



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:17 AM UTC

PDB ID : 8OLB / pdb_00008olb
EMDB ID : EMD-16954
Title : SA11 Rotavirus Non-trypsinized Triple Layered Particle
Authors : Asensio-Cob, D.; Perez-Mata, C.; Gomez-Blanco, J.; Vargas, J.; Rodriguez, J.M.; Luque, D.
Deposited on : 2023-03-30
Resolution : 3.40 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
Mogul : 2022.3.0, CSD as543be (2022)
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

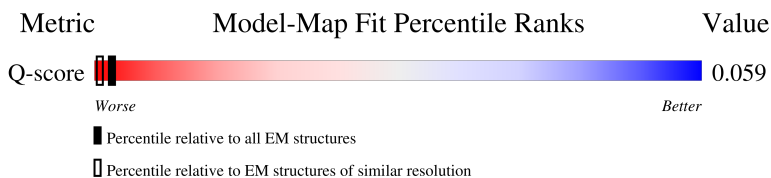
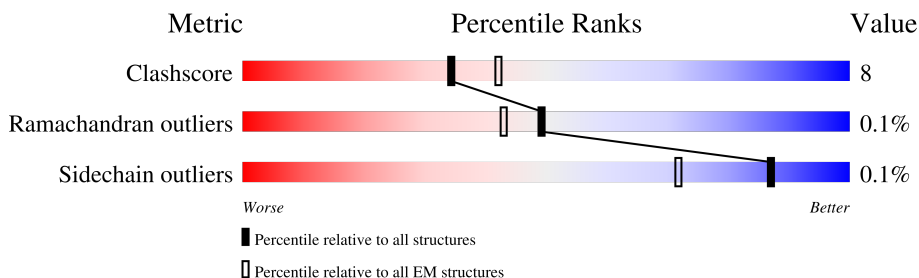
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	882	13% 70% 18% 11%
1	B	882	15% 71% 20% 9%
2	c	326	7% 63% 21% 16%
2	d	326	• 60% 19% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	e	326	
2	f	326	
2	g	326	
2	h	326	
2	i	326	
2	j	326	
2	k	326	
2	l	326	
2	m	326	
2	n	326	
2	o	326	
3	C	397	
3	D	397	
3	E	397	
3	F	397	
3	G	397	
3	H	397	
3	I	397	
3	J	397	
3	K	397	
3	L	397	
3	M	397	
3	N	397	
3	O	397	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	h	401	-	-	X	-
5	NAG	l	401	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 82097 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 Inner capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	781	Total	C	N	O	S	0	0
			6377	4051	1100	1189	37		
1	B	800	Total	C	N	O	S	0	0
			6540	4155	1126	1222	37		

- Molecule 2 is a protein called Outer capsid glycoprotein VP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	274	Total	C	N	O	S	0	0
			2167	1377	342	432	16		
2	d	258	Total	C	N	O	S	0	0
			2039	1295	320	408	16		
2	e	270	Total	C	N	O	S	0	0
			2141	1361	339	425	16		
2	f	275	Total	C	N	O	S	0	0
			2181	1386	346	433	16		
2	g	276	Total	C	N	O	S	0	0
			2185	1388	347	434	16		
2	h	277	Total	C	N	O	S	0	0
			2190	1391	348	435	16		
2	i	273	Total	C	N	O	S	0	0
			2163	1375	341	431	16		
2	j	270	Total	C	N	O	S	0	0
			2141	1361	339	425	16		
2	k	275	Total	C	N	O	S	0	0
			2181	1386	346	433	16		
2	l	276	Total	C	N	O	S	0	0
			2190	1391	348	435	16		
2	m	260	Total	C	N	O	S	0	0
			2053	1304	323	410	16		
2	n	277	Total	C	N	O	S	0	0
			2190	1391	348	435	16		
2	o	261	Total	C	N	O	S	0	0
			2059	1307	324	412	16		

- Molecule 3 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	397	Total 3163	C 2007	N 550	O 592	S 14	0	0
3	D	397	Total 3163	C 2007	N 550	O 592	S 14	0	0
3	E	397	Total 3163	C 2007	N 550	O 592	S 14	0	0
3	F	397	Total 3163	C 2007	N 550	O 592	S 14	0	0
3	G	397	Total 3163	C 2007	N 550	O 592	S 14	0	0
3	H	397	Total 3163	C 2007	N 550	O 592	S 14	0	0
3	I	397	Total 3163	C 2007	N 550	O 592	S 14	0	0
3	J	397	Total 3163	C 2007	N 550	O 592	S 14	0	0
3	K	397	Total 3163	C 2007	N 550	O 592	S 14	0	0
3	L	397	Total 3163	C 2007	N 550	O 592	S 14	0	0
3	M	397	Total 3163	C 2007	N 550	O 592	S 14	0	0
3	N	397	Total 3163	C 2007	N 550	O 592	S 14	0	0
3	O	397	Total 3163	C 2007	N 550	O 592	S 14	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

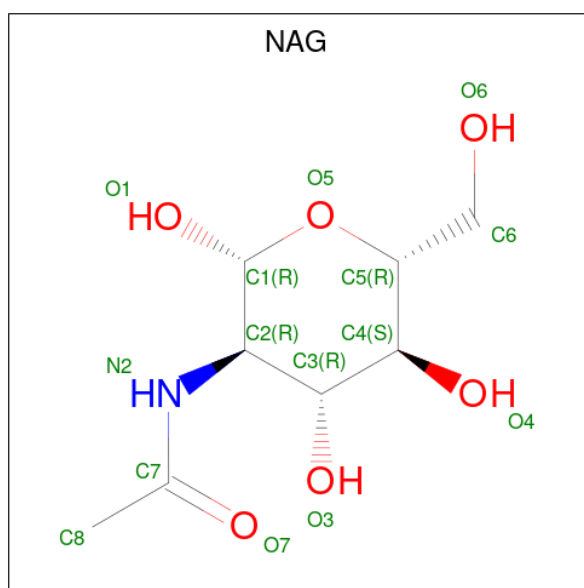
Mol	Chain	Residues	Atoms		AltConf
4	c	2	Total 2	Ca 2	0
4	d	2	Total 2	Ca 2	0
4	e	2	Total 2	Ca 2	0
4	f	2	Total 2	Ca 2	0
4	g	2	Total 2	Ca 2	0
4	h	2	Total 2	Ca 2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
4	i	2	Total	Ca	0
			2	2	
4	j	2	Total	Ca	0
			2	2	
4	k	2	Total	Ca	0
			2	2	
4	l	2	Total	Ca	0
			2	2	
4	m	2	Total	Ca	0
			2	2	
4	n	2	Total	Ca	0
			2	2	
4	o	2	Total	Ca	0
			2	2	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
5	d	1	Total	C	N	O	0
			15	8	1	6	
5	e	1	Total	C	N	O	0
			15	8	1	6	
5	f	1	Total	C	N	O	0
			15	8	1	6	
5	h	1	Total	C	N	O	0
			15	8	1	6	

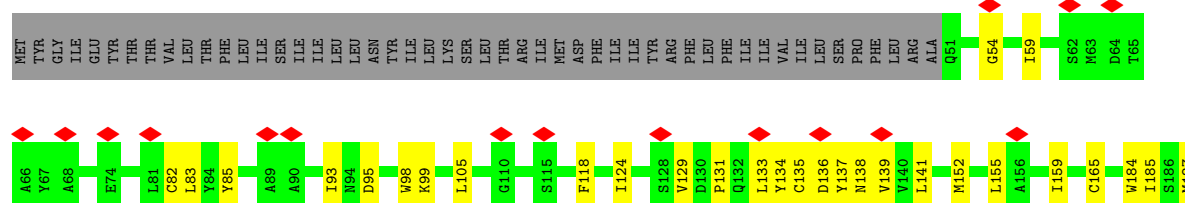
Continued on next page...

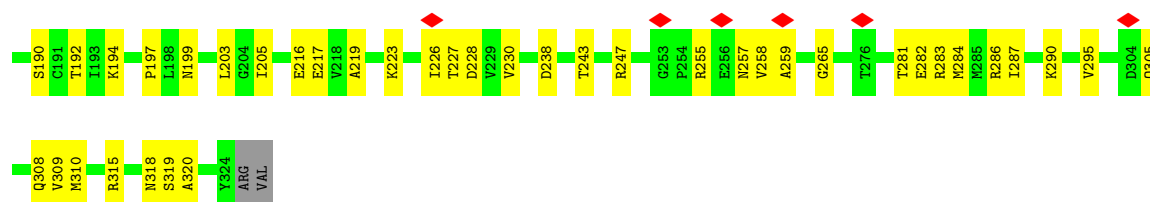
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
5	j	1	Total	C	N	O	0
			15	8	1	6	
5	k	1	Total	C	N	O	0
			15	8	1	6	
5	l	1	Total	C	N	O	0
			15	8	1	6	
5	m	1	Total	C	N	O	0
			15	8	1	6	
5	n	1	Total	C	N	O	0
			15	8	1	6	
5	o	1	Total	C	N	O	0
			15	8	1	6	

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

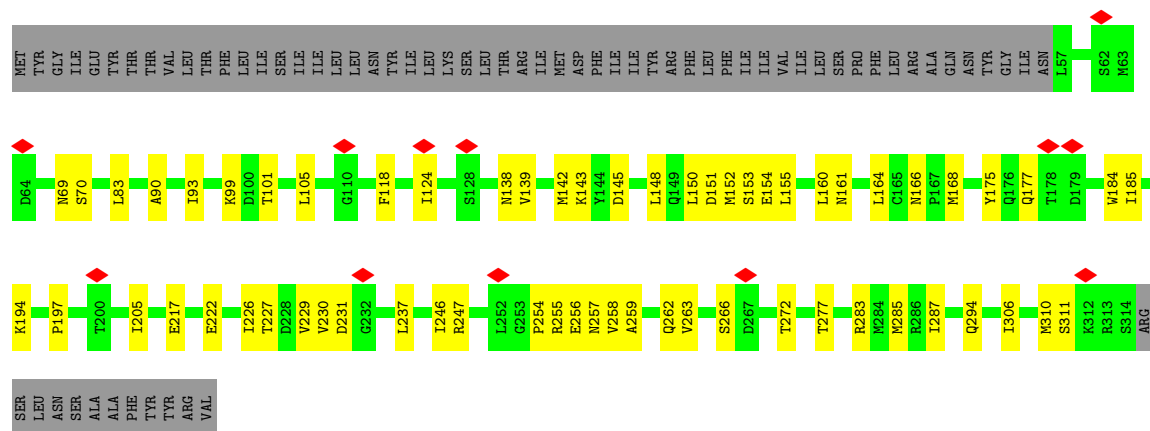
Mol	Chain	Residues	Atoms		AltConf
6	C	1	Total	Zn	0
			1	1	
6	H	1	Total	Zn	0
			1	1	
6	I	1	Total	Zn	0
			1	1	
6	L	1	Total	Zn	0
			1	1	
6	O	1	Total	Zn	0
			1	1	





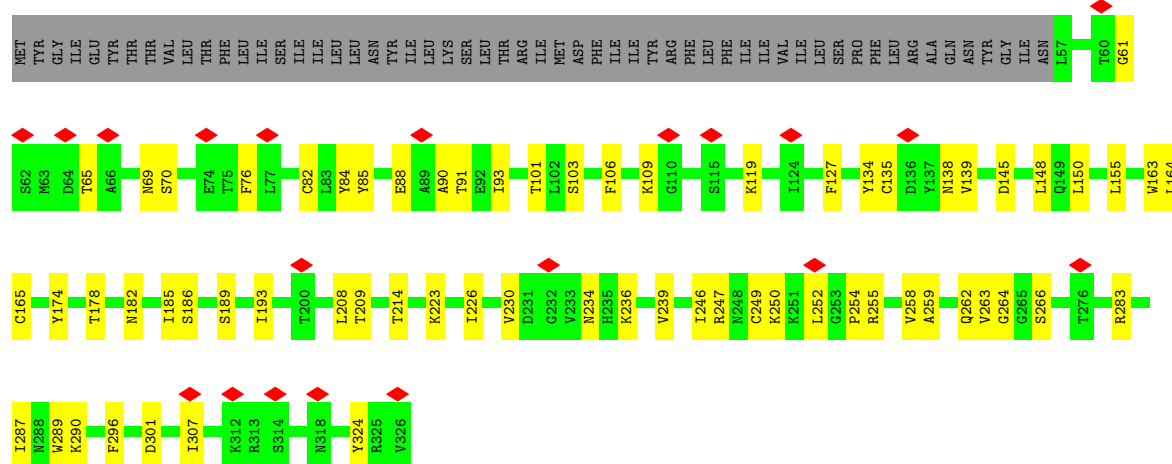
• Molecule 2: Outer capsid glycoprotein VP7

Chain d: 60% 19% 21%



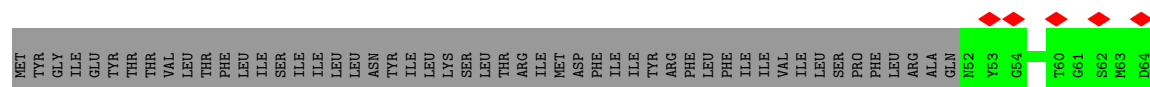
• Molecule 2: Outer capsid glycoprotein VP7

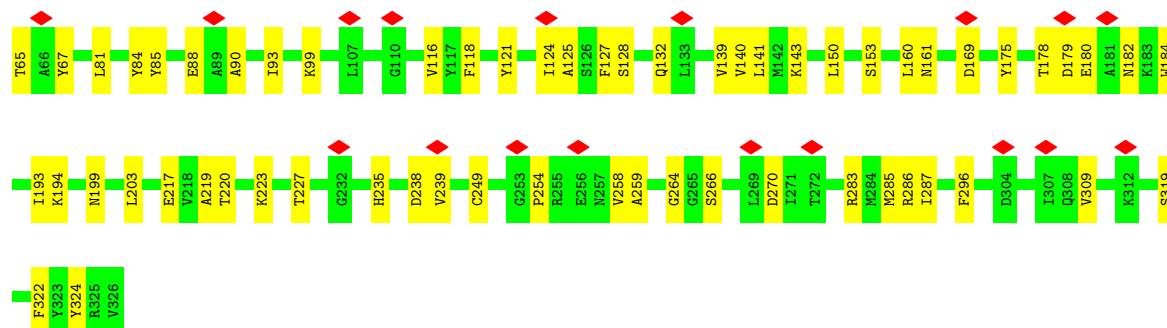
Chain e: 6% 63% 20% 17%



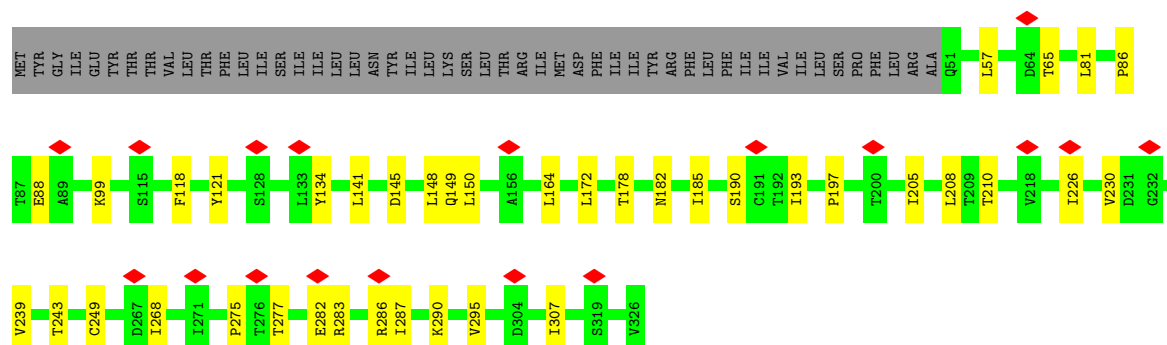
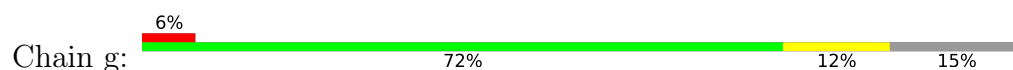
• Molecule 2: Outer capsid glycoprotein VP7

Chain f: 7% 66% 18% 16%

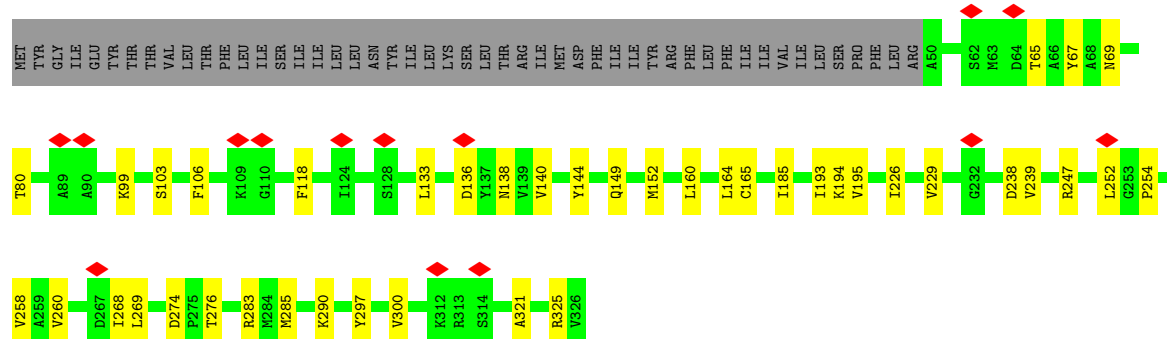




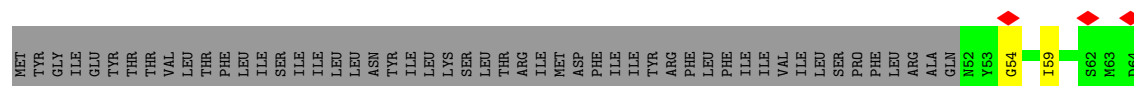
• Molecule 2: Outer capsid glycoprotein VP7

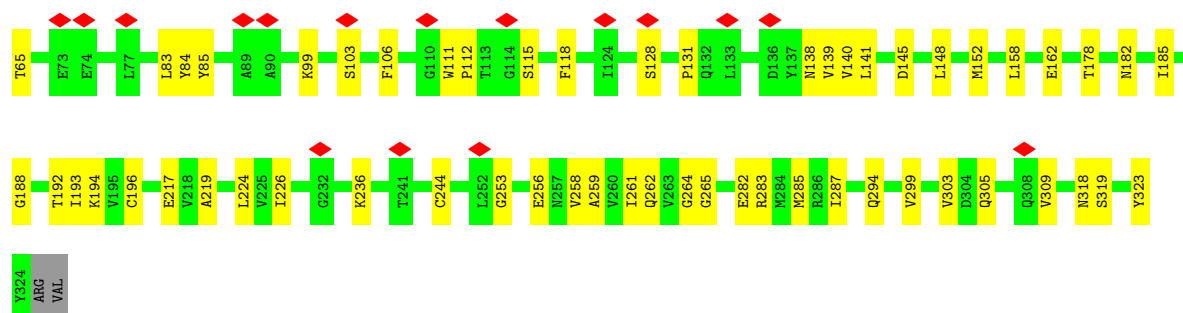


• Molecule 2: Outer capsid glycoprotein VP7



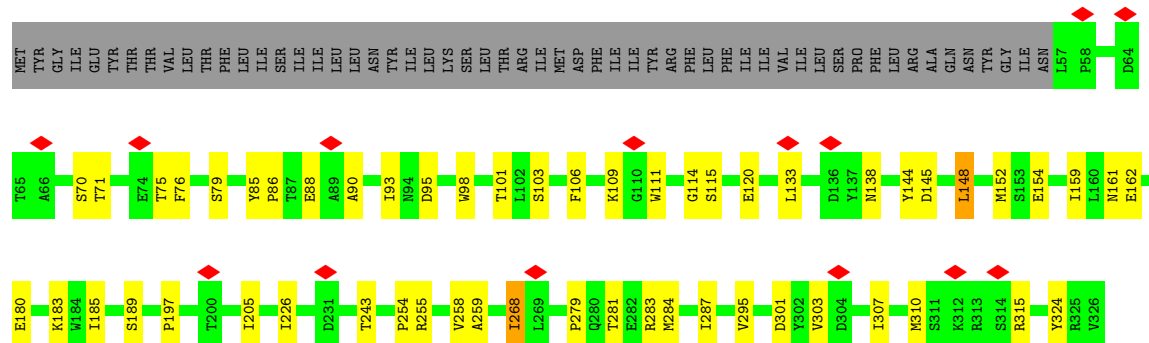
• Molecule 2: Outer capsid glycoprotein VP7





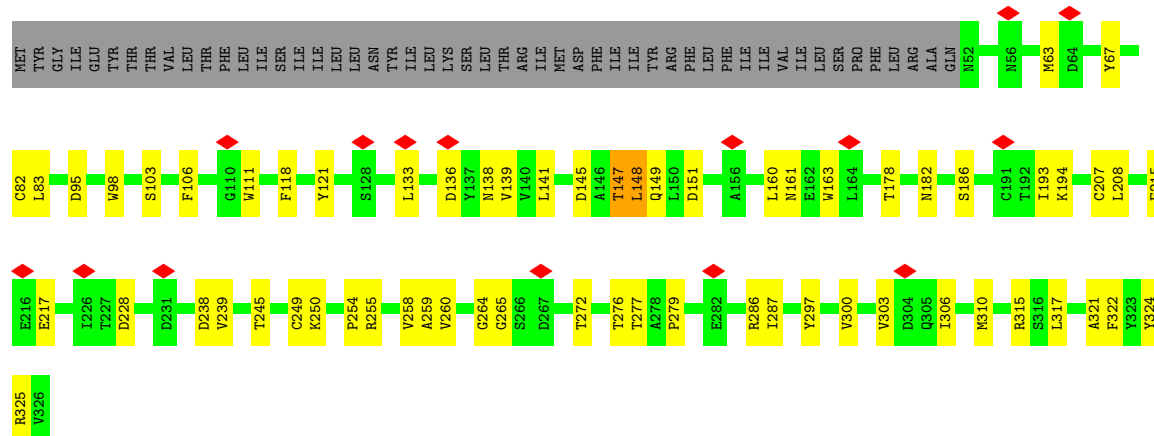
• Molecule 2: Outer capsid glycoprotein VP7

Chain j: 66% 16% 17%



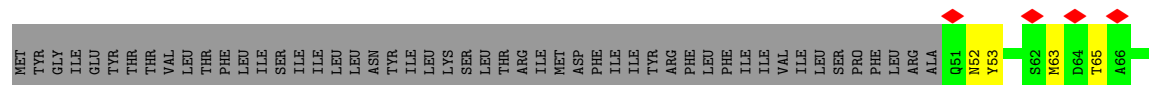
• Molecule 2: Outer capsid glycoprotein VP7

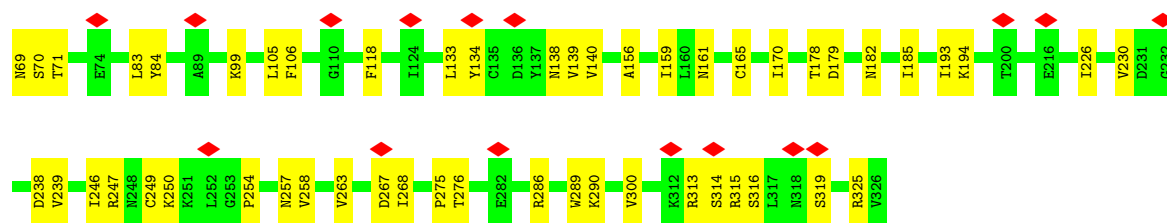
Chain k: 5% 65% 19% 16%



• Molecule 2: Outer capsid glycoprotein VP7

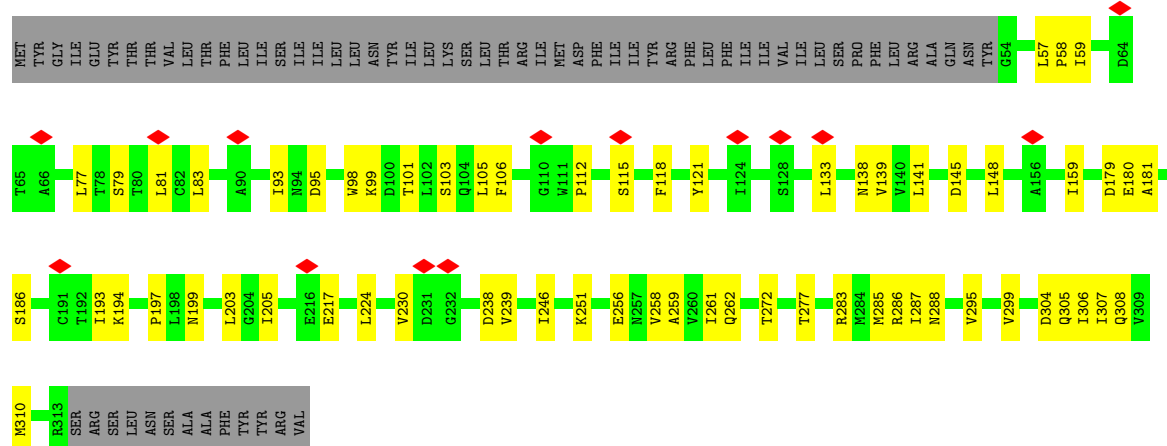
Chain l: 6% 68% 17% 15%





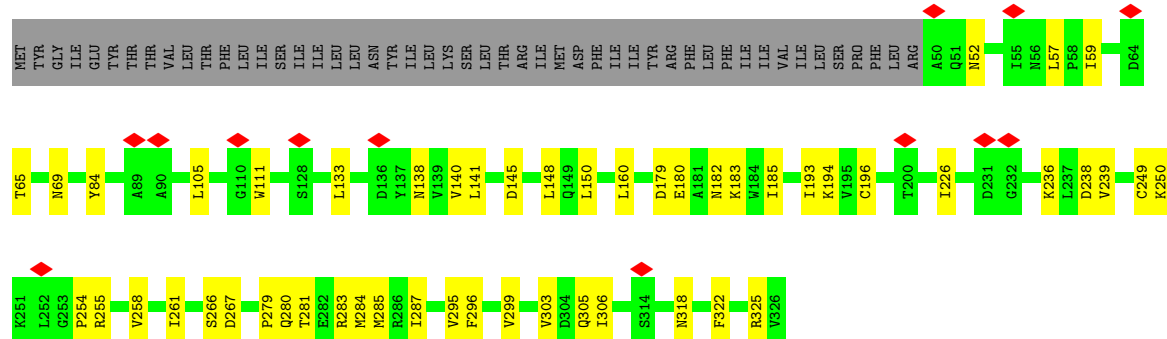
• Molecule 2: Outer capsid glycoprotein VP7

Chain m: 60% 19% 20%



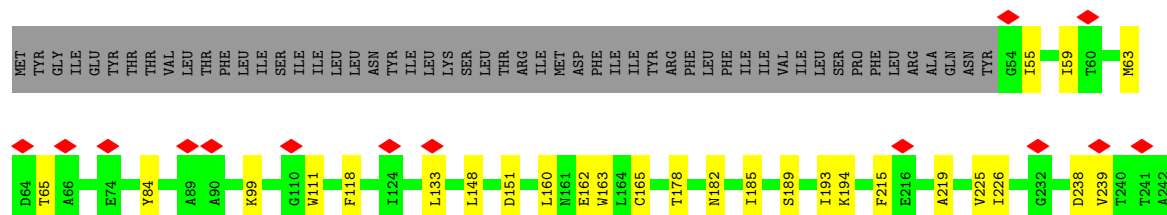
• Molecule 2: Outer capsid glycoprotein VP7

Chain n: 69% 16% 15%



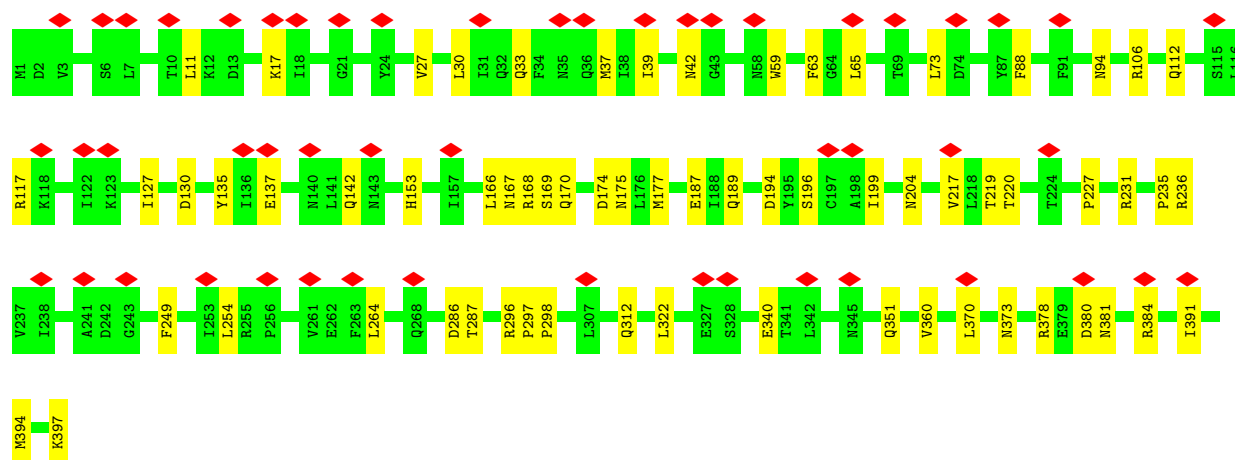
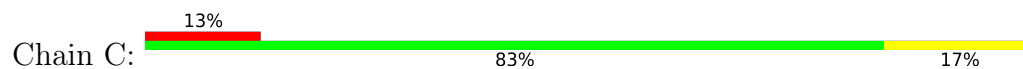
• Molecule 2: Outer capsid glycoprotein VP7

Chain o: 5% 67% 20%

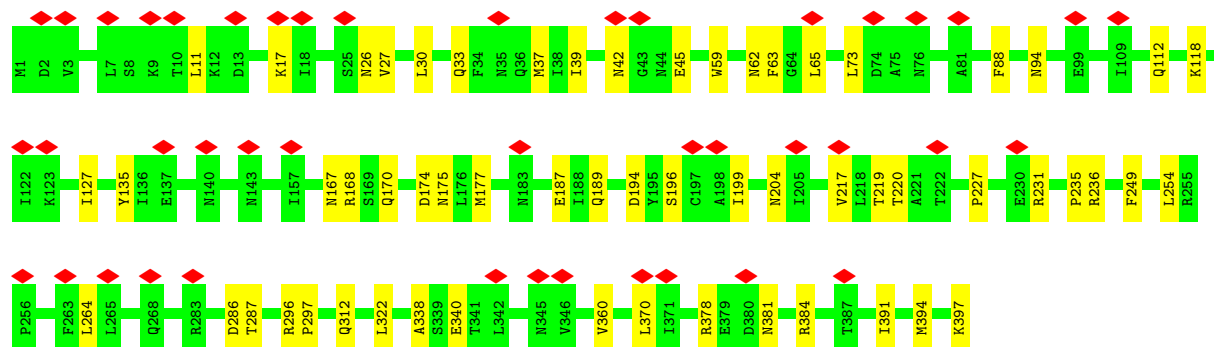
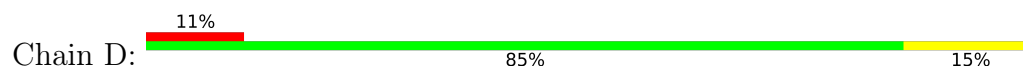




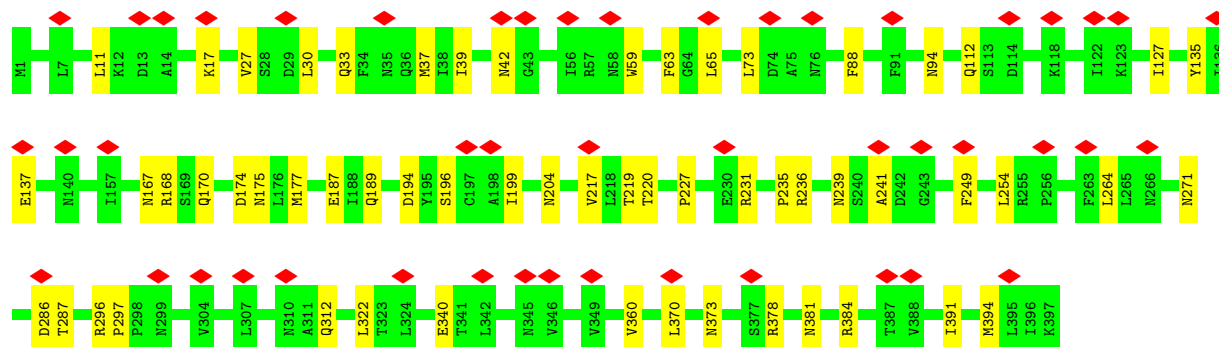
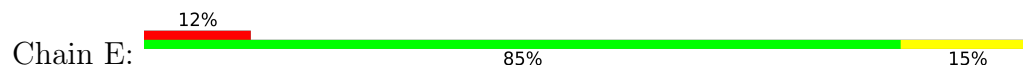
• Molecule 3: Intermediate capsid protein VP6



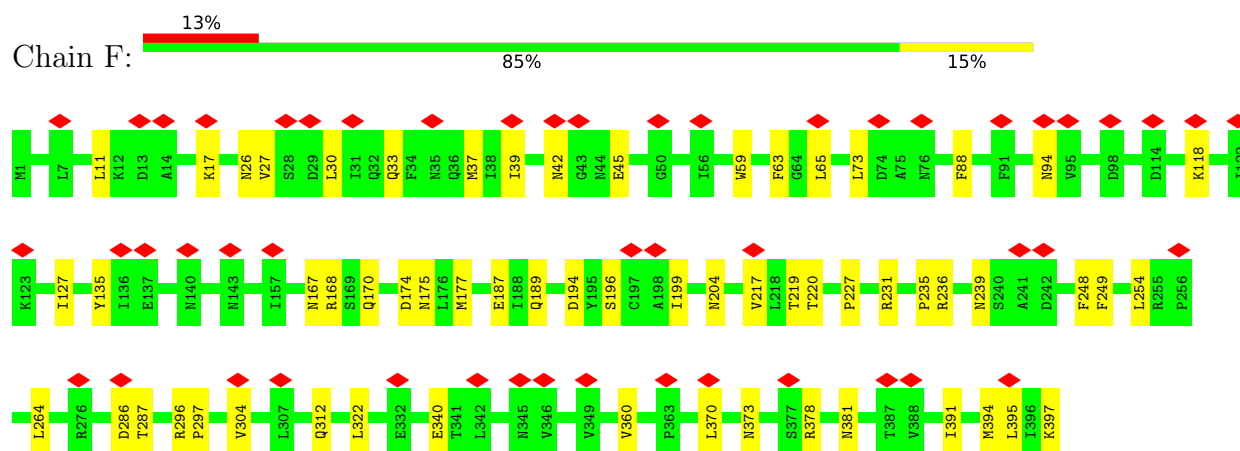
• Molecule 3: Intermediate capsid protein VP6



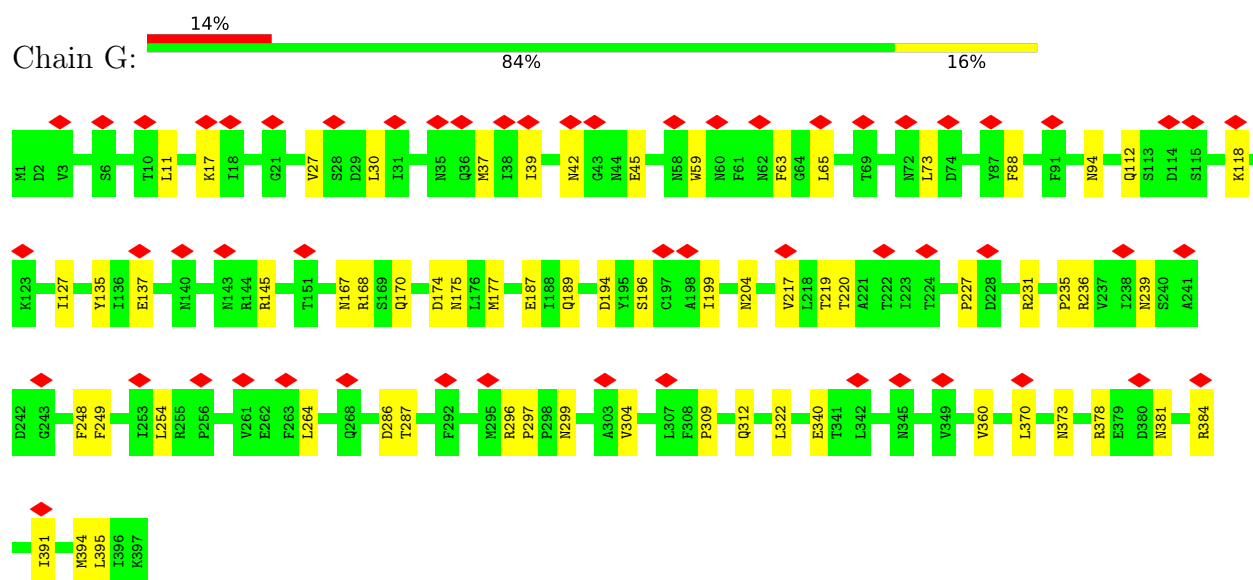
• Molecule 3: Intermediate capsid protein VP6



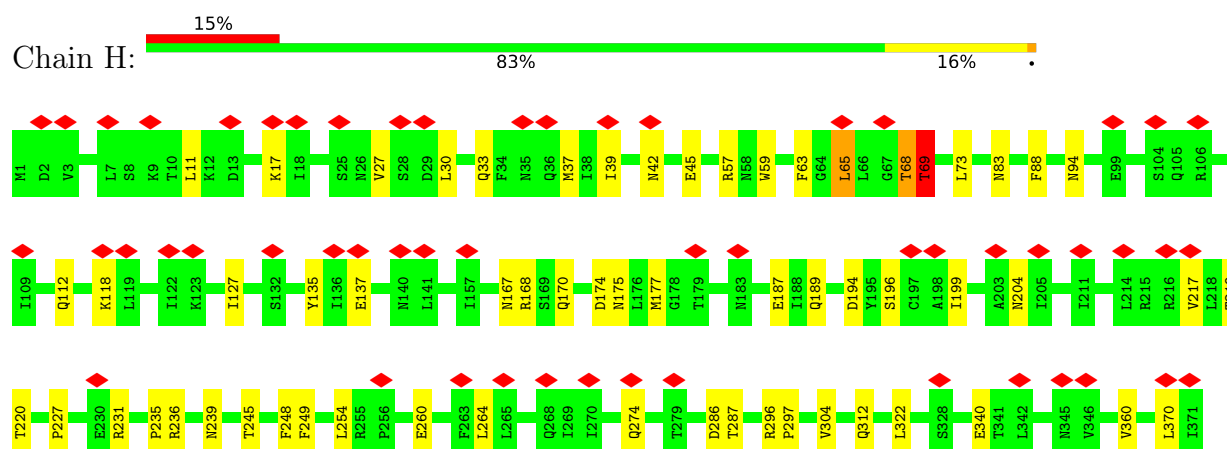
- Molecule 3: Intermediate capsid protein VP6

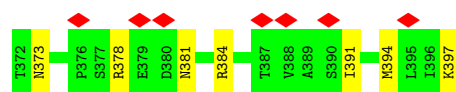


- Molecule 3: Intermediate capsid protein VP6

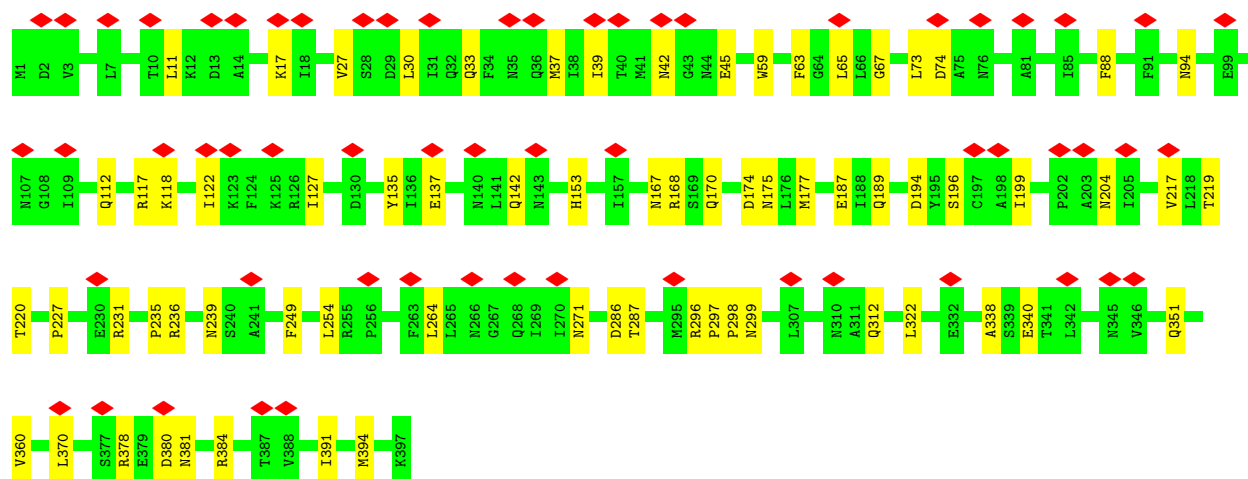
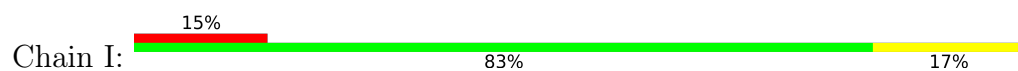


- Molecule 3: Intermediate capsid protein VP6

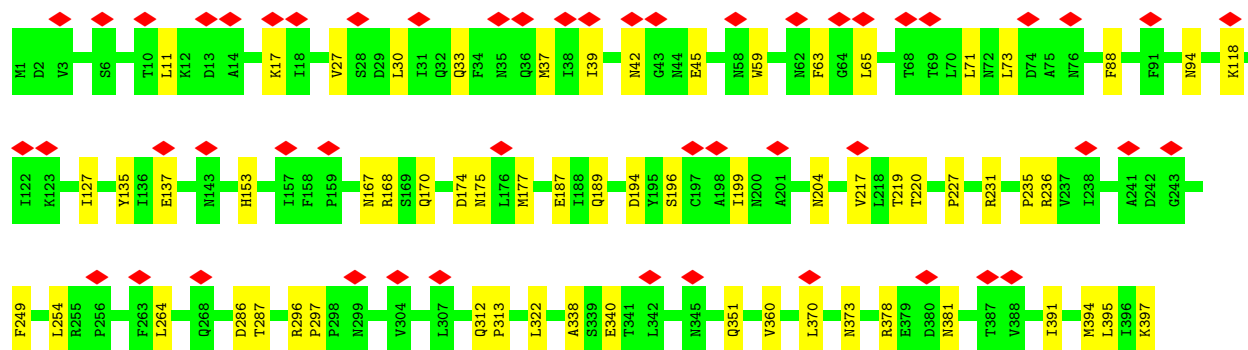
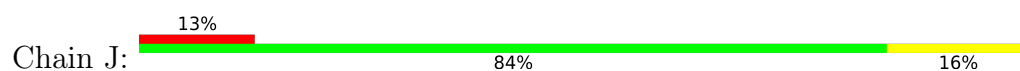




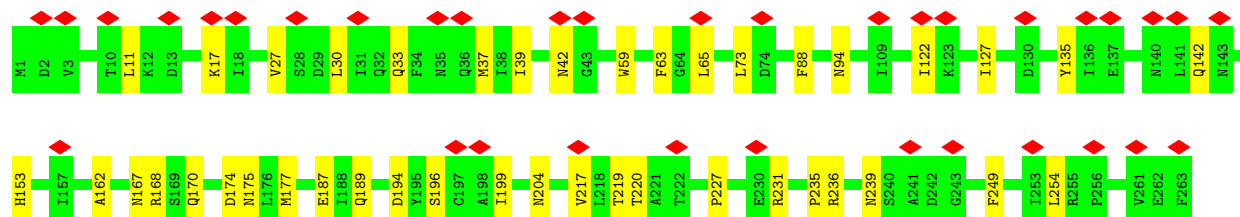
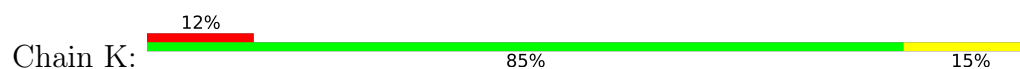
• Molecule 3: Intermediate capsid protein VP6

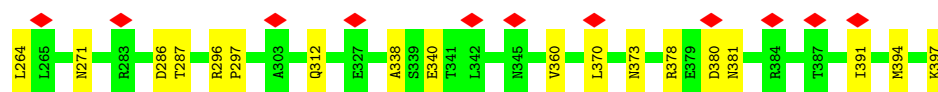


• Molecule 3: Intermediate capsid protein VP6

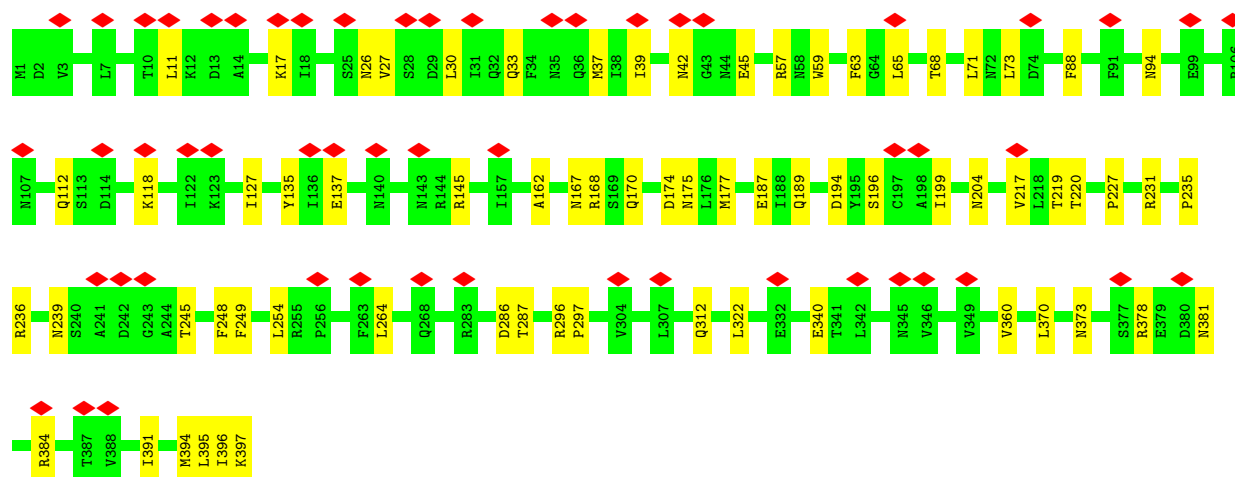
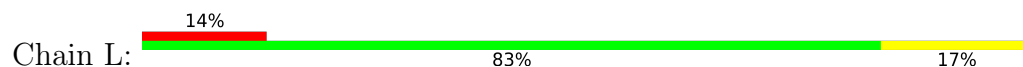


• Molecule 3: Intermediate capsid protein VP6

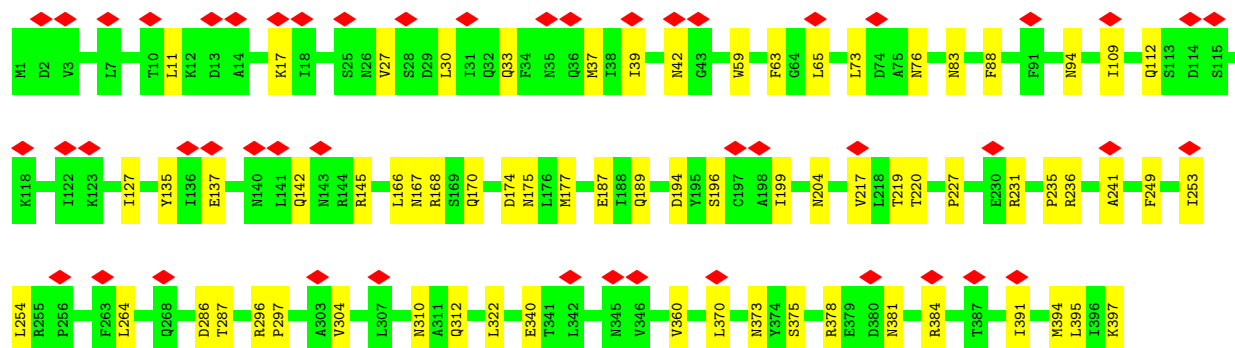
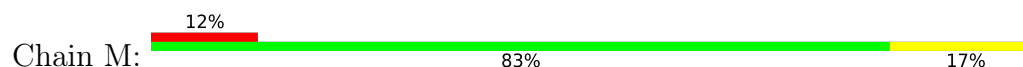




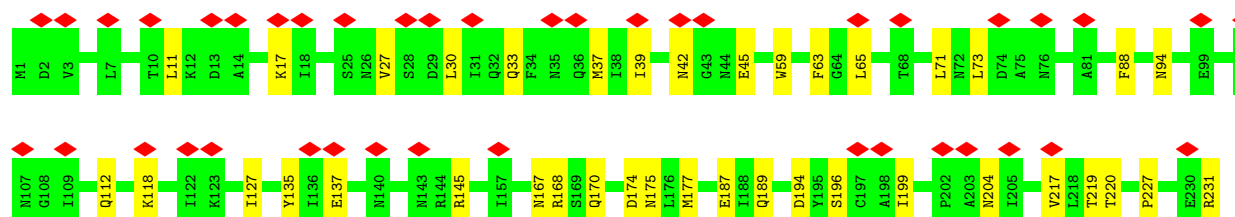
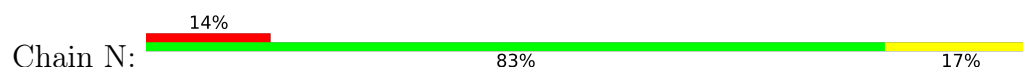
• Molecule 3: Intermediate capsid protein VP6

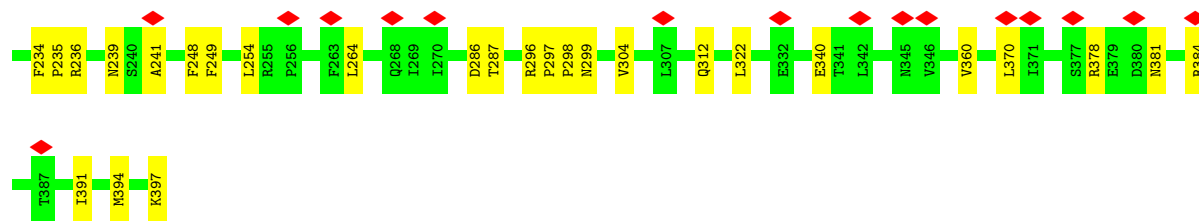


• Molecule 3: Intermediate capsid protein VP6

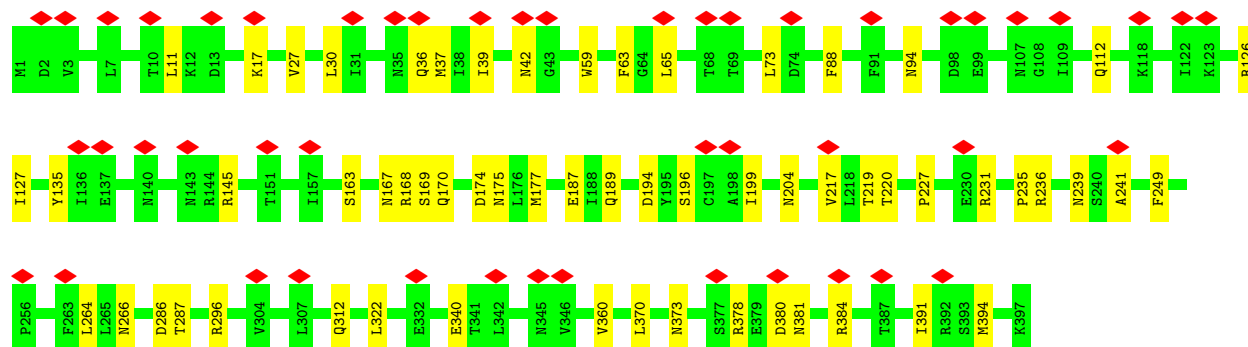
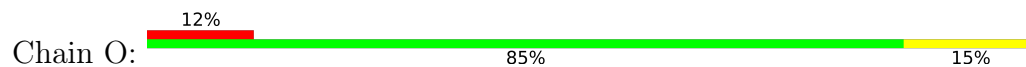


• Molecule 3: Intermediate capsid protein VP6





• Molecule 3: Intermediate capsid protein VP6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	10815	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	1072.0, 1072.0, 1072.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, ZN

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	0.31	0/6494	0.62	3/8806 (0.0%)
1	B	0.32	0/6661	0.65	2/9033 (0.0%)
2	c	0.29	0/2213	0.59	2/3023 (0.1%)
2	d	0.33	0/2081	0.60	0/2844
2	e	0.25	0/2186	0.55	0/2986
2	f	0.24	0/2227	0.55	0/3042
2	g	0.23	0/2231	0.52	0/3047
2	h	0.25	0/2236	0.56	0/3054
2	i	0.26	0/2209	0.57	0/3018
2	j	0.33	0/2186	0.67	2/2986 (0.1%)
2	k	0.29	0/2227	0.54	0/3042
2	l	0.28	0/2236	0.60	0/3054
2	m	0.27	0/2095	0.56	2/2863 (0.1%)
2	n	0.26	0/2236	0.54	0/3054
2	o	0.23	0/2101	0.55	0/2871
3	C	0.24	0/3234	0.49	0/4402
3	D	0.24	0/3234	0.49	0/4402
3	E	0.24	0/3234	0.49	0/4402
3	F	0.24	0/3234	0.49	0/4402
3	G	0.24	0/3234	0.49	0/4402
3	H	0.26	0/3234	0.54	1/4402 (0.0%)
3	I	0.24	0/3234	0.49	0/4402
3	J	0.24	0/3234	0.49	0/4402
3	K	0.24	0/3234	0.49	0/4402
3	L	0.24	0/3234	0.49	0/4402
3	M	0.24	0/3234	0.49	0/4402
3	N	0.24	0/3234	0.49	0/4402
3	O	0.25	0/3234	0.49	0/4402
All	All	0.27	0/83661	0.55	12/113949 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	69	THR	CA-CB-OG1	-6.00	100.61	109.60
2	j	95	ASP	CA-C-N	5.70	129.36	120.82
2	j	95	ASP	C-N-CA	5.70	129.36	120.82
1	A	219	THR	CA-C-N	5.48	132.00	121.54
1	A	219	THR	C-N-CA	5.48	132.00	121.54
2	c	93	ILE	CA-C-N	5.33	131.72	121.54
2	c	93	ILE	C-N-CA	5.33	131.72	121.54
2	m	93	ILE	CA-C-N	5.09	131.27	121.54
2	m	93	ILE	C-N-CA	5.09	131.27	121.54
1	B	808	SER	CA-C-N	5.08	131.24	121.54
1	B	808	SER	C-N-CA	5.08	131.24	121.54
1	A	219	THR	O-C-N	5.04	127.89	122.15

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	6377	0	6399	108	0
1	B	6540	0	6550	159	0
2	c	2167	0	2100	58	0
2	d	2039	0	1987	76	0
2	e	2141	0	2086	45	0
2	f	2181	0	2119	38	0
2	g	2185	0	2124	26	0
2	h	2190	0	2127	34	0
2	i	2163	0	2099	35	0
2	j	2141	0	2086	47	0
2	k	2181	0	2122	48	0
2	l	2190	0	2129	63	0
2	m	2053	0	2001	61	0
2	n	2190	0	2125	51	0
2	o	2059	0	2007	39	0
3	C	3163	0	3114	47	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	3163	0	3114	37	0
3	E	3163	0	3114	37	0
3	F	3163	0	3114	40	0
3	G	3163	0	3114	43	0
3	H	3163	0	3114	51	0
3	I	3163	0	3114	50	0
3	J	3163	0	3114	40	0
3	K	3163	0	3114	41	0
3	L	3163	0	3114	48	0
3	M	3163	0	3114	51	0
3	N	3163	0	3114	47	0
3	O	3163	0	3114	73	0
4	c	2	0	0	1	0
4	d	2	0	0	0	0
4	e	2	0	0	0	0
4	f	2	0	0	0	0
4	g	2	0	0	0	0
4	h	2	0	0	0	0
4	i	2	0	0	0	0
4	j	2	0	0	0	0
4	k	2	0	0	0	0
4	l	2	0	0	0	0
4	m	2	0	0	0	0
4	n	2	0	0	0	0
4	o	2	0	0	0	0
5	d	15	0	15	4	0
5	e	15	0	14	2	0
5	f	15	0	14	0	0
5	h	15	0	15	10	0
5	j	15	0	15	0	0
5	k	15	0	14	0	0
5	l	15	0	15	20	0
5	m	15	0	14	0	0
5	n	15	0	15	5	0
5	o	15	0	15	2	0
6	C	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	L	1	0	0	0	0
6	O	1	0	0	0	0
All	All	82097	0	80689	1315	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1315) 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:j:145:ASP:HB3	2:j:148:LEU:CD2	1.45	1.47
2:l:69:ASN:CG	5:l:401:NAG:H2	1.41	1.46
2:l:69:ASN:ND2	5:l:401:NAG:H2	1.19	1.43
2:l:69:ASN:OD1	5:l:401:NAG:C1	1.66	1.42
2:j:145:ASP:CB	2:j:148:LEU:HD21	1.51	1.38
1:B:838:ARG:HD3	3:O:126:ARG:NH1	1.35	1.37
2:d:145:ASP:CB	2:d:148:LEU:HD21	1.55	1.35
2:d:145:ASP:HB2	2:d:148:LEU:CD2	1.58	1.30
2:l:69:ASN:HD21	5:l:401:NAG:C2	1.50	1.25
2:m:261:ILE:HG12	2:m:285:MET:SD	1.78	1.22
2:l:69:ASN:ND2	5:l:401:NAG:C2	2.02	1.22
1:B:310:LEU:CD1	1:B:312:LEU:HG	1.73	1.19
1:A:213:ILE:O	1:A:219:THR:HG21	1.42	1.18
2:l:69:ASN:OD1	5:l:401:NAG:O1	1.61	1.15
1:B:838:ARG:CD	3:O:126:ARG:NH1	2.08	1.14
2:n:280:GLN:HA	2:n:284:MET:HE1	1.29	1.14
2:l:69:ASN:OD1	5:l:401:NAG:C2	1.94	1.14
2:d:83:LEU:HD21	2:d:118:PHE:CD1	1.82	1.14
1:B:838:ARG:NH2	3:O:36:GLN:HE22	1.46	1.13
2:l:69:ASN:CG	5:l:401:NAG:C2	2.21	1.13
2:n:280:GLN:HA	2:n:284:MET:CE	1.80	1.12
2:n:281:THR:H	2:n:284:MET:HE2	1.17	1.09
2:o:65:THR:HG22	3:O:239:ASN:ND2	1.66	1.09
2:o:65:THR:CG2	3:O:239:ASN:ND2	2.16	1.08
1:B:473:TRP:NE1	1:B:508:LEU:HD13	1.69	1.07
2:o:254:PRO:HD3	3:O:312:GLN:HG2	1.41	1.02
5:d:401:NAG:H82	5:d:401:NAG:H1	1.41	1.02
1:B:310:LEU:HD11	1:B:312:LEU:HG	1.43	1.00
1:B:355:LEU:HD23	1:B:355:LEU:H	1.27	0.99
2:o:65:THR:HG22	3:O:239:ASN:HD21	1.17	0.99
2:l:69:ASN:OD1	5:l:401:NAG:H2	1.54	0.98
2:d:145:ASP:CB	2:d:148:LEU:CD2	2.28	0.97
2:d:83:LEU:HD23	2:d:83:LEU:H	1.31	0.96
3:M:145:ARG:NH2	3:O:380:ASP:OD1	1.99	0.96
2:h:69:ASN:ND2	5:h:401:NAG:C1	2.29	0.95
1:B:714:LEU:CD2	1:B:722:TYR:HB3	1.97	0.95
2:j:148:LEU:HD23	2:j:148:LEU:H	1.28	0.95
1:B:310:LEU:HD12	1:B:312:LEU:HG	1.46	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:838:ARG:HH22	3:O:36:GLN:HE22	1.00	0.94
2:n:281:THR:N	2:n:284:MET:HE2	1.81	0.93
2:h:69:ASN:CG	5:h:401:NAG:HO1	1.76	0.93
2:k:83:LEU:HD21	2:k:118:PHE:CE1	2.03	0.93
1:B:838:ARG:HH22	3:O:36:GLN:NE2	1.67	0.92
2:d:148:LEU:HD23	2:d:148:LEU:H	1.32	0.92
2:m:261:ILE:CG1	2:m:285:MET:SD	2.58	0.92
2:o:59:ILE:HG22	3:O:241:ALA:HB2	1.52	0.92
1:B:128:PHE:CE1	1:B:152:LEU:HD13	2.06	0.90
2:m:59:ILE:HG13	3:M:241:ALA:CB	2.04	0.88
1:A:801:LEU:HD21	1:A:829:LYS:HZ3	1.37	0.87
2:d:83:LEU:HD21	2:d:118:PHE:HD1	1.39	0.87
2:l:69:ASN:ND2	5:l:401:NAG:C3	2.38	0.86
1:B:473:TRP:CE2	1:B:508:LEU:HD13	2.11	0.86
2:o:59:ILE:CG2	3:O:241:ALA:CB	2.54	0.85
2:l:69:ASN:OD1	5:l:401:NAG:O5	1.93	0.85
1:B:838:ARG:HD3	3:O:126:ARG:HH11	1.05	0.84
2:d:166:ASN:O	2:d:247:ARG:HB2	1.78	0.84
2:c:83:LEU:H	2:c:83:LEU:HD23	1.41	0.83
2:e:69:ASN:OD1	2:e:70:SER:N	2.12	0.83
1:B:310:LEU:HD11	1:B:312:LEU:CG	2.08	0.82
2:k:138:ASN:O	2:k:258:VAL:HA	1.80	0.82
2:l:268:ILE:HG12	2:m:286:ARG:HH22	1.44	0.81
2:j:76:PHE:CE1	2:j:307:ILE:CD1	2.63	0.81
2:o:65:THR:HG23	3:O:239:ASN:ND2	1.96	0.81
2:h:69:ASN:ND2	5:h:401:NAG:O5	2.13	0.80
1:B:310:LEU:CD1	1:B:312:LEU:CG	2.58	0.80
2:o:59:ILE:CG2	3:O:241:ALA:HB2	2.11	0.80
2:d:168:MET:HE3	2:d:175:TYR:CG	2.16	0.80
2:m:261:ILE:HA	2:m:285:MET:HG3	1.63	0.79
1:B:838:ARG:CD	3:O:126:ARG:HH12	1.93	0.79
2:j:145:ASP:CB	2:j:148:LEU:CD2	2.30	0.79
2:o:55:ILE:HA	3:O:169:SER:O	1.83	0.79
2:l:69:ASN:HD21	5:l:401:NAG:C3	1.95	0.78
3:H:39:ILE:HD11	3:H:65:LEU:HD11	1.65	0.78
3:M:375:SER:HB3	3:O:266:ASN:OD1	1.83	0.78
2:j:303:VAL:O	2:j:307:ILE:HG13	1.83	0.77
2:l:69:ASN:HD21	5:l:401:NAG:H2	0.95	0.77
2:d:150:LEU:HD22	2:d:153:SER:HB3	1.66	0.77
2:h:69:ASN:HD21	5:h:401:NAG:C1	1.94	0.77
2:j:148:LEU:CD2	2:j:148:LEU:H	1.98	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:838:ARG:CB	3:O:126:ARG:HH12	1.98	0.77
1:A:801:LEU:HD21	1:A:829:LYS:NZ	2.00	0.77
2:d:83:LEU:HD21	2:d:118:PHE:CE1	2.19	0.77
2:c:216:GLU:OE2	4:c:401:CA:CA	1.61	0.76
1:B:714:LEU:HD21	1:B:722:TYR:HB3	1.66	0.76
2:d:83:LEU:H	2:d:83:LEU:CD2	1.99	0.76
2:n:69:ASN:OD1	5:n:401:NAG:H1	1.85	0.76
2:o:59:ILE:HG22	3:O:241:ALA:CB	2.15	0.76
2:j:76:PHE:CE1	2:j:307:ILE:HD12	2.20	0.76
2:k:317:LEU:O	2:k:317:LEU:HD23	1.85	0.75
3:H:39:ILE:HG13	3:H:65:LEU:HD21	1.68	0.75
2:e:69:ASN:HD22	5:e:401:NAG:H5	1.52	0.75
1:B:128:PHE:CD1	1:B:152:LEU:HD13	2.21	0.74
2:d:148:LEU:CD2	2:d:148:LEU:H	1.99	0.74
2:k:83:LEU:CD2	2:k:118:PHE:CE1	2.70	0.74
2:m:286:ARG:HD2	2:m:286:ARG:C	2.13	0.74
1:B:128:PHE:HE1	1:B:152:LEU:HD13	1.51	0.73
2:h:133:LEU:HD12	2:h:133:LEU:O	1.89	0.73
1:B:355:LEU:H	1:B:355:LEU:CD2	2.00	0.72
2:c:139:VAL:HG12	2:c:259:ALA:HB3	1.72	0.72
2:d:150:LEU:HD13	2:d:154:GLU:HG2	1.71	0.72
2:j:76:PHE:CZ	2:j:307:ILE:HD12	2.23	0.72
2:o:65:THR:CG2	3:O:239:ASN:HD21	1.90	0.71
1:B:127:ILE:HG22	1:B:152:LEU:CD1	2.20	0.71
2:n:280:GLN:CA	2:n:284:MET:CE	2.66	0.71
1:B:272:ILE:HG12	1:B:856:LEU:CD1	2.19	0.71
1:A:740:LEU:HD21	1:A:749:ILE:HD13	1.71	0.71
2:e:164:LEU:O	2:e:249:CYS:HA	1.90	0.71
2:d:150:LEU:CD1	2:d:154:GLU:HG2	2.20	0.71
1:B:355:LEU:HD22	1:B:537:LEU:HD11	1.71	0.71
3:C:33:GLN:OE1	3:D:26:ASN:ND2	2.24	0.70
2:d:150:LEU:HD13	2:d:150:LEU:O	1.92	0.70
2:n:69:ASN:OD1	5:n:401:NAG:C1	2.38	0.70
1:B:272:ILE:HG12	1:B:856:LEU:HD11	1.73	0.70
2:j:148:LEU:HD23	2:j:148:LEU:N	2.05	0.70
2:k:111:TRP:HE1	2:k:303:VAL:HG11	1.56	0.69
2:n:194:LYS:HB2	2:n:238:ASP:HB3	1.74	0.69
2:o:111:TRP:HE1	2:o:303:VAL:HG11	1.58	0.69
5:d:401:NAG:H1	5:d:401:NAG:C8	2.09	0.69
2:m:194:LYS:HB2	2:m:238:ASP:HB3	1.75	0.68
1:B:194:ASN:HD21	1:B:227:ILE:HG22	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:83:LEU:HD23	2:c:83:LEU:N	2.08	0.68
2:e:185:ILE:HG12	2:e:226:ILE:HG12	1.75	0.68
2:j:138:ASN:O	2:j:258:VAL:HA	1.94	0.68
3:C:380:ASP:OD1	3:N:145:ARG:NH2	2.27	0.68
1:A:430:GLN:O	1:A:434:ILE:HG12	1.93	0.68
2:c:185:ILE:HG12	2:c:226:ILE:HG12	1.75	0.68
1:A:491:LEU:HD21	1:A:493:GLN:HE21	1.59	0.67
2:l:69:ASN:ND2	5:l:401:NAG:O3	2.27	0.67
5:l:401:NAG:O1	5:l:401:NAG:O7	2.12	0.67
1:B:746:TYR:CE2	1:B:792:ARG:HB3	2.29	0.67
5:d:401:NAG:H82	5:d:401:NAG:C1	2.23	0.67
2:n:148:LEU:HD12	2:n:148:LEU:O	1.94	0.67
2:o:194:LYS:HB2	2:o:238:ASP:HB3	1.77	0.67
1:A:696:ARG:HD3	1:A:830:GLN:HG3	1.77	0.66
2:k:317:LEU:HD23	2:k:317:LEU:C	2.20	0.66
1:B:619:ARG:HE	1:B:650:ARG:HB3	1.60	0.66
3:G:304:VAL:HG22	3:H:248:PHE:HB2	1.78	0.66
2:n:138:ASN:O	2:n:258:VAL:HA	1.95	0.66
2:d:145:ASP:HB3	2:d:148:LEU:CD2	2.25	0.66
2:d:145:ASP:HB2	2:d:148:LEU:HD21	0.73	0.66
2:i:138:ASN:O	2:i:258:VAL:HA	1.96	0.66
2:k:194:LYS:HB2	2:k:238:ASP:HB3	1.76	0.66
1:A:435:ASN:ND2	1:A:446:ARG:O	2.29	0.65
2:d:184:TRP:HB2	2:d:227:THR:HB	1.78	0.65
2:m:57:LEU:HD12	2:m:58:PRO:HD2	1.77	0.65
2:m:58:PRO:HA	3:M:166:LEU:O	1.96	0.65
2:o:65:THR:HG23	3:O:239:ASN:HD22	1.61	0.65
1:A:397:ASP:HB2	1:A:577:LYS:HD2	1.78	0.65
2:c:83:LEU:HB3	2:c:139:VAL:HG23	1.77	0.65
3:L:397:LYS:NZ	3:N:137:GLU:OE1	2.30	0.65
2:d:83:LEU:CD2	2:d:118:PHE:CD1	2.72	0.65
1:B:838:ARG:NH2	3:O:36:GLN:NE2	2.30	0.65
2:g:185:ILE:HG12	2:g:226:ILE:HG12	1.79	0.65
2:d:139:VAL:HG12	2:d:259:ALA:HB3	1.79	0.65
1:A:130:PRO:HA	1:A:149:TYR:O	1.97	0.65
2:k:83:LEU:HD12	2:k:83:LEU:O	1.97	0.65
2:d:151:ASP:OD1	2:e:290:LYS:NZ	2.28	0.65
2:l:179:ASP:OD1	2:l:250:LYS:NZ	2.30	0.64
2:o:55:ILE:HG13	3:O:169:SER:O	1.97	0.64
2:d:185:ILE:HG12	2:d:226:ILE:HG12	1.78	0.64
1:B:765:LEU:HD13	1:B:799:PRO:HD2	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:76:PHE:HE1	2:j:307:ILE:CD1	2.08	0.64
2:j:148:LEU:HG	2:j:148:LEU:O	1.98	0.64
2:f:139:VAL:HG12	2:f:259:ALA:HB3	1.80	0.64
2:j:76:PHE:HE1	2:j:307:ILE:HD13	1.62	0.64
2:j:145:ASP:CG	2:j:148:LEU:CD2	2.70	0.64
3:I:137:GLU:OE1	3:J:397:LYS:NZ	2.30	0.64
1:B:355:LEU:HD23	1:B:355:LEU:N	2.08	0.63
3:M:375:SER:CB	3:O:266:ASN:OD1	2.46	0.63
2:c:228:ASP:H	2:d:294:GLN:HE22	1.44	0.63
2:j:162:GLU:HB3	2:j:315:ARG:HH11	1.62	0.63
1:B:467:ASN:HD21	1:B:514:GLN:HG2	1.63	0.63
3:F:26:ASN:ND2	3:H:33:GLN:OE1	2.30	0.63
2:d:150:LEU:HD22	2:d:150:LEU:O	1.99	0.63
1:A:687:ILE:O	1:A:691:MET:HB2	1.99	0.63
2:k:145:ASP:OD1	2:k:148:LEU:HD11	1.98	0.62
1:B:838:ARG:CD	3:O:126:ARG:HH11	1.87	0.62
3:H:175:ASN:HB2	3:H:312:GLN:HE22	1.65	0.62
3:M:175:ASN:HB2	3:M:312:GLN:HE22	1.65	0.62
1:B:220:GLU:OE2	3:O:39:ILE:HG21	2.00	0.62
3:L:175:ASN:HB2	3:L:312:GLN:HE22	1.65	0.62
1:B:124:LEU:HD11	1:B:202:VAL:HG13	1.81	0.62
1:B:285:ASN:HD21	1:B:871:VAL:H	1.46	0.62
3:K:175:ASN:HB2	3:K:312:GLN:HE22	1.65	0.62
3:N:175:ASN:HB2	3:N:312:GLN:HE22	1.65	0.62
1:B:127:ILE:O	1:B:152:LEU:HD12	2.00	0.62
2:o:133:LEU:O	2:o:255:ARG:NH2	2.32	0.62
3:O:175:ASN:HB2	3:O:312:GLN:HE22	1.65	0.62
2:n:69:ASN:CG	5:n:401:NAG:O1	2.43	0.62
3:G:175:ASN:HB2	3:G:312:GLN:HE22	1.65	0.62
2:c:258:VAL:O	2:c:283:ARG:NH1	2.33	0.62
2:e:258:VAL:O	2:e:283:ARG:NH1	2.33	0.62
1:A:121:GLN:HB2	1:A:180:PRO:HB3	1.81	0.62
2:c:59:ILE:HD11	3:C:166:LEU:HD12	1.82	0.62
2:m:59:ILE:CG1	3:M:241:ALA:CB	2.78	0.62
2:k:145:ASP:OD1	2:k:148:LEU:CD1	2.47	0.61
3:E:175:ASN:HB2	3:E:312:GLN:HE22	1.65	0.61
3:J:175:ASN:HB2	3:J:312:GLN:HE22	1.64	0.61
1:A:126:ARG:HG3	1:A:153:LYS:HD2	1.82	0.61
2:n:69:ASN:OD1	5:n:401:NAG:O1	2.18	0.61
3:F:397:LYS:NZ	3:H:137:GLU:OE1	2.31	0.61
2:d:148:LEU:HD23	2:d:148:LEU:N	2.07	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:175:ASN:HB2	3:F:312:GLN:HE22	1.65	0.61
1:A:434:ILE:HG22	1:A:439:TYR:CE2	2.35	0.61
1:B:380:CYS:HB2	1:B:582:SER:HB3	1.83	0.61
2:h:69:ASN:ND2	5:h:401:NAG:H1	2.11	0.61
2:h:194:LYS:HB2	2:h:238:ASP:HB3	1.83	0.61
2:j:111:TRP:HZ2	2:j:307:ILE:HD11	1.66	0.61
3:C:175:ASN:HB2	3:C:312:GLN:HE22	1.65	0.61
3:F:304:VAL:HG22	3:G:248:PHE:HB2	1.82	0.61
2:n:69:ASN:CG	5:n:401:NAG:HO1	2.08	0.61
2:m:59:ILE:HG13	3:M:241:ALA:HB2	1.82	0.61
3:C:137:GLU:OE1	3:D:397:LYS:NZ	2.33	0.61
3:D:175:ASN:HB2	3:D:312:GLN:HE22	1.65	0.61
3:I:175:ASN:HB2	3:I:312:GLN:HE22	1.65	0.61
2:j:76:PHE:CE1	2:j:307:ILE:HD13	2.34	0.61
3:N:264:LEU:HB2	3:N:287:THR:HB	1.83	0.61
3:G:264:LEU:HB2	3:G:287:THR:HB	1.83	0.60
1:B:444:MET:HE1	1:B:464:GLN:HB3	1.83	0.60
3:D:264:LEU:HB2	3:D:287:THR:HB	1.83	0.60
3:L:264:LEU:HB2	3:L:287:THR:HB	1.83	0.60
3:O:264:LEU:HB2	3:O:287:THR:HB	1.83	0.60
2:g:150:LEU:HB3	2:h:290:LYS:HE2	1.83	0.60
2:c:184:TRP:HB2	2:c:227:THR:HB	1.83	0.60
3:H:264:LEU:HB2	3:H:287:THR:HB	1.83	0.60
3:E:264:LEU:HB2	3:E:287:THR:HB	1.83	0.60
3:J:264:LEU:HB2	3:J:287:THR:HB	1.83	0.60
3:M:370:LEU:HG	3:M:378:ARG:HD3	1.84	0.60
1:B:312:LEU:HD23	1:B:316:PHE:HD2	1.66	0.60
2:l:178:THR:H	2:l:182:ASN:HD22	1.49	0.60
3:O:370:LEU:HG	3:O:378:ARG:HD3	1.84	0.60
2:c:281:THR:HG22	2:c:284:MET:HE2	1.83	0.60
2:n:180:GLU:O	2:n:183:LYS:NZ	2.35	0.60
3:D:370:LEU:HG	3:D:378:ARG:HD3	1.84	0.60
3:M:264:LEU:HB2	3:M:287:THR:HB	1.83	0.60
3:C:370:LEU:HG	3:C:378:ARG:HD3	1.84	0.60
3:G:235:PRO:HA	3:G:249:PHE:O	2.02	0.60
3:M:235:PRO:HA	3:M:249:PHE:O	2.02	0.60
3:E:370:LEU:HG	3:E:378:ARG:HD3	1.84	0.60
3:L:235:PRO:HA	3:L:249:PHE:O	2.02	0.60
2:d:83:LEU:HD23	2:d:83:LEU:N	2.10	0.60
2:f:193:ILE:HG12	2:f:239:VAL:HG22	1.84	0.60
3:H:370:LEU:HG	3:H:378:ARG:HD3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HE2	1:A:849:THR:HG22	1.84	0.59
2:l:290:LYS:HE2	2:n:150:LEU:HB3	1.84	0.59
3:F:264:LEU:HB2	3:F:287:THR:HB	1.83	0.59
2:d:83:LEU:CD2	2:d:118:PHE:HD1	2.10	0.59
3:J:370:LEU:HG	3:J:378:ARG:HD3	1.84	0.59
3:K:235:PRO:HA	3:K:249:PHE:O	2.02	0.59
3:L:248:PHE:HB2	3:N:304:VAL:HG22	1.82	0.59
1:A:396:LEU:HD23	1:A:580:LEU:HD11	1.83	0.59
2:e:178:THR:H	2:e:182:ASN:HD21	1.50	0.59
3:H:235:PRO:HA	3:H:249:PHE:O	2.02	0.59
3:O:235:PRO:HA	3:O:249:PHE:O	2.02	0.59
2:e:138:ASN:O	2:e:258:VAL:HA	2.02	0.59
2:i:162:GLU:HB3	2:i:253:GLY:H	1.67	0.59
3:D:59:TRP:HZ2	3:D:94:ASN:HD22	1.51	0.59
3:J:235:PRO:HA	3:J:249:PHE:O	2.02	0.59
3:K:264:LEU:HB2	3:K:287:THR:HB	1.83	0.59
1:B:276:ILE:O	1:B:281:ARG:NH1	2.35	0.59
2:i:111:TRP:HE1	2:i:303:VAL:HG11	1.68	0.59
3:C:264:LEU:HB2	3:C:287:THR:HB	1.83	0.59
3:I:235:PRO:HA	3:I:249:PHE:O	2.02	0.59
3:N:235:PRO:HA	3:N:249:PHE:O	2.02	0.59
2:j:279:PRO:HB3	3:J:313:PRO:HG2	1.83	0.59
3:F:235:PRO:HA	3:F:249:PHE:O	2.02	0.59
3:G:59:TRP:HZ2	3:G:94:ASN:HD22	1.50	0.59
3:H:59:TRP:HZ2	3:H:94:ASN:HD22	1.51	0.59
3:K:370:LEU:HG	3:K:378:ARG:HD3	1.84	0.59
3:N:59:TRP:HZ2	3:N:94:ASN:HD22	1.51	0.59
2:c:137:TYR:HD1	2:c:310:MET:HE2	1.67	0.59
2:e:109:LYS:HE3	2:e:301:ASP:HA	1.84	0.59
2:g:145:ASP:HB2	2:g:148:LEU:HB2	1.85	0.59
2:m:287:ILE:HD11	2:m:295:VAL:HG13	1.85	0.59
3:C:59:TRP:HZ2	3:C:94:ASN:HD22	1.51	0.59
3:E:235:PRO:HA	3:E:249:PHE:O	2.02	0.59
3:L:231:ARG:HH12	3:N:227:PRO:HG2	1.66	0.59
2:h:65:THR:O	3:H:239:ASN:ND2	2.36	0.59
3:K:59:TRP:HZ2	3:K:94:ASN:HD22	1.51	0.59
3:L:370:LEU:HG	3:L:378:ARG:HD3	1.84	0.59
2:d:148:LEU:O	2:d:148:LEU:HG	2.03	0.59
3:C:235:PRO:HA	3:C:249:PHE:O	2.02	0.59
3:G:370:LEU:HG	3:G:378:ARG:HD3	1.84	0.59
3:D:235:PRO:HA	3:D:249:PHE:O	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:59:TRP:HZ2	3:F:94:ASN:HD22	1.51	0.58
3:I:370:LEU:HG	3:I:378:ARG:HD3	1.84	0.58
3:M:59:TRP:HZ2	3:M:94:ASN:HD22	1.51	0.58
2:h:321:ALA:HA	2:h:325:ARG:HD3	1.84	0.58
2:n:280:GLN:CA	2:n:284:MET:HE1	2.19	0.58
3:O:59:TRP:HZ2	3:O:94:ASN:HD22	1.51	0.58
1:B:392:ARG:NH2	1:B:574:THR:OG1	2.37	0.58
2:d:255:ARG:HH21	2:d:257:ASN:HD21	1.49	0.58
2:j:283:ARG:HD3	2:j:310:MET:HB3	1.85	0.58
3:I:264:LEU:HB2	3:I:287:THR:HB	1.83	0.58
2:c:199:ASN:HD22	2:c:203:LEU:HB2	1.67	0.58
2:m:59:ILE:HG23	2:m:59:ILE:O	2.02	0.58
3:E:59:TRP:HZ2	3:E:94:ASN:HD22	1.51	0.58
1:A:434:ILE:HD11	1:A:458:PHE:CD1	2.39	0.58
1:B:310:LEU:HD12	1:B:310:LEU:O	2.04	0.58
2:l:69:ASN:CG	5:l:401:NAG:H4	2.28	0.58
1:B:310:LEU:HD21	1:B:616:TYR:OH	2.03	0.58
2:c:59:ILE:HG22	2:n:57:LEU:HD21	1.86	0.58
3:N:370:LEU:HG	3:N:378:ARG:HD3	1.84	0.58
1:B:468:PHE:O	1:B:472:ASN:ND2	2.37	0.58
2:k:207:CYS:SG	2:k:208:LEU:N	2.77	0.58
1:A:418:ASN:ND2	1:A:477:VAL:O	2.37	0.58
2:c:187:MET:HE2	2:c:247:ARG:HH22	1.68	0.58
2:l:268:ILE:HD13	2:m:286:ARG:HH21	1.68	0.58
2:o:285:MET:HE1	2:o:306:ILE:HG12	1.85	0.58
3:F:370:LEU:HG	3:F:378:ARG:HD3	1.84	0.58
1:A:649:LYS:HD3	1:A:656:VAL:HG11	1.86	0.58
2:f:132:GLN:HB3	2:f:319:SER:HB2	1.86	0.58
1:A:547:ASP:HB3	1:A:879:MET:HG2	1.85	0.58
1:B:308:ASP:CG	1:B:310:LEU:O	2.46	0.58
2:d:150:LEU:HD13	2:d:150:LEU:C	2.28	0.58
2:c:83:LEU:HB3	2:c:139:VAL:CG2	2.33	0.57
2:c:83:LEU:CB	2:c:139:VAL:HG23	2.34	0.57
2:d:184:TRP:HB3	2:d:246:ILE:HD11	1.86	0.57
3:I:59:TRP:HZ2	3:I:94:ASN:HD22	1.51	0.57
1:A:619:ARG:HE	1:A:650:ARG:HB3	1.68	0.57
1:B:714:LEU:HD21	1:B:722:TYR:CB	2.34	0.57
2:l:268:ILE:CG1	2:m:286:ARG:HH22	2.16	0.57
2:e:163:TRP:HB3	2:e:249:CYS:HB3	1.85	0.57
2:o:63:MET:HG2	3:O:163:SER:CA	2.34	0.57
3:F:37:MET:HE2	3:F:127:ILE:HG23	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:59:TRP:HZ2	3:L:94:ASN:HD22	1.51	0.57
1:A:444:MET:HE1	1:A:465:ILE:HA	1.87	0.57
1:B:838:ARG:CB	3:O:126:ARG:NH1	2.67	0.57
2:c:136:ASP:HA	2:c:315:ARG:HD2	1.85	0.57
2:i:178:THR:H	2:i:182:ASN:HD22	1.52	0.57
2:m:261:ILE:HG12	2:m:285:MET:CG	2.34	0.57
3:G:137:GLU:OE1	3:H:397:LYS:NZ	2.36	0.57
3:N:37:MET:HE2	3:N:127:ILE:HG23	1.87	0.57
1:B:714:LEU:HD23	1:B:722:TYR:HB3	1.84	0.57
2:m:57:LEU:HD22	2:o:59:ILE:HG12	1.86	0.57
2:l:99:LYS:HG2	2:l:118:PHE:HD2	1.69	0.57
3:H:37:MET:HE2	3:H:127:ILE:HG23	1.87	0.57
3:E:37:MET:HE2	3:E:127:ILE:HG23	1.87	0.57
1:B:487:ILE:HD12	1:B:487:ILE:O	2.05	0.57
1:B:714:LEU:HB3	1:B:821:PRO:HB2	1.87	0.57
3:D:42:ASN:HD21	3:D:63:PHE:H	1.53	0.57
3:E:42:ASN:HD21	3:E:63:PHE:H	1.53	0.57
3:H:42:ASN:HD21	3:H:63:PHE:H	1.53	0.56
3:J:59:TRP:HZ2	3:J:94:ASN:HD22	1.51	0.56
3:M:37:MET:HE2	3:M:127:ILE:HG23	1.87	0.56
1:A:441:ALA:HB1	1:A:518:GLN:HG3	1.86	0.56
1:B:441:ALA:HB1	1:B:518:GLN:HG2	1.87	0.56
2:f:67:TYR:HE1	3:F:239:ASN:HB3	1.70	0.56
2:g:149:GLN:HE22	2:g:268:ILE:HB	1.68	0.56
3:I:37:MET:HE2	3:I:127:ILE:HG23	1.87	0.56
3:K:37:MET:HE2	3:K:127:ILE:HG23	1.87	0.56
2:d:150:LEU:CD1	2:d:154:GLU:CG	2.83	0.56
2:j:86:PRO:HB2	2:j:88:GLU:HG2	1.86	0.56
2:k:139:VAL:HG12	2:k:259:ALA:HB3	1.86	0.56
2:l:165:CYS:HB3	2:l:247:ARG:HD3	1.86	0.56
2:m:230:VAL:HG11	2:n:105:LEU:HD22	1.87	0.56
2:n:193:ILE:HG12	2:n:239:VAL:HG22	1.87	0.56
3:J:42:ASN:HD21	3:J:63:PHE:H	1.53	0.56
3:J:153:HIS:ND1	3:K:338:ALA:O	2.35	0.56
3:L:37:MET:HE2	3:L:127:ILE:HG23	1.87	0.56
2:l:268:ILE:HG12	2:m:286:ARG:NH2	2.18	0.56
3:N:219:THR:HG22	3:N:220:THR:HG23	1.88	0.56
1:A:110:LEU:HD13	1:A:653:ILE:HD11	1.87	0.56
2:n:305:GLN:NE2	3:M:310:ASN:OD1	2.38	0.56
3:J:219:THR:HG22	3:J:220:THR:HG23	1.88	0.56
3:O:42:ASN:HD21	3:O:63:PHE:H	1.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:194:LYS:HB2	2:l:238:ASP:HB3	1.87	0.56
3:C:37:MET:HE2	3:C:127:ILE:HG23	1.87	0.56
3:G:219:THR:HG22	3:G:220:THR:HG23	1.88	0.56
3:J:37:MET:HE2	3:J:127:ILE:HG23	1.87	0.56
2:f:199:ASN:HD22	2:f:203:LEU:HB3	1.70	0.56
2:n:52:ASN:H	3:C:169:SER:H	1.52	0.56
3:N:42:ASN:HD21	3:N:63:PHE:H	1.53	0.56
2:n:59:ILE:HD13	3:N:241:ALA:HB2	1.88	0.56
2:o:63:MET:HG2	3:O:163:SER:HA	1.88	0.56
3:C:42:ASN:HD21	3:C:63:PHE:H	1.53	0.56
3:F:248:PHE:HB2	3:H:304:VAL:HG22	1.86	0.56
3:G:42:ASN:HD21	3:G:63:PHE:H	1.53	0.56
3:J:170:GLN:NE2	3:J:174:ASP:OD1	2.39	0.56
3:L:170:GLN:NE2	3:L:174:ASP:OD1	2.39	0.56
3:O:219:THR:HG22	3:O:220:THR:HG23	1.87	0.56
2:d:160:LEU:HD23	2:d:258:VAL:HG13	1.87	0.56
2:m:139:VAL:HG12	2:m:259:ALA:HB3	1.87	0.56
3:G:170:GLN:NE2	3:G:174:ASP:OD1	2.39	0.56
3:H:219:THR:HG22	3:H:220:THR:HG23	1.88	0.56
2:d:143:LYS:HA	2:d:263:VAL:HB	1.87	0.56
3:D:37:MET:HE2	3:D:127:ILE:HG23	1.87	0.56
3:F:42:ASN:HD21	3:F:63:PHE:H	1.53	0.56
3:G:227:PRO:HG2	3:H:231:ARG:HH12	1.70	0.56
3:K:219:THR:HG22	3:K:220:THR:HG23	1.88	0.56
3:E:170:GLN:NE2	3:E:174:ASP:OD1	2.39	0.55
1:B:279:ARG:NH1	1:B:557:GLU:O	2.36	0.55
2:k:178:THR:H	2:k:182:ASN:HD21	1.54	0.55
2:m:138:ASN:O	2:m:258:VAL:HA	2.06	0.55
3:O:37:MET:HE2	3:O:127:ILE:HG23	1.87	0.55
2:h:138:ASN:O	2:h:258:VAL:HA	2.06	0.55
2:n:145:ASP:HB3	2:n:148:LEU:HG	1.87	0.55
3:K:42:ASN:HD21	3:K:63:PHE:H	1.53	0.55
3:D:170:GLN:NE2	3:D:174:ASP:OD1	2.39	0.55
3:F:170:GLN:NE2	3:F:174:ASP:OD1	2.39	0.55
3:I:42:ASN:HD21	3:I:63:PHE:H	1.53	0.55
3:I:219:THR:HG22	3:I:220:THR:HG23	1.88	0.55
3:O:170:GLN:NE2	3:O:174:ASP:OD1	2.39	0.55
2:c:134:TYR:O	2:c:315:ARG:NH2	2.40	0.55
2:i:185:ILE:HG12	2:i:226:ILE:HG12	1.87	0.55
2:l:65:THR:O	3:L:239:ASN:ND2	2.40	0.55
3:C:170:GLN:NE2	3:C:174:ASP:OD1	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:219:THR:HG22	3:F:220:THR:HG23	1.88	0.55
3:G:37:MET:HE2	3:G:127:ILE:HG23	1.87	0.55
3:K:122:ILE:H	3:M:83:ASN:ND2	2.04	0.55
3:M:219:THR:HG22	3:M:220:THR:HG23	1.88	0.55
2:c:192:THR:HA	2:c:219:ALA:O	2.06	0.55
2:n:279:PRO:O	2:n:284:MET:HE1	2.06	0.55
2:m:286:ARG:HH12	2:m:288:ASN:ND2	2.05	0.55
3:D:219:THR:HG22	3:D:220:THR:HG23	1.88	0.55
3:H:170:GLN:NE2	3:H:174:ASP:OD1	2.39	0.55
3:L:219:THR:HG22	3:L:220:THR:HG23	1.88	0.55
3:N:170:GLN:NE2	3:N:174:ASP:OD1	2.39	0.55
1:B:306:LEU:O	1:B:613:HIS:NE2	2.40	0.55
2:c:136:ASP:OD1	2:c:315:ARG:NH1	2.36	0.55
3:C:106:ARG:HH11	3:L:396:ILE:HG22	1.70	0.55
3:K:142:GLN:OE1	3:L:145:ARG:NH1	2.36	0.55
3:L:42:ASN:HD21	3:L:63:PHE:H	1.53	0.55
1:B:555:ASN:HD22	1:B:597:PRO:HD3	1.71	0.55
2:f:160:LEU:HD23	2:f:258:VAL:HG13	1.89	0.55
2:l:83:LEU:HD11	2:l:106:PHE:HZ	1.72	0.55
2:o:162:GLU:HG3	2:o:252:LEU:HB2	1.87	0.55
3:E:219:THR:HG22	3:E:220:THR:HG23	1.88	0.55
3:I:170:GLN:NE2	3:I:174:ASP:OD1	2.39	0.55
3:K:39:ILE:HG13	3:K:65:LEU:HD11	1.89	0.55
3:M:42:ASN:HD21	3:M:63:PHE:H	1.53	0.55
3:C:219:THR:HG22	3:C:220:THR:HG23	1.88	0.54
3:F:39:ILE:HG13	3:F:65:LEU:HD11	1.89	0.54
3:I:39:ILE:HG13	3:I:65:LEU:HD11	1.89	0.54
1:A:436:THR:O	1:A:527:TYR:OH	2.25	0.54
2:e:182:ASN:HA	2:e:249:CYS:O	2.07	0.54
3:M:39:ILE:HG13	3:M:65:LEU:HD11	1.89	0.54
2:c:265:GLY:O	2:c:286:ARG:NH1	2.41	0.54
2:h:185:ILE:HG12	2:h:226:ILE:HG12	1.89	0.54
2:k:136:ASP:OD1	2:k:315:ARG:NH1	2.40	0.54
2:l:193:ILE:HG12	2:l:239:VAL:HG22	1.89	0.54
3:C:39:ILE:HG13	3:C:65:LEU:HD11	1.89	0.54
3:L:39:ILE:HG13	3:L:65:LEU:HD11	1.89	0.54
1:A:276:ILE:HD13	1:A:288:LEU:HD13	1.89	0.54
3:L:137:GLU:OE1	3:M:397:LYS:NZ	2.40	0.54
3:M:170:GLN:NE2	3:M:174:ASP:OD1	2.39	0.54
3:N:39:ILE:HG13	3:N:65:LEU:HD11	1.89	0.54
2:m:304:ASP:O	2:m:308:GLN:HB2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:281:THR:H	2:n:284:MET:CE	2.06	0.54
2:o:148:LEU:HD13	2:o:151:ASP:HB2	1.89	0.54
1:A:722:TYR:HB2	1:A:804:ILE:HB	1.90	0.54
1:B:220:GLU:CD	3:O:39:ILE:HD13	2.33	0.54
1:B:548:LEU:HD13	1:B:590:ILE:HG12	1.90	0.54
2:c:105:LEU:HD22	2:e:230:VAL:HG21	1.87	0.54
2:k:272:THR:OG1	2:k:277:THR:O	2.26	0.54
2:o:272:THR:HG21	2:o:277:THR:HG23	1.88	0.54
3:J:39:ILE:HG13	3:J:65:LEU:HD11	1.89	0.54
2:f:184:TRP:HB2	2:f:227:THR:HB	1.90	0.54
2:o:194:LYS:HE3	2:o:215:PHE:HB2	1.89	0.54
3:D:39:ILE:HG13	3:D:65:LEU:HD11	1.89	0.54
3:I:231:ARG:O	3:I:236:ARG:NH2	2.41	0.54
1:A:191:GLU:OE2	1:A:200:LYS:NZ	2.40	0.54
1:B:128:PHE:CD1	1:B:152:LEU:CD1	2.91	0.54
1:B:130:PRO:HA	1:B:149:TYR:O	2.08	0.54
1:B:165:ARG:HA	1:B:168:PHE:HD2	1.73	0.54
2:c:124:ILE:HG23	2:c:155:LEU:HD22	1.89	0.54
2:i:265:GLY:O	2:k:149:GLN:NE2	2.41	0.54
2:k:265:GLY:O	2:k:286:ARG:NH2	2.41	0.54
3:F:231:ARG:O	3:F:236:ARG:NH2	2.41	0.54
3:L:231:ARG:O	3:L:236:ARG:NH2	2.41	0.54
3:L:245:THR:HG22	3:N:299:ASN:HB3	1.90	0.54
1:B:704:GLY:HA2	1:B:761:LEU:O	2.08	0.54
2:f:65:THR:OG1	3:F:239:ASN:ND2	2.41	0.54
3:H:231:ARG:O	3:H:236:ARG:NH2	2.41	0.54
1:A:201:VAL:HA	1:A:244:PRO:HG2	1.89	0.54
2:g:65:THR:OG1	3:G:239:ASN:ND2	2.40	0.54
2:i:139:VAL:HG12	2:i:259:ALA:HB3	1.90	0.54
3:E:231:ARG:O	3:E:236:ARG:NH2	2.41	0.54
3:G:231:ARG:O	3:G:236:ARG:NH2	2.41	0.54
3:M:231:ARG:O	3:M:236:ARG:NH2	2.41	0.54
2:d:168:MET:HE3	2:d:175:TYR:CD2	2.42	0.53
2:g:57:LEU:HB2	2:i:54:GLY:HA3	1.91	0.53
3:G:39:ILE:HG13	3:G:65:LEU:HD11	1.89	0.53
3:J:231:ARG:O	3:J:236:ARG:NH2	2.41	0.53
2:h:160:LEU:HD23	2:h:258:VAL:HG13	1.90	0.53
2:o:185:ILE:HG12	2:o:226:ILE:HG12	1.88	0.53
3:O:39:ILE:HG13	3:O:65:LEU:HD11	1.89	0.53
3:O:187:GLU:OE2	3:O:189:GLN:NE2	2.42	0.53
1:A:434:ILE:CG2	1:A:439:TYR:CE2	2.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:672:ARG:O	3:L:68:THR:OG1	2.24	0.53
3:D:231:ARG:O	3:D:236:ARG:NH2	2.41	0.53
1:A:462:GLU:OE1	1:A:478:ASN:ND2	2.42	0.53
2:d:150:LEU:HD11	2:d:154:GLU:CG	2.39	0.53
2:i:256:GLU:OE1	2:i:283:ARG:NH1	2.42	0.53
2:o:189:SER:OG	2:o:243:THR:OG1	2.26	0.53
3:E:39:ILE:HG13	3:E:65:LEU:HD11	1.90	0.53
3:G:145:ARG:NH1	3:I:142:GLN:OE1	2.39	0.53
3:K:231:ARG:O	3:K:236:ARG:NH2	2.41	0.53
2:e:139:VAL:HG12	2:e:259:ALA:HB3	1.90	0.53
5:h:401:NAG:H5	5:h:401:NAG:N2	2.22	0.53
2:j:144:TYR:HE1	2:j:268:ILE:HG12	1.74	0.53
3:C:231:ARG:O	3:C:236:ARG:NH2	2.41	0.53
3:K:391:ILE:HA	3:K:394:MET:HE2	1.91	0.53
3:O:231:ARG:O	3:O:236:ARG:NH2	2.41	0.53
2:e:208:LEU:HD23	2:e:214:THR:HG21	1.89	0.53
2:j:71:THR:HG23	3:I:299:ASN:HD21	1.73	0.53
2:n:254:PRO:HD3	3:N:312:GLN:HG2	1.89	0.53
5:o:401:NAG:O7	5:o:401:NAG:O3	2.23	0.53
3:C:391:ILE:HA	3:C:394:MET:HE2	1.91	0.53
3:N:187:GLU:OE2	3:N:189:GLN:NE2	2.42	0.53
3:F:391:ILE:HA	3:F:394:MET:HE2	1.91	0.53
2:k:161:ASN:HA	2:k:254:PRO:HA	1.91	0.53
2:l:156:ALA:HA	2:l:159:ILE:HG22	1.90	0.53
3:D:391:ILE:HA	3:D:394:MET:HE2	1.91	0.53
3:I:391:ILE:HA	3:I:394:MET:HE2	1.91	0.53
3:M:187:GLU:OE2	3:M:189:GLN:NE2	2.42	0.53
3:N:391:ILE:HA	3:N:394:MET:HE2	1.91	0.53
1:B:355:LEU:O	1:B:355:LEU:HG	2.09	0.53
2:i:196:CYS:HB3	2:i:236:LYS:HB3	1.91	0.53
2:m:83:LEU:HD21	2:m:299:VAL:HG11	1.90	0.53
3:N:231:ARG:O	3:N:236:ARG:NH2	2.41	0.53
1:A:216:ASP:O	1:A:224:ARG:NH2	2.38	0.53
1:B:473:TRP:CD1	1:B:508:LEU:HD13	2.41	0.53
1:B:838:ARG:CZ	3:O:36:GLN:HE22	2.16	0.53
3:C:187:GLU:OE2	3:C:189:GLN:NE2	2.42	0.53
3:E:187:GLU:OE2	3:E:189:GLN:NE2	2.42	0.53
3:G:391:ILE:HA	3:G:394:MET:HE2	1.91	0.53
3:I:74:ASP:HB2	3:M:76:ASN:OD1	2.09	0.53
1:A:619:ARG:HD2	1:A:650:ARG:HE	1.75	0.52
1:B:733:GLN:HB2	3:D:62:ASN:HD21	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:83:LEU:HB2	2:c:139:VAL:O	2.09	0.52
2:c:159:ILE:O	2:c:255:ARG:NH1	2.42	0.52
3:H:391:ILE:HA	3:H:394:MET:HE2	1.91	0.52
3:L:187:GLU:OE2	3:L:189:GLN:NE2	2.42	0.52
1:A:637:GLN:HE21	1:B:869:ASN:HD21	1.55	0.52
2:i:193:ILE:H	2:i:219:ALA:HB3	1.75	0.52
2:k:193:ILE:HG12	2:k:239:VAL:HG22	1.91	0.52
2:m:239:VAL:HG11	2:m:246:ILE:HG21	1.92	0.52
2:n:84:TYR:HB2	2:n:140:VAL:HG12	1.92	0.52
1:A:475:HIS:HA	1:A:478:ASN:HD22	1.74	0.52
1:B:290:MET:HE1	1:B:860:VAL:HG22	1.91	0.52
1:A:216:ASP:HB3	1:A:219:THR:CG2	2.40	0.52
2:j:197:PRO:HB2	2:j:205:ILE:HD12	1.92	0.52
2:k:322:PHE:HE2	2:k:324:TYR:HB2	1.74	0.52
3:H:57:ARG:HE	3:I:117:ARG:HH22	1.57	0.52
3:I:351:GLN:OE1	3:K:271:ASN:ND2	2.42	0.52
3:M:168:ARG:NH2	3:M:194:ASP:OD1	2.42	0.52
2:d:142:MET:HE2	2:d:155:LEU:HD23	1.92	0.52
2:d:168:MET:CE	2:d:175:TYR:CD2	2.93	0.52
2:j:145:ASP:HB3	2:j:148:LEU:HD21	0.62	0.52
2:j:154:GLU:HB2	2:j:226:ILE:HD12	1.91	0.52
2:k:83:LEU:HD21	2:k:118:PHE:CZ	2.43	0.52
3:C:117:ARG:HH22	3:L:57:ARG:HE	1.56	0.52
3:E:168:ARG:NH2	3:E:194:ASP:OD1	2.42	0.52
3:I:153:HIS:ND1	3:J:338:ALA:O	2.39	0.52
3:N:168:ARG:NH2	3:N:194:ASP:OD1	2.42	0.52
3:O:391:ILE:HA	3:O:394:MET:HE2	1.91	0.52
1:B:838:ARG:HB3	3:O:126:ARG:HH22	1.74	0.52
2:f:270:ASP:HB2	2:g:286:ARG:HH12	1.74	0.52
2:k:277:THR:HG22	2:k:279:PRO:HD3	1.91	0.52
3:D:187:GLU:OE2	3:D:189:GLN:NE2	2.42	0.52
3:F:187:GLU:OE2	3:F:189:GLN:NE2	2.42	0.52
1:A:740:LEU:HG	1:A:746:TYR:HE1	1.74	0.52
2:e:135:CYS:HB3	2:e:324:TYR:HB3	1.92	0.52
2:n:318:ASN:OD1	2:n:325:ARG:NH2	2.42	0.52
3:H:17:LYS:HD2	3:H:30:LEU:HD22	1.92	0.52
3:L:391:ILE:HA	3:L:394:MET:HE2	1.91	0.52
1:B:233:ARG:HB3	1:B:242:ASN:HB2	1.92	0.52
2:c:194:LYS:HB2	2:c:238:ASP:HB3	1.91	0.52
2:n:196:CYS:HB3	2:n:236:LYS:HB3	1.92	0.52
1:A:351:MET:HG3	1:A:537:LEU:HD11	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:ILE:O	1:B:758:PRO:HA	2.10	0.52
3:I:74:ASP:HB2	3:M:76:ASN:HD21	1.74	0.52
3:K:187:GLU:OE2	3:K:189:GLN:NE2	2.42	0.52
3:O:17:LYS:HD2	3:O:30:LEU:HD22	1.92	0.52
1:B:838:ARG:HB3	3:O:126:ARG:NH2	2.25	0.52
2:f:182:ASN:HA	2:f:249:CYS:O	2.10	0.52
2:i:282:GLU:HG2	2:i:283:ARG:HG3	1.91	0.52
3:D:17:LYS:HD2	3:D:30:LEU:HD22	1.92	0.52
3:J:187:GLU:OE2	3:J:189:GLN:NE2	2.42	0.52
1:A:483:ARG:HH11	1:A:485:VAL:HG22	1.75	0.51
2:c:99:LYS:HG2	2:c:118:PHE:HD2	1.75	0.51
3:C:153:HIS:ND1	3:D:338:ALA:O	2.39	0.51
3:H:187:GLU:OE2	3:H:189:GLN:NE2	2.42	0.51
3:I:17:LYS:HD2	3:I:30:LEU:HD22	1.92	0.51
3:J:17:LYS:HD2	3:J:30:LEU:HD22	1.92	0.51
3:K:170:GLN:NE2	3:K:174:ASP:OD1	2.39	0.51
3:M:17:LYS:HD2	3:M:30:LEU:HD22	1.92	0.51
1:A:848:LEU:HG	1:A:849:THR:HG23	1.92	0.51
2:c:82:CYS:N	2:c:135:CYS:SG	2.83	0.51
3:J:27:VAL:HG21	3:J:73:LEU:HD11	1.93	0.51
3:M:391:ILE:HA	3:M:394:MET:HE2	1.91	0.51
1:A:195:SER:HA	1:A:228:ALA:HA	1.92	0.51
2:d:145:ASP:O	2:d:148:LEU:HD23	2.10	0.51
5:h:401:NAG:N2	5:h:401:NAG:C5	2.73	0.51
3:K:17:LYS:HD2	3:K:30:LEU:HD22	1.92	0.51
3:L:168:ARG:NH2	3:L:194:ASP:OD1	2.42	0.51
1:B:272:ILE:HG12	1:B:856:LEU:HD12	1.90	0.51
2:c:230:VAL:HG11	2:d:105:LEU:HD22	1.91	0.51
2:j:133:LEU:HD12	2:j:255:ARG:HH11	1.75	0.51
2:n:182:ASN:HA	2:n:249:CYS:O	2.10	0.51
3:L:27:VAL:HG21	3:L:73:LEU:HD11	1.93	0.51
1:A:202:VAL:HG21	1:A:844:LEU:HD12	1.92	0.51
1:A:342:VAL:HG22	1:A:589:LEU:HA	1.92	0.51
1:B:704:GLY:CA	1:B:761:LEU:O	2.59	0.51
2:l:138:ASN:O	2:l:258:VAL:HA	2.11	0.51
3:G:145:ARG:HH11	3:I:142:GLN:HB3	1.76	0.51
3:G:187:GLU:OE2	3:G:189:GLN:NE2	2.42	0.51
3:K:168:ARG:NH2	3:K:194:ASP:OD1	2.42	0.51
1:A:484:GLN:HE21	1:A:491:LEU:HD11	1.76	0.51
1:A:512:LEU:HG	1:A:535:ILE:HG23	1.93	0.51
1:B:310:LEU:HD23	1:B:620:ILE:HD13	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:93:ILE:HD11	2:f:296:PHE:HE2	1.76	0.51
2:i:85:TYR:HE1	2:i:118:PHE:HB3	1.76	0.51
2:l:105:LEU:HB3	2:l:300:VAL:HG11	1.93	0.51
2:o:165:CYS:HB3	2:o:247:ARG:HD3	1.92	0.51
3:E:391:ILE:HA	3:E:394:MET:HE2	1.91	0.51
3:F:27:VAL:HG21	3:F:73:LEU:HD11	1.93	0.51
3:I:187:GLU:OE2	3:I:189:GLN:NE2	2.42	0.51
3:L:17:LYS:HD2	3:L:30:LEU:HD22	1.92	0.51
1:B:417:PRO:HB3	1:B:481:GLN:HA	1.92	0.51
3:G:27:VAL:HG21	3:G:73:LEU:HD11	1.93	0.51
2:e:262:GLN:NE2	2:e:266:SER:O	2.43	0.51
2:k:322:PHE:CE2	2:k:324:TYR:HB2	2.46	0.51
2:m:95:ASP:HB3	2:m:98:TRP:HB3	1.93	0.51
3:N:17:LYS:HD2	3:N:30:LEU:HD22	1.92	0.51
3:O:27:VAL:HG21	3:O:73:LEU:HD11	1.93	0.51
1:A:740:LEU:HG	1:A:746:TYR:CE1	2.45	0.51
1:B:308:ASP:OD2	1:B:310:LEU:O	2.29	0.51
1:B:641:LYS:HE3	1:B:664:MET:HG2	1.92	0.51
2:c:287:ILE:HD11	2:c:295:VAL:HG13	1.93	0.51
2:e:193:ILE:HG12	2:e:239:VAL:HG22	1.93	0.51
2:m:256:GLU:OE1	2:m:283:ARG:NH1	2.38	0.51
2:m:286:ARG:NH1	2:m:288:ASN:OD1	2.44	0.51
2:o:59:ILE:HG21	3:O:241:ALA:CB	2.40	0.51
3:C:17:LYS:HD2	3:C:30:LEU:HD22	1.92	0.51
3:G:17:LYS:HD2	3:G:30:LEU:HD22	1.92	0.51
1:B:632:ARG:HB3	3:L:71:LEU:HD12	1.93	0.51
2:d:145:ASP:CA	2:d:148:LEU:HD21	2.34	0.51
2:n:185:ILE:HG12	2:n:226:ILE:HG12	1.93	0.51
3:C:27:VAL:HG21	3:C:73:LEU:HD11	1.93	0.51
1:A:447:MET:HE1	1:A:457:PRO:HB3	1.92	0.50
2:c:165:CYS:HB3	2:c:247:ARG:HD3	1.92	0.50
3:F:17:LYS:HD2	3:F:30:LEU:HD22	1.92	0.50
3:I:168:ARG:NH2	3:I:194:ASP:OD1	2.42	0.50
3:J:391:ILE:HA	3:J:394:MET:HE2	1.91	0.50
2:d:69:ASN:HD21	5:d:401:NAG:H81	1.75	0.50
2:g:282:GLU:HG2	2:g:283:ARG:HG3	1.92	0.50
2:j:161:ASN:HA	2:j:254:PRO:HA	1.93	0.50
2:k:255:ARG:HH22	2:k:321:ALA:HA	1.75	0.50
1:B:838:ARG:HH11	3:O:126:ARG:HD3	1.75	0.50
2:c:83:LEU:N	2:c:83:LEU:CD2	2.74	0.50
2:d:177:GLN:HB2	2:d:231:ASP:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:85:TYR:HE2	2:e:90:ALA:HB2	1.76	0.50
3:C:227:PRO:HG2	3:D:231:ARG:HH12	1.76	0.50
3:E:27:VAL:HG21	3:E:73:LEU:HD11	1.93	0.50
2:d:148:LEU:CD2	2:d:148:LEU:N	2.73	0.50
2:f:85:TYR:OH	2:f:99:LYS:NZ	2.40	0.50
2:j:189:SER:HB2	2:j:243:THR:HB	1.93	0.50
2:o:178:THR:H	2:o:182:ASN:HD21	1.59	0.50
3:G:168:ARG:NH2	3:G:194:ASP:OD1	2.42	0.50
3:I:27:VAL:HG21	3:I:73:LEU:HD11	1.93	0.50
3:J:168:ARG:NH2	3:J:194:ASP:OD1	2.42	0.50
3:K:380:ASP:OD1	3:L:145:ARG:NH2	2.42	0.50
1:B:127:ILE:HG22	1:B:152:LEU:HD13	1.92	0.50
2:i:131:PRO:HG2	2:i:158:LEU:HD23	1.92	0.50
2:j:145:ASP:H	2:j:152:MET:HE1	1.76	0.50
2:j:185:ILE:HG12	2:j:226:ILE:HG12	1.93	0.50
2:l:70:SER:HA	3:N:298:PRO:HB2	1.93	0.50
3:E:17:LYS:HD2	3:E:30:LEU:HD22	1.92	0.50
3:F:231:ARG:HH12	3:H:227:PRO:HG2	1.75	0.50
1:B:720:TYR:HD2	1:B:723:VAL:HG21	1.76	0.50
2:h:195:VAL:HG11	2:h:229:VAL:HG11	1.94	0.50
1:B:838:ARG:CG	3:O:126:ARG:NH1	2.72	0.50
2:j:114:GLY:O	2:j:324:TYR:OH	2.30	0.50
2:j:133:LEU:HD11	2:j:159:ILE:HG23	1.94	0.50
2:l:268:ILE:CG1	2:m:286:ARG:NH2	2.75	0.50
2:m:286:ARG:NH1	2:m:288:ASN:CG	2.70	0.50
3:H:27:VAL:HG21	3:H:73:LEU:HD11	1.93	0.50
3:M:27:VAL:HG21	3:M:73:LEU:HD11	1.93	0.50
1:A:737:LEU:HD21	1:A:761:LEU:HB3	1.92	0.50
1:B:330:LEU:HD11	1:B:608:VAL:HG21	1.94	0.50
2:l:185:ILE:HD13	2:l:249:CYS:HB2	1.93	0.50
2:l:230:VAL:HG11	2:m:105:LEU:HD22	1.94	0.50
3:F:168:ARG:NH2	3:F:194:ASP:OD1	2.42	0.50
3:K:27:VAL:HG21	3:K:73:LEU:HD11	1.93	0.50
3:N:135:TYR:OH	3:N:340:GLU:OE1	2.29	0.50
2:l:268:ILE:HD13	2:m:286:ARG:NH2	2.27	0.49
3:N:27:VAL:HG21	3:N:73:LEU:HD11	1.93	0.49
1:A:124:LEU:O	1:A:255:ASN:ND2	2.27	0.49
1:A:241:VAL:HG11	1:A:848:LEU:HD13	1.95	0.49
3:D:27:VAL:HG21	3:D:73:LEU:HD11	1.93	0.49
3:J:135:TYR:OH	3:J:340:GLU:OE1	2.29	0.49
2:i:294:GLN:HE22	2:k:228:ASP:H	1.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:83:LEU:HD12	2:l:118:PHE:CE1	2.47	0.49
3:H:168:ARG:NH2	3:H:194:ASP:OD1	2.42	0.49
2:e:103:SER:HA	2:e:106:PHE:HD2	1.78	0.49
2:n:145:ASP:HB3	2:n:148:LEU:CD2	2.43	0.49
2:d:138:ASN:H	2:d:310:MET:HE1	1.78	0.49
2:f:125:ALA:HB1	2:f:223:LYS:HG3	1.92	0.49
2:i:145:ASP:HB3	2:i:148:LEU:HB2	1.94	0.49
1:B:297:THR:HB	1:B:850:PHE:HA	1.94	0.49
2:j:98:TRP:HA	2:j:101:THR:HG22	1.94	0.49
2:j:180:GLU:O	2:j:183:LYS:NZ	2.45	0.49
1:B:363:GLN:HE22	1:B:367:GLN:H	1.60	0.49
2:d:168:MET:HE3	2:d:175:TYR:CD1	2.47	0.49
2:n:287:ILE:HD11	2:n:295:VAL:HG13	1.94	0.49
3:D:168:ARG:NH2	3:D:194:ASP:OD1	2.42	0.49
2:d:150:LEU:HD11	2:d:154:GLU:HG2	1.94	0.49
2:d:263:VAL:HG22	2:d:287:ILE:HD11	1.95	0.49
2:l:83:LEU:HD23	2:l:139:VAL:CG1	2.43	0.49
2:m:194:LYS:HA	2:m:217:GLU:HA	1.95	0.49
3:H:135:TYR:OH	3:H:340:GLU:OE1	2.29	0.49
2:e:255:ARG:O	2:e:283:ARG:NH2	2.45	0.49
2:k:83:LEU:HG	2:k:118:PHE:CD1	2.48	0.49
2:k:264:GLY:N	2:k:287:ILE:O	2.46	0.49
1:B:733:GLN:HE22	1:B:748:GLN:NE2	2.11	0.49
2:e:127:PHE:HD2	2:e:155:LEU:HD21	1.78	0.49
2:g:134:TYR:HB3	2:i:323:TYR:CE2	2.46	0.49
2:g:277:THR:HG21	3:G:309:PRO:HB3	1.94	0.49
2:l:276:THR:HG21	2:m:305:GLN:HB3	1.95	0.49
3:G:135:TYR:OH	3:G:340:GLU:OE1	2.29	0.49
1:B:507:GLN:HB2	3:J:71:LEU:HB2	1.95	0.48
1:A:141:GLU:HA	1:A:806:SER:HB2	1.95	0.48
1:B:483:ARG:HB3	3:I:67:GLY:HA2	1.95	0.48
3:D:227:PRO:HG2	3:E:231:ARG:HH12	1.78	0.48
3:F:17:LYS:HB3	3:F:27:VAL:HG12	1.95	0.48
3:G:17:LYS:HB3	3:G:27:VAL:HG12	1.96	0.48
3:K:17:LYS:HB3	3:K:27:VAL:HG12	1.95	0.48
1:A:320:TRP:HA	1:A:323:ILE:HD12	1.95	0.48
2:i:192:THR:HA	2:i:219:ALA:O	2.12	0.48
3:C:17:LYS:HB3	3:C:27:VAL:HG12	1.95	0.48
3:H:17:LYS:HB3	3:H:27:VAL:HG12	1.95	0.48
3:N:17:LYS:HB3	3:N:27:VAL:HG12	1.95	0.48
1:B:398:PHE:HB3	1:B:580:LEU:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:209:THR:HG23	2:e:236:LYS:HE2	1.95	0.48
3:F:135:TYR:OH	3:F:340:GLU:OE1	2.29	0.48
3:M:37:MET:HE3	3:M:37:MET:HB2	1.71	0.48
1:A:869:ASN:HD22	1:A:877:ARG:HE	1.61	0.48
3:I:135:TYR:OH	3:I:340:GLU:OE1	2.29	0.48
3:K:37:MET:HE3	3:K:37:MET:HB2	1.71	0.48
1:A:351:MET:HE3	1:A:537:LEU:HD21	1.95	0.48
2:e:164:LEU:HB2	2:e:252:LEU:HD11	1.95	0.48
2:o:84:TYR:HE2	2:o:133:LEU:HG	1.79	0.48
3:O:17:LYS:HB3	3:O:27:VAL:HG12	1.95	0.48
2:e:82:CYS:N	2:e:135:CYS:SG	2.87	0.48
2:f:264:GLY:N	2:f:287:ILE:O	2.40	0.48
2:g:287:ILE:HD11	2:g:295:VAL:HG13	1.95	0.48
2:i:83:LEU:HD21	2:i:299:VAL:HG11	1.96	0.48
2:m:99:LYS:HG2	2:m:118:PHE:HD2	1.79	0.48
3:E:17:LYS:HB3	3:E:27:VAL:HG12	1.95	0.48
3:O:168:ARG:NH2	3:O:194:ASP:OD1	2.42	0.48
2:d:194:LYS:HG2	2:d:217:GLU:HB3	1.96	0.48
2:e:174:TYR:HE2	2:e:234:ASN:HB3	1.77	0.48
2:g:197:PRO:HB2	2:g:205:ILE:HD12	1.95	0.48
2:j:70:SER:HB2	3:I:298:PRO:HB2	1.95	0.48
2:j:281:THR:OG1	2:j:284:MET:HE3	2.14	0.48
2:o:193:ILE:HG12	2:o:239:VAL:HG22	1.96	0.48
1:B:242:ASN:ND2	1:B:845:THR:OG1	2.47	0.48
2:m:121:TYR:OH	2:m:141:LEU:O	2.25	0.48
3:C:135:TYR:OH	3:C:340:GLU:OE1	2.29	0.48
3:C:231:ARG:HH12	3:E:227:PRO:HG2	1.79	0.48
1:A:541:ARG:HH21	1:A:590:ILE:HG22	1.79	0.48
1:A:667:LEU:O	1:A:671:LEU:HB2	2.14	0.48
2:h:103:SER:HA	2:h:106:PHE:HD2	1.79	0.48
2:l:185:ILE:HG13	2:l:226:ILE:HG12	1.94	0.48
2:l:257:ASN:HB3	2:l:313:ARG:HB2	1.96	0.48
2:n:145:ASP:HB3	2:n:148:LEU:CG	2.44	0.48
2:o:163:TRP:HB3	2:o:249:CYS:HB3	1.96	0.48
3:L:231:ARG:NH1	3:N:227:PRO:HG2	2.28	0.48
2:k:121:TYR:OH	2:k:141:LEU:O	2.29	0.47
2:m:262:GLN:O	2:m:286:ARG:HA	2.14	0.47
3:F:227:PRO:HG2	3:G:231:ARG:HH12	1.78	0.47
1:A:434:ILE:HG22	1:A:439:TYR:CD2	2.48	0.47
2:c:85:TYR:HE1	2:c:118:PHE:HB3	1.79	0.47
2:c:282:GLU:HB3	2:c:309:VAL:CG1	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:230:VAL:HA	2:e:301:ASP:HB3	1.95	0.47
2:h:144:TYR:HA	2:h:152:MET:HE1	1.95	0.47
2:k:133:LEU:HD12	2:k:255:ARG:HH11	1.79	0.47
2:o:99:LYS:HG2	2:o:118:PHE:HD2	1.78	0.47
3:J:17:LYS:HB3	3:J:27:VAL:HG12	1.95	0.47
1:A:692:GLU:HG2	1:A:696:ARG:HH21	1.78	0.47
2:k:306:ILE:HG22	2:k:310:MET:HE2	1.95	0.47
3:C:168:ARG:NH2	3:C:194:ASP:OD1	2.42	0.47
3:L:135:TYR:OH	3:L:340:GLU:OE1	2.29	0.47
1:B:737:LEU:HD12	1:B:763:GLY:HA3	1.97	0.47
2:c:83:LEU:CB	2:c:139:VAL:O	2.62	0.47
2:c:190:SER:O	2:c:243:THR:OG1	2.28	0.47
2:f:150:LEU:HB3	2:g:290:LYS:HE2	1.95	0.47
2:l:313:ARG:NH2	2:l:316:SER:OG	2.40	0.47
3:L:17:LYS:HB3	3:L:27:VAL:HG12	1.96	0.47
1:B:161:ASP:HB3	1:B:738:GLU:HB2	1.97	0.47
1:B:729:LEU:HD22	1:B:760:ALA:HB1	1.97	0.47
2:j:79:SER:O	2:j:115:SER:OG	2.32	0.47
3:M:17:LYS:HB3	3:M:27:VAL:HG12	1.95	0.47
3:M:135:TYR:OH	3:M:340:GLU:OE1	2.29	0.47
1:B:233:ARG:HE	1:B:235:GLN:HE21	1.62	0.47
1:B:838:ARG:HB3	3:O:126:ARG:NH1	2.29	0.47
2:h:258:VAL:O	2:h:283:ARG:NH1	2.44	0.47
3:I:74:ASP:HB2	3:M:76:ASN:ND2	2.30	0.47
3:L:37:MET:HE3	3:L:37:MET:HB2	1.70	0.47
1:A:705:VAL:HG11	1:A:785:PHE:HZ	1.79	0.47
2:c:83:LEU:HD12	2:c:141:LEU:CD1	2.45	0.47
2:f:85:TYR:HE1	2:f:118:PHE:HB3	1.80	0.47
2:f:161:ASN:HA	2:f:254:PRO:HA	1.96	0.47
2:k:182:ASN:HB3	2:k:250:LYS:HG3	1.97	0.47
2:l:69:ASN:CG	5:l:401:NAG:C4	2.87	0.47
2:o:254:PRO:CD	3:O:312:GLN:HG2	2.29	0.47
3:D:17:LYS:HB3	3:D:27:VAL:HG12	1.95	0.47
1:A:541:ARG:HA	1:A:544:GLN:HE21	1.80	0.47
1:B:630:ALA:HB3	1:B:640:MET:HE1	1.97	0.47
2:c:159:ILE:HG22	2:c:258:VAL:HG21	1.97	0.47
2:k:194:LYS:HA	2:k:217:GLU:HA	1.97	0.47
2:m:145:ASP:HB3	2:m:148:LEU:HB2	1.97	0.47
3:C:130:ASP:HB3	3:D:17:LYS:HG2	1.95	0.47
3:E:135:TYR:OH	3:E:340:GLU:OE1	2.29	0.47
3:I:17:LYS:HB3	3:I:27:VAL:HG12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:LEU:CG	1:B:722:TYR:HB3	2.45	0.47
2:k:95:ASP:HB3	2:k:98:TRP:HB3	1.97	0.47
2:l:69:ASN:ND2	5:l:401:NAG:H4	2.30	0.47
2:o:160:LEU:HD23	2:o:258:VAL:HG23	1.96	0.47
2:j:109:LYS:HE3	2:j:301:ASP:HA	1.95	0.47
2:m:59:ILE:CG1	3:M:241:ALA:HB3	2.45	0.47
3:G:227:PRO:HG2	3:H:231:ARG:NH1	2.30	0.47
1:B:838:ARG:HB3	3:O:126:ARG:HH12	1.79	0.46
2:d:205:ILE:HG22	2:e:101:THR:HG23	1.96	0.46
2:n:52:ASN:ND2	3:C:169:SER:OG	2.48	0.46
2:n:281:THR:N	2:n:284:MET:CE	2.67	0.46
3:N:11:LEU:HD11	3:N:88:PHE:HB3	1.98	0.46
1:B:487:ILE:HG13	1:B:492:ASN:OD1	2.15	0.46
2:d:161:ASN:HA	2:d:254:PRO:HA	1.98	0.46
1:A:316:PHE:HE2	1:A:670:ARG:HD2	1.80	0.46
2:d:150:LEU:HD11	2:d:154:GLU:OE2	2.15	0.46
2:e:119:LYS:NZ	2:e:134:TYR:OH	2.49	0.46
3:E:11:LEU:HD11	3:E:88:PHE:HB3	1.97	0.46
2:f:90:ALA:HA	2:f:93:ILE:HD12	1.97	0.46
2:f:266:SER:HA	2:f:286:ARG:HH11	1.80	0.46
2:k:148:LEU:HB2	2:k:151:ASP:HB2	1.97	0.46
3:J:11:LEU:HD11	3:J:88:PHE:HB3	1.98	0.46
2:h:69:ASN:ND2	5:h:401:NAG:HO1	2.07	0.46
3:O:11:LEU:HD11	3:O:88:PHE:HB3	1.97	0.46
1:A:423:ARG:O	1:A:427:VAL:HB	2.16	0.46
1:A:538:LEU:HD11	1:A:545:LEU:HD11	1.97	0.46
1:B:838:ARG:NH1	3:O:126:ARG:HD3	2.31	0.46
2:d:83:LEU:CD2	2:d:83:LEU:N	2.73	0.46
2:i:285:MET:HE1	2:i:309:VAL:HG11	1.98	0.46
3:C:11:LEU:HD11	3:C:88:PHE:HB3	1.98	0.46
1:A:487:ILE:HB	1:A:492:ASN:HD21	1.80	0.46
1:B:267:LEU:HB2	1:B:300:TYR:HD1	1.80	0.46
1:B:484:GLN:HB3	1:B:491:LEU:HD11	1.98	0.46
2:f:81:LEU:HB3	2:f:116:VAL:HG22	1.98	0.46
2:m:81:LEU:HD13	2:m:307:ILE:HD11	1.97	0.46
2:m:186:SER:O	2:m:224:LEU:HA	2.15	0.46
3:G:11:LEU:HD11	3:G:88:PHE:HB3	1.98	0.46
1:B:145:ARG:HH12	1:B:147:ARG:HH21	1.63	0.46
2:f:258:VAL:O	2:f:283:ARG:NH1	2.49	0.46
3:D:135:TYR:OH	3:D:340:GLU:OE1	2.29	0.46
3:J:137:GLU:OE1	3:K:397:LYS:NZ	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HG13	1:A:143:GLU:HB2	1.96	0.46
1:A:398:PHE:HB3	1:A:580:LEU:HD13	1.97	0.46
2:d:197:PRO:HG2	2:d:205:ILE:HB	1.98	0.46
2:g:172:LEU:HD11	2:i:99:LYS:HB3	1.98	0.46
2:k:145:ASP:OD2	2:k:147:THR:CG2	2.64	0.46
1:A:407:ILE:HG22	1:A:538:LEU:HD22	1.97	0.45
2:k:194:LYS:HB3	2:k:215:PHE:HB3	1.98	0.45
2:l:69:ASN:ND2	5:l:401:NAG:C4	2.78	0.45
2:n:141:LEU:HD23	2:n:261:ILE:HB	1.98	0.45
3:I:11:LEU:HD11	3:I:88:PHE:HB3	1.98	0.45
1:A:801:LEU:CD2	1:A:829:LYS:NZ	2.77	0.45
1:B:637:GLN:NE2	1:B:742:ARG:HH12	2.14	0.45
2:d:168:MET:SD	2:d:184:TRP:HD1	2.40	0.45
2:g:208:LEU:HD23	2:g:210:THR:H	1.80	0.45
2:h:69:ASN:ND2	5:h:401:NAG:O1	2.47	0.45
2:h:140:VAL:HG13	2:h:260:VAL:HG23	1.99	0.45
2:l:63:MET:HE3	3:L:162:ALA:HB1	1.97	0.45
2:m:197:PRO:HG2	2:m:205:ILE:HB	1.98	0.45
3:K:11:LEU:HD11	3:K:88:PHE:HB3	1.98	0.45
3:M:196:SER:HB2	3:M:199:ILE:HG22	1.98	0.45
3:M:227:PRO:HG2	3:N:231:ARG:HH12	1.80	0.45
1:A:687:ILE:O	1:A:691:MET:CB	2.64	0.45
1:B:318:SER:H	1:B:663:GLN:HE22	1.64	0.45
1:B:714:LEU:CD2	1:B:722:TYR:CB	2.82	0.45
2:f:217:GLU:OE2	2:f:220:THR:OG1	2.33	0.45
3:E:196:SER:HB2	3:E:199:ILE:HG22	1.98	0.45
3:H:83:ASN:HD22	3:I:122:ILE:HG12	1.81	0.45
2:c:124:ILE:HD13	2:c:152:MET:HG2	1.98	0.45
2:c:282:GLU:HB3	2:c:309:VAL:HG13	1.99	0.45
2:o:255:ARG:HG3	2:o:313:ARG:HH11	1.82	0.45
3:C:196:SER:HB2	3:C:199:ILE:HG22	1.98	0.45
3:C:397:LYS:NZ	3:E:137:GLU:OE1	2.48	0.45
3:J:37:MET:HB2	3:J:37:MET:HE3	1.70	0.45
1:B:305:LEU:HD21	1:B:610:VAL:HG13	1.97	0.45
2:c:133:LEU:HD11	2:c:159:ILE:HG23	1.97	0.45
2:f:84:TYR:HB2	2:f:140:VAL:HA	1.97	0.45
3:F:11:LEU:HD11	3:F:88:PHE:HB3	1.98	0.45
3:G:196:SER:HB2	3:G:199:ILE:HG22	1.99	0.45
1:B:339:LYS:HG2	1:B:340:GLU:HG2	1.97	0.45
1:B:787:GLN:HB3	1:B:791:LEU:HD13	1.99	0.45
2:f:121:TYR:HB2	2:f:127:PHE:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:196:SER:HB2	3:F:199:ILE:HG22	1.99	0.45
3:N:196:SER:HB2	3:N:199:ILE:HG22	1.99	0.45
1:B:128:PHE:HD1	1:B:152:LEU:CD1	2.29	0.45
1:B:355:LEU:CD2	1:B:355:LEU:N	2.73	0.45
1:B:393:THR:HG21	1:B:571:GLN:HA	1.99	0.45
2:e:189:SER:HA	2:e:223:LYS:HE3	1.98	0.45
2:i:65:THR:OG1	3:I:239:ASN:ND2	2.50	0.45
3:H:37:MET:HB2	3:H:37:MET:HE3	1.71	0.45
3:L:11:LEU:HD11	3:L:88:PHE:HB3	1.98	0.45
3:L:196:SER:HB2	3:L:199:ILE:HG22	1.99	0.45
3:M:11:LEU:HD11	3:M:88:PHE:HB3	1.97	0.45
3:O:135:TYR:OH	3:O:340:GLU:OE1	2.29	0.45
2:f:184:TRP:HH2	2:f:235:HIS:HB2	1.82	0.45
2:h:165:CYS:HB3	2:h:247:ARG:HD3	1.98	0.45
2:i:264:GLY:N	2:i:287:ILE:O	2.43	0.45
2:n:179:ASP:OD1	2:n:250:LYS:NZ	2.50	0.45
3:G:217:VAL:HG22	3:G:286:ASP:HB3	1.99	0.45
3:H:11:LEU:HD11	3:H:88:PHE:HB3	1.98	0.45
3:I:217:VAL:HG22	3:I:286:ASP:HB3	1.99	0.45
3:J:196:SER:HB2	3:J:199:ILE:HG22	1.98	0.45
1:A:245:SER:O	1:A:841:MET:HA	2.17	0.45
2:d:222:GLU:OE2	2:e:290:LYS:NZ	2.48	0.45
2:i:83:LEU:HD12	2:i:118:PHE:HE1	1.82	0.45
3:D:11:LEU:HD11	3:D:88:PHE:HB3	1.98	0.45
3:G:145:ARG:NH2	3:I:380:ASP:OD1	2.50	0.45
3:K:217:VAL:HG22	3:K:286:ASP:HB3	1.99	0.45
3:N:45:GLU:O	3:N:118:LYS:NZ	2.47	0.45
1:A:110:LEU:HD22	1:A:326:SER:HB3	1.97	0.45
1:A:136:TYR:N	1:A:718:GLU:O	2.39	0.45
1:B:363:GLN:OE1	1:B:365:GLU:N	2.50	0.45
1:B:412:LEU:HD22	1:B:583:VAL:HG21	1.99	0.45
2:l:69:ASN:CG	5:l:401:NAG:C1	2.62	0.45
3:G:299:ASN:HB3	3:H:245:THR:HG22	1.98	0.45
3:I:196:SER:HB2	3:I:199:ILE:HG22	1.98	0.45
1:B:411:TRP:HA	1:B:414:THR:HG22	1.99	0.44
1:B:705:VAL:HG11	1:B:785:PHE:HZ	1.82	0.44
2:f:193:ILE:H	2:f:219:ALA:HB3	1.81	0.44
2:f:285:MET:HE1	2:f:309:VAL:HG11	1.99	0.44
2:n:84:TYR:HE2	2:n:133:LEU:HG	1.82	0.44
3:C:217:VAL:HG22	3:C:286:ASP:HB3	1.99	0.44
1:A:216:ASP:HB3	1:A:219:THR:HG23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:MET:HE2	1:B:689:MET:HB3	1.90	0.44
2:f:169:ASP:N	2:f:175:TYR:OH	2.50	0.44
2:f:194:LYS:HB2	2:f:238:ASP:HB3	1.99	0.44
2:g:164:LEU:O	2:g:249:CYS:HA	2.17	0.44
3:N:217:VAL:HG22	3:N:286:ASP:HB3	1.99	0.44
1:B:363:GLN:NE2	1:B:367:GLN:H	2.15	0.44
1:B:669:ASP:HA	1:B:672:ARG:HE	1.83	0.44
2:i:188:GLY:HA3	2:i:244:CYS:HA	2.00	0.44
3:K:196:SER:HB2	3:K:199:ILE:HG22	1.99	0.44
1:A:724:ASN:HB2	1:A:826:LYS:HA	1.98	0.44
1:B:335:VAL:HG21	1:B:382:LYS:HA	1.99	0.44
2:k:325:ARG:HH11	2:l:134:TYR:HB2	1.82	0.44
3:D:196:SER:HB2	3:D:199:ILE:HG22	1.99	0.44
1:A:434:ILE:HD11	1:A:458:PHE:HD1	1.82	0.44
2:e:69:ASN:ND2	5:e:401:NAG:H5	2.27	0.44
2:h:69:ASN:CG	5:h:401:NAG:C1	2.91	0.44
2:h:254:PRO:HD3	3:H:312:GLN:HG2	1.99	0.44
2:l:84:TYR:HB2	2:l:140:VAL:HG12	1.99	0.44
3:G:37:MET:HE3	3:G:37:MET:HB2	1.70	0.44
3:H:196:SER:HB2	3:H:199:ILE:HG22	1.98	0.44
3:K:135:TYR:OH	3:K:340:GLU:OE1	2.29	0.44
1:B:216:ASP:O	1:B:224:ARG:NH2	2.50	0.44
2:e:264:GLY:N	2:e:287:ILE:O	2.42	0.44
2:f:153:SER:OG	2:f:270:ASP:O	2.35	0.44
2:l:83:LEU:HD11	2:l:106:PHE:CZ	2.51	0.44
1:A:338:LEU:HB3	1:A:341:LEU:HD21	2.00	0.44
1:B:182:TYR:HB2	1:B:850:PHE:HZ	1.82	0.44
1:B:838:ARG:CG	3:O:126:ARG:HH12	2.29	0.44
2:c:194:LYS:HA	2:c:217:GLU:HA	1.98	0.44
2:f:121:TYR:OH	2:f:141:LEU:O	2.31	0.44
2:g:86:PRO:HB2	2:g:88:GLU:HG2	2.00	0.44
2:l:268:ILE:HG21	2:m:286:ARG:NH2	2.33	0.44
2:m:193:ILE:HG12	2:m:239:VAL:HG12	1.99	0.44
3:J:360:VAL:HG11	3:J:381:ASN:HD22	1.83	0.44
3:N:360:VAL:HG11	3:N:381:ASN:HD22	1.83	0.44
3:O:196:SER:HB2	3:O:199:ILE:HG22	1.98	0.44
1:A:203:ASP:HB3	1:A:206:THR:H	1.82	0.44
1:A:315:ASN:ND2	1:B:540:ASN:OD1	2.39	0.44
1:B:705:VAL:HG23	1:B:765:LEU:HD21	2.00	0.44
2:d:99:LYS:HG2	2:d:118:PHE:HD2	1.83	0.44
2:l:275:PRO:HB2	2:m:285:MET:SD	2.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:145:ASP:HB3	2:n:148:LEU:HD21	1.99	0.44
3:D:217:VAL:HG22	3:D:286:ASP:HB3	1.99	0.44
3:F:37:MET:HE3	3:F:37:MET:HB2	1.71	0.44
3:M:360:VAL:HG11	3:M:381:ASN:HD22	1.83	0.44
2:c:129:VAL:HG12	2:c:223:LYS:HD2	1.99	0.44
2:d:194:LYS:O	2:d:237:LEU:HA	2.18	0.44
2:d:229:VAL:HG12	2:d:230:VAL:H	1.83	0.44
2:l:267:ASP:HB2	2:l:286:ARG:HE	1.83	0.44
3:M:109:ILE:HD13	3:O:145:ARG:NH2	2.33	0.44
3:M:217:VAL:HG22	3:M:286:ASP:HB3	1.99	0.44
1:A:644:VAL:HG23	1:A:667:LEU:HD22	1.99	0.43
1:B:127:ILE:CG2	1:B:152:LEU:HD11	2.48	0.43
1:B:310:LEU:CD1	1:B:312:LEU:CD2	2.96	0.43
1:B:437:ILE:HG12	1:B:531:ILE:HD11	1.98	0.43
2:d:145:ASP:O	2:d:148:LEU:CD2	2.65	0.43
2:e:186:SER:HB3	2:e:246:ILE:HG13	2.00	0.43
2:e:254:PRO:HD3	3:E:312:GLN:HG2	1.99	0.43
2:l:268:ILE:CD1	2:m:286:ARG:NH2	2.81	0.43
3:D:360:VAL:HG11	3:D:381:ASN:HD22	1.83	0.43
3:K:360:VAL:HG11	3:K:381:ASN:HD22	1.83	0.43
3:O:37:MET:HE3	3:O:37:MET:HB2	1.70	0.43
2:d:256:GLU:HB3	2:d:311:SER:HB2	2.00	0.43
2:i:84:TYR:HD2	2:i:140:VAL:HG12	1.83	0.43
2:k:103:SER:HA	2:k:106:PHE:HD2	1.83	0.43
2:l:170:ILE:HD11	2:l:246:ILE:HG21	2.00	0.43
3:E:37:MET:HB2	3:E:37:MET:HE3	1.71	0.43
3:J:217:VAL:HG22	3:J:286:ASP:HB3	1.99	0.43
3:L:217:VAL:HG22	3:L:286:ASP:HB3	1.99	0.43
3:L:360:VAL:HG11	3:L:381:ASN:HD22	1.83	0.43
3:O:217:VAL:HG22	3:O:286:ASP:HB3	1.99	0.43
1:A:343:SER:HB3	1:A:346:ALA:HB3	2.00	0.43
1:B:548:LEU:HD21	1:B:586:LEU:HG	1.99	0.43
2:m:286:ARG:C	2:m:286:ARG:CD	2.85	0.43
3:E:217:VAL:HG22	3:E:286:ASP:HB3	1.99	0.43
3:I:231:ARG:HH12	3:K:227:PRO:HG2	1.84	0.43
3:M:204:ASN:HB3	3:M:296:ARG:HB3	2.01	0.43
1:A:103:LYS:HD3	1:A:106:ILE:HD12	2.00	0.43
1:A:183:LEU:HD21	1:A:259:LEU:HD23	2.00	0.43
1:B:304:ASN:O	1:B:617:ASN:ND2	2.45	0.43
2:d:124:ILE:HD12	2:d:148:LEU:HD11	1.99	0.43
2:f:179:ASP:OD1	2:f:180:GLU:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:85:TYR:CZ	2:j:120:GLU:HB3	2.53	0.43
2:l:53:TYR:HE1	2:l:319:SER:HA	1.82	0.43
2:m:262:GLN:HB3	2:m:286:ARG:HB2	1.99	0.43
3:C:142:GLN:OE1	3:N:145:ARG:NH1	2.51	0.43
1:A:473:TRP:CE2	1:A:508:LEU:HD13	2.53	0.43
1:A:714:LEU:HD12	1:A:821:PRO:HB2	2.01	0.43
1:B:749:ILE:O	1:B:753:LEU:HB2	2.18	0.43
2:d:152:MET:HE1	2:d:262:GLN:HG3	2.00	0.43
2:e:165:CYS:HB3	2:e:247:ARG:HD3	2.00	0.43
2:j:103:SER:HA	2:j:106:PHE:HD2	1.83	0.43
1:A:740:LEU:HD21	1:A:749:ILE:CD1	2.44	0.43
1:B:372:ILE:HG21	1:B:375:GLN:HB2	1.99	0.43
2:c:131:PRO:HB3	2:c:320:ALA:HB3	2.01	0.43
2:j:259:ALA:HA	2:j:283:ARG:HB3	2.00	0.43
2:o:219:ALA:HB2	2:o:225:VAL:HG11	2.00	0.43
3:C:204:ASN:HB3	3:C:296:ARG:HB3	2.01	0.43
3:F:217:VAL:HG22	3:F:286:ASP:HB3	1.99	0.43
3:H:204:ASN:HB3	3:H:296:ARG:HB3	2.01	0.43
3:I:204:ASN:HB3	3:I:296:ARG:HB3	2.01	0.43
3:O:360:VAL:HG11	3:O:381:ASN:HD22	1.83	0.43
1:A:729:LEU:HD12	1:A:760:ALA:HB1	2.00	0.43
1:B:443:GLY:HA2	1:B:521:PRO:HG2	2.00	0.43
1:B:746:TYR:CZ	1:B:792:ARG:HB3	2.51	0.43
2:c:54:GLY:HA3	2:n:57:LEU:HB2	2.00	0.43
2:j:90:ALA:HA	2:j:93:ILE:HB	2.01	0.43
2:m:306:ILE:HG22	2:m:310:MET:HE2	2.01	0.43
2:n:285:MET:HE1	2:n:306:ILE:HG12	1.99	0.43
3:G:204:ASN:HB3	3:G:296:ARG:HB3	2.01	0.43
3:G:360:VAL:HG11	3:G:381:ASN:HD22	1.83	0.43
3:H:360:VAL:HG11	3:H:381:ASN:HD22	1.83	0.43
3:I:360:VAL:HG11	3:I:381:ASN:HD22	1.83	0.43
1:A:248:HIS:CD2	1:A:250:ILE:H	2.37	0.43
1:A:248:HIS:HD2	1:A:250:ILE:HB	1.83	0.43
1:A:332:ARG:HH12	1:A:383:THR:HB	1.84	0.43
1:A:462:GLU:HB3	1:A:478:ASN:HD21	1.84	0.43
2:j:71:THR:HG23	3:I:299:ASN:ND2	2.33	0.43
2:m:181:ALA:HB1	2:m:251:LYS:HB3	2.00	0.43
2:n:322:PHE:HE2	3:C:170:GLN:HB2	1.83	0.43
3:C:37:MET:HE3	3:C:37:MET:HB2	1.70	0.43
3:H:217:VAL:HG22	3:H:286:ASP:HB3	1.99	0.43
1:B:124:LEU:O	1:B:255:ASN:ND2	2.40	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:80:THR:H	2:h:136:ASP:HB2	1.83	0.43
3:E:360:VAL:HG11	3:E:381:ASN:HD22	1.83	0.43
3:N:204:ASN:HB3	3:N:296:ARG:HB3	2.01	0.43
3:O:204:ASN:HB3	3:O:296:ARG:HB3	2.01	0.43
1:A:136:TYR:OH	1:A:807:ASP:OD2	2.33	0.43
1:A:330:LEU:HD11	1:A:608:VAL:HG21	2.01	0.43
2:c:197:PRO:HG2	2:c:205:ILE:HB	2.00	0.43
2:d:160:LEU:HD22	2:d:283:ARG:HE	1.84	0.43
2:f:99:LYS:HG2	2:f:118:PHE:HD2	1.84	0.43
2:f:322:PHE:HE2	2:f:324:TYR:HB2	1.83	0.43
2:l:315:ARG:HB3	2:l:325:ARG:HB3	2.00	0.43
2:m:77:LEU:HD13	2:m:112:PRO:HG3	2.01	0.43
2:n:111:TRP:HE1	2:n:303:VAL:HG11	1.83	0.43
2:n:133:LEU:HB2	2:n:255:ARG:HH12	1.84	0.43
3:H:45:GLU:O	3:H:118:LYS:NZ	2.47	0.43
1:B:396:LEU:H	1:B:425:SER:HB3	1.84	0.42
2:e:145:ASP:HB2	2:e:148:LEU:HB2	2.01	0.42
2:g:193:ILE:HG12	2:g:239:VAL:HG22	2.01	0.42
2:i:152:MET:HE1	2:i:262:GLN:HG3	2.01	0.42
3:F:204:ASN:HB3	3:F:296:ARG:HB3	2.01	0.42
1:B:418:ASN:HB2	1:B:426:LEU:HD21	2.01	0.42
1:B:705:VAL:HG21	1:B:799:PRO:HG2	2.01	0.42
2:h:164:LEU:HB2	2:h:252:LEU:HD11	2.00	0.42
2:k:63:MET:HE3	3:K:162:ALA:HB1	2.02	0.42
1:B:172:TYR:HD1	1:B:687:ILE:HD12	1.83	0.42
2:c:305:GLN:HA	2:c:308:GLN:NE2	2.35	0.42
2:h:99:LYS:HG2	2:h:118:PHE:HD2	1.84	0.42
2:m:98:TRP:HA	2:m:101:THR:HG22	2.00	0.42
2:m:272:THR:OG1	2:m:277:THR:O	2.38	0.42
3:M:227:PRO:HA	3:M:322:LEU:HD23	2.02	0.42
2:g:121:TYR:OH	2:g:141:LEU:O	2.33	0.42
5:o:401:NAG:HO3	5:o:401:NAG:C7	2.28	0.42
3:D:227:PRO:HA	3:D:322:LEU:HD23	2.02	0.42
3:K:142:GLN:HB3	3:L:145:ARG:HH11	1.85	0.42
3:L:395:LEU:HD23	3:L:395:LEU:HA	1.93	0.42
3:M:304:VAL:HG22	3:N:248:PHE:HB2	2.00	0.42
1:B:248:HIS:CD2	1:B:249:PRO:HD2	2.54	0.42
2:c:205:ILE:HG22	2:d:101:THR:HG23	2.02	0.42
2:g:81:LEU:HD13	2:g:307:ILE:HD11	2.01	0.42
2:g:275:PRO:HB2	2:h:285:MET:HB3	2.02	0.42
2:n:160:LEU:HD23	2:n:258:VAL:HG13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:PRO:HA	3:C:322:LEU:HD23	2.02	0.42
3:E:227:PRO:HA	3:E:322:LEU:HD23	2.02	0.42
3:F:360:VAL:HG11	3:F:381:ASN:HD22	1.83	0.42
3:J:204:ASN:HB3	3:J:296:ARG:HB3	2.01	0.42
3:M:142:GLN:O	3:O:145:ARG:HD2	2.20	0.42
2:d:150:LEU:HD13	2:d:154:GLU:CG	2.44	0.42
3:L:26:ASN:ND2	3:N:33:GLN:OE1	2.49	0.42
3:L:204:ASN:HB3	3:L:296:ARG:HB3	2.01	0.42
1:B:599:PRO:HA	1:B:602:LEU:HB3	2.02	0.42
2:l:161:ASN:HA	2:l:254:PRO:HA	2.01	0.42
3:G:227:PRO:HA	3:G:322:LEU:HD23	2.02	0.42
3:K:204:ASN:HB3	3:K:296:ARG:HB3	2.01	0.42
1:A:242:ASN:HA	1:A:844:LEU:O	2.20	0.42
1:B:749:ILE:O	1:B:753:LEU:CB	2.68	0.42
2:c:305:GLN:CD	2:c:308:GLN:NE2	2.77	0.42
2:d:90:ALA:HA	2:d:93:ILE:HD12	2.01	0.42
2:f:67:TYR:CE1	3:F:239:ASN:HB3	2.54	0.42
2:n:296:PHE:HA	2:n:299:VAL:HG12	2.02	0.42
3:D:37:MET:HE3	3:D:37:MET:HB2	1.70	0.42
3:D:204:ASN:HB3	3:D:296:ARG:HB3	2.01	0.42
3:J:45:GLU:O	3:J:118:LYS:NZ	2.47	0.42
3:O:227:PRO:HA	3:O:322:LEU:HD23	2.02	0.42
1:A:437:ILE:HG12	1:A:531:ILE:HD12	2.01	0.42
2:d:145:ASP:CB	2:d:148:LEU:HD22	2.40	0.42
2:k:182:ASN:HA	2:k:250:LYS:HA	2.02	0.42
2:h:149:GLN:HE21	2:h:268:ILE:HB	1.85	0.42
2:k:186:SER:HA	2:k:245:THR:O	2.20	0.42
3:C:351:GLN:OE1	3:E:271:ASN:ND2	2.52	0.42
1:A:233:ARG:HH12	1:A:235:GLN:NE2	2.17	0.41
1:B:357:LEU:HD11	1:B:367:GLN:HG2	2.01	0.41
2:d:194:LYS:HA	2:d:217:GLU:HA	2.01	0.41
2:e:93:ILE:HD11	2:e:296:PHE:CE2	2.55	0.41
2:e:182:ASN:HB3	2:e:250:LYS:HG2	2.02	0.41
2:h:297:TYR:HA	2:h:300:VAL:HG22	2.01	0.41
2:j:133:LEU:HB3	2:j:138:ASN:ND2	2.35	0.41
2:l:161:ASN:HD22	2:l:254:PRO:HA	1.84	0.41
2:m:141:LEU:HD23	2:m:261:ILE:HB	2.00	0.41
3:D:45:GLU:O	3:D:118:LYS:NZ	2.47	0.41
1:A:335:VAL:HG11	1:A:382:LYS:HA	2.01	0.41
1:A:547:ASP:OD2	1:A:881:GLU:HB2	2.20	0.41
1:B:420:MET:HE3	1:B:420:MET:HB3	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:g:57:LEU:HD11	2:i:59:ILE:HG22	2.02	0.41
3:C:360:VAL:HG11	3:C:381:ASN:HD22	1.83	0.41
3:G:395:LEU:HD23	3:G:395:LEU:HA	1.93	0.41
3:N:254:LEU:HD21	3:N:297:PRO:HD3	2.02	0.41
2:d:262:GLN:NE2	2:d:266:SER:O	2.52	0.41
2:f:178:THR:H	2:f:182:ASN:HD21	1.67	0.41
2:m:179:ASP:OD1	2:m:180:GLU:N	2.53	0.41
2:n:266:SER:OG	2:n:267:ASP:N	2.52	0.41
3:E:204:ASN:HB3	3:E:296:ARG:HB3	2.01	0.41
3:F:395:LEU:HD23	3:F:395:LEU:HA	1.93	0.41
3:K:394:MET:HE3	3:K:394:MET:HB2	1.90	0.41
1:B:310:LEU:HD23	1:B:620:ILE:CD1	2.50	0.41
2:e:263:VAL:HG12	2:e:289:TRP:CD1	2.55	0.41
3:C:254:LEU:HD21	3:C:297:PRO:HD3	2.03	0.41
3:L:167:ASN:N	3:L:177:MET:O	2.54	0.41
2:e:61:GLY:HA3	3:E:241:ALA:HA	2.03	0.41
2:e:65:THR:OG1	3:E:239:ASN:ND2	2.54	0.41
2:e:76:PHE:HE1	2:e:307:ILE:HG12	1.85	0.41
2:g:99:LYS:HG2	2:g:118:PHE:HD2	1.85	0.41
2:k:67:TYR:HE1	3:K:239:ASN:HB3	1.86	0.41
2:l:263:VAL:HG12	2:l:289:TRP:CD1	2.55	0.41
2:m:79:SER:O	2:m:115:SER:OG	2.38	0.41
3:I:227:PRO:HA	3:I:322:LEU:HD23	2.02	0.41
3:I:227:PRO:HG2	3:J:231:ARG:HH12	1.86	0.41
3:M:167:ASN:N	3:M:177:MET:O	2.54	0.41
3:O:167:ASN:N	3:O:177:MET:O	2.54	0.41
1:A:441:ALA:HA	1:A:520:PHE:CD1	2.56	0.41
1:B:768:ILE:HG13	1:B:798:LYS:HG2	2.02	0.41
2:c:309:VAL:O	2:c:309:VAL:HG12	2.21	0.41
2:g:230:VAL:HB	2:h:300:VAL:HG23	2.01	0.41
2:i:141:LEU:HD23	2:i:261:ILE:HB	2.02	0.41
2:i:194:LYS:HG2	2:i:217:GLU:HA	2.01	0.41
2:k:297:TYR:HA	2:k:300:VAL:HG12	2.02	0.41
2:k:317:LEU:C	2:k:317:LEU:CD2	2.93	0.41
2:o:160:LEU:HD21	2:o:260:VAL:HG23	2.02	0.41
3:C:112:GLN:HG2	3:C:384:ARG:HH12	1.86	0.41
3:F:254:LEU:HD21	3:F:297:PRO:HD3	2.02	0.41
3:G:167:ASN:N	3:G:177:MET:O	2.54	0.41
3:H:112:GLN:HG2	3:H:384:ARG:HH12	1.86	0.41
3:M:373:ASN:O	3:M:378:ARG:NH1	2.54	0.41
1:B:442:PHE:CE1	3:H:68:THR:HA	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:PHE:CE2	1:B:504:VAL:HG21	2.56	0.41
2:c:95:ASP:HB3	2:c:98:TRP:HB3	2.01	0.41
2:h:193:ILE:HG12	2:h:239:VAL:HG22	2.02	0.41
2:m:133:LEU:HD11	2:m:159:ILE:HG23	2.03	0.41
2:n:65:THR:O	3:N:239:ASN:ND2	2.53	0.41
2:o:182:ASN:HB3	2:o:250:LYS:HG2	2.03	0.41
3:D:33:GLN:NE2	3:D:127:ILE:O	2.54	0.41
3:D:112:GLN:HG2	3:D:384:ARG:HH12	1.86	0.41
3:E:254:LEU:HD21	3:E:297:PRO:HD3	2.02	0.41
3:F:45:GLU:O	3:F:118:LYS:NZ	2.47	0.41
3:H:227:PRO:HA	3:H:322:LEU:HD23	2.02	0.41
3:I:338:ALA:O	3:K:153:HIS:ND1	2.48	0.41
1:A:627:ILE:HD12	1:A:671:LEU:HD23	2.02	0.41
1:A:708:ALA:HB3	1:A:712:MET:HE2	2.02	0.41
1:A:735:ILE:HD13	1:A:749:ILE:HG22	2.03	0.41
2:c:290:LYS:HG2	2:e:150:LEU:HD13	2.03	0.41
2:c:318:ASN:OD1	2:c:319:SER:N	2.53	0.41
2:d:70:SER:HB2	3:C:298:PRO:HB2	2.02	0.41
2:f:124:ILE:O	2:f:128:SER:HB2	2.20	0.41
2:i:128:SER:HB3	2:i:224:LEU:HB2	2.02	0.41
2:m:199:ASN:HD21	2:m:203:LEU:HB2	1.86	0.41
3:C:167:ASN:N	3:C:177:MET:O	2.53	0.41
3:D:167:ASN:N	3:D:177:MET:O	2.54	0.41
3:E:112:GLN:HG2	3:E:384:ARG:HH12	1.86	0.41
3:G:112:GLN:HG2	3:G:384:ARG:HH12	1.86	0.41
3:H:83:ASN:ND2	3:I:122:ILE:HG23	2.35	0.41
3:H:167:ASN:N	3:H:177:MET:O	2.54	0.41
3:J:167:ASN:N	3:J:177:MET:O	2.54	0.41
3:N:227:PRO:HA	3:N:322:LEU:HD23	2.02	0.41
1:A:437:ILE:HG22	1:A:515:LEU:HD13	2.03	0.41
1:A:723:VAL:HB	1:A:725:ILE:HG13	2.03	0.41
1:A:768:ILE:HG12	1:A:800:ILE:HG12	2.02	0.41
1:B:220:GLU:OE2	3:O:39:ILE:HD13	2.21	0.41
2:c:83:LEU:HA	2:c:139:VAL:O	2.21	0.41
2:i:318:ASN:OD1	2:i:319:SER:N	2.54	0.41
2:k:82:CYS:HB2	2:k:138:ASN:HD22	1.86	0.41
3:E:167:ASN:N	3:E:177:MET:O	2.54	0.41
3:F:33:GLN:NE2	3:F:127:ILE:O	2.54	0.41
3:F:167:ASN:N	3:F:177:MET:O	2.54	0.41
3:G:373:ASN:O	3:G:378:ARG:NH1	2.54	0.41
3:H:254:LEU:HD21	3:H:297:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:394:MET:HE3	3:H:394:MET:HB2	1.90	0.41
3:J:33:GLN:NE2	3:J:127:ILE:O	2.54	0.41
3:K:167:ASN:N	3:K:177:MET:O	2.54	0.41
3:L:33:GLN:NE2	3:L:127:ILE:O	2.54	0.41
3:L:373:ASN:O	3:L:378:ARG:NH1	2.54	0.41
3:M:33:GLN:NE2	3:M:127:ILE:O	2.54	0.41
3:M:112:GLN:HG2	3:M:384:ARG:HH12	1.86	0.41
3:N:112:GLN:HG2	3:N:384:ARG:HH12	1.86	0.41
3:N:167:ASN:N	3:N:177:MET:O	2.54	0.41
3:O:373:ASN:O	3:O:378:ARG:NH1	2.54	0.41
1:A:372:ILE:HA	1:A:585:SER:HB3	2.02	0.41
1:A:773:VAL:HG22	1:A:804:ILE:HD12	2.01	0.41
1:B:266:PRO:HA	1:B:299:ARG:HD3	2.02	0.41
1:B:555:ASN:ND2	1:B:597:PRO:HD3	2.36	0.41
2:d:272:THR:OG1	2:d:277:THR:O	2.39	0.41
2:m:103:SER:HA	2:m:106:PHE:HD2	1.86	0.41
2:m:286:ARG:HH12	2:m:288:ASN:HD21	1.69	0.41
3:F:227:PRO:HA	3:F:322:LEU:HD23	2.02	0.41
3:H:69:THR:O	3:H:69:THR:CG2	2.69	0.41
3:N:394:MET:HE3	3:N:394:MET:HB2	1.90	0.41
1:B:520:PHE:H	1:B:528:LYS:HD2	1.86	0.40
2:g:178:THR:H	2:g:182:ASN:HD22	1.69	0.40
2:h:268:ILE:HG13	2:h:269:LEU:HD12	2.03	0.40
2:h:274:ASP:OD2	2:h:276:THR:OG1	2.38	0.40
2:j:254:PRO:HD3	3:J:312:GLN:HG2	2.03	0.40
3:C:33:GLN:NE2	3:C:127:ILE:O	2.54	0.40
3:E:33:GLN:NE2	3:E:127:ILE:O	2.54	0.40
3:H:373:ASN:O	3:H:378:ARG:NH1	2.54	0.40
3:I:45:GLU:O	3:I:118:LYS:NZ	2.47	0.40
3:J:227:PRO:HA	3:J:322:LEU:HD23	2.02	0.40
3:K:33:GLN:NE2	3:K:127:ILE:O	2.54	0.40
3:K:254:LEU:HD21	3:K:297:PRO:HD3	2.02	0.40
3:K:373:ASN:O	3:K:378:ARG:NH1	2.54	0.40
3:L:227:PRO:HA	3:L:322:LEU:HD23	2.02	0.40
3:M:137:GLU:OE1	3:N:397:LYS:NZ	2.52	0.40
3:N:33:GLN:NE2	3:N:127:ILE:O	2.54	0.40
3:O:112:GLN:HG2	3:O:384:ARG:HH12	1.86	0.40
1:B:260:GLN:HB3	3:N:71:LEU:HB2	2.04	0.40
2:e:88:GLU:HA	2:e:91:THR:HG22	2.03	0.40
2:i:103:SER:HA	2:i:106:PHE:HD2	1.85	0.40
2:k:163:TRP:HB3	2:k:249:CYS:SG	2.61	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:133:LEU:HB3	2:l:138:ASN:ND2	2.36	0.40
2:m:194:LYS:HG2	2:m:217:GLU:HB3	2.03	0.40
3:F:373:ASN:O	3:F:378:ARG:NH1	2.54	0.40
3:I:33:GLN:NE2	3:I:127:ILE:O	2.54	0.40
3:I:271:ASN:ND2	3:J:351:GLN:OE1	2.54	0.40
3:J:395:LEU:HD23	3:J:395:LEU:HA	1.93	0.40
1:B:641:LYS:HD2	1:B:665:TYR:HE1	1.86	0.40
2:c:138:ASN:H	2:c:310:MET:HE1	1.87	0.40
2:c:257:ASN:OD1	2:c:258:VAL:N	2.52	0.40
2:e:84:TYR:CE1	2:e:119:LYS:HB3	2.56	0.40
2:f:88:GLU:OE2	2:f:143:LYS:NZ	2.40	0.40
2:g:190:SER:O	2:g:243:THR:OG1	2.33	0.40
2:h:67:TYR:CE1	3:H:239:ASN:HB3	2.56	0.40
2:k:160:LEU:HD21	2:k:260:VAL:HG23	2.04	0.40
2:l:52:ASN:H	3:K:168:ARG:HA	1.86	0.40
2:l:83:LEU:HD23	2:l:139:VAL:HG13	2.04	0.40
2:n:255:ARG:O	2:n:283:ARG:NH2	2.53	0.40
3:C:373:ASN:O	3:C:378:ARG:NH1	2.54	0.40
3:G:254:LEU:HD21	3:G:297:PRO:HD3	2.02	0.40
3:J:254:LEU:HD21	3:J:297:PRO:HD3	2.02	0.40
3:L:112:GLN:HG2	3:L:384:ARG:HH12	1.86	0.40
3:L:254:LEU:HD21	3:L:297:PRO:HD3	2.03	0.40
1:A:380:CYS:HB2	1:A:582:SER:HB2	2.02	0.40
1:B:484:GLN:HG3	1:B:493:GLN:OE1	2.22	0.40
2:d:285:MET:HE1	2:d:306:ILE:HG23	2.02	0.40
2:i:112:PRO:HG2	2:i:115:SER:HB3	2.04	0.40
2:j:287:ILE:HD11	2:j:295:VAL:HG13	2.03	0.40
3:D:254:LEU:HD21	3:D:297:PRO:HD3	2.02	0.40
3:G:45:GLU:O	3:G:118:LYS:NZ	2.47	0.40
3:L:45:GLU:O	3:L:118:LYS:NZ	2.47	0.40
3:M:254:LEU:HD21	3:M:297:PRO:HD3	2.03	0.40
3:M:395:LEU:HD23	3:M:395:LEU:HA	1.93	0.40
1:A:191:GLU:HA	1:A:200:LYS:HA	2.03	0.40
1:B:501:ASN:HB3	1:B:873:PHE:CZ	2.57	0.40
1:B:706:ILE:HB	1:B:826:LYS:HB2	2.03	0.40
2:c:305:GLN:O	2:c:309:VAL:HG23	2.21	0.40
2:d:168:MET:CE	2:d:175:TYR:CG	2.98	0.40
2:i:305:GLN:HB3	2:k:276:THR:HG21	2.04	0.40
2:n:145:ASP:OD2	2:n:148:LEU:HD23	2.21	0.40
3:E:373:ASN:O	3:E:378:ARG:NH1	2.54	0.40
3:H:33:GLN:NE2	3:H:127:ILE:O	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:260:GLU:HG2	3:H:274:GLN:HG2	2.04	0.40
3:I:112:GLN:HG2	3:I:384:ARG:HH12	1.86	0.40
3:I:167:ASN:N	3:I:177:MET:O	2.54	0.40
3:I:254:LEU:HD21	3:I:297:PRO:HD3	2.02	0.40
3:J:373:ASN:O	3:J:378:ARG:NH1	2.54	0.40
3:M:253:ILE:HG13	3:N:234:PHE:CE1	2.57	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	779/882 (88%)	728 (94%)	50 (6%)	1 (0%)	48	78
1	B	798/882 (90%)	753 (94%)	42 (5%)	3 (0%)	30	59
2	c	272/326 (83%)	251 (92%)	21 (8%)	0	100	100
2	d	256/326 (78%)	243 (95%)	13 (5%)	0	100	100
2	e	268/326 (82%)	251 (94%)	17 (6%)	0	100	100
2	f	273/326 (84%)	252 (92%)	21 (8%)	0	100	100
2	g	274/326 (84%)	264 (96%)	10 (4%)	0	100	100
2	h	275/326 (84%)	255 (93%)	20 (7%)	0	100	100
2	i	271/326 (83%)	253 (93%)	18 (7%)	0	100	100
2	j	268/326 (82%)	246 (92%)	22 (8%)	0	100	100
2	k	273/326 (84%)	251 (92%)	22 (8%)	0	100	100
2	l	274/326 (84%)	252 (92%)	20 (7%)	2 (1%)	18	47
2	m	258/326 (79%)	242 (94%)	16 (6%)	0	100	100
2	n	275/326 (84%)	253 (92%)	22 (8%)	0	100	100
2	o	259/326 (79%)	238 (92%)	21 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	D	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	E	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	F	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	G	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	H	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	I	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	J	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	K	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	L	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	M	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	N	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
3	O	395/397 (100%)	380 (96%)	15 (4%)	0	100	100
All	All	10208/11163 (91%)	9672 (95%)	530 (5%)	6 (0%)	49	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	746	TYR
1	A	220	GLU
2	l	71	THR
1	B	747	ALA
1	B	809	ASN
2	l	314	SER

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	714/812 (88%)	712 (100%)	2 (0%)	86	84
1	B	732/812 (90%)	732 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	c	245/296 (83%)	245 (100%)	0	100	100
2	d	233/296 (79%)	232 (100%)	1 (0%)	84	83
2	e	243/296 (82%)	243 (100%)	0	100	100
2	f	247/296 (83%)	247 (100%)	0	100	100
2	g	247/296 (83%)	247 (100%)	0	100	100
2	h	247/296 (83%)	247 (100%)	0	100	100
2	i	245/296 (83%)	245 (100%)	0	100	100
2	j	243/296 (82%)	240 (99%)	3 (1%)	63	72
2	k	247/296 (83%)	245 (99%)	2 (1%)	73	77
2	l	248/296 (84%)	248 (100%)	0	100	100
2	m	234/296 (79%)	234 (100%)	0	100	100
2	n	247/296 (83%)	247 (100%)	0	100	100
2	o	235/296 (79%)	235 (100%)	0	100	100
3	C	351/351 (100%)	351 (100%)	0	100	100
3	D	351/351 (100%)	351 (100%)	0	100	100
3	E	351/351 (100%)	351 (100%)	0	100	100
3	F	351/351 (100%)	351 (100%)	0	100	100
3	G	351/351 (100%)	351 (100%)	0	100	100
3	H	351/351 (100%)	348 (99%)	3 (1%)	70	76
3	I	351/351 (100%)	351 (100%)	0	100	100
3	J	351/351 (100%)	351 (100%)	0	100	100
3	K	351/351 (100%)	351 (100%)	0	100	100
3	L	351/351 (100%)	351 (100%)	0	100	100
3	M	351/351 (100%)	351 (100%)	0	100	100
3	N	351/351 (100%)	351 (100%)	0	100	100
3	O	351/351 (100%)	351 (100%)	0	100	100
All	All	9170/10035 (91%)	9159 (100%)	11 (0%)	87	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	GLU
1	A	220	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	d	164	LEU
2	j	75	THR
2	j	148	LEU
2	j	268	ILE
2	k	147	THR
2	k	148	LEU
3	H	65	LEU
3	H	68	THR
3	H	69	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (218) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	GLN
1	A	248	HIS
1	A	269	ASN
1	A	307	GLN
1	A	367	GLN
1	A	391	GLN
1	A	402	ASN
1	A	435	ASN
1	A	466	GLN
1	A	478	ASN
1	A	484	GLN
1	A	492	ASN
1	A	493	GLN
1	A	569	HIS
1	A	615	ASN
1	A	869	ASN
1	B	89	GLN
1	B	215	GLN
1	B	235	GLN
1	B	242	ASN
1	B	252	HIS
1	B	260	GLN
1	B	261	HIS
1	B	269	ASN
1	B	285	ASN
1	B	307	GLN
1	B	327	ASN
1	B	467	ASN
1	B	475	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	506	ASN
1	B	544	GLN
1	B	555	ASN
1	B	637	GLN
1	B	733	GLN
1	B	734	GLN
1	B	842	HIS
1	B	869	ASN
2	c	138	ASN
2	c	166	ASN
2	c	199	ASN
2	c	294	GLN
2	c	308	GLN
2	d	166	ASN
2	d	257	ASN
2	d	294	GLN
2	e	161	ASN
2	e	182	ASN
2	e	235	HIS
2	e	294	GLN
2	f	182	ASN
2	f	199	ASN
2	f	235	HIS
2	g	138	ASN
2	g	149	GLN
2	g	177	GLN
2	g	235	HIS
2	g	294	GLN
2	i	72	GLN
2	i	235	HIS
2	i	294	GLN
2	i	305	GLN
2	j	161	ASN
2	j	176	GLN
2	j	305	GLN
2	k	72	GLN
2	k	235	HIS
2	k	248	ASN
2	l	138	ASN
2	l	161	ASN
2	l	280	GLN
2	l	294	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	l	305	GLN
2	l	308	GLN
2	m	161	ASN
2	m	305	GLN
2	n	52	ASN
2	n	182	ASN
2	n	201	GLN
2	n	235	HIS
2	n	294	GLN
2	n	305	GLN
2	n	308	GLN
2	o	132	GLN
2	o	161	ASN
2	o	177	GLN
2	o	201	GLN
2	o	235	HIS
2	o	248	ASN
3	C	36	GLN
3	C	42	ASN
3	C	94	ASN
3	C	173	HIS
3	C	207	GLN
3	C	210	HIS
3	C	312	GLN
3	C	345	ASN
3	C	381	ASN
3	D	36	GLN
3	D	42	ASN
3	D	94	ASN
3	D	173	HIS
3	D	207	GLN
3	D	210	HIS
3	D	312	GLN
3	D	345	ASN
3	D	381	ASN
3	E	36	GLN
3	E	42	ASN
3	E	94	ASN
3	E	173	HIS
3	E	207	GLN
3	E	210	HIS
3	E	239	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	312	GLN
3	E	345	ASN
3	E	381	ASN
3	F	36	GLN
3	F	42	ASN
3	F	94	ASN
3	F	173	HIS
3	F	207	GLN
3	F	210	HIS
3	F	239	ASN
3	F	284	ASN
3	F	312	GLN
3	F	345	ASN
3	F	381	ASN
3	G	36	GLN
3	G	42	ASN
3	G	94	ASN
3	G	173	HIS
3	G	207	GLN
3	G	210	HIS
3	G	239	ASN
3	G	312	GLN
3	G	345	ASN
3	G	381	ASN
3	H	36	GLN
3	H	42	ASN
3	H	83	ASN
3	H	94	ASN
3	H	173	HIS
3	H	207	GLN
3	H	210	HIS
3	H	312	GLN
3	H	345	ASN
3	H	381	ASN
3	I	36	GLN
3	I	42	ASN
3	I	94	ASN
3	I	207	GLN
3	I	210	HIS
3	I	239	ASN
3	I	312	GLN
3	I	345	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	381	ASN
3	J	36	GLN
3	J	42	ASN
3	J	72	ASN
3	J	94	ASN
3	J	207	GLN
3	J	210	HIS
3	J	312	GLN
3	J	345	ASN
3	J	381	ASN
3	K	36	GLN
3	K	42	ASN
3	K	94	ASN
3	K	173	HIS
3	K	207	GLN
3	K	210	HIS
3	K	284	ASN
3	K	312	GLN
3	K	345	ASN
3	K	381	ASN
3	L	36	GLN
3	L	42	ASN
3	L	83	ASN
3	L	94	ASN
3	L	207	GLN
3	L	210	HIS
3	L	312	GLN
3	L	345	ASN
3	L	381	ASN
3	M	36	GLN
3	M	42	ASN
3	M	83	ASN
3	M	94	ASN
3	M	173	HIS
3	M	207	GLN
3	M	210	HIS
3	M	284	ASN
3	M	310	ASN
3	M	312	GLN
3	M	345	ASN
3	M	381	ASN
3	N	36	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	N	42	ASN
3	N	94	ASN
3	N	173	HIS
3	N	207	GLN
3	N	210	HIS
3	N	312	GLN
3	N	345	ASN
3	N	381	ASN
3	O	33	GLN
3	O	36	GLN
3	O	42	ASN
3	O	94	ASN
3	O	173	HIS
3	O	207	GLN
3	O	210	HIS
3	O	239	ASN
3	O	284	ASN
3	O	312	GLN
3	O	345	ASN
3	O	366	ASN
3	O	381	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](#)

Of 41 ligands modelled in this entry, 31 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	h	401	-	15,15,15	0.46	0	21,21,21	0.86	0
5	NAG	l	401	-	15,15,15	0.49	0	21,21,21	1.29	4 (19%)
5	NAG	n	401	-	15,15,15	0.43	0	21,21,21	0.57	0
5	NAG	d	401	-	15,15,15	0.55	0	21,21,21	1.31	3 (14%)
5	NAG	j	401	-	15,15,15	0.51	0	21,21,21	1.23	3 (14%)
5	NAG	k	401	-	15,15,15	0.50	0	21,21,21	0.99	1 (4%)
5	NAG	f	401	2	15,15,15	0.49	0	21,21,21	0.77	0
5	NAG	e	401	-	15,15,15	0.37	0	21,21,21	1.04	2 (9%)
5	NAG	m	401	2	15,15,15	0.52	0	21,21,21	0.76	0
5	NAG	o	401	-	15,15,15	0.41	0	21,21,21	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	h	401	-	-	4/6/26/26	0/1/1/1
5	NAG	l	401	-	-	4/6/26/26	0/1/1/1
5	NAG	n	401	-	-	2/6/26/26	0/1/1/1
5	NAG	d	401	-	-	3/6/26/26	0/1/1/1
5	NAG	j	401	-	-	6/6/26/26	0/1/1/1
5	NAG	k	401	-	-	2/6/26/26	0/1/1/1
5	NAG	f	401	2	-	5/6/26/26	0/1/1/1
5	NAG	e	401	-	-	2/6/26/26	0/1/1/1
5	NAG	m	401	2	-	0/6/26/26	0/1/1/1
5	NAG	o	401	-	-	4/6/26/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	d	401	NAG	O5-C1-C2	3.20	112.73	109.52
5	d	401	NAG	C1-C2-N2	-2.82	107.46	110.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	l	401	NAG	O5-C5-C6	2.67	113.05	106.44
5	j	401	NAG	C1-C2-C3	2.48	113.93	110.54
5	j	401	NAG	C3-C4-C5	-2.45	105.79	110.23
5	d	401	NAG	C1-C2-C3	2.42	113.84	110.54
5	l	401	NAG	C3-C4-C5	-2.35	105.98	110.23
5	k	401	NAG	O5-C5-C4	2.25	113.75	109.70
5	l	401	NAG	O5-C1-C2	2.21	111.73	109.52
5	e	401	NAG	O5-C5-C6	2.21	111.91	106.44
5	l	401	NAG	C1-C2-C3	2.05	113.34	110.54
5	e	401	NAG	C3-C4-C5	-2.04	106.53	110.23
5	j	401	NAG	O5-C5-C6	2.03	111.47	106.44

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	d	401	NAG	C1-C2-N2-C7
5	d	401	NAG	C8-C7-N2-C2
5	d	401	NAG	O7-C7-N2-C2
5	f	401	NAG	C3-C2-N2-C7
5	f	401	NAG	C8-C7-N2-C2
5	f	401	NAG	O7-C7-N2-C2
5	h	401	NAG	C1-C2-N2-C7
5	h	401	NAG	C8-C7-N2-C2
5	h	401	NAG	O7-C7-N2-C2
5	j	401	NAG	C1-C2-N2-C7
5	j	401	NAG	C8-C7-N2-C2
5	j	401	NAG	O7-C7-N2-C2
5	n	401	NAG	C8-C7-N2-C2
5	n	401	NAG	O7-C7-N2-C2
5	o	401	NAG	C1-C2-N2-C7
5	o	401	NAG	C3-C2-N2-C7
5	o	401	NAG	C8-C7-N2-C2
5	o	401	NAG	O7-C7-N2-C2
5	l	401	NAG	C3-C2-N2-C7
5	e	401	NAG	C8-C7-N2-C2
5	j	401	NAG	O5-C5-C6-O6
5	e	401	NAG	O7-C7-N2-C2
5	l	401	NAG	C4-C5-C6-O6
5	k	401	NAG	C4-C5-C6-O6
5	l	401	NAG	O5-C5-C6-O6
5	f	401	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	j	401	NAG	C3-C2-N2-C7
5	j	401	NAG	C4-C5-C6-O6
5	l	401	NAG	C1-C2-N2-C7
5	k	401	NAG	O5-C5-C6-O6
5	f	401	NAG	C1-C2-N2-C7
5	h	401	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	h	401	NAG	10	0
5	l	401	NAG	20	0
5	n	401	NAG	5	0
5	d	401	NAG	4	0
5	e	401	NAG	2	0
5	o	401	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

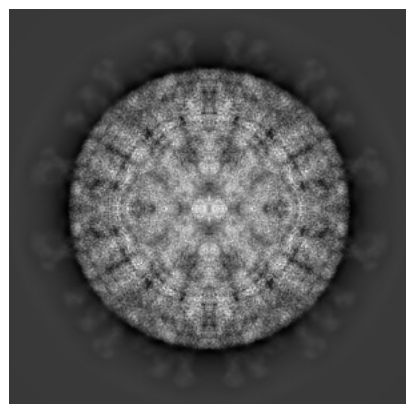
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16954. These allow visual inspection of the internal detail of the map and identification of artifacts.

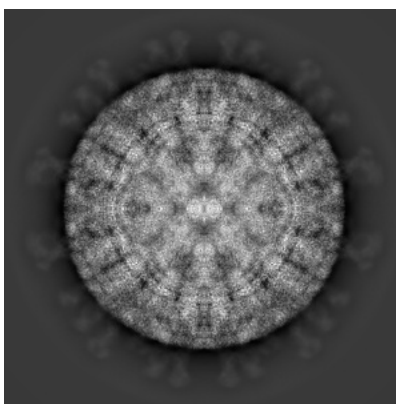
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

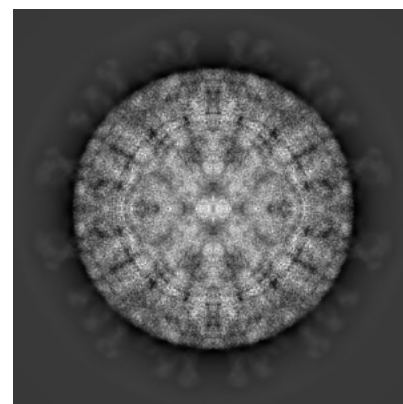
6.1.1 Primary map



X

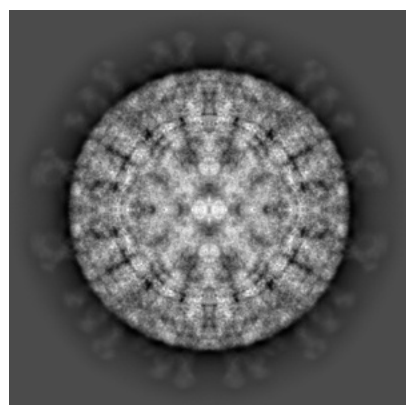


Y

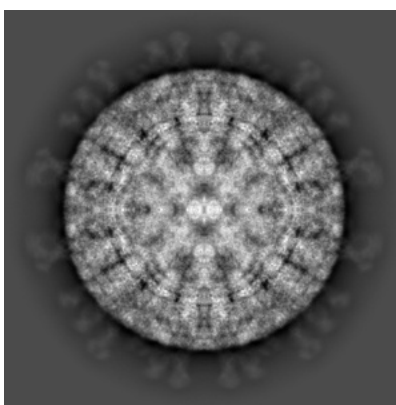


Z

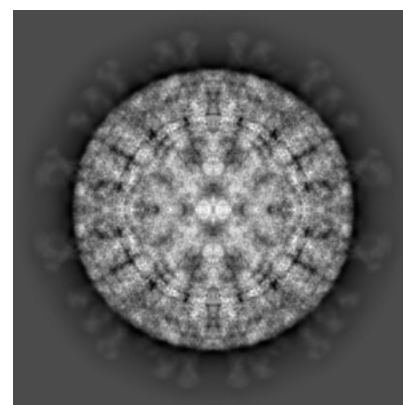
6.1.2 Raw map



X



Y

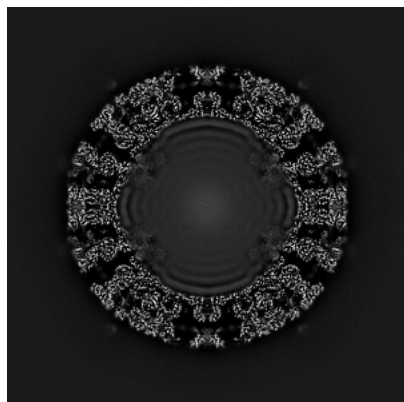


Z

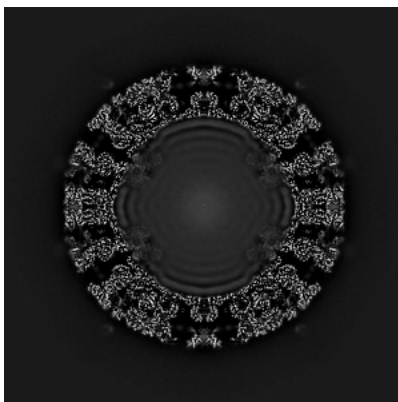
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

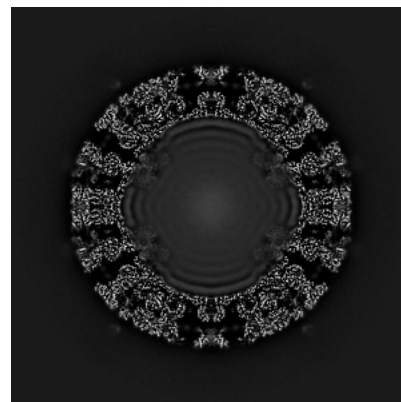
6.2.1 Primary map



X Index: 400

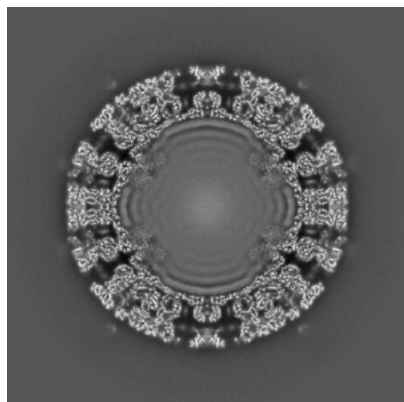


Y Index: 400

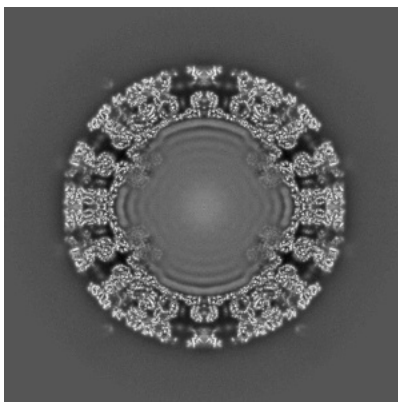


Z Index: 400

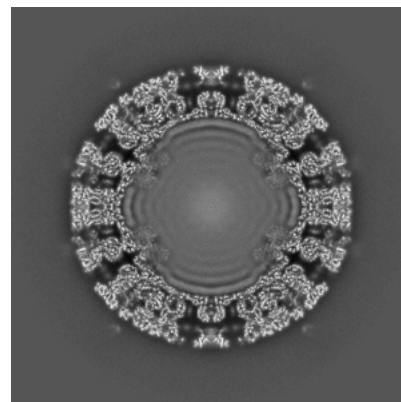
6.2.2 Raw map



X Index: 400



Y Index: 400

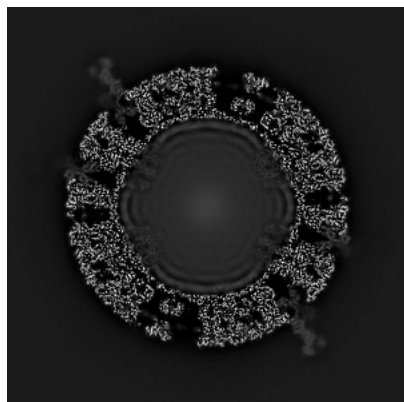


Z Index: 400

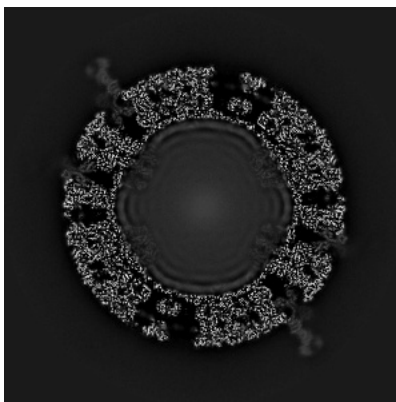
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

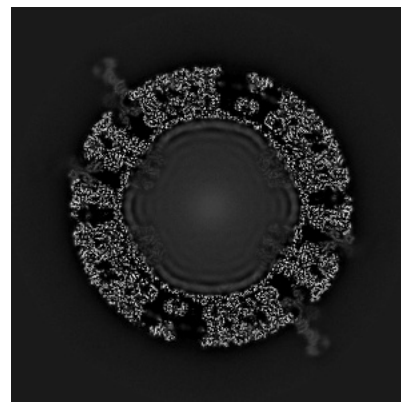
6.3.1 Primary map



X Index: 380

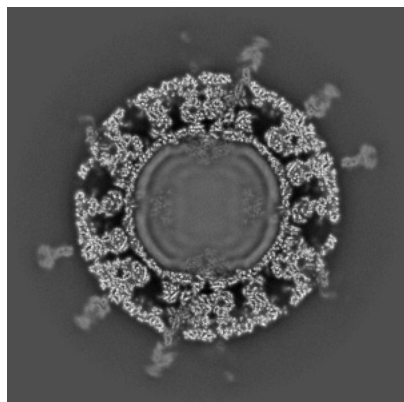


Y Index: 380

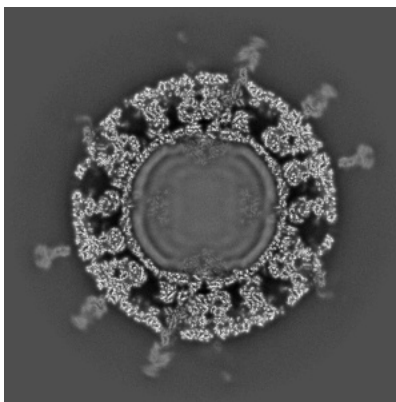


Z Index: 380

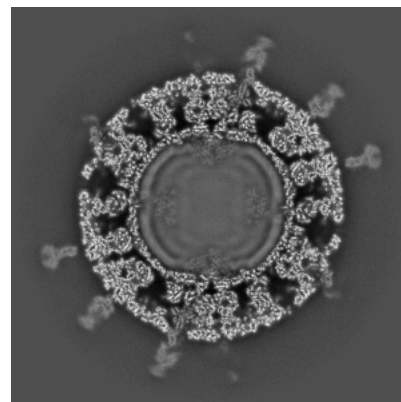
6.3.2 Raw map



X Index: 304



Y Index: 304

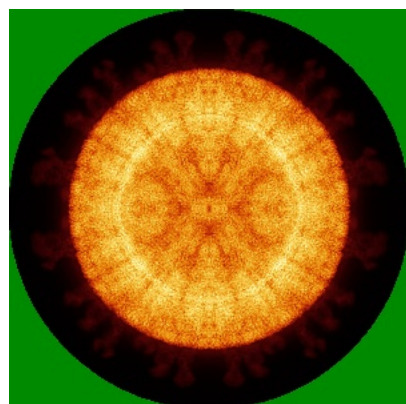


Z Index: 304

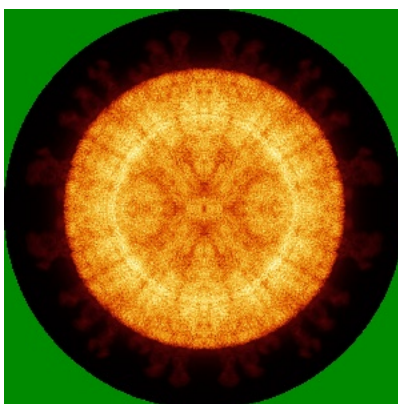
The images above show the largest variance slices of the map in three orthogonal directions.

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

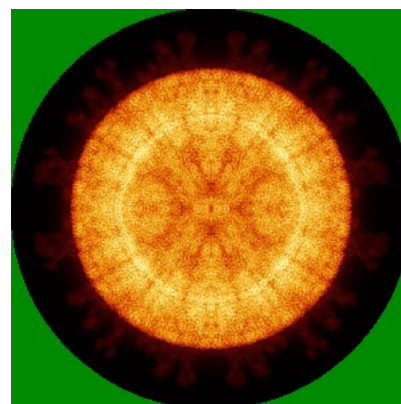
6.4.1 Primary map



X

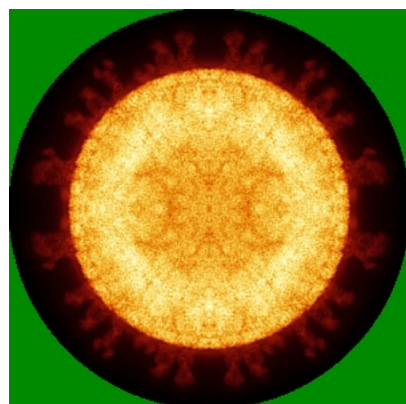


Y

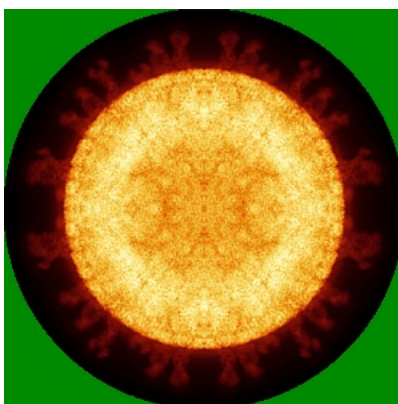


Z

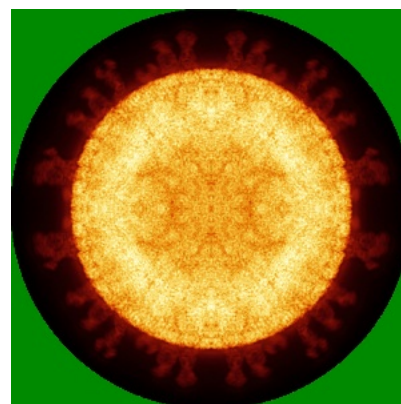
6.4.2 Raw map



X



Y

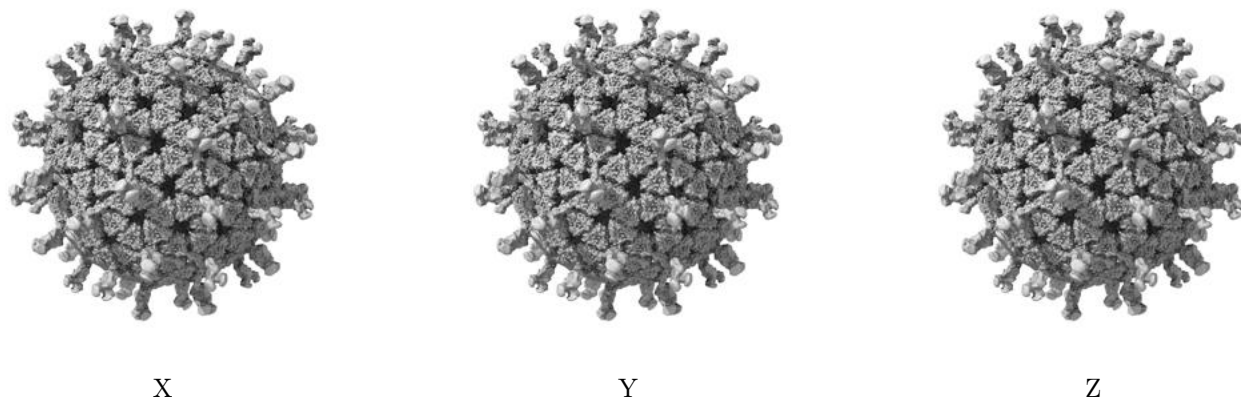


Z

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

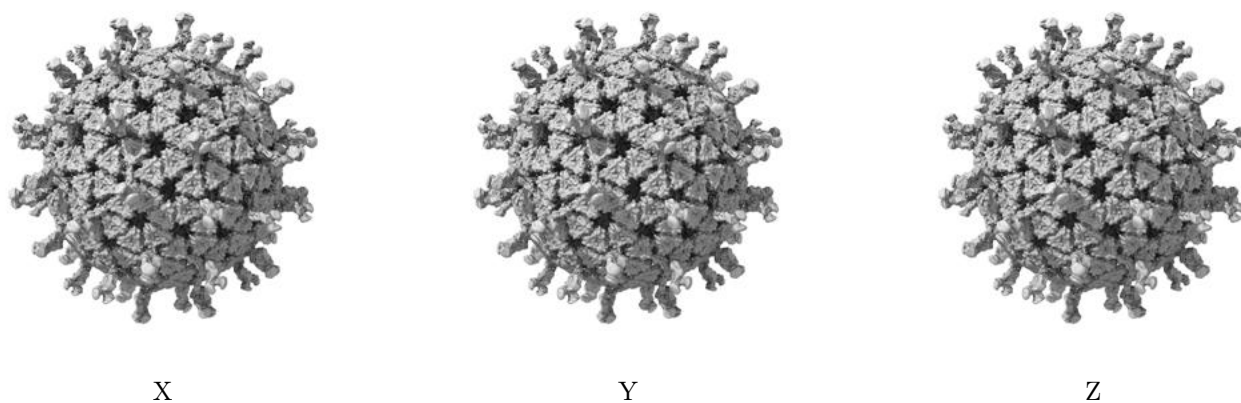
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

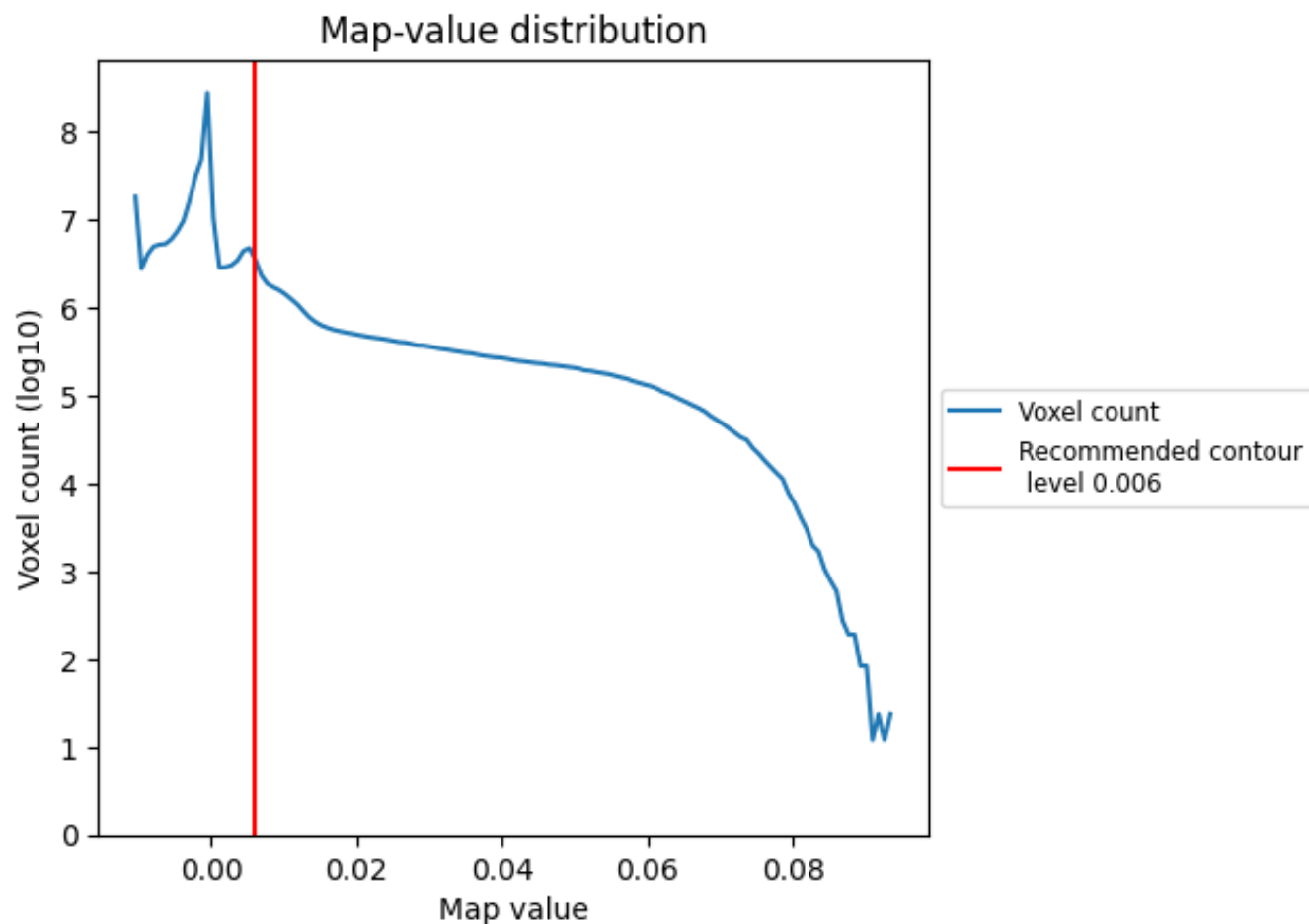
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

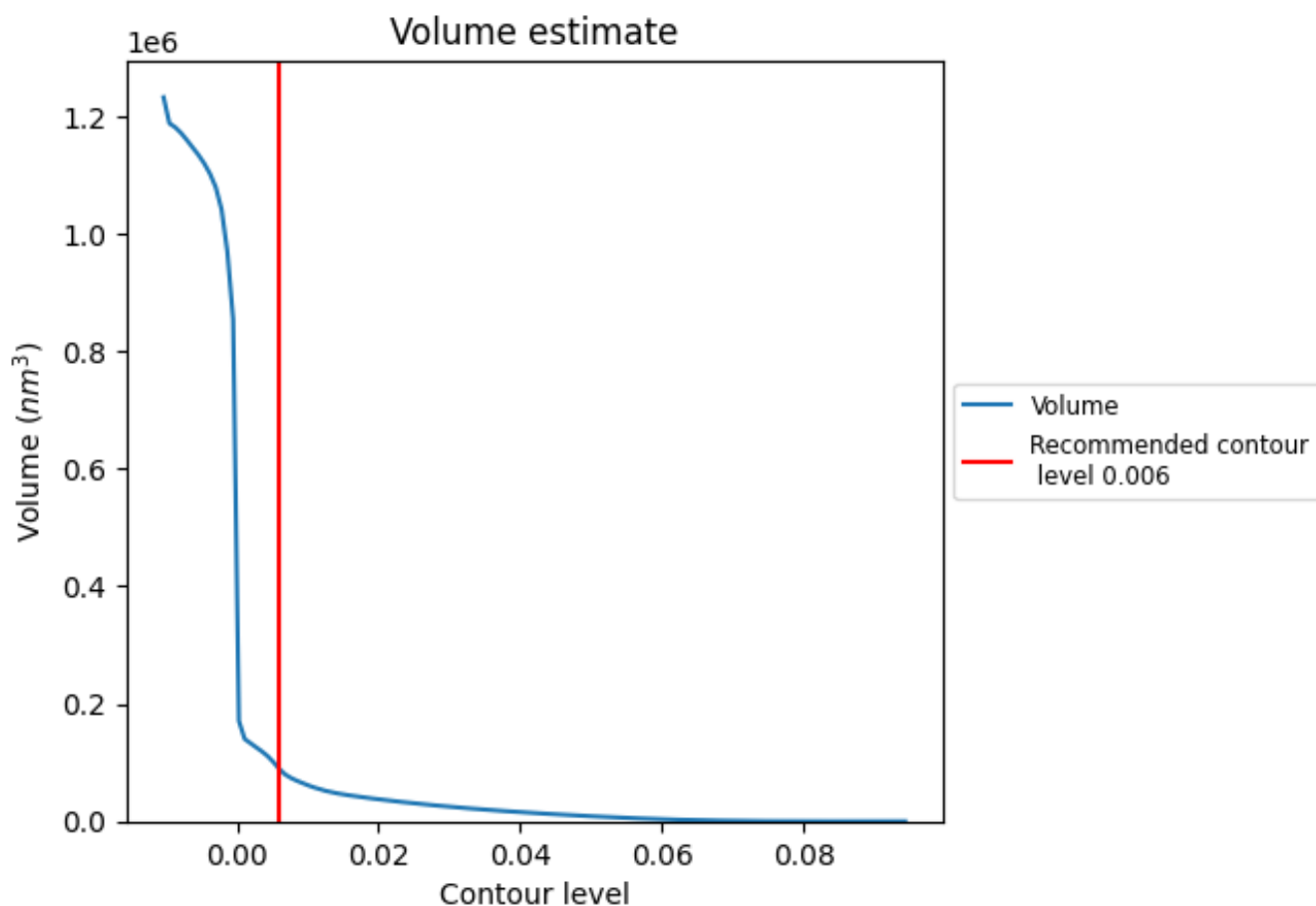
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

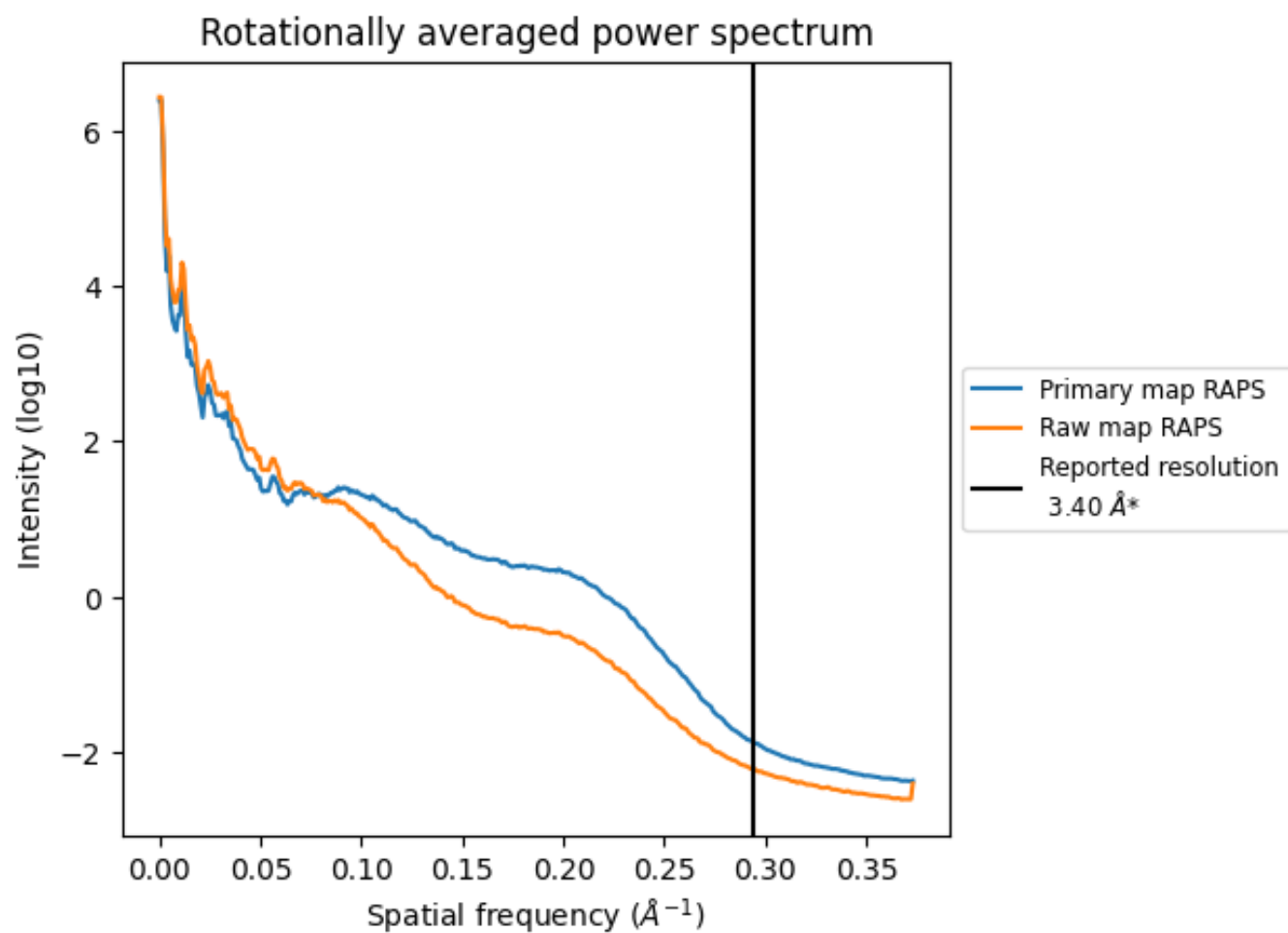
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89021 nm³; this corresponds to an approximate mass of 80415 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 ⓘ

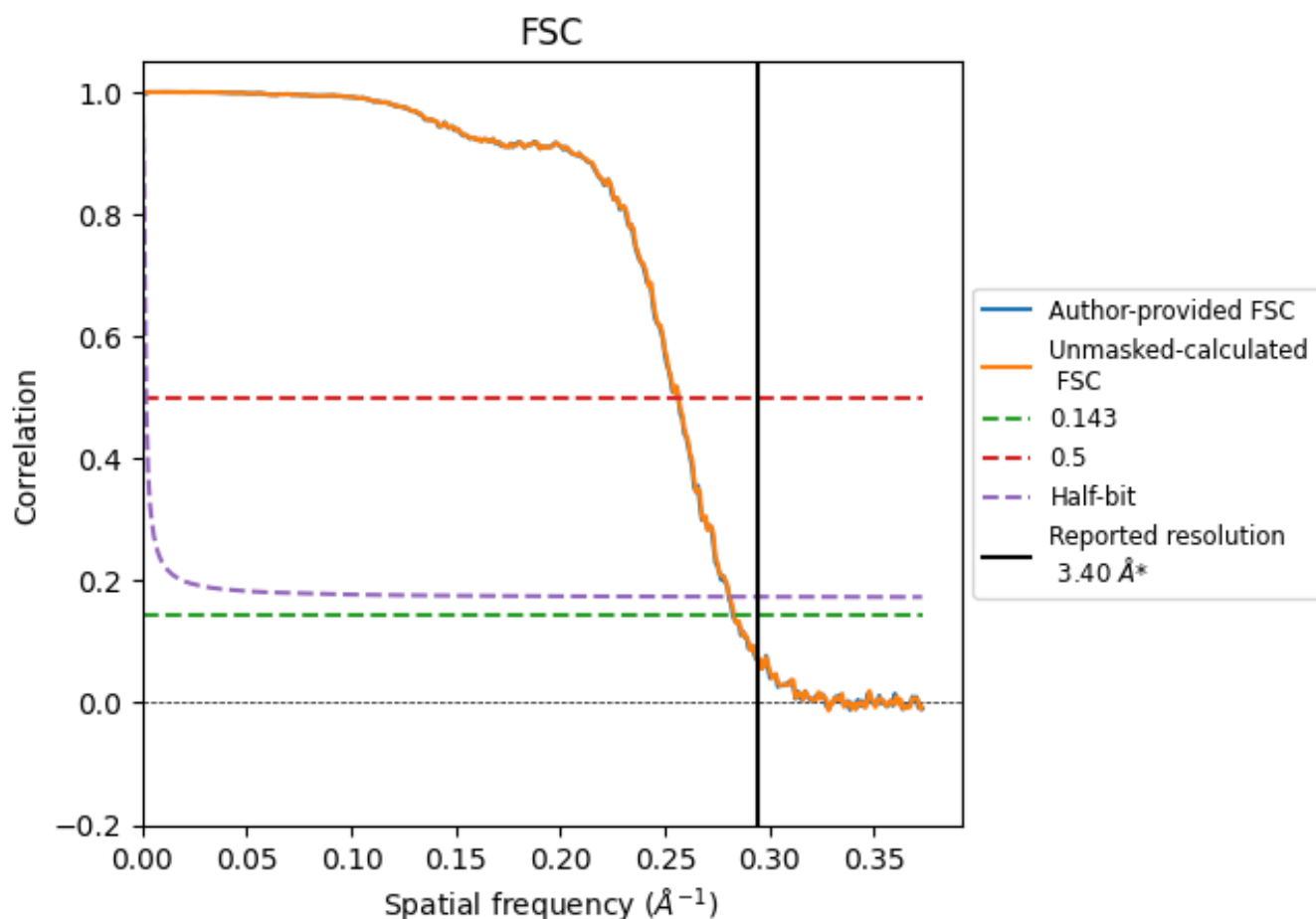


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.54	3.90	3.56
Unmasked-calculated*	3.53	3.89	3.56

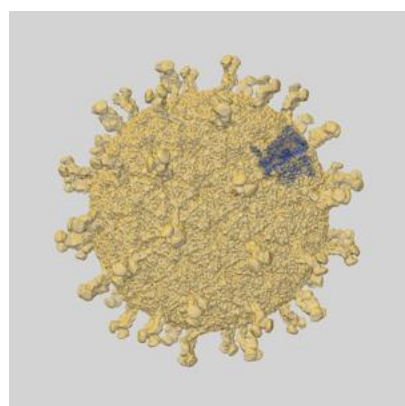
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

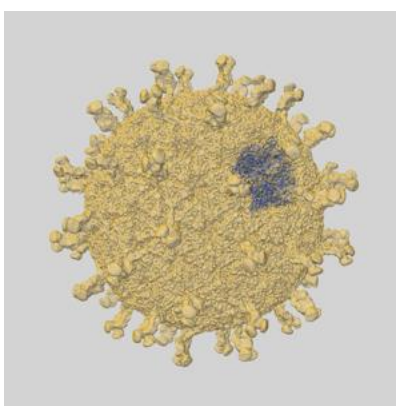
This section contains information regarding the fit between EMDB map EMD-16954 and PDB model 8OLB. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

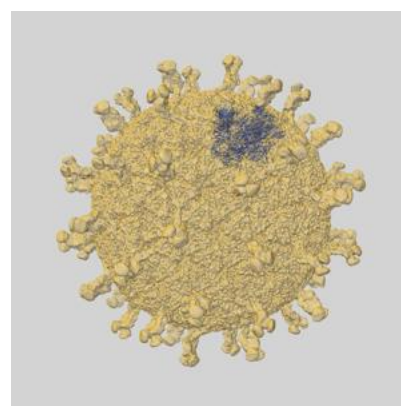
9.1.1 Map-model overlay [i](#)



X

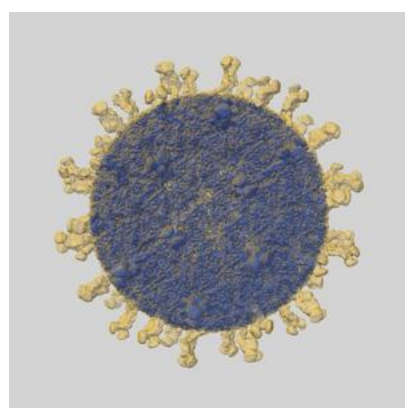


Y

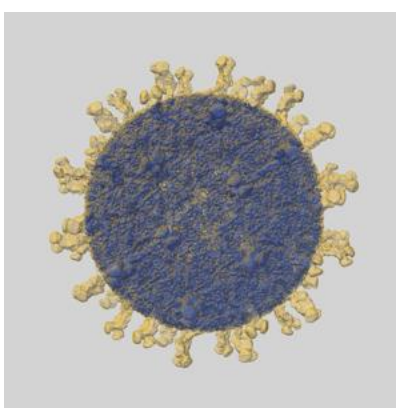


Z

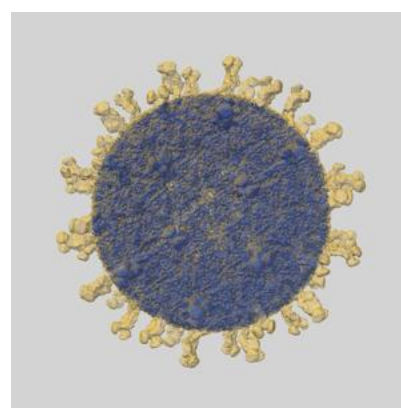
9.1.2 Map-model assembly overlay [i](#)



X



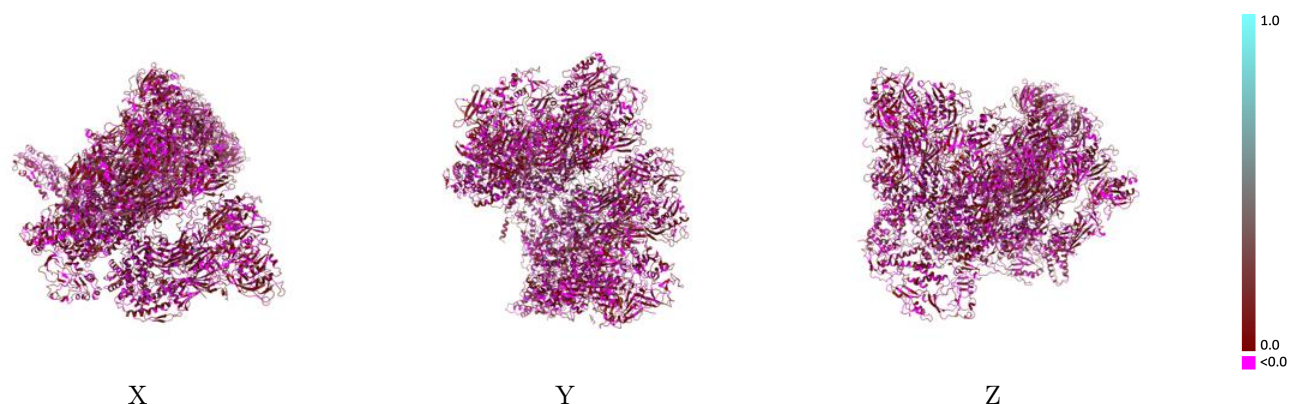
Y



Z

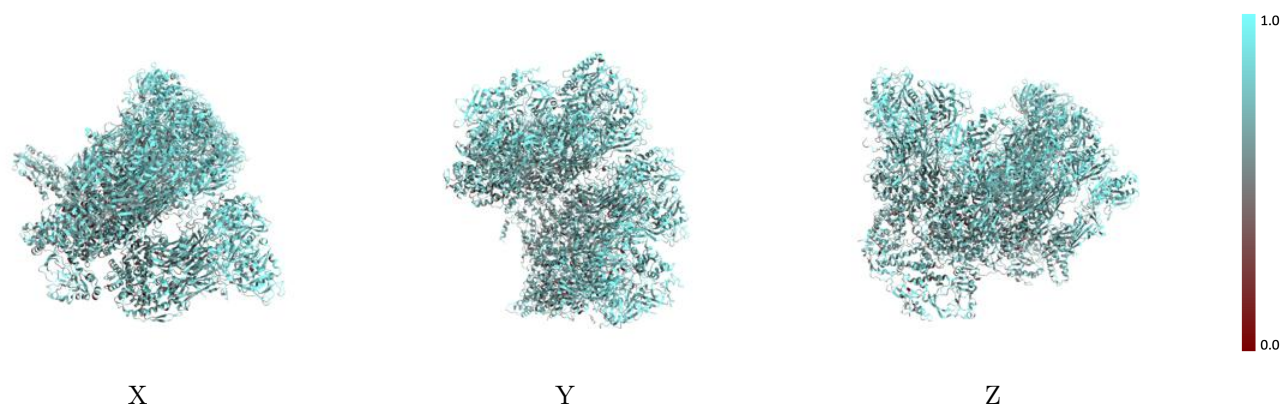
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



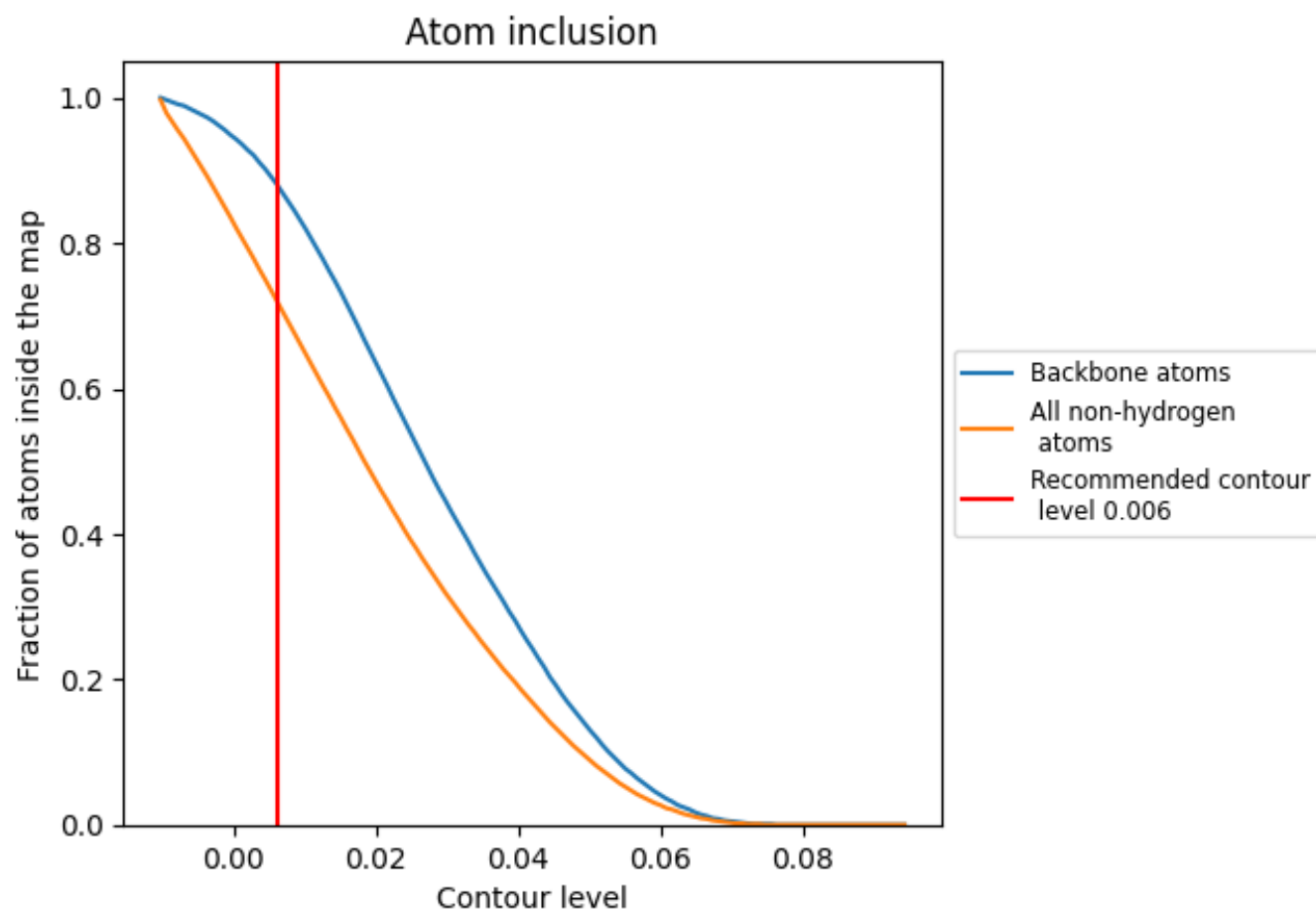
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 72% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7210	 0.0590
A	 0.6810	 0.0430
B	 0.6700	 0.0470
C	 0.6880	 0.0470
D	 0.7090	 0.0570
E	 0.6980	 0.0580
F	 0.6830	 0.0610
G	 0.6790	 0.0440
H	 0.6880	 0.0500
I	 0.6850	 0.0590
J	 0.6910	 0.0590
K	 0.6980	 0.0510
L	 0.6920	 0.0620
M	 0.6970	 0.0560
N	 0.6980	 0.0620
O	 0.7030	 0.0610
c	 0.7800	 0.0730
d	 0.7930	 0.0690
e	 0.7780	 0.0690
f	 0.7770	 0.0680
g	 0.7770	 0.0650
h	 0.7750	 0.0620
i	 0.7790	 0.0660
j	 0.7940	 0.0820
k	 0.7790	 0.0680
l	 0.7670	 0.0520
m	 0.7900	 0.0730
n	 0.7880	 0.0690
o	 0.7930	 0.0740

