



Full wwPDB EM Validation Report ⓘ

May 14, 2025 – 02:19 AM EDT

PDB ID : 6PO2 / pdb_00006po2
EMDB ID : EMD-20407
Title : In situ structure of BTV RNA-dependent RNA polymerase in BTV core
Authors : He, Y.; Shivakoti, S.; Ding, K.; Cui, Y.; Roy, P.; Zhou, Z.H.
Deposited on : 2019-07-03
Resolution : 3.60 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

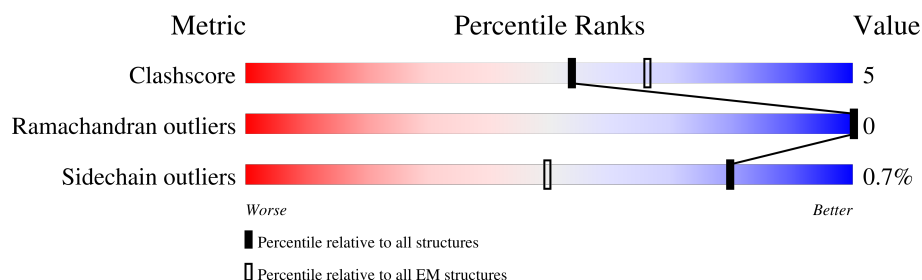
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1302	<div> <div>61%</div> <div>79%</div> <div>16%</div> <div>.</div> </div>
2	B	901	<div> <div>27%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
2	C	901	<div> <div>52%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
2	D	901	<div> <div>30%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
2	E	901	<div> <div>52%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
2	F	901	<div> <div>31%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
2	G	901	<div> <div>53%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
2	H	901	<div> <div>30%</div> <div>83%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	901	<div><div></div><div>51%</div><div></div><div>85%</div><div></div><div>13%</div><div></div></div>
2	J	901	<div><div></div><div>29%</div><div></div><div>83%</div><div></div><div>13%</div><div></div></div>
2	K	901	<div><div></div><div>51%</div><div></div><div>88%</div><div></div><div>10%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 80873 atoms, of which 0 are hydrogens and 0 are deuteriums.

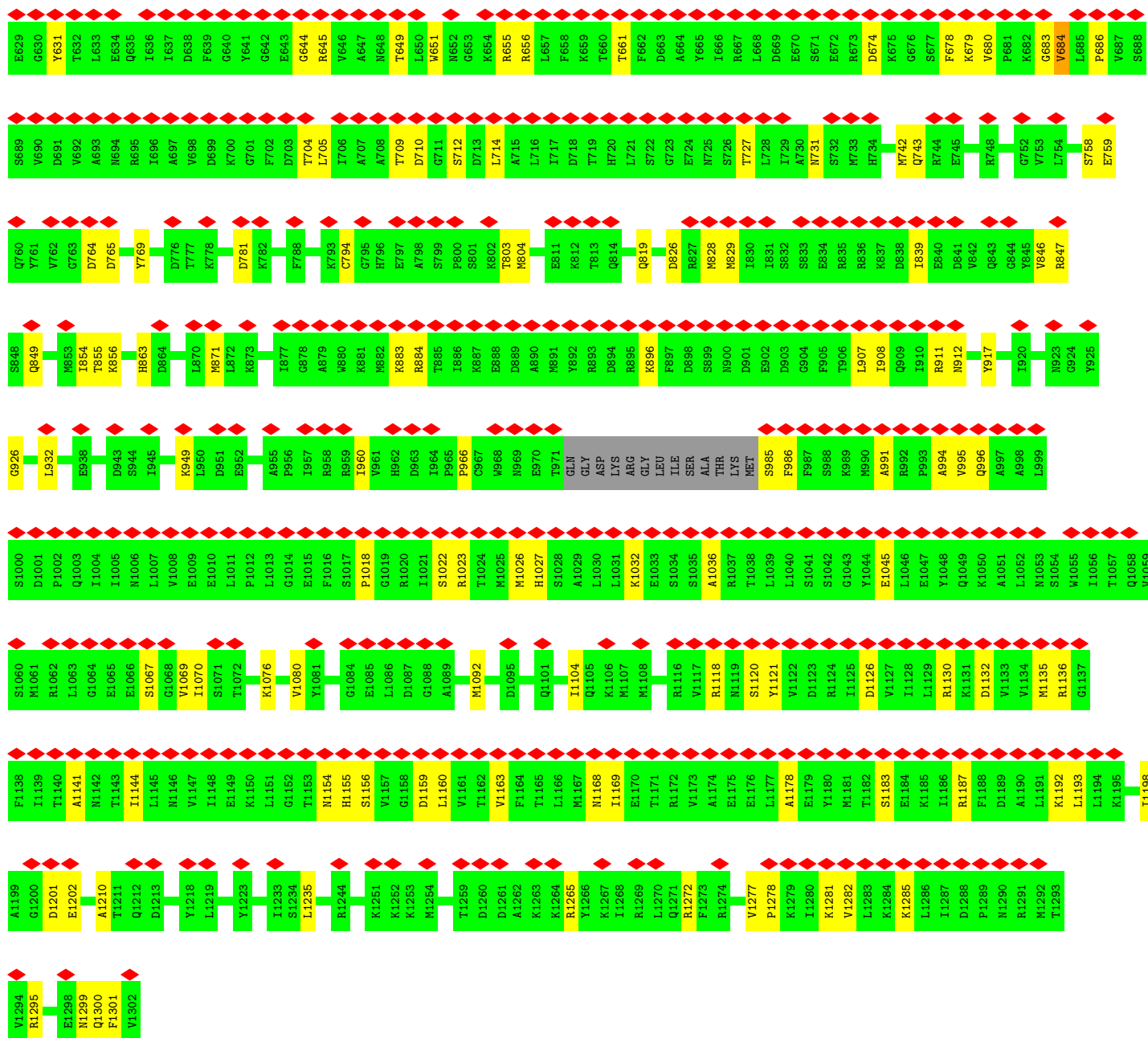
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RNA-directed RNA polymerase.

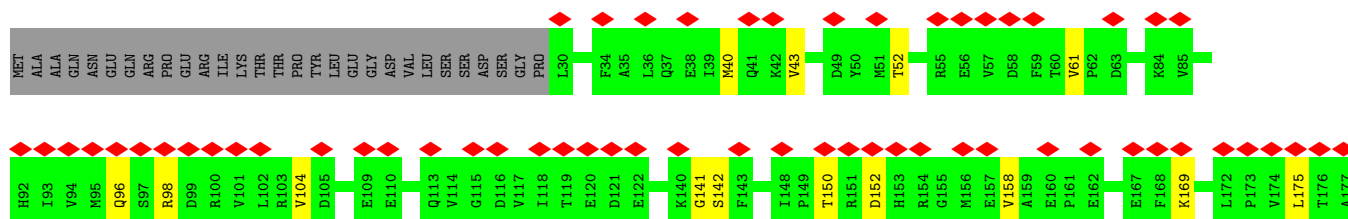
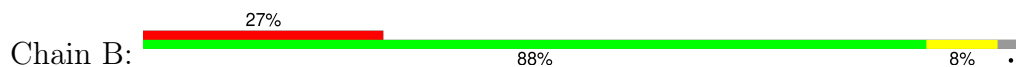
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1244	Total	C	N	O	S	0	0
			10062	6417	1720	1865	60		

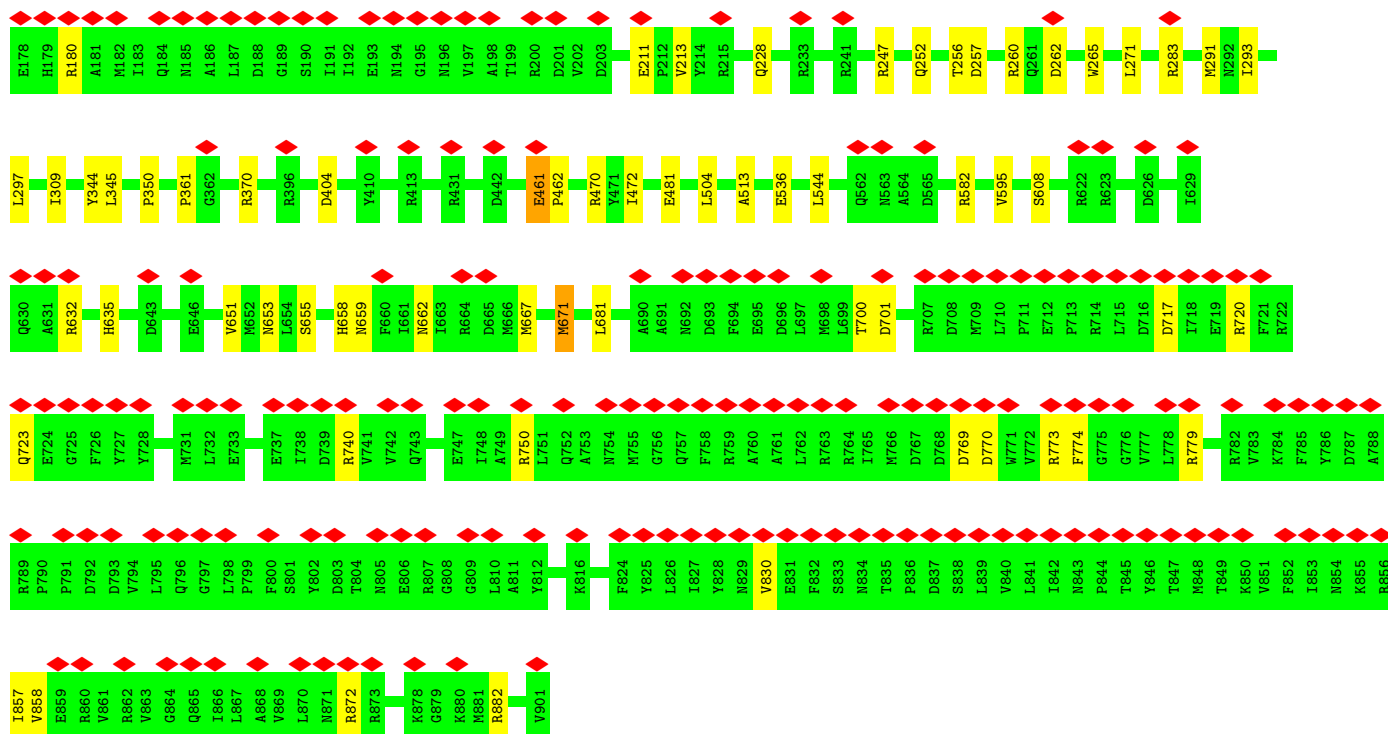
- Molecule 2 is a protein called Inner core structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	872	Total	C	N	O	S	0	0
			7046	4496	1222	1287	41		
2	C	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
2	D	863	Total	C	N	O	S	0	0
			6968	4448	1209	1271	40		
2	E	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
2	F	868	Total	C	N	O	S	0	0
			6995	4463	1209	1283	40		
2	G	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
2	H	868	Total	C	N	O	S	0	0
			7017	4476	1218	1282	41		
2	I	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		
2	J	870	Total	C	N	O	S	0	0
			7030	4484	1220	1285	41		
2	K	885	Total	C	N	O	S	0	0
			7151	4561	1239	1310	41		

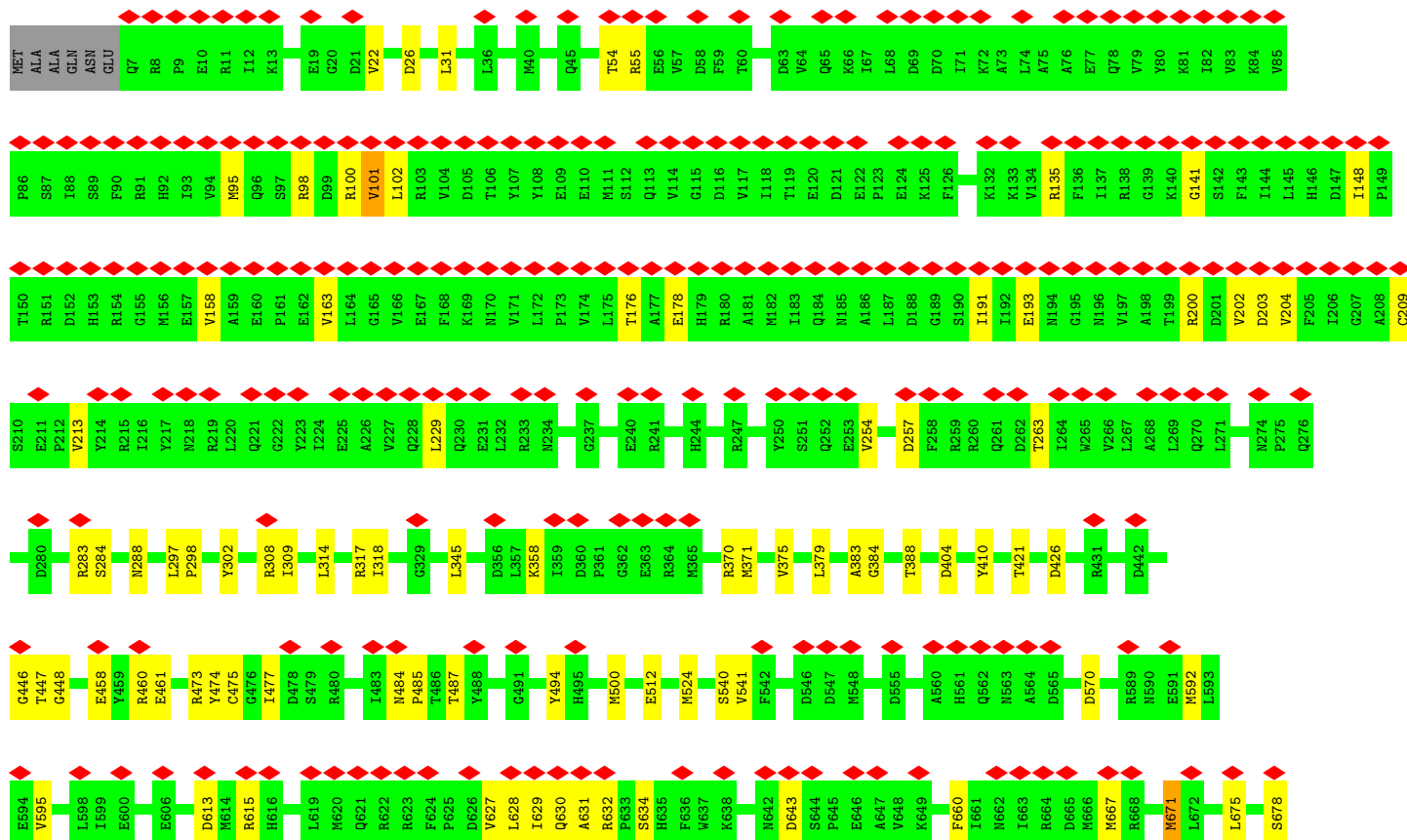
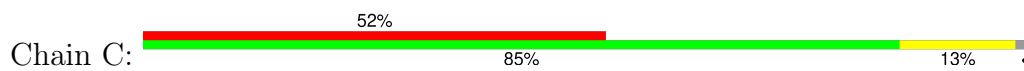


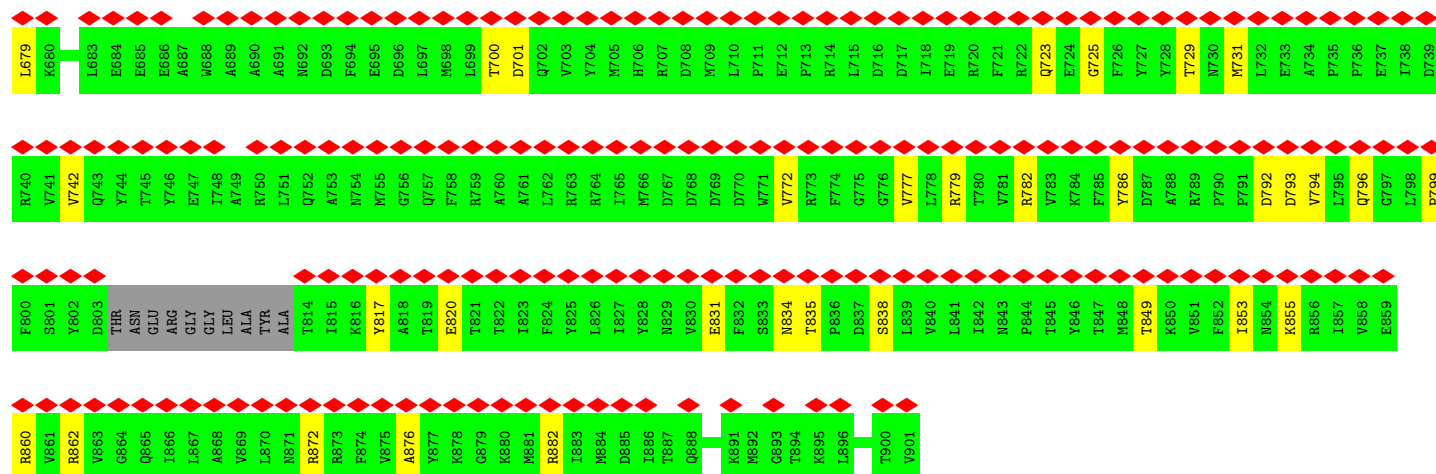
• Molecule 2: Inner core structural protein VP3



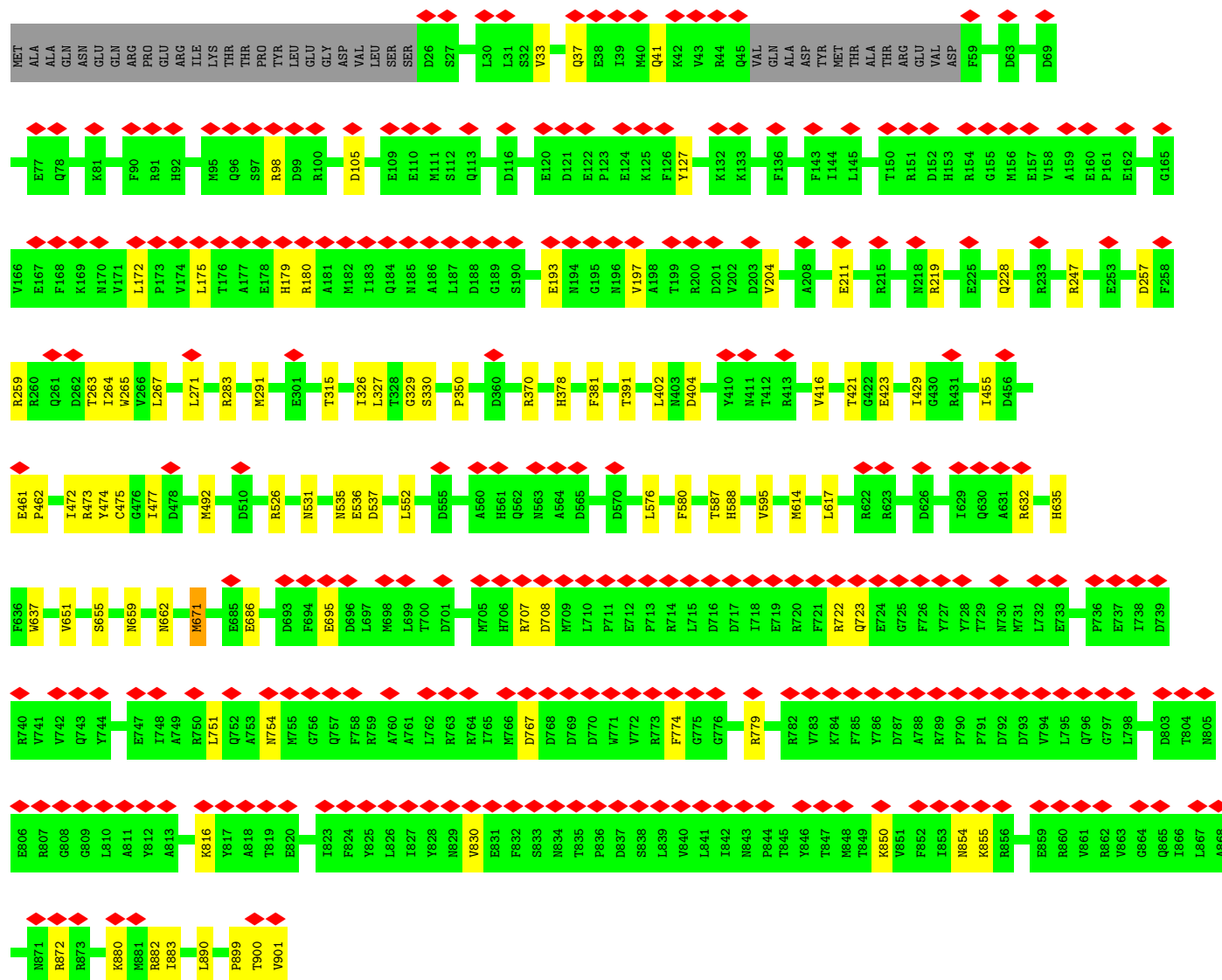
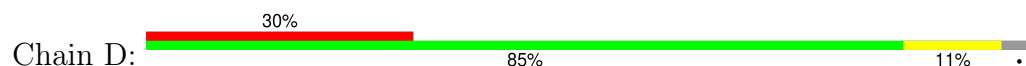


• Molecule 2: Inner core structural protein VP3



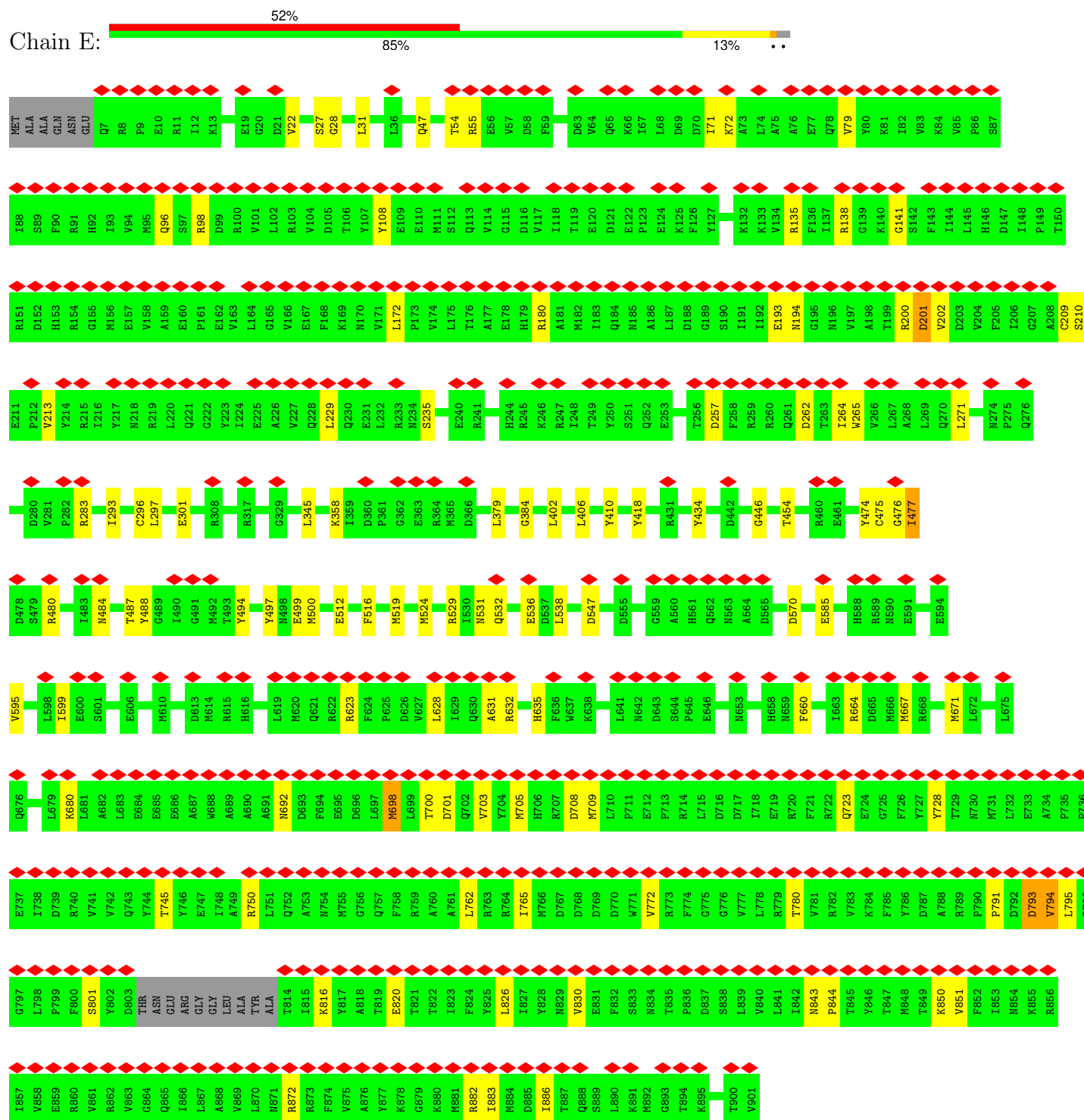


• Molecule 2: Inner core structural protein VP3



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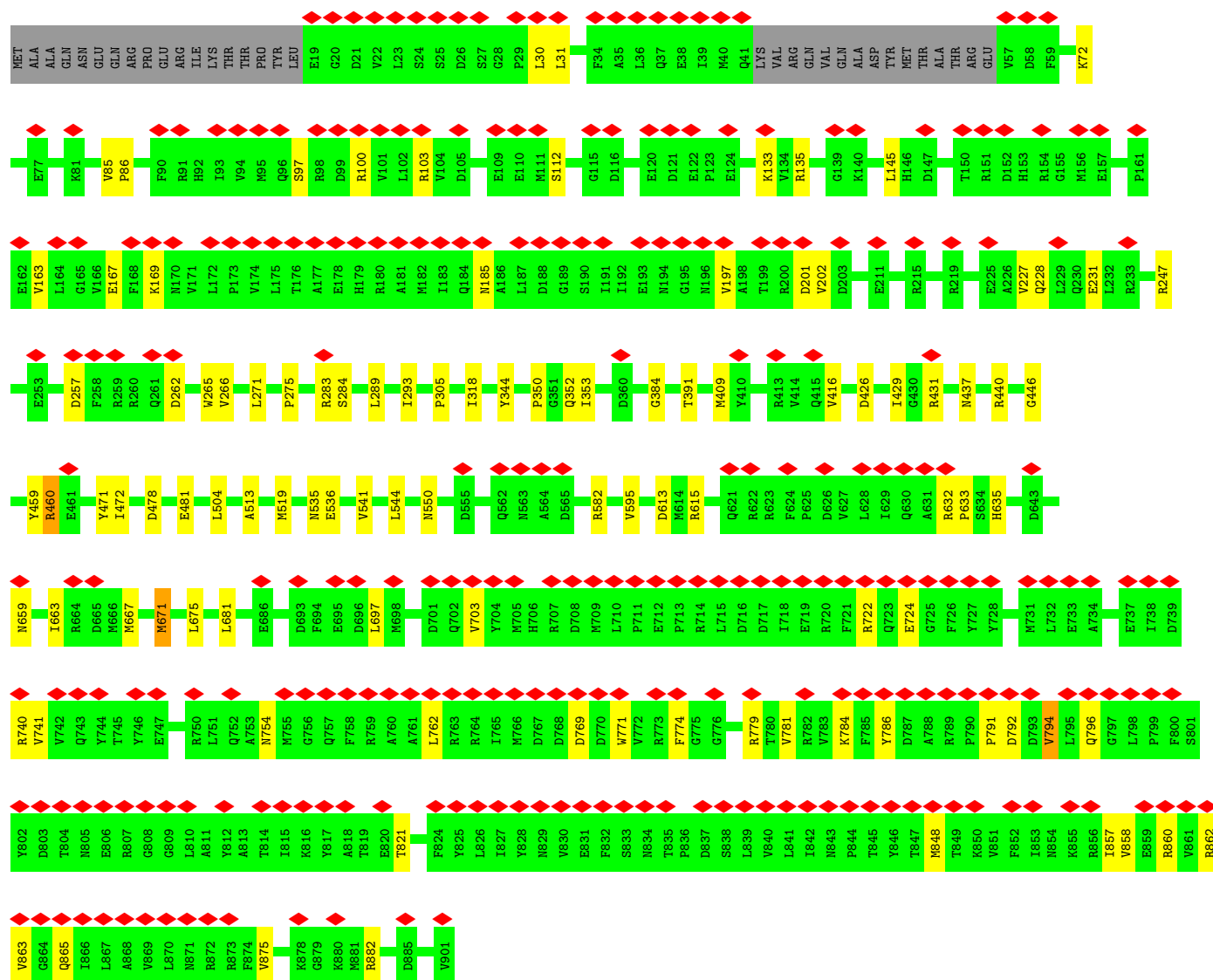
Chain E:



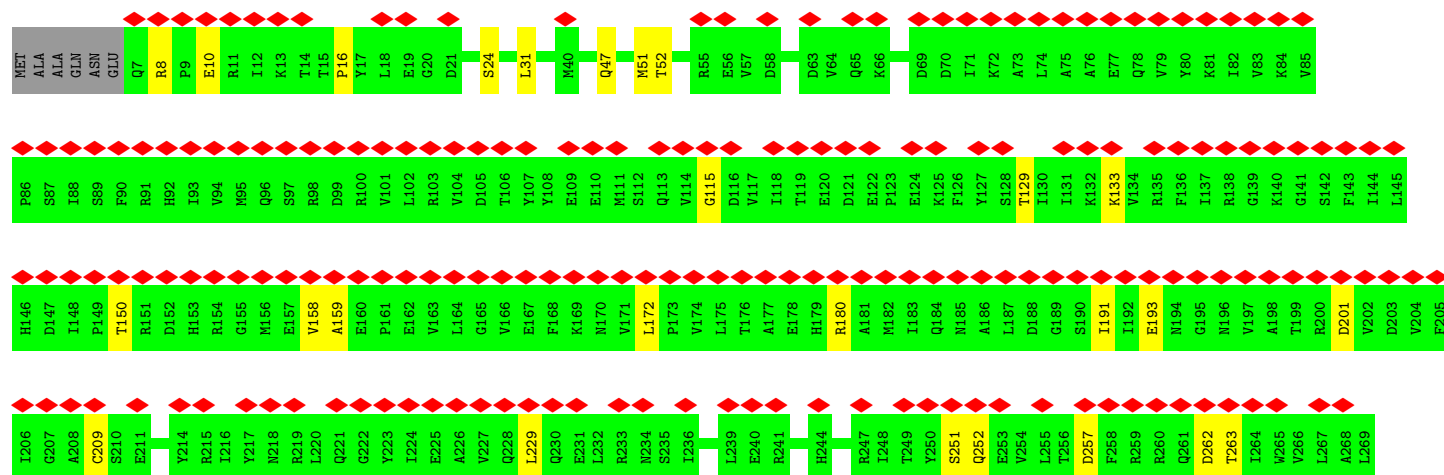
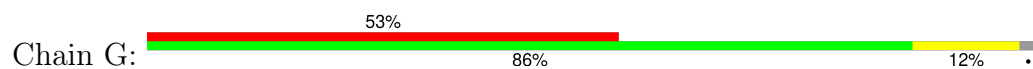
• Molecule 2: Inner core structural protein VP3

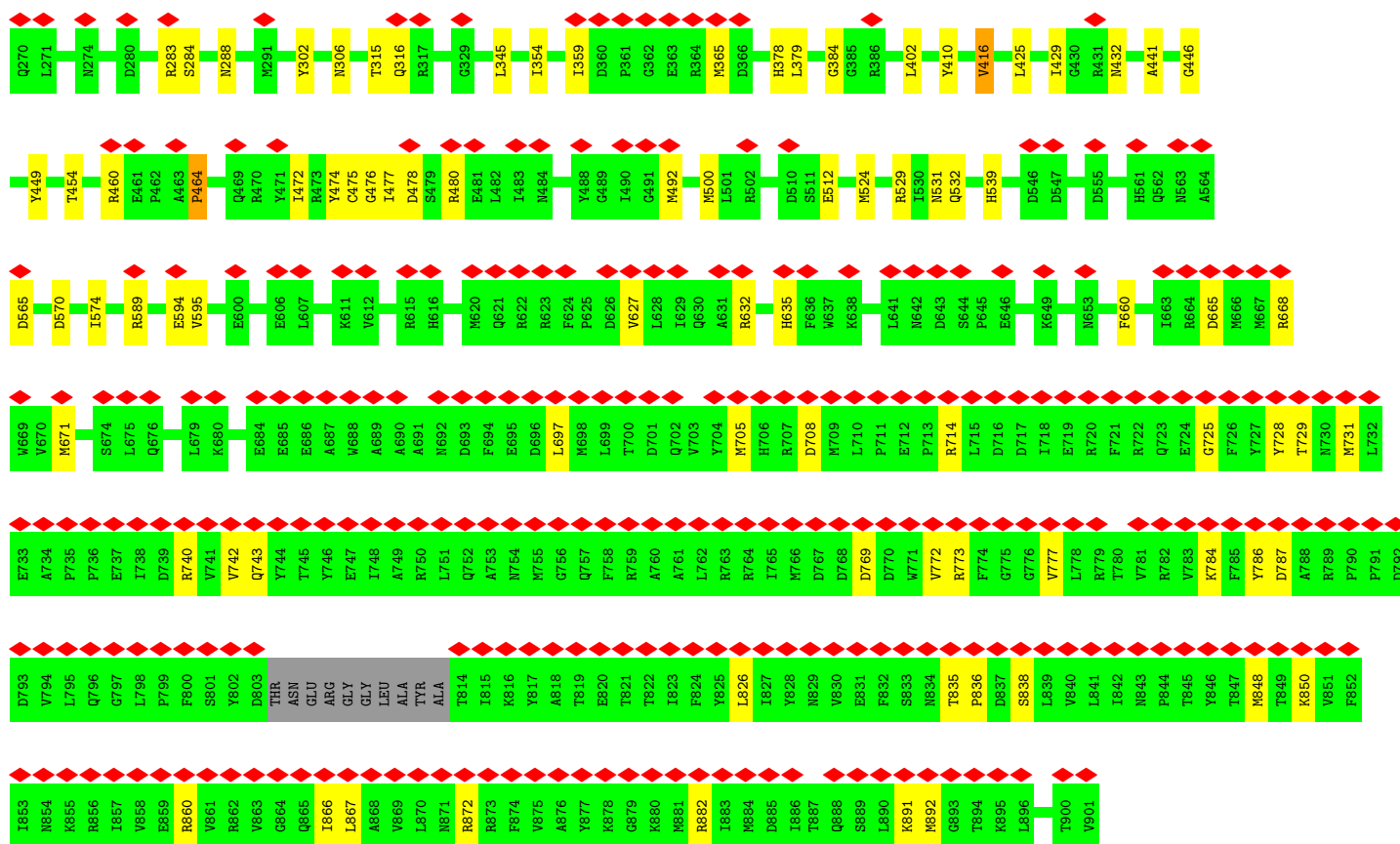
Chain F:



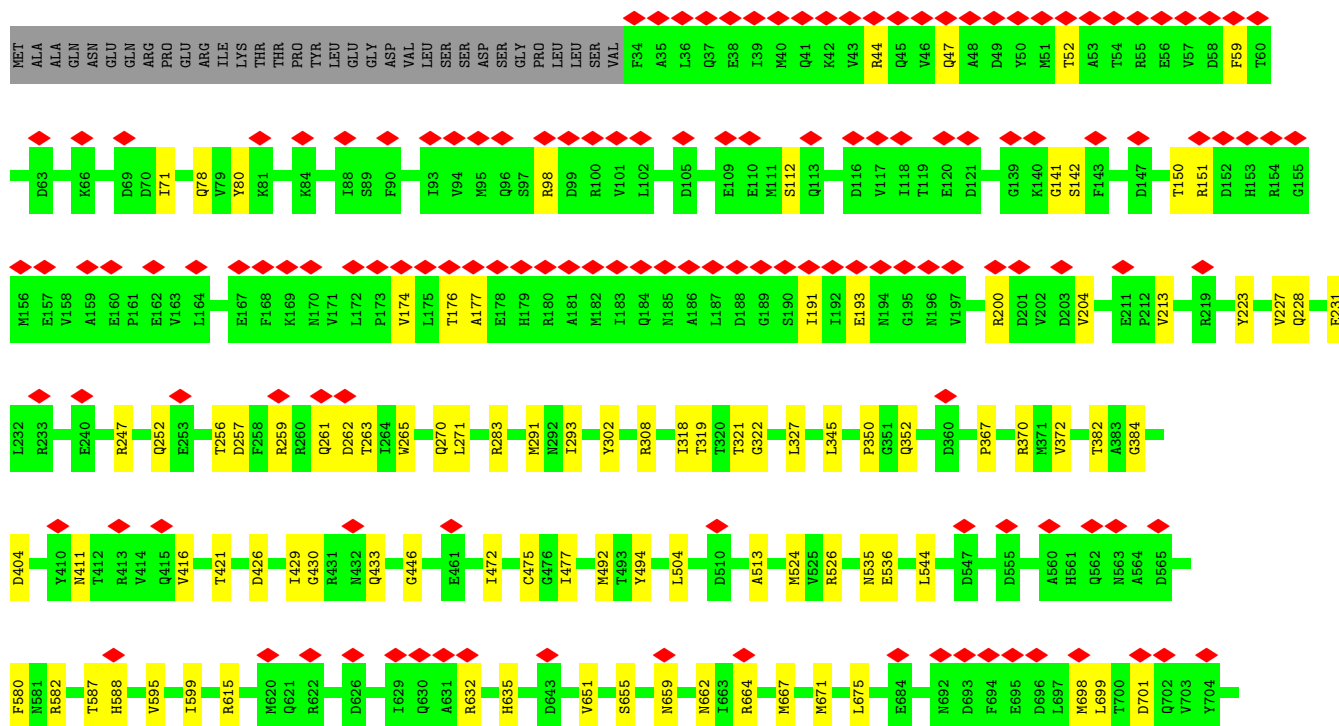
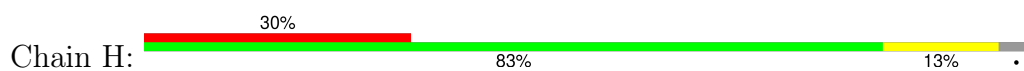


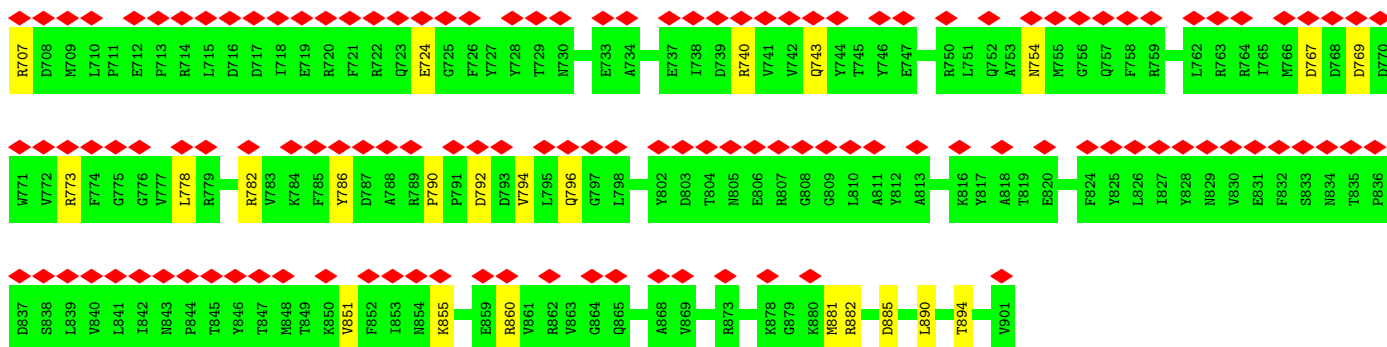
• Molecule 2: Inner core structural protein VP3



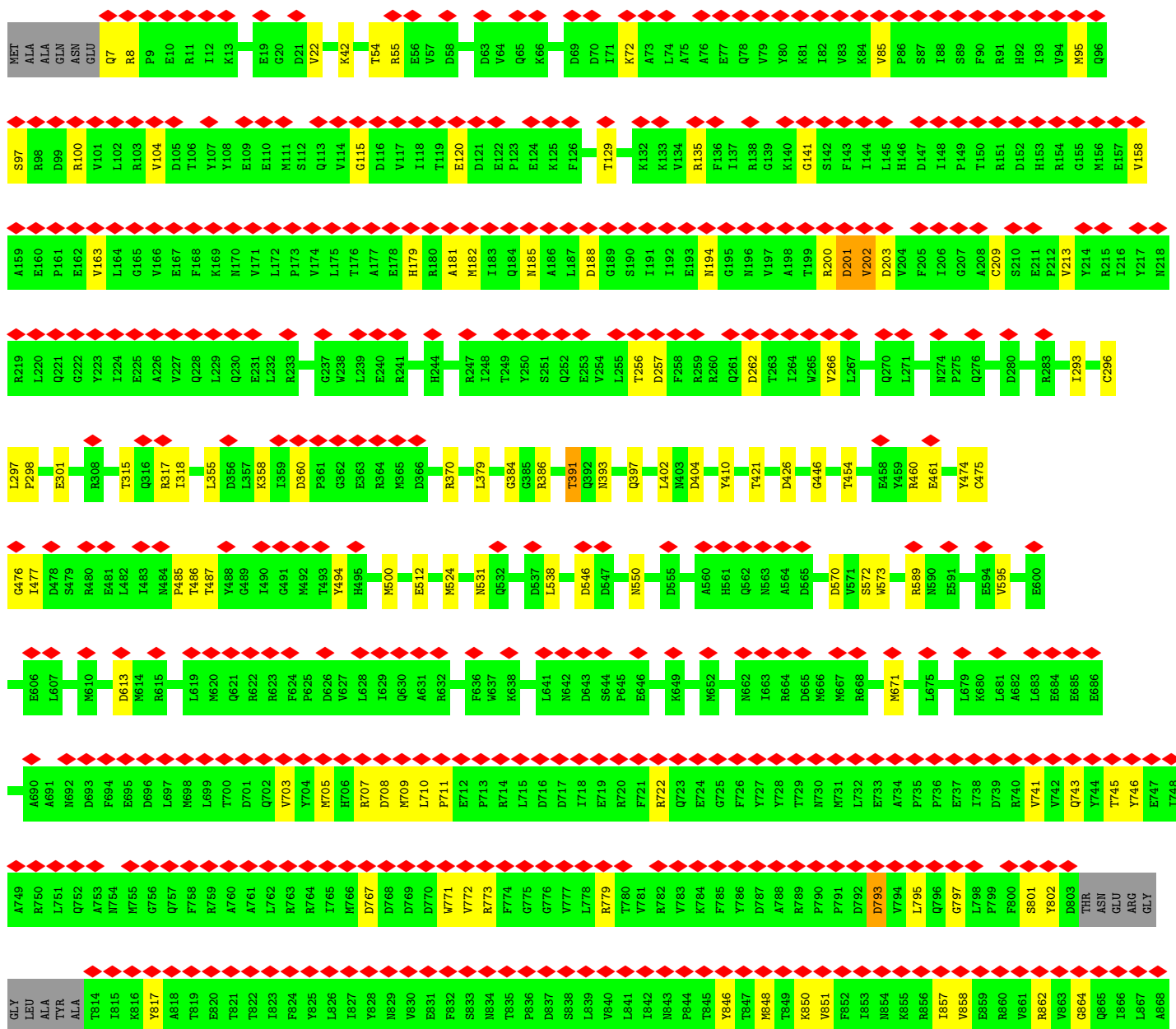
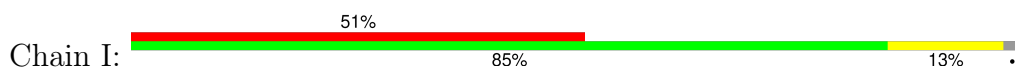


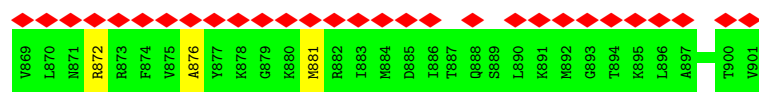
• Molecule 2: Inner core structural protein VP3



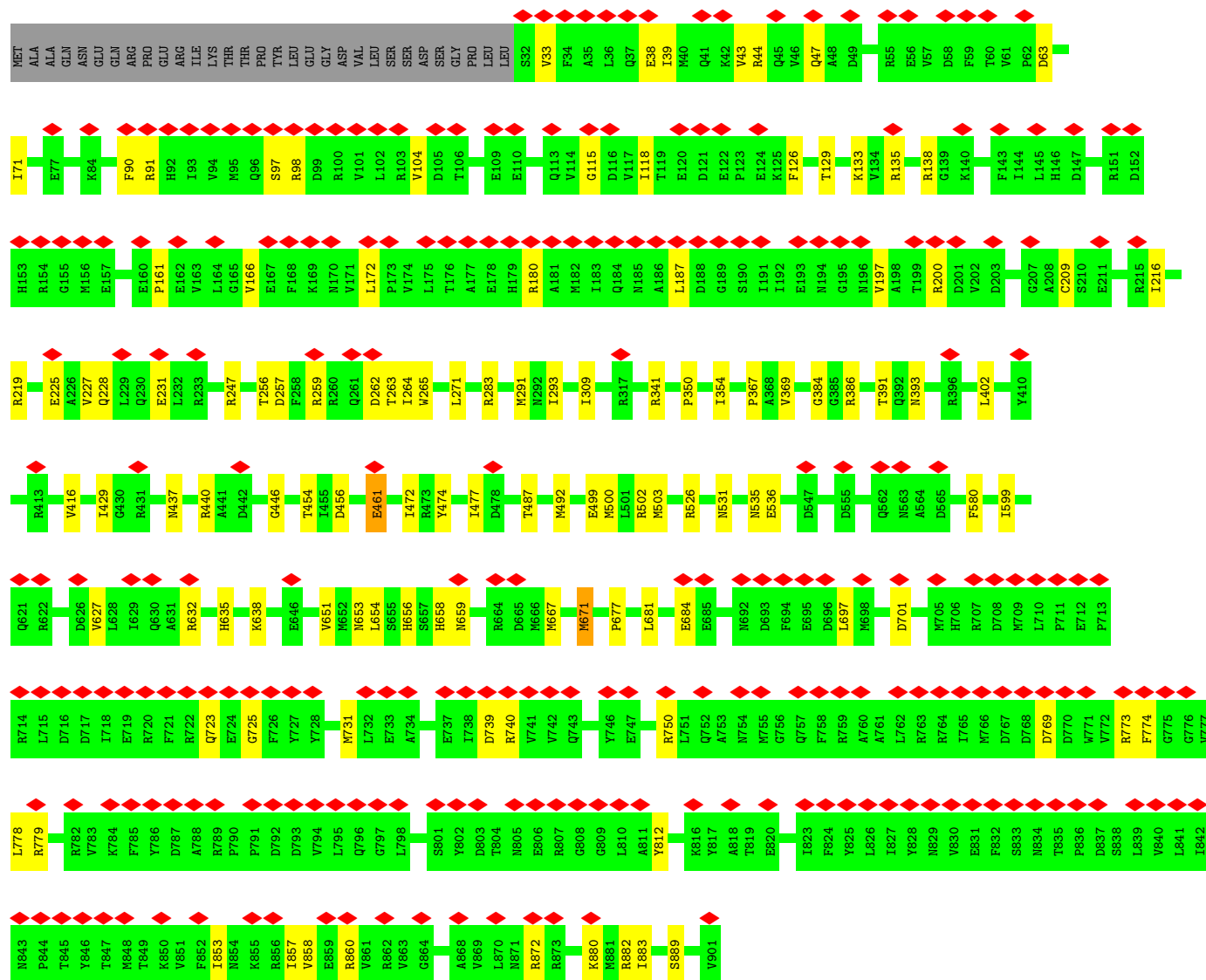
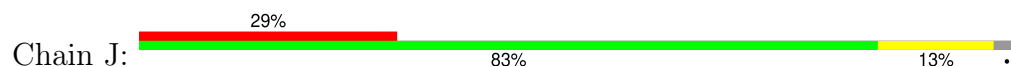


• Molecule 2: Inner core structural protein VP3

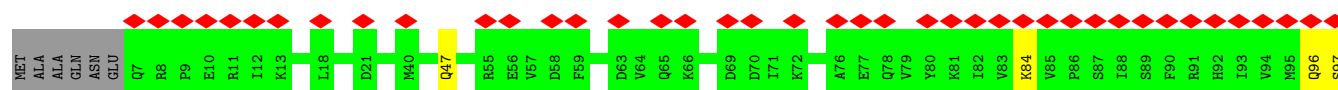
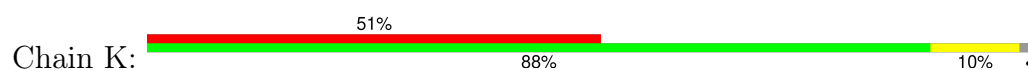




• Molecule 2: Inner core structural protein VP3



• Molecule 2: Inner core structural protein VP3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	150346	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 ($e^-/\text{\AA}^2$)	32.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.076	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	348.16, 348.16, 348.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/10268	0.51	2/13862 (0.0%)
2	B	0.30	0/7203	0.47	0/9782
2	C	0.25	0/7310	0.44	0/9927
2	D	0.31	0/7124	0.48	2/9673 (0.0%)
2	E	0.26	0/7310	0.45	0/9927
2	F	0.32	0/7151	0.49	0/9712
2	G	0.28	0/7310	0.47	3/9927 (0.0%)
2	H	0.32	0/7174	0.50	0/9742
2	I	0.28	0/7310	0.48	0/9927
2	J	0.32	0/7187	0.49	1/9760 (0.0%)
2	K	0.27	0/7310	0.47	0/9927
All	All	0.29	0/82657	0.48	8/112166 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	369	VAL	N-CA-C	-5.82	107.14	112.96
2	G	193	GLU	CA-C-N	5.61	130.36	122.46
2	G	193	GLU	C-N-CA	5.61	130.36	122.46
2	D	105	ASP	CA-C-N	5.60	132.24	121.54
2	D	105	ASP	C-N-CA	5.60	132.24	121.54
2	G	464	PRO	N-CA-C	-5.58	105.77	113.53
1	A	530	LEU	CA-C-N	5.42	123.66	120.24
1	A	530	LEU	C-N-CA	5.42	123.66	120.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10062	0	10106	135	0
2	B	7046	0	7032	59	0
2	C	7151	0	7137	79	0
2	D	6968	0	6955	71	0
2	E	7151	0	7137	69	0
2	F	6995	0	6968	71	0
2	G	7151	0	7137	71	0
2	H	7017	0	6996	82	0
2	I	7151	0	7137	76	0
2	J	7030	0	7010	77	0
2	K	7151	0	7137	78	0
All	All	80873	0	80752	807	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 5.

All (807) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:438:VAL:HG11	2:K:452:TRP:CZ2	1.57	1.37
2:K:438:VAL:HG11	2:K:452:TRP:CH2	1.65	1.32
2:D:461:GLU:CG	2:D:462:PRO:HD3	1.67	1.23
2:K:438:VAL:CG1	2:K:452:TRP:CZ2	2.23	1.21
2:G:595:VAL:HG22	2:G:891:LYS:NZ	1.60	1.16
2:C:475:CYS:SG	2:C:477:ILE:HG12	1.88	1.12
2:K:438:VAL:CG1	2:K:452:TRP:CH2	2.31	1.12
2:D:461:GLU:HG3	2:D:462:PRO:HD3	1.12	1.12
2:K:477:ILE:HD11	2:K:524:MET:HE2	1.12	1.11
2:K:477:ILE:HD11	2:K:524:MET:CE	1.84	1.07
2:E:477:ILE:HD11	2:E:524:MET:HE2	1.12	1.05
2:D:461:GLU:HG3	2:D:462:PRO:CD	1.86	1.04
2:F:671:MET:HE3	2:F:671:MET:HA	1.38	1.03
2:G:477:ILE:HD11	2:G:524:MET:HE2	1.06	1.03
2:G:595:VAL:CG2	2:G:891:LYS:NZ	2.22	1.02
2:J:667:MET:CE	2:J:671:MET:HE2	1.94	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:667:MET:HE3	2:J:671:MET:HE2	1.47	0.96
2:K:671:MET:HA	2:K:671:MET:HE3	1.44	0.96
2:E:477:ILE:CD1	2:E:524:MET:HE2	1.98	0.94
2:G:477:ILE:HD11	2:G:524:MET:CE	1.97	0.93
2:C:667:MET:SD	2:C:671:MET:HE1	2.12	0.88
2:K:141:GLY:HA2	2:K:213:VAL:HG13	1.56	0.88
2:H:475:CYS:SG	2:H:477:ILE:HD11	2.14	0.88
2:D:461:GLU:HG2	2:D:462:PRO:HD3	1.56	0.87
2:E:477:ILE:HD11	2:E:524:MET:CE	2.04	0.86
2:G:595:VAL:CG2	2:G:891:LYS:HZ1	1.90	0.84
2:C:101:VAL:C	2:C:102:LEU:HD12	2.02	0.84
2:G:595:VAL:HG22	2:G:891:LYS:HZ2	1.40	0.83
2:K:438:VAL:HG11	2:K:452:TRP:HZ2	1.42	0.81
2:D:461:GLU:CG	2:D:462:PRO:CD	2.52	0.80
2:B:671:MET:HE3	2:B:671:MET:HA	1.62	0.79
2:H:475:CYS:SG	2:H:477:ILE:HG13	2.24	0.78
2:D:475:CYS:SG	2:D:477:ILE:HG13	2.23	0.78
2:E:141:GLY:HA2	2:E:213:VAL:HG13	1.66	0.77
2:H:475:CYS:SG	2:H:477:ILE:CD1	2.72	0.77
2:E:791:PRO:O	2:E:794:VAL:HG23	1.86	0.76
2:K:671:MET:HE3	2:K:671:MET:CA	2.16	0.75
2:K:438:VAL:HG12	2:K:452:TRP:CH2	2.22	0.74
2:C:475:CYS:SG	2:C:477:ILE:CG1	2.72	0.73
2:E:793:ASP:OD1	2:E:793:ASP:N	2.20	0.73
1:A:1160:LEU:O	1:A:1163:VAL:HG22	1.87	0.73
2:D:671:MET:HA	2:D:671:MET:HE3	1.70	0.72
2:H:667:MET:O	2:H:671:MET:HG3	1.89	0.72
2:C:475:CYS:HG	2:C:477:ILE:HG12	1.53	0.71
2:K:438:VAL:HG11	2:K:452:TRP:HH2	1.54	0.69
2:D:283:ARG:HE	2:D:659:ASN:HB3	1.56	0.69
2:D:474:TYR:O	2:D:475:CYS:SG	2.51	0.69
2:H:475:CYS:SG	2:H:477:ILE:CG1	2.80	0.69
2:F:667:MET:O	2:F:671:MET:HG2	1.92	0.69
2:G:209:CYS:H	2:G:872:ARG:HG3	1.59	0.67
2:D:472:ILE:H	2:D:535:ASN:HD21	1.41	0.67
2:J:461:GLU:HA	2:J:461:GLU:OE1	1.93	0.67
2:I:793:ASP:O	2:I:797:GLY:HA3	1.95	0.66
2:B:667:MET:O	2:B:671:MET:HG2	1.95	0.66
1:A:230:LEU:HD11	1:A:368:ILE:HB	1.78	0.65
2:I:793:ASP:O	2:I:797:GLY:CA	2.44	0.65
2:C:102:LEU:HD12	2:C:102:LEU:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:474:TYR:H	2:E:531:ASN:HD21	1.45	0.64
1:A:884:ARG:HE	1:A:896:LYS:HZ2	1.45	0.64
2:E:135:ARG:HD2	2:E:138:ARG:HH21	1.61	0.64
2:G:595:VAL:HG22	2:G:891:LYS:HZ3	1.58	0.64
2:D:474:TYR:H	2:D:531:ASN:HD21	1.46	0.63
2:D:632:ARG:H	2:D:635:HIS:HD2	1.45	0.63
2:H:472:ILE:H	2:H:535:ASN:HD21	1.46	0.63
2:C:375:VAL:HG13	2:C:500:MET:HE2	1.81	0.62
2:F:671:MET:HE3	2:F:671:MET:CA	2.18	0.62
2:F:632:ARG:H	2:F:635:HIS:HD2	1.46	0.62
2:E:201:ASP:OD1	2:E:202:VAL:HG13	1.99	0.62
2:J:474:TYR:H	2:J:531:ASN:HD21	1.47	0.62
1:A:499:LYS:HG3	1:A:644:GLY:HA3	1.82	0.62
2:C:384:GLY:HA2	2:C:446:GLY:HA3	1.82	0.62
2:K:477:ILE:CD1	2:K:524:MET:HE2	2.08	0.61
1:A:96:GLU:O	1:A:100:ASN:ND2	2.32	0.61
2:E:728:TYR:HB3	2:E:826:LEU:HB3	1.83	0.61
1:A:764:ASP:O	1:A:765:ASP:OD1	2.18	0.61
2:E:791:PRO:O	2:E:795:LEU:HD23	2.00	0.61
2:D:526:ARG:HH12	2:D:580:PHE:HA	1.63	0.61
2:H:327:LEU:HG	2:H:372:VAL:HG11	1.82	0.61
2:H:59:PHE:HD2	2:I:317:ARG:HH22	1.49	0.61
2:E:31:LEU:HD13	2:E:345:LEU:HD13	1.82	0.61
2:I:474:TYR:H	2:I:531:ASN:HD21	1.48	0.61
2:J:135:ARG:NH1	2:J:684:GLU:OE2	2.33	0.61
1:A:406:VAL:HG13	1:A:607:ASN:HD22	1.65	0.60
2:F:671:MET:HA	2:F:671:MET:CE	2.23	0.60
2:D:472:ILE:O	2:D:531:ASN:ND2	2.34	0.60
1:A:995:VAL:HG22	1:A:1168:ASN:HB3	1.83	0.60
2:J:526:ARG:NH2	2:J:580:PHE:O	2.35	0.60
2:F:416:VAL:HG22	2:F:429:ILE:HG13	1.84	0.60
2:K:141:GLY:CA	2:K:213:VAL:HG13	2.30	0.60
2:B:671:MET:HE3	2:B:671:MET:CA	2.32	0.59
2:J:857:ILE:HG12	2:J:858:VAL:HG23	1.84	0.59
2:K:293:ILE:HG23	2:K:297:LEU:HD12	1.82	0.59
2:B:247:ARG:NH1	2:B:536:GLU:OE1	2.35	0.59
2:E:801:SER:HB2	2:E:816:LYS:HB2	1.84	0.59
2:E:108:TYR:HB3	2:E:698:MET:HE2	1.84	0.59
2:E:667:MET:O	2:E:671:MET:HG2	2.02	0.59
2:E:750:ARG:HH22	2:F:185:ASN:HD21	1.49	0.59
1:A:1265:ARG:NH2	1:A:1301:PHE:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1281:LYS:HB3	1:A:1285:LYS:HE2	1.84	0.59
2:C:370:ARG:NH2	2:C:404:ASP:OD2	2.36	0.59
2:C:667:MET:SD	2:C:671:MET:CE	2.88	0.58
2:I:358:LYS:HB2	2:I:570:ASP:HB3	1.84	0.58
2:F:283:ARG:HD3	2:F:659:ASN:HB3	1.86	0.58
2:F:460:ARG:NH1	2:F:478:ASP:OD1	2.35	0.58
2:G:475:CYS:O	2:G:475:CYS:SG	2.62	0.58
2:G:474:TYR:H	2:G:531:ASN:HD21	1.51	0.58
2:D:37:GLN:O	2:D:41:GLN:NE2	2.37	0.58
1:A:397:GLN:OE1	1:A:606:HIS:ND1	2.36	0.58
2:F:460:ARG:HG2	2:F:460:ARG:HH21	1.68	0.58
2:F:791:PRO:HD2	2:F:794:VAL:HG21	1.85	0.58
2:J:209:CYS:H	2:J:872:ARG:HG3	1.69	0.58
2:I:386:ARG:NH2	2:I:454:THR:O	2.37	0.58
2:B:96:GLN:HE22	2:B:830:VAL:H	1.52	0.57
2:C:263:THR:HG1	2:C:882:ARG:HH21	1.52	0.57
2:D:774:PHE:O	2:D:779:ARG:NH2	2.37	0.57
1:A:1160:LEU:CD2	1:A:1178:ALA:HA	2.33	0.57
2:F:437:ASN:OD1	2:F:440:ARG:NH2	2.35	0.57
1:A:1154:ASN:ND2	1:A:1156:SER:O	2.37	0.57
2:B:774:PHE:O	2:B:779:ARG:NH2	2.38	0.57
2:I:370:ARG:NH2	2:I:404:ASP:OD2	2.37	0.57
2:I:475:CYS:O	2:I:475:CYS:SG	2.62	0.57
2:K:200:ARG:NH1	2:K:203:ASP:OD1	2.36	0.57
2:G:595:VAL:CG2	2:G:891:LYS:HZ2	2.05	0.57
2:H:141:GLY:HA3	2:H:213:VAL:HG13	1.86	0.57
2:F:472:ILE:H	2:F:535:ASN:HD21	1.53	0.57
2:G:16:PRO:O	2:G:306:ASN:ND2	2.37	0.57
2:H:350:PRO:HG2	2:H:472:ILE:HD13	1.86	0.57
2:J:283:ARG:HE	2:J:659:ASN:HB3	1.69	0.57
2:I:7:GLN:HG3	2:I:8:ARG:HG3	1.87	0.57
2:I:201:ASP:OD2	2:I:881:MET:HE2	2.05	0.57
2:B:632:ARG:NH2	2:C:484:ASN:OD1	2.37	0.57
1:A:656:ARG:NH2	1:A:712:SER:OG	2.38	0.57
2:E:293:ILE:HG23	2:E:297:LEU:HD12	1.85	0.57
2:H:227:VAL:HA	2:H:231:GLU:HB2	1.86	0.57
2:J:416:VAL:HG22	2:J:429:ILE:HG13	1.87	0.57
2:B:595:VAL:HG12	2:B:595:VAL:O	2.04	0.56
2:C:95:MET:SD	2:C:102:LEU:HD11	2.45	0.56
2:D:614:MET:HE1	2:D:637:TRP:HA	1.86	0.56
2:G:384:GLY:HA2	2:G:446:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:259:ARG:NH2	2:J:880:LYS:O	2.38	0.56
2:K:370:ARG:NH2	2:K:404:ASP:OD2	2.38	0.56
2:H:247:ARG:NH1	2:H:536:GLU:OE2	2.37	0.56
2:H:370:ARG:NH2	2:H:404:ASP:OD2	2.38	0.56
2:H:786:TYR:OH	2:H:794:VAL:HG21	2.05	0.56
2:K:793:ASP:OD1	2:K:793:ASP:N	2.38	0.56
2:F:352:GLN:HE21	2:F:544:LEU:HB2	1.70	0.56
2:D:475:CYS:SG	2:D:477:ILE:CG1	2.93	0.56
2:D:259:ARG:NH2	2:D:880:LYS:O	2.39	0.56
2:J:750:ARG:HD3	2:K:254:VAL:HG11	1.87	0.56
1:A:1272:ARG:HH22	1:A:1300:GLN:HE21	1.53	0.56
2:D:526:ARG:NH2	2:D:580:PHE:O	2.38	0.56
2:K:835:THR:HB	2:K:838:SER:HB3	1.87	0.56
2:G:714:ARG:NH2	2:G:836:PRO:O	2.39	0.56
2:K:452:TRP:HD1	2:K:452:TRP:O	1.89	0.56
2:K:104:VAL:HG22	2:K:858:VAL:HG22	1.88	0.56
1:A:758:SER:HB3	1:A:769:TYR:HB2	1.88	0.56
2:C:729:THR:HG22	2:C:731:MET:H	1.71	0.56
2:J:384:GLY:HA2	2:J:446:GLY:HA3	1.88	0.56
2:B:632:ARG:H	2:B:635:HIS:HD2	1.53	0.55
2:F:247:ARG:NH1	2:F:536:GLU:OE2	2.39	0.55
2:D:475:CYS:SG	2:D:477:ILE:CD1	2.94	0.55
2:F:133:LYS:HG2	2:F:697:LEU:HD22	1.88	0.55
2:G:47:GLN:HG2	2:G:52:THR:HG21	1.88	0.55
2:H:262:ASP:HB2	2:H:881:MET:HG2	1.87	0.55
2:G:454:THR:HG21	2:G:476:GLY:N	2.21	0.55
2:J:172:LEU:O	2:J:180:ARG:NH2	2.39	0.55
2:H:271:LEU:HD22	2:H:890:LEU:HD13	1.88	0.55
2:C:742:VAL:HB	2:C:772:VAL:HG23	1.89	0.55
2:J:667:MET:CE	2:J:671:MET:CE	2.77	0.55
1:A:1299:ASN:ND2	2:D:315:THR:O	2.40	0.55
2:B:361:PRO:HG3	2:D:901:VAL:HB	1.88	0.55
2:F:85:VAL:HG23	2:F:163:VAL:HA	1.88	0.55
2:G:594:GLU:HA	2:G:892:MET:HE3	1.88	0.55
2:I:410:TYR:OH	2:I:512:GLU:OE2	2.23	0.55
2:J:161:PRO:HB3	2:J:187:LEU:HD21	1.88	0.55
1:A:994:ALA:HA	2:H:47:GLN:HE22	1.71	0.55
2:G:632:ARG:H	2:G:635:HIS:HD2	1.54	0.55
2:F:595:VAL:HG12	2:F:595:VAL:O	2.07	0.54
2:J:291:MET:HE3	2:J:651:VAL:HG13	1.90	0.54
1:A:1155:HIS:O	2:H:308:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:ARG:NH1	2:C:202:VAL:O	2.40	0.54
2:C:570:ASP:OD1	2:C:570:ASP:N	2.40	0.54
2:G:570:ASP:N	2:G:570:ASP:OD1	2.38	0.54
1:A:130:PHE:HB2	1:A:683:GLY:HA3	1.90	0.54
2:C:100:ARG:HA	2:C:862:ARG:HA	1.89	0.54
2:E:475:CYS:SG	2:E:475:CYS:O	2.66	0.54
2:E:632:ARG:H	2:E:635:HIS:HD2	1.55	0.54
2:E:664:ARG:NH2	2:F:201:ASP:OD1	2.39	0.54
2:H:475:CYS:SG	2:H:475:CYS:O	2.65	0.54
2:K:671:MET:CA	2:K:671:MET:CE	2.86	0.54
1:A:496:LEU:O	1:A:645:ARG:NH1	2.41	0.54
1:A:535:ILE:HG13	1:A:536:VAL:HG13	1.88	0.54
2:F:740:ARG:NH1	2:F:769:ASP:O	2.40	0.54
2:I:141:GLY:CA	2:I:213:VAL:HG13	2.37	0.54
1:A:492:THR:HB	1:A:495:GLU:HB2	1.90	0.54
2:B:350:PRO:HG2	2:B:472:ILE:HD13	1.89	0.54
2:I:384:GLY:HA2	2:I:446:GLY:HA3	1.90	0.54
2:J:350:PRO:HG2	2:J:472:ILE:HD13	1.89	0.54
2:J:386:ARG:NH2	2:J:454:THR:O	2.41	0.54
2:J:701:ASP:OD2	2:J:773:ARG:NH2	2.40	0.54
1:A:854:ILE:HG21	1:A:1201:ASP:HB2	1.90	0.54
2:I:360:ASP:OD1	2:I:360:ASP:N	2.39	0.54
2:G:51:MET:SD	2:H:78:GLN:NE2	2.75	0.54
2:H:504:LEU:HB3	2:H:513:ALA:HB2	1.88	0.54
2:I:181:ALA:O	2:I:185:ASN:ND2	2.41	0.54
2:K:315:THR:OG1	2:K:316:GLN:N	2.41	0.54
2:I:595:VAL:HG12	2:I:595:VAL:O	2.08	0.54
2:K:263:THR:HG22	2:K:882:ARG:HE	1.73	0.54
2:C:209:CYS:H	2:C:872:ARG:HG3	1.73	0.53
2:K:115:GLY:HA3	2:K:129:THR:HG23	1.90	0.53
2:I:201:ASP:OD2	2:I:881:MET:CE	2.56	0.53
2:K:475:CYS:O	2:K:475:CYS:SG	2.66	0.53
2:F:792:ASP:O	2:F:796:GLN:NE2	2.42	0.53
2:G:729:THR:HG22	2:G:731:MET:H	1.73	0.53
2:F:227:VAL:HA	2:F:231:GLU:HB2	1.90	0.53
2:D:98:ARG:HB2	2:D:723:GLN:HE22	1.73	0.53
2:D:291:MET:HE3	2:D:651:VAL:HG13	1.90	0.53
2:G:784:LYS:HB3	2:G:786:TYR:CE2	2.43	0.53
2:H:302:TYR:HB3	2:H:582:ARG:HB3	1.90	0.53
2:C:595:VAL:HG12	2:C:595:VAL:O	2.09	0.53
2:E:708:ASP:OD2	2:E:850:LYS:NZ	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:200:ARG:HB3	2:H:881:MET:HE1	1.91	0.53
2:J:200:ARG:NH2	2:J:263:THR:O	2.42	0.53
1:A:223:ARG:HH11	2:J:33:VAL:HG22	1.74	0.53
2:J:257:ASP:OD1	2:J:257:ASP:N	2.41	0.53
2:J:264:ILE:HB	2:J:883:ILE:HG12	1.91	0.53
2:K:454:THR:HG21	2:K:476:GLY:N	2.24	0.53
2:D:264:ILE:HB	2:D:883:ILE:HG12	1.91	0.53
2:E:265:TRP:HB3	2:E:886:ILE:HD13	1.91	0.53
2:D:175:LEU:HD11	2:D:179:HIS:HB3	1.91	0.53
1:A:194:ASP:N	1:A:194:ASP:OD1	2.42	0.52
1:A:1070:ILE:HB	1:A:1192:LYS:HD2	1.91	0.52
2:B:283:ARG:HE	2:B:659:ASN:HB3	1.73	0.52
2:H:291:MET:HE3	2:H:651:VAL:HG13	1.90	0.52
2:J:658:HIS:HB2	2:K:309:ILE:HA	1.91	0.52
2:C:158:VAL:HG12	2:C:191:ILE:HG22	1.91	0.52
2:E:762:LEU:HA	2:E:765:ILE:HD12	1.92	0.52
2:G:315:THR:OG1	2:G:316:GLN:N	2.41	0.52
2:H:699:LEU:HD12	2:H:778:LEU:HB3	1.91	0.52
1:A:343:ARG:NH2	1:A:348:GLU:OE2	2.42	0.52
1:A:424:ALA:HB1	1:A:429:GLU:HB2	1.91	0.52
2:B:175:LEU:O	2:B:180:ARG:NH2	2.42	0.52
2:D:326:ILE:HA	2:F:31:LEU:HD22	1.91	0.52
2:F:384:GLY:HA2	2:F:446:GLY:HA3	1.90	0.52
2:G:708:ASP:HB2	2:G:850:LYS:HZ1	1.73	0.52
2:C:358:LYS:HB2	2:C:570:ASP:HB2	1.91	0.52
2:J:90:PHE:HB2	2:J:166:VAL:HG12	1.91	0.52
2:E:229:LEU:HD21	2:E:257:ASP:HB2	1.91	0.52
2:K:632:ARG:H	2:K:635:HIS:HD2	1.58	0.52
1:A:285:THR:HG23	2:K:317:ARG:HD2	1.91	0.52
1:A:411:ASP:OD2	1:A:414:ARG:NH1	2.43	0.52
2:H:367:PRO:HG3	2:J:309:ILE:HG13	1.92	0.52
2:B:141:GLY:HA3	2:B:213:VAL:HG13	1.92	0.52
2:E:454:THR:HG21	2:E:476:GLY:N	2.25	0.52
2:H:283:ARG:HE	2:H:659:ASN:HB3	1.74	0.52
2:H:662:ASN:ND2	2:I:487:THR:O	2.43	0.52
2:J:677:PRO:HA	2:J:681:LEU:HD23	1.90	0.52
2:J:725:GLY:O	2:J:860:ARG:NH2	2.42	0.52
2:E:358:LYS:HB2	2:E:570:ASP:HB3	1.91	0.52
2:E:410:TYR:OH	2:E:512:GLU:OE2	2.28	0.52
2:I:572:SER:OG	2:I:573:TRP:N	2.43	0.52
1:A:280:VAL:HG21	1:A:362:HIS:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:SER:HB3	1:A:555:TYR:HB2	1.91	0.51
2:C:98:ARG:HG3	2:C:723:GLN:HE22	1.75	0.51
2:I:421:THR:OG1	2:I:426:ASP:OD2	2.28	0.51
1:A:826:ASP:OD1	1:A:826:ASP:N	2.39	0.51
2:B:750:ARG:HD3	2:C:254:VAL:HG11	1.91	0.51
2:H:176:THR:OG1	2:H:177:ALA:N	2.44	0.51
2:J:283:ARG:HH11	2:K:490:ILE:HG12	1.75	0.51
2:C:475:CYS:SG	2:C:475:CYS:O	2.68	0.51
2:G:262:ASP:N	2:G:262:ASP:OD1	2.43	0.51
2:K:671:MET:HA	2:K:671:MET:CE	2.29	0.51
2:B:262:ASP:OD1	2:B:262:ASP:N	2.42	0.51
2:C:835:THR:HB	2:C:838:SER:HB3	1.92	0.51
2:D:267:LEU:HD11	2:D:890:LEU:HD11	1.92	0.51
2:I:741:VAL:HG12	2:I:771:TRP:HB2	1.91	0.51
2:H:252:GLN:O	2:H:256:THR:OG1	2.25	0.51
1:A:27:ILE:O	1:A:912:ASN:ND2	2.40	0.51
1:A:1159:ASP:OD1	2:H:44:ARG:NH1	2.44	0.51
2:D:211:GLU:OE1	2:D:872:ARG:NH2	2.43	0.51
2:D:707:ARG:NH2	2:D:767:ASP:OD1	2.38	0.51
2:I:95:MET:HG3	2:I:97:SER:H	1.76	0.51
2:J:44:ARG:HA	2:J:47:GLN:HB2	1.92	0.51
2:B:104:VAL:HG22	2:B:858:VAL:HG22	1.93	0.51
2:C:135:ARG:NH2	2:C:613:ASP:OD2	2.44	0.51
2:F:671:MET:CA	2:F:671:MET:CE	2.86	0.51
2:G:10:GLU:OE1	2:G:529:ARG:NH2	2.44	0.51
2:H:384:GLY:HA2	2:H:446:GLY:HA3	1.91	0.51
2:J:115:GLY:HA3	2:J:129:THR:HG23	1.93	0.51
2:B:40:MET:HA	2:B:43:VAL:HG12	1.92	0.51
2:C:229:LEU:HD21	2:C:257:ASP:HB2	1.92	0.51
2:E:595:VAL:HG12	2:E:595:VAL:O	2.11	0.51
2:E:780:THR:HB	2:E:820:GLU:HG2	1.91	0.51
1:A:594:ILE:HG22	1:A:803:THR:HG23	1.93	0.51
1:A:1018:PRO:HB2	1:A:1169:ILE:HD11	1.93	0.51
2:E:172:LEU:O	2:E:180:ARG:NH2	2.44	0.51
2:I:779:ARG:NH2	2:I:817:TYR:O	2.43	0.51
1:A:985:SER:OG	1:A:986:PHE:N	2.42	0.50
2:B:257:ASP:OD2	2:B:882:ARG:NH1	2.41	0.50
2:C:283:ARG:NH2	2:C:660:PHE:O	2.43	0.50
2:D:695:GLU:OE2	2:D:854:ASN:N	2.45	0.50
2:E:384:GLY:HA2	2:E:446:GLY:HA3	1.92	0.50
2:C:678:SER:OG	2:C:679:LEU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:410:TYR:OH	2:G:512:GLU:OE2	2.30	0.50
1:A:115:LEU:HD23	1:A:116:ARG:H	1.76	0.50
2:B:291:MET:HE3	2:B:651:VAL:HG13	1.93	0.50
2:F:135:ARG:NH2	2:F:613:ASP:OD2	2.44	0.50
2:F:633:PRO:HB2	2:F:663:ILE:HG12	1.93	0.50
2:H:430:GLY:O	2:H:433:GLN:NE2	2.45	0.50
2:I:857:ILE:HG22	2:I:858:VAL:HG23	1.92	0.50
2:K:375:VAL:HG13	2:K:500:MET:HE2	1.91	0.50
1:A:911:ARG:NH2	1:A:966:PRO:O	2.44	0.50
2:G:402:LEU:HD23	2:G:425:LEU:HD21	1.92	0.50
2:H:318:ILE:HG13	2:H:319:THR:HG23	1.94	0.50
2:I:703:VAL:HG23	2:I:851:VAL:HG22	1.94	0.50
1:A:3:ALA:HB3	1:A:6:VAL:HG12	1.93	0.50
1:A:546:ARG:NH2	1:A:559:GLY:O	2.44	0.50
2:H:141:GLY:CA	2:H:213:VAL:HG13	2.41	0.50
2:K:384:GLY:HA2	2:K:446:GLY:HA3	1.94	0.50
2:F:262:ASP:OD1	2:F:262:ASP:N	2.40	0.50
2:I:85:VAL:HG12	2:I:163:VAL:HG12	1.93	0.50
2:J:477:ILE:HG23	2:J:492:MET:HE1	1.93	0.50
2:C:135:ARG:NH1	2:C:643:ASP:OD2	2.45	0.50
2:C:494:TYR:HD1	2:C:524:MET:HE3	1.77	0.50
1:A:949:LYS:NZ	2:J:38:GLU:OE2	2.44	0.50
1:A:1141:ALA:HA	1:A:1144:ILE:HG22	1.94	0.50
2:C:203:ASP:HB2	2:C:876:ALA:HB3	1.93	0.50
2:D:421:THR:HB	2:D:423:GLU:HG3	1.94	0.50
2:F:86:PRO:HD3	2:F:145:LEU:HD21	1.94	0.50
2:G:472:ILE:O	2:G:531:ASN:ND2	2.45	0.50
2:J:654:LEU:HA	2:K:308:ARG:HH22	1.77	0.50
2:E:703:VAL:HG23	2:E:851:VAL:HG12	1.92	0.50
1:A:432:VAL:O	1:A:628:TYR:OH	2.30	0.49
2:C:421:THR:OG1	2:C:426:ASP:OD2	2.28	0.49
2:D:263:THR:HG22	2:D:882:ARG:HG2	1.93	0.49
2:E:529:ARG:NE	2:E:585:GLU:OE2	2.46	0.49
2:H:754:ASN:ND2	2:I:257:ASP:OD1	2.45	0.49
1:A:313:SER:OG	1:A:314:SER:N	2.45	0.49
2:C:700:THR:OG1	2:C:701:ASP:N	2.45	0.49
2:K:715:LEU:HG	2:K:836:PRO:HB3	1.93	0.49
1:A:35:TYR:HA	1:A:908:ILE:HG12	1.92	0.49
1:A:104:PRO:HB3	1:A:118:TYR:HB3	1.95	0.49
2:D:193:GLU:HB3	2:D:204:VAL:HG23	1.93	0.49
2:H:259:ARG:O	2:H:263:THR:OG1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:499:GLU:OE2	2:J:502:ARG:NH2	2.45	0.49
2:K:229:LEU:HD21	2:K:257:ASP:HB2	1.95	0.49
1:A:1120:SER:OG	1:A:1121:TYR:N	2.46	0.49
2:B:658:HIS:HB2	2:C:309:ILE:HA	1.94	0.49
2:C:540:SER:OG	2:C:541:VAL:N	2.45	0.49
2:D:475:CYS:SG	2:D:477:ILE:HD11	2.52	0.49
2:G:379:LEU:HD23	2:G:500:MET:HG2	1.94	0.49
2:I:179:HIS:HA	2:I:182:MET:HB2	1.94	0.49
1:A:273:GLY:O	1:A:819:GLN:NE2	2.45	0.49
2:B:370:ARG:NH2	2:B:404:ASP:OD2	2.44	0.49
2:C:632:ARG:HG2	2:C:634:SER:H	1.78	0.49
2:C:792:ASP:HB3	2:C:796:GLN:HE21	1.77	0.49
2:F:305:PRO:HG3	2:F:519:MET:HE1	1.94	0.49
2:I:454:THR:HG21	2:I:476:GLY:N	2.28	0.49
2:B:211:GLU:OE1	2:B:872:ARG:NH2	2.46	0.49
2:B:283:ARG:O	2:B:655:SER:OG	2.30	0.49
2:G:665:ASP:OD1	2:G:668:ARG:NH2	2.45	0.49
2:I:708:ASP:HB3	2:I:850:LYS:HZ1	1.77	0.49
2:I:710:LEU:HD12	2:I:711:PRO:HD2	1.95	0.49
2:K:382:THR:HG22	2:K:384:GLY:H	1.77	0.49
2:B:701:ASP:OD2	2:B:773:ARG:NH2	2.45	0.49
2:K:452:TRP:CD1	2:K:452:TRP:C	2.90	0.49
1:A:379:ILE:HG13	1:A:380:THR:HG23	1.94	0.49
2:E:96:GLN:NE2	2:E:830:VAL:O	2.42	0.49
2:K:358:LYS:HB2	2:K:570:ASP:HB2	1.95	0.49
2:C:615:ARG:HH12	2:C:675:LEU:HD21	1.78	0.49
2:C:628:LEU:HB3	2:C:631:ALA:HB2	1.95	0.49
2:H:263:THR:HG23	2:H:882:ARG:HG3	1.94	0.49
2:H:595:VAL:O	2:H:595:VAL:HG12	2.13	0.49
1:A:863:HIS:HE1	1:A:932:LEU:H	1.61	0.48
2:B:662:ASN:HB2	2:C:485:PRO:HG3	1.93	0.48
2:J:293:ILE:HG21	2:K:315:THR:HG22	1.95	0.48
2:K:84:LYS:NZ	2:K:147:ASP:O	2.40	0.48
2:J:71:ILE:HG21	2:J:599:ILE:HG23	1.95	0.48
2:K:251:SER:OG	2:K:252:GLN:N	2.46	0.48
1:A:224:GLU:O	2:J:44:ARG:NH2	2.40	0.48
2:F:504:LEU:HB3	2:F:513:ALA:HB2	1.95	0.48
2:H:475:CYS:HG	2:H:477:ILE:CG1	2.25	0.48
2:I:801:SER:OG	2:I:802:TYR:N	2.46	0.48
1:A:134:ARG:HE	1:A:138:GLU:HB2	1.79	0.48
2:H:223:TYR:OH	2:H:270:GLN:NE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:724:GLU:HB2	2:H:860:ARG:HH12	1.78	0.48
2:K:354:ILE:CG2	2:K:391:THR:HG23	2.43	0.48
2:K:707:ARG:NH1	2:K:767:ASP:OD1	2.47	0.48
1:A:1132:ASP:HB2	1:A:1135:MET:HB2	1.96	0.48
2:E:27:SER:OG	2:E:28:GLY:N	2.46	0.48
2:F:103:ARG:NH1	2:F:865:GLN:O	2.47	0.48
2:J:402:LEU:HD11	2:J:500:MET:HE1	1.95	0.48
2:B:293:ILE:HG23	2:B:297:LEU:HD12	1.96	0.48
2:C:54:THR:HB	2:D:882:ARG:HB2	1.94	0.48
2:H:283:ARG:O	2:H:655:SER:OG	2.31	0.48
2:H:421:THR:OG1	2:H:426:ASP:OD2	2.29	0.48
2:J:472:ILE:H	2:J:535:ASN:HD21	1.61	0.48
2:K:725:GLY:O	2:K:860:ARG:NH1	2.46	0.48
2:B:653:ASN:O	2:C:308:ARG:NH2	2.47	0.48
2:D:228:GLN:OE1	2:D:265:TRP:N	2.44	0.48
2:F:284:SER:O	2:F:284:SER:OG	2.32	0.48
2:G:284:SER:O	2:G:288:ASN:ND2	2.47	0.48
2:I:743:GLN:OE1	2:I:773:ARG:NH1	2.46	0.48
2:F:133:LYS:HD3	2:F:697:LEU:HB3	1.94	0.48
2:F:754:ASN:ND2	2:G:257:ASP:OD1	2.40	0.48
2:H:112:SER:O	2:H:782:ARG:NH1	2.46	0.48
1:A:572:SER:OG	1:A:573:ARG:N	2.46	0.48
1:A:655:ARG:HH22	1:A:678:PHE:HB3	1.79	0.48
2:C:725:GLY:O	2:C:860:ARG:NH1	2.42	0.48
2:E:209:CYS:H	2:E:872:ARG:HG3	1.78	0.48
2:I:202:VAL:HG13	2:I:203:ASP:N	2.29	0.48
2:K:135:ARG:HD2	2:K:138:ARG:HH21	1.78	0.48
2:H:740:ARG:NH1	2:H:769:ASP:O	2.47	0.47
2:I:705:MET:HG3	2:I:848:MET:HB3	1.96	0.47
2:J:393:ASN:OD1	2:K:411:ASN:ND2	2.47	0.47
1:A:1278:PRO:HB2	1:A:1281:LYS:HB2	1.95	0.47
2:G:464:PRO:HG2	2:G:539:HIS:CE1	2.49	0.47
1:A:656:ARG:HH22	1:A:714:LEU:HA	1.78	0.47
2:C:193:GLU:HB3	2:C:204:VAL:HB	1.95	0.47
2:D:722:ARG:NH1	2:D:830:VAL:O	2.46	0.47
2:E:532:GLN:NE2	2:E:536:GLU:OE2	2.48	0.47
2:K:456:ASP:OD1	2:K:456:ASP:N	2.45	0.47
1:A:572:SER:HA	1:A:1202:GLU:HB2	1.96	0.47
1:A:255:LYS:O	1:A:259:ASN:ND2	2.47	0.47
2:E:418:TYR:OH	2:F:481:GLU:OE1	2.33	0.47
2:I:793:ASP:OD1	2:I:793:ASP:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:138:ARG:HA	2:J:216:ILE:HG21	1.96	0.47
2:J:197:VAL:HG13	2:J:225:GLU:HG3	1.97	0.47
1:A:655:ARG:NH2	1:A:679:LYS:O	2.48	0.47
2:J:91:ARG:HG3	2:J:104:VAL:HB	1.96	0.47
2:K:96:GLN:NE2	2:K:830:VAL:O	2.41	0.47
1:A:1201:ASP:OD1	1:A:1201:ASP:N	2.47	0.47
2:D:172:LEU:O	2:D:180:ARG:NH2	2.47	0.47
2:F:857:ILE:HG13	2:F:858:VAL:HG23	1.96	0.47
2:H:321:THR:OG1	2:H:322:GLY:N	2.47	0.47
2:I:120:GLU:OE2	2:I:817:TYR:N	2.48	0.47
2:K:354:ILE:HG22	2:K:391:THR:HG23	1.97	0.47
1:A:674:ASP:OD1	1:A:674:ASP:N	2.48	0.47
2:B:470:ARG:NH1	2:B:544:LEU:O	2.44	0.47
2:D:754:ASN:ND2	2:E:257:ASP:OD1	2.48	0.47
2:H:615:ARG:HH12	2:H:675:LEU:HD21	1.80	0.47
2:H:707:ARG:NH1	2:H:767:ASP:OD1	2.42	0.47
1:A:35:TYR:HB3	1:A:907:LEU:HD23	1.96	0.47
2:B:52:THR:O	2:C:317:ARG:NH1	2.48	0.47
2:B:882:ARG:HH21	2:K:47:GLN:HE21	1.62	0.47
2:F:197:VAL:HG22	2:F:202:VAL:HG21	1.97	0.47
2:K:141:GLY:HA2	2:K:213:VAL:CG1	2.38	0.47
1:A:335:GLN:HE22	1:A:341:ASP:HA	1.80	0.47
2:E:98:ARG:H	2:E:723:GLN:HE22	1.62	0.47
2:H:345:LEU:HD22	2:I:318:ILE:HD13	1.96	0.47
2:H:416:VAL:HG22	2:H:429:ILE:HG13	1.97	0.47
1:A:267:TRP:HA	1:A:270:LYS:HD2	1.97	0.46
2:F:350:PRO:HG2	2:F:472:ILE:HD13	1.98	0.46
2:F:460:ARG:HH21	2:F:460:ARG:CG	2.25	0.46
2:G:743:GLN:OE1	2:G:773:ARG:NH1	2.42	0.46
2:H:150:THR:OG1	2:H:151:ARG:N	2.48	0.46
2:B:152:ASP:OD1	2:B:152:ASP:N	2.48	0.46
2:D:587:THR:OG1	2:D:588:HIS:N	2.48	0.46
1:A:286:ALA:O	2:J:341:ARG:NH1	2.47	0.46
1:A:294:ASP:OD1	1:A:294:ASP:N	2.44	0.46
2:E:22:VAL:HG13	2:E:301:GLU:HB3	1.96	0.46
2:F:293:ILE:HG21	2:G:315:THR:HG22	1.97	0.46
2:J:247:ARG:NH1	2:J:536:GLU:OE2	2.48	0.46
2:J:774:PHE:HB2	2:J:779:ARG:HH22	1.81	0.46
1:A:306:ARG:NH1	2:J:63:ASP:OD2	2.40	0.46
2:I:100:ARG:HH21	2:I:862:ARG:HH22	1.63	0.46
2:I:262:ASP:OD1	2:I:262:ASP:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:745:THR:OG1	2:I:746:TYR:N	2.48	0.46
2:J:627:VAL:HG21	2:J:778:LEU:HG	1.97	0.46
2:F:675:LEU:HD12	2:F:681:LEU:HD11	1.98	0.46
2:G:565:ASP:HB2	2:H:261:GLN:HE21	1.80	0.46
2:K:209:CYS:SG	2:K:210:SER:N	2.88	0.46
1:A:138:GLU:HG2	1:A:139:MET:HG3	1.98	0.46
1:A:226:GLU:HG2	2:J:44:ARG:HH21	1.79	0.46
1:A:995:VAL:HA	1:A:1168:ASN:HD22	1.80	0.46
2:C:799:PRO:HG3	2:C:849:THR:HG23	1.98	0.46
2:E:480:ARG:O	2:E:484:ASN:N	2.46	0.46
2:J:437:ASN:HD22	2:J:440:ARG:HH21	1.62	0.46
2:G:441:ALA:HB2	2:G:449:TYR:HE1	1.80	0.46
2:J:739:ASP:OD1	2:J:739:ASP:N	2.40	0.46
1:A:173:ASP:HA	1:A:176:ASN:HD21	1.80	0.46
1:A:546:ARG:HH12	1:A:563:ILE:HD13	1.81	0.46
2:B:671:MET:CA	2:B:671:MET:CE	2.94	0.46
2:B:740:ARG:NH1	2:B:770:ASP:OD1	2.49	0.46
2:C:141:GLY:HA2	2:C:213:VAL:HG13	1.98	0.46
2:D:416:VAL:HG22	2:D:429:ILE:HG13	1.98	0.46
2:E:402:LEU:HG	2:E:406:LEU:HD23	1.98	0.46
2:G:866:ILE:HG22	2:G:867:LEU:HD12	1.97	0.46
2:K:257:ASP:N	2:K:257:ASP:OD1	2.40	0.46
1:A:1132:ASP:O	1:A:1136:ARG:N	2.49	0.46
2:F:275:PRO:HB3	2:F:541:VAL:HG12	1.98	0.46
2:G:150:THR:HG22	2:G:159:ALA:HA	1.97	0.46
2:H:352:GLN:HE21	2:H:544:LEU:HD13	1.81	0.46
2:K:699:LEU:HD13	2:K:778:LEU:HD13	1.97	0.46
1:A:431:ILE:HD11	1:A:536:VAL:HA	1.97	0.45
2:B:141:GLY:CA	2:B:213:VAL:HG13	2.47	0.45
2:F:97:SER:OG	2:F:722:ARG:O	2.32	0.45
2:I:546:ASP:O	2:I:550:ASN:ND2	2.49	0.45
2:K:741:VAL:HG22	2:K:771:TRP:HB2	1.97	0.45
2:K:745:THR:OG1	2:K:746:TYR:N	2.48	0.45
1:A:991:ALA:O	1:A:996:GLN:NE2	2.49	0.45
2:B:700:THR:OG1	2:B:701:ASP:N	2.49	0.45
2:E:79:VAL:HG21	2:E:680:LYS:HG3	1.98	0.45
2:E:235:SER:HB3	2:E:271:LEU:HD23	1.97	0.45
2:G:595:VAL:HG12	2:G:595:VAL:O	2.15	0.45
1:A:144:ASP:OD1	1:A:144:ASP:N	2.49	0.45
2:E:283:ARG:NH2	2:E:660:PHE:O	2.49	0.45
2:F:426:ASP:OD1	2:F:437:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:158:VAL:HG21	2:I:188:ASP:HA	1.99	0.45
2:K:283:ARG:NH2	2:K:660:PHE:O	2.50	0.45
1:A:684:VAL:HG13	1:A:705:LEU:HB3	1.99	0.45
1:A:1076:LYS:HG3	2:D:33:VAL:HG13	1.98	0.45
2:B:98:ARG:H	2:B:723:GLN:HE22	1.65	0.45
2:I:42:LYS:NZ	2:J:256:THR:O	2.49	0.45
2:I:203:ASP:HB2	2:I:876:ALA:HB3	1.99	0.45
2:K:97:SER:OG	2:K:98:ARG:N	2.49	0.45
2:E:709:MET:HE3	2:E:844:PRO:HB3	1.98	0.45
2:G:742:VAL:HG23	2:G:772:VAL:HG23	1.98	0.45
1:A:221:ARG:NH2	1:A:225:GLU:OE1	2.45	0.45
2:D:247:ARG:NH1	2:D:536:GLU:OE2	2.50	0.45
2:I:296:CYS:HB2	2:I:538:LEU:HD23	1.98	0.45
1:A:742:MET:HB2	1:A:742:MET:HE2	1.77	0.45
2:B:252:GLN:O	2:B:256:THR:OG1	2.34	0.45
2:G:263:THR:HG22	2:G:882:ARG:HE	1.81	0.45
2:H:228:GLN:OE1	2:H:265:TRP:N	2.50	0.45
1:A:1183:SER:O	1:A:1187:ARG:N	2.38	0.45
2:B:150:THR:OG1	2:B:158:VAL:O	2.33	0.45
2:C:148:ILE:HB	2:C:163:VAL:HG11	1.99	0.45
2:H:754:ASN:HA	2:I:256:THR:HG23	1.99	0.45
1:A:46:MET:HE3	1:A:46:MET:HB3	1.85	0.45
1:A:605:ARG:NH1	1:A:794:CYS:O	2.49	0.45
2:B:662:ASN:ND2	2:C:487:THR:O	2.49	0.45
2:B:671:MET:HE2	2:B:671:MET:HB3	1.81	0.45
2:D:855:LYS:HA	2:D:855:LYS:HD3	1.79	0.45
2:F:741:VAL:HG12	2:F:771:TRP:HB2	1.98	0.45
2:I:862:ARG:HG3	2:I:864:GLY:H	1.82	0.45
1:A:245:GLU:HG3	1:A:344:LEU:HD23	1.98	0.45
1:A:829:MET:HE2	1:A:829:MET:HB3	1.77	0.45
2:B:257:ASP:OD1	2:B:257:ASP:N	2.45	0.45
2:B:309:ILE:HG13	2:J:367:PRO:HG3	1.99	0.45
2:F:112:SER:OG	2:F:781:VAL:O	2.33	0.45
2:F:784:LYS:CE	2:F:786:TYR:OH	2.65	0.45
1:A:1198:ILE:HD11	1:A:1235:LEU:HB3	1.99	0.44
2:H:142:SER:O	2:H:142:SER:OG	2.32	0.44
2:K:146:HIS:NE2	2:K:881:MET:O	2.51	0.44
2:K:470:ARG:NH1	2:K:544:LEU:O	2.48	0.44
2:K:510:ASP:N	2:K:510:ASP:OD1	2.44	0.44
1:A:804:MET:HE3	1:A:804:MET:HB3	1.82	0.44
2:G:728:TYR:HB3	2:G:826:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:257:ASP:OD1	2:H:257:ASP:N	2.40	0.44
1:A:242:LEU:HD23	1:A:373:LEU:HD21	1.99	0.44
1:A:709:THR:OG1	1:A:710:ASP:N	2.51	0.44
2:C:102:LEU:N	2:C:102:LEU:CD1	2.80	0.44
2:C:786:TYR:OH	2:C:794:VAL:HG21	2.18	0.44
2:D:455:ILE:HB	2:D:473:ARG:HH21	1.81	0.44
2:G:595:VAL:HG23	2:G:891:LYS:NZ	2.22	0.44
2:I:54:THR:OG1	2:I:55:ARG:N	2.50	0.44
2:J:227:VAL:HA	2:J:231:GLU:HB2	1.98	0.44
2:D:381:PHE:HE2	2:D:576:LEU:HD11	1.82	0.44
2:E:434:TYR:OH	2:E:499:GLU:OE1	2.33	0.44
2:G:229:LEU:HD11	2:G:257:ASP:HB2	1.99	0.44
2:K:474:TYR:H	2:K:531:ASN:HD21	1.66	0.44
1:A:210:MET:HG2	1:A:379:ILE:HA	1.99	0.44
1:A:680:VAL:HG21	1:A:686:PRO:HB3	1.99	0.44
2:C:410:TYR:OH	2:C:512:GLU:OE2	2.35	0.44
2:D:315:THR:O	2:D:315:THR:OG1	2.36	0.44
2:D:595:VAL:HG12	2:D:595:VAL:O	2.17	0.44
2:I:293:ILE:HG23	2:I:297:LEU:HD12	2.00	0.44
2:J:731:MET:HE3	2:J:853:ILE:HB	2.00	0.44
2:B:142:SER:O	2:B:142:SER:OG	2.34	0.44
2:D:900:THR:OG1	2:D:901:VAL:N	2.49	0.44
2:E:547:ASP:OD1	2:E:547:ASP:N	2.47	0.44
2:F:257:ASP:OD1	2:F:257:ASP:N	2.39	0.44
2:G:24:SER:HB3	2:G:302:TYR:HD2	1.81	0.44
2:I:72:LYS:HD3	2:I:595:VAL:HG11	2.00	0.44
2:J:98:ARG:HB2	2:J:723:GLN:HE22	1.83	0.44
1:A:655:ARG:HH12	1:A:678:PHE:HB3	1.83	0.44
1:A:1092:MET:HE3	1:A:1092:MET:HB3	1.83	0.44
2:B:169:LYS:HE3	2:B:169:LYS:HB3	1.80	0.44
2:B:481:GLU:OE1	2:K:418:TYR:OH	2.30	0.44
2:D:655:SER:O	2:D:659:ASN:N	2.49	0.44
1:A:109:ASP:OD1	1:A:109:ASP:N	2.30	0.44
2:B:461:GLU:CB	2:B:462:PRO:HD3	2.48	0.44
2:H:662:ASN:HB2	2:I:485:PRO:HG2	1.99	0.44
2:I:141:GLY:HA2	2:I:213:VAL:HG13	1.99	0.44
2:D:219:ARG:HG2	2:D:686:GLU:HG3	2.00	0.43
2:F:228:GLN:OE1	2:F:265:TRP:N	2.49	0.43
2:G:115:GLY:HA3	2:G:129:THR:HG23	2.00	0.43
2:I:707:ARG:NH1	2:I:767:ASP:OD1	2.51	0.43
2:J:812:TYR:HE1	2:K:255:LEU:HD12	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:477:ILE:HD11	2:C:524:MET:HE2	1.99	0.43
2:H:80:TYR:OH	2:H:885:ASP:OD2	2.27	0.43
2:H:494:TYR:HD1	2:H:524:MET:HE1	1.83	0.43
2:I:115:GLY:HA3	2:I:129:THR:HG23	1.98	0.43
1:A:273:GLY:HA3	1:A:359:PHE:HB3	1.99	0.43
1:A:1032:LYS:HA	1:A:1036:ALA:HB3	2.01	0.43
2:B:260:ARG:NH2	2:K:565:ASP:OD1	2.51	0.43
2:B:740:ARG:NH1	2:B:769:ASP:O	2.48	0.43
2:D:671:MET:HE3	2:D:671:MET:CA	2.40	0.43
2:J:774:PHE:O	2:J:779:ARG:NH2	2.51	0.43
1:A:395:ASP:OD1	1:A:395:ASP:N	2.52	0.43
1:A:1295:ARG:HD2	2:F:318:ILE:HD13	2.01	0.43
2:C:458:GLU:OE2	2:C:460:ARG:NE	2.51	0.43
2:I:257:ASP:OD1	2:I:257:ASP:N	2.44	0.43
2:I:298:PRO:HB3	2:I:589:ARG:HA	2.01	0.43
1:A:165:PRO:HD2	1:A:168:MET:HE2	2.00	0.43
2:B:671:MET:HA	2:B:671:MET:CE	2.40	0.43
2:F:100:ARG:HE	2:F:862:ARG:HG2	1.84	0.43
2:G:158:VAL:HA	2:G:191:ILE:HA	1.99	0.43
2:G:172:LEU:O	2:G:180:ARG:NH2	2.52	0.43
2:K:386:ARG:HG2	2:K:457:VAL:HG12	2.01	0.43
1:A:1295:ARG:HG2	2:F:30:LEU:HG	2.00	0.43
2:C:284:SER:O	2:C:288:ASN:ND2	2.52	0.43
2:J:740:ARG:NH1	2:J:769:ASP:O	2.43	0.43
2:K:200:ARG:HH22	2:K:203:ASP:HA	1.84	0.43
2:C:54:THR:OG1	2:C:55:ARG:N	2.51	0.43
2:C:627:VAL:HG22	2:C:777:VAL:HA	2.00	0.43
2:E:193:GLU:HG3	2:E:194:ASN:HD22	1.83	0.43
2:E:494:TYR:HD1	2:E:524:MET:HE3	1.83	0.43
2:E:628:LEU:HD12	2:E:631:ALA:HB2	1.99	0.43
2:G:283:ARG:NH2	2:G:660:PHE:O	2.52	0.43
2:I:97:SER:OG	2:I:722:ARG:O	2.31	0.43
2:I:795:LEU:HD23	2:I:795:LEU:HA	1.84	0.43
1:A:123:GLU:HB3	1:A:128:GLU:HG3	2.00	0.43
1:A:502:SER:HB2	1:A:505:LEU:HD23	2.01	0.43
1:A:1069:VAL:HG12	1:A:1193:LEU:HB2	2.01	0.43
2:C:782:ARG:NE	2:C:820:GLU:OE2	2.52	0.43
2:F:724:GLU:HG3	2:F:860:ARG:HH12	1.83	0.43
2:G:595:VAL:HG23	2:G:891:LYS:HZ1	1.76	0.43
2:H:792:ASP:O	2:H:796:GLN:NE2	2.52	0.43
2:I:379:LEU:HD23	2:I:500:MET:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:627:VAL:HG22	2:G:777:VAL:HA	2.00	0.43
2:K:552:LEU:HD23	2:K:552:LEU:HA	1.87	0.43
2:K:787:ASP:OD1	2:K:787:ASP:N	2.48	0.43
1:A:871:MET:SD	1:A:917:TYR:OH	2.71	0.43
1:A:1118:ARG:HG3	1:A:1210:ALA:HB1	2.01	0.43
2:I:402:LEU:HD11	2:I:500:MET:HE1	2.00	0.43
2:J:97:SER:OG	2:J:98:ARG:N	2.52	0.43
2:B:293:ILE:HD12	2:C:314:LEU:HD12	2.01	0.42
2:G:251:SER:OG	2:G:252:GLN:N	2.52	0.42
2:J:118:ILE:HD12	2:J:126:PHE:HD1	1.84	0.42
1:A:97:VAL:HG21	1:A:248:ILE:HD11	2.01	0.42
1:A:211:GLU:HG2	1:A:243:LEU:HD21	2.01	0.42
1:A:847:ARG:NH1	1:A:926:GLY:O	2.50	0.42
2:G:705:MET:HE2	2:G:848:MET:HE3	2.01	0.42
2:H:664:ARG:NE	2:I:486:THR:O	2.52	0.42
2:J:386:ARG:HE	2:J:456:ASP:HB2	1.84	0.42
2:C:297:LEU:HD12	2:C:298:PRO:HD2	2.01	0.42
2:D:378:HIS:CD2	2:D:402:LEU:HD22	2.53	0.42
2:F:352:GLN:NE2	2:F:544:LEU:HB2	2.33	0.42
2:H:587:THR:OG1	2:H:588:HIS:N	2.52	0.42
2:I:460:ARG:O	2:I:461:GLU:HG3	2.19	0.42
2:J:43:VAL:HG12	2:J:47:GLN:HG3	2.01	0.42
1:A:599:TYR:HE2	1:A:731:ASN:HB2	1.84	0.42
2:C:474:TYR:O	2:C:475:CYS:SG	2.77	0.42
2:D:816:LYS:HB2	2:D:816:LYS:HE3	1.86	0.42
2:E:47:GLN:HE21	2:F:882:ARG:HH21	1.66	0.42
2:H:632:ARG:H	2:H:635:HIS:HD2	1.66	0.42
2:J:228:GLN:OE1	2:J:265:TRP:N	2.53	0.42
2:K:333:THR:HG23	2:K:336:GLN:H	1.85	0.42
2:C:31:LEU:HD13	2:C:345:LEU:HD13	2.02	0.42
2:C:592:MET:HE2	2:C:592:MET:HB3	1.92	0.42
2:E:262:ASP:O	2:E:882:ARG:N	2.51	0.42
2:F:703:VAL:HG21	2:F:821:THR:HG21	2.01	0.42
2:G:416:VAL:HB	2:G:429:ILE:HD12	2.00	0.42
2:B:608:SER:HB3	2:B:681:LEU:HD13	2.00	0.42
2:G:478:ASP:OD2	2:G:480:ARG:NE	2.48	0.42
2:H:526:ARG:NH2	2:H:580:PHE:O	2.52	0.42
2:H:743:GLN:HE22	2:H:773:ARG:HH11	1.67	0.42
2:J:133:LYS:NZ	2:J:697:LEU:O	2.50	0.42
1:A:207:MET:HE3	1:A:207:MET:HB2	1.88	0.42
1:A:314:SER:OG	1:A:781:ASP:OD1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:ARG:O	1:A:1027:HIS:N	2.45	0.42
2:D:751:LEU:HD23	2:D:751:LEU:HA	1.92	0.42
2:E:519:MET:HE3	2:E:519:MET:HB3	1.79	0.42
2:G:359:ILE:HG23	2:H:894:THR:HG23	2.02	0.42
1:A:743:GLN:NE2	1:A:759:GLU:OE2	2.36	0.42
2:B:344:TYR:OH	2:B:582:ARG:O	2.27	0.42
2:C:383:ALA:HA	2:C:388:THR:HG22	2.01	0.42
2:D:475:CYS:HG	2:D:477:ILE:HG13	1.81	0.42
2:E:72:LYS:HE2	2:E:72:LYS:HB3	1.89	0.42
2:F:289:LEU:HD21	2:F:353:ILE:HD11	2.02	0.42
2:F:762:LEU:HD23	2:F:762:LEU:HA	1.93	0.42
2:G:464:PRO:HG2	2:G:539:HIS:HE1	1.84	0.42
2:I:393:ASN:HD21	2:I:397:GLN:HE21	1.66	0.42
2:J:257:ASP:OD2	2:J:882:ARG:NH1	2.44	0.42
2:J:262:ASP:OD1	2:J:262:ASP:N	2.52	0.42
2:D:257:ASP:N	2:D:257:ASP:OD1	2.53	0.42
2:E:209:CYS:SG	2:E:210:SER:N	2.93	0.42
2:G:365:MET:HE1	2:G:574:ILE:HD12	2.01	0.42
2:G:492:MET:HE2	2:G:492:MET:HB3	1.81	0.42
2:G:725:GLY:O	2:G:860:ARG:NH1	2.53	0.42
2:G:787:ASP:OD1	2:G:787:ASP:N	2.44	0.42
2:I:194:ASN:O	2:I:200:ARG:HD3	2.20	0.42
2:K:447:THR:O	2:K:452:TRP:CD2	2.73	0.42
2:C:779:ARG:NH2	2:C:817:TYR:O	2.53	0.42
2:D:327:LEU:O	2:D:330:SER:OG	2.37	0.42
2:D:477:ILE:HG23	2:D:492:MET:HE1	2.02	0.42
2:F:796:GLN:HA	2:F:848:MET:HB2	2.02	0.42
2:H:701:ASP:OD1	2:H:701:ASP:N	2.50	0.42
2:K:402:LEU:HD11	2:K:500:MET:HE1	2.01	0.42
1:A:605:ARG:CZ	1:A:607:ASN:HD21	2.32	0.41
1:A:1022:SER:O	1:A:1026:MET:N	2.45	0.41
1:A:1104:ILE:HD12	2:J:39:ILE:HG23	2.02	0.41
2:D:370:ARG:NH2	2:D:404:ASP:OD2	2.38	0.41
2:E:487:THR:OG1	2:E:488:TYR:N	2.53	0.41
2:G:8:ARG:HH22	2:G:589:ARG:HH21	1.68	0.41
2:K:379:LEU:HD23	2:K:500:MET:HG2	2.01	0.41
1:A:883:LYS:HA	1:A:883:LYS:HD2	1.93	0.41
2:C:26:ASP:OD2	2:C:302:TYR:OH	2.30	0.41
2:F:459:TYR:OH	2:F:550:ASN:OD1	2.37	0.41
2:H:193:GLU:HB2	2:H:204:VAL:HG13	2.01	0.41
2:I:202:VAL:CG1	2:I:203:ASP:N	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:853:ILE:HG22	2:C:855:LYS:HB2	2.02	0.41
2:D:350:PRO:HG2	2:D:472:ILE:HD13	2.01	0.41
2:E:200:ARG:O	2:E:201:ASP:HB3	2.20	0.41
2:H:855:LYS:HA	2:H:855:LYS:HD3	1.89	0.41
1:A:649:THR:OG1	1:A:651:TRP:NE1	2.51	0.41
1:A:1155:HIS:HB2	2:H:308:ARG:HH12	1.85	0.41
2:C:371:MET:HE1	2:D:899:PRO:HG3	2.03	0.41
2:E:54:THR:OG1	2:E:55:ARG:N	2.53	0.41
2:E:296:CYS:HB2	2:E:538:LEU:HD23	2.02	0.41
2:G:432:ASN:OD1	2:G:432:ASN:N	2.48	0.41
2:I:104:VAL:HG22	2:I:858:VAL:HG22	2.02	0.41
2:I:135:ARG:NH2	2:I:613:ASP:OD2	2.47	0.41
2:I:209:CYS:H	2:I:872:ARG:HG3	1.85	0.41
1:A:628:TYR:N	1:A:631:TYR:O	2.54	0.41
2:B:345:LEU:HD22	2:C:318:ILE:HD13	2.03	0.41
2:D:461:GLU:HG2	2:D:462:PRO:CD	2.37	0.41
2:D:662:ASN:OD1	2:D:662:ASN:N	2.45	0.41
2:F:615:ARG:HH12	2:F:675:LEU:HD21	1.84	0.41
2:G:133:LYS:HD3	2:G:697:LEU:HB3	2.03	0.41
2:I:355:LEU:O	2:I:391:THR:OG1	2.31	0.41
1:A:883:LYS:HB2	1:A:1045:GLU:HG2	2.02	0.41
1:A:1067:SER:HB3	1:A:1278:PRO:HG3	2.03	0.41
1:A:1126:ASP:O	1:A:1130:ARG:N	2.53	0.41
2:B:291:MET:HE2	2:B:291:MET:HB2	1.85	0.41
2:C:379:LEU:HD21	2:C:500:MET:HG2	2.03	0.41
2:E:700:THR:OG1	2:E:701:ASP:N	2.53	0.41
2:H:71:ILE:HG21	2:H:599:ILE:HG23	2.03	0.41
2:H:698:MET:HE3	2:H:698:MET:HB3	1.96	0.41
2:J:219:ARG:HD2	2:J:219:ARG:HA	1.86	0.41
1:A:828:MET:HG3	1:A:856:LYS:HD3	2.02	0.41
2:C:831:GLU:H	2:C:834:ASN:ND2	2.18	0.41
2:D:552:LEU:HD23	2:D:552:LEU:HA	1.90	0.41
2:E:71:ILE:HG21	2:E:599:ILE:HG23	2.02	0.41
2:G:31:LEU:HD13	2:G:345:LEU:HD13	2.03	0.41
2:H:411:ASN:OD1	2:H:411:ASN:N	2.53	0.41
2:H:786:TYR:CD1	2:H:790:PRO:HB3	2.55	0.41
2:J:354:ILE:HD12	2:J:391:THR:HG22	2.01	0.41
1:A:105:TRP:HD1	1:A:127:VAL:HG11	1.85	0.41
1:A:846:VAL:HA	1:A:849:GLN:HB3	2.02	0.41
2:C:95:MET:SD	2:C:102:LEU:CD1	3.08	0.41
2:D:127:TYR:HD1	2:D:617:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:264:ILE:HB	2:E:883:ILE:HG12	2.03	0.41
2:F:167:GLU:HG2	2:F:169:LYS:HG2	2.03	0.41
2:F:409:MET:HE3	2:F:409:MET:HB2	1.96	0.41
2:J:503:MET:HB3	2:J:503:MET:HE2	1.80	0.41
1:A:280:VAL:HG21	1:A:362:HIS:CD2	2.55	0.41
1:A:828:MET:SD	1:A:855:THR:OG1	2.79	0.41
1:A:1070:ILE:HD12	1:A:1070:ILE:HA	1.87	0.41
2:B:504:LEU:HB3	2:B:513:ALA:HB2	2.02	0.41
2:C:176:THR:HG22	2:C:178:GLU:H	1.86	0.41
2:C:460:ARG:HH21	2:C:473:ARG:HD2	1.84	0.41
2:E:379:LEU:HD23	2:E:500:MET:HG2	2.02	0.41
2:G:740:ARG:NH2	2:G:769:ASP:O	2.54	0.41
2:H:778:LEU:HD23	2:H:778:LEU:HA	1.89	0.41
2:I:494:TYR:HD1	2:I:524:MET:HE3	1.86	0.41
2:J:632:ARG:H	2:J:635:HIS:HD2	1.68	0.41
2:J:653:ASN:HA	2:J:656:HIS:HB2	2.02	0.41
2:B:228:GLN:OE1	2:B:265:TRP:N	2.54	0.41
2:E:843:ASN:HD22	2:E:843:ASN:HA	1.69	0.41
2:F:431:ARG:HE	2:F:431:ARG:HB3	1.67	0.41
2:G:835:THR:HB	2:G:838:SER:HB3	2.02	0.41
2:B:857:ILE:HG22	2:B:858:VAL:HG23	2.03	0.40
2:C:447:THR:OG1	2:C:448:GLY:N	2.54	0.40
2:C:629:ILE:HG13	2:C:630:GLN:HG3	2.03	0.40
2:E:497:TYR:OH	2:E:516:PHE:O	2.37	0.40
2:E:623:ARG:NH2	2:E:692:ASN:O	2.40	0.40
2:F:344:TYR:OH	2:F:582:ARG:O	2.31	0.40
2:H:98:ARG:HG2	2:H:174:VAL:HG12	2.03	0.40
2:J:638:LYS:HA	2:J:638:LYS:HD2	1.83	0.40
1:A:1154:ASN:HD22	1:A:1159:ASP:HB3	1.85	0.40
2:B:717:ASP:HB3	2:B:720:ARG:HB3	2.03	0.40
2:D:708:ASP:OD2	2:D:850:LYS:NZ	2.40	0.40
2:F:72:LYS:HE2	2:F:72:LYS:HB3	1.80	0.40
2:F:774:PHE:O	2:F:779:ARG:NH1	2.54	0.40
2:G:378:HIS:CD2	2:G:402:LEU:HD22	2.56	0.40
2:I:297:LEU:HD23	2:I:297:LEU:HA	1.93	0.40
2:K:378:HIS:CD2	2:K:402:LEU:HD22	2.56	0.40
1:A:661:THR:O	1:A:704:THR:OG1	2.39	0.40
2:C:793:ASP:OD1	2:C:793:ASP:N	2.53	0.40
2:E:705:MET:HB3	2:E:772:VAL:HG13	2.02	0.40
2:F:460:ARG:CG	2:F:460:ARG:NH2	2.81	0.40
2:F:784:LYS:HE3	2:F:786:TYR:OH	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:293:ILE:HG21	2:I:315:THR:HG22	2.03	0.40
2:H:492:MET:HE2	2:H:492:MET:HB3	1.95	0.40
2:I:460:ARG:HD3	2:I:460:ARG:HA	1.90	0.40
2:J:889:SER:O	2:J:889:SER:OG	2.37	0.40
2:D:671:MET:HE2	2:D:671:MET:HB3	1.92	0.40
2:I:22:VAL:HG13	2:I:301:GLU:HB3	2.04	0.40
2:D:329:GLY:HA3	2:F:31:LEU:HB2	2.03	0.40
2:G:10:GLU:HG2	2:G:532:GLN:HE22	1.86	0.40
2:H:191:ILE:HD12	2:H:191:ILE:HA	1.86	0.40
2:H:382:THR:HG22	2:H:384:GLY:H	1.87	0.40
2:I:709:MET:HA	2:I:846:TYR:HA	2.04	0.40
2:K:474:TYR:H	2:K:531:ASN:ND2	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1238/1302 (95%)	1153 (93%)	85 (7%)	0	100	100
2	B	870/901 (97%)	829 (95%)	41 (5%)	0	100	100
2	C	881/901 (98%)	825 (94%)	56 (6%)	0	100	100
2	D	859/901 (95%)	828 (96%)	31 (4%)	0	100	100
2	E	881/901 (98%)	828 (94%)	53 (6%)	0	100	100
2	F	864/901 (96%)	822 (95%)	42 (5%)	0	100	100
2	G	881/901 (98%)	836 (95%)	45 (5%)	0	100	100
2	H	866/901 (96%)	813 (94%)	53 (6%)	0	100	100
2	I	881/901 (98%)	829 (94%)	52 (6%)	0	100	100
2	J	868/901 (96%)	821 (95%)	47 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	881/901 (98%)	830 (94%)	51 (6%)	0	100	100
All	All	9970/10312 (97%)	9414 (94%)	556 (6%)	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	A	1110/1161 (96%)	1101 (99%)	9 (1%)	79	88
2	B	767/792 (97%)	763 (100%)	4 (0%)	86	93
2	C	782/792 (99%)	778 (100%)	4 (0%)	86	93
2	D	759/792 (96%)	754 (99%)	5 (1%)	81	90
2	E	782/792 (99%)	776 (99%)	6 (1%)	79	88
2	F	763/792 (96%)	754 (99%)	9 (1%)	67	82
2	G	782/792 (99%)	777 (99%)	5 (1%)	84	92
2	H	763/792 (96%)	761 (100%)	2 (0%)	91	96
2	I	782/792 (99%)	774 (99%)	8 (1%)	73	85
2	J	765/792 (97%)	761 (100%)	4 (0%)	86	93
2	K	782/792 (99%)	778 (100%)	4 (0%)	86	93
All	All	8837/9081 (97%)	8777 (99%)	60 (1%)	80	90

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ASP
1	A	115	LEU
1	A	684	VAL
1	A	727	THR
1	A	839	ILE
1	A	960	ILE

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Mol	Chain	Res	Type
1	A	1080	VAL
1	A	1277	VAL
1	A	1282	VAL
2	B	61	VAL
2	B	271	LEU
2	B	461	GLU
2	B	671	MET
2	C	22	VAL
2	C	101	VAL
2	C	461	GLU
2	C	671	MET
2	D	197	VAL
2	D	271	LEU
2	D	391	THR
2	D	537	ASP
2	D	671	MET
2	E	201	ASP
2	E	477	ILE
2	E	698	MET
2	E	745	THR
2	E	793	ASP
2	E	794	VAL
2	F	266	VAL
2	F	271	LEU
2	F	391	THR
2	F	460	ARG
2	F	471	TYR
2	F	671	MET
2	F	794	VAL
2	F	863	VAL
2	F	875	VAL
2	G	201	ASP
2	G	354	ILE
2	G	416	VAL
2	G	460	ARG
2	G	671	MET
2	H	52	THR
2	H	851	VAL
2	I	201	ASP
2	I	202	VAL
2	I	266	VAL
2	I	391	THR

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Mol	Chain	Res	Type
2	I	477	ILE
2	I	671	MET
2	I	772	VAL
2	I	793	ASP
2	J	271	LEU
2	J	461	GLU
2	J	487	THR
2	J	671	MET
2	K	354	ILE
2	K	570	ASP
2	K	671	MET
2	K	794	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (210) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	55	GLN
1	A	91	GLN
1	A	176	ASN
1	A	217	ASN
1	A	259	ASN
1	A	283	GLN
1	A	335	GLN
1	A	377	GLN
1	A	507	GLN
1	A	648	ASN
1	A	843	GLN
1	A	851	GLN
1	A	863	HIS
1	A	867	GLN
1	A	923	ASN
1	A	996	GLN
1	A	1003	GLN
1	A	1296	ASN
1	A	1299	ASN
1	A	1300	GLN
2	B	45	GLN
2	B	96	GLN
2	B	288	ASN
2	B	338	ASN
2	B	389	ASN

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Mol	Chain	Res	Type
2	B	437	ASN
2	B	450	ASN
2	B	467	HIS
2	B	531	ASN
2	B	550	ASN
2	B	635	HIS
2	B	656	HIS
2	B	676	GLN
2	B	692	ASN
2	B	702	GLN
2	B	723	GLN
2	B	757	GLN
2	B	834	ASN
2	B	865	GLN
2	C	45	GLN
2	C	78	GLN
2	C	92	HIS
2	C	179	HIS
2	C	244	HIS
2	C	276	GLN
2	C	288	ASN
2	C	378	HIS
2	C	393	ASN
2	C	531	ASN
2	C	539	HIS
2	C	561	HIS
2	C	563	ASN
2	C	588	HIS
2	C	635	HIS
2	C	642	ASN
2	C	653	ASN
2	C	676	GLN
2	C	723	GLN
2	C	754	ASN
2	C	796	GLN
2	C	834	ASN
2	C	854	ASN
2	D	37	GLN
2	D	41	GLN
2	D	65	GLN
2	D	153	HIS
2	D	276	GLN

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Mol	Chain	Res	Type
2	D	352	GLN
2	D	417	ASN
2	D	428	GLN
2	D	437	ASN
2	D	450	ASN
2	D	467	HIS
2	D	531	ASN
2	D	535	ASN
2	D	539	HIS
2	D	550	ASN
2	D	635	HIS
2	D	659	ASN
2	D	676	GLN
2	D	723	GLN
2	D	752	GLN
2	D	757	GLN
2	D	805	ASN
2	D	829	ASN
2	E	47	GLN
2	E	113	GLN
2	E	146	HIS
2	E	194	ASN
2	E	221	GLN
2	E	228	GLN
2	E	276	GLN
2	E	389	ASN
2	E	467	HIS
2	E	531	ASN
2	E	581	ASN
2	E	635	HIS
2	E	653	ASN
2	E	692	ASN
2	E	723	GLN
2	E	754	ASN
2	E	843	ASN
2	F	92	HIS
2	F	185	ASN
2	F	276	GLN
2	F	352	GLN
2	F	417	ASN
2	F	450	ASN
2	F	495	HIS

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Mol	Chain	Res	Type
2	F	531	ASN
2	F	532	GLN
2	F	535	ASN
2	F	539	HIS
2	F	550	ASN
2	F	635	HIS
2	F	676	GLN
2	F	702	GLN
2	F	752	GLN
2	F	805	ASN
2	F	829	ASN
2	G	218	ASN
2	G	234	ASN
2	G	270	GLN
2	G	288	ASN
2	G	378	HIS
2	G	467	HIS
2	G	531	ASN
2	G	532	GLN
2	G	539	HIS
2	G	588	HIS
2	G	635	HIS
2	G	642	ASN
2	G	692	ASN
2	G	706	HIS
2	H	47	GLN
2	H	153	HIS
2	H	221	GLN
2	H	276	GLN
2	H	288	ASN
2	H	392	GLN
2	H	450	ASN
2	H	532	GLN
2	H	535	ASN
2	H	550	ASN
2	H	635	HIS
2	H	642	ASN
2	H	659	ASN
2	H	702	GLN
2	H	743	GLN
2	H	752	GLN
2	H	754	ASN

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Mol	Chain	Res	Type
2	H	757	GLN
2	H	796	GLN
2	H	829	ASN
2	H	834	ASN
2	I	47	GLN
2	I	92	HIS
2	I	179	HIS
2	I	194	ASN
2	I	276	GLN
2	I	389	ASN
2	I	393	ASN
2	I	415	GLN
2	I	467	HIS
2	I	484	ASN
2	I	495	HIS
2	I	531	ASN
2	I	550	ASN
2	I	635	HIS
2	I	642	ASN
2	I	653	ASN
2	I	752	GLN
2	I	843	ASN
2	J	37	GLN
2	J	47	GLN
2	J	179	HIS
2	J	196	ASN
2	J	276	GLN
2	J	292	ASN
2	J	352	GLN
2	J	389	ASN
2	J	417	ASN
2	J	433	GLN
2	J	437	ASN
2	J	531	ASN
2	J	535	ASN
2	J	550	ASN
2	J	635	HIS
2	J	659	ASN
2	J	702	GLN
2	J	743	GLN
2	J	805	ASN
2	J	834	ASN

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Mol	Chain	Res	Type
2	K	47	GLN
2	K	65	GLN
2	K	92	HIS
2	K	170	ASN
2	K	228	GLN
2	K	276	GLN
2	K	389	ASN
2	K	393	ASN
2	K	433	GLN
2	K	484	ASN
2	K	635	HIS
2	K	642	ASN
2	K	653	ASN
2	K	706	HIS
2	K	723	GLN
2	K	834	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 ⓘ

There are no chain breaks in this entry.

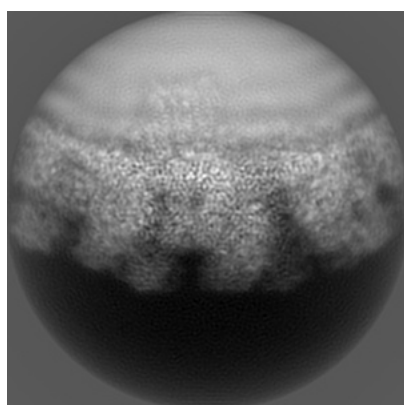
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20407. These allow visual inspection of the internal detail of the map and identification of artifacts.

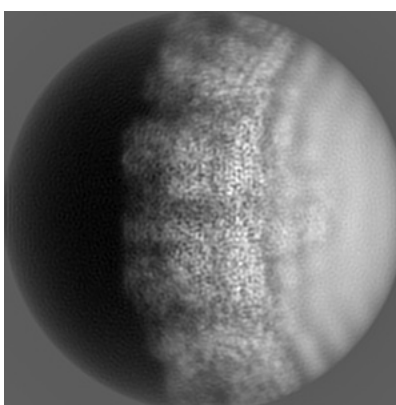
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

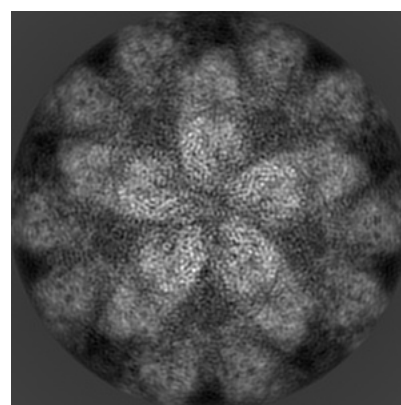
6.1.1 Primary map



X



Y

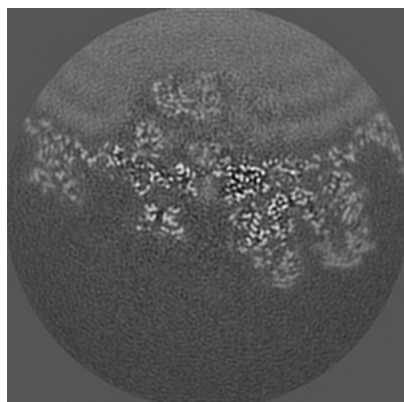


Z

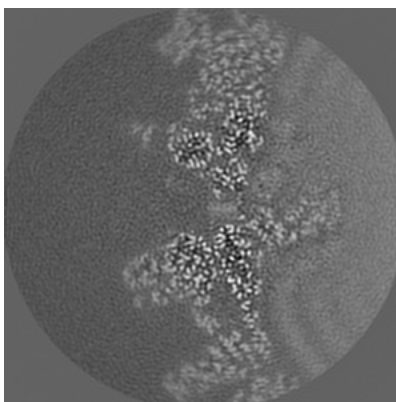
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

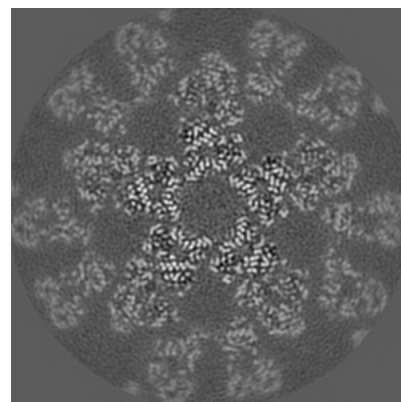
6.2.1 Primary map



X Index: 128



Y Index: 128

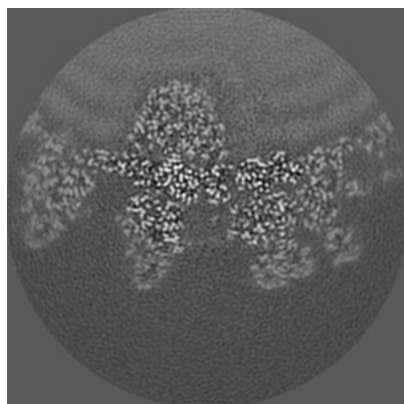


Z Index: 128

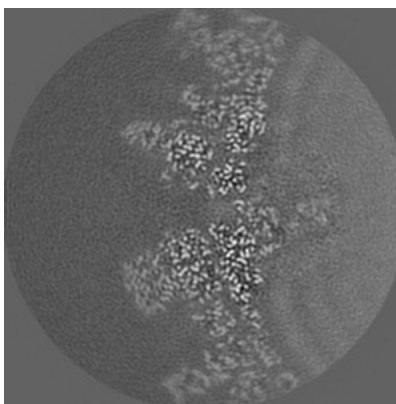
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

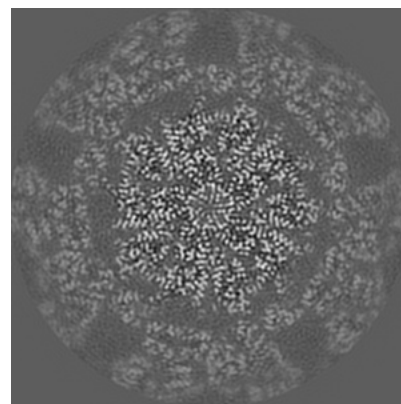
6.3.1 Primary map



X Index: 114



Y Index: 132

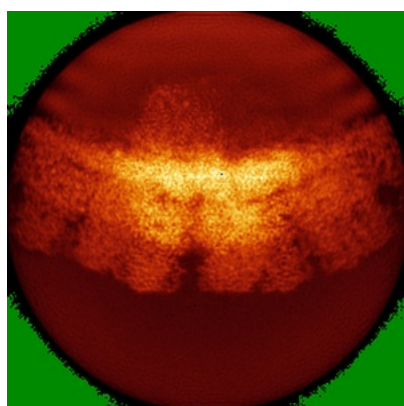


Z Index: 149

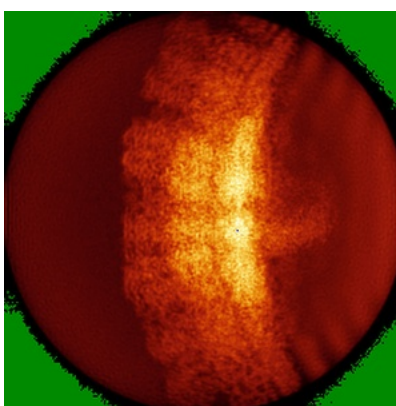
The images above show the largest variance slices of the map in three orthogonal directions.

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

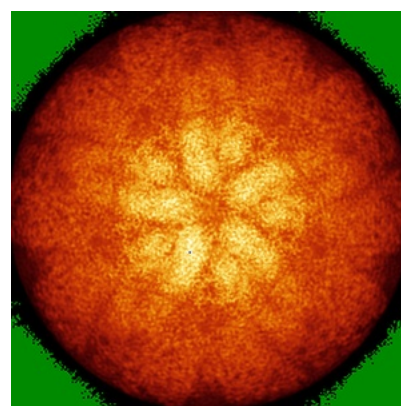
6.4.1 Primary map



X



Y

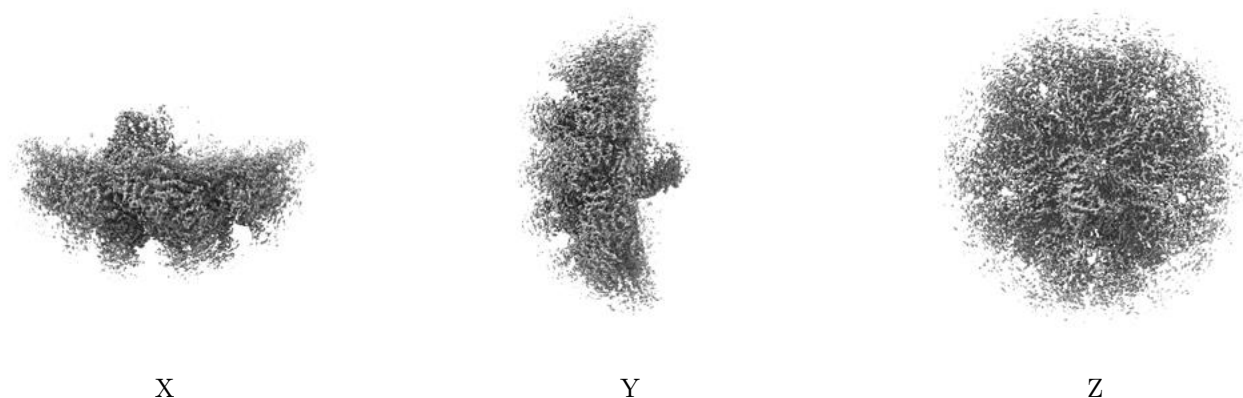


Z

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

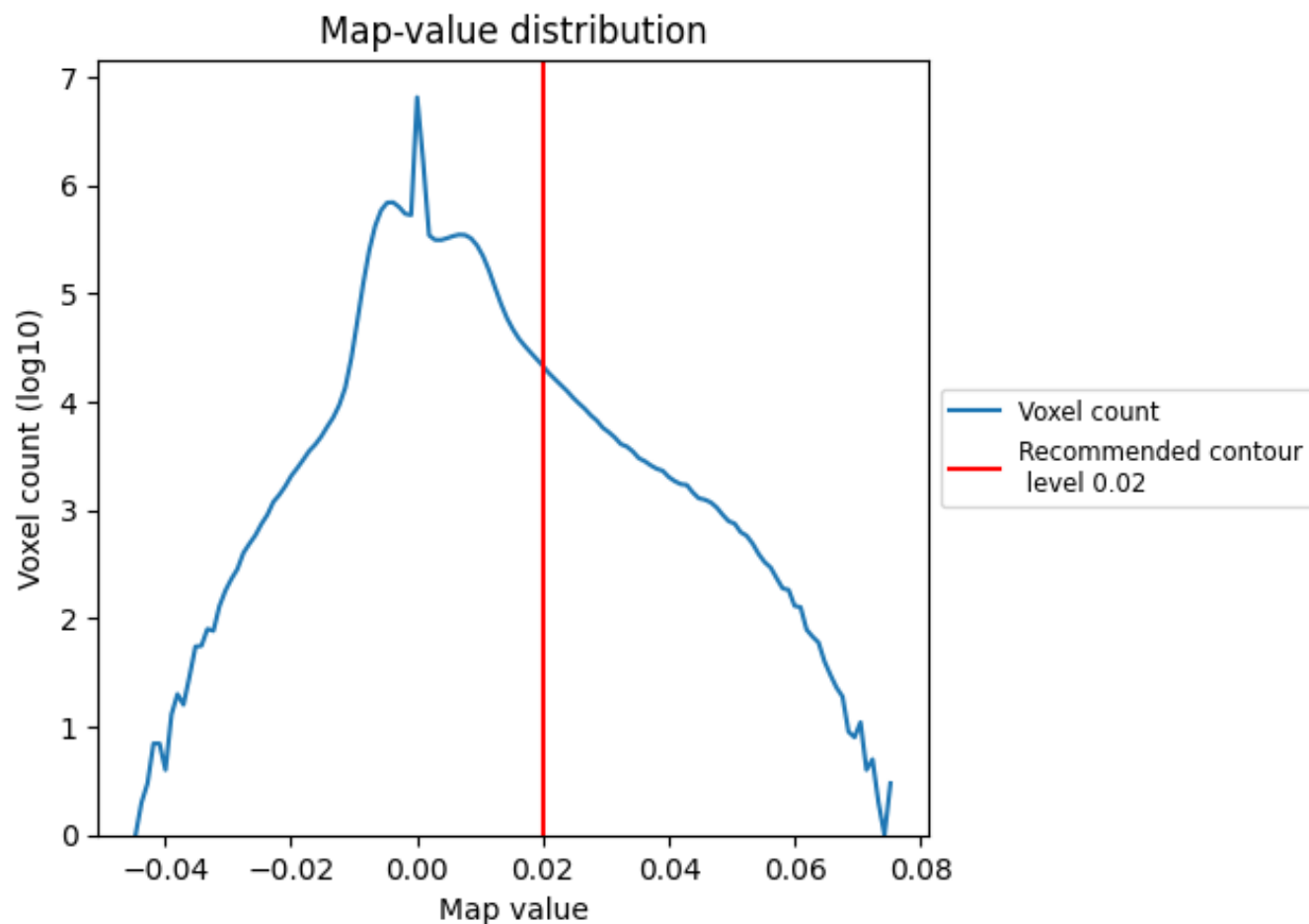
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

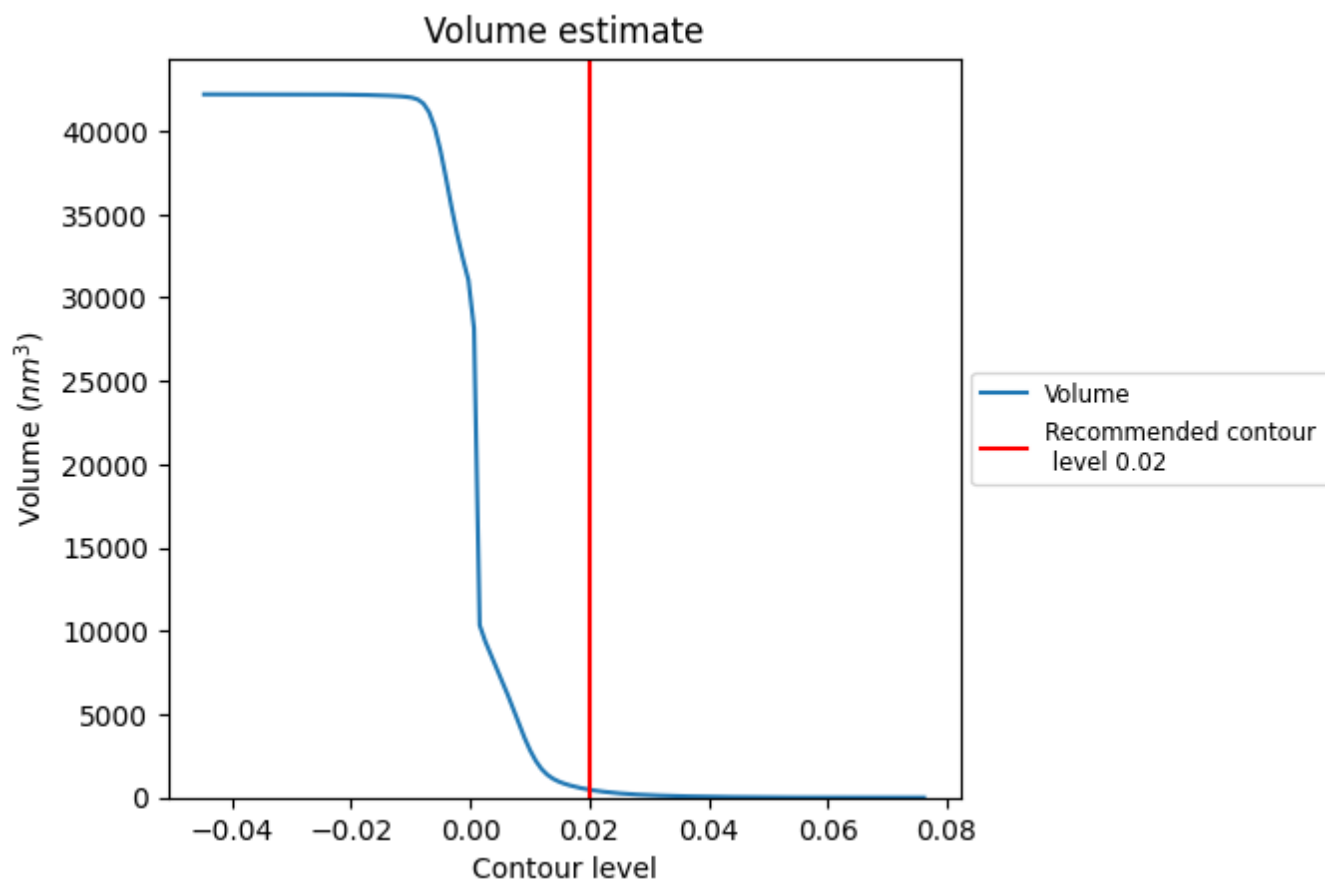
This section contains the results of statistical analysis of the map.

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.

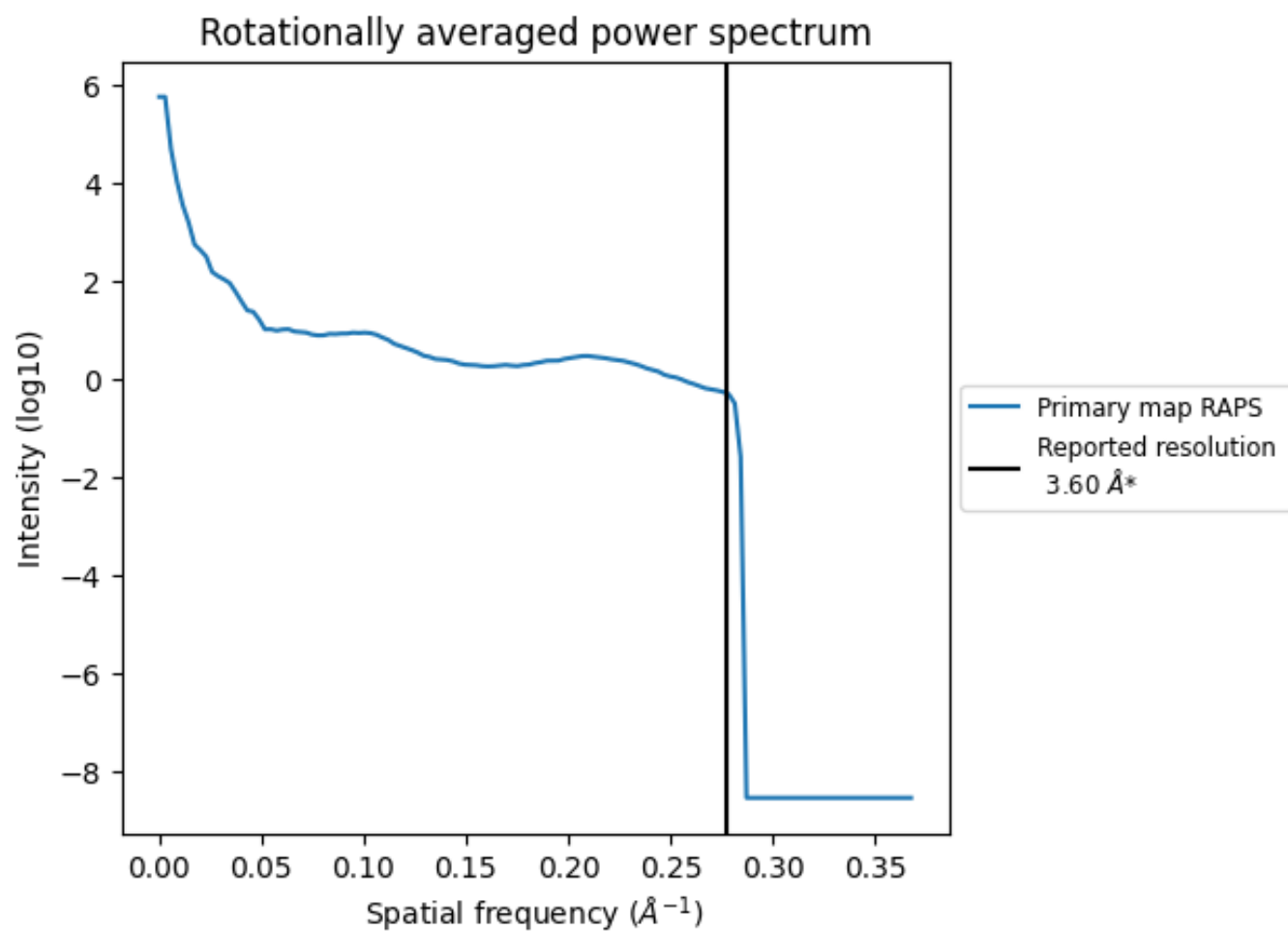
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 474 nm³; this corresponds to an approximate mass of 428 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 0.278 Å⁻¹

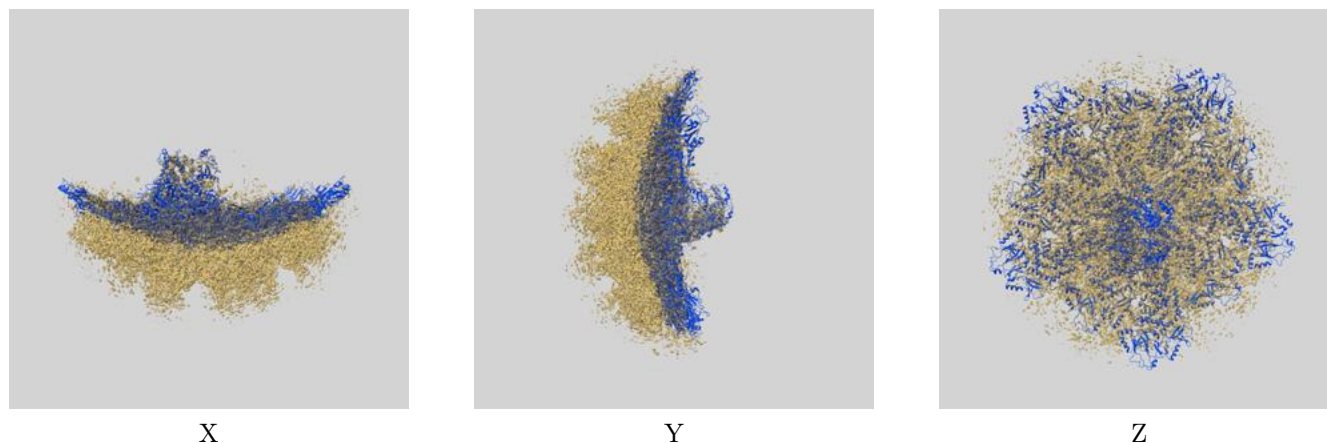
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

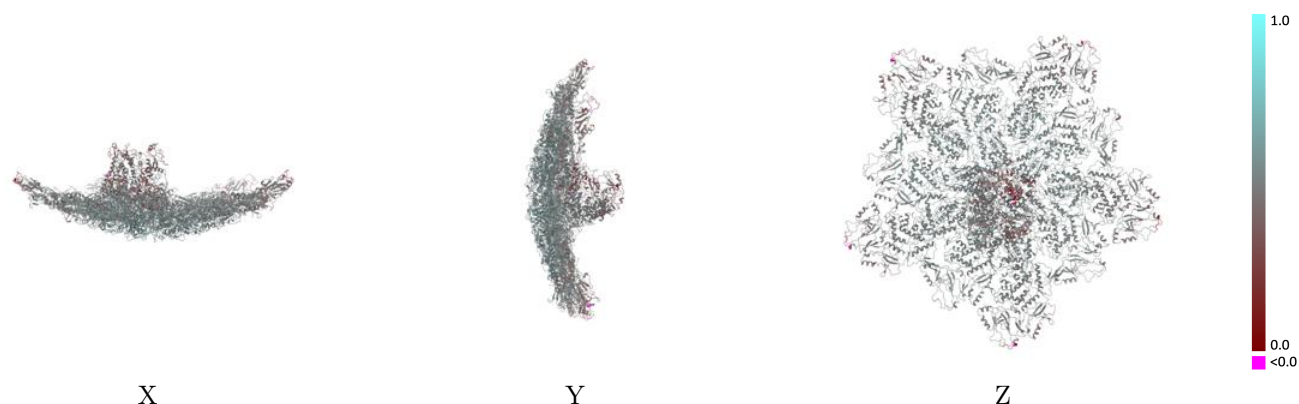
This section contains information regarding the fit between EMDB map EMD-20407 and PDB model 6PO2. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



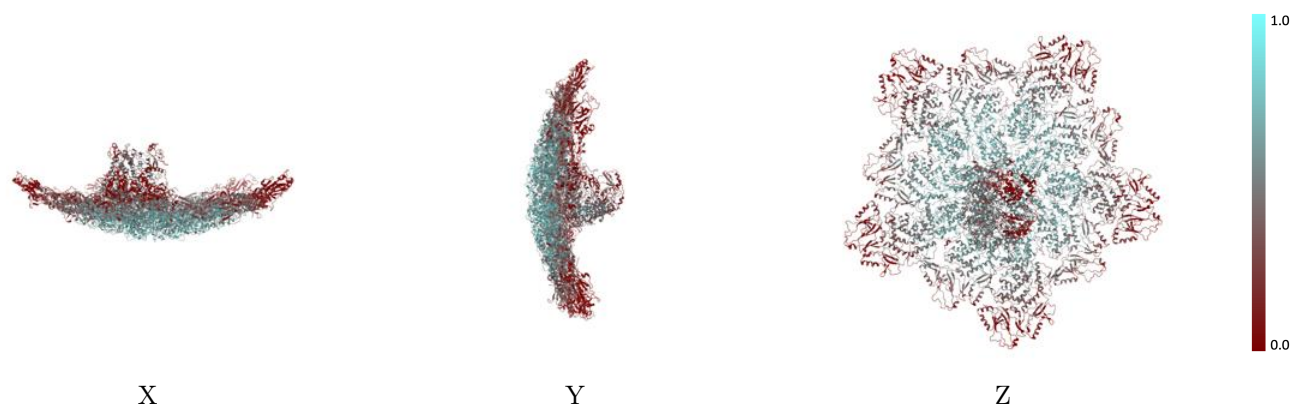
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



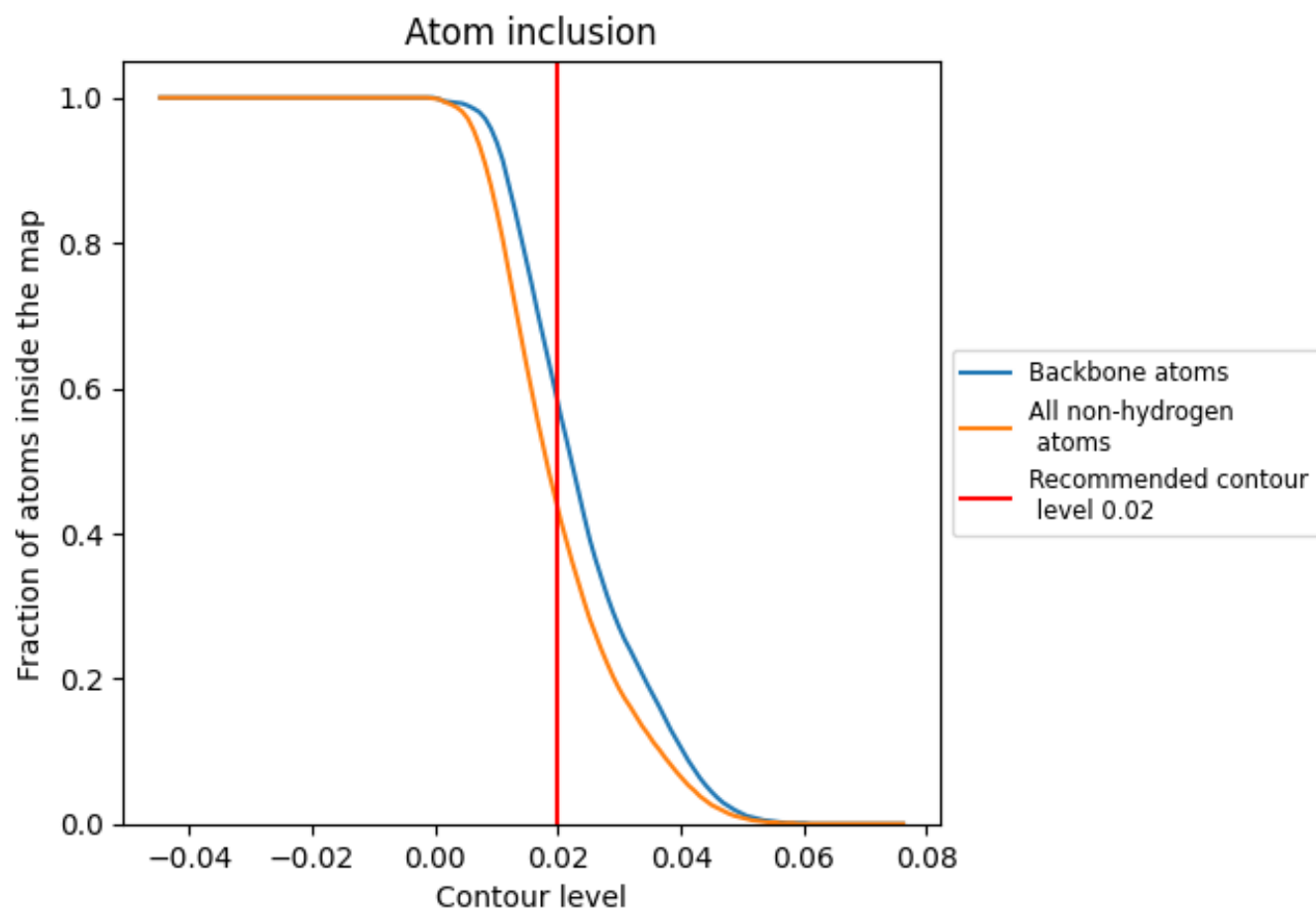
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4340	<div></div> 0.4970
A	<div></div> 0.3050	<div></div> 0.4370
B	<div></div> 0.5430	<div></div> 0.5230
C	<div></div> 0.3780	<div></div> 0.4900
D	<div></div> 0.5320	<div></div> 0.5200
E	<div></div> 0.3720	<div></div> 0.4890
F	<div></div> 0.5140	<div></div> 0.5160
G	<div></div> 0.3700	<div></div> 0.4880
H	<div></div> 0.5190	<div></div> 0.5150
I	<div></div> 0.3790	<div></div> 0.4930
J	<div></div> 0.5410	<div></div> 0.5240
K	<div></div> 0.3820	<div></div> 0.4920

1.0

0.0

<0.0