:N:28:GLU:HG2	6:O:2:SER:HB3	1.82	0.62
8:a:794:ASN:ND2	8:a:998:CYS:SG	2.72	0.62
8:B:702:PRO:HB3	8:C:965:HIS:HB3	1.82	0.62
8:B:1054:CYS:SG	8:B:1055:THR:N	2.73	0.62
8:D:820:MET:SD	8:D:877:ARG:NH1	2.73	0.62
8:C:534:HIS:HD2	8:C:536:PHE:H	1.47	0.61
8:Z:756:ARG:HH22	8:Z:887:GLY:HA2	1.64	0.61
2:o:188:VAL:HG22	2:o:193:LEU:HD13	1.82	0.61
7:R:62:LEU:HD11	8:B:805:LYS:HA	1.82	0.61
8:Y:798:CYS:SG	8:Y:799:GLY:N	2.73	0.61
1:1:248:ASN:HD22	7:S:73:THR:HG23	1.64	0.61
8:A:1189:PRO:HB3	8:A:1321:ALA:HA	1.82	0.61
2:n:10:CYS:HB3	2:n:81:ILE:HB	1.82	0.61
8:D:981:HIS:HB3	8:D:984:HIS:HB2	1.82	0.61
2:I:78:GLY:HA3	8:B:86:LEU:HA	1.82	0.61
8:A:392:THR:HG22	8:A:1039:THR:HG22	1.82	0.61
8:Z:1228:THR:OG1	8:Z:1229:HIS:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:715:LEU:HA	8:A:914:GLN:HE22	1.66	0.61
8:C:604:PRO:HA	8:C:925:THR:HG21	1.83	0.60
2:h:193:LEU:HG	2:h:197:MET:HE3	1.83	0.60
8:Z:1195:ARG:NH1	8:Z:1227:ALA:O	2.33	0.60
2:I:113:PRO:HB2	2:I:116:HIS:HB2	1.81	0.60
8:B:1330:LEU:HD21	8:C:1183:VAL:HG11	1.83	0.60
8:C:472:GLU:HB3	8:C:475:MET:HB2	1.84	0.60
8:D:139:LEU:HD22	8:D:160:VAL:HG21	1.83	0.60
8:B:617:VAL:HG13	8:B:619:GLY:H	1.66	0.60
8:C:92:LEU:HB3	8:Z:7:LEU:HD13	1.83	0.60
8:C:441:ASP:HB2	8:C:443:VAL:HG22	1.83	0.60
8:D:1244:TYR:HA	8:D:1249:ARG:HH11	1.66	0.60
2:I:109:CYS:SG	2:I:110:VAL:N	2.75	0.60
8:a:146:THR:HG23	8:a:148:LEU:H	1.66	0.60
8:A:812:PHE:HE1	8:A:857:LEU:HD21	1.67	0.60
8:a:936:PRO:HD3	8:a:952:LEU:HD22	1.84	0.60
8:Z:245:ARG:O	8:Z:249:ALA:HB2	2.02	0.60
5:M:121:ARG:HE	5:M:123:ARG:HH22	1.49	0.60
2:h:34:ILE:HD12	2:h:35:PRO:HD2	1.82	0.60
8:a:317:SER:O	8:Z:3:ASN:ND2	2.34	0.60
6:O:59:ARG:HE	6:O:63:GLN:HG3	1.66	0.59
2:h:277:GLN:HG2	4:g:290:VAL:HG22	1.82	0.59
8:a:149:ASP:OD1	8:a:149:ASP:N	2.35	0.59
8:A:478:LEU:HB2	8:A:506:PRO:HD2	1.84	0.59
8:C:641:THR:HG23	8:C:642:ARG:HG3	1.84	0.59
8:Y:310:GLU:OE2	8:Y:326:ASN:ND2	2.36	0.59
7:R:72:ARG:HB3	8:B:820:MET:HE3	1.85	0.59
8:A:553:THR:HG21	8:A:983:TYR:HB3	1.85	0.59
8:Y:1101:ARG:NH1	8:Z:199:ASN:OD1	2.35	0.59
8:Z:1324:ILE:HA	8:Z:1358:GLU:HG3	1.84	0.59
2:h:93:THR:HA	2:h:301:THR:HA	1.84	0.59
2:h:110:VAL:HG23	2:h:287:VAL:HG11	1.85	0.59
8:a:101:ALA:HB3	8:Z:174:GLY:HA3	1.83	0.59
8:a:1285:TYR:HA	8:a:1289:ALA:HB3	1.83	0.59
8:Y:580:GLU:HG2	8:Y:585:ARG:HB2	1.85	0.59
8:B:485:GLN:HE22	8:B:896:ARG:HH22	1.50	0.59
8:B:554:PRO:O	8:B:988:ARG:NH2	2.36	0.59
8:Y:628:ARG:NH2	8:Y:663:ASP:OD2	2.36	0.58
8:Y:1156:MET:SD	8:Y:1156:MET:N	2.76	0.58
8:Z:888:GLU:O	8:Z:919:ASN:ND2	2.36	0.58
5:M:93:CYS:SG	5:M:94:PHE:N	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:1034:LEU:HD12	8:a:1173:GLU:HG3	1.85	0.58
8:B:871:PRO:O	8:B:874:GLN:NE2	2.35	0.58
8:C:225:ALA:O	8:C:232:ARG:NH1	2.36	0.58
8:C:804:LEU:HB2	8:C:808:LEU:HD23	1.85	0.58
5:M:481:VAL:HG13	5:M:482:ARG:HG2	1.85	0.58
8:A:480:GLU:HB2	8:A:543:GLN:HG2	1.85	0.58
2:n:116:HIS:HE1	2:n:133:VAL:HG13	1.67	0.58
5:M:71:ASP:O	5:M:431:ARG:NH2	2.35	0.58
8:Y:703:LEU:HD12	8:Y:1022:LEU:HD11	1.85	0.58
8:Y:1054:CYS:SG	8:Y:1055:THR:N	2.75	0.58
8:Z:447:LYS:HE3	8:Z:1112:ASP:HB3	1.84	0.58
8:B:1193:ARG:HH22	8:B:1197:SER:HB3	1.67	0.58
7:S:14:ARG:O	7:S:18:HIS:ND1	2.37	0.58
8:C:151:ILE:HD12	8:D:332:LEU:HG	1.86	0.58
2:o:24:LEU:HD13	2:o:125:LEU:HD22	1.86	0.58
6:N:30:VAL:HA	6:N:33:ARG:HE	1.69	0.58
8:a:1360:ILE:HG23	8:a:1362:LEU:HD22	1.85	0.58
8:C:1336:LYS:NZ	8:C:1346:THR:OG1	2.37	0.58
8:D:1329:THR:HG23	8:D:1332:LEU:H	1.68	0.58
8:a:798:CYS:SG	8:a:799:GLY:N	2.77	0.58
8:Y:389:VAL:HG23	8:Y:1044:VAL:HG11	1.84	0.58
2:h:103:GLU:OE2	2:h:178:ARG:NH1	2.36	0.58
8:a:222:LYS:NZ	8:Z:1370:SER:O	2.37	0.58
2:h:36:GLN:HG3	2:h:38:LEU:HD23	1.85	0.57
2:I:173:GLN:NE2	2:I:184:ILE:O	2.37	0.57
8:B:252:ASP:OD1	8:B:252:ASP:N	2.36	0.57
8:B:514:GLN:HE22	8:B:562:PRO:HA	1.69	0.57
8:B:1110:VAL:HA	8:B:1171:ALA:HB3	1.86	0.57
8:C:968:ARG:HG3	8:C:970:ASP:H	1.69	0.57
8:Y:1104:THR:OG1	8:Y:1300:GLN:NE2	2.37	0.57
1:1:136:ALA:HB1	1:1:157:VAL:HG11	1.87	0.57
8:B:22:HIS:NE2	8:Z:379:THR:O	2.37	0.57
8:C:761:ASP:OD1	8:C:889:HIS:ND1	2.29	0.57
5:M:163:PHE:HA	5:M:320:VAL:HG13	1.85	0.57
5:M:167:ASP:N	5:M:167:ASP:OD1	2.36	0.57
8:A:182:THR:HG21	8:A:1083:THR:HG21	1.85	0.57
8:C:1157:SER:OG	8:C:1255:ASN:ND2	2.37	0.57
8:Z:795:ASN:ND2	8:Z:995:SER:OG	2.37	0.57
2:I:113:PRO:HD3	2:I:135:PRO:HA	1.87	0.57
5:M:365:TYR:HA	5:M:368:ILE:HD12	1.87	0.57
7:Q:56:ASP:OD2	7:Q:56:ASP:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:66:ARG:NH1	8:A:751:VAL:O	2.37	0.57
8:A:1288:ARG:NH1	8:A:1299:THR:O	2.38	0.57
8:D:58:CYS:SG	8:D:59:ASN:N	2.77	0.57
8:a:968:ARG:NH1	8:Z:694:ASN:O	2.38	0.57
8:A:760:MET:HG3	8:A:805:LYS:HE3	1.85	0.57
8:B:505:VAL:HG11	8:B:974:PRO:HB3	1.86	0.57
8:D:534:HIS:HD2	8:D:536:PHE:H	1.53	0.57
8:Y:534:HIS:HD2	8:Y:536:PHE:H	1.52	0.57
1:x:52:LEU:HG	1:x:234:LEU:HD22	1.86	0.57
2:n:279:ASP:OD2	2:o:283:ARG:NH2	2.38	0.57
2:o:101:THR:OG1	2:o:297:ASN:ND2	2.37	0.57
4:g:220:ARG:NH1	4:g:290:VAL:OXT	2.37	0.57
8:B:140:ARG:NH2	8:B:321:ILE:O	2.38	0.57
8:a:687:ILE:HG21	8:a:1006:MET:HE3	1.87	0.56
3:H:2236:ARG:HD2	6:N:62:ARG:HG3	1.87	0.56
4:g:170:ASP:OD1	4:g:170:ASP:N	2.36	0.56
8:a:1327:THR:HG23	8:a:1355:VAL:HG22	1.87	0.56
8:B:747:ARG:HB2	8:B:767:PHE:HB3	1.88	0.56
8:Y:324:ASP:OD2	8:Y:346:GLN:NE2	2.38	0.56
8:Y:638:MET:SD	8:Y:642:ARG:NH2	2.75	0.56
2:h:186:ASP:OD1	5:M:576:ARG:NH1	2.38	0.56
2:n:277:GLN:HE22	4:m:220:ARG:HH21	1.53	0.56
4:m:69:ARG:NH1	4:m:130:GLU:OE1	2.38	0.56
8:A:236:ARG:NH1	8:A:286:LEU:O	2.38	0.56
8:A:554:PRO:O	8:A:988:ARG:NH2	2.38	0.56
8:C:1139:ARG:HE	8:C:1140:PRO:HD2	1.70	0.56
8:C:626:LEU:HD23	8:C:881:LEU:HB3	1.86	0.56
1:x:87:VAL:HG13	1:x:109:LEU:HD21	1.87	0.56
2:h:195:ILE:HA	2:h:198:LYS:HD2	1.86	0.56
2:o:149:ARG:NH1	2:o:174:THR:O	2.38	0.56
7:Q:14:ARG:O	7:Q:18:HIS:ND1	2.38	0.56
8:A:847:ALA:O	8:A:851:GLN:NE2	2.38	0.56
8:C:118:LYS:NZ	8:C:1087:GLY:O	2.39	0.56
8:D:99:ARG:NH2	8:D:111:GLN:OE1	2.38	0.56
8:D:485:GLN:OE1	8:D:896:ARG:NH2	2.38	0.56
7:R:14:ARG:O	7:R:18:HIS:ND1	2.34	0.56
8:A:579:MET:HG2	8:A:584:LEU:HD11	1.88	0.56
8:B:1245:ASN:HB3	8:B:1248:HIS:HB2	1.87	0.56
8:a:895:VAL:HB	8:a:914:GLN:HB3	1.87	0.56
8:C:220:LYS:NZ	8:C:1320:GLU:OE1	2.39	0.56
8:C:1054:CYS:SG	8:C:1055:THR:N	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:760:MET:HB2	8:Z:888:GLU:HA	1.87	0.56
1:x:49:ARG:HH21	1:x:283:PRO:HD3	1.70	0.56
4:m:137:THR:HG1	4:m:147:THR:HG1	1.52	0.56
5:M:409:HIS:NE2	6:O:38:ALA:O	2.38	0.56
8:A:1037:VAL:HG21	8:A:1262:CYS:HB3	1.86	0.56
8:C:258:PRO:O	8:C:268:LYS:NZ	2.38	0.56
2:o:278:LEU:HD12	2:o:281:LEU:HD13	1.86	0.56
8:a:1109:ARG:HD2	8:a:1169:LYS:HD2	1.86	0.56
8:B:544:GLU:HB3	8:B:547:GLU:HG2	1.88	0.56
2:h:62:ARG:NH1	2:h:147:ASN:OD1	2.39	0.56
8:a:721:THR:HG1	8:a:722:HIS:HD1	1.54	0.56
8:A:1312:GLU:HG3	8:A:1315:CYS:HB2	1.88	0.56
8:B:668:PRO:O	8:B:672:PHE:HB2	2.06	0.56
8:D:733:VAL:HG22	8:D:894:GLU:HB2	1.87	0.56
8:D:1155:SER:HA	8:D:1255:ASN:HD21	1.70	0.56
8:Z:870:THR:OG1	8:Z:874:GLN:NE2	2.38	0.56
8:a:1191:ASN:ND2	8:a:1195:ARG:O	2.37	0.55
8:A:562:PRO:HD2	8:A:565:LEU:HD22	1.88	0.55
8:B:174:GLY:HA3	8:C:101:ALA:HB3	1.87	0.55
8:D:953:SER:OG	8:D:954:ASP:N	2.39	0.55
8:Y:681:LEU:HD22	8:Y:783:VAL:HG13	1.88	0.55
1:x:26:LYS:HD2	1:x:27:PRO:HD2	1.87	0.55
2:h:274:MET:HE1	4:g:290:VAL:HG21	1.87	0.55
8:B:575:THR:HA	8:B:578:ILE:HD12	1.88	0.55
8:D:1292:CYS:HB3	8:D:1310:LEU:HD12	1.87	0.55
2:o:104:LYS:NZ	2:o:292:ASP:OD2	2.39	0.55
8:C:1211:THR:HA	8:C:1214:ILE:HG22	1.88	0.55
8:Y:470:PRO:O	8:Y:476:GLN:NE2	2.39	0.55
8:Y:553:THR:HG21	8:Y:983:TYR:HB3	1.89	0.55
5:M:163:PHE:HB3	5:M:319:ASP:HA	1.88	0.55
7:j:15:ASP:OD1	7:j:19:ARG:NH1	2.39	0.55
8:a:440:ILE:HD12	8:a:1108:VAL:HB	1.87	0.55
8:D:99:ARG:NH1	8:D:109:SER:O	2.39	0.55
8:D:1060:ASN:O	8:D:1079:GLN:NE2	2.33	0.55
5:M:64:ASP:HB3	5:M:553:ARG:HB3	1.89	0.55
8:A:1217:HIS:NE2	8:A:1235:GLN:OE1	2.40	0.55
8:B:594:LEU:HD12	8:B:792:MET:HE3	1.87	0.55
8:Y:785:TYR:O	8:Y:943:TYR:OH	2.23	0.55
8:Y:1246:THR:N	8:Y:1267:ASN:OD1	2.40	0.55
2:h:149:ARG:NH1	2:h:174:THR:O	2.40	0.55
5:M:162:GLU:OE2	5:M:360:ARG:NH1	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:207:LEU:HD13	8:Y:212:ARG:HB3	1.89	0.55
8:Y:1110:VAL:HA	8:Y:1171:ALA:HB3	1.88	0.55
8:a:86:LEU:HA	8:Z:50:PHE:HB2	1.89	0.55
2:I:62:ARG:NH2	2:I:283:ARG:O	2.39	0.55
8:a:472:GLU:O	8:a:476:GLN:NE2	2.36	0.55
8:Y:289:SER:HG	8:Y:290:HIS:HD1	1.55	0.55
2:h:224:LEU:HD11	2:h:253:PRO:HD2	1.89	0.55
8:a:715:LEU:O	8:a:782:LYS:NZ	2.36	0.55
8:Z:798:CYS:SG	8:Z:799:GLY:N	2.80	0.55
8:Z:1290:LYS:HG2	8:Z:1312:GLU:HA	1.89	0.55
8:A:901:HIS:HA	8:A:904:ARG:HG2	1.88	0.55
8:Y:1329:THR:HG23	8:Y:1332:LEU:H	1.72	0.55
8:B:470:PRO:HB3	8:B:475:MET:HE3	1.90	0.54
8:Y:377:LYS:NZ	8:Y:378:ASN:OD1	2.39	0.54
8:Y:404:ASP:OD1	8:Y:405:ARG:NH2	2.40	0.54
2:o:35:PRO:HD3	2:o:50:GLN:HE22	1.72	0.54
5:M:524:TYR:HB2	5:M:532:TYR:HB2	1.88	0.54
8:B:392:THR:HG22	8:B:1039:THR:HG22	1.89	0.54
8:C:731:GLN:HG2	8:C:740:ASN:HD21	1.72	0.54
8:D:277:ALA:HA	8:D:371:ASN:HD22	1.72	0.54
8:D:463:THR:HG21	8:D:1237:GLY:HA3	1.90	0.54
7:T:26:LEU:O	8:D:813:TYR:OH	2.24	0.54
8:Y:1360:ILE:HD12	8:Y:1361:PRO:HD2	1.89	0.54
8:A:1023:GLN:HA	8:A:1028:ILE:HD12	1.89	0.54
8:C:514:GLN:HE22	8:C:562:PRO:HA	1.72	0.54
8:D:389:VAL:HG13	8:D:1044:VAL:HG21	1.90	0.54
8:a:387:ARG:NH1	8:a:1309:GLN:OE1	2.40	0.54
8:B:870:THR:HB	8:B:874:GLN:HE22	1.73	0.54
8:D:1316:ARG:O	8:D:1319:GLN:NE2	2.40	0.54
8:Y:610:CYS:HB3	8:Y:649:HIS:HE1	1.71	0.54
8:Z:694:ASN:HA	8:Z:703:LEU:HD23	1.88	0.54
8:Z:1347:SER:HB3	8:Z:1357:GLY:H	1.71	0.54
5:M:45:TYR:HB3	5:M:132:LEU:HD22	1.88	0.54
1:1:88:ALA:HA	1:1:106:LEU:HD11	1.90	0.54
1:1:230:GLU:OE2	1:1:231:ARG:NH1	2.41	0.54
7:Q:37:HIS:HD2	7:Q:40:LEU:HB2	1.72	0.54
8:a:383:ASP:HB2	8:a:386:GLU:HB2	1.89	0.54
8:a:1064:VAL:HG12	8:a:1077:VAL:HG12	1.89	0.54
8:A:97:VAL:O	8:A:112:THR:OG1	2.25	0.54
8:A:534:HIS:HD2	8:A:536:PHE:H	1.54	0.54
8:A:541:HIS:HA	8:A:550:ALA:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:575:THR:HA	8:A:578:ILE:HG22	1.90	0.54
8:C:232:ARG:HG2	8:C:233:THR:HG23	1.89	0.54
8:C:691:PRO:HB3	8:D:968:ARG:HH21	1.72	0.54
8:C:936:PRO:HB3	8:C:952:LEU:HD23	1.88	0.54
8:D:58:CYS:O	8:D:60:ARG:NH1	2.41	0.54
5:M:108:ARG:NH2	5:M:114:VAL:O	2.41	0.54
5:M:314:LEU:HD11	5:M:327:ARG:HB3	1.89	0.54
8:Y:478:LEU:HD11	8:Y:527:ILE:HG22	1.89	0.54
8:Y:574:ARG:NH1	8:Y:1023:GLN:OE1	2.41	0.54
2:I:35:PRO:HA	2:I:68:MET:HG2	1.89	0.54
8:a:293:LYS:HD2	8:a:358:ASP:HB3	1.90	0.54
8:B:1069:ARG:NH1	8:B:1074:THR:OG1	2.40	0.54
8:C:900:ASP:OD2	8:C:1014:LYS:NZ	2.40	0.54
8:D:1106:MET:SD	8:D:1363:GLN:NE2	2.81	0.54
8:D:1247:ARG:NH1	8:D:1250:GLU:OE1	2.41	0.54
8:Y:130:GLU:O	8:Z:111:GLN:NE2	2.41	0.54
8:Z:681:LEU:HD22	8:Z:783:VAL:HG13	1.90	0.54
2:o:74:ARG:NH2	8:C:1070:ASP:OD1	2.41	0.54
8:a:768:VAL:HG23	8:a:770:ASP:H	1.72	0.54
8:C:93:PHE:HB2	8:C:116:VAL:HB	1.90	0.54
8:Y:96:GLN:HB3	8:Y:113:THR:HG22	1.89	0.54
8:Y:618:HIS:NE2	8:Y:886:VAL:O	2.41	0.54
8:A:630:PHE:HA	8:A:633:ARG:HH21	1.72	0.53
8:C:31:MET:HG2	8:C:32:PHE:HD1	1.73	0.53
8:C:359:VAL:HG12	8:C:368:ILE:HG12	1.90	0.53
8:C:950:ALA:HB1	8:C:957:LYS:HG3	1.90	0.53
8:Z:681:LEU:HB3	8:Z:780:LEU:HD22	1.91	0.53
8:Z:1032:PHE:HA	8:Z:1178:PRO:HD3	1.90	0.53
8:Z:1104:THR:HG22	8:Z:1168:GLN:HE21	1.73	0.53
1:x:83:ARG:NH1	1:x:206:THR:OG1	2.41	0.53
2:h:147:ASN:ND2	2:h:284:GLU:OE2	2.40	0.53
1:1:83:ARG:NH1	1:1:206:THR:OG1	2.41	0.53
8:B:472:GLU:HB3	8:B:475:MET:HE2	1.90	0.53
8:Y:747:ARG:NH1	8:Y:767:PHE:O	2.41	0.53
8:Z:575:THR:HG21	8:Z:1007:THR:HA	1.90	0.53
7:R:72:ARG:NE	8:B:820:MET:O	2.41	0.53
8:B:444:ASP:OD1	8:B:444:ASP:N	2.35	0.53
8:B:494:ARG:HA	8:B:497:HIS:HD2	1.73	0.53
1:x:99:ARG:O	1:x:103:ARG:HB2	2.08	0.53
2:n:34:ILE:HD12	2:n:35:PRO:HD2	1.90	0.53
2:o:13:ASP:OD2	2:o:42:LYS:NZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:414:TRP:HB2	5:M:478:VAL:HG11	1.89	0.53
7:j:52:SER:OG	7:j:53:LEU:N	2.41	0.53
8:a:115:MET:HB2	8:B:36:ARG:HB3	1.90	0.53
8:A:424:LEU:HB3	8:A:573:LEU:HD21	1.89	0.53
8:Y:20:LEU:HG	8:Y:21:THR:HG23	1.89	0.53
8:Z:121:GLU:O	8:Z:1082:ASN:ND2	2.42	0.53
3:H:2228:VAL:HA	3:H:2231:THR:HG22	1.89	0.53
8:Z:1185:TYR:O	8:Z:1190:ASN:ND2	2.41	0.53
8:C:1161:ALA:O	8:D:209:ARG:NH1	2.37	0.53
8:C:1290:LYS:HB2	8:C:1310:LEU:HD12	1.89	0.53
8:D:310:GLU:HB3	8:D:325:PHE:HD2	1.73	0.53
8:D:438:GLN:HE22	8:D:1107:GLY:HA2	1.74	0.53
8:Z:1060:ASN:ND2	8:Z:1061:ASN:O	2.41	0.53
2:h:223:ALA:HB1	2:h:235:GLN:HE21	1.73	0.53
4:m:185:VAL:HG23	4:m:251:LEU:HB3	1.90	0.53
5:M:478:VAL:HG12	5:M:485:VAL:HG23	1.91	0.53
7:Q:26:LEU:HD23	7:Q:64:LEU:HD22	1.89	0.53
7:i:33:SER:OG	7:i:34:GLU:N	2.40	0.53
8:a:334:SER:OG	8:a:335:GLY:N	2.42	0.53
8:B:1336:LYS:NZ	8:B:1346:THR:OG1	2.38	0.53
8:D:800:LEU:HD22	8:D:923:VAL:HB	1.90	0.53
8:Y:537:PHE:O	8:Y:555:ARG:NH2	2.42	0.53
2:n:276:ARG:NH1	4:m:288:GLU:OE2	2.42	0.53
4:m:262:SER:OG	4:m:263:PHE:N	2.42	0.53
5:M:46:ARG:HB2	5:M:89:TRP:HD1	1.74	0.53
5:M:322:HIS:O	8:a:737:GLN:NE2	2.42	0.53
8:B:1199:MET:HE3	8:B:1214:ILE:HD12	1.89	0.53
8:C:776:ASP:OD1	8:C:776:ASP:N	2.37	0.53
5:M:62:ASP:OD1	5:M:62:ASP:N	2.40	0.53
1:1:129:LEU:HD11	1:1:204:VAL:HA	1.91	0.53
8:a:404:ASP:OD1	8:a:404:ASP:N	2.42	0.53
8:a:510:ASN:OD1	8:a:989:SER:OG	2.27	0.53
8:D:609:LEU:HD11	8:D:630:PHE:HZ	1.74	0.53
8:Z:905:GLN:HA	8:Z:1123:ARG:HD3	1.91	0.53
1:1:171:LEU:O	1:1:212:ASN:ND2	2.41	0.53
8:A:954:ASP:N	8:A:954:ASP:OD1	2.41	0.53
8:B:743:ASN:OD1	8:B:743:ASN:N	2.42	0.53
8:B:1104:THR:OG1	8:B:1105:ASP:N	2.42	0.53
8:C:1124:HIS:HB3	8:C:1127:VAL:HG12	1.91	0.53
8:D:275:SER:OG	8:D:276:THR:N	2.42	0.53
7:Q:61:LYS:HG2	8:A:813:TYR:OH	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:510:ASN:ND2	8:C:989:SER:OG	2.42	0.52
8:C:614:ASP:OD1	8:C:649:HIS:NE2	2.42	0.52
8:Y:1336:LYS:NZ	8:Y:1346:THR:OG1	2.42	0.52
2:h:157:SER:HB2	5:M:566:LEU:HD12	1.91	0.52
5:M:54:SER:OG	5:M:57:ARG:NH2	2.42	0.52
8:a:1316:ARG:O	8:a:1319:GLN:NE2	2.43	0.52
8:A:209:ARG:HE	8:A:210:ILE:HG13	1.74	0.52
8:C:231:ASN:ND2	8:C:1099:VAL:O	2.42	0.52
8:Y:475:MET:HG3	8:Y:1218:ARG:HE	1.74	0.52
1:l:250:CYS:HA	1:l:253:ILE:HD12	1.91	0.52
8:A:478:LEU:HD22	8:A:505:VAL:HG22	1.91	0.52
8:C:791:ALA:O	8:C:1000:ASN:ND2	2.43	0.52
8:Y:686:ARG:NH2	8:Z:996:ALA:O	2.43	0.52
2:n:261:PRO:HB2	2:o:172:LEU:HD21	1.90	0.52
7:j:66:ARG:NH2	8:a:884:GLN:O	2.42	0.52
8:A:712:ASP:O	8:A:782:LYS:NZ	2.34	0.52
2:o:93:THR:HG22	8:C:1070:ASP:HB3	1.92	0.52
4:m:42:ASP:O	4:m:159:LYS:NZ	2.35	0.52
8:a:275:SER:HB3	8:a:280:MET:HE3	1.91	0.52
8:D:615:VAL:HG21	8:D:802:LEU:HD12	1.91	0.52
8:Y:1182:ASP:OD1	8:Y:1182:ASP:N	2.42	0.52
8:Z:275:SER:OG	8:Z:276:THR:N	2.42	0.52
6:O:34:LEU:HD21	8:a:503:ARG:HH11	1.75	0.52
8:a:237:ASP:OD1	8:a:237:ASP:N	2.39	0.52
8:A:1057:VAL:HG12	8:A:1083:THR:HG22	1.91	0.52
8:B:308:SER:OG	8:B:346:GLN:NE2	2.43	0.52
8:C:663:ASP:O	8:D:642:ARG:NH1	2.42	0.52
8:D:507:ARG:HE	8:D:512:MET:HE2	1.75	0.52
8:D:1185:TYR:OH	8:D:1193:ARG:O	2.27	0.52
8:Z:1157:SER:HB3	8:Z:1258:PHE:HE2	1.75	0.52
8:C:203:ALA:O	8:Z:25:THR:OG1	2.28	0.52
8:C:513:LYS:NZ	8:C:532:GLU:OE1	2.43	0.52
8:Y:532:GLU:OE2	8:Y:555:ARG:NH1	2.40	0.52
8:Z:120:SER:OG	8:Z:121:GLU:N	2.42	0.52
8:D:970:ASP:N	8:D:970:ASP:OD1	2.42	0.52
8:Y:622:ASP:N	8:Y:622:ASP:OD1	2.41	0.52
8:Z:1285:TYR:HA	8:Z:1289:ALA:HB3	1.91	0.52
5:M:96:VAL:HA	5:M:128:VAL:HA	1.92	0.52
8:a:1059:ILE:HG22	8:a:1081:ILE:HG12	1.91	0.52
8:A:1267:ASN:HD22	8:A:1270:GLU:HB2	1.74	0.52
8:B:716:TRP:O	8:B:914:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1231:PRO:O	8:B:1235:GLN:NE2	2.42	0.52
8:C:1193:ARG:NH2	8:C:1214:ILE:O	2.36	0.52
8:D:454:LEU:HD12	8:D:1239:LEU:HD11	1.92	0.52
8:D:529:LEU:O	8:D:1235:GLN:NE2	2.40	0.52
8:D:1157:SER:OG	8:D:1158:GLU:N	2.41	0.52
8:Y:433:ARG:HD3	8:Y:1105:ASP:HA	1.92	0.52
8:Y:790:PRO:HA	8:Y:793:THR:HG22	1.92	0.52
8:a:714:ARG:NH1	8:a:900:ASP:OD1	2.43	0.52
8:a:941:ARG:HH12	8:a:982:GLU:HG2	1.75	0.52
8:A:209:ARG:HD3	8:A:1201:ALA:HA	1.91	0.52
8:C:502:ARG:NH1	8:C:962:GLU:OE1	2.43	0.52
8:C:694:ASN:HA	8:C:703:LEU:HD23	1.92	0.52
2:I:66:ARG:HH11	2:I:285:GLN:HG3	1.75	0.51
4:m:234:ARG:NH1	4:m:240:GLN:O	2.43	0.51
8:a:403:GLU:OE1	8:Z:417:ASN:ND2	2.43	0.51
8:A:454:LEU:HD22	8:A:1239:LEU:HD11	1.91	0.51
8:A:638:MET:SD	8:A:642:ARG:NH1	2.83	0.51
8:Y:1038:ARG:NH1	8:Y:1107:GLY:O	2.42	0.51
8:Z:1113:LEU:HA	8:Z:1116:VAL:HG22	1.91	0.51
5:M:302:ARG:O	5:M:306:TRP:HB2	2.09	0.51
8:B:414:VAL:HG12	8:C:409:THR:HG22	1.91	0.51
8:D:475:MET:SD	8:D:1218:ARG:NH1	2.82	0.51
8:a:451:HIS:HE2	8:a:1114:PHE:HA	1.75	0.51
8:a:575:THR:HG22	8:a:1010:ALA:HB3	1.92	0.51
8:a:816:ALA:O	8:a:877:ARG:NH1	2.39	0.51
8:Y:662:ALA:HB1	8:Z:605:ASN:HD22	1.76	0.51
8:Y:895:VAL:HB	8:Y:914:GLN:HB3	1.92	0.51
2:I:103:GLU:OE1	2:I:178:ARG:NH1	2.43	0.51
8:a:1230:ASN:HB2	8:a:1233:ALA:HB3	1.92	0.51
8:A:507:ARG:HG3	8:A:511:GLU:HB2	1.92	0.51
8:B:276:THR:HG22	8:B:278:ASN:H	1.75	0.51
8:B:472:GLU:HG3	8:B:474:ALA:H	1.74	0.51
8:C:180:LEU:HD23	8:C:384:PRO:HG2	1.92	0.51
8:C:380:ASP:OD1	8:C:380:ASP:N	2.40	0.51
8:D:558:ILE:HD11	8:D:1031:GLY:H	1.75	0.51
8:Z:1336:LYS:NZ	8:Z:1346:THR:OG1	2.40	0.51
5:M:34:ASN:ND2	5:M:38:GLU:OE1	2.43	0.51
8:D:64:VAL:HG21	8:D:375:VAL:HG23	1.92	0.51
8:Y:427:THR:HG22	8:Y:441:ASP:HB3	1.93	0.51
8:Y:845:SER:OG	8:Y:846:ILE:N	2.43	0.51
8:Y:1257:LYS:NZ	8:Y:1302:VAL:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:1264:GLN:OE1	8:Y:1313:ASN:ND2	2.43	0.51
2:h:159:ASP:OD1	5:M:91:ARG:NH2	2.44	0.51
1:1:227:ARG:HH11	1:1:231:ARG:HH12	1.57	0.51
8:a:575:THR:HG21	8:a:1007:THR:HA	1.91	0.51
8:A:235:ASP:OD1	8:A:235:ASP:N	2.42	0.51
8:D:582:MET:HE3	8:D:691:PRO:HD2	1.92	0.51
8:D:635:ILE:HD13	8:D:646:VAL:HB	1.92	0.51
8:D:846:ILE:O	8:D:849:GLN:NE2	2.43	0.51
3:H:2238:LEU:HD22	7:j:53:LEU:HD11	1.93	0.51
8:A:432:ASN:HB3	8:A:436:ALA:H	1.76	0.51
8:B:820:MET:HG2	8:B:877:ARG:HE	1.75	0.51
8:C:1268:THR:HA	8:C:1271:ILE:HB	1.92	0.51
8:D:451:HIS:HE1	8:D:1120:ASN:HB2	1.75	0.51
8:Y:609:LEU:HD11	8:Y:630:PHE:HZ	1.76	0.51
8:Y:756:ARG:HD2	8:Y:767:PHE:HZ	1.76	0.51
8:Z:122:LYS:HG3	8:Z:1082:ASN:HD21	1.75	0.51
1:x:50:THR:O	1:x:54:ASN:ND2	2.44	0.51
8:B:83:LEU:HG	8:B:85:LYS:HG2	1.93	0.51
1:x:129:LEU:HD11	1:x:204:VAL:HA	1.91	0.51
6:O:2:SER:OG	6:O:3:LEU:N	2.38	0.51
8:a:1336:LYS:NZ	8:a:1346:THR:OG1	2.44	0.51
8:A:757:LEU:HD22	8:A:805:LYS:HZ1	1.76	0.51
8:B:263:THR:HA	8:B:296:VAL:HA	1.92	0.51
8:D:807:LEU:HG	8:D:811:LEU:HD23	1.93	0.51
8:D:1110:VAL:HA	8:D:1171:ALA:HB3	1.91	0.51
8:D:1128:ASP:OD2	8:D:1139:ARG:NH2	2.44	0.51
4:m:93:ASN:ND2	4:m:170:ASP:O	2.44	0.51
8:a:92:LEU:HA	8:a:117:THR:HA	1.92	0.51
8:C:949:CYS:HB3	8:C:956:ILE:HG21	1.93	0.51
8:D:718:PRO:HD2	8:D:785:TYR:HB3	1.93	0.51
8:Y:225:ALA:O	8:Y:232:ARG:NH1	2.44	0.51
2:h:62:ARG:HG2	2:h:66:ARG:HH22	1.76	0.50
2:n:4:MET:SD	2:n:4:MET:N	2.84	0.50
8:A:578:ILE:HG23	8:A:687:ILE:HD11	1.94	0.50
8:A:1244:TYR:HA	8:A:1249:ARG:HH21	1.75	0.50
8:C:543:GLN:HG2	8:C:548:THR:HG22	1.92	0.50
8:C:755:PRO:O	8:C:759:ALA:N	2.44	0.50
8:C:1057:VAL:HG12	8:C:1083:THR:HG22	1.93	0.50
8:C:1295:GLY:O	8:D:208:ASN:ND2	2.44	0.50
8:D:552:CYS:SG	8:D:553:THR:N	2.84	0.50
8:Y:463:THR:HA	8:Y:466:GLU:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:58:CYS:SG	8:Z:59:ASN:N	2.83	0.50
2:h:158:LEU:O	2:I:221:LYS:NZ	2.39	0.50
8:a:1290:LYS:HG2	8:a:1312:GLU:HA	1.94	0.50
8:A:941:ARG:NE	8:A:987:LEU:O	2.44	0.50
8:B:1191:ASN:ND2	8:B:1319:GLN:O	2.42	0.50
8:C:215:ILE:HG21	8:C:1278:LEU:HD11	1.93	0.50
8:C:804:LEU:HD23	8:C:889:HIS:HD2	1.77	0.50
8:C:927:PRO:HB2	8:C:930:LEU:HB2	1.93	0.50
8:Z:263:THR:HB	8:Z:267:ALA:HB3	1.92	0.50
1:x:240:ARG:HA	1:x:251:ARG:HH21	1.76	0.50
7:S:62:LEU:HA	7:S:65:LEU:HD12	1.93	0.50
8:A:257:ASN:O	8:A:260:THR:OG1	2.29	0.50
8:Z:970:ASP:HB3	8:Z:996:ALA:HB2	1.93	0.50
7:S:28:LEU:HD12	7:S:29:PRO:HD2	1.93	0.50
8:a:1239:LEU:HA	8:a:1242:VAL:HG12	1.94	0.50
8:A:256:ASP:OD1	8:A:256:ASP:N	2.45	0.50
8:B:927:PRO:HD2	8:B:952:LEU:HD21	1.94	0.50
8:C:375:VAL:HG13	8:C:376:TYR:HD1	1.77	0.50
8:Y:900:ASP:OD2	8:Y:1014:LYS:NZ	2.45	0.50
8:Z:1199:MET:HB3	8:Z:1275:ASN:HB3	1.94	0.50
2:I:102:TRP:O	2:I:297:ASN:ND2	2.45	0.50
8:a:216:LEU:HD21	8:a:1200:LEU:HB3	1.93	0.50
8:A:510:ASN:ND2	8:A:989:SER:OG	2.44	0.50
8:A:1325:LEU:HD12	8:A:1357:GLY:HA2	1.93	0.50
8:B:510:ASN:ND2	8:B:538:ASP:OD2	2.45	0.50
8:C:197:VAL:HG23	8:Z:20:LEU:HD11	1.94	0.50
8:D:697:GLN:HB2	8:D:702:PRO:HA	1.92	0.50
8:Z:1284:GLU:OE2	8:Z:1288:ARG:NH1	2.43	0.50
5:M:423:CYS:SG	5:M:424:ILE:N	2.84	0.50
8:a:495:ILE:HG23	8:a:496:PRO:HD3	1.94	0.50
8:A:903:GLN:NE2	8:A:1015:ILE:O	2.44	0.50
8:B:1211:THR:HA	8:B:1214:ILE:HG22	1.94	0.50
8:C:1182:ASP:N	8:C:1182:ASP:OD1	2.43	0.50
8:Y:292:THR:HG21	8:Y:361:ARG:HH22	1.77	0.50
8:Z:1110:VAL:HA	8:Z:1171:ALA:HB3	1.94	0.50
8:a:1245:ASN:HD21	8:a:1247:ARG:HB3	1.77	0.50
8:A:450:CYS:HB3	8:A:1131:ILE:HD11	1.93	0.50
8:B:82:ASP:OD1	8:B:82:ASP:N	2.45	0.50
8:B:619:GLY:HA3	8:B:652:ALA:HB1	1.94	0.50
2:h:152:ILE:HD12	2:I:268:LEU:HB3	1.94	0.50
8:B:795:ASN:ND2	8:B:969:HIS:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:535:PRO:HG3	8:C:1175:ILE:HG21	1.94	0.50
8:C:1263:ALA:O	8:C:1267:ASN:ND2	2.45	0.50
1:x:253:ILE:HD11	1:x:270:LEU:HB3	1.92	0.49
2:h:62:ARG:O	2:h:66:ARG:NH1	2.45	0.49
5:M:168:LEU:HD23	5:M:317:VAL:HG21	1.93	0.49
7:Q:73:THR:O	7:Q:74:ARG:NH1	2.45	0.49
8:A:642:ARG:HB3	8:A:644:LEU:HD13	1.94	0.49
8:B:796:ARG:O	8:B:945:ASN:ND2	2.36	0.49
8:C:599:THR:O	8:C:603:SER:OG	2.29	0.49
8:D:526:ASN:HB2	8:D:528:THR:HG22	1.94	0.49
8:Y:672:PHE:HA	8:Y:675:ARG:HG2	1.93	0.49
8:Y:675:ARG:HA	8:Y:678:VAL:HG12	1.93	0.49
2:h:220:ARG:NH2	2:h:242:ASP:OD2	2.44	0.49
2:n:209:ASN:HA	2:o:241:LEU:HD13	1.93	0.49
2:o:41:ILE:HD11	2:o:45:GLN:HB2	1.93	0.49
4:g:241:ILE:HD12	4:g:242:PRO:HD2	1.94	0.49
8:a:513:LYS:NZ	8:a:532:GLU:OE1	2.44	0.49
8:A:1337:LEU:HD12	8:A:1338:LYS:HG3	1.94	0.49
2:h:160:ARG:NH2	2:I:264:GLU:OE2	2.45	0.49
5:M:471:GLN:OE1	5:M:473:TRP:NE1	2.41	0.49
8:a:557:VAL:HG23	8:a:559:GLY:H	1.77	0.49
8:D:606:TYR:OH	8:D:648:ALA:N	2.45	0.49
8:D:800:LEU:HB3	8:D:923:VAL:HG11	1.95	0.49
8:Z:449:LEU:HD12	8:Z:1020:LEU:HD21	1.94	0.49
8:Z:855:GLU:O	8:Z:858:THR:OG1	2.29	0.49
2:n:255:ARG:NH2	1:I:194:THR:OG1	2.46	0.49
5:M:320:VAL:O	6:N:59:ARG:NH2	2.38	0.49
8:a:310:GLU:HB2	8:C:325:PHE:HE2	1.77	0.49
8:A:314:THR:O	8:A:317:SER:OG	2.30	0.49
8:D:934:SER:HB2	8:D:952:LEU:HD11	1.95	0.49
2:I:152:ILE:HD13	2:I:155:LEU:HD12	1.95	0.49
2:n:126:THR:HG23	2:n:131:GLU:HG2	1.93	0.49
5:M:368:ILE:HG22	5:M:415:MET:HE1	1.94	0.49
8:a:405:ARG:NH1	8:Z:421:ARG:O	2.46	0.49
8:B:74:ALA:HA	8:B:1053:SER:H	1.77	0.49
8:B:615:VAL:HG11	8:B:802:LEU:HD12	1.93	0.49
8:D:317:SER:OG	8:D:318:TYR:N	2.46	0.49
8:Z:558:ILE:HD11	8:Z:1031:GLY:HA3	1.93	0.49
8:Z:698:LEU:HD11	8:Z:1018:VAL:HG21	1.94	0.49
2:n:280:ASP:HB2	4:m:213:GLN:HE21	1.76	0.49
8:a:87:THR:OG1	8:a:88:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:357:MET:HE3	8:a:368:ILE:HD13	1.94	0.49
8:B:109:SER:OG	8:B:111:GLN:O	2.31	0.49
8:C:432:ASN:ND2	8:C:436:ALA:O	2.46	0.49
8:D:536:PHE:HD1	8:D:1015:ILE:HD12	1.76	0.49
8:Y:801:GLY:HA3	8:Y:890:VAL:HB	1.94	0.49
2:n:262:ASP:N	2:n:262:ASP:OD1	2.46	0.49
5:M:316:GLU:HA	5:M:327:ARG:HA	1.95	0.49
1:1:239:LEU:O	1:1:251:ARG:NH2	2.44	0.49
8:a:432:ASN:ND2	8:a:436:ALA:O	2.45	0.49
8:a:599:THR:O	8:a:603:SER:OG	2.28	0.49
8:C:716:TRP:H	8:C:914:GLN:HE22	1.61	0.49
8:C:1018:VAL:HG12	8:C:1131:ILE:HD11	1.94	0.49
8:C:1191:ASN:ND2	8:C:1197:SER:OG	2.45	0.49
8:D:387:ARG:NH2	8:D:1310:LEU:O	2.46	0.49
8:D:507:ARG:HH21	8:D:512:MET:HG3	1.77	0.49
8:D:682:ARG:HE	8:D:780:LEU:HD11	1.77	0.49
2:o:236:GLU:HG3	6:O:10:LEU:HG	1.95	0.49
4:m:69:ARG:HH21	4:m:79:HIS:CG	2.30	0.49
1:1:99:ARG:O	1:1:103:ARG:HB2	2.12	0.49
8:a:230:LEU:HD21	8:a:282:ILE:HB	1.95	0.49
8:a:1293:ILE:HD12	8:a:1300:GLN:HB3	1.95	0.49
8:A:714:ARG:HH12	8:A:900:ASP:HB2	1.77	0.49
8:A:1112:ASP:OD2	8:A:1112:ASP:N	2.37	0.49
8:B:488:MET:HE3	8:B:894:GLU:HB2	1.95	0.49
8:C:1289:ALA:O	8:C:1316:ARG:NH1	2.46	0.49
8:Y:121:GLU:HB2	8:Y:1083:THR:HG23	1.93	0.49
8:Y:970:ASP:OD1	8:Y:970:ASP:N	2.42	0.49
1:x:239:LEU:O	1:x:251:ARG:NH2	2.46	0.49
2:h:8:ILE:HG13	2:h:83:LEU:HB2	1.95	0.49
5:M:136:CYS:HB3	5:M:141:LEU:HD12	1.94	0.49
7:T:75:ARG:HH12	8:D:625:LEU:HB3	1.76	0.49
8:A:773:ALA:HB1	8:A:777:GLU:HG3	1.94	0.49
8:D:79:LYS:HE2	8:D:302:TYR:HD2	1.76	0.49
8:D:1265:TYR:OH	8:D:1320:GLU:O	2.28	0.49
8:Y:983:TYR:O	8:Y:988:ARG:NH2	2.41	0.49
8:Z:274:VAL:HG12	8:Z:370:GLU:HB3	1.94	0.49
8:Z:820:MET:HE3	8:Z:877:ARG:HD3	1.95	0.49
8:Z:1245:ASN:HB2	8:Z:1248:HIS:HB2	1.95	0.49
8:Z:1330:LEU:HA	8:Z:1333:MET:HB3	1.94	0.49
2:h:33:PRO:HB2	2:h:68:MET:HE2	1.95	0.49
4:m:188:ILE:HG12	4:m:248:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:22:VAL:HA	7:S:26:LEU:HB3	1.95	0.49
8:a:1193:ARG:NH2	8:a:1214:ILE:O	2.39	0.49
8:C:86:LEU:HD11	8:C:1082:ASN:HD21	1.77	0.49
8:Y:102:SER:OG	8:Y:103:GLY:N	2.45	0.49
8:B:71:LEU:HD11	8:B:372:LEU:HD11	1.95	0.48
8:Y:18:ASP:OD1	8:Y:18:ASP:N	2.46	0.48
1:x:45:ARG:HG3	1:x:46:LEU:HD12	1.95	0.48
2:h:35:PRO:HD3	2:h:68:MET:HE3	1.94	0.48
5:M:560:GLN:NE2	5:M:561:ASN:O	2.46	0.48
6:N:30:VAL:HG23	6:N:33:ARG:HH21	1.79	0.48
8:B:527:ILE:HG22	8:B:1218:ARG:HH22	1.78	0.48
8:Z:954:ASP:HA	8:Z:957:LYS:HB3	1.94	0.48
5:M:55:THR:OG1	5:M:135:ARG:NH2	2.44	0.48
7:T:22:VAL:HA	7:T:26:LEU:HB2	1.95	0.48
8:A:717:PRO:HB3	8:A:782:LYS:HA	1.94	0.48
8:C:186:LYS:O	8:C:1092:SER:OG	2.32	0.48
8:D:404:ASP:OD1	8:D:404:ASP:N	2.47	0.48
8:Y:940:HIS:O	8:Y:944:SER:OG	2.30	0.48
8:Y:1173:GLU:O	8:Y:1244:TYR:OH	2.30	0.48
8:Z:699:ALA:HB3	8:Z:701:GLU:HG2	1.95	0.48
2:h:71:THR:OG1	2:h:72:LEU:N	2.46	0.48
4:m:17:ASP:N	4:m:17:ASP:OD1	2.43	0.48
5:M:388:GLN:HA	5:M:539:PHE:HA	1.94	0.48
1:1:119:ARG:NH2	1:1:218:GLU:OE1	2.46	0.48
7:i:66:ARG:HB2	8:Z:884:GLN:HA	1.96	0.48
8:B:558:ILE:HG21	8:B:574:ARG:HH22	1.78	0.48
8:C:538:ASP:OD1	8:C:538:ASP:N	2.44	0.48
8:C:714:ARG:NH1	8:C:900:ASP:OD1	2.46	0.48
8:C:719:PHE:HD1	8:C:917:LEU:HD22	1.78	0.48
8:D:275:SER:HB3	8:D:280:MET:HE2	1.96	0.48
1:x:3:LEU:HD11	1:x:61:GLY:HA3	1.95	0.48
8:a:534:HIS:HD2	8:a:536:PHE:H	1.60	0.48
8:a:717:PRO:HB3	8:a:782:LYS:HA	1.95	0.48
8:a:861:VAL:HA	8:a:864:VAL:HG22	1.95	0.48
8:A:5:SER:N	8:A:8:GLU:OE2	2.43	0.48
8:A:724:PRO:HG2	8:A:727:MET:HG2	1.95	0.48
8:D:521:PHE:O	8:D:526:ASN:ND2	2.46	0.48
8:B:905:GLN:O	8:B:1123:ARG:NH2	2.47	0.48
8:C:720:VAL:HG23	8:C:918:TYR:HD1	1.78	0.48
8:C:1329:THR:HG23	8:C:1332:LEU:H	1.79	0.48
8:D:704:SER:HA	8:D:707:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:866:THR:OG1	8:Y:870:THR:O	2.30	0.48
8:Y:1176:LEU:HD21	8:Y:1233:ALA:HB2	1.95	0.48
2:o:91:LEU:HA	2:o:303:ILE:HA	1.96	0.48
8:a:85:LYS:NZ	8:B:138:TYR:OH	2.46	0.48
8:a:488:MET:HE1	8:a:978:ALA:HB1	1.96	0.48
8:a:605:ASN:OD1	8:a:605:ASN:N	2.45	0.48
8:Z:1217:HIS:HE1	8:Z:1228:THR:HB	1.78	0.48
2:I:240:ARG:NH1	4:g:235:ILE:O	2.46	0.48
8:a:358:ASP:N	8:a:358:ASP:OD1	2.43	0.48
8:A:1029:HIS:ND1	8:A:1030:PRO:O	2.46	0.48
8:B:622:ASP:OD1	8:B:622:ASP:N	2.46	0.48
8:B:1285:TYR:HA	8:B:1289:ALA:HB3	1.96	0.48
8:Y:1032:PHE:HA	8:Y:1178:PRO:HD3	1.95	0.48
8:Z:617:VAL:HG12	8:Z:619:GLY:H	1.79	0.48
5:M:65:ASP:N	5:M:65:ASP:OD1	2.47	0.48
5:M:484:GLN:NE2	8:a:484:GLN:OE1	2.47	0.48
8:A:301:THR:OG1	8:A:302:TYR:N	2.47	0.48
8:B:734:ALA:H	8:B:739:LEU:HD23	1.77	0.48
8:Y:417:ASN:O	8:Y:422:ASN:ND2	2.39	0.48
8:Y:454:LEU:HD22	8:Y:1239:LEU:HD11	1.96	0.48
7:S:26:LEU:HD11	7:S:64:LEU:HD22	1.96	0.48
8:a:275:SER:OG	8:a:276:THR:N	2.46	0.48
8:a:1038:ARG:NH1	8:a:1107:GLY:O	2.47	0.48
8:B:1162:ALA:O	8:C:209:ARG:NH2	2.47	0.48
8:D:597:PHE:HA	8:D:600:THR:HG22	1.96	0.48
8:Y:688:SER:OG	8:Y:711:HIS:NE2	2.41	0.48
8:Y:1195:ARG:NH1	8:Y:1227:ALA:O	2.46	0.48
1:x:271:LEU:O	1:x:278:TYR:OH	2.29	0.47
4:m:249:GLN:HB3	4:m:286:PHE:HA	1.96	0.47
1:l:161:ASP:HA	1:l:164:VAL:HG12	1.96	0.47
7:Q:26:LEU:O	8:A:813:TYR:OH	2.30	0.47
7:S:75:ARG:NH1	8:C:625:LEU:O	2.46	0.47
7:T:66:ARG:HH12	8:D:756:ARG:HH21	1.62	0.47
8:a:342:ASP:O	8:a:346:GLN:NE2	2.47	0.47
8:A:389:VAL:HG12	8:A:1311:ILE:HA	1.96	0.47
8:C:1196:ALA:HB2	8:C:1223:GLN:HB2	1.96	0.47
8:C:1318:THR:OG1	8:C:1320:GLU:OE1	2.25	0.47
8:Z:785:TYR:O	8:Z:943:TYR:OH	2.26	0.47
8:Z:895:VAL:HB	8:Z:914:GLN:HB2	1.96	0.47
2:h:18:ILE:HD11	8:Z:51:GLU:HG2	1.95	0.47
5:M:319:ASP:OD2	5:M:324:VAL:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:889:HIS:O	8:A:919:ASN:ND2	2.43	0.47
8:D:654:VAL:HG11	8:D:677:LEU:HD23	1.95	0.47
8:Y:717:PRO:HB3	8:Y:782:LYS:HA	1.95	0.47
8:Z:1045:ASP:OD1	8:Z:1045:ASP:N	2.38	0.47
1:1:194:THR:HB	1:1:197:VAL:HG23	1.97	0.47
7:Q:61:LYS:HD2	8:A:813:TYR:CZ	2.50	0.47
8:a:1329:THR:HG23	8:a:1332:LEU:H	1.79	0.47
8:A:127:ILE:HD12	8:A:128:PRO:HD2	1.97	0.47
8:C:675:ARG:HE	8:D:603:SER:HA	1.79	0.47
8:D:858:THR:HA	8:D:861:VAL:HG12	1.96	0.47
8:Y:712:ASP:O	8:Y:782:LYS:NZ	2.33	0.47
8:Z:625:LEU:HD13	8:Z:628:ARG:HD2	1.96	0.47
8:a:390:ASP:HB3	8:a:1041:THR:HG22	1.96	0.47
8:a:1132:ARG:HH12	8:a:1140:PRO:HB3	1.79	0.47
8:A:481:CYS:SG	8:A:482:ARG:N	2.87	0.47
8:B:684:VAL:HA	8:B:687:ILE:HG22	1.97	0.47
8:B:1101:ARG:HE	8:C:214:ASN:HB3	1.79	0.47
8:B:1164:THR:HG21	8:C:209:ARG:HE	1.78	0.47
8:B:1185:TYR:OH	8:B:1191:ASN:O	2.23	0.47
8:C:718:PRO:HA	8:C:916:VAL:HG23	1.96	0.47
8:B:424:LEU:HD12	8:B:425:PRO:HD2	1.97	0.47
8:C:804:LEU:HA	8:C:807:LEU:HB3	1.96	0.47
8:Y:1183:VAL:HA	8:Y:1187:LYS:HD2	1.96	0.47
8:Z:109:SER:OG	8:Z:110:ARG:N	2.47	0.47
1:x:166:ARG:HD2	1:x:186:LEU:HD21	1.97	0.47
2:h:206:MET:HE1	2:I:237:LEU:HD13	1.96	0.47
7:Q:22:VAL:HG13	7:Q:28:LEU:HD12	1.96	0.47
8:a:146:THR:O	8:a:150:LYS:NZ	2.44	0.47
8:a:514:GLN:HE22	8:a:563:ASP:H	1.62	0.47
8:a:584:LEU:HD21	8:a:683:LEU:HD11	1.94	0.47
8:a:807:LEU:HD11	8:a:930:LEU:HD23	1.96	0.47
8:B:263:THR:OG1	8:B:264:SER:N	2.47	0.47
8:B:1345:ALA:HA	8:B:1358:GLU:HB3	1.96	0.47
8:B:1367:LEU:O	8:B:1370:SER:OG	2.31	0.47
8:Z:138:TYR:O	8:Z:153:ASN:ND2	2.40	0.47
2:n:108:LEU:HB2	2:n:288:PHE:HB2	1.97	0.47
2:n:191:GLN:HA	2:n:194:LEU:HD12	1.96	0.47
4:g:186:TYR:N	4:g:205:LEU:O	2.47	0.47
7:Q:66:ARG:NH2	8:A:884:GLN:O	2.39	0.47
8:a:195:THR:O	8:a:199:ASN:ND2	2.41	0.47
8:a:803:ASN:OD1	8:a:889:HIS:NE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:1234:SER:OG	8:a:1235:GLN:OE1	2.32	0.47
8:A:723:LEU:HG	8:A:768:VAL:HG21	1.96	0.47
8:Y:775:ASP:N	8:Y:775:ASP:OD1	2.40	0.47
8:Z:317:SER:OG	8:Z:318:TYR:N	2.47	0.47
1:1:111:ARG:NH2	1:1:113:GLU:OE2	2.48	0.47
8:B:520:ASP:HA	8:B:523:LYS:HG2	1.96	0.47
8:C:135:CYS:O	8:C:139:LEU:HB2	2.14	0.47
8:D:315:ALA:HB2	8:D:321:ILE:HD11	1.96	0.47
8:D:575:THR:HG21	8:D:1007:THR:HA	1.96	0.47
8:D:790:PRO:HA	8:D:793:THR:HG22	1.96	0.47
8:D:1290:LYS:HE2	8:D:1310:LEU:HB3	1.97	0.47
8:Z:379:THR:OG1	8:Z:380:ASP:N	2.48	0.47
8:Z:1132:ARG:NH2	8:Z:1138:GLU:O	2.48	0.47
7:T:67:MET:HA	7:T:70:VAL:HG12	1.97	0.47
8:A:87:THR:OG1	8:A:88:THR:N	2.47	0.47
8:A:508:THR:OG1	8:A:509:VAL:N	2.45	0.47
8:A:1182:ASP:O	8:A:1186:PHE:N	2.45	0.47
8:C:1173:GLU:O	8:C:1244:TYR:OH	2.32	0.47
8:D:761:ASP:HB3	8:D:889:HIS:HD1	1.80	0.47
8:Y:428:ALA:HB3	8:Y:440:ILE:HG23	1.96	0.47
8:Z:212:ARG:NH1	8:Z:1203:ASP:OD1	2.48	0.47
2:n:40:LEU:O	8:a:105:GLY:N	2.48	0.47
8:a:790:PRO:HA	8:a:793:THR:HG22	1.97	0.47
8:A:646:VAL:O	8:A:674:TYR:OH	2.32	0.47
8:A:798:CYS:SG	8:A:945:ASN:N	2.88	0.47
8:D:534:HIS:CE1	8:D:1239:LEU:HD13	2.50	0.47
8:Y:1016:SER:O	8:Y:1019:SER:OG	2.32	0.47
8:Y:1176:LEU:HD13	8:Y:1176:LEU:HA	1.76	0.47
8:Z:442:PHE:HB3	8:Z:1024:THR:HG23	1.96	0.47
8:Z:446:LEU:HD11	8:Z:1021:VAL:HG22	1.96	0.47
2:I:79:ASN:HB3	8:B:122:LYS:HD2	1.98	0.46
2:n:59:VAL:HG12	2:n:62:ARG:HH21	1.81	0.46
5:M:312:SER:OG	5:M:313:ARG:N	2.48	0.46
8:C:690:LEU:HD22	8:C:707:VAL:HG21	1.96	0.46
8:C:1185:TYR:OH	8:C:1191:ASN:O	2.24	0.46
8:D:1057:VAL:HG12	8:D:1083:THR:HG22	1.96	0.46
8:D:1144:ASP:OD1	8:D:1144:ASP:N	2.48	0.46
8:Y:641:THR:HG23	8:Y:642:ARG:HG3	1.96	0.46
8:Z:351:SER:OG	8:Z:352:LEU:N	2.48	0.46
2:h:88:HIS:HA	2:h:305:LYS:HB3	1.97	0.46
2:o:71:THR:HG21	2:o:83:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:71:SER:OG	7:i:72:ARG:NH1	2.48	0.46
8:B:1091:THR:OG1	8:B:1092:SER:N	2.48	0.46
5:M:528:ASP:OD1	5:M:528:ASP:N	2.45	0.46
6:N:26:CYS:O	6:O:2:SER:N	2.49	0.46
7:Q:59:ALA:HA	8:A:805:LYS:HZ2	1.80	0.46
7:R:55:ASN:OD1	7:R:55:ASN:N	2.49	0.46
7:T:21:VAL:O	7:T:25:VAL:HB	2.15	0.46
7:i:32:ILE:HD11	7:i:37:HIS:HB2	1.96	0.46
8:a:507:ARG:NH1	8:Z:695:ASN:OD1	2.48	0.46
8:a:532:GLU:OE1	8:a:555:ARG:NH1	2.38	0.46
8:a:646:VAL:O	8:a:674:TYR:OH	2.33	0.46
8:a:1203:ASP:OD1	8:a:1203:ASP:N	2.48	0.46
8:C:69:SER:HB2	8:C:374:ARG:HH22	1.79	0.46
8:D:1059:ILE:HB	8:D:1079:GLN:HE21	1.81	0.46
8:D:1104:THR:HG22	8:D:1168:GLN:HB2	1.97	0.46
8:Y:688:SER:OG	8:Y:689:ALA:N	2.46	0.46
8:Y:747:ARG:NH1	8:Y:888:GLU:OE2	2.48	0.46
8:Z:488:MET:HE2	8:Z:894:GLU:HG2	1.97	0.46
8:Z:540:THR:OG1	8:Z:541:HIS:N	2.48	0.46
8:Z:856:MET:HE3	8:Z:856:MET:HB2	1.89	0.46
1:x:244:SER:OG	1:x:246:ASP:OD1	2.32	0.46
2:I:279:ASP:OD1	2:I:279:ASP:N	2.46	0.46
2:n:204:MET:HA	2:n:207:VAL:HG12	1.97	0.46
4:m:101:LEU:HD11	4:m:269:LEU:HB3	1.97	0.46
8:a:807:LEU:HD12	8:a:933:TYR:HB2	1.96	0.46
8:D:900:ASP:OD1	8:D:900:ASP:N	2.44	0.46
5:M:321:GLN:NE2	5:M:357:TYR:OH	2.34	0.46
7:Q:72:ARG:NE	8:A:820:MET:O	2.38	0.46
8:a:718:PRO:HA	8:a:916:VAL:HG23	1.98	0.46
8:B:14:GLY:HA3	8:Z:60:ARG:HH21	1.79	0.46
8:C:120:SER:HB3	8:C:1084:VAL:HG22	1.97	0.46
8:C:1109:ARG:HH11	8:C:1169:LYS:HB3	1.81	0.46
8:D:87:THR:OG1	8:D:88:THR:N	2.49	0.46
1:x:136:ALA:HB2	1:x:200:VAL:HG11	1.98	0.46
2:I:270:ALA:HA	2:I:273:VAL:HG12	1.98	0.46
8:a:607:PRO:HD3	8:a:638:MET:HE2	1.98	0.46
8:a:1020:LEU:HA	8:a:1023:GLN:HE21	1.81	0.46
8:a:1125:ASP:OD1	8:a:1129:ARG:NH2	2.49	0.46
8:C:502:ARG:O	8:C:503:ARG:NE	2.48	0.46
8:C:796:ARG:O	8:C:945:ASN:ND2	2.49	0.46
8:Y:668:PRO:HB3	8:Z:642:ARG:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:387:ARG:N	8:Z:1044:VAL:O	2.48	0.46
1:x:118:VAL:HB	1:x:214:ARG:HE	1.80	0.46
2:I:88:HIS:ND1	2:I:306:GLY:OXT	2.44	0.46
8:A:131:LEU:O	8:A:1072:SER:OG	2.32	0.46
8:A:513:LYS:HE2	8:A:562:PRO:HG3	1.97	0.46
8:B:601:VAL:HG13	8:B:924:VAL:HG21	1.98	0.46
8:D:276:THR:OG1	8:D:277:ALA:N	2.48	0.46
8:D:424:LEU:HD13	8:D:573:LEU:HD23	1.97	0.46
8:D:1269:GLU:HA	8:D:1272:ILE:HG22	1.97	0.46
8:Z:269:ILE:HD13	8:Z:368:ILE:HD11	1.97	0.46
2:n:8:ILE:HB	2:n:83:LEU:HB2	1.97	0.46
2:n:194:LEU:HA	2:n:197:MET:HE3	1.96	0.46
5:M:3:THR:OG1	5:M:93:CYS:SG	2.67	0.46
5:M:55:THR:HG1	5:M:135:ARG:HH21	1.64	0.46
8:B:641:THR:HG23	8:B:642:ARG:HG3	1.98	0.46
8:C:263:THR:HG22	8:C:296:VAL:HG12	1.98	0.46
8:D:1332:LEU:HD13	8:D:1355:VAL:HG23	1.98	0.46
8:Z:1316:ARG:O	8:Z:1319:GLN:NE2	2.46	0.46
1:1:223:LYS:HA	1:1:223:LYS:HD2	1.84	0.46
1:1:223:LYS:HE2	1:1:227:ARG:HG2	1.97	0.46
8:B:1112:ASP:OD2	8:B:1112:ASP:N	2.49	0.46
8:C:1064:VAL:HG22	8:C:1077:VAL:HG12	1.98	0.46
8:D:661:LEU:HB3	8:D:666:LEU:HD11	1.97	0.46
8:Y:894:GLU:HG3	8:Y:896:ARG:HG3	1.98	0.46
4:g:251:LEU:O	4:g:282:GLU:N	2.43	0.46
4:m:148:CYS:SG	4:m:149:VAL:N	2.88	0.46
8:A:1067:GLU:OE1	8:A:1074:THR:OG1	2.30	0.46
8:C:681:LEU:HB3	8:C:780:LEU:HD22	1.98	0.46
8:C:1195:ARG:NH2	8:C:1219:GLU:O	2.44	0.46
8:D:424:LEU:HD12	8:D:425:PRO:HD2	1.98	0.46
8:Y:66:PHE:HA	8:Y:176:ILE:HD11	1.98	0.46
8:Y:1168:GLN:NE2	8:Y:1297:THR:O	2.40	0.46
8:a:273:MET:HE2	8:a:369:MET:HE1	1.97	0.45
8:a:307:LEU:HD11	8:a:321:ILE:HD12	1.98	0.45
8:a:953:SER:OG	8:a:954:ASP:N	2.49	0.45
8:a:1032:PHE:HA	8:a:1178:PRO:HD3	1.98	0.45
8:a:1036:ALA:HA	8:a:1173:GLU:HA	1.98	0.45
8:A:180:LEU:HD11	8:A:372:LEU:HD13	1.98	0.45
8:A:562:PRO:HG2	8:A:565:LEU:HD13	1.99	0.45
8:B:269:ILE:HG22	8:B:271:GLY:H	1.81	0.45
8:B:1040:ASP:HA	8:B:1104:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:295:THR:HA	8:C:356:SER:HA	1.97	0.45
8:D:360:ILE:HG23	8:D:367:VAL:HG23	1.98	0.45
8:D:435:ARG:HH21	8:D:1364:GLN:HA	1.81	0.45
8:D:614:ASP:OD2	8:D:649:HIS:NE2	2.49	0.45
8:D:662:ALA:HA	8:D:671:LEU:HD21	1.97	0.45
8:D:1023:GLN:HE21	8:D:1030:PRO:HB3	1.80	0.45
8:Y:1039:THR:HG21	8:Y:1259:TYR:HE2	1.81	0.45
8:Y:1143:LEU:O	8:Y:1147:THR:OG1	2.29	0.45
8:Z:609:LEU:HD21	8:Z:630:PHE:HE2	1.81	0.45
3:H:2225:ALA:HB1	6:N:72:VAL:HG22	1.98	0.45
2:n:277:GLN:NE2	4:m:220:ARG:HH21	2.15	0.45
5:M:23:LEU:HD21	5:M:168:LEU:HD13	1.97	0.45
5:M:422:SER:OG	5:M:476:ASP:OD2	2.30	0.45
8:a:782:LYS:O	8:a:786:LEU:HB2	2.16	0.45
8:A:770:ASP:OD1	8:A:770:ASP:N	2.41	0.45
8:D:1336:LYS:NZ	8:D:1348:GLU:OE1	2.44	0.45
4:m:89:ILE:HD12	4:m:115:LEU:HD22	1.98	0.45
7:Q:61:LYS:HD2	8:A:813:TYR:CE2	2.52	0.45
7:R:72:ARG:HH21	8:B:821:PRO:HA	1.82	0.45
8:A:1204:PRO:HB3	8:A:1279:PHE:HD2	1.79	0.45
8:B:628:ARG:NH2	8:B:663:ASP:OD2	2.48	0.45
8:B:924:VAL:HG13	8:B:925:THR:HG23	1.97	0.45
8:C:1039:THR:HG21	8:C:1259:TYR:HE2	1.80	0.45
8:D:601:VAL:HG13	8:D:924:VAL:HG11	1.98	0.45
8:Y:795:ASN:HD21	8:Y:942:PHE:HD1	1.64	0.45
8:Y:941:ARG:NH1	8:Y:982:GLU:OE1	2.49	0.45
8:Y:1044:VAL:HG21	8:Y:1096:VAL:HG13	1.98	0.45
8:Y:1172:CYS:SG	8:Y:1173:GLU:N	2.88	0.45
2:h:239:MET:HG2	2:h:243:ARG:HD3	1.98	0.45
2:o:105:GLY:H	2:o:290:VAL:HB	1.82	0.45
8:B:786:LEU:HD22	8:B:987:LEU:HD11	1.97	0.45
8:B:798:CYS:SG	8:B:799:GLY:N	2.89	0.45
8:D:481:CYS:SG	8:D:482:ARG:N	2.89	0.45
8:Y:311:ASN:HA	8:Y:314:THR:HG22	1.98	0.45
8:Z:1245:ASN:O	8:Z:1249:ARG:N	2.40	0.45
2:I:293:VAL:HG23	2:I:300:ALA:HB2	1.98	0.45
8:a:300:ALA:N	8:a:351:SER:OG	2.48	0.45
8:A:134:ALA:O	8:A:137:THR:OG1	2.35	0.45
8:C:173:ARG:NH2	8:C:375:VAL:O	2.49	0.45
8:Y:142:THR:HA	8:Y:153:ASN:HD21	1.82	0.45
8:Y:638:MET:HA	8:Y:641:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:1347:SER:HB2	8:Y:1357:GLY:H	1.82	0.45
5:M:422:SER:OG	5:M:423:CYS:N	2.39	0.45
7:Q:45:SER:OG	7:Q:49:ARG:NH2	2.47	0.45
8:a:1346:THR:HB	8:Z:1338:LYS:HG2	1.98	0.45
8:B:1287:LEU:HD12	8:B:1288:ARG:HB2	1.98	0.45
8:D:182:THR:HG21	8:D:1083:THR:HG21	1.99	0.45
2:o:113:PRO:HD3	2:o:135:PRO:HA	1.99	0.45
4:g:245:THR:HB	4:g:290:VAL:HA	1.98	0.45
7:R:72:ARG:HG3	8:B:820:MET:HB3	1.98	0.45
8:A:237:ASP:OD1	8:A:237:ASP:N	2.48	0.45
8:B:596:LEU:HD23	8:B:596:LEU:HA	1.79	0.45
7:S:66:ARG:HG3	7:S:67:MET:HE2	1.98	0.45
7:T:28:LEU:HD12	7:T:32:ILE:HD13	1.98	0.45
8:D:747:ARG:NH1	8:D:769:ASP:OD1	2.50	0.45
8:Y:1293:ILE:HG12	8:Y:1311:ILE:HD11	1.99	0.45
8:Z:284:MET:HG2	8:Z:291:ILE:HG21	1.97	0.45
8:Z:452:PRO:HB3	8:Z:905:GLN:HE22	1.82	0.45
8:Z:596:LEU:HD12	8:Z:596:LEU:HA	1.80	0.45
1:x:246:ASP:HB2	1:x:278:TYR:HA	1.99	0.45
1:x:270:LEU:HD12	1:x:270:LEU:HA	1.88	0.45
4:m:101:LEU:O	4:m:104:SER:OG	2.30	0.45
1:l:19:PHE:HE1	1:l:26:LYS:HZ3	1.63	0.45
8:a:180:LEU:HD21	8:a:385:LEU:HG	1.98	0.45
8:a:280:MET:HB3	8:a:284:MET:HE3	1.99	0.45
8:a:1004:SER:HA	8:a:1007:THR:HG22	1.99	0.45
8:a:1228:THR:OG1	8:a:1229:HIS:N	2.50	0.45
8:C:174:GLY:HA3	8:D:101:ALA:HB3	1.97	0.45
8:Y:646:VAL:O	8:Y:674:TYR:OH	2.34	0.45
8:Z:84:ASN:HB3	8:Z:1080:ASN:HD22	1.82	0.45
8:Z:173:ARG:NH2	8:Z:375:VAL:O	2.49	0.45
8:Z:611:TYR:CZ	8:Z:923:VAL:HG13	2.52	0.45
2:n:153:MET:HG2	2:n:172:LEU:HD23	1.99	0.45
2:o:127:LEU:HB2	2:o:130:TRP:HB3	1.98	0.45
7:S:52:SER:OG	7:S:53:LEU:N	2.45	0.45
8:A:1322:LEU:HD21	8:A:1360:ILE:HG12	1.98	0.45
8:B:22:HIS:CE1	8:B:24:LYS:HB2	2.51	0.45
8:B:419:THR:HG22	8:B:421:ARG:H	1.81	0.45
8:B:561:LEU:HD23	8:B:561:LEU:HA	1.87	0.45
8:C:534:HIS:CD2	8:C:536:PHE:H	2.32	0.45
8:C:686:ARG:HG3	8:D:968:ARG:HH22	1.82	0.45
8:D:488:MET:HE1	8:D:978:ALA:HB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:1307:THR:OG1	8:Z:1308:GLU:OE1	2.35	0.45
5:M:40:LEU:HD21	5:M:151:LEU:HD12	1.98	0.44
8:B:1057:VAL:HG12	8:B:1083:THR:HB	1.98	0.44
8:C:1086:MET:HE3	8:C:1086:MET:HB2	1.89	0.44
8:D:1217:HIS:NE2	8:D:1234:SER:O	2.41	0.44
8:Y:596:LEU:HD21	8:Y:639:PHE:HE1	1.82	0.44
7:R:33:SER:H	7:R:36:THR:HG1	1.63	0.44
7:i:40:LEU:O	7:i:44:LEU:HB2	2.17	0.44
8:A:1336:LYS:HG3	8:A:1355:VAL:HG11	1.99	0.44
8:C:79:LYS:HG3	8:C:302:TYR:HB2	1.99	0.44
8:Y:846:ILE:HA	8:Y:849:GLN:HE21	1.82	0.44
8:Z:454:LEU:HD23	8:Z:1239:LEU:HD11	1.99	0.44
1:x:129:LEU:HB3	1:x:154:ILE:HD12	1.99	0.44
8:C:459:PRO:HB2	8:C:1242:VAL:HG21	1.99	0.44
8:C:1002:LEU:HG	8:C:1006:MET:HE3	2.00	0.44
8:Z:857:LEU:HA	8:Z:860:LEU:HB2	2.00	0.44
8:Z:1081:ILE:O	8:Z:1082:ASN:ND2	2.51	0.44
8:Z:1297:THR:OG1	8:Z:1298:ASP:N	2.51	0.44
4:m:90:ARG:HH22	4:m:199:ARG:HA	1.83	0.44
7:Q:62:LEU:HA	7:Q:62:LEU:HD12	1.77	0.44
8:A:811:LEU:HB3	8:A:857:LEU:HD11	1.99	0.44
8:B:235:ASP:OD2	8:B:238:TYR:N	2.42	0.44
8:B:744:ILE:HG22	8:B:765:PRO:HA	1.99	0.44
8:B:785:TYR:O	8:B:943:TYR:OH	2.29	0.44
8:B:846:ILE:HG13	8:B:850:ARG:HH21	1.82	0.44
8:C:79:LYS:N	8:C:303:GLY:O	2.48	0.44
8:C:810:ASP:OD2	8:C:933:TYR:OH	2.34	0.44
8:Y:1316:ARG:O	8:Y:1319:GLN:NE2	2.44	0.44
2:n:71:THR:OG1	2:n:72:LEU:N	2.51	0.44
2:o:13:ASP:H	2:o:43:HIS:CE1	2.36	0.44
4:m:134:CYS:O	4:m:149:VAL:N	2.41	0.44
5:M:27:LEU:HD22	5:M:31:VAL:HG11	2.00	0.44
1:1:138:MET:HE1	1:1:144:LEU:HD22	1.98	0.44
8:a:1182:ASP:HA	8:a:1186:PHE:HD2	1.82	0.44
8:A:264:SER:OG	8:A:295:THR:OG1	2.31	0.44
8:A:747:ARG:HD2	8:A:747:ARG:HA	1.82	0.44
8:D:724:PRO:HG2	8:D:727:MET:HE3	1.99	0.44
8:Y:1292:CYS:HB3	8:Y:1310:LEU:HD23	1.98	0.44
8:Z:130:GLU:HA	8:Z:1074:THR:HA	2.00	0.44
8:Z:245:ARG:O	8:Z:249:ALA:CB	2.66	0.44
8:Z:311:ASN:ND2	8:Z:322:LEU:O	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:488:MET:HE3	8:Z:488:MET:HB3	1.76	0.44
4:m:39:TYR:HB3	4:m:40:HIS:HD2	1.82	0.44
5:M:505:ARG:HA	5:M:512:ARG:H	1.83	0.44
5:M:558:ARG:HD2	5:M:558:ARG:HA	1.70	0.44
6:N:25:ARG:HA	6:N:25:ARG:HD3	1.86	0.44
7:S:18:HIS:HD2	7:S:44:LEU:HB3	1.82	0.44
8:a:991:PHE:HE1	8:a:1011:MET:HB3	1.82	0.44
8:a:1144:ASP:OD1	8:a:1144:ASP:N	2.50	0.44
8:a:1285:TYR:OH	8:a:1312:GLU:OE1	2.36	0.44
8:C:1163:ALA:HB2	8:D:1202:VAL:HG12	1.98	0.44
8:Y:1092:SER:O	8:Y:1093:ASN:ND2	2.50	0.44
8:Y:1336:LYS:HE3	8:Y:1355:VAL:HG11	2.00	0.44
8:Z:554:PRO:O	8:Z:988:ARG:NH2	2.50	0.44
8:a:80:PHE:HB2	8:a:305:PHE:HD2	1.83	0.44
8:a:731:GLN:HB3	8:a:738:PRO:HB3	1.99	0.44
8:C:404:ASP:N	8:C:404:ASP:OD1	2.51	0.44
8:D:180:LEU:HD23	8:D:384:PRO:HG2	2.00	0.44
1:1:236:VAL:HG23	1:1:251:ARG:HG3	1.99	0.44
7:Q:61:LYS:CD	8:A:813:TYR:CZ	3.00	0.44
8:a:690:LEU:HD12	8:a:690:LEU:HA	1.89	0.44
8:A:223:MET:SD	8:A:1313:ASN:ND2	2.73	0.44
8:A:881:LEU:HD23	8:A:881:LEU:HA	1.87	0.44
8:C:1338:LYS:HE2	8:C:1338:LYS:HB3	1.80	0.44
8:D:123:SER:O	8:D:123:SER:OG	2.31	0.44
8:Z:387:ARG:HB3	8:Z:1044:VAL:HG13	2.00	0.44
1:x:127:ARG:HA	1:x:130:VAL:HG22	2.00	0.44
2:n:278:LEU:HG	2:o:275:LEU:HD22	1.99	0.44
7:i:26:LEU:O	8:Z:813:TYR:OH	2.27	0.44
7:i:72:ARG:NE	8:Z:820:MET:O	2.45	0.44
8:a:772:ARG:HA	8:a:772:ARG:HD3	1.74	0.44
8:a:1292:CYS:HB3	8:a:1303:CYS:HB3	1.72	0.44
8:B:96:GLN:HA	8:B:113:THR:HA	1.99	0.44
8:C:909:ASP:OD1	8:C:909:ASP:N	2.42	0.44
8:D:514:GLN:HE22	8:D:562:PRO:HA	1.83	0.44
8:D:712:ASP:OD1	8:D:712:ASP:N	2.47	0.44
8:Y:385:LEU:HD23	8:Y:385:LEU:HA	1.84	0.44
8:Y:782:LYS:O	8:Y:786:LEU:HB2	2.18	0.44
8:Z:177:HIS:ND1	8:Z:376:TYR:OH	2.36	0.44
8:Z:747:ARG:CZ	8:Z:756:ARG:HH21	2.30	0.44
8:a:92:LEU:HG	8:B:7:LEU:HD13	1.99	0.43
8:a:1222:ALA:HB1	8:Z:1165:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:637:ASN:ND2	8:A:866:THR:O	2.51	0.43
8:A:1327:THR:HG22	8:A:1355:VAL:HG22	1.98	0.43
8:B:243:LEU:HD22	8:B:273:MET:HE1	1.99	0.43
8:C:779:THR:HA	8:C:782:LYS:HE3	2.00	0.43
8:D:391:LEU:HD12	8:D:1042:PHE:HE2	1.82	0.43
8:D:494:ARG:HG2	8:D:497:HIS:HD2	1.83	0.43
8:Z:518:VAL:HG13	8:Z:519:THR:HG23	2.00	0.43
8:A:497:HIS:CG	8:A:500:ARG:HH12	2.37	0.43
8:A:856:MET:HE2	8:A:856:MET:HB3	1.83	0.43
8:A:1350:HIS:N	8:A:1353:ASN:O	2.47	0.43
8:C:1327:THR:HG22	8:C:1329:THR:H	1.83	0.43
8:C:1366:MET:HE2	8:C:1366:MET:HB3	1.77	0.43
8:D:600:THR:OG1	8:D:645:LEU:O	2.27	0.43
8:Y:457:PRO:O	8:Y:461:LEU:N	2.48	0.43
8:Y:584:LEU:HD12	8:Y:687:ILE:HD12	1.99	0.43
8:Y:1048:LEU:HD12	8:Y:1048:LEU:HA	1.90	0.43
8:Z:646:VAL:O	8:Z:674:TYR:OH	2.34	0.43
2:h:199:THR:HG22	4:g:227:ARG:HH22	1.82	0.43
7:i:43:MET:HG3	7:i:67:MET:HG2	2.00	0.43
8:C:422:ASN:O	8:C:1353:ASN:ND2	2.40	0.43
8:D:1191:ASN:ND2	8:D:1196:ALA:HA	2.33	0.43
8:Y:310:GLU:HA	8:Y:313:VAL:HG22	2.00	0.43
8:Z:440:ILE:HD13	8:Z:1108:VAL:HB	2.00	0.43
8:Z:820:MET:HE3	8:Z:877:ARG:HB3	2.00	0.43
3:H:2224:LEU:O	3:H:2227:SER:OG	2.36	0.43
7:Q:72:ARG:HG3	8:A:820:MET:HB2	1.99	0.43
7:T:37:HIS:HD2	7:T:38:PRO:HD2	1.82	0.43
8:a:1366:MET:HE3	8:a:1366:MET:HB3	1.93	0.43
8:A:1273:ALA:HA	8:A:1276:LYS:HG2	2.01	0.43
8:B:553:THR:HG21	8:B:983:TYR:HB3	2.00	0.43
8:C:472:GLU:O	8:C:476:GLN:N	2.52	0.43
8:D:578:ILE:HG12	8:D:1028:ILE:HG12	1.99	0.43
8:Y:936:PRO:HB3	8:Y:952:LEU:HD22	2.00	0.43
8:Z:1085:ASP:OD1	8:Z:1086:MET:N	2.51	0.43
2:I:279:ASP:HA	2:I:282:ILE:HG12	2.00	0.43
2:n:276:ARG:NH2	2:o:282:ILE:O	2.41	0.43
8:a:820:MET:HE3	8:a:820:MET:HB2	1.86	0.43
8:a:1153:PHE:HB2	8:a:1304:VAL:HG11	1.99	0.43
8:B:9:LEU:HD23	8:Z:155:GLU:HG3	2.00	0.43
8:B:1124:HIS:HB3	8:B:1127:VAL:HG12	2.00	0.43
8:Y:717:PRO:HG3	8:Y:781:GLN:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:1233:ALA:HA	8:Y:1240:SER:HB2	2.00	0.43
8:Z:66:PHE:N	8:Z:172:GLU:OE1	2.52	0.43
8:Z:970:ASP:N	8:Z:970:ASP:OD1	2.44	0.43
8:a:793:THR:HG23	8:a:796:ARG:H	1.83	0.43
8:C:472:GLU:OE1	8:C:475:MET:N	2.48	0.43
8:C:1035:THR:HG23	8:C:1174:LEU:HB2	2.01	0.43
8:Y:681:LEU:HB3	8:Y:780:LEU:HD22	2.01	0.43
8:Z:273:MET:HB3	8:Z:273:MET:HE2	1.78	0.43
8:Z:639:PHE:CG	8:Z:670:LEU:HD11	2.54	0.43
8:Z:651:TYR:HA	8:Z:654:VAL:HG12	2.00	0.43
2:n:7:ASN:HB3	2:n:82:LEU:HD11	2.01	0.43
4:g:182:LEU:HD12	4:g:182:LEU:HA	1.89	0.43
4:m:23:ALA:HB2	8:C:139:LEU:HD21	2.00	0.43
1:1:24:THR:HB	1:1:69:HIS:CE1	2.53	0.43
8:a:1289:ALA:HB1	8:a:1316:ARG:HD2	2.01	0.43
8:Z:529:LEU:HD12	8:Z:529:LEU:HA	1.86	0.43
7:Q:61:LYS:HG2	8:A:813:TYR:CZ	2.54	0.43
8:A:121:GLU:OE1	8:A:123:SER:OG	2.35	0.43
8:A:393:PHE:O	8:A:1038:ARG:N	2.46	0.43
8:B:529:LEU:HD23	8:B:529:LEU:HA	1.89	0.43
8:B:610:CYS:HB3	8:B:649:HIS:HE1	1.84	0.43
8:C:282:ILE:O	8:C:286:LEU:HB2	2.19	0.43
8:C:785:TYR:O	8:C:943:TYR:OH	2.29	0.43
8:C:1307:THR:OG1	8:C:1308:GLU:N	2.51	0.43
8:D:212:ARG:HH22	8:D:1203:ASP:HA	1.84	0.43
8:D:1291:ASP:O	8:D:1311:ILE:N	2.49	0.43
2:o:34:ILE:N	2:o:69:THR:O	2.50	0.43
2:o:216:MET:HE3	2:o:220:ARG:HB2	2.00	0.43
4:m:245:THR:HG23	4:m:290:VAL:HG22	1.99	0.43
8:a:393:PHE:HZ	8:a:1362:LEU:HD11	1.83	0.43
8:B:554:PRO:HD3	8:B:907:LEU:HD12	2.00	0.43
8:C:636:VAL:O	8:C:640:HIS:HB2	2.18	0.43
8:C:724:PRO:HA	8:C:773:ALA:HB3	2.00	0.43
8:C:1183:VAL:HG23	8:C:1187:LYS:HD2	2.01	0.43
8:D:1124:HIS:HB3	8:D:1127:VAL:HG12	2.00	0.43
2:o:160:ARG:HA	2:o:160:ARG:HD3	1.85	0.43
5:M:53:ARG:NH2	5:M:58:ALA:O	2.52	0.43
5:M:477:VAL:HG22	5:M:522:VAL:HG12	2.00	0.43
8:a:64:VAL:HG11	8:a:375:VAL:HG23	2.01	0.43
8:a:996:ALA:O	8:Z:686:ARG:NH2	2.51	0.43
8:A:677:LEU:HD11	8:A:788:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1020:LEU:HD11	8:B:1032:PHE:HZ	1.83	0.43
8:B:1257:LYS:HD3	8:B:1257:LYS:HA	1.89	0.43
8:C:934:SER:OG	8:C:935:LEU:N	2.50	0.43
8:C:1143:LEU:HD23	8:C:1143:LEU:HA	1.90	0.43
8:Y:84:ASN:OD1	8:Y:1080:ASN:ND2	2.52	0.43
8:Z:1338:LYS:HB3	8:Z:1338:LYS:HE2	1.85	0.43
2:I:223:ALA:O	2:I:227:SER:OG	2.38	0.42
2:o:66:ARG:HH22	2:o:284:GLU:HA	1.83	0.42
2:o:73:MET:HA	2:o:83:LEU:HD23	2.00	0.42
5:M:41:ARG:HA	5:M:41:ARG:HD3	1.82	0.42
5:M:393:HIS:HA	6:N:18:PRO:HD3	2.00	0.42
8:a:92:LEU:HD21	8:Z:56:THR:HG22	2.01	0.42
8:a:662:ALA:HA	8:a:671:LEU:HD21	2.01	0.42
8:a:1181:MET:HG2	8:a:1183:VAL:HG12	2.01	0.42
8:A:186:LYS:O	8:A:1092:SER:OG	2.35	0.42
8:A:597:PHE:HA	8:A:600:THR:HG22	2.01	0.42
8:C:226:THR:HB	8:C:229:LEU:HD21	2.01	0.42
8:C:1344:PHE:HB2	8:C:1364:GLN:HE21	1.84	0.42
8:D:263:THR:HG22	8:D:296:VAL:HG12	2.01	0.42
8:D:553:THR:HG21	8:D:983:TYR:HB3	2.01	0.42
8:Y:495:ILE:HG13	8:Y:976:PRO:HG2	2.01	0.42
8:Y:1033:ALA:N	8:Y:1176:LEU:O	2.45	0.42
8:Z:780:LEU:HA	8:Z:783:VAL:HG12	2.01	0.42
8:Z:1183:VAL:HA	8:Z:1187:LYS:HE2	2.01	0.42
1:x:47:HIS:CE1	1:x:283:PRO:HB2	2.54	0.42
1:x:184:LEU:HD13	1:x:184:LEU:HA	1.87	0.42
1:x:243:LEU:HD12	1:x:243:LEU:HA	1.87	0.42
2:h:151:LEU:HD23	2:h:151:LEU:HA	1.83	0.42
2:o:146:ILE:HD13	2:o:146:ILE:HA	1.89	0.42
1:1:52:LEU:HB3	1:1:235:LEU:HD13	2.00	0.42
1:1:244:SER:N	1:1:247:SER:OG	2.51	0.42
7:i:28:LEU:HD12	7:i:32:ILE:HG21	2.00	0.42
8:a:610:CYS:O	8:a:649:HIS:NE2	2.50	0.42
8:A:547:GLU:HG3	8:A:549:VAL:HG13	2.01	0.42
8:A:791:ALA:HB2	8:A:1008:LEU:HD12	2.00	0.42
8:Z:522:TYR:OH	8:Z:1179:VAL:O	2.33	0.42
8:Z:733:VAL:HG13	8:Z:894:GLU:HB2	2.01	0.42
8:Z:981:HIS:O	8:Z:985:ASN:N	2.52	0.42
5:M:368:ILE:HD13	5:M:418:ALA:HB1	2.01	0.42
7:T:75:ARG:NH2	8:D:625:LEU:O	2.45	0.42
8:a:596:LEU:HD23	8:a:596:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:216:LEU:HD11	8:B:1200:LEU:HB3	2.00	0.42
8:B:373:ARG:HD2	8:B:373:ARG:HA	1.75	0.42
8:B:458:ALA:O	8:B:462:GLN:HB2	2.20	0.42
8:B:1018:VAL:HA	8:B:1021:VAL:HG12	2.01	0.42
8:C:268:LYS:O	8:C:366:THR:OG1	2.35	0.42
8:C:1032:PHE:HA	8:C:1178:PRO:HD3	2.01	0.42
8:Y:192:VAL:HG21	8:Y:1282:ILE:HD13	2.01	0.42
8:Y:811:LEU:HD12	8:Y:857:LEU:HD11	2.01	0.42
8:Y:1298:ASP:OD1	8:Y:1298:ASP:N	2.49	0.42
8:Z:771:TYR:OH	8:Z:777:GLU:OE1	2.35	0.42
5:M:39:THR:HG23	5:M:153:TRP:HD1	1.85	0.42
8:a:329:LYS:HE2	8:a:329:LYS:HB3	1.93	0.42
8:a:624:PHE:HE2	8:a:660:HIS:HB2	1.85	0.42
8:a:999:PRO:HB2	8:a:1001:VAL:HG23	2.01	0.42
8:C:291:ILE:HG12	8:C:360:ILE:HG22	2.01	0.42
8:C:745:GLU:HG3	8:C:766:LEU:HB3	2.01	0.42
8:D:689:ALA:O	8:D:694:ASN:ND2	2.53	0.42
8:Y:341:ASN:ND2	8:Y:345:SER:OG	2.52	0.42
8:Y:514:GLN:OE1	8:Y:563:ASP:N	2.52	0.42
8:Y:1342:GLY:N	8:Y:1364:GLN:OE1	2.52	0.42
4:g:258:ASP:OD2	4:g:277:ASP:N	2.52	0.42
8:a:1284:GLU:O	8:a:1289:ALA:N	2.48	0.42
8:A:1189:PRO:HG3	8:A:1359:ILE:HG21	2.01	0.42
8:B:183:LEU:HD23	8:B:183:LEU:HA	1.82	0.42
8:B:597:PHE:HA	8:B:600:THR:HG22	2.01	0.42
8:C:1191:ASN:ND2	8:C:1195:ARG:O	2.43	0.42
4:g:196:PRO:O	4:g:233:ARG:NH2	2.52	0.42
8:a:91:MET:HE2	8:a:91:MET:HB3	1.89	0.42
8:a:717:PRO:HA	8:a:718:PRO:HD3	1.82	0.42
8:B:12:LYS:HE3	8:Z:58:CYS:HB2	2.01	0.42
8:C:119:TYR:OH	8:Z:2:GLU:OE2	2.28	0.42
8:C:216:LEU:HD11	8:C:1198:CYS:HB2	2.02	0.42
2:h:88:HIS:HB2	2:h:305:LYS:HD3	2.00	0.42
4:m:69:ARG:NH2	4:m:71:GLU:OE2	2.51	0.42
5:M:459:PHE:CG	8:C:1250:GLU:HB3	2.54	0.42
1:1:178:MET:HB2	1:1:213:VAL:HG23	2.02	0.42
8:a:139:LEU:HD12	8:a:140:ARG:HE	1.85	0.42
8:A:701:GLU:HB3	8:A:706:TYR:HE1	1.85	0.42
8:A:914:GLN:HE21	8:A:986:TRP:CD1	2.37	0.42
8:B:1158:GLU:N	8:B:1301:TYR:OH	2.49	0.42
8:C:392:THR:OG1	8:C:1264:GLN:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:515:ASP:OD1	8:C:515:ASP:N	2.48	0.42
8:D:502:ARG:HD3	8:D:502:ARG:HA	1.80	0.42
8:D:532:GLU:OE1	8:D:555:ARG:NH1	2.52	0.42
8:D:698:LEU:HB3	8:D:699:ALA:H	1.67	0.42
8:Y:1085:ASP:OD1	8:Y:1085:ASP:N	2.45	0.42
8:Z:1068:GLU:HA	8:Z:1073:THR:HG22	2.01	0.42
1:x:160:LYS:HB2	1:x:190:ARG:HH12	1.85	0.42
4:g:211:HIS:CD2	4:g:213:GLN:H	2.38	0.42
4:g:234:ARG:HA	4:g:234:ARG:HD2	1.75	0.42
4:m:234:ARG:HH11	4:m:242:PRO:HD2	1.85	0.42
7:S:67:MET:HA	7:S:70:VAL:HG12	2.02	0.42
8:a:514:GLN:HE22	8:a:562:PRO:HA	1.85	0.42
8:A:401:LEU:HD21	8:A:1183:VAL:HG21	2.02	0.42
8:A:653:LEU:HD23	8:A:653:LEU:HA	1.91	0.42
8:A:721:THR:HG22	8:A:781:GLN:HE22	1.84	0.42
8:C:711:HIS:HA	8:C:779:THR:HG22	2.00	0.42
8:Y:495:ILE:HD13	8:Y:937:VAL:HA	2.01	0.42
8:Y:1358:GLU:OE1	8:Y:1358:GLU:N	2.51	0.42
2:n:22:GLY:O	2:n:25:THR:OG1	2.36	0.42
7:i:75:ARG:HA	7:i:75:ARG:HD3	1.86	0.42
8:a:252:ASP:OD1	8:a:252:ASP:N	2.52	0.42
8:a:311:ASN:ND2	8:a:322:LEU:O	2.40	0.42
8:A:1200:LEU:HD22	8:A:1223:GLN:HE22	1.85	0.42
8:D:502:ARG:NH1	8:D:962:GLU:OE2	2.53	0.42
8:D:641:THR:OG1	8:D:642:ARG:N	2.53	0.42
8:D:1033:ALA:HB3	8:D:1176:LEU:HB3	2.02	0.42
8:Y:688:SER:HB2	8:Y:708:ASN:HD22	1.83	0.42
1:x:27:PRO:HA	1:x:177:ASN:HD22	1.85	0.42
2:n:195:ILE:HA	2:n:198:LYS:HD3	2.01	0.42
5:M:439:ALA:HA	5:M:442:ARG:HH21	1.85	0.42
1:1:125:VAL:O	1:1:129:LEU:HB2	2.20	0.42
7:j:13:LYS:HG3	7:j:15:ASP:H	1.84	0.42
8:A:899:LEU:HG	8:A:903:GLN:HB3	2.02	0.42
8:B:668:PRO:HB2	8:C:643:GLN:HB2	2.02	0.42
8:B:692:GLY:HA2	8:C:993:ARG:HH12	1.84	0.42
8:C:195:THR:O	8:C:199:ASN:ND2	2.53	0.42
8:Y:59:ASN:HB2	8:Z:95:VAL:HG13	2.01	0.42
8:Y:180:LEU:HD23	8:Y:384:PRO:HG2	2.02	0.42
8:Y:223:MET:HE2	8:Y:223:MET:HB3	1.88	0.42
8:Y:700:GLU:HG2	8:Y:701:GLU:HG3	2.02	0.42
8:Z:42:ASP:OD1	8:Z:42:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:1196:ALA:HB3	8:Z:1222:ALA:HB3	2.01	0.42
2:I:24:LEU:HD13	2:I:125:LEU:HD12	2.02	0.41
2:n:23:LYS:NZ	2:n:123:ASN:O	2.41	0.41
5:M:517:GLN:HA	5:M:518:PRO:HD3	1.90	0.41
7:T:19:ARG:HD3	7:T:19:ARG:HA	1.95	0.41
8:a:82:ASP:OD2	8:B:146:THR:OG1	2.30	0.41
8:a:263:THR:HG22	8:a:296:VAL:HG12	2.01	0.41
8:a:482:ARG:NH1	8:a:543:GLN:OE1	2.52	0.41
8:a:941:ARG:NE	8:a:987:LEU:O	2.40	0.41
8:A:611:TYR:CZ	8:A:923:VAL:HG13	2.55	0.41
8:A:1008:LEU:HD23	8:A:1008:LEU:HA	1.92	0.41
8:A:1366:MET:HE2	8:A:1366:MET:HB3	1.92	0.41
8:C:186:LYS:HD3	8:C:186:LYS:HA	1.96	0.41
8:C:385:LEU:HD23	8:C:385:LEU:HA	1.86	0.41
8:D:522:TYR:OH	8:D:1177:THR:OG1	2.27	0.41
8:Y:1004:SER:O	8:Y:1007:THR:OG1	2.38	0.41
8:Z:807:LEU:O	8:Z:811:LEU:HB2	2.20	0.41
8:Z:1149:SER:O	8:Z:1149:SER:OG	2.31	0.41
3:P:2236:ARG:NH2	6:N:64:GLU:HB3	2.35	0.41
5:M:150:ARG:NH2	5:M:160:ASP:OD2	2.53	0.41
1:1:30:ASP:OD1	1:1:31:LEU:N	2.53	0.41
1:1:118:VAL:HB	1:1:119:ARG:HH21	1.84	0.41
8:a:155:GLU:O	8:a:159:THR:OG1	2.32	0.41
8:a:635:ILE:HD13	8:a:635:ILE:HA	1.89	0.41
8:A:300:ALA:HA	8:A:353:THR:HG23	2.02	0.41
8:B:818:LEU:HD13	8:B:818:LEU:HA	1.93	0.41
8:C:388:ASN:OD1	8:C:388:ASN:N	2.52	0.41
8:Y:798:CYS:HA	8:Y:943:TYR:HB3	2.02	0.41
8:Z:225:ALA:O	8:Z:232:ARG:NH1	2.53	0.41
8:Z:968:ARG:HE	8:Z:972:GLY:HA3	1.85	0.41
1:1:32:GLU:OE2	1:1:223:LYS:NZ	2.46	0.41
8:a:1139:ARG:HD2	8:a:1139:ARG:HA	1.77	0.41
8:a:1287:LEU:HD23	8:a:1288:ARG:HG3	2.02	0.41
8:A:177:HIS:ND1	8:A:376:TYR:OH	2.40	0.41
8:A:297:SER:O	8:A:297:SER:OG	2.38	0.41
8:B:246:LEU:HD23	8:B:246:LEU:HA	1.84	0.41
8:C:694:ASN:ND2	8:C:704:SER:OG	2.54	0.41
8:Z:369:MET:HB3	8:Z:369:MET:HE2	1.73	0.41
2:h:96:ASN:HB3	2:h:102:TRP:CZ2	2.55	0.41
2:o:33:PRO:HD3	2:o:135:PRO:HG3	2.03	0.41
5:M:388:GLN:OE1	6:N:22:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:52:SER:OG	7:Q:53:LEU:N	2.52	0.41
7:R:28:LEU:HD12	7:R:29:PRO:HD2	2.01	0.41
8:a:79:LYS:N	8:a:303:GLY:O	2.44	0.41
8:a:180:LEU:HD23	8:a:384:PRO:HG2	2.01	0.41
8:A:428:ALA:HB3	8:A:440:ILE:HG23	2.02	0.41
8:A:578:ILE:HD12	8:A:578:ILE:HA	1.93	0.41
8:A:801:GLY:HA3	8:A:890:VAL:HB	2.03	0.41
8:B:639:PHE:CG	8:B:670:LEU:HD11	2.56	0.41
8:B:1113:LEU:HA	8:B:1116:VAL:HG12	2.03	0.41
8:C:410:VAL:HG21	8:C:1332:LEU:HD21	2.03	0.41
8:D:720:VAL:HG13	8:D:918:TYR:HD1	1.84	0.41
8:Y:15:ILE:HD12	8:Y:16:PRO:HD2	2.02	0.41
8:Y:79:LYS:HG3	8:Y:302:TYR:HB2	2.02	0.41
8:Y:458:ALA:HA	8:Y:461:LEU:HB3	2.02	0.41
2:h:127:LEU:HD23	2:h:127:LEU:HA	1.87	0.41
2:n:108:LEU:HD22	2:n:137:ILE:HG22	2.02	0.41
4:m:183:GLN:HG2	4:m:256:ALA:HB2	2.03	0.41
5:M:367:LEU:HG	5:M:424:ILE:HD12	2.01	0.41
8:A:687:ILE:HD12	8:A:687:ILE:HA	1.89	0.41
8:A:1332:LEU:HD23	8:A:1332:LEU:HA	1.95	0.41
8:B:139:LEU:HD12	8:B:139:LEU:HA	1.91	0.41
8:B:184:LEU:HD23	8:B:184:LEU:HA	1.89	0.41
8:C:600:THR:OG1	8:C:645:LEU:O	2.34	0.41
8:C:1280:LYS:HD2	8:C:1280:LYS:HA	1.93	0.41
8:D:243:LEU:HD23	8:D:243:LEU:HA	1.87	0.41
8:D:307:LEU:HD23	8:D:307:LEU:HA	1.88	0.41
8:Y:698:LEU:HD12	8:Y:706:TYR:CZ	2.56	0.41
8:Y:1007:THR:O	8:Y:1011:MET:N	2.50	0.41
8:Y:1212:LYS:HE3	8:Y:1212:LYS:HB2	1.95	0.41
8:Z:647:PHE:HD1	8:Z:653:LEU:HD13	1.85	0.41
8:Z:945:ASN:HA	8:Z:946:PRO:HD3	1.94	0.41
2:I:232:VAL:HG22	5:M:6:TYR:HB2	2.03	0.41
2:o:75:ARG:H	2:o:82:LEU:HB2	1.86	0.41
4:m:135:VAL:HA	4:m:148:CYS:HA	2.01	0.41
5:M:535:LEU:HD11	5:M:539:PHE:HB2	2.02	0.41
7:Q:65:LEU:HD11	8:A:813:TYR:HD1	1.85	0.41
8:A:283:ILE:HG21	8:A:369:MET:HE3	2.01	0.41
8:A:455:HIS:CE1	8:A:1017:PRO:HG3	2.56	0.41
8:A:523:LYS:HD3	8:A:523:LYS:HA	1.88	0.41
8:B:3:ASN:OD1	8:B:5:SER:OG	2.30	0.41
8:B:935:LEU:HD12	8:B:935:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:1156:MET:HG3	8:C:1257:LYS:HE2	2.03	0.41
8:D:180:LEU:HD12	8:D:180:LEU:HA	1.94	0.41
8:D:455:HIS:CD2	8:D:1017:PRO:HG3	2.56	0.41
8:Y:627:ILE:HG22	8:Y:630:PHE:HB3	2.03	0.41
8:Y:701:GLU:OE2	8:Y:714:ARG:NH1	2.52	0.41
8:Y:766:LEU:HD11	8:Y:893:LEU:HD21	2.02	0.41
8:Y:1243:LEU:HD12	8:Y:1243:LEU:HA	1.92	0.41
2:I:62:ARG:NE	2:I:280:ASP:O	2.39	0.41
5:M:453:LYS:HA	5:M:453:LYS:HD3	1.89	0.41
1:l:178:MET:SD	1:l:216:SER:OG	2.71	0.41
8:a:842:PRO:HB2	8:a:843:GLU:H	1.61	0.41
8:a:1113:LEU:HA	8:a:1116:VAL:HG22	2.01	0.41
8:A:779:THR:HA	8:A:782:LYS:HE3	2.01	0.41
8:B:122:LYS:HD3	8:B:1080:ASN:HD21	1.84	0.41
8:B:702:PRO:HG3	8:C:964:PRO:HD2	2.03	0.41
8:B:810:ASP:OD2	8:B:933:TYR:OH	2.32	0.41
8:C:390:ASP:OD1	8:C:1039:THR:OG1	2.38	0.41
8:C:1014:LYS:HE2	8:C:1014:LYS:HB3	1.92	0.41
8:D:658:ALA:HB2	8:D:674:TYR:HB3	2.03	0.41
8:D:1326:SER:O	8:D:1326:SER:OG	2.33	0.41
8:Y:173:ARG:HD3	8:Z:100:VAL:HG12	2.02	0.41
8:Z:1125:ASP:OD1	8:Z:1125:ASP:N	2.43	0.41
1:x:130:VAL:HA	1:x:133:VAL:HG12	2.03	0.41
2:h:108:LEU:HB2	2:h:288:PHE:HB2	2.02	0.41
7:j:72:ARG:NH2	8:a:820:MET:O	2.44	0.41
8:A:348:GLY:O	8:A:351:SER:OG	2.39	0.41
8:B:387:ARG:HB2	8:B:1046:MET:HE3	2.03	0.41
8:C:315:ALA:HB2	8:C:321:ILE:HD11	2.03	0.41
8:C:1218:ARG:HD2	8:C:1218:ARG:HA	1.95	0.41
8:D:401:LEU:HD11	8:D:1354:TYR:HB3	2.02	0.41
8:D:1263:ALA:O	8:D:1267:ASN:ND2	2.54	0.41
8:D:1361:PRO:HB2	8:D:1364:GLN:HB3	2.03	0.41
8:Y:372:LEU:HD23	8:Y:372:LEU:HA	1.86	0.41
8:Y:820:MET:HE2	8:Y:820:MET:HB2	1.96	0.41
8:Y:1248:HIS:HA	8:Y:1251:ARG:HH11	1.86	0.41
8:Z:324:ASP:HB3	8:Z:327:SER:HB3	2.03	0.41
1:x:246:ASP:OD1	1:x:246:ASP:N	2.50	0.41
1:x:250:CYS:HA	1:x:253:ILE:HG22	2.02	0.41
2:h:34:ILE:HG23	2:h:69:THR:HG23	2.01	0.41
2:I:56:ARG:HA	2:I:56:ARG:HD3	1.81	0.41
3:P:2232:ILE:O	3:P:2235:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:92:TYR:HA	8:C:1070:ASP:HB2	2.02	0.41
2:o:125:LEU:HB3	2:o:132:LEU:HB3	2.02	0.41
4:m:91:ALA:O	4:m:99:ARG:NH2	2.53	0.41
4:m:132:LEU:HD23	4:m:132:LEU:HA	1.88	0.41
5:M:149:LEU:HA	5:M:149:LEU:HD23	1.88	0.41
7:i:21:VAL:O	7:i:26:LEU:N	2.51	0.41
8:a:127:ILE:HD12	8:a:128:PRO:HD2	2.01	0.41
8:a:184:LEU:HD13	8:a:387:ARG:HE	1.86	0.41
8:a:337:PRO:HA	8:B:11:PRO:HB3	2.03	0.41
8:a:715:LEU:HD23	8:a:782:LYS:HD3	2.03	0.41
8:B:157:MET:HE3	8:B:157:MET:HB2	1.92	0.41
8:B:1055:THR:OG1	8:B:1056:SER:N	2.54	0.41
8:C:78:ILE:HB	8:C:1058:ILE:HG22	2.03	0.41
8:C:399:LEU:HA	8:C:399:LEU:HD23	1.83	0.41
8:C:469:PRO:HA	8:C:470:PRO:HD3	1.93	0.41
8:C:1187:LYS:NZ	8:C:1355:VAL:O	2.53	0.41
8:C:1327:THR:HG23	8:C:1355:VAL:HG22	2.03	0.41
8:D:392:THR:HG21	8:D:1265:TYR:HE2	1.85	0.41
8:D:502:ARG:HH22	8:D:958:ARG:HD2	1.86	0.41
8:D:681:LEU:HD21	8:D:788:LEU:HD22	2.03	0.41
8:D:1336:LYS:NZ	8:D:1346:THR:O	2.44	0.41
8:D:1350:HIS:CD2	8:D:1351:PHE:H	2.39	0.41
8:Y:892:VAL:HG21	8:Y:979:PHE:HZ	1.86	0.41
8:Y:1146:GLU:HB3	8:Y:1150:MET:HE1	2.01	0.41
8:Y:1155:SER:O	8:Y:1255:ASN:ND2	2.43	0.41
8:Z:310:GLU:HB3	8:Z:325:PHE:HD2	1.86	0.41
8:Z:454:LEU:HD21	8:Z:1175:ILE:HD13	2.03	0.41
8:Z:514:GLN:HE22	8:Z:990:PRO:HD3	1.85	0.41
8:Z:753:ASP:OD1	8:Z:753:ASP:N	2.47	0.41
8:Z:820:MET:HG3	8:Z:877:ARG:HD3	2.03	0.41
2:I:218:TYR:HD1	2:I:218:TYR:HA	1.72	0.41
4:g:186:TYR:CE1	4:g:250:LYS:HB3	2.55	0.41
1:1:235:LEU:HD12	1:1:235:LEU:HA	1.93	0.41
8:a:146:THR:OG1	8:a:147:ILE:N	2.51	0.41
8:a:268:LYS:HE2	8:a:268:LYS:HB3	1.93	0.41
8:a:457:PRO:O	8:a:461:LEU:N	2.43	0.41
8:a:1182:ASP:N	8:a:1182:ASP:OD1	2.54	0.41
8:B:144:GLU:N	8:B:149:ASP:OD2	2.54	0.41
8:B:1199:MET:HB3	8:B:1275:ASN:HB3	2.02	0.41
8:C:433:ARG:NH2	8:C:1166:HIS:O	2.36	0.41
8:D:136:LEU:HD23	8:D:136:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:1272:ILE:HD12	8:D:1272:ILE:HA	1.91	0.41
8:Z:387:ARG:HD3	8:Z:387:ARG:HA	1.80	0.41
8:Z:798:CYS:O	8:Z:923:VAL:N	2.39	0.41
8:Z:800:LEU:HD22	8:Z:952:LEU:HD21	2.01	0.41
2:h:52:VAL:HG21	2:h:133:VAL:HG11	2.03	0.40
2:h:59:VAL:HG11	2:h:193:LEU:HD22	2.02	0.40
5:M:451:ALA:HA	5:M:452:PRO:HD3	1.93	0.40
1:l:99:ARG:HD2	1:l:99:ARG:HA	1.84	0.40
7:j:73:THR:OG1	7:j:75:ARG:O	2.39	0.40
8:a:669:GLN:O	8:a:673:HIS:ND1	2.54	0.40
8:A:122:LYS:HD3	8:A:1082:ASN:HB3	2.02	0.40
8:A:268:LYS:HE2	8:A:268:LYS:HB3	1.77	0.40
8:A:681:LEU:HD22	8:A:783:VAL:HG13	2.03	0.40
8:B:756:ARG:HH22	8:B:887:GLY:HA2	1.86	0.40
8:B:1008:LEU:HD23	8:B:1008:LEU:HA	1.82	0.40
8:B:1317:LEU:HD23	8:B:1317:LEU:HA	1.89	0.40
8:C:820:MET:HA	8:C:877:ARG:HH21	1.86	0.40
8:D:495:ILE:HD12	8:D:937:VAL:HG12	2.03	0.40
8:D:944:SER:O	8:D:944:SER:OG	2.36	0.40
8:Y:246:LEU:HD23	8:Y:246:LEU:HA	1.96	0.40
8:Y:955:ASP:OD1	8:Y:958:ARG:NH2	2.53	0.40
8:Z:534:HIS:HD2	8:Z:537:PHE:H	1.70	0.40
8:Z:1182:ASP:OD1	8:Z:1182:ASP:N	2.52	0.40
2:h:138:VAL:HG21	2:h:142:LEU:HD22	2.03	0.40
2:n:111:LEU:HD22	2:n:138:VAL:HG21	2.04	0.40
4:g:197:GLU:O	4:g:233:ARG:NH2	2.45	0.40
4:m:38:LEU:HD21	8:C:1066:LYS:HD2	2.04	0.40
4:m:126:HIS:CG	4:m:247:VAL:HG21	2.56	0.40
7:Q:44:LEU:HD23	7:Q:44:LEU:HA	1.93	0.40
8:a:184:LEU:HD23	8:a:184:LEU:HA	1.85	0.40
8:A:884:GLN:H	8:A:884:GLN:HG2	1.59	0.40
8:B:874:GLN:H	8:B:874:GLN:HG3	1.70	0.40
8:C:478:LEU:HD21	8:C:528:THR:HG22	2.03	0.40
8:C:1048:LEU:HD13	8:C:1094:THR:HB	2.03	0.40
8:D:545:ASN:OD1	8:D:545:ASN:N	2.54	0.40
8:D:1041:THR:HG21	8:D:1103:ARG:HH21	1.85	0.40
8:Y:1086:MET:HE2	8:Y:1086:MET:HB3	1.93	0.40
2:I:206:MET:HE2	2:I:206:MET:HB2	1.98	0.40
2:I:219:VAL:HG13	2:I:231:LEU:HD22	2.02	0.40
2:I:222:LEU:HA	2:I:222:LEU:HD12	1.85	0.40
2:n:234:CYS:HB2	2:o:206:MET:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:190:ASP:O	2:o:192:HIS:ND1	2.55	0.40
7:T:47:TYR:OH	7:T:63:ASP:OD2	2.38	0.40
8:a:121:GLU:OE1	8:a:123:SER:OG	2.38	0.40
8:A:1064:VAL:HG12	8:A:1077:VAL:HG22	2.02	0.40
8:A:1359:ILE:HG23	8:A:1360:ILE:HG23	2.02	0.40
8:C:1279:PHE:HE2	8:Z:26:SER:HA	1.85	0.40
8:Y:591:GLU:OE2	8:Y:595:ARG:NH2	2.48	0.40
8:Y:734:ALA:HB2	8:Y:893:LEU:HD13	2.02	0.40
8:Z:184:LEU:HD23	8:Z:184:LEU:HA	1.92	0.40
8:Z:512:MET:HE2	8:Z:512:MET:HB2	1.90	0.40
8:Z:690:LEU:HD23	8:Z:690:LEU:HA	1.88	0.40
1:x:3:LEU:HD23	1:x:57:MET:HE3	2.04	0.40
2:n:159:ASP:HB3	2:o:221:LYS:HE3	2.04	0.40
2:n:210:LEU:HD12	2:n:210:LEU:HA	1.97	0.40
2:o:280:ASP:OD2	2:o:280:ASP:N	2.47	0.40
4:m:90:ARG:HH12	4:m:199:ARG:HE	1.69	0.40
8:A:277:ALA:HB2	8:A:373:ARG:HB2	2.04	0.40
8:A:789:MET:HB2	8:A:789:MET:HE2	1.79	0.40
8:A:975:LEU:HB2	8:A:980:ALA:HB2	2.02	0.40
8:A:1282:ILE:HD13	8:A:1282:ILE:HA	1.86	0.40
8:B:136:LEU:HD23	8:B:136:LEU:HA	1.90	0.40
8:C:774:THR:OG1	8:C:777:GLU:OE2	2.40	0.40
8:C:804:LEU:HD23	8:C:889:HIS:CD2	2.54	0.40
8:C:1244:TYR:O	8:C:1249:ARG:NH2	2.43	0.40
8:D:78:ILE:HG12	8:D:348:GLY:HA2	2.03	0.40
8:D:717:PRO:HA	8:D:718:PRO:HD3	1.95	0.40
8:Y:1006:MET:HB3	8:Y:1006:MET:HE3	1.83	0.40
8:Y:1176:LEU:HD13	8:Y:1232:TRP:HB2	2.02	0.40
8:Z:749:HIS:NE2	8:Z:885:PHE:HA	2.37	0.40
1:x:20:LEU:HA	1:x:23:LEU:HG	2.04	0.40
2:h:222:LEU:HD23	2:h:222:LEU:HA	1.89	0.40
2:h:226:ASP:OD1	2:h:227:SER:N	2.53	0.40
2:n:66:ARG:HB3	4:m:211:HIS:CG	2.56	0.40
7:Q:65:LEU:HD11	8:A:813:TYR:CD1	2.57	0.40
7:S:72:ARG:NE	8:C:820:MET:O	2.42	0.40
7:i:19:ARG:HA	7:i:22:VAL:HG22	2.03	0.40
8:a:667:PRO:HA	8:a:668:PRO:HD3	1.94	0.40
8:B:321:ILE:HD13	8:B:321:ILE:HA	1.89	0.40
8:B:1211:THR:O	8:B:1215:TYR:HB2	2.21	0.40
8:Y:274:VAL:HG13	8:Y:385:LEU:HD11	2.04	0.40
8:Z:1366:MET:HE3	8:Z:1366:MET:HB3	1.99	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	1	283/1048 (27%)	268 (95%)	15 (5%)	0	100	100
1	x	283/1048 (27%)	268 (95%)	15 (5%)	0	100	100
2	I	292/306 (95%)	279 (96%)	13 (4%)	0	100	100
2	h	300/306 (98%)	278 (93%)	22 (7%)	0	100	100
2	n	291/306 (95%)	271 (93%)	20 (7%)	0	100	100
2	o	285/306 (93%)	274 (96%)	11 (4%)	0	100	100
3	H	18/2241 (1%)	18 (100%)	0	0	100	100
3	P	18/2241 (1%)	18 (100%)	0	0	100	100
4	g	108/290 (37%)	98 (91%)	10 (9%)	0	100	100
4	m	288/290 (99%)	268 (93%)	20 (7%)	0	100	100
5	M	462/594 (78%)	424 (92%)	38 (8%)	0	100	100
6	N	64/642 (10%)	63 (98%)	1 (2%)	0	100	100
6	O	65/642 (10%)	63 (97%)	2 (3%)	0	100	100
7	Q	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	R	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
7	S	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	T	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	i	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
7	j	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
8	A	1255/1370 (92%)	1163 (93%)	92 (7%)	0	100	100
8	B	1329/1370 (97%)	1227 (92%)	102 (8%)	0	100	100
8	C	1323/1370 (97%)	1250 (94%)	73 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	D	1293/1370 (94%)	1201 (93%)	92 (7%)	0	100	100
8	Y	1343/1370 (98%)	1253 (93%)	90 (7%)	0	100	100
8	Z	1325/1370 (97%)	1223 (92%)	102 (8%)	0	100	100
8	a	1293/1370 (94%)	1205 (93%)	88 (7%)	0	100	100
All	All	12284/20300 (60%)	11468 (93%)	816 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	1	256/883 (29%)	255 (100%)	1 (0%)	84	84
1	x	256/883 (29%)	255 (100%)	1 (0%)	84	84
2	I	266/273 (97%)	264 (99%)	2 (1%)	73	77
2	h	271/273 (99%)	271 (100%)	0	100	100
2	n	263/273 (96%)	261 (99%)	2 (1%)	73	77
2	o	259/273 (95%)	257 (99%)	2 (1%)	73	77
3	H	19/1941 (1%)	19 (100%)	0	100	100
3	P	19/1941 (1%)	18 (95%)	1 (5%)	20	44
4	g	101/252 (40%)	101 (100%)	0	100	100
4	m	252/252 (100%)	251 (100%)	1 (0%)	84	84
5	M	395/500 (79%)	388 (98%)	7 (2%)	51	68
6	N	59/526 (11%)	59 (100%)	0	100	100
6	O	64/526 (12%)	64 (100%)	0	100	100
7	Q	59/68 (87%)	58 (98%)	1 (2%)	53	68
7	R	59/68 (87%)	59 (100%)	0	100	100
7	S	59/68 (87%)	59 (100%)	0	100	100
7	T	59/68 (87%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	i	59/68 (87%)	59 (100%)	0	100	100
7	j	59/68 (87%)	59 (100%)	0	100	100
8	A	1109/1192 (93%)	1103 (100%)	6 (0%)	81	82
8	B	1162/1192 (98%)	1156 (100%)	6 (0%)	81	82
8	C	1159/1192 (97%)	1147 (99%)	12 (1%)	68	76
8	D	1130/1192 (95%)	1126 (100%)	4 (0%)	84	84
8	Y	1174/1192 (98%)	1166 (99%)	8 (1%)	76	79
8	Z	1159/1192 (97%)	1150 (99%)	9 (1%)	73	77
8	a	1130/1192 (95%)	1117 (99%)	13 (1%)	63	73
All	All	10857/17548 (62%)	10781 (99%)	76 (1%)	73	79

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	x	258	VAL
2	I	133	VAL
2	I	188	VAL
3	P	2240	LEU
2	n	85	VAL
2	n	127	LEU
2	o	31	VAL
2	o	241	LEU
4	m	35	VAL
5	M	44	TYR
5	M	76	VAL
5	M	113	THR
5	M	114	VAL
5	M	131	THR
5	M	164	LEU
5	M	584	VAL
1	1	73	LEU
7	Q	24	VAL
8	a	95	VAL
8	a	446	LEU
8	a	589	ASP
8	a	609	LEU
8	a	646	VAL
8	a	751	VAL
8	a	861	VAL

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Mol	Chain	Res	Type
8	a	935	LEU
8	a	937	VAL
8	a	1001	VAL
8	a	1179	VAL
8	a	1278	LEU
8	a	1307	THR
8	A	97	VAL
8	A	100	VAL
8	A	375	VAL
8	A	545	ASN
8	A	872	LEU
8	A	889	HIS
8	B	446	LEU
8	B	703	LEU
8	B	892	VAL
8	B	937	VAL
8	B	977	THR
8	B	1360	ILE
8	C	388	ASN
8	C	509	VAL
8	C	517	VAL
8	C	616	LEU
8	C	754	VAL
8	C	761	ASP
8	C	861	VAL
8	C	870	THR
8	C	937	VAL
8	C	1015	ILE
8	C	1035	THR
8	C	1297	THR
8	D	388	ASN
8	D	937	VAL
8	D	1077	VAL
8	D	1303	CYS
8	Y	272	VAL
8	Y	397	VAL
8	Y	655	THR
8	Y	786	LEU
8	Y	1001	VAL
8	Y	1044	VAL
8	Y	1083	THR
8	Y	1176	LEU

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Mol	Chain	Res	Type
8	Z	227	LEU
8	Z	739	LEU
8	Z	864	VAL
8	Z	870	THR
8	Z	956	ILE
8	Z	1045	ASP
8	Z	1077	VAL
8	Z	1112	ASP
8	Z	1356	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (203) such sidechains are listed below:

Mol	Chain	Res	Type
1	x	34	HIS
1	x	170	ASN
1	x	177	ASN
1	x	193	ASN
1	x	198	ASN
1	x	201	ASN
2	h	36	GLN
2	h	84	HIS
2	h	209	ASN
2	h	235	GLN
2	I	14	HIS
2	I	79	ASN
2	I	170	GLN
2	I	257	GLN
2	n	79	ASN
2	n	116	HIS
2	n	147	ASN
2	n	170	GLN
2	n	171	GLN
2	n	209	ASN
2	n	277	GLN
2	n	297	ASN
2	o	88	HIS
2	o	147	ASN
2	o	297	ASN
4	g	213	GLN
4	g	278	ASN
4	m	18	ASN
4	m	40	HIS

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Mol	Chain	Res	Type
4	m	183	GLN
4	m	240	GLN
5	M	34	ASN
5	M	322	HIS
5	M	463	ASN
5	M	561	ASN
5	M	571	HIS
6	N	73	GLN
1	1	150	GLN
1	1	158	HIS
7	Q	23	ASN
7	Q	37	HIS
7	S	37	HIS
7	T	37	HIS
7	T	55	ASN
7	i	37	HIS
8	a	94	HIS
8	a	346	GLN
8	a	510	ASN
8	a	514	GLN
8	a	534	HIS
8	a	618	HIS
8	a	694	ASN
8	a	749	HIS
8	a	794	ASN
8	a	849	GLN
8	a	940	HIS
8	a	945	ASN
8	a	1000	ASN
8	a	1023	GLN
8	a	1076	HIS
8	a	1111	GLN
8	a	1230	ASN
8	a	1245	ASN
8	a	1248	HIS
8	a	1267	ASN
8	a	1319	GLN
8	a	1353	ASN
8	A	3	ASN
8	A	181	GLN
8	A	199	ASN
8	A	231	ASN

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Mol	Chain	Res	Type
8	A	319	HIS
8	A	510	ASN
8	A	543	GLN
8	A	581	HIS
8	A	618	HIS
8	A	643	GLN
8	A	676	ASN
8	A	749	HIS
8	A	967	HIS
8	A	981	HIS
8	A	1023	GLN
8	A	1079	GLN
8	A	1191	ASN
8	A	1275	ASN
8	A	1363	GLN
8	A	1369	ASN
8	B	319	HIS
8	B	346	GLN
8	B	371	ASN
8	B	455	HIS
8	B	484	GLN
8	B	485	GLN
8	B	497	HIS
8	B	514	GLN
8	B	534	HIS
8	B	560	ASN
8	B	571	HIS
8	B	694	ASN
8	B	740	ASN
8	B	1027	HIS
8	B	1029	HIS
8	B	1079	GLN
8	B	1082	ASN
8	B	1111	GLN
8	B	1255	ASN
8	B	1369	ASN
8	C	311	ASN
8	C	510	ASN
8	C	514	GLN
8	C	534	HIS
8	C	676	ASN
8	C	726	ASN

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Mol	Chain	Res	Type
8	C	737	GLN
8	C	849	GLN
8	C	903	GLN
8	C	914	GLN
8	C	919	ASN
8	C	1027	HIS
8	C	1079	GLN
8	C	1124	HIS
8	C	1184	ASN
8	C	1191	ASN
8	C	1223	GLN
8	C	1229	HIS
8	C	1245	ASN
8	D	214	ASN
8	D	346	GLN
8	D	371	ASN
8	D	438	GLN
8	D	476	GLN
8	D	484	GLN
8	D	514	GLN
8	D	534	HIS
8	D	640	HIS
8	D	643	GLN
8	D	795	ASN
8	D	914	GLN
8	D	981	HIS
8	D	1023	GLN
8	D	1080	ASN
8	D	1120	ASN
8	D	1191	ASN
8	D	1245	ASN
8	D	1313	ASN
8	D	1350	HIS
8	Y	22	HIS
8	Y	81	HIS
8	Y	153	ASN
8	Y	208	ASN
8	Y	211	GLN
8	Y	231	ASN
8	Y	257	ASN
8	Y	326	ASN
8	Y	388	ASN

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Mol	Chain	Res	Type
8	Y	432	ASN
8	Y	510	ASN
8	Y	534	HIS
8	Y	560	ASN
8	Y	708	ASN
8	Y	794	ASN
8	Y	849	GLN
8	Y	889	HIS
8	Y	914	GLN
8	Y	1029	HIS
8	Y	1061	ASN
8	Y	1093	ASN
8	Y	1120	ASN
8	Y	1141	GLN
8	Y	1229	HIS
8	Y	1264	GLN
8	Y	1300	GLN
8	Y	1313	ASN
8	Y	1369	ASN
8	Z	49	HIS
8	Z	96	GLN
8	Z	111	GLN
8	Z	181	GLN
8	Z	462	GLN
8	Z	543	GLN
8	Z	618	HIS
8	Z	660	HIS
8	Z	676	ASN
8	Z	722	HIS
8	Z	748	HIS
8	Z	795	ASN
8	Z	874	GLN
8	Z	905	GLN
8	Z	914	GLN
8	Z	985	ASN
8	Z	1000	ASN
8	Z	1060	ASN
8	Z	1061	ASN
8	Z	1082	ASN
8	Z	1111	GLN
8	Z	1120	ASN
8	Z	1166	HIS

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Mol	Chain	Res	Type
8	Z	1168	GLN
8	Z	1230	ASN
8	Z	1309	GLN
8	Z	1313	ASN
8	Z	1363	GLN
8	Z	1369	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

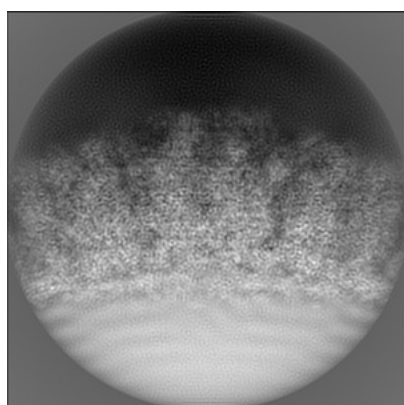
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31301. These allow visual inspection of the internal detail of the map and identification of artifacts.

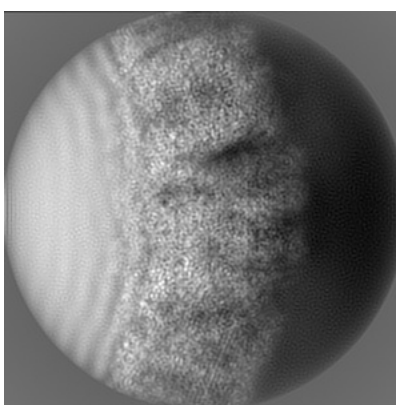
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

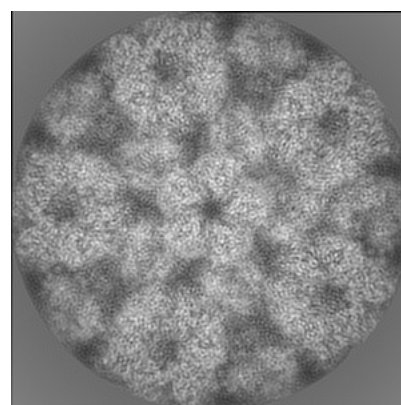
6.1.1 Primary map



X



Y

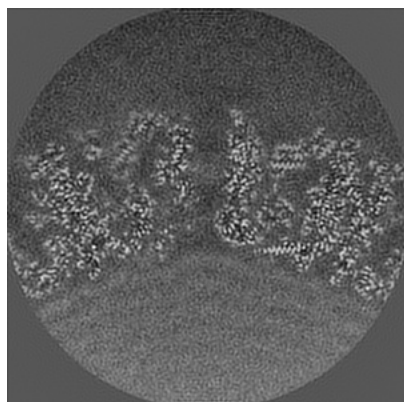


Z

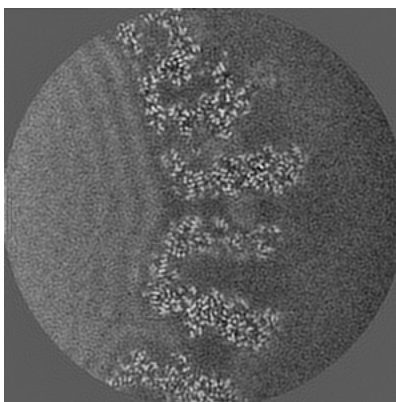
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

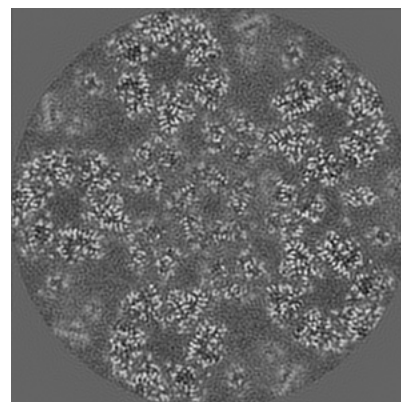
6.2.1 Primary map



X Index: 128



Y Index: 128

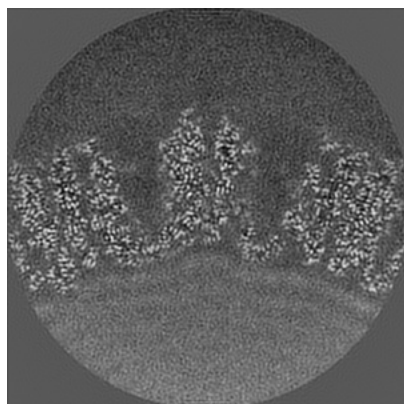


Z Index: 128

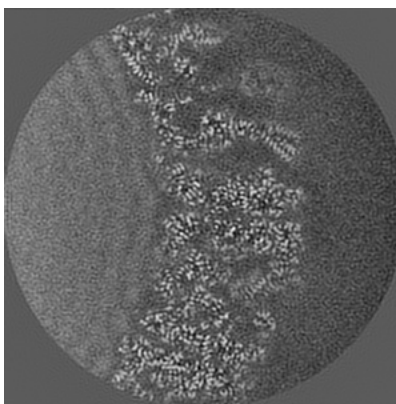
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

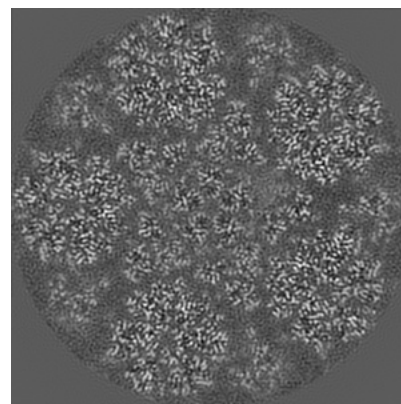
6.3.1 Primary map



X Index: 117



Y Index: 113

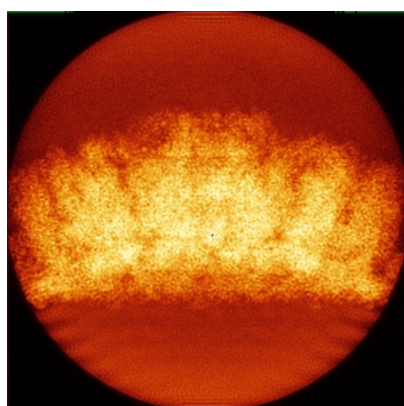


Z Index: 118

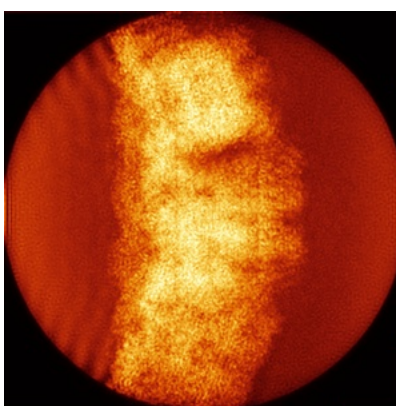
The images above show the largest variance slices of the map in three orthogonal directions.

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

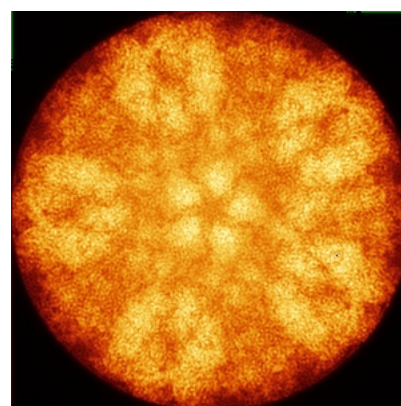
6.4.1 Primary map



X



Y

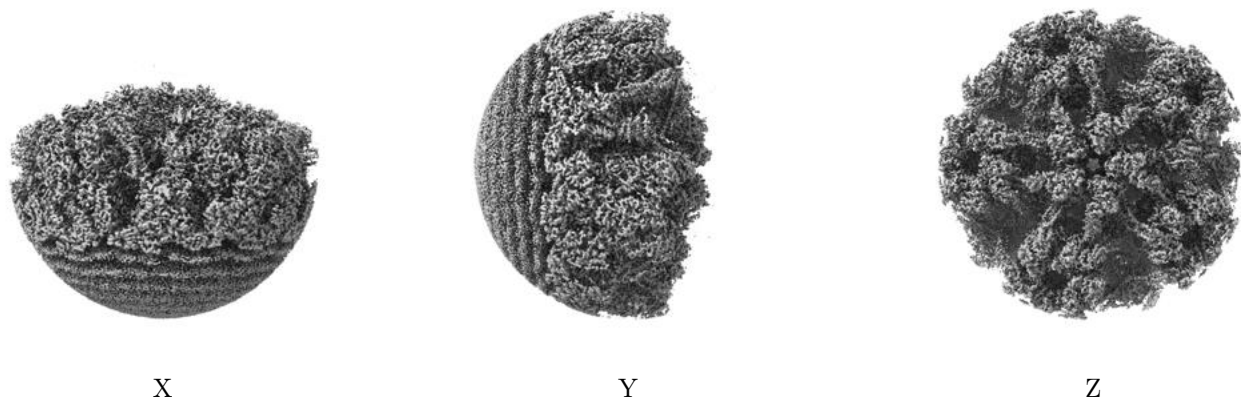


Z

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 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

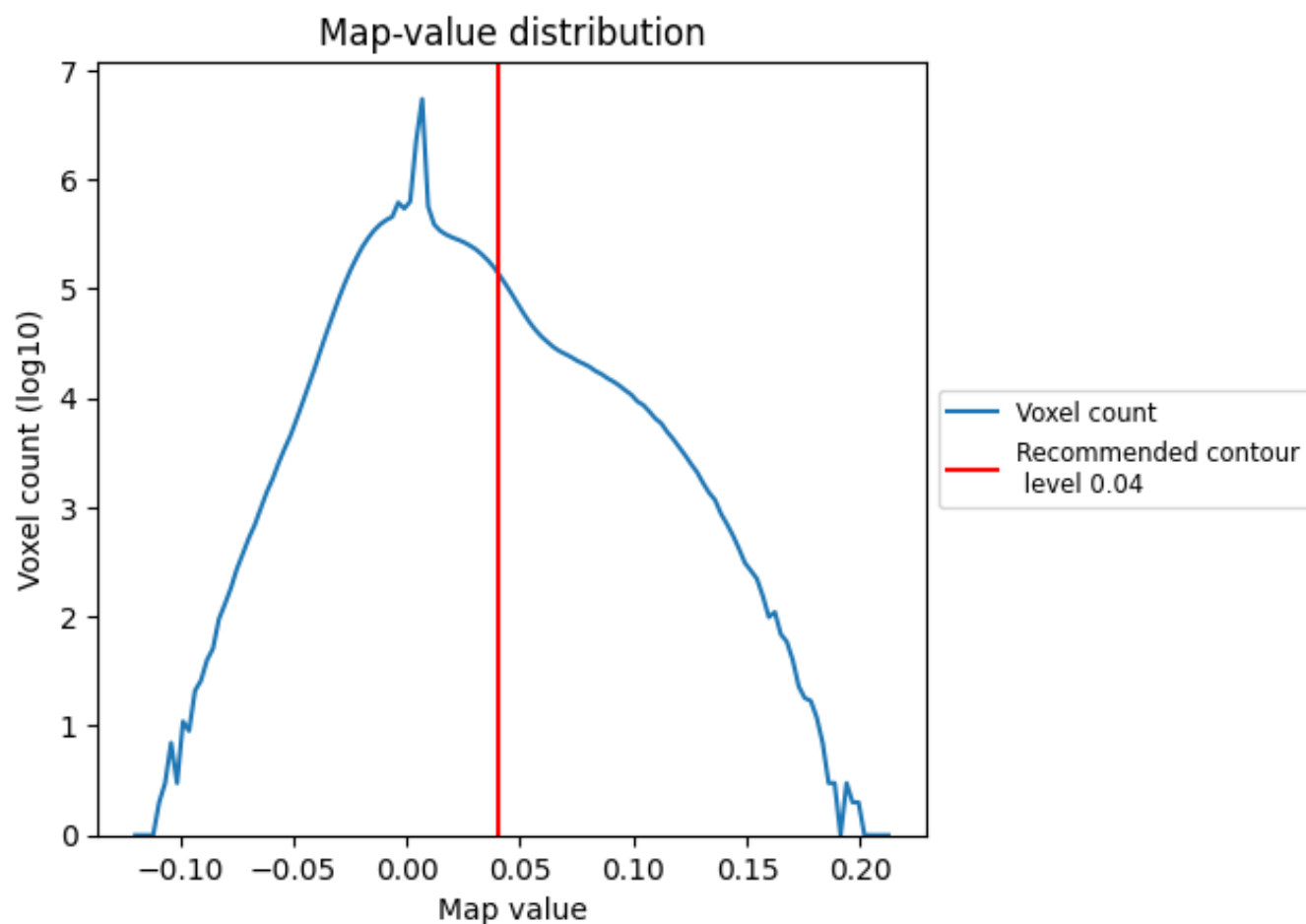
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

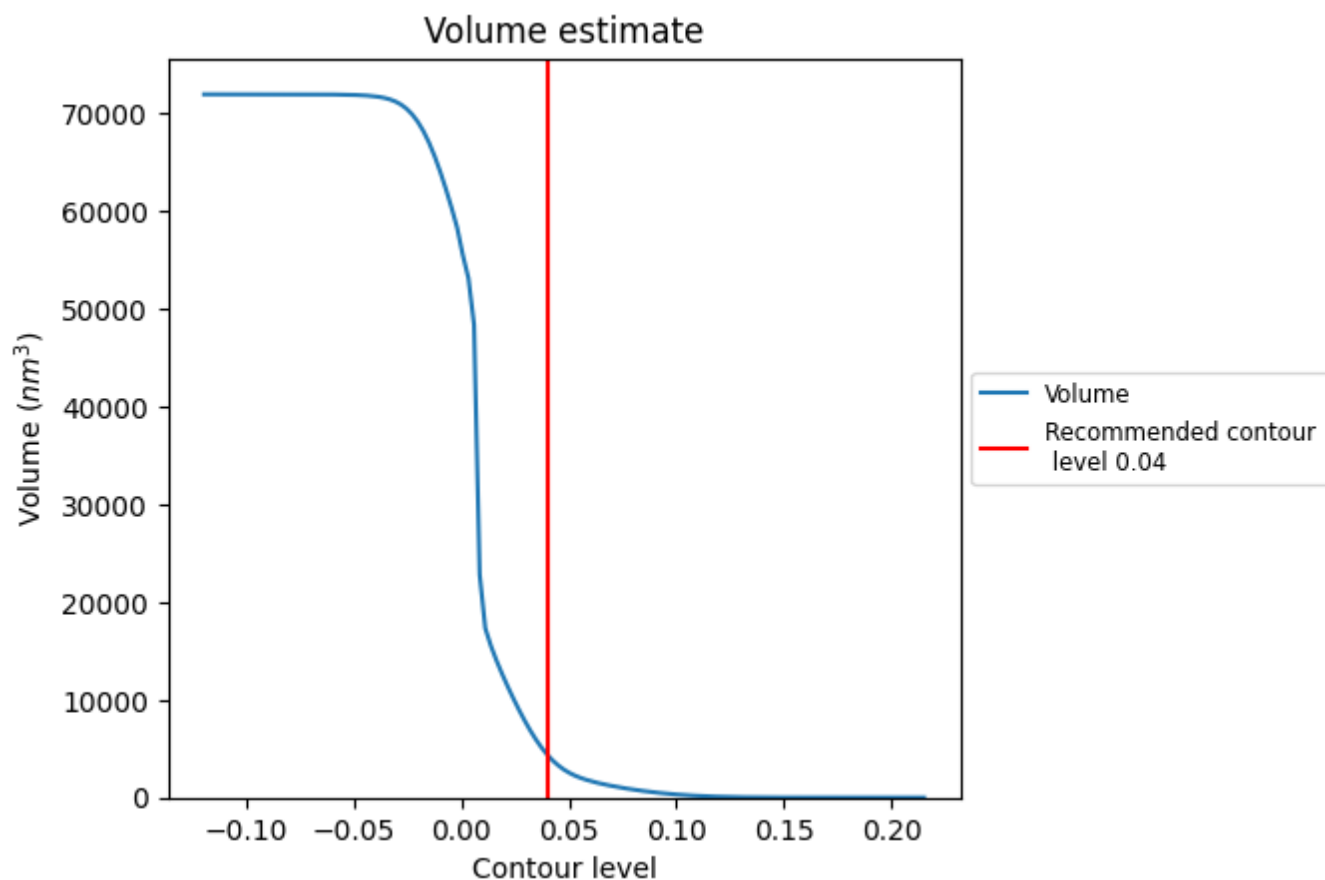
This section contains the results of statistical analysis of the map.

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.

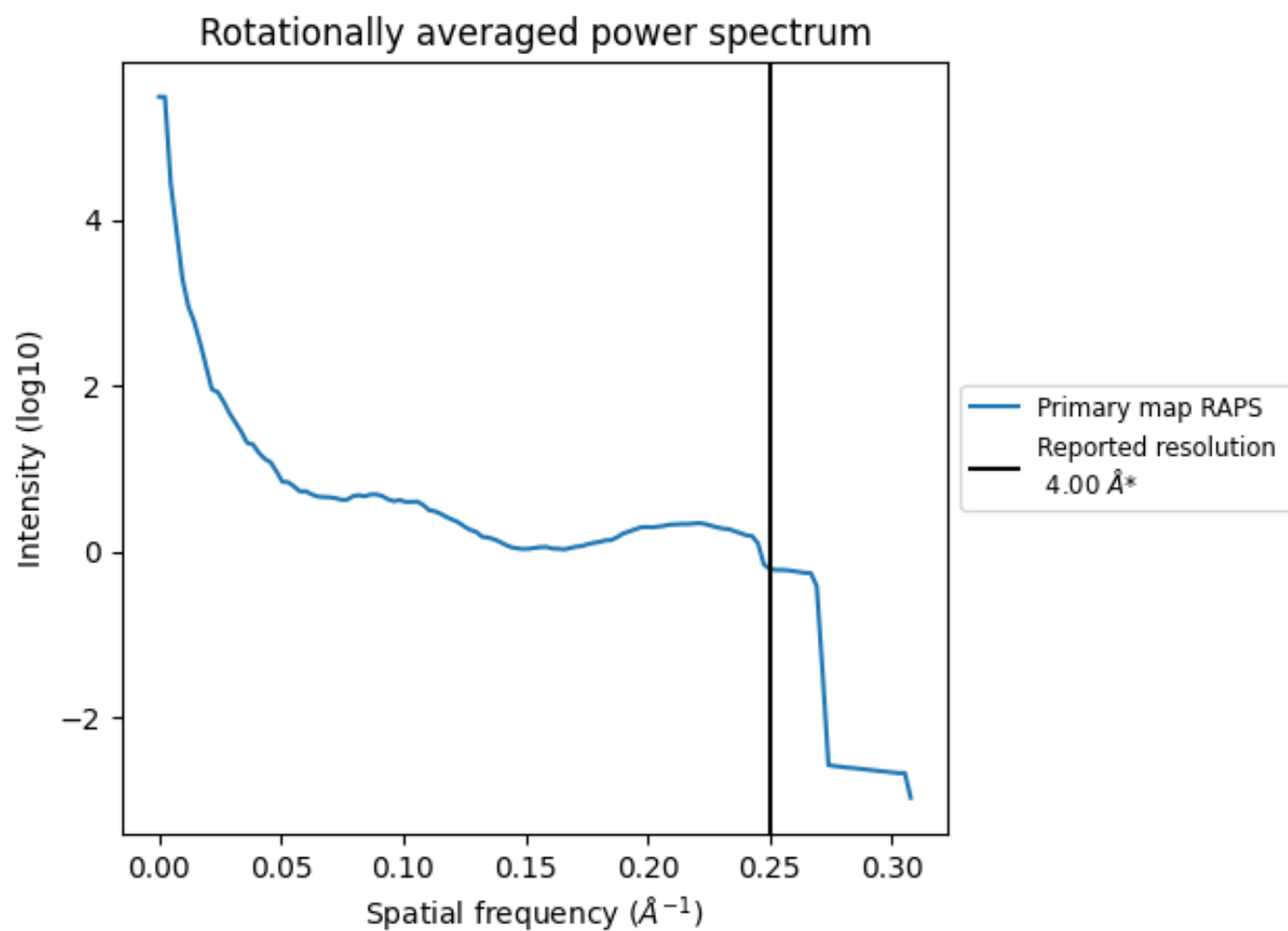
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4382 nm³; this corresponds to an approximate mass of 3958 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 0.250 Å⁻¹

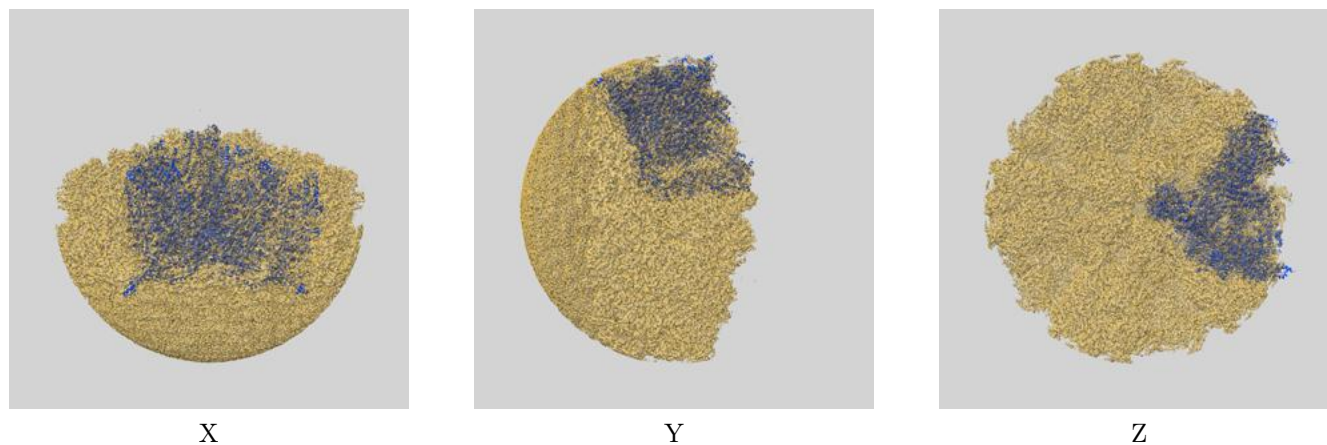
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

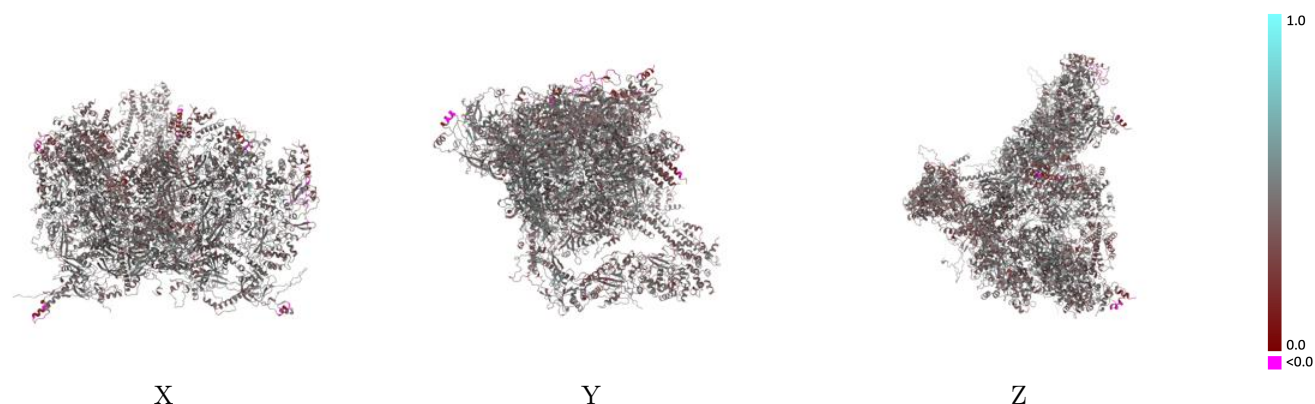
This section contains information regarding the fit between EMDB map EMD-31301 and PDB model 7ETO. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



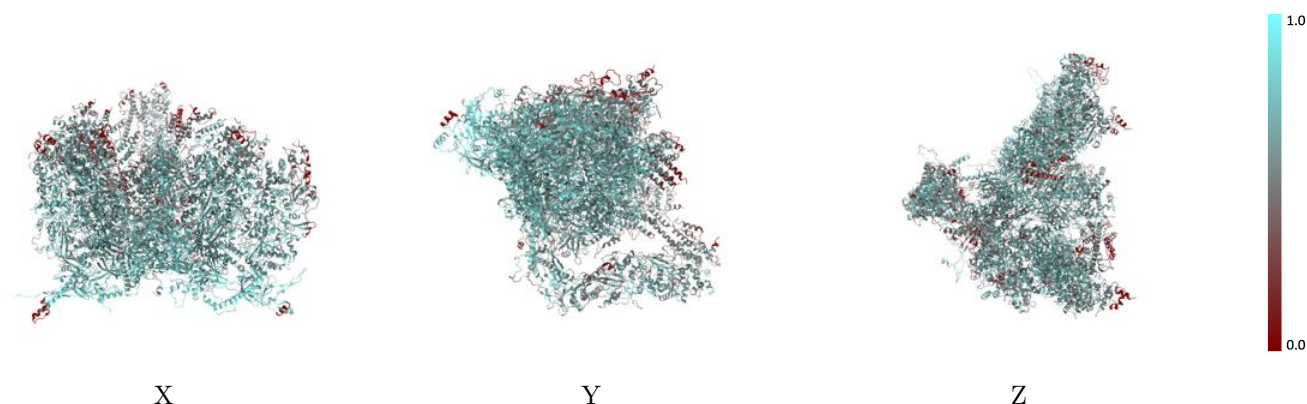
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



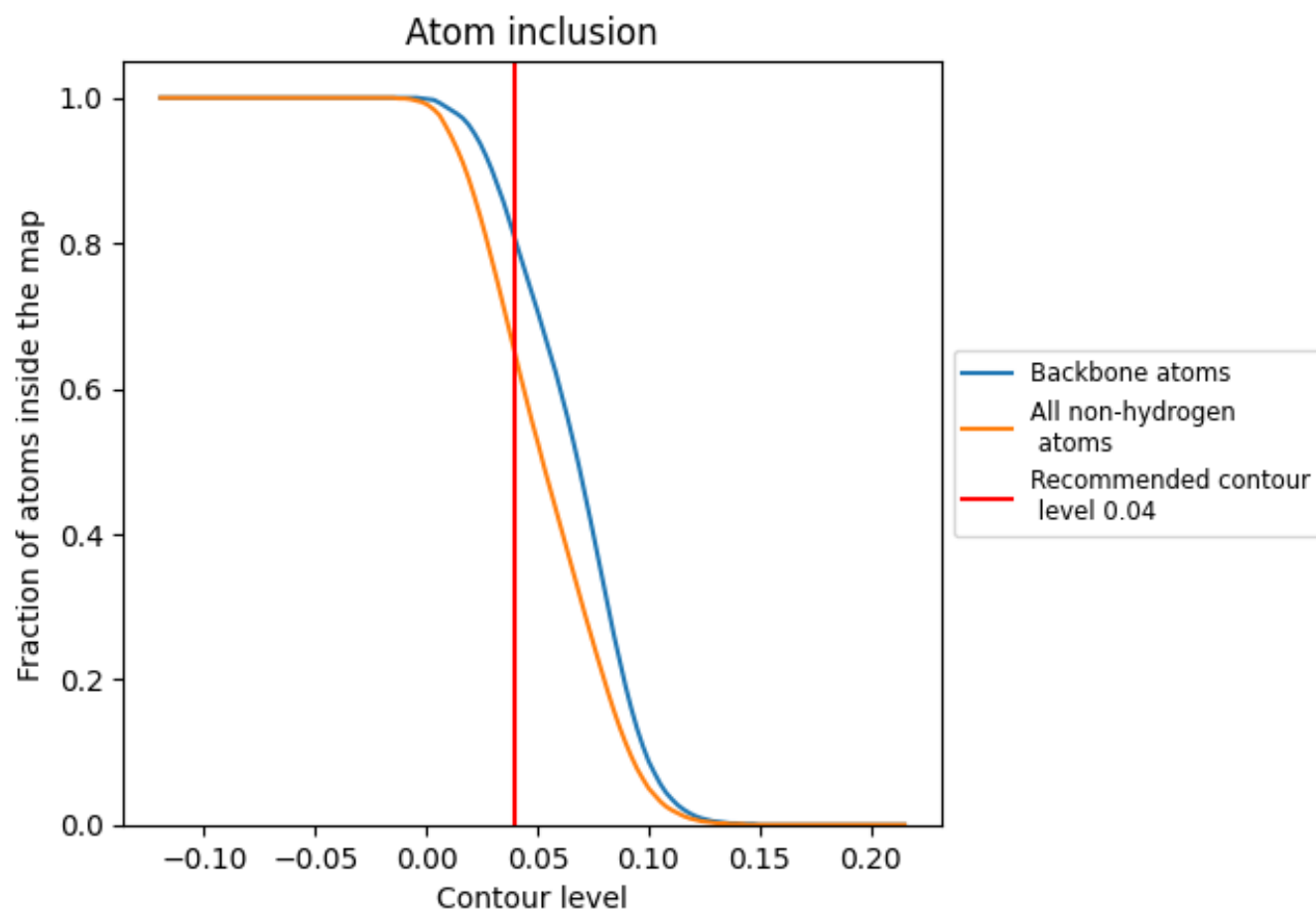
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 65% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6470	 0.4280
1	 0.4150	 0.3720
A	 0.5930	 0.4080
B	 0.6670	 0.4410
C	 0.7080	 0.4480
D	 0.6840	 0.4390
H	 0.3530	 0.3050
I	 0.5970	 0.4120
M	 0.6780	 0.4310
N	 0.5460	 0.3660
O	 0.4110	 0.2970
P	 0.3890	 0.3220
Q	 0.4600	 0.3810
R	 0.4180	 0.3790
S	 0.4740	 0.3990
T	 0.2530	 0.2760
Y	 0.6620	 0.4200
Z	 0.6920	 0.4480
a	 0.7010	 0.4510
g	 0.6250	 0.4060
h	 0.6610	 0.4150
i	 0.3270	 0.3450
j	 0.4020	 0.3890
m	 0.7070	 0.4510
n	 0.6530	 0.4190
o	 0.6500	 0.4240
x	 0.4650	 0.3860

