



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:40 AM UTC

PDB ID : 8XA3 / pdb_00008xa3
EMDB ID : EMD-38193
Title : C-hexon capsomer of the VZV B-Capsid
Authors : Wang, N.; Cao, L.; Wang, X.
Deposited on : 2023-12-01
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

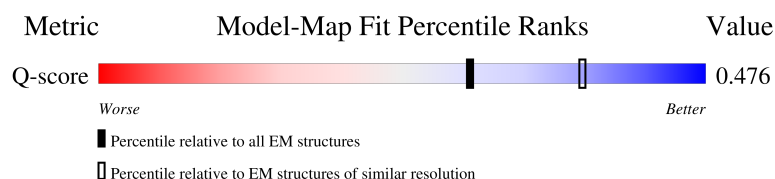
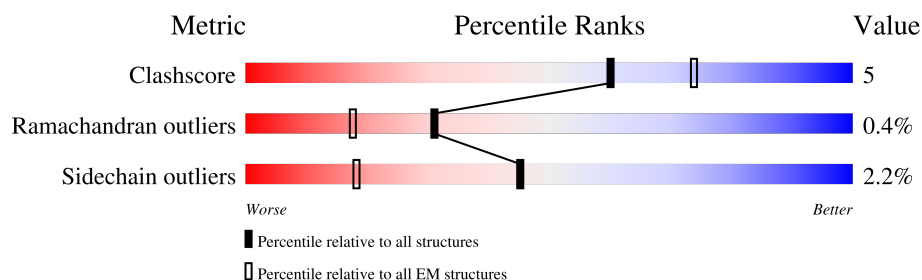
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	1381	
1	C	1381	
1	D	1381	
1	E	1381	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	1381	
1	H	1381	
2	B	94	
2	G	94	
2	L	94	
2	Q	94	
2	V	94	
2	g	94	
3	I	256	
3	K	256	
4	N	263	
4	P	263	
5	S	392	
5	U	392	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 81795 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1381	Total	C	N	O	S	0	0
			10675	6757	1870	1981	67		
1	C	1381	Total	C	N	O	S	0	0
			10675	6757	1870	1981	67		
1	D	1381	Total	C	N	O	S	0	0
			10680	6759	1873	1981	67		
1	E	1381	Total	C	N	O	S	0	0
			10675	6757	1870	1981	67		
1	F	1381	Total	C	N	O	S	0	0
			10675	6757	1870	1981	67		
1	H	1381	Total	C	N	O	S	0	0
			10675	6757	1870	1981	67		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	LEU	conflict	UNP Q6QCL5
A	814	ALA	GLY	conflict	UNP Q6QCL5
C	22	ILE	LEU	conflict	UNP Q6QCL5
C	814	ALA	GLY	conflict	UNP Q6QCL5
D	22	ILE	LEU	conflict	UNP Q6QCL5
D	814	ALA	GLY	conflict	UNP Q6QCL5
E	22	ILE	LEU	conflict	UNP Q6QCL5
E	814	ALA	GLY	conflict	UNP Q6QCL5
F	22	ILE	LEU	conflict	UNP Q6QCL5
F	814	ALA	GLY	conflict	UNP Q6QCL5
H	22	ILE	LEU	conflict	UNP Q6QCL5
H	814	ALA	GLY	conflict	UNP Q6QCL5

- Molecule 2 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	G	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	B	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	g	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	V	94	Total	C	N	O	S	0	0
			699	437	135	125	2		
2	Q	94	Total	C	N	O	S	0	0
			699	437	135	125	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	95	ARG	LYS	conflict	UNP U5NQG6
G	95	ARG	LYS	conflict	UNP U5NQG6
B	95	ARG	LYS	conflict	UNP U5NQG6
g	95	ARG	LYS	conflict	UNP U5NQG6
V	95	ARG	LYS	conflict	UNP U5NQG6
Q	95	ARG	LYS	conflict	UNP U5NQG6

- Molecule 3 is a protein called Tri2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	256	Total	C	N	O	S	0	0
			1847	1191	315	333	8		
3	K	256	Total	C	N	O	S	0	0
			1847	1191	315	333	8		

- Molecule 4 is a protein called Tri2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	263	Total	C	N	O	S	0	0
			1975	1269	339	358	9		
4	P	263	Total	C	N	O	S	0	0
			1975	1269	339	358	9		

- Molecule 5 is a protein called Tri1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	392	Total 2951	C 1854	N 552	O 529	S 16	0	0
5	U	392	Total 2951	C 1854	N 552	O 529	S 16	0	0

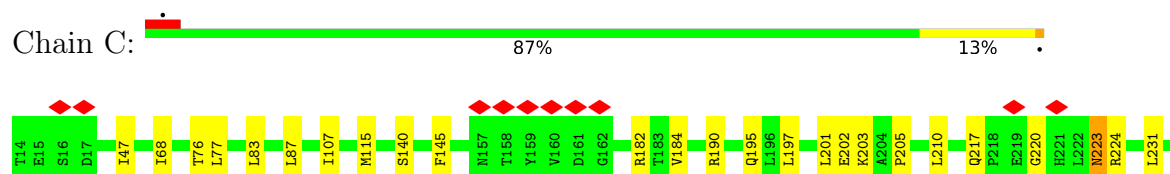
3 Residue-property plots

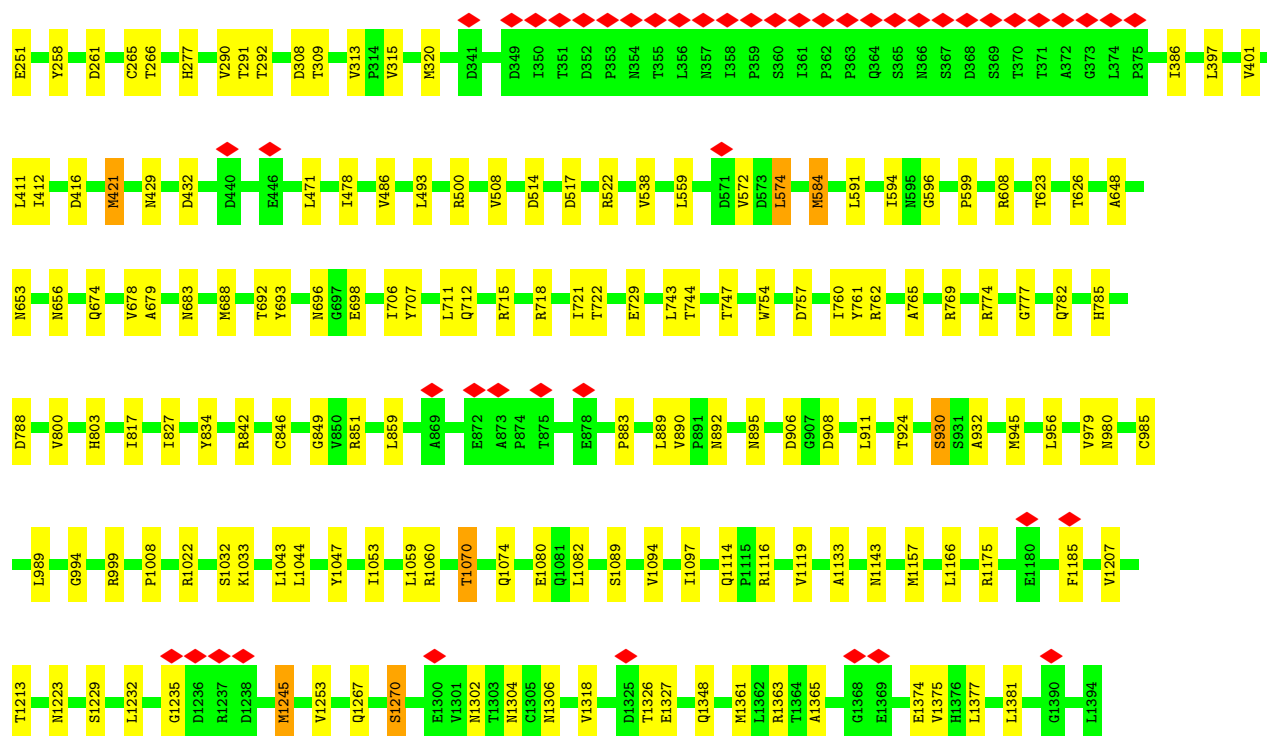
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Major capsid protein

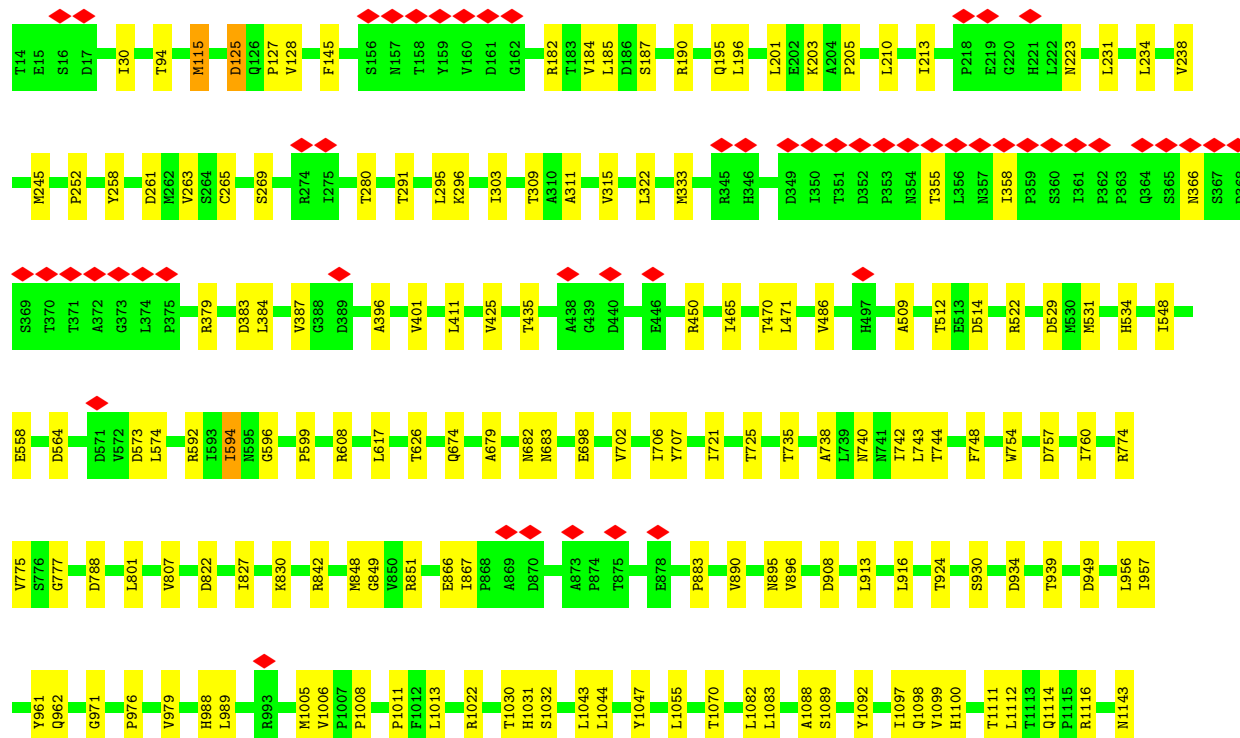
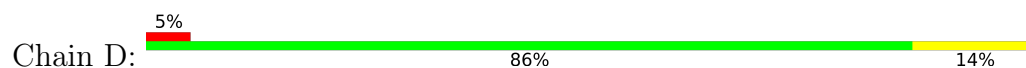


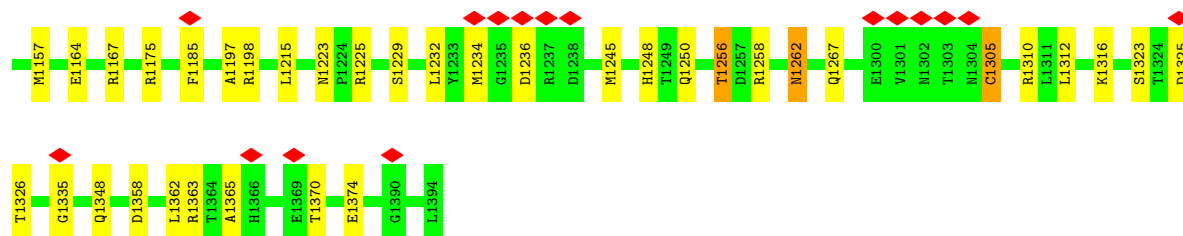
• Molecule 1: Major capsid protein



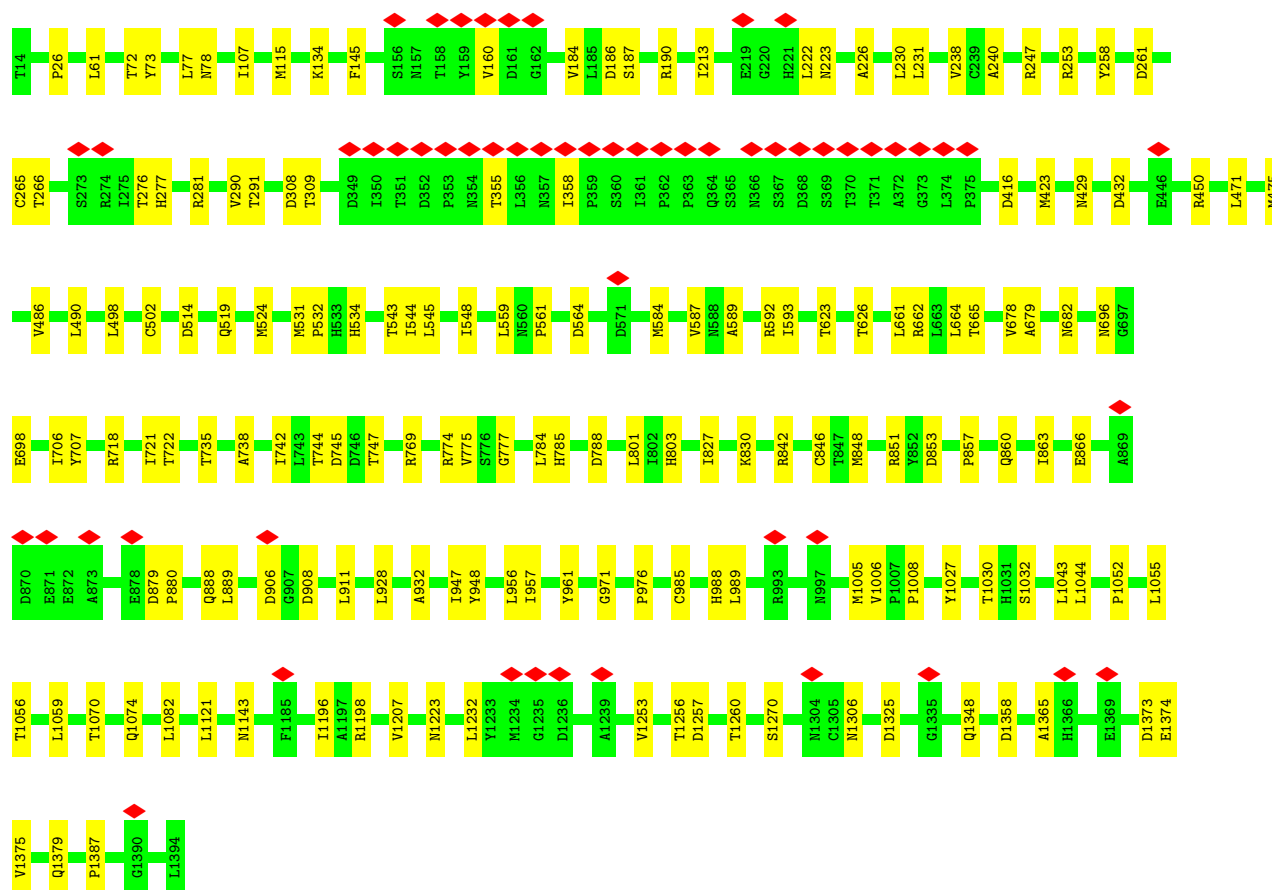
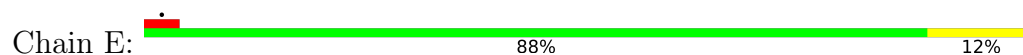


• Molecule 1: Major capsid protein

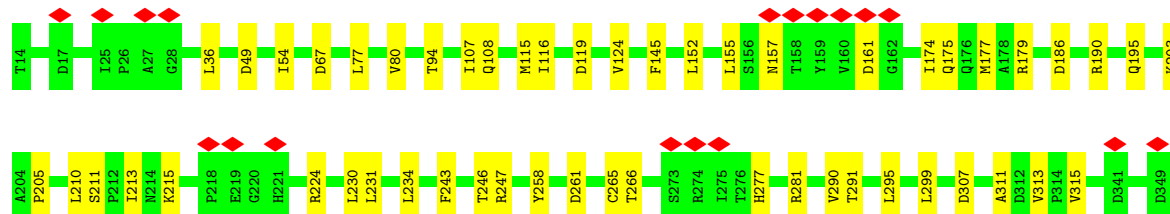
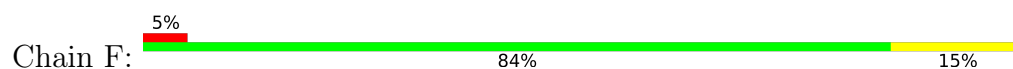


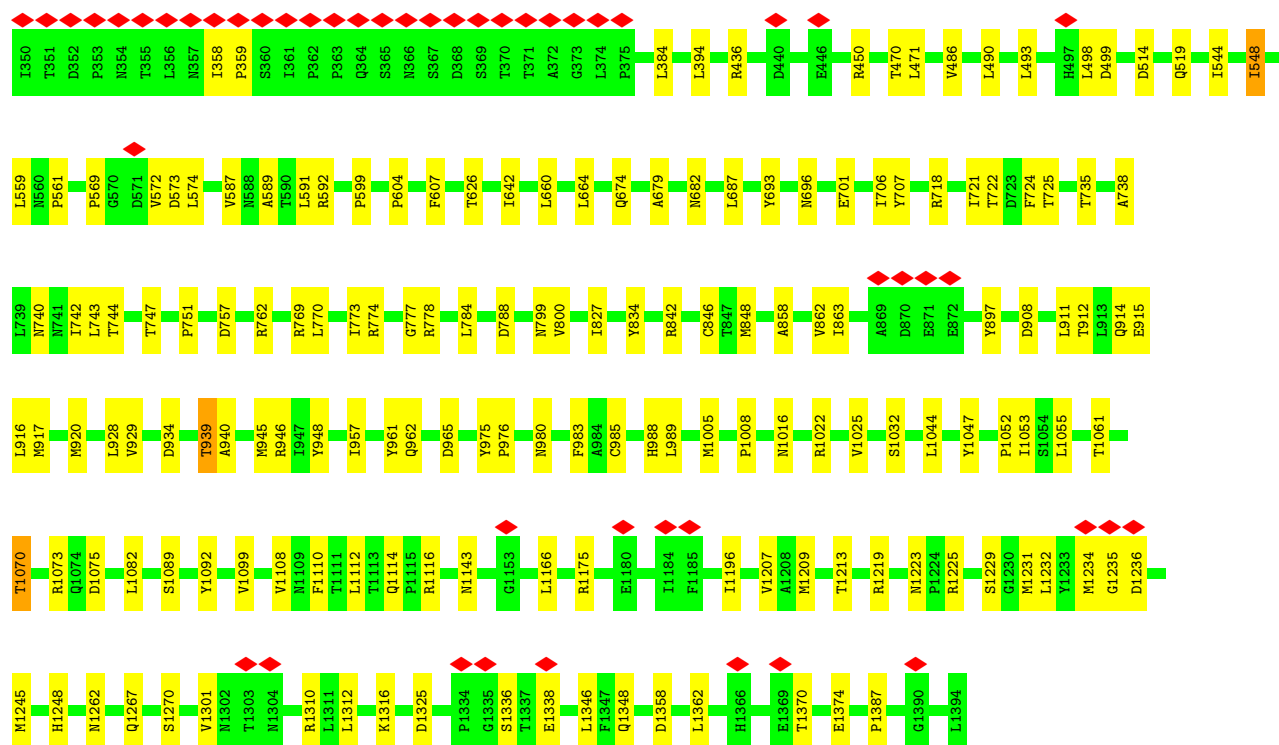


• Molecule 1: Major capsid protein

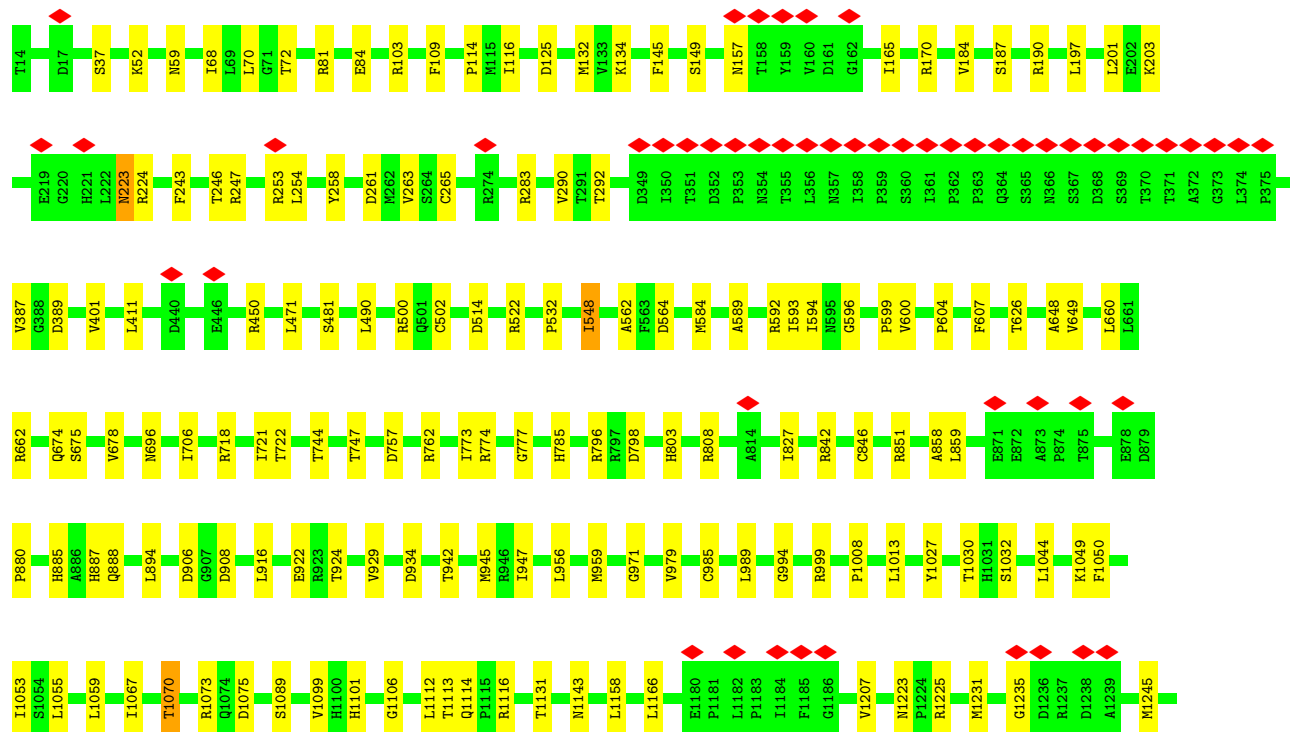
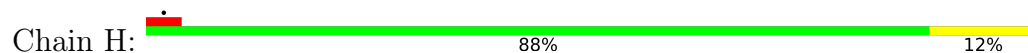


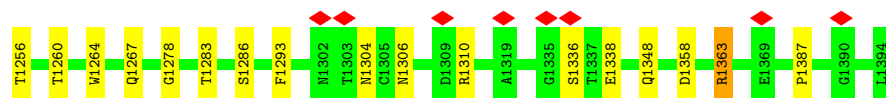
• Molecule 1: Major capsid protein



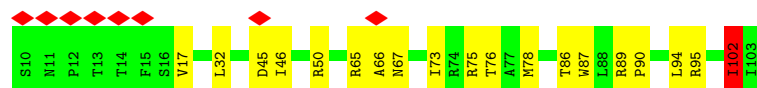
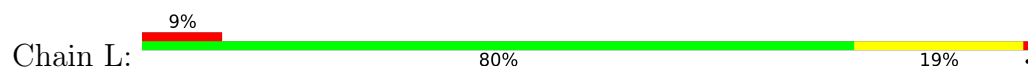


• Molecule 1: Major capsid protein

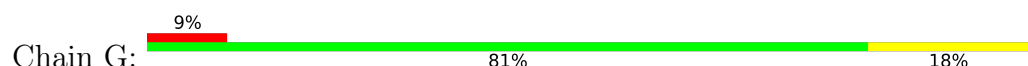




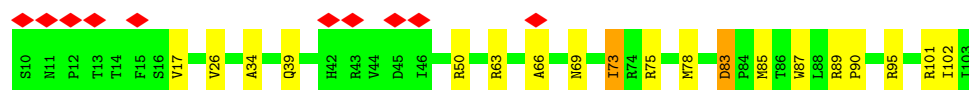
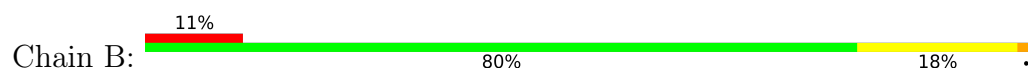
- Molecule 2: Small capsomere-interacting protein



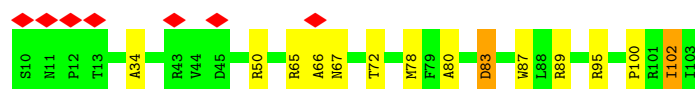
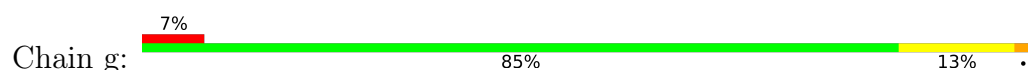
- Molecule 2: Small capsomere-interacting protein



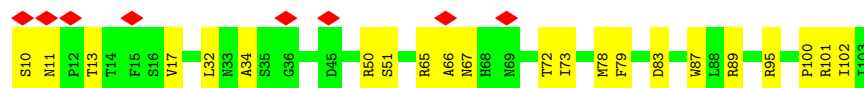
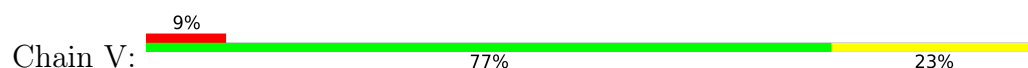
- Molecule 2: Small capsomere-interacting protein



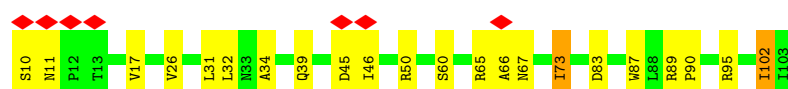
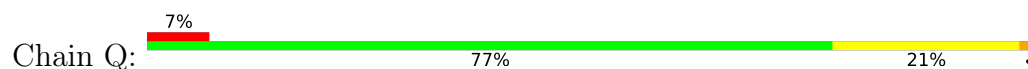
- Molecule 2: Small capsomere-interacting protein



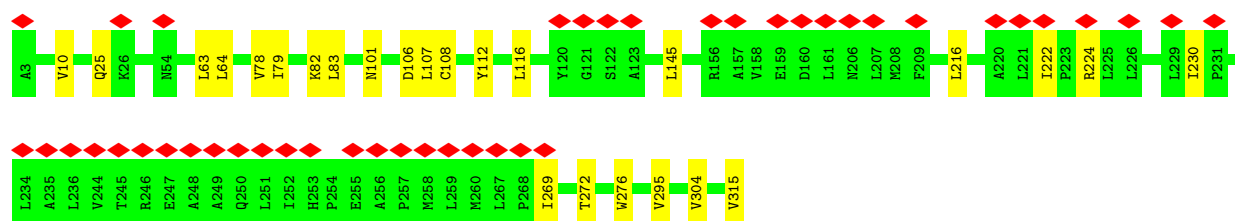
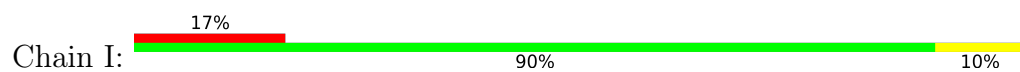
- Molecule 2: Small capsomere-interacting protein



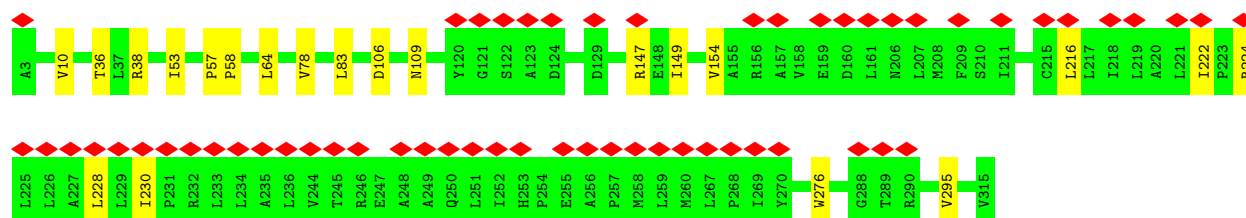
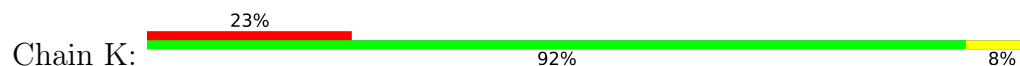
- Molecule 2: Small capsomere-interacting protein



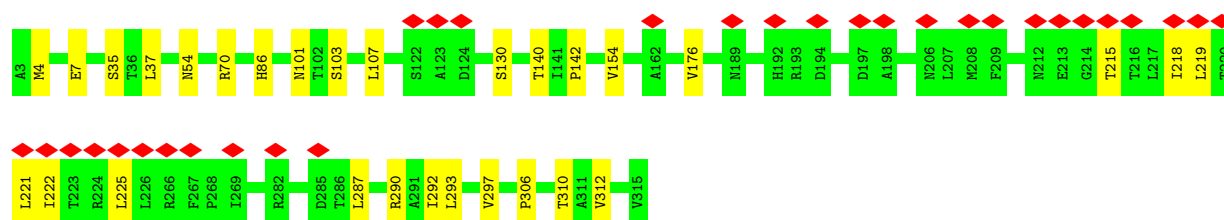
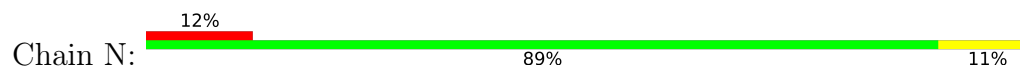
- Molecule 3: Tri2A



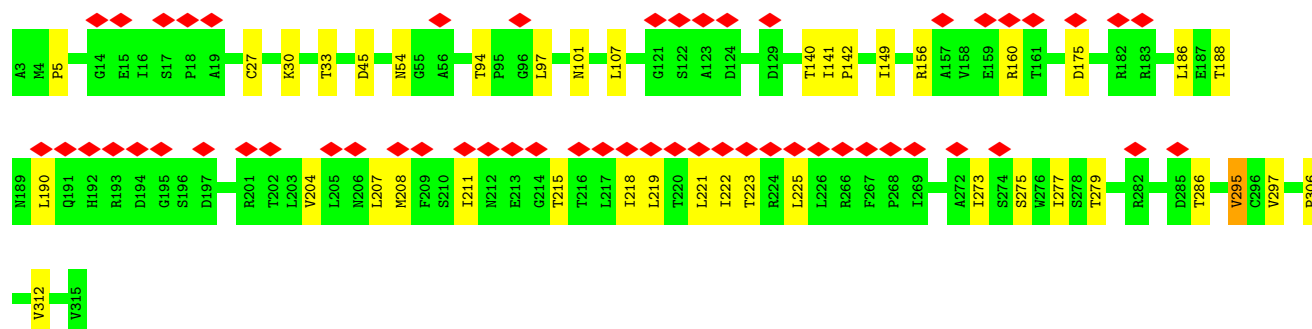
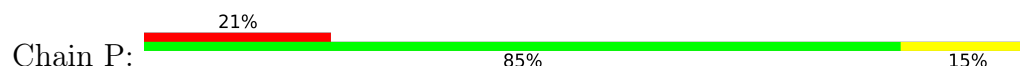
• Molecule 3: Tri2A



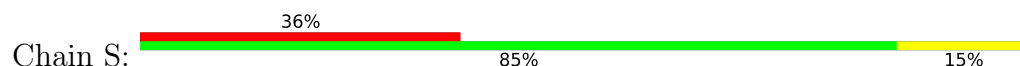
• Molecule 4: Tri2B

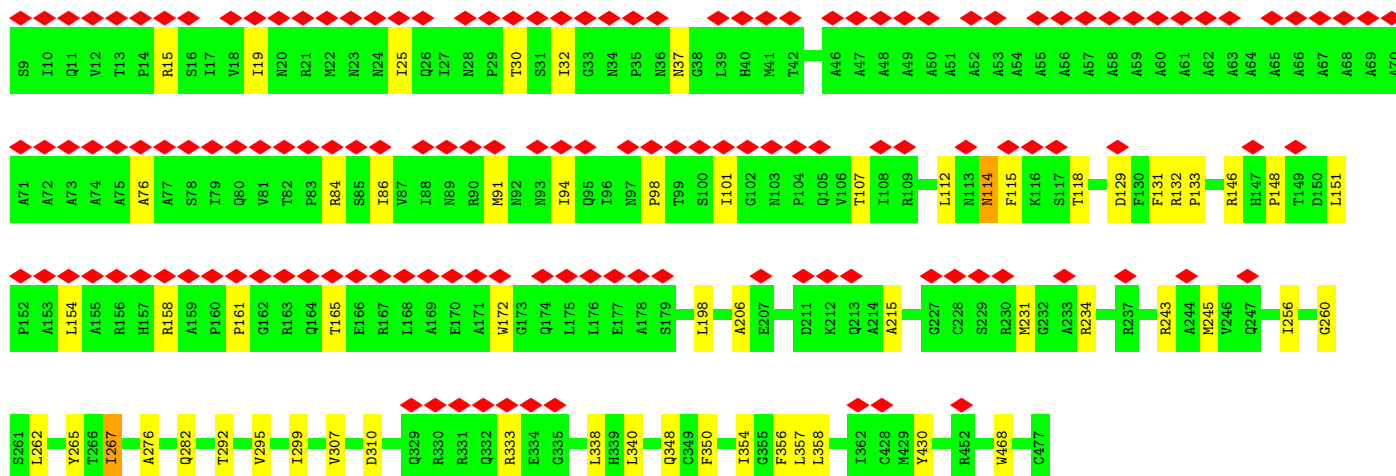


• Molecule 4: Tri2B

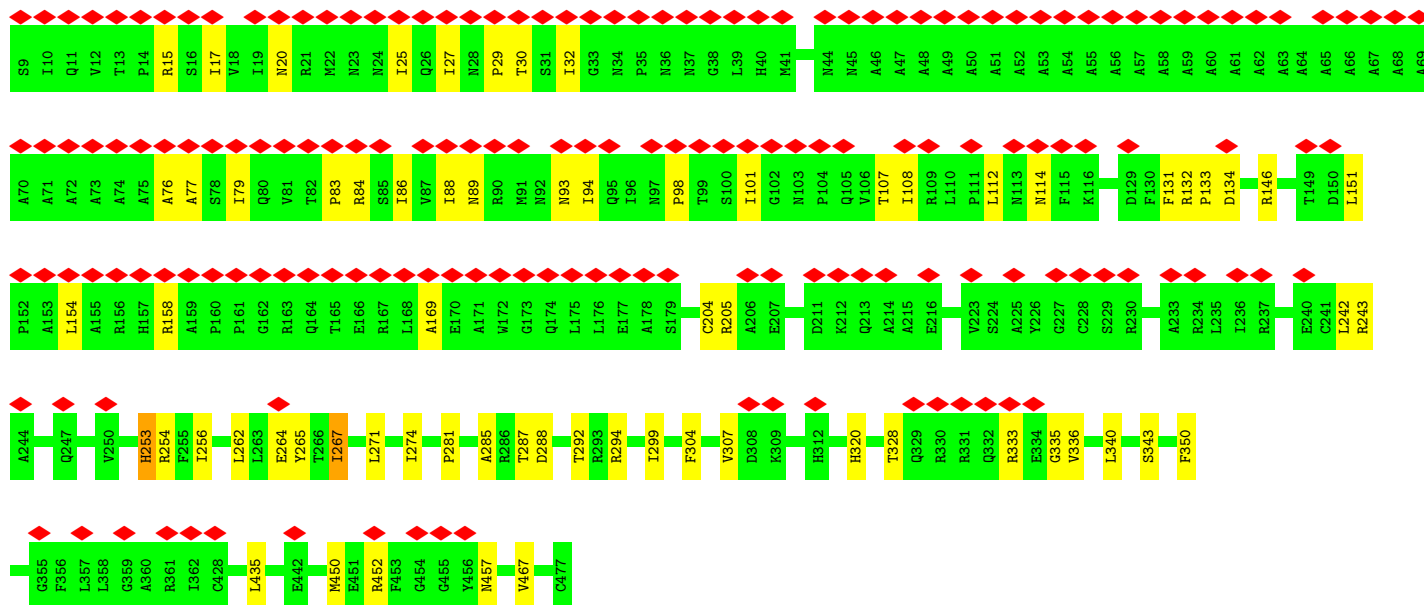
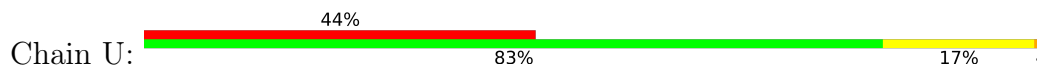


• Molecule 5: Tri1





• Molecule 5: Tri1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1442742	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.267	Depositor
Minimum map value	-0.201	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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	0.19	0/10933	0.47	0/14911
1	C	0.18	0/10933	0.47	4/14911 (0.0%)
1	D	0.19	0/10938	0.49	2/14917 (0.0%)
1	E	0.19	0/10933	0.47	1/14911 (0.0%)
1	F	0.19	0/10933	0.47	2/14911 (0.0%)
1	H	0.19	0/10933	0.49	3/14911 (0.0%)
2	B	0.31	0/714	0.84	3/978 (0.3%)
2	G	0.33	0/714	0.93	5/978 (0.5%)
2	L	0.35	0/714	0.86	3/978 (0.3%)
2	Q	0.32	0/714	0.85	3/978 (0.3%)
2	V	0.35	0/714	0.85	1/978 (0.1%)
2	g	0.32	0/714	0.77	0/978
3	I	0.17	0/1878	0.45	0/2568
3	K	0.19	0/1878	0.52	0/2568
4	N	0.18	0/2010	0.43	0/2743
4	P	0.17	0/2010	0.45	0/2743
5	S	0.24	0/3008	0.59	0/4097
5	U	0.25	0/3008	0.60	2/4097 (0.0%)
All	All	0.20	0/83679	0.51	29/114156 (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
1	A	0	1
1	F	0	1
2	B	0	1
2	G	0	1
2	Q	0	1
All	All	0	5

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	599	PRO	CA-C-N	9.23	126.05	120.24
1	C	599	PRO	C-N-CA	9.23	126.05	120.24
1	F	599	PRO	CA-C-N	8.98	125.90	120.24
1	F	599	PRO	C-N-CA	8.98	125.90	120.24
1	H	599	PRO	CA-C-N	8.95	125.88	120.24
1	H	599	PRO	C-N-CA	8.95	125.88	120.24
1	D	599	PRO	CA-C-N	8.91	125.86	120.24
1	D	599	PRO	C-N-CA	8.91	125.86	120.24
2	G	82	THR	CA-C-N	7.20	131.62	120.68
2	G	82	THR	C-N-CA	7.20	131.62	120.68
2	L	17	VAL	N-CA-C	-6.58	106.72	113.10
1	E	160	VAL	N-CA-C	-6.24	107.17	113.47
1	H	165	ILE	N-CA-C	-6.17	107.48	113.53
2	B	17	VAL	N-CA-C	-5.79	107.11	112.43
2	Q	17	VAL	N-CA-C	-5.70	107.73	113.20
1	C	412	ILE	CG1-CB-CG2	-5.67	93.69	110.70
2	V	17	VAL	N-CA-C	-5.66	107.22	112.43
5	U	253	HIS	CA-C-N	5.59	136.34	126.45
5	U	253	HIS	C-N-CA	5.59	136.34	126.45
2	B	101	ARG	CA-C-N	5.39	131.68	121.97
2	B	101	ARG	C-N-CA	5.39	131.68	121.97
2	G	101	ARG	CA-C-N	5.39	131.67	121.97
2	G	101	ARG	C-N-CA	5.39	131.67	121.97
2	L	45	ASP	CA-C-N	5.32	131.54	121.97
2	L	45	ASP	C-N-CA	5.32	131.54	121.97
2	Q	45	ASP	CA-C-N	5.27	131.46	121.97
2	Q	45	ASP	C-N-CA	5.27	131.46	121.97
2	G	17	VAL	N-CA-C	-5.15	108.26	113.20
1	C	397	LEU	CA-CB-CG	5.14	134.27	116.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	ILE	Peptide
2	B	39	GLN	Peptide
1	F	573	ASP	Peptide
2	G	39	GLN	Peptide
2	Q	39	GLN	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	A	10675	0	10419	97	0
1	C	10675	0	10419	102	0
1	D	10680	0	10428	111	0
1	E	10675	0	10419	95	0
1	F	10675	0	10419	117	0
1	H	10675	0	10419	96	0
2	B	699	0	696	12	0
2	G	699	0	696	8	0
2	L	699	0	696	11	0
2	Q	699	0	696	12	0
2	V	699	0	696	13	0
2	g	699	0	696	9	0
3	I	1847	0	1851	13	0
3	K	1847	0	1851	13	0
4	N	1975	0	2031	15	0
4	P	1975	0	2031	21	0
5	S	2951	0	2928	34	0
5	U	2951	0	2928	43	0
All	All	81795	0	80319	733	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 (733) 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)
1:F:261:ASP:O	1:F:265:CYS:HB2	1.79	0.82
1:E:261:ASP:O	1:E:265:CYS:HB2	1.88	0.74
1:A:261:ASP:O	1:A:265:CYS:HB2	1.89	0.73
1:C:261:ASP:O	1:C:265:CYS:HB2	1.88	0.73
1:D:261:ASP:O	1:D:265:CYS:HB2	1.89	0.72
1:C:594:ILE:HG22	1:C:596:GLY:H	1.54	0.71
4:P:215:THR:O	4:P:219:LEU:HB2	1.91	0.70
5:U:77:ALA:HB1	5:U:88:ILE:HB	1.74	0.69
1:H:594:ILE:HG22	1:H:596:GLY:H	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:261:ASP:O	1:H:265:CYS:HB2	1.95	0.67
1:D:145:PHE:HB2	1:D:184:VAL:HG21	1.78	0.66
1:H:885:HIS:HD2	1:H:887:HIS:H	1.46	0.64
1:D:725:THR:HG22	1:D:740:ASN:HD22	1.63	0.63
1:H:145:PHE:HB2	1:H:184:VAL:HG21	1.81	0.63
1:H:1231:MET:HG3	1:H:1310:ARG:HH21	1.63	0.63
1:D:115:MET:HE2	1:D:127:PRO:HD3	1.79	0.63
4:N:290:ARG:HD3	5:S:348:GLN:HB2	1.81	0.63
1:C:889:LEU:HD21	2:G:94:LEU:HD21	1.80	0.63
2:G:89:ARG:NH2	2:B:34:ALA:O	2.32	0.63
1:E:1005:MET:HG3	1:E:1006:VAL:HG23	1.83	0.61
1:E:880:PRO:O	1:E:888:GLN:NE2	2.34	0.61
4:N:215:THR:O	4:N:219:LEU:HB2	2.00	0.61
3:K:222:ILE:HG21	3:K:276:TRP:HB2	1.83	0.60
1:F:1231:MET:HG3	1:F:1301:VAL:HG21	1.82	0.60
1:A:1175:ARG:NH1	1:D:1256:THR:OG1	2.35	0.60
2:B:89:ARG:NH2	2:g:34:ALA:O	2.35	0.59
1:A:859:LEU:HD23	1:A:917:MET:HE1	1.83	0.59
3:K:149:ILE:HD13	5:U:158:ARG:HH22	1.67	0.59
1:D:231:LEU:HD21	1:D:1232:LEU:HB3	1.85	0.59
1:C:1175:ARG:NH2	1:C:1327:GLU:OE2	2.36	0.59
1:E:848:MET:HG2	1:E:976:PRO:HA	1.84	0.59
1:F:569:PRO:HG2	1:F:572:VAL:HG11	1.85	0.58
1:C:892:ASN:HD21	2:G:91:THR:HG23	1.66	0.58
4:N:107:LEU:HD23	4:N:142:PRO:HG3	1.86	0.58
3:K:10:VAL:HB	3:K:83:LEU:HB3	1.84	0.58
1:D:1223:ASN:ND2	1:D:1348:GLN:O	2.36	0.58
1:H:880:PRO:O	1:H:888:GLN:NE2	2.37	0.58
2:g:87:TRP:O	2:V:50:ARG:NH1	2.37	0.58
1:D:1092:TYR:HE1	1:D:1116:ARG:HH11	1.52	0.58
1:H:197:LEU:HD21	1:H:290:VAL:HG11	1.86	0.58
1:E:145:PHE:HB2	1:E:184:VAL:HG21	1.85	0.57
1:H:224:ARG:HE	1:H:1235:GLY:HA3	1.69	0.57
1:A:1114:GLN:OE1	1:A:1116:ARG:NH2	2.37	0.57
1:E:531:MET:HE1	1:E:1006:VAL:HG21	1.85	0.57
1:D:1114:GLN:OE1	1:D:1116:ARG:NH2	2.37	0.57
1:D:1197:ALA:HB2	1:E:1253:VAL:HG12	1.87	0.57
5:U:204:CYS:O	5:U:205:ARG:NH1	2.37	0.57
1:F:186:ASP:OD2	1:F:190:ARG:NH1	2.38	0.57
1:H:157:ASN:OD1	1:H:170:ARG:NH1	2.37	0.57
5:S:154:LEU:HD21	5:S:158:ARG:HB3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:674:GLN:NE2	1:H:696:ASN:O	2.38	0.56
1:D:744:THR:HA	1:D:827:ILE:HD12	1.88	0.56
1:F:842:ARG:NH1	1:F:1032:SER:O	2.38	0.56
1:D:1175:ARG:NH1	1:E:1256:THR:OG1	2.38	0.56
1:F:195:GLN:NE2	1:F:1092:TYR:OH	2.35	0.56
1:F:311:ALA:HB2	1:F:384:LEU:HD11	1.87	0.56
1:A:842:ARG:NH1	1:A:1032:SER:O	2.39	0.56
2:g:89:ARG:NH2	2:V:34:ALA:O	2.35	0.56
1:A:231:LEU:HD21	1:A:1232:LEU:HB3	1.86	0.56
1:D:1305:CYS:O	1:D:1310:ARG:NH2	2.39	0.56
1:F:696:ASN:O	1:H:674:GLN:NE2	2.39	0.56
1:C:626:THR:HG22	1:C:706:ILE:HG12	1.88	0.56
1:H:744:THR:HA	1:H:827:ILE:HD12	1.87	0.56
5:S:243:ARG:NH1	5:S:333:ARG:O	2.39	0.56
1:D:683:ASN:OD1	1:D:754:TRP:NE1	2.35	0.56
1:A:450:ARG:NH1	1:A:1358:ASP:OD2	2.39	0.56
1:D:842:ARG:NH1	1:D:1032:SER:O	2.39	0.55
1:E:842:ARG:NH1	1:E:1032:SER:O	2.39	0.55
1:C:729:GLU:OE2	1:C:1060:ARG:NH2	2.40	0.55
1:C:1223:ASN:ND2	1:C:1348:GLN:O	2.39	0.55
1:E:745:ASP:O	1:E:830:LYS:NZ	2.39	0.55
1:D:1097:ILE:HD11	1:D:1112:LEU:HB3	1.88	0.55
1:H:247:ARG:NH2	1:H:1387:PRO:O	2.39	0.55
4:P:107:LEU:HD23	4:P:142:PRO:HG3	1.89	0.55
5:S:133:PRO:HD2	5:S:267:ILE:HD12	1.89	0.55
1:C:842:ARG:NH1	1:C:1032:SER:O	2.40	0.55
1:F:744:THR:HA	1:F:827:ILE:HD12	1.88	0.55
1:F:1223:ASN:ND2	1:F:1348:GLN:O	2.39	0.55
5:U:27:ILE:HG22	5:U:29:PRO:HD3	1.87	0.55
1:E:1365:ALA:HB2	1:F:436:ARG:HH11	1.71	0.55
2:B:87:TRP:O	2:g:50:ARG:NH1	2.39	0.55
1:C:1097:ILE:HG22	1:C:1114:GLN:HB2	1.88	0.55
1:F:660:LEU:HB3	1:F:664:LEU:HD23	1.89	0.55
1:E:187:SER:HB2	1:F:115:MET:HG3	1.89	0.54
1:C:517:ASP:OD2	1:C:851:ARG:NH1	2.40	0.54
1:D:1363:ARG:NH1	1:E:1374:GLU:OE1	2.39	0.54
5:U:452:ARG:NH1	5:U:457:ASN:OD1	2.40	0.54
1:E:358:ILE:HD11	5:U:76:ALA:H	1.72	0.54
1:D:450:ARG:NH1	1:D:1358:ASP:OD2	2.41	0.54
1:E:682:ASN:ND2	1:E:957:ILE:O	2.29	0.54
1:C:1374:GLU:OE1	1:H:1363:ARG:NH1	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1236:ASP:OD1	1:D:1236:ASP:N	2.41	0.54
1:H:1073:ARG:NH1	1:H:1075:ASP:OD2	2.41	0.54
4:N:35:SER:HB2	4:N:70:ARG:HG2	1.88	0.54
1:C:217:GLN:HE21	1:C:220:GLY:HA2	1.72	0.54
1:D:531:MET:HE1	1:D:1006:VAL:HG21	1.90	0.54
1:E:416:ASP:OD1	1:E:1074:GLN:NE2	2.41	0.54
1:C:698:GLU:OE2	2:B:95:ARG:NH2	2.41	0.54
1:E:698:GLU:OE2	2:Q:95:ARG:NH2	2.41	0.54
1:F:1234:MET:SD	1:F:1235:GLY:N	2.81	0.54
1:H:1114:GLN:OE1	1:H:1116:ARG:NH2	2.40	0.54
5:U:281:PRO:HA	5:U:467:VAL:HA	1.90	0.54
2:V:89:ARG:NH2	2:Q:34:ALA:O	2.41	0.54
1:D:851:ARG:NH1	1:D:971:GLY:O	2.41	0.53
1:E:247:ARG:NH2	1:E:1387:PRO:O	2.40	0.53
1:F:247:ARG:NH2	1:F:1387:PRO:O	2.41	0.53
2:L:87:TRP:O	2:G:50:ARG:NH1	2.41	0.53
1:C:1326:THR:OG1	1:C:1327:GLU:N	2.40	0.53
1:F:231:LEU:HD11	1:F:1232:LEU:HD23	1.89	0.53
1:H:450:ARG:NH1	1:H:1358:ASP:OD2	2.41	0.53
1:F:693:TYR:O	2:L:95:ARG:NH1	2.42	0.53
1:H:203:LYS:NZ	1:H:1089:SER:OG	2.42	0.53
1:H:773:ILE:HG23	1:H:929:VAL:HG12	1.90	0.53
1:H:851:ARG:NH1	1:H:971:GLY:O	2.41	0.53
4:P:149:ILE:HD12	4:P:186:LEU:HD21	1.88	0.53
1:A:109:PHE:HE2	1:A:134:LYS:HD2	1.73	0.53
1:E:423:MET:HE2	1:E:471:LEU:HD23	1.90	0.53
1:H:514:ASP:OD2	1:H:522:ARG:NH1	2.41	0.53
1:A:718:ARG:NH1	1:A:722:THR:OG1	2.42	0.53
1:A:744:THR:HA	1:A:827:ILE:HD12	1.89	0.53
1:C:688:MET:HE2	1:C:711:LEU:HD11	1.91	0.53
1:D:682:ASN:ND2	1:D:957:ILE:O	2.35	0.53
1:D:934:ASP:OD1	1:D:934:ASP:N	2.42	0.53
1:F:718:ARG:NH1	1:F:722:THR:OG1	2.42	0.53
1:H:934:ASP:N	1:H:934:ASP:OD1	2.40	0.53
5:S:129:ASP:O	5:S:234:ARG:NH1	2.42	0.53
5:U:89:ASN:ND2	5:U:93:ASN:O	2.42	0.53
1:C:757:ASP:HA	1:C:760:ILE:HD12	1.90	0.53
1:E:744:THR:HA	1:E:827:ILE:HD12	1.89	0.53
1:E:908:ASP:OD1	1:E:908:ASP:N	2.41	0.53
1:E:1257:ASP:OD1	1:E:1257:ASP:N	2.41	0.53
1:D:311:ALA:HB2	1:D:384:LEU:HD11	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:564:ASP:OD2	1:D:1022:ARG:NH1	2.42	0.53
1:D:1005:MET:HG3	1:D:1006:VAL:HG23	1.91	0.53
1:F:682:ASN:ND2	1:F:957:ILE:O	2.30	0.53
2:V:72:THR:HB	2:V:100:PRO:HB2	1.89	0.53
1:D:1099:VAL:HG12	1:D:1112:LEU:HG	1.91	0.53
1:E:450:ARG:NH1	1:E:1358:ASP:OD2	2.42	0.53
1:E:774:ARG:NH2	1:E:777:GLY:O	2.42	0.53
1:F:773:ILE:HG23	1:F:929:VAL:HG12	1.90	0.53
1:F:908:ASP:OD1	1:F:908:ASP:N	2.41	0.53
1:H:626:THR:HG22	1:H:706:ILE:HG12	1.92	0.53
1:C:416:ASP:OD2	1:C:1074:GLN:NE2	2.42	0.52
1:C:762:ARG:NH2	1:C:930:SER:O	2.42	0.52
1:A:279:ASN:HD21	1:A:283:ARG:HB3	1.74	0.52
1:C:782:GLN:HB2	1:C:800:VAL:HA	1.90	0.52
1:H:942:THR:HA	1:H:945:MET:HG3	1.91	0.52
1:D:514:ASP:OD2	1:D:522:ARG:NH1	2.43	0.52
1:D:679:ALA:O	1:D:707:TYR:OH	2.26	0.52
1:D:883:PRO:O	1:D:895:ASN:ND2	2.41	0.52
1:F:660:LEU:HD11	1:F:916:LEU:HB2	1.91	0.52
1:E:1223:ASN:ND2	1:E:1348:GLN:O	2.40	0.52
1:A:626:THR:HG22	1:A:706:ILE:HG12	1.91	0.52
1:E:696:ASN:O	1:F:674:GLN:NE2	2.43	0.52
1:F:1219:ARG:NH1	1:F:1374:GLU:OE1	2.42	0.52
2:V:87:TRP:O	2:Q:50:ARG:NH1	2.43	0.52
1:E:851:ARG:NH2	1:E:971:GLY:O	2.43	0.52
1:F:725:THR:HG22	1:F:740:ASN:HD22	1.75	0.52
1:F:1114:GLN:OE1	1:F:1116:ARG:NH2	2.43	0.52
2:Q:26:VAL:HG23	2:Q:60:SER:HB3	1.92	0.52
1:D:788:ASP:OD1	1:D:788:ASP:N	2.39	0.52
1:F:213:ILE:HD13	1:F:230:LEU:HD21	1.92	0.52
3:I:10:VAL:HB	3:I:83:LEU:HB3	1.90	0.52
1:A:989:LEU:HD11	1:A:1008:PRO:HG3	1.92	0.52
1:C:190:ARG:HG2	1:C:401:VAL:HG23	1.90	0.52
1:D:203:LYS:NZ	1:D:1089:SER:OG	2.43	0.52
1:F:1073:ARG:NH1	1:F:1075:ASP:OD2	2.43	0.52
1:A:358:ILE:HD11	5:S:76:ALA:H	1.74	0.52
1:A:1312:LEU:O	1:A:1316:LYS:NZ	2.43	0.52
1:C:653:ASN:HB3	1:C:656:ASN:HB2	1.92	0.52
1:F:679:ALA:O	1:F:707:TYR:OH	2.24	0.52
5:S:299:ILE:HD13	5:S:340:LEU:HD22	1.92	0.52
1:F:498:LEU:HD11	1:F:587:VAL:HG23	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ASP:OD2	1:A:851:ARG:NH1	2.43	0.51
1:F:747:THR:HA	1:F:762:ARG:HG3	1.92	0.51
1:F:915:GLU:OE2	2:L:75:ARG:NH1	2.44	0.51
1:H:502:CYS:HB2	1:H:532:PRO:HD2	1.90	0.51
3:K:147:ARG:HG3	4:P:277:ILE:HD11	1.93	0.51
1:A:247:ARG:NH1	1:A:1387:PRO:O	2.44	0.51
1:C:785:HIS:HB3	1:C:803:HIS:HB3	1.93	0.51
1:C:788:ASP:OD1	1:C:788:ASP:N	2.44	0.51
5:U:299:ILE:HD11	5:U:304:PHE:HD1	1.75	0.51
1:A:994:GLY:O	1:A:999:ARG:NH1	2.44	0.51
1:E:788:ASP:N	1:E:788:ASP:OD1	2.43	0.51
5:S:282:GLN:OE1	5:S:468:TRP:NE1	2.42	0.51
2:G:87:TRP:O	2:B:50:ARG:NH1	2.44	0.51
1:E:1358:ASP:HB2	1:E:1379:GLN:HG2	1.92	0.51
1:F:295:LEU:HD23	1:F:1082:LEU:HD12	1.93	0.51
4:N:7:GLU:OE2	4:N:86:HIS:NE2	2.41	0.51
1:A:283:ARG:NH2	1:A:389:ASP:O	2.43	0.51
1:C:596:GLY:O	1:C:608:ARG:NH2	2.44	0.51
1:C:908:ASP:HA	1:C:911:LEU:HB2	1.93	0.51
1:F:770:LEU:HB2	1:F:946:ARG:HH12	1.75	0.51
1:A:848:MET:HB3	1:A:976:PRO:HA	1.93	0.51
1:A:619:ARG:NH2	1:A:723:ASP:OD2	2.43	0.51
1:C:115:MET:HB3	1:H:187:SER:HB2	1.93	0.51
1:E:866:GLU:OE1	2:Q:67:ASN:ND2	2.42	0.51
1:F:989:LEU:HD11	1:F:1008:PRO:HG3	1.91	0.51
4:N:54:ASN:N	4:N:54:ASN:OD1	2.44	0.51
1:A:674:GLN:NE2	1:C:696:ASN:O	2.44	0.50
1:C:1229:SER:HB2	1:C:1245:MET:HG3	1.92	0.50
1:F:701:GLU:HG3	1:H:675:SER:HA	1.94	0.50
1:C:678:VAL:HG21	1:C:706:ILE:HG21	1.92	0.50
1:D:269:SER:HB2	1:D:1088:ALA:HB3	1.93	0.50
4:P:156:ARG:NH1	4:P:175:ASP:OD2	2.44	0.50
1:C:145:PHE:HB2	1:C:184:VAL:HG21	1.92	0.50
1:C:994:GLY:O	1:C:999:ARG:NH1	2.45	0.50
1:C:1143:ASN:OD1	1:C:1143:ASN:N	2.45	0.50
1:D:245:MET:HE3	1:D:295:LEU:HD22	1.94	0.50
1:E:276:THR:OG1	1:E:277:HIS:N	2.45	0.50
1:E:718:ARG:NH1	1:E:722:THR:OG1	2.44	0.50
2:L:50:ARG:NH1	2:Q:87:TRP:O	2.45	0.50
1:D:355:THR:HA	1:D:358:ILE:HG12	1.92	0.50
1:D:1262:ASN:C	1:D:1262:ASN:HD22	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:20:ASN:H	5:U:25:ILE:HG22	1.76	0.50
1:C:693:TYR:O	2:B:95:ARG:NH1	2.44	0.50
1:E:785:HIS:HB3	1:E:803:HIS:HB3	1.92	0.50
1:E:853:ASP:OD1	1:E:853:ASP:N	2.44	0.50
3:K:109:ASN:O	5:U:146:ARG:NH2	2.43	0.50
1:A:307:ASP:HB2	1:A:386:ILE:HG13	1.92	0.50
1:E:857:PRO:HA	1:E:860:GLN:HG2	1.93	0.50
1:F:735:THR:HG23	1:F:738:ALA:H	1.76	0.50
1:F:980:ASN:HB3	1:F:983:PHE:H	1.76	0.50
1:D:185:LEU:HD22	5:U:107:THR:HG21	1.94	0.50
1:E:186:ASP:OD1	1:E:190:ARG:NH1	2.44	0.50
1:E:1143:ASN:OD1	1:E:1143:ASN:N	2.45	0.50
1:C:774:ARG:NH2	1:C:777:GLY:O	2.45	0.50
1:D:757:ASP:HA	1:D:760:ILE:HD12	1.94	0.50
1:D:848:MET:HG2	1:D:976:PRO:HA	1.94	0.50
4:P:207:LEU:HD22	4:P:211:ILE:HD11	1.93	0.50
1:A:280:THR:HG23	1:A:379:ARG:HH21	1.76	0.49
1:A:264:SER:O	1:A:264:SER:OG	2.27	0.49
1:A:721:ILE:HG13	1:A:1044:LEU:HD11	1.93	0.49
1:F:788:ASP:OD1	1:F:788:ASP:N	2.42	0.49
1:A:243:PHE:HB3	1:A:246:THR:HG22	1.93	0.49
1:E:661:LEU:O	1:E:665:THR:OG1	2.27	0.49
1:F:243:PHE:HB3	1:F:246:THR:HG22	1.94	0.49
4:P:101:ASN:HB3	4:P:306:PRO:HA	1.93	0.49
1:A:725:THR:HG22	1:A:740:ASN:HD22	1.76	0.49
1:D:908:ASP:N	1:D:908:ASP:OD1	2.44	0.49
1:F:962:GLN:HG2	1:F:965:ASP:HB2	1.94	0.49
5:S:231:MET:SD	5:S:231:MET:N	2.85	0.49
1:H:796:ARG:NE	1:H:922:GLU:OE1	2.38	0.49
1:H:908:ASP:OD1	1:H:908:ASP:N	2.45	0.49
1:A:908:ASP:OD1	1:A:908:ASP:N	2.38	0.49
1:C:1114:GLN:OE1	1:C:1116:ARG:NH2	2.45	0.49
2:B:69:ASN:OD1	2:B:75:ARG:NH1	2.43	0.49
1:A:427:GLN:HE21	1:A:1215:LEU:HD23	1.78	0.49
1:A:908:ASP:HA	1:A:911:LEU:HB2	1.95	0.49
1:C:744:THR:HA	1:C:827:ILE:HD12	1.94	0.49
1:D:949:ASP:OD1	1:D:949:ASP:N	2.45	0.49
1:E:662:ARG:NH2	1:E:906:ASP:OD2	2.43	0.49
5:S:15:ARG:NE	5:S:30:THR:O	2.46	0.49
1:A:698:GLU:OE2	2:g:95:ARG:NH2	2.45	0.49
1:A:1147:ASN:OD1	1:A:1177:ASN:ND2	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:648:ALA:HB2	1:C:956:LEU:HD11	1.94	0.49
1:D:263:VAL:HG21	1:D:387:VAL:HG21	1.94	0.49
1:H:600:VAL:HG21	1:H:1027:TYR:HD2	1.78	0.49
4:N:218:ILE:HA	4:N:221:LEU:HB2	1.94	0.49
4:P:27:CYS:SG	4:P:30:LYS:NZ	2.86	0.49
1:A:1143:ASN:OD1	1:A:1143:ASN:N	2.42	0.49
2:V:10:SER:N	2:V:13:THR:HG1	2.10	0.49
1:C:182:ARG:HD2	5:S:84:ARG:HH21	1.78	0.49
1:D:182:ARG:HE	5:U:83:PRO:HB3	1.78	0.49
1:D:596:GLY:O	1:D:608:ARG:NH2	2.45	0.49
1:F:774:ARG:NH2	1:F:777:GLY:O	2.46	0.49
4:P:160:ARG:NH1	4:P:190:LEU:O	2.46	0.49
1:A:775:VAL:HG11	1:A:801:LEU:HD21	1.94	0.48
1:A:1363:ARG:NH1	1:D:1374:GLU:OE1	2.44	0.48
1:C:514:ASP:OD2	1:C:522:ARG:NH1	2.46	0.48
1:D:509:ALA:N	1:D:1011:PRO:O	2.45	0.48
1:D:1143:ASN:OD1	1:D:1143:ASN:N	2.47	0.48
1:F:559:LEU:HB3	1:F:1270:SER:HA	1.95	0.48
5:U:132:ARG:NH2	5:U:134:ASP:OD2	2.46	0.48
1:A:291:THR:HG22	1:A:1082:LEU:HG	1.94	0.48
1:D:1164:GLU:OE2	1:D:1167:ARG:NH2	2.45	0.48
1:E:564:ASP:OD1	1:E:592:ARG:NE	2.46	0.48
1:E:678:VAL:HG21	1:E:706:ILE:HG21	1.94	0.48
3:I:25:GLN:NE2	3:I:78:VAL:O	2.44	0.48
5:S:146:ARG:HH22	5:S:151:LEU:HD11	1.78	0.48
1:F:145:PHE:HB3	1:F:1110:PHE:HB2	1.95	0.48
1:F:157:ASN:ND2	1:F:161:ASP:OD2	2.46	0.48
1:F:928:LEU:HD11	1:F:948:TYR:HB3	1.94	0.48
1:H:660:LEU:HD11	1:H:916:LEU:HB2	1.95	0.48
1:H:1306:ASN:OD1	1:H:1306:ASN:N	2.45	0.48
1:E:769:ARG:HB3	1:E:932:ALA:HB3	1.96	0.48
1:E:928:LEU:HD11	1:E:948:TYR:HB3	1.96	0.48
1:F:1143:ASN:OD1	1:F:1143:ASN:N	2.45	0.48
1:F:1175:ARG:HD3	1:H:1256:THR:HG22	1.96	0.48
3:K:106:ASP:HB2	5:U:151:LEU:HD22	1.96	0.48
1:D:534:HIS:ND1	1:D:1005:MET:SD	2.86	0.48
1:D:465:ILE:HG13	1:D:1198:ARG:HH12	1.79	0.48
1:D:1312:LEU:O	1:D:1316:LYS:NZ	2.47	0.48
1:F:281:ARG:NH2	1:F:307:ASP:OD1	2.46	0.48
1:D:1335:GLY:HA3	5:U:271:LEU:HD23	1.96	0.48
1:H:785:HIS:HB3	1:H:803:HIS:HB3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:218:ILE:HA	4:P:221:LEU:HB2	1.94	0.48
1:A:658:CYS:HA	1:A:661:LEU:HG	1.96	0.48
1:C:224:ARG:HE	1:C:1235:GLY:HA3	1.79	0.48
1:H:757:ASP:OD1	1:H:757:ASP:N	2.41	0.48
1:C:559:LEU:HB3	1:C:1270:SER:HA	1.96	0.48
1:D:213:ILE:HG13	1:D:234:LEU:HD11	1.94	0.48
1:H:718:ARG:NH1	1:H:722:THR:OG1	2.46	0.48
2:L:86:THR:O	2:L:86:THR:OG1	2.28	0.48
5:S:282:GLN:HE21	5:S:295:VAL:HG13	1.79	0.48
4:P:5:PRO:HB3	4:P:94:THR:HG22	1.96	0.48
2:V:83:ASP:OD2	2:V:89:ARG:NH1	2.41	0.48
1:A:355:THR:HA	5:S:76:ALA:HB2	1.96	0.47
1:A:1150:PHE:HD2	1:A:1288:ILE:HD13	1.80	0.47
1:F:277:HIS:HD2	1:F:313:VAL:HG22	1.78	0.47
3:I:79:ILE:HD11	3:I:82:LYS:HE2	1.96	0.47
1:A:934:ASP:OD1	1:A:934:ASP:N	2.41	0.47
1:C:486:VAL:HG11	1:C:945:MET:HE1	1.96	0.47
1:C:721:ILE:HG13	1:C:1044:LEU:HD11	1.95	0.47
1:E:559:LEU:HB3	1:E:1270:SER:HA	1.97	0.47
1:F:152:LEU:HD11	1:F:1108:VAL:HG22	1.96	0.47
1:H:842:ARG:NH1	1:H:1032:SER:O	2.47	0.47
1:A:531:MET:HE1	1:A:1006:VAL:HG21	1.95	0.47
1:C:1185:PHE:HZ	5:S:172:TRP:HD1	1.62	0.47
1:E:775:VAL:HG11	1:E:801:LEU:HD21	1.95	0.47
1:F:561:PRO:O	1:F:592:ARG:NH1	2.47	0.47
1:F:1092:TYR:HE2	1:F:1116:ARG:HH11	1.61	0.47
1:C:989:LEU:HD11	1:C:1008:PRO:HG3	1.96	0.47
1:E:534:HIS:ND1	1:E:1005:MET:SD	2.83	0.47
1:F:175:GLN:OE1	1:F:179:ARG:NH2	2.48	0.47
1:C:679:ALA:O	1:C:707:TYR:OH	2.29	0.47
1:C:1070:THR:HG23	1:C:1207:VAL:HB	1.96	0.47
1:E:584:MET:HE3	1:E:584:MET:HB3	1.80	0.47
1:F:778:ARG:HB2	1:F:799:ASN:HD22	1.79	0.47
1:F:1312:LEU:O	1:F:1316:LYS:NZ	2.48	0.47
1:A:490:LEU:HD21	1:A:589:ALA:HB2	1.97	0.47
1:A:1373:ASP:HA	1:C:1365:ALA:HB1	1.96	0.47
1:E:543:THR:OG1	1:E:544:ILE:N	2.47	0.47
1:A:1306:ASN:OD1	1:A:1306:ASN:N	2.43	0.47
1:F:591:LEU:O	1:F:1022:ARG:NH2	2.47	0.47
1:H:934:ASP:OD2	1:H:1049:LYS:NZ	2.46	0.47
1:H:994:GLY:O	1:H:999:ARG:NH1	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:222:ILE:HA	4:N:225:LEU:HB2	1.97	0.47
5:S:198:LEU:HD11	5:S:338:LEU:HD22	1.97	0.47
4:P:222:ILE:HA	4:P:225:LEU:HB2	1.95	0.47
1:D:748:PHE:O	1:D:830:LYS:NZ	2.42	0.47
1:E:514:ASP:HB2	1:E:519:GLN:HG3	1.96	0.47
5:U:17:ILE:HG22	5:U:27:ILE:HG23	1.96	0.47
1:E:190:ARG:HB3	1:F:116:ILE:HG22	1.96	0.47
5:U:328:THR:OG1	5:U:335:GLY:O	2.33	0.47
1:A:770:LEU:HB2	1:A:946:ARG:HH12	1.79	0.47
1:A:876:THR:OG1	1:A:878:GLU:OE2	2.33	0.47
1:H:649:VAL:HG23	1:H:916:LEU:HD21	1.97	0.47
5:U:205:ARG:HH21	5:U:243:ARG:HD3	1.80	0.47
1:C:291:THR:HG22	1:C:1082:LEU:HG	1.97	0.46
1:D:698:GLU:OE2	2:V:95:ARG:NH2	2.40	0.46
1:E:721:ILE:HG13	1:E:1044:LEU:HD11	1.96	0.46
1:H:721:ILE:HG13	1:H:1044:LEU:HD11	1.97	0.46
1:A:145:PHE:HB2	1:A:184:VAL:HG21	1.96	0.46
1:H:243:PHE:HB3	1:H:246:THR:HG22	1.96	0.46
1:H:283:ARG:NH2	1:H:389:ASP:O	2.49	0.46
3:I:222:ILE:HG21	3:I:276:TRP:HB2	1.96	0.46
1:A:773:ILE:HG23	1:A:929:VAL:HG12	1.96	0.46
1:E:1070:THR:HG23	1:E:1207:VAL:HB	1.97	0.46
1:F:721:ILE:HG13	1:F:1044:LEU:HD11	1.97	0.46
1:H:648:ALA:HB2	1:H:956:LEU:HD11	1.97	0.46
1:C:761:TYR:O	1:C:765:ALA:CB	2.63	0.46
1:D:1248:HIS:CD2	1:D:1267:GLN:HG3	2.51	0.46
1:A:59:ASN:O	5:U:292:THR:OG1	2.33	0.46
1:A:94:THR:OG1	1:A:318:GLY:O	2.30	0.46
1:D:201:LEU:HD23	1:D:1083:LEU:HD13	1.97	0.46
1:F:203:LYS:NZ	1:F:1089:SER:OG	2.44	0.46
1:F:770:LEU:O	1:F:946:ARG:NH2	2.49	0.46
1:F:1362:LEU:O	1:F:1370:THR:OG1	2.34	0.46
1:H:1283:THR:OG1	1:H:1286:SER:OG	2.30	0.46
1:E:471:LEU:HB3	1:E:1059:LEU:HD22	1.97	0.46
1:F:299:LEU:HD23	1:F:394:LEU:HD11	1.97	0.46
1:F:920:MET:HE3	1:F:920:MET:HB3	1.83	0.46
2:V:65:ARG:O	2:V:67:ASN:N	2.48	0.46
1:A:696:ASN:O	1:D:674:GLN:NE2	2.49	0.46
1:C:308:ASP:OD1	1:C:309:THR:N	2.49	0.46
1:C:421:MET:HE2	1:C:421:MET:HB2	1.80	0.46
1:D:735:THR:HG23	1:D:738:ALA:H	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:PHE:HB2	1:H:132:MET:HB2	1.98	0.46
1:D:775:VAL:HG11	1:D:801:LEU:HD21	1.98	0.46
1:D:866:GLU:OE1	2:V:67:ASN:ND2	2.43	0.46
2:L:65:ARG:O	2:L:67:ASN:N	2.49	0.46
4:P:219:LEU:HA	4:P:222:ILE:HG12	1.98	0.46
1:A:332:VAL:HG13	1:A:333:MET:HG3	1.97	0.46
1:A:1325:ASP:OD1	1:A:1325:ASP:N	2.48	0.46
1:C:1304:ASN:N	1:C:1304:ASN:OD1	2.47	0.46
1:F:1070:THR:HG23	1:F:1207:VAL:HB	1.96	0.46
1:F:1301:VAL:HG23	1:F:1310:ARG:HE	1.79	0.46
2:B:83:ASP:OD1	2:B:89:ARG:NH2	2.49	0.46
1:D:1325:ASP:OD1	1:D:1325:ASP:N	2.49	0.45
1:E:73:TYR:HE2	1:F:107:ILE:HD11	1.81	0.45
1:F:450:ARG:NH1	1:F:1358:ASP:OD2	2.49	0.45
3:I:108:CYS:SG	5:S:146:ARG:NH1	2.90	0.45
1:A:277:HIS:HD2	1:A:313:VAL:HG22	1.81	0.45
1:A:1053:ILE:HD13	1:A:1166:LEU:HD13	1.98	0.45
1:D:190:ARG:HG2	1:D:401:VAL:HG23	1.98	0.45
1:E:679:ALA:O	1:E:707:TYR:OH	2.28	0.45
5:U:133:PRO:HD2	5:U:267:ILE:HD12	1.97	0.45
5:U:205:ARG:HD3	5:U:205:ARG:HA	1.74	0.45
5:U:299:ILE:HD13	5:U:340:LEU:HD22	1.97	0.45
1:D:913:LEU:HD13	1:D:916:LEU:HD23	1.98	0.45
1:H:959:MET:SD	1:H:959:MET:N	2.89	0.45
3:I:112:TYR:HE2	3:I:315:VAL:HG21	1.80	0.45
1:C:205:PRO:HG2	1:C:210:LEU:HD22	1.98	0.45
1:E:908:ASP:HA	1:E:911:LEU:HB2	1.97	0.45
5:S:206:ALA:HB1	5:S:215:ALA:HB1	1.99	0.45
5:S:307:VAL:HG21	5:S:350:PHE:HE1	1.82	0.45
1:A:383:ASP:OD1	1:A:383:ASP:N	2.39	0.45
1:A:596:GLY:O	1:A:608:ARG:NH2	2.50	0.45
1:D:470:THR:OG1	1:D:471:LEU:N	2.49	0.45
1:D:1185:PHE:HB2	5:U:169:ALA:HB1	1.99	0.45
1:F:724:PHE:HA	1:F:1061:THR:HG21	1.98	0.45
5:S:94:ILE:HG12	5:S:112:LEU:HB2	1.98	0.45
1:A:806:PRO:HD2	1:A:811:THR:HG22	1.99	0.45
1:F:358:ILE:HG13	1:F:359:PRO:HD3	1.98	0.45
1:F:1196:ILE:HD11	1:H:224:ARG:HB3	1.98	0.45
1:F:1325:ASP:OD1	1:F:1325:ASP:N	2.50	0.45
1:F:1336:SER:OG	1:F:1338:GLU:OE1	2.33	0.45
1:H:1053:ILE:HD13	1:H:1166:LEU:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:ALA:HB2	2:B:90:PRO:HD2	1.99	0.45
1:A:980:ASN:HB3	1:A:983:PHE:H	1.81	0.45
1:C:471:LEU:HB3	1:C:1059:LEU:HD22	1.99	0.45
1:C:698:GLU:N	1:C:698:GLU:OE1	2.49	0.45
4:N:101:ASN:OD1	4:N:103:SER:OG	2.29	0.45
5:S:310:ASP:HB3	5:S:357:LEU:HD11	1.99	0.45
1:A:1374:GLU:OE1	1:C:1363:ARG:NH1	2.46	0.45
1:C:277:HIS:HD2	1:C:313:VAL:HG22	1.82	0.45
1:D:252:PRO:HB3	1:D:303:ILE:HG12	1.99	0.45
1:D:594:ILE:HG13	1:D:742:ILE:HD12	1.99	0.45
1:E:240:ALA:O	1:E:247:ARG:NH1	2.50	0.45
1:F:205:PRO:HG2	1:F:210:LEU:HD22	1.99	0.45
1:H:662:ARG:HH12	1:H:906:ASP:HB3	1.82	0.45
1:H:846:CYS:HB2	1:H:985:CYS:HB3	1.38	0.45
5:S:114:ASN:HA	5:S:115:PHE:HA	1.60	0.45
1:A:336:ALA:HB3	1:C:68:ILE:HG22	1.98	0.45
1:A:760:ILE:HD11	1:A:817:ILE:HD12	1.99	0.45
1:D:425:VAL:HG11	1:D:1215:LEU:HD13	1.99	0.45
1:H:1099:VAL:HG22	1:H:1112:LEU:HG	1.98	0.45
4:N:293:LEU:HD13	4:N:312:VAL:HG11	1.99	0.45
1:F:834:TYR:HE1	1:F:980:ASN:HD21	1.65	0.44
1:H:564:ASP:OD1	1:H:592:ARG:NE	2.48	0.44
5:S:161:PRO:HB2	5:S:165:THR:HG21	1.97	0.44
2:Q:65:ARG:O	2:Q:67:ASN:N	2.49	0.44
1:A:962:GLN:OE1	1:A:962:GLN:N	2.49	0.44
1:D:979:VAL:HB	1:D:1013:LEU:HD13	1.99	0.44
1:D:1100:HIS:HB2	1:D:1111:THR:HB	1.98	0.44
1:A:296:LYS:HD2	1:A:396:ALA:HB3	1.98	0.44
1:F:626:THR:HG22	1:F:706:ILE:HG12	1.99	0.44
1:F:751:PRO:HD3	1:F:834:TYR:CZ	2.53	0.44
1:C:223:ASN:OD1	1:C:223:ASN:N	2.45	0.44
1:D:187:SER:HB2	1:E:115:MET:HG3	1.99	0.44
1:E:231:LEU:HD11	1:E:1232:LEU:HD23	1.99	0.44
1:H:1070:THR:HG23	1:H:1207:VAL:HB	1.99	0.44
5:U:134:ASP:OD1	5:U:134:ASP:N	2.49	0.44
2:Q:83:ASP:OD2	2:Q:89:ARG:NH1	2.51	0.44
1:A:635:GLU:OE1	1:C:712:GLN:NE2	2.51	0.44
1:A:1238:ASP:OD2	1:A:1303:THR:OG1	2.36	0.44
1:C:201:LEU:HD21	1:C:411:LEU:HD23	1.98	0.44
1:C:769:ARG:HB3	1:C:932:ALA:HB3	2.00	0.44
1:C:846:CYS:HB2	1:C:985:CYS:HB3	1.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:908:ASP:OD1	1:C:908:ASP:N	2.47	0.44
1:D:626:THR:HG22	1:D:706:ILE:HG12	1.98	0.44
1:F:642:ILE:HD11	1:F:897:TYR:HB3	1.99	0.44
1:F:848:MET:HG2	1:F:976:PRO:HA	2.00	0.44
1:H:548:ILE:HD13	1:H:548:ILE:HA	1.87	0.44
4:N:101:ASN:HB3	4:N:306:PRO:HA	1.98	0.44
1:E:1306:ASN:OD1	1:E:1306:ASN:N	2.51	0.44
1:H:1225:ARG:NH2	1:H:1245:MET:O	2.48	0.44
1:A:1004:LYS:HA	1:A:1004:LYS:HD3	1.78	0.44
1:D:223:ASN:OD1	1:D:223:ASN:N	2.50	0.44
1:E:213:ILE:HD13	1:E:230:LEU:HD21	1.99	0.44
1:D:280:THR:HG22	1:D:379:ARG:HE	1.82	0.44
1:D:757:ASP:N	1:D:757:ASP:OD1	2.48	0.44
1:E:848:MET:O	1:E:956:LEU:N	2.49	0.44
1:F:858:ALA:HB2	2:Q:90:PRO:HD2	2.00	0.44
1:F:939:THR:OG1	1:F:940:ALA:N	2.41	0.44
2:V:10:SER:OG	2:V:11:ASN:N	2.51	0.44
1:D:939:THR:HA	1:D:1157:MET:HA	2.00	0.44
1:H:109:PHE:HE2	1:H:134:LYS:HD2	1.82	0.44
1:H:774:ARG:NH2	1:H:777:GLY:O	2.51	0.44
1:H:1158:LEU:HD23	1:H:1158:LEU:HA	1.90	0.44
5:U:15:ARG:NE	5:U:30:THR:O	2.51	0.44
5:U:264:GLU:HB3	5:U:287:THR:HG23	2.00	0.44
1:D:195:GLN:OE1	1:D:1092:TYR:OH	2.36	0.43
1:D:962:GLN:OE1	1:D:962:GLN:N	2.47	0.43
3:I:216:LEU:HD23	4:N:218:ILE:HD12	2.00	0.43
4:N:4:MET:HE3	4:N:4:MET:HB2	1.82	0.43
3:K:78:VAL:HG22	3:K:83:LEU:HD12	1.99	0.43
1:A:891:PRO:HA	1:A:896:VAL:HG21	2.00	0.43
1:A:1248:HIS:CD2	1:A:1267:GLN:HG3	2.52	0.43
1:E:222:LEU:HB3	1:E:226:ALA:HB3	2.00	0.43
1:E:889:LEU:HD12	1:E:889:LEU:HA	1.84	0.43
1:H:678:VAL:HG21	1:H:706:ILE:HG21	2.00	0.43
5:S:84:ARG:HD2	5:S:98:PRO:HB3	2.00	0.43
1:A:95:LYS:HB2	1:A:319:GLU:HB2	1.99	0.43
1:A:808:ARG:NE	2:g:80:ALA:O	2.44	0.43
1:D:743:LEU:HD11	1:D:1047:TYR:HD2	1.83	0.43
1:E:863:ILE:HD12	1:E:863:ILE:HG23	1.80	0.43
1:F:934:ASP:OD1	1:F:934:ASP:N	2.49	0.43
1:F:1225:ARG:HH21	1:F:1229:SER:HB3	1.83	0.43
1:H:604:PRO:HD2	1:H:607:PHE:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1143:ASN:OD1	1:H:1143:ASN:N	2.47	0.43
1:A:514:ASP:HB2	1:A:519:GLN:HG3	1.99	0.43
1:C:182:ARG:HD3	1:C:182:ARG:HA	1.78	0.43
1:F:224:ARG:HH21	1:F:1236:ASP:HB3	1.84	0.43
1:F:604:PRO:HD2	1:F:607:PHE:HB3	2.00	0.43
1:H:201:LEU:HD11	1:H:411:LEU:HD23	2.01	0.43
3:K:36:THR:OG1	3:K:38:ARG:NH2	2.51	0.43
2:g:65:ARG:O	2:g:67:ASN:N	2.51	0.43
1:A:849:GLY:HA3	1:A:924:THR:HG21	2.00	0.43
1:C:718:ARG:NH1	1:C:722:THR:OG1	2.52	0.43
1:C:883:PRO:O	1:C:895:ASN:ND2	2.51	0.43
1:D:291:THR:HG22	1:D:1082:LEU:HD12	1.99	0.43
1:D:721:ILE:HG13	1:D:1044:LEU:HD11	2.00	0.43
1:E:291:THR:HG22	1:E:1082:LEU:HG	2.00	0.43
1:F:1209:MET:HE3	1:F:1213:THR:HG21	2.00	0.43
1:H:81:ARG:HB2	1:H:84:GLU:HG2	2.01	0.43
1:H:808:ARG:HH12	2:G:80:ALA:H	1.65	0.43
2:L:76:THR:HG21	2:L:94:LEU:HD12	2.00	0.43
1:C:834:TYR:HE1	1:C:980:ASN:HD21	1.66	0.43
1:F:291:THR:HG22	1:F:1082:LEU:HG	1.99	0.43
1:F:914:GLN:OE1	2:L:65:ARG:NH2	2.51	0.43
1:F:1245:MET:HE3	1:F:1245:MET:HB2	1.84	0.43
1:D:201:LEU:HD11	1:D:411:LEU:HD23	2.01	0.43
1:D:1225:ARG:HH21	1:D:1229:SER:HB3	1.84	0.43
1:E:561:PRO:O	1:E:592:ARG:NH1	2.52	0.43
1:E:1027:TYR:HA	1:E:1030:THR:HG22	2.01	0.43
1:H:490:LEU:HD21	1:H:589:ALA:HB2	2.00	0.43
1:C:849:GLY:HA3	1:C:924:THR:HG21	2.00	0.43
1:D:1098:GLN:NE2	5:U:288:ASP:OD2	2.51	0.43
1:E:593:ILE:HD11	1:E:947:ILE:HG21	2.01	0.43
1:F:1099:VAL:HG22	1:F:1112:LEU:HG	2.01	0.43
1:H:190:ARG:HG2	1:H:401:VAL:HG23	2.01	0.43
2:L:102:ILE:HD12	2:L:102:ILE:HA	1.87	0.43
5:U:450:MET:HE3	5:U:457:ASN:HB3	2.00	0.43
2:g:83:ASP:OD1	2:g:89:ARG:NH2	2.52	0.43
1:C:761:TYR:O	1:C:765:ALA:HB2	2.18	0.43
1:D:529:ASP:N	1:D:529:ASP:OD1	2.51	0.43
1:E:490:LEU:HD21	1:E:589:ALA:HB2	2.01	0.43
1:A:548:ILE:HG22	1:A:1258:ARG:HB2	2.00	0.43
1:A:1027:TYR:HA	1:A:1030:THR:HG22	2.01	0.43
1:A:1362:LEU:O	1:A:1370:THR:OG1	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:ASP:OD1	1:F:119:ASP:N	2.49	0.43
1:F:155:LEU:HD21	1:F:174:ILE:HG22	2.01	0.43
1:F:493:LEU:HD23	1:F:493:LEU:HA	1.92	0.43
4:P:97:LEU:HD23	4:P:97:LEU:HA	1.92	0.43
1:E:429:ASN:HB3	1:E:432:ASP:HB2	2.01	0.42
1:E:1052:PRO:HA	1:E:1055:LEU:HB2	2.01	0.42
1:H:562:ALA:HB2	1:H:1050:PHE:HD2	1.84	0.42
3:K:57:PRO:HA	3:K:58:PRO:HD3	1.87	0.42
5:U:320:HIS:N	5:U:343:SER:O	2.52	0.42
1:A:213:ILE:HD13	1:A:230:LEU:HD21	2.02	0.42
1:A:757:ASP:OD1	1:A:757:ASP:N	2.50	0.42
1:C:107:ILE:HG22	1:H:70:LEU:HB2	2.01	0.42
1:C:683:ASN:OD1	1:C:754:TRP:NE1	2.44	0.42
1:C:747:THR:HA	1:C:762:ARG:HG3	2.01	0.42
1:F:1052:PRO:HA	1:F:1055:LEU:HB2	2.00	0.42
1:H:1027:TYR:HA	1:H:1030:THR:HG22	2.01	0.42
5:S:132:ARG:HA	5:S:133:PRO:HD3	1.91	0.42
1:C:591:LEU:O	1:C:1022:ARG:NH2	2.52	0.42
1:D:1055:LEU:HD23	1:D:1055:LEU:HA	1.88	0.42
1:D:1362:LEU:O	1:D:1370:THR:OG1	2.37	0.42
1:D:1365:ALA:HB1	1:E:1373:ASP:HA	2.01	0.42
1:E:544:ILE:O	1:E:548:ILE:HB	2.19	0.42
1:E:989:LEU:HD11	1:E:1008:PRO:HG3	2.01	0.42
1:F:211:SER:O	1:F:215:LYS:HB2	2.18	0.42
1:H:223:ASN:OD1	1:H:223:ASN:N	2.48	0.42
4:N:219:LEU:HA	4:N:222:ILE:HG12	2.01	0.42
4:P:219:LEU:O	4:P:223:THR:OG1	2.32	0.42
2:B:73:ILE:H	2:B:73:ILE:HG12	1.44	0.42
2:g:72:THR:HG23	2:g:100:PRO:HB2	2.01	0.42
1:A:451:GLN:H	1:A:451:GLN:HG3	1.66	0.42
1:D:125:ASP:OD1	1:D:125:ASP:N	2.43	0.42
1:E:281:ARG:NH1	1:E:308:ASP:OD2	2.52	0.42
1:E:355:THR:HA	5:U:76:ALA:HB2	2.00	0.42
1:F:514:ASP:HB2	1:F:519:GLN:HG3	2.01	0.42
1:H:263:VAL:HG21	1:H:387:VAL:HG21	2.01	0.42
1:H:858:ALA:HB2	2:L:90:PRO:HD2	2.01	0.42
1:H:1278:GLY:HA3	1:H:1293:PHE:HE1	1.85	0.42
3:K:154:VAL:HG11	4:P:273:ILE:HG21	2.01	0.42
1:A:729:GLU:O	1:A:736:SER:OG	2.35	0.42
1:A:864:VAL:HA	1:A:865:PRO:HD3	1.91	0.42
1:H:859:LEU:HD12	1:H:894:LEU:HD21	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1304:ASN:OD1	1:H:1304:ASN:N	2.52	0.42
1:A:203:LYS:NZ	1:A:1089:SER:OG	2.52	0.42
1:D:774:ARG:NH2	1:D:777:GLY:O	2.53	0.42
1:D:1262:ASN:C	1:D:1262:ASN:ND2	2.77	0.42
1:E:846:CYS:HB2	1:E:985:CYS:HB3	1.46	0.42
3:K:222:ILE:HG22	3:K:228:LEU:HD11	2.01	0.42
1:A:1055:LEU:HD23	1:A:1055:LEU:HA	1.93	0.42
1:C:140:SER:O	1:C:195:GLN:NE2	2.53	0.42
1:C:493:LEU:HD23	1:C:493:LEU:HA	1.94	0.42
1:C:1043:LEU:HD23	1:C:1043:LEU:HA	1.89	0.42
1:D:558:GLU:OE1	1:D:592:ARG:NH2	2.51	0.42
1:D:848:MET:O	1:D:956:LEU:N	2.53	0.42
1:E:626:THR:HB	1:E:706:ILE:HG23	2.02	0.42
1:F:490:LEU:HD21	1:F:589:ALA:HB2	2.02	0.42
1:F:1053:ILE:HD13	1:F:1166:LEU:HD13	2.02	0.42
1:H:149:SER:HB3	1:H:1106:GLY:HA3	2.02	0.42
5:U:84:ARG:HD2	5:U:98:PRO:HB3	2.01	0.42
1:A:637:ARG:HG3	1:C:715:ARG:HH12	1.85	0.42
1:A:747:THR:HA	1:A:762:ARG:HG3	2.01	0.42
1:C:182:ARG:HH22	5:S:86:ILE:HB	1.84	0.42
1:E:735:THR:HG23	1:E:738:ALA:H	1.84	0.42
2:B:26:VAL:O	2:B:63:ARG:NH1	2.53	0.42
1:C:688:MET:O	1:C:692:THR:OG1	2.30	0.42
1:C:1053:ILE:HD13	1:C:1166:LEU:HD13	2.02	0.42
1:D:201:LEU:HD23	1:D:201:LEU:HA	1.86	0.42
1:F:470:THR:OG1	1:F:471:LEU:N	2.53	0.42
1:F:846:CYS:HB2	1:F:985:CYS:HB3	1.45	0.42
1:F:908:ASP:HA	1:F:911:LEU:HB2	2.02	0.42
1:F:917:MET:HE2	1:F:917:MET:HB2	1.57	0.42
1:F:1025:VAL:HG21	1:F:1047:TYR:HE1	1.84	0.42
5:S:19:ILE:HA	5:S:25:ILE:HG22	2.01	0.42
1:D:617:LEU:HD12	1:D:617:LEU:HA	1.94	0.41
1:E:1198:ARG:HE	1:E:1198:ARG:HB3	1.69	0.41
1:H:471:LEU:HB3	1:H:1059:LEU:HD22	2.02	0.41
4:P:54:ASN:OD1	4:P:54:ASN:N	2.53	0.41
5:U:307:VAL:HG21	5:U:350:PHE:HE1	1.85	0.41
1:C:1302:ASN:ND2	1:C:1304:ASN:OD1	2.53	0.41
1:D:296:LYS:HD2	1:D:396:ALA:HB3	2.02	0.41
1:H:989:LEU:HD11	1:H:1008:PRO:HG3	2.02	0.41
3:K:216:LEU:HD23	4:P:218:ILE:HD12	2.03	0.41
1:C:760:ILE:HD11	1:C:817:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1361:MET:HG3	1:C:1381:LEU:HD12	2.02	0.41
1:H:253:ARG:HA	1:H:253:ARG:HD2	1.82	0.41
2:L:89:ARG:NH2	2:G:34:ALA:O	2.54	0.41
5:S:243:ARG:HA	5:S:243:ARG:HD3	1.90	0.41
5:S:260:GLY:HA3	5:S:276:ALA:HB1	2.02	0.41
1:A:883:PRO:O	1:A:895:ASN:ND2	2.51	0.41
1:A:1358:ASP:HB3	1:A:1361:MET:HG2	2.01	0.41
1:C:203:LYS:NZ	1:C:1089:SER:OG	2.53	0.41
1:D:548:ILE:HG22	1:D:1258:ARG:HB2	2.02	0.41
1:D:867:ILE:HG21	2:V:101:ARG:HH12	1.86	0.41
1:E:961:TYR:HB2	1:E:988:HIS:CE1	2.55	0.41
1:E:1325:ASP:OD1	1:E:1325:ASP:N	2.47	0.41
1:F:499:ASP:OD1	1:F:499:ASP:N	2.48	0.41
1:H:796:ARG:HG2	1:H:798:ASP:H	1.86	0.41
1:H:1067:ILE:HG13	1:H:1264:TRP:HZ3	1.84	0.41
3:I:222:ILE:O	3:I:224:ARG:NE	2.53	0.41
1:A:846:CYS:HB2	1:A:985:CYS:HB3	1.44	0.41
1:D:205:PRO:HG2	1:D:210:LEU:HD22	2.02	0.41
1:F:486:VAL:HG11	1:F:945:MET:HE1	2.03	0.41
1:F:1236:ASP:OD1	1:F:1236:ASP:N	2.53	0.41
1:F:1248:HIS:CD2	1:F:1267:GLN:HG3	2.55	0.41
1:H:52:LYS:HB3	1:H:52:LYS:HE2	1.87	0.41
1:H:500:ARG:NH2	1:H:584:MET:SD	2.81	0.41
1:H:1223:ASN:ND2	1:H:1348:GLN:O	2.45	0.41
3:I:106:ASP:HB2	5:S:151:LEU:HD22	2.02	0.41
3:I:145:LEU:HD21	5:S:148:PRO:HB3	2.03	0.41
5:U:243:ARG:NH2	5:U:333:ARG:O	2.53	0.41
1:C:320:MET:HE1	1:H:68:ILE:HD11	2.02	0.41
1:C:500:ARG:NH1	1:C:584:MET:SD	2.83	0.41
1:C:743:LEU:HD11	1:C:1047:TYR:HD2	1.86	0.41
1:D:182:ARG:HH21	5:U:83:PRO:HG3	1.85	0.41
1:D:1323:SER:HG	1:D:1326:THR:HG1	1.66	0.41
1:E:502:CYS:HB2	1:E:532:PRO:HD2	2.03	0.41
1:F:213:ILE:HG12	1:F:234:LEU:HD11	2.02	0.41
1:A:363:PRO:HB2	1:C:76:THR:HG22	2.02	0.41
1:D:196:LEU:HD23	1:D:196:LEU:HA	1.95	0.41
1:H:593:ILE:HD11	1:H:947:ILE:HG21	2.02	0.41
1:H:979:VAL:HB	1:H:1013:LEU:HD13	2.01	0.41
5:U:154:LEU:HD21	5:U:158:ARG:HB3	2.02	0.41
1:E:1043:LEU:HD23	1:E:1043:LEU:HA	1.94	0.41
1:H:201:LEU:HD23	1:H:201:LEU:HA	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:224:ARG:NH2	3:K:228:LEU:O	2.53	0.41
4:P:295:VAL:HA	4:P:312:VAL:HG12	2.02	0.41
2:Q:73:ILE:H	2:Q:73:ILE:HG12	1.64	0.41
1:A:735:THR:HG23	1:A:738:ALA:H	1.86	0.41
1:C:231:LEU:HD11	1:C:1232:LEU:HD23	2.02	0.41
1:C:842:ARG:HH12	1:C:1033:LYS:HA	1.85	0.41
1:C:1306:ASN:OD1	1:C:1306:ASN:N	2.53	0.41
1:D:961:TYR:HB2	1:D:988:HIS:CE1	2.56	0.41
1:D:1030:THR:HG23	1:D:1031:HIS:ND1	2.36	0.41
1:D:1245:MET:HE2	1:D:1245:MET:HB2	1.90	0.41
1:E:26:PRO:HG3	1:E:61:LEU:HG	2.02	0.41
1:E:253:ARG:HD3	1:E:253:ARG:HA	1.92	0.41
1:E:879:ASP:OD1	1:E:879:ASP:N	2.51	0.41
1:F:544:ILE:O	1:F:548:ILE:HB	2.21	0.41
1:F:961:TYR:HB2	1:F:988:HIS:CE1	2.56	0.41
1:H:59:ASN:O	5:S:292:THR:OG1	2.28	0.41
1:H:747:THR:HA	1:H:762:ARG:HG3	2.01	0.41
1:H:1055:LEU:HD23	1:H:1055:LEU:HA	1.89	0.41
4:N:154:VAL:HG21	4:N:287:LEU:HD13	2.02	0.41
5:S:354:ILE:HG22	5:S:430:TYR:HE2	1.85	0.41
5:U:242:LEU:HD12	5:U:336:VAL:HG21	2.03	0.41
1:A:275:ILE:HD13	1:A:375:PRO:HA	2.03	0.41
1:C:87:LEU:HD21	1:C:197:LEU:HG	2.03	0.41
1:F:743:LEU:HD11	1:F:1047:TYR:HD2	1.85	0.41
5:U:108:ILE:H	5:U:108:ILE:HG13	1.68	0.41
5:U:253:HIS:O	5:U:254:ARG:HG2	2.20	0.41
1:C:1377:LEU:HD12	1:C:1377:LEU:HA	1.92	0.40
1:D:822:ASP:N	1:D:822:ASP:OD1	2.54	0.40
1:E:747:THR:OG1	1:E:769:ARG:NH1	2.52	0.40
1:F:77:LEU:HD21	1:H:114:PRO:HD3	2.02	0.40
1:F:757:ASP:N	1:F:757:ASP:OD1	2.53	0.40
4:P:215:THR:O	4:P:219:LEU:CB	2.67	0.40
5:U:83:PRO:HB2	5:U:86:ILE:HD12	2.03	0.40
5:U:94:ILE:HD11	5:U:112:LEU:HD22	2.03	0.40
1:H:1336:SER:OG	1:H:1338:GLU:OE1	2.39	0.40
3:I:107:LEU:HB2	3:I:304:VAL:HB	2.02	0.40
2:G:48:ASP:O	2:G:52:ILE:HD12	2.21	0.40
2:B:85:MET:HE3	2:B:85:MET:HB3	1.95	0.40
2:Q:10:SER:OG	2:Q:11:ASN:N	2.54	0.40
1:A:311:ALA:HB2	1:A:384:LEU:HD11	2.04	0.40
1:A:785:HIS:HB3	1:A:803:HIS:HB3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:VAL:HG23	1:C:574:LEU:HD12	2.02	0.40
1:D:807:VAL:HG21	2:V:79:PHE:HD2	1.86	0.40
1:D:849:GLY:HA3	1:D:924:THR:HG21	2.02	0.40
1:D:989:LEU:HD11	1:D:1008:PRO:HG3	2.02	0.40
1:E:664:LEU:HD23	1:E:664:LEU:HA	1.89	0.40
1:H:254:LEU:HD23	1:H:254:LEU:HA	1.94	0.40
3:I:269:ILE:HA	3:I:272:THR:HG22	2.02	0.40
4:P:204:VAL:O	4:P:208:MET:HG2	2.21	0.40
5:U:132:ARG:HA	5:U:133:PRO:HD3	1.92	0.40
5:U:285:ALA:O	5:U:294:ARG:NE	2.47	0.40
1:A:114:PRO:HD3	1:C:77:LEU:HD21	2.03	0.40
1:A:196:LEU:HD23	1:A:196:LEU:HA	1.91	0.40
1:C:429:ASN:HB3	1:C:432:ASP:HB2	2.03	0.40
1:C:1080:GLU:HB2	1:C:1133:ALA:HB3	2.03	0.40
1:D:1043:LEU:HD23	1:D:1043:LEU:HA	1.85	0.40
1:E:72:THR:HG22	1:F:108:GLN:HB2	2.04	0.40
1:F:67:ASP:OD2	1:H:103:ARG:NH1	2.54	0.40
3:I:63:LEU:HD12	3:I:63:LEU:HA	1.94	0.40
5:S:356:PHE:O	5:S:358:LEU:N	2.55	0.40
1:C:231:LEU:HD21	1:C:1232:LEU:HB3	2.04	0.40
1:E:77:LEU:HD23	1:E:77:LEU:HA	1.90	0.40
1:E:107:ILE:HG22	1:E:134:LYS:HB2	2.04	0.40
1:E:498:LEU:HD11	1:E:587:VAL:HG23	2.04	0.40
1:E:623:THR:HG23	1:E:626:THR:HG23	2.03	0.40
1:F:784:LEU:HB3	1:F:800:VAL:HG13	2.03	0.40
1:F:848:MET:HB3	1:F:975:TYR:O	2.20	0.40
2:Q:11:ASN:N	2:Q:11:ASN:OD1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1379/1381 (100%)	1278 (93%)	101 (7%)	0	100	100
1	C	1379/1381 (100%)	1271 (92%)	108 (8%)	0	100	100
1	D	1379/1381 (100%)	1281 (93%)	97 (7%)	1 (0%)	48	78
1	E	1379/1381 (100%)	1276 (92%)	103 (8%)	0	100	100
1	F	1379/1381 (100%)	1261 (91%)	118 (9%)	0	100	100
1	H	1379/1381 (100%)	1268 (92%)	111 (8%)	0	100	100
2	B	92/94 (98%)	72 (78%)	17 (18%)	3 (3%)	3	25
2	G	92/94 (98%)	72 (78%)	18 (20%)	2 (2%)	5	31
2	L	92/94 (98%)	69 (75%)	19 (21%)	4 (4%)	2	19
2	Q	92/94 (98%)	70 (76%)	19 (21%)	3 (3%)	3	25
2	V	92/94 (98%)	72 (78%)	17 (18%)	3 (3%)	3	25
2	g	92/94 (98%)	71 (77%)	18 (20%)	3 (3%)	3	25
3	I	248/256 (97%)	234 (94%)	13 (5%)	1 (0%)	30	60
3	K	248/256 (97%)	232 (94%)	15 (6%)	1 (0%)	30	60
4	N	257/263 (98%)	238 (93%)	19 (7%)	0	100	100
4	P	257/263 (98%)	241 (94%)	16 (6%)	0	100	100
5	S	386/392 (98%)	322 (83%)	55 (14%)	9 (2%)	5	30
5	U	386/392 (98%)	320 (83%)	58 (15%)	8 (2%)	5	31
All	All	10608/10672 (99%)	9648 (91%)	922 (9%)	38 (0%)	31	60

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	46	ILE
2	L	66	ALA
2	L	102	ILE
5	S	267	ILE
5	U	267	ILE
2	G	102	ILE
2	B	102	ILE
2	g	66	ALA
2	g	102	ILE
2	V	66	ALA
2	V	102	ILE
2	Q	46	ILE
2	Q	66	ALA
2	Q	102	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	230	ILE
5	S	265	TYR
3	K	230	ILE
5	U	265	TYR
2	G	66	ALA
2	B	66	ALA
5	U	131	PHE
2	V	78	MET
5	S	131	PHE
5	S	114	ASN
5	S	262	LEU
5	U	114	ASN
2	g	78	MET
1	D	366	ASN
2	L	78	MET
5	S	118	THR
5	U	262	LEU
2	B	78	MET
5	U	101	ILE
5	U	256	ILE
5	S	101	ILE
5	S	256	ILE
5	U	32	ILE
5	S	32	ILE

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	1141/1168 (98%)	1123 (98%)	18 (2%)	55	68
1	C	1141/1168 (98%)	1107 (97%)	34 (3%)	36	57
1	D	1142/1168 (98%)	1114 (98%)	28 (2%)	42	61
1	E	1141/1168 (98%)	1123 (98%)	18 (2%)	55	68
1	F	1141/1168 (98%)	1116 (98%)	25 (2%)	45	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	1141/1168 (98%)	1124 (98%)	17 (2%)	57	68
2	B	69/73 (94%)	67 (97%)	2 (3%)	37	57
2	G	69/73 (94%)	65 (94%)	4 (6%)	18	45
2	L	69/73 (94%)	66 (96%)	3 (4%)	26	50
2	Q	69/73 (94%)	65 (94%)	4 (6%)	18	45
2	V	69/73 (94%)	66 (96%)	3 (4%)	26	50
2	g	69/73 (94%)	67 (97%)	2 (3%)	37	57
3	I	188/218 (86%)	184 (98%)	4 (2%)	47	64
3	K	188/218 (86%)	185 (98%)	3 (2%)	55	68
4	N	214/224 (96%)	207 (97%)	7 (3%)	33	55
4	P	214/224 (96%)	204 (95%)	10 (5%)	23	48
5	S	295/309 (96%)	291 (99%)	4 (1%)	59	70
5	U	295/309 (96%)	292 (99%)	3 (1%)	68	74
All	All	8655/8948 (97%)	8466 (98%)	189 (2%)	45	63

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	136	ILE
1	A	208	SER
1	A	258	TYR
1	A	292	THR
1	A	325	THR
1	A	467	THR
1	A	481	SER
1	A	498	LEU
1	A	548	ILE
1	A	642	ILE
1	A	675	SER
1	A	817	ILE
1	A	930	SER
1	A	979	VAL
1	A	1061	THR
1	A	1306	ASN
1	A	1375	VAL
1	C	47	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	83	LEU
1	C	202	GLU
1	C	223	ASN
1	C	251	GLU
1	C	258	TYR
1	C	266	THR
1	C	290	VAL
1	C	292	THR
1	C	315	VAL
1	C	386	ILE
1	C	421	MET
1	C	478	ILE
1	C	538	VAL
1	C	572	VAL
1	C	574	LEU
1	C	584	MET
1	C	623	THR
1	C	859	LEU
1	C	890	VAL
1	C	906	ASP
1	C	930	SER
1	C	979	VAL
1	C	1070	THR
1	C	1094	VAL
1	C	1119	VAL
1	C	1157	MET
1	C	1213	THR
1	C	1245	MET
1	C	1253	VAL
1	C	1267	GLN
1	C	1270	SER
1	C	1318	VAL
1	C	1375	VAL
1	D	30	ILE
1	D	94	THR
1	D	115	MET
1	D	125	ASP
1	D	128	VAL
1	D	238	VAL
1	D	258	TYR
1	D	309	THR
1	D	315	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	322	LEU
1	D	333	MET
1	D	383	ASP
1	D	435	THR
1	D	486	VAL
1	D	512	THR
1	D	573	ASP
1	D	574	LEU
1	D	594	ILE
1	D	702	VAL
1	D	890	VAL
1	D	896	VAL
1	D	930	SER
1	D	1070	THR
1	D	1234	MET
1	D	1250	GLN
1	D	1256	THR
1	D	1262	ASN
1	D	1305	CYS
1	E	78	ASN
1	E	223	ASN
1	E	238	VAL
1	E	258	TYR
1	E	266	THR
1	E	290	VAL
1	E	309	THR
1	E	475	MET
1	E	486	VAL
1	E	524	MET
1	E	545	LEU
1	E	742	ILE
1	E	784	LEU
1	E	1056	THR
1	E	1121	LEU
1	E	1196	ILE
1	E	1260	THR
1	E	1375	VAL
1	F	36	LEU
1	F	49	ASP
1	F	54	ILE
1	F	80	VAL
1	F	94	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	124	VAL
1	F	177	MET
1	F	258	TYR
1	F	266	THR
1	F	290	VAL
1	F	315	VAL
1	F	548	ILE
1	F	574	LEU
1	F	687	LEU
1	F	742	ILE
1	F	769	ARG
1	F	862	VAL
1	F	863	ILE
1	F	912	THR
1	F	939	THR
1	F	1005	MET
1	F	1016	ASN
1	F	1070	THR
1	F	1262	ASN
1	F	1346	LEU
1	H	37	SER
1	H	72	THR
1	H	116	ILE
1	H	125	ASP
1	H	223	ASN
1	H	258	TYR
1	H	292	THR
1	H	481	SER
1	H	548	ILE
1	H	924	THR
1	H	1070	THR
1	H	1101	HIS
1	H	1113	THR
1	H	1131	THR
1	H	1260	THR
1	H	1267	GLN
1	H	1363	ARG
2	L	32	LEU
2	L	73	ILE
2	L	102	ILE
3	I	64	LEU
3	I	101	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	116	LEU
3	I	295	VAL
4	N	37	LEU
4	N	130	SER
4	N	140	THR
4	N	176	VAL
4	N	292	ILE
4	N	297	VAL
4	N	310	THR
5	S	37	ASN
5	S	91	MET
5	S	107	THR
5	S	245	MET
3	K	53	ILE
3	K	64	LEU
3	K	295	VAL
4	P	33	THR
4	P	45	ASP
4	P	140	THR
4	P	141	ILE
4	P	188	THR
4	P	275	SER
4	P	279	THR
4	P	286	THR
4	P	295	VAL
4	P	297	VAL
5	U	79	ILE
5	U	274	ILE
5	U	435	LEU
2	G	16	SER
2	G	20	ILE
2	G	32	LEU
2	G	102	ILE
2	B	73	ILE
2	B	83	ASP
2	g	83	ASP
2	g	102	ILE
2	V	32	LEU
2	V	51	SER
2	V	73	ILE
2	Q	31	LEU
2	Q	32	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Q	73	ILE
2	Q	102	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	326	ASN
1	A	541	HIS
1	A	674	GLN
1	A	712	GLN
1	A	821	HIS
1	A	1018	HIS
1	A	1177	ASN
1	A	1321	GLN
1	A	1329	GLN
1	C	326	ASN
1	C	364	GLN
1	C	455	GLN
1	C	595	ASN
1	C	727	GLN
1	C	892	ASN
1	C	899	HIS
1	C	1329	GLN
1	D	65	GLN
1	D	157	ASN
1	D	501	GLN
1	D	536	HIS
1	D	666	GLN
1	D	674	GLN
1	D	740	ASN
1	D	899	HIS
1	D	1016	ASN
1	D	1058	GLN
1	D	1262	ASN
1	D	1329	GLN
1	D	1341	GLN
1	E	447	GLN
1	E	595	ASN
1	E	674	GLN
1	E	683	ASN
1	E	782	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	888	GLN
1	E	954	HIS
1	E	1081	GLN
1	E	1109	ASN
1	E	1329	GLN
1	F	65	GLN
1	F	108	GLN
1	F	157	ASN
1	F	195	GLN
1	F	217	GLN
1	F	326	ASN
1	F	364	GLN
1	F	674	GLN
1	F	676	HIS
1	F	696	ASN
1	F	731	HIS
1	F	740	ASN
1	F	892	ASN
1	F	1058	GLN
1	F	1250	GLN
1	F	1281	ASN
1	F	1329	GLN
1	F	1341	GLN
1	F	1348	GLN
1	H	113	GLN
1	H	130	ASN
1	H	180	ASN
1	H	674	GLN
1	H	782	GLN
1	H	1037	ASN
1	H	1100	HIS
1	H	1250	GLN
1	H	1329	GLN
1	H	1348	GLN
2	L	11	ASN
4	N	143	GLN
4	N	206	ASN
5	S	105	GLN
5	S	213	GLN
4	P	143	GLN
5	U	137	HIS
5	U	312	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	68	HIS
2	g	68	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	K	3
3	I	3
4	N	2
4	P	2
5	U	2
5	S	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	226:LEU	C	266:ARG	N	28.83
1	P	226:LEU	C	266:ARG	N	28.15
1	K	236:LEU	C	244:VAL	N	20.36
1	I	236:LEU	C	244:VAL	N	20.15
1	K	260:MET	C	267:LEU	N	18.69
1	I	260:MET	C	267:LEU	N	18.64
1	P	163:ALA	C	175:ASP	N	17.41
1	N	163:ALA	C	175:ASP	N	16.34
1	U	362:ILE	C	428:CYS	N	13.65
1	U	179:SER	C	192:ARG	N	12.91
1	S	179:SER	C	192:ARG	N	12.72
1	I	161:LEU	C	206:ASN	N	12.20
1	K	161:LEU	C	206:ASN	N	12.13
1	S	362:ILE	C	428:CYS	N	12.04

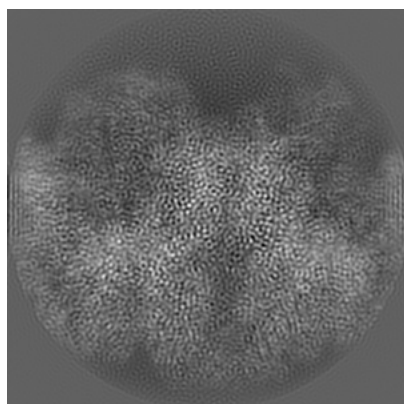
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38193. These allow visual inspection of the internal detail of the map and identification of artifacts.

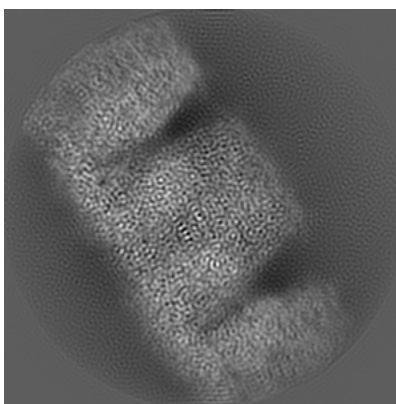
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

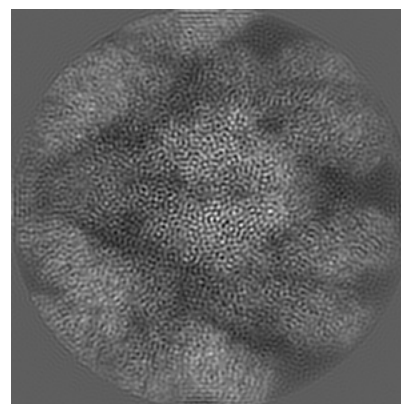
6.1.1 Primary map



X

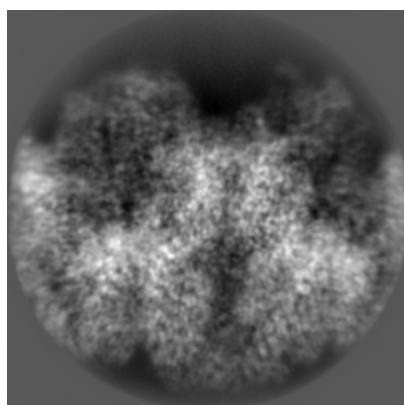


Y

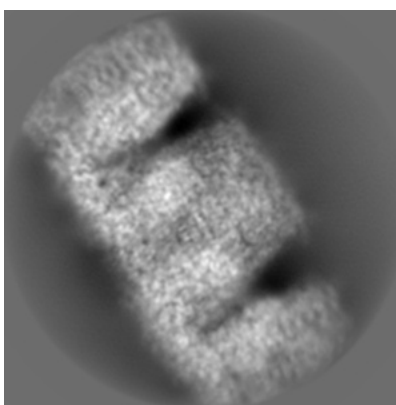


Z

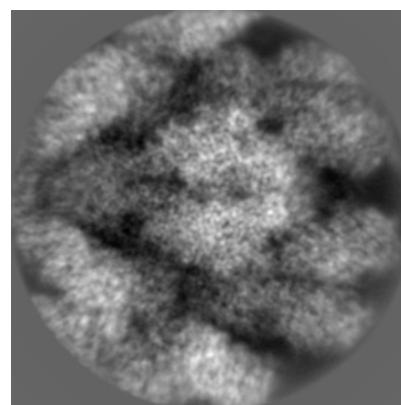
6.1.2 Raw map



X



Y

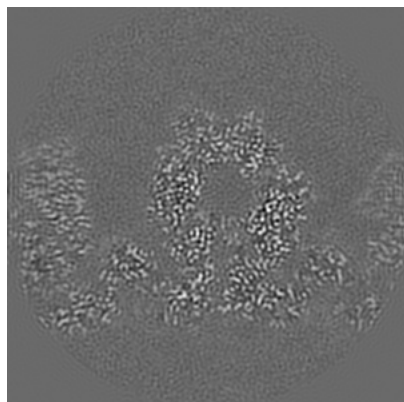


Z

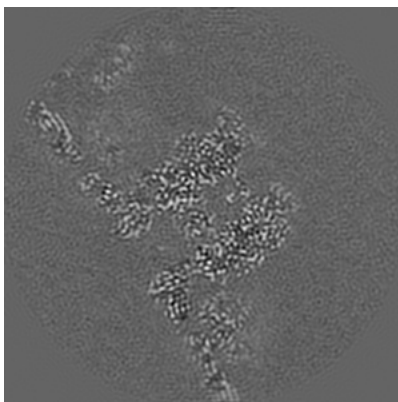
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

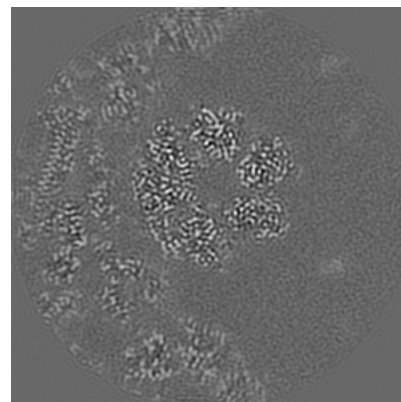
6.2.1 Primary map



X Index: 120

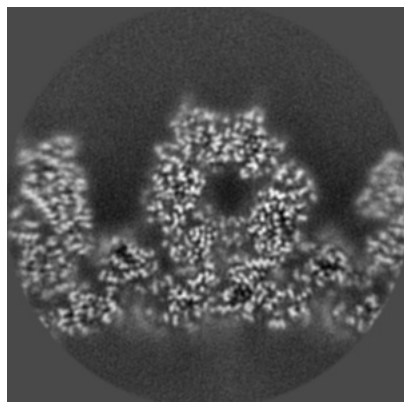


Y Index: 120

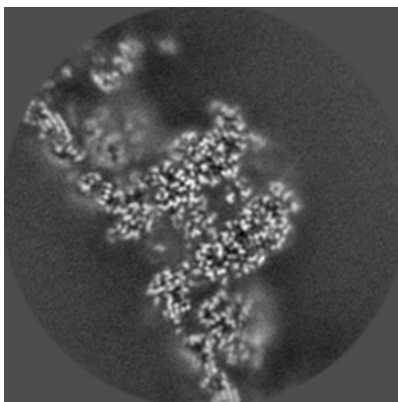


Z Index: 120

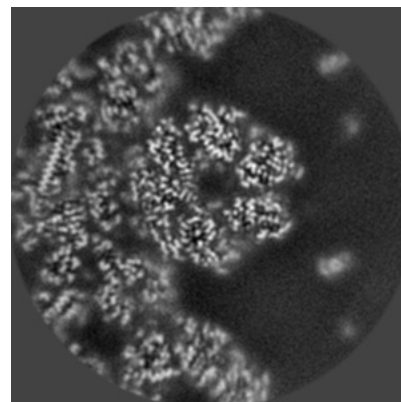
6.2.2 Raw map



X Index: 120



Y Index: 120

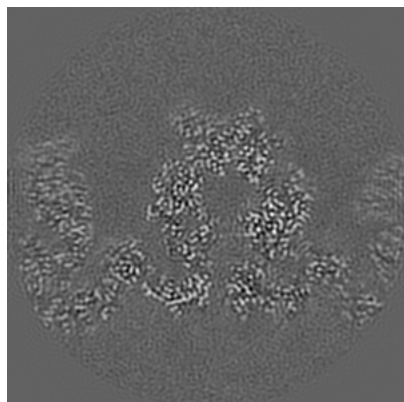


Z Index: 120

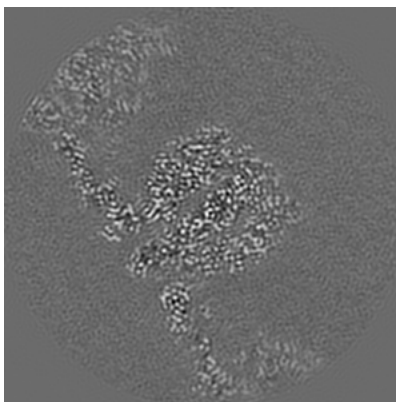
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

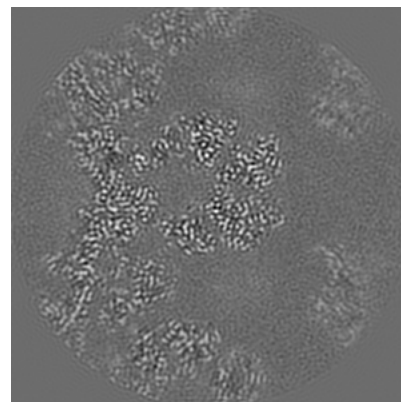
6.3.1 Primary map



X Index: 117

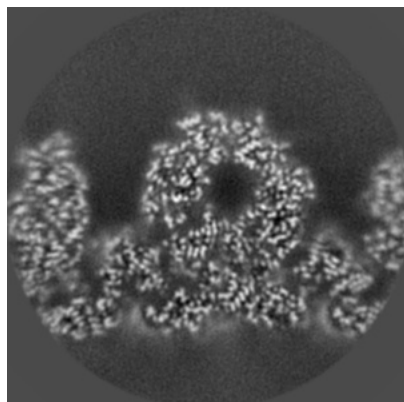


Y Index: 109

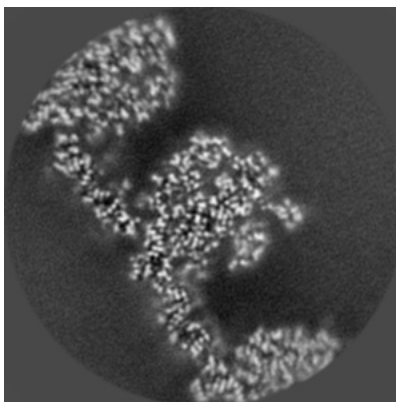


Z Index: 106

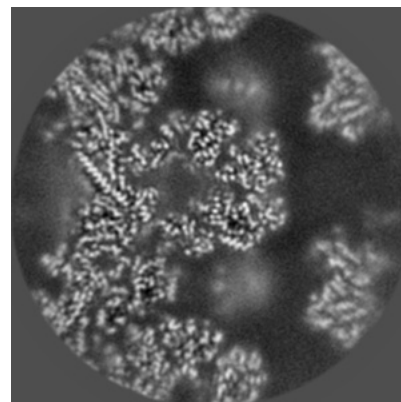
6.3.2 Raw map



X Index: 123



Y Index: 103

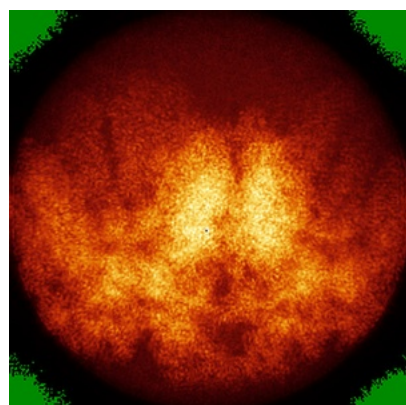


Z Index: 105

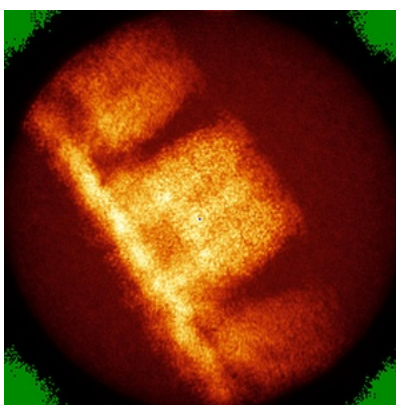
The images above show the largest variance slices of the map in three orthogonal directions.

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

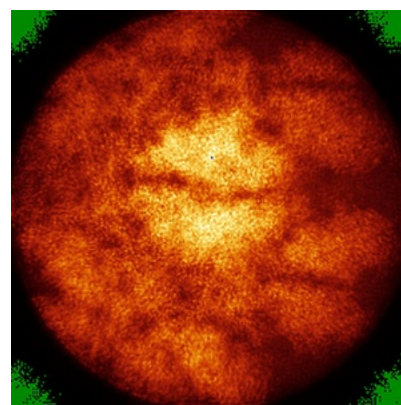
6.4.1 Primary map



X

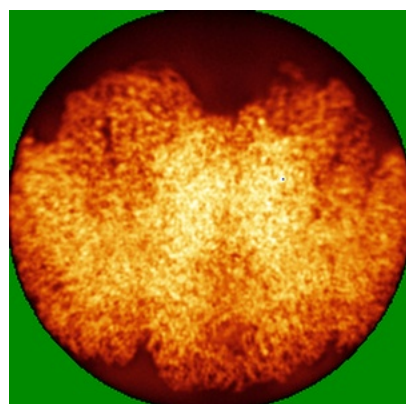


Y

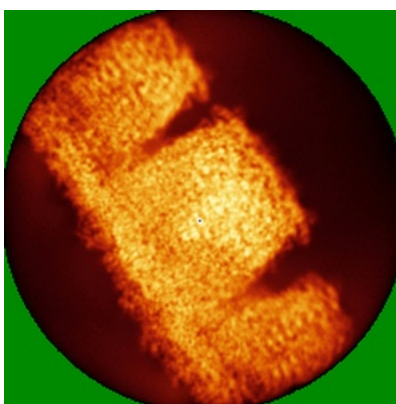


Z

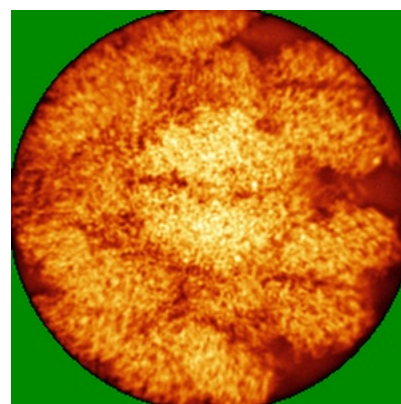
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

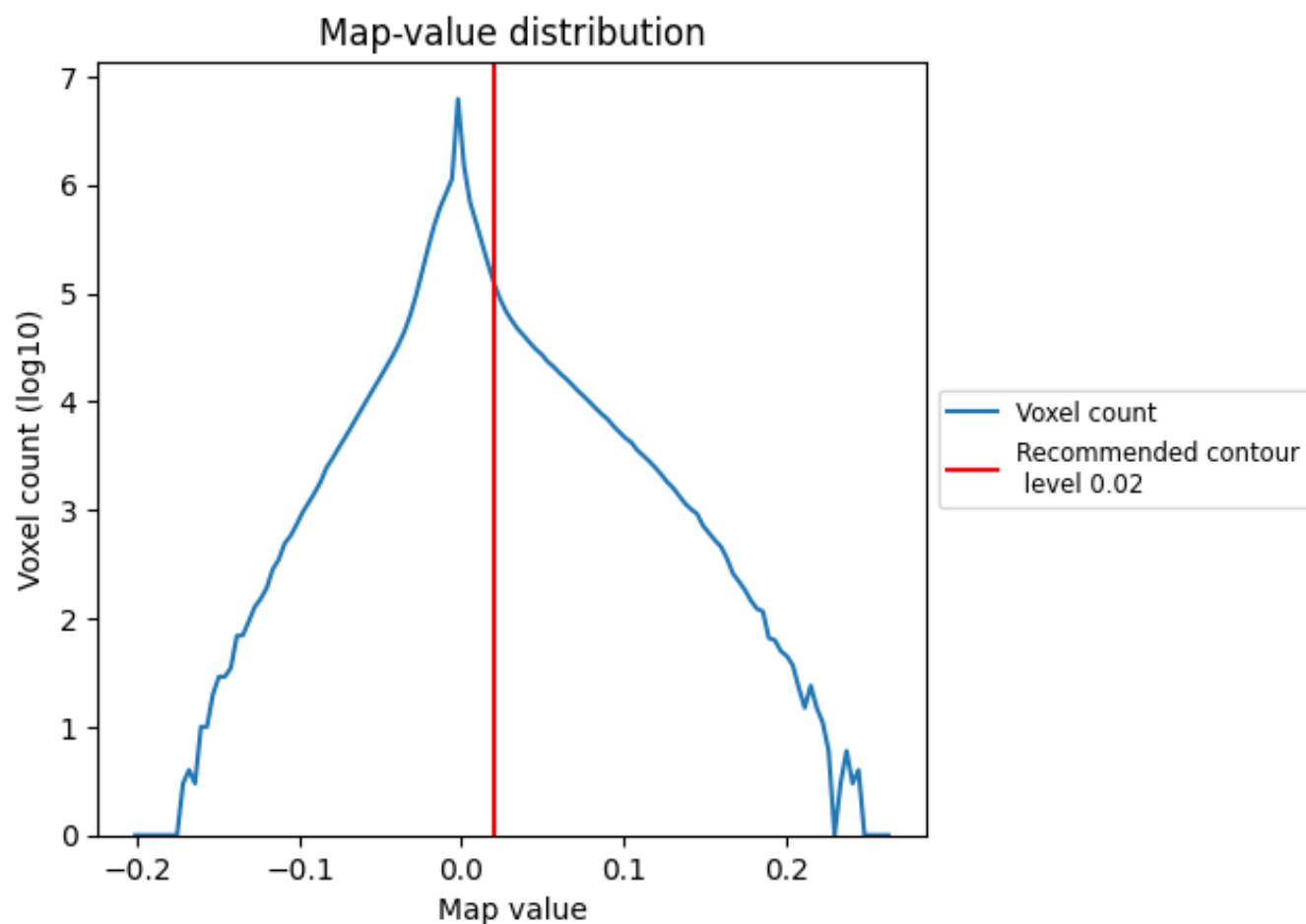
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

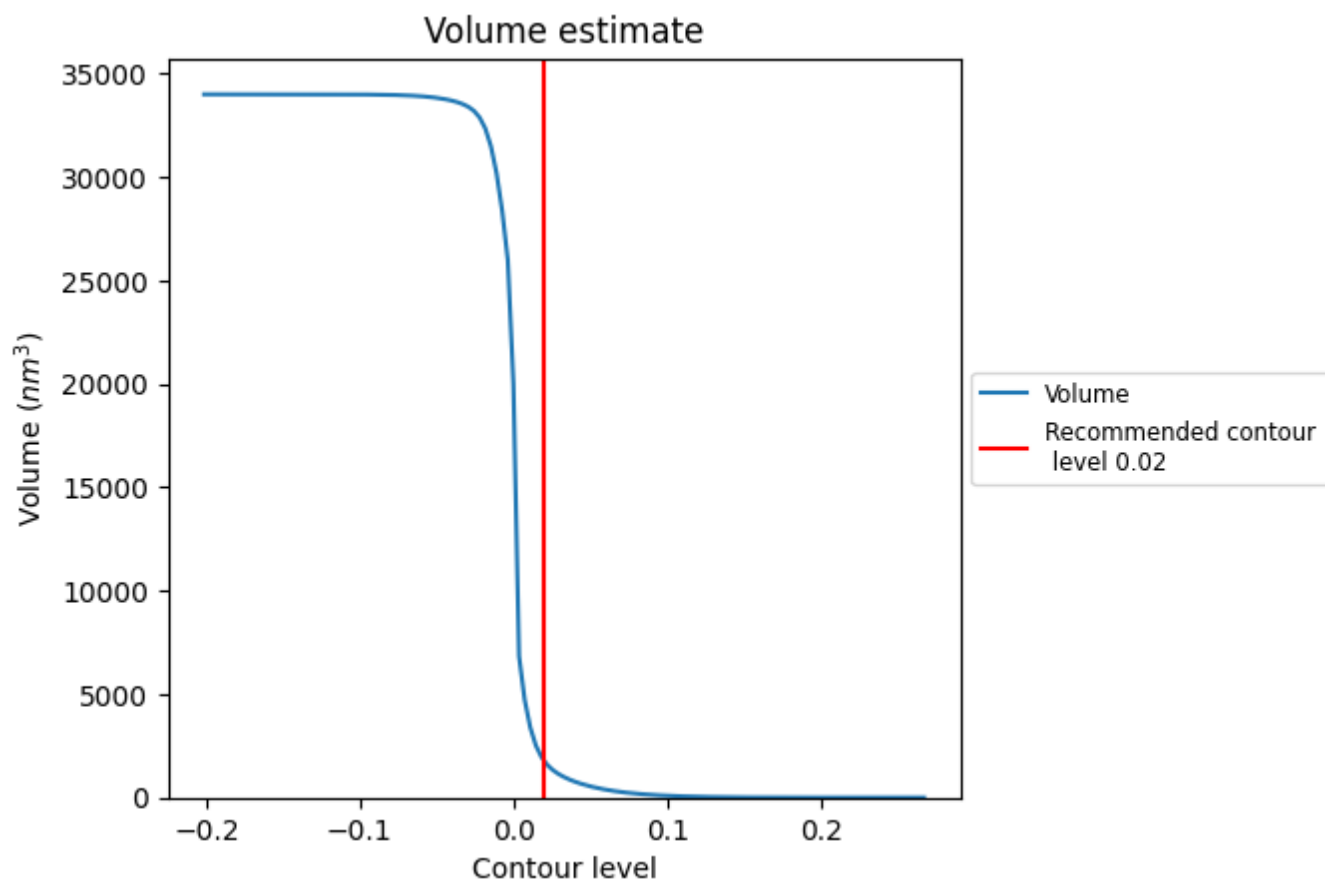
This section contains the results of statistical analysis of the map.

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.

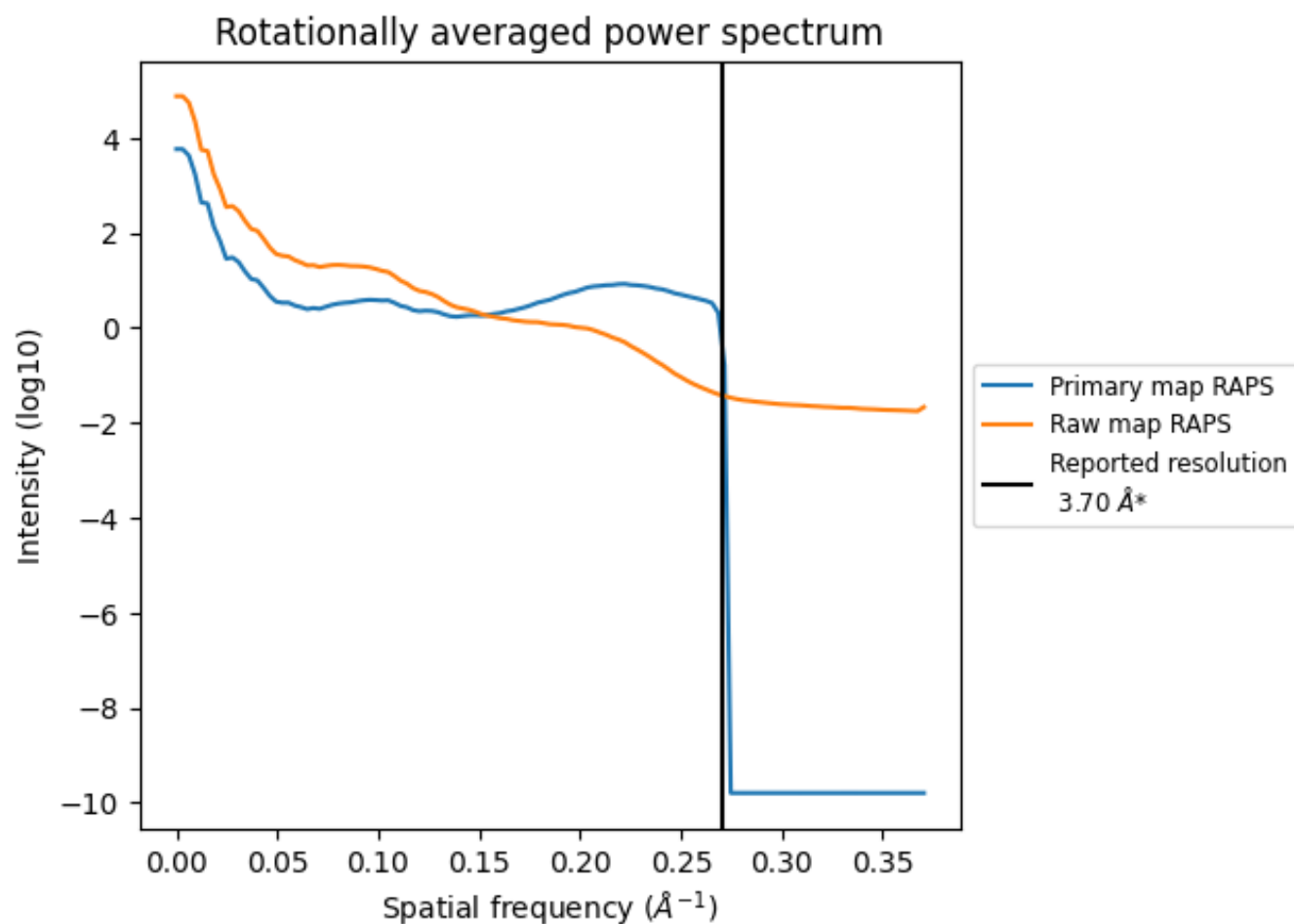
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1774 nm^3 ; this corresponds to an approximate mass of 1603 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 ⓘ

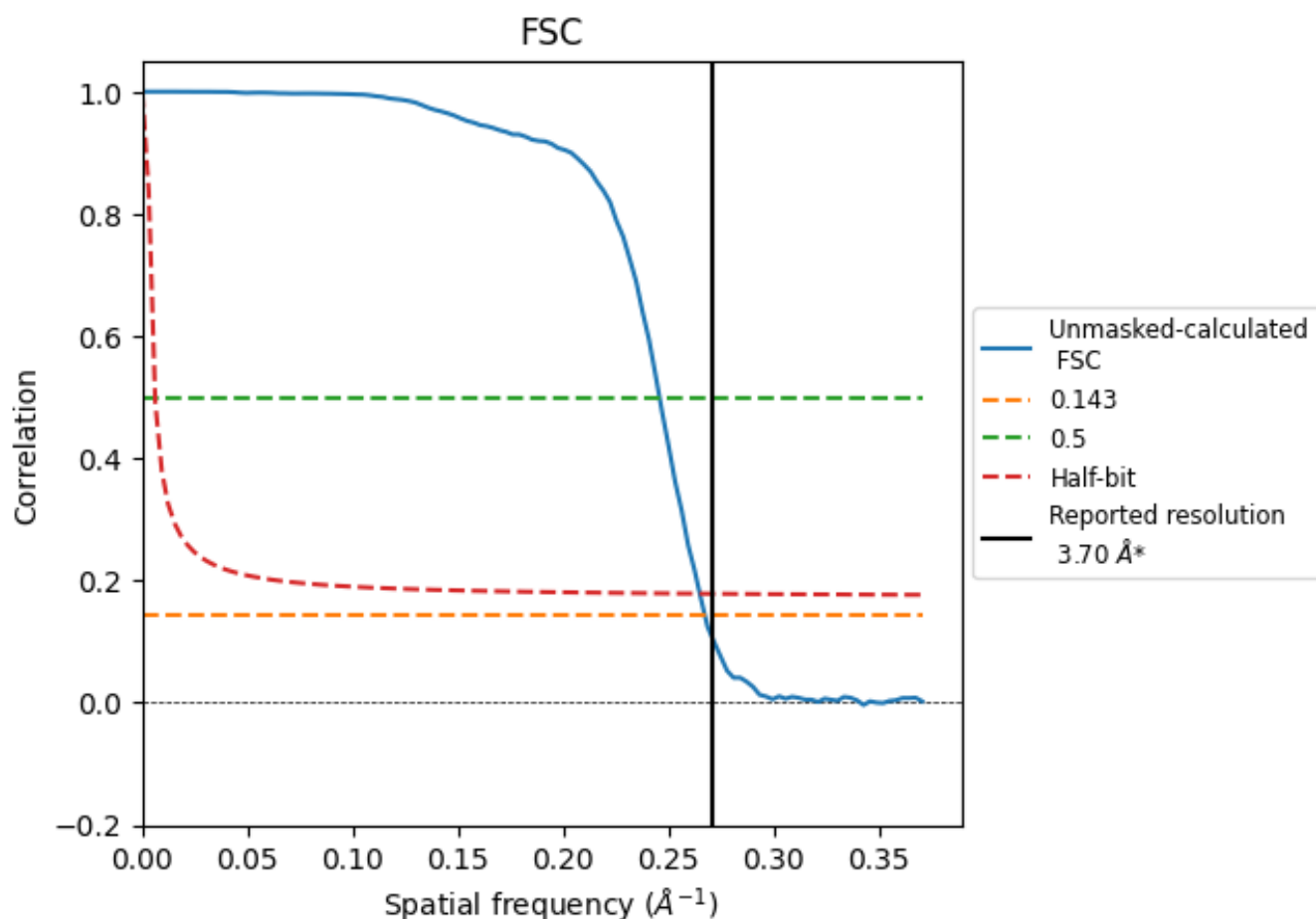


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

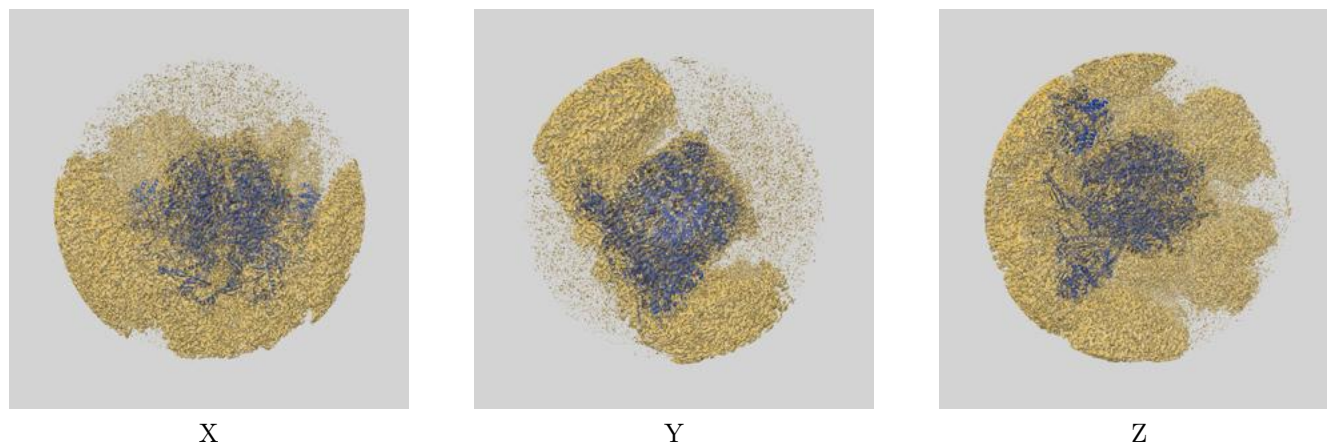
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	4.07	3.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

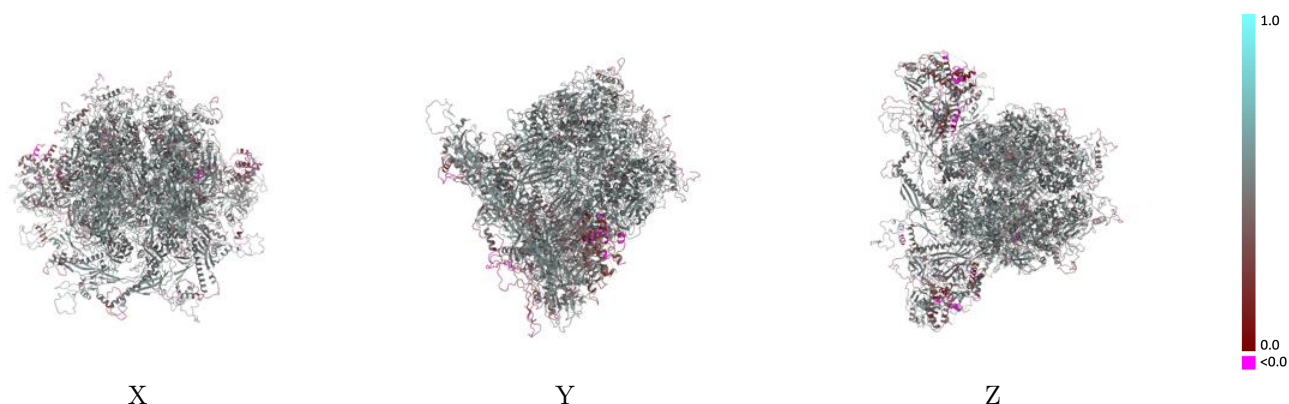
This section contains information regarding the fit between EMDB map EMD-38193 and PDB model 8XA3. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



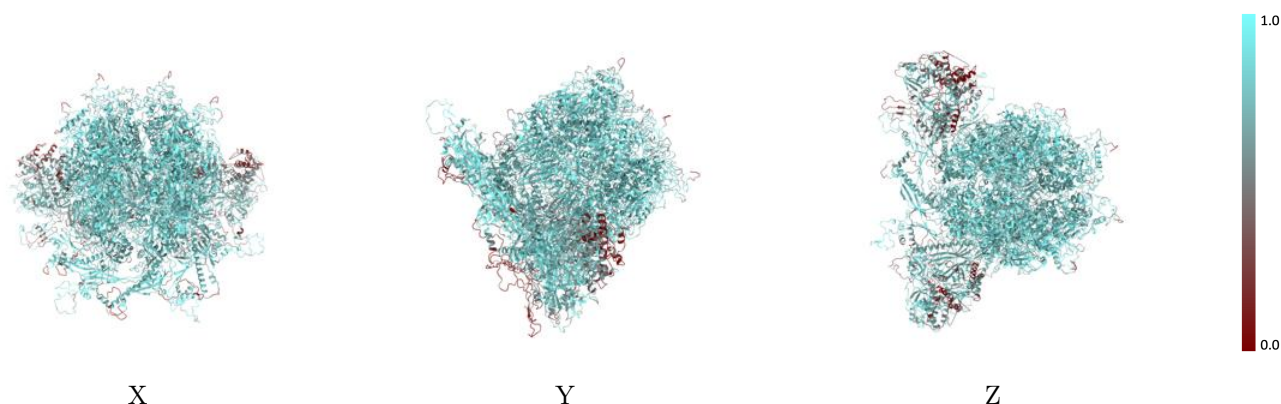
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



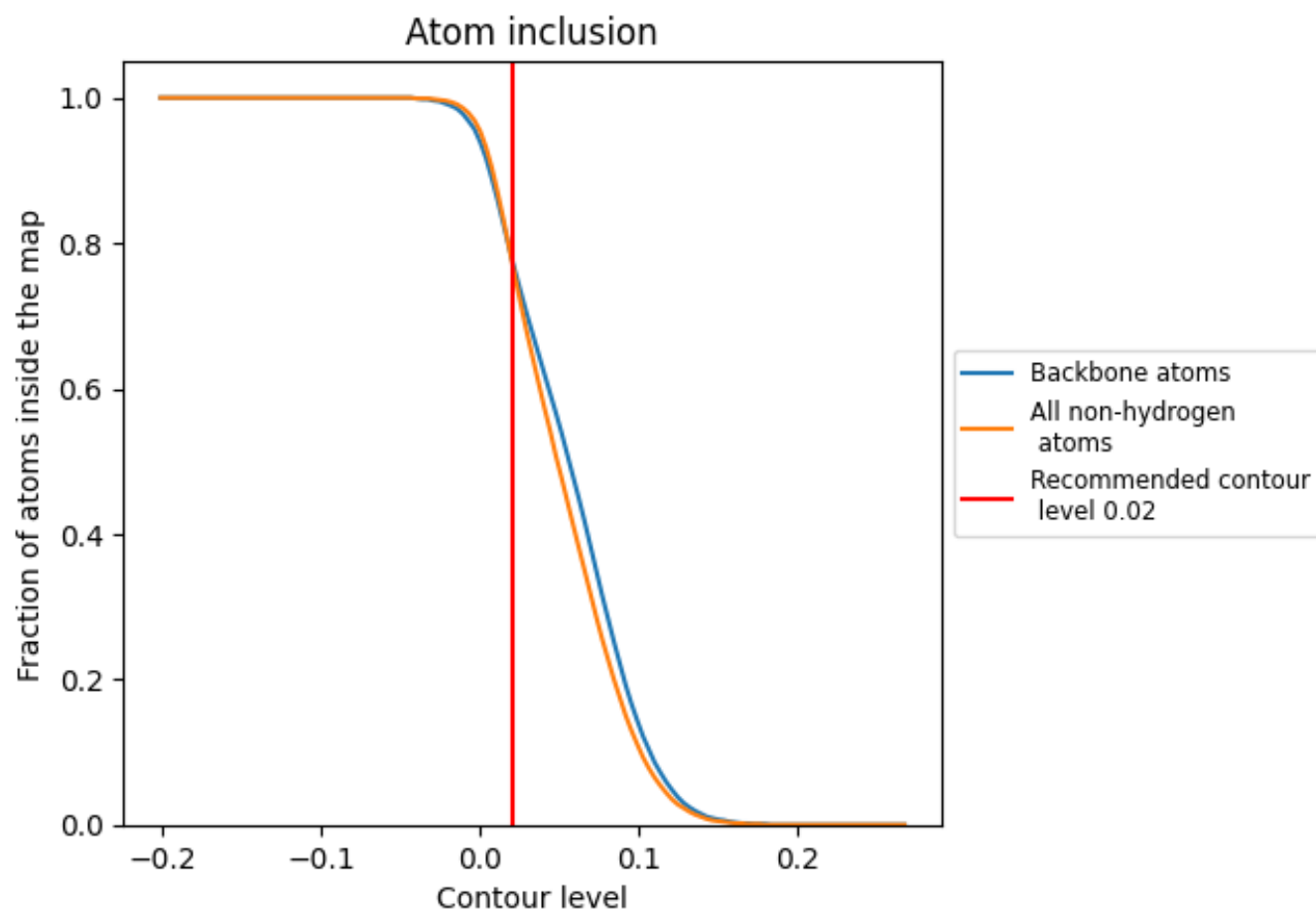
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 78% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.7730	 0.4760
A	 0.8180	 0.5000
B	 0.7340	 0.4090
C	 0.8190	 0.4980
D	 0.8140	 0.4980
E	 0.8150	 0.4970
F	 0.8090	 0.4940
G	 0.7310	 0.4020
H	 0.8120	 0.4970
I	 0.6900	 0.4310
K	 0.6190	 0.4160
L	 0.7370	 0.4280
N	 0.6960	 0.4470
P	 0.6010	 0.4120
Q	 0.7310	 0.4230
S	 0.5390	 0.3640
U	 0.4770	 0.3320
V	 0.7400	 0.4200
g	 0.7600	 0.4070

