



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:02 AM UTC

PDB ID : 8CXG / pdb_00008cxg
EMDB ID : EMD-27055
Title : Structures of Zika Virus in Complex with Antibodies Targeting E Dimer Epitopes and Basis for Neutralization Efficacy
Authors : Liu, W.; Zhang, X.K.; Gong, D.Y.; Dai, X.H.; Sharma, A.; Zhang, T.H.; Rey, F.; Zhou, Z.H.
Deposited on : 2022-05-21
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

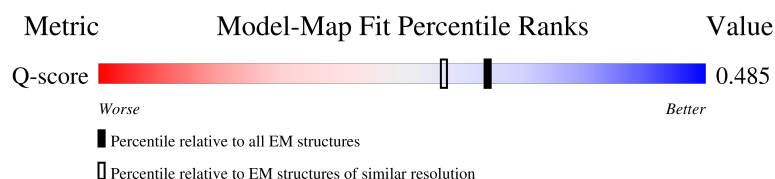
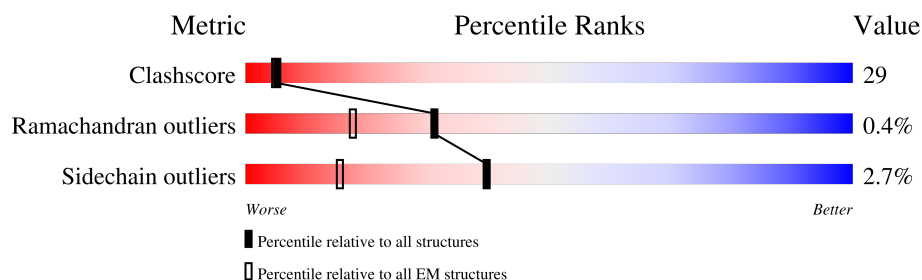
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	1	122	
1	H	122	
1	h	122	
2	2	109	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	L	109	
2	l	109	
3	A	639	
3	B	639	
3	C	639	
4	D	3423	
4	E	3423	
4	F	3423	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18381 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 C8 scFv heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	121	Total	C	N	O	S	0	0
			933	591	151	186	5		
1	h	121	Total	C	N	O	S	0	0
			933	591	151	186	5		
1	1	121	Total	C	N	O	S	0	0
			933	591	151	186	5		

- Molecule 2 is a protein called C8 scFv light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	109	Total	C	N	O	S	0	0
			852	541	145	164	2		
2	1	109	Total	C	N	O	S	0	0
			852	541	145	164	2		
2	2	108	Total	C	N	O	S	0	0
			846	538	144	162	2		

- Molecule 3 is a protein called Ankyrin repeat family A protein 2,Envelope E protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	492	Total	C	N	O	S	0	0
			3721	2343	645	703	30		
3	B	492	Total	C	N	O	S	0	0
			3721	2343	645	703	30		
3	C	501	Total	C	N	O	S	0	0
			3790	2384	657	718	31		

- Molecule 4 is a protein called Membrane M protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	75	Total	C	N	O	S	0	0
			600	391	105	103	1		

Continued on next page...

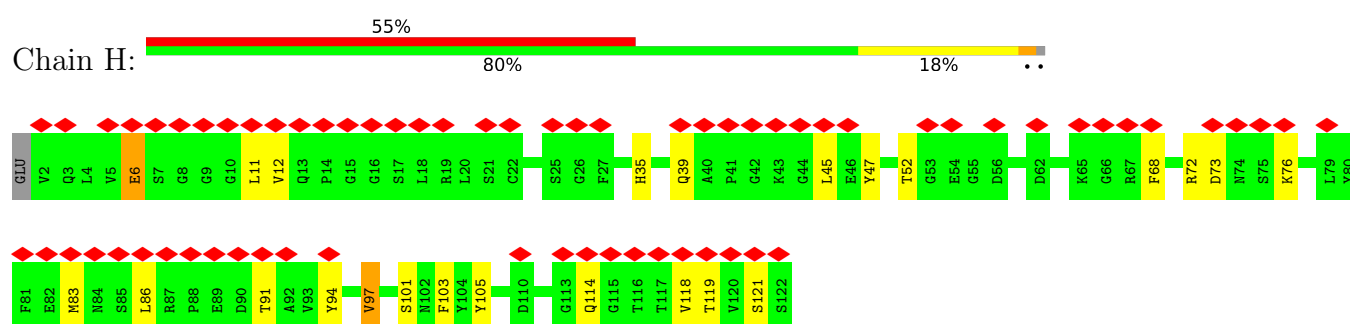
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	75	Total	C	N	O	S	0	0
			600	391	105	103	1		
4	F	75	Total	C	N	O	S	0	0
			600	391	105	103	1		

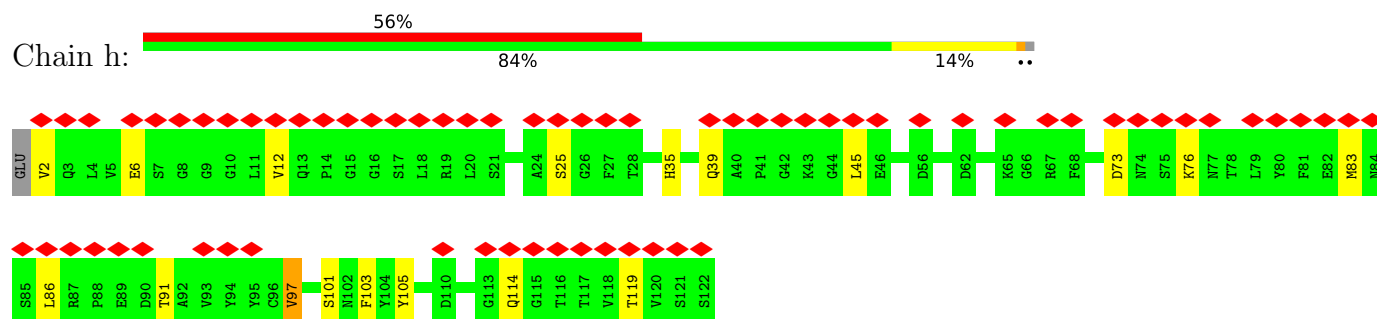
3 Residue-property plots [i](#)

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

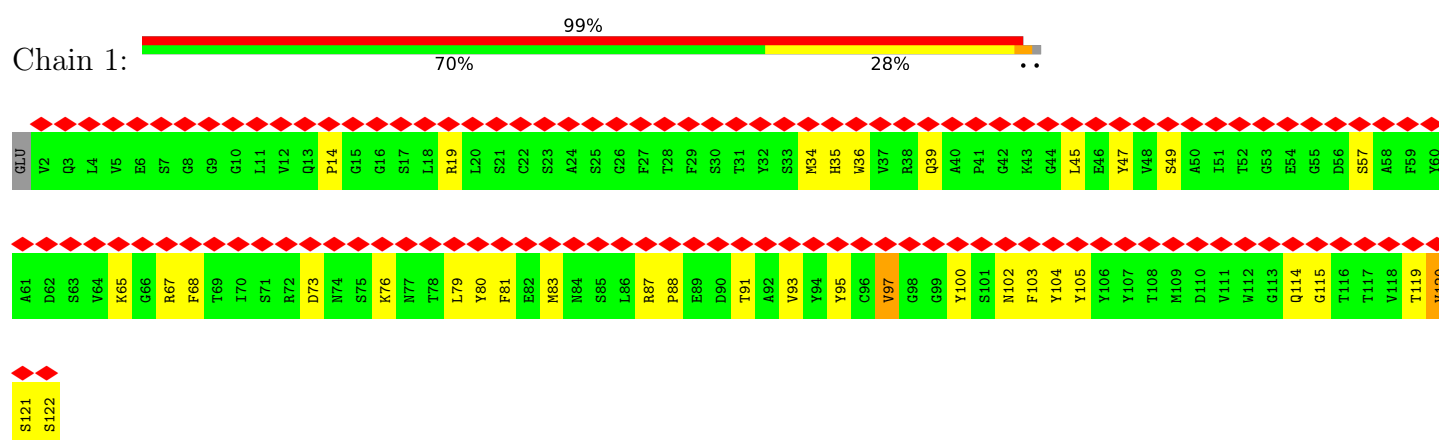
- Molecule 1: C8 scFv heavy chain



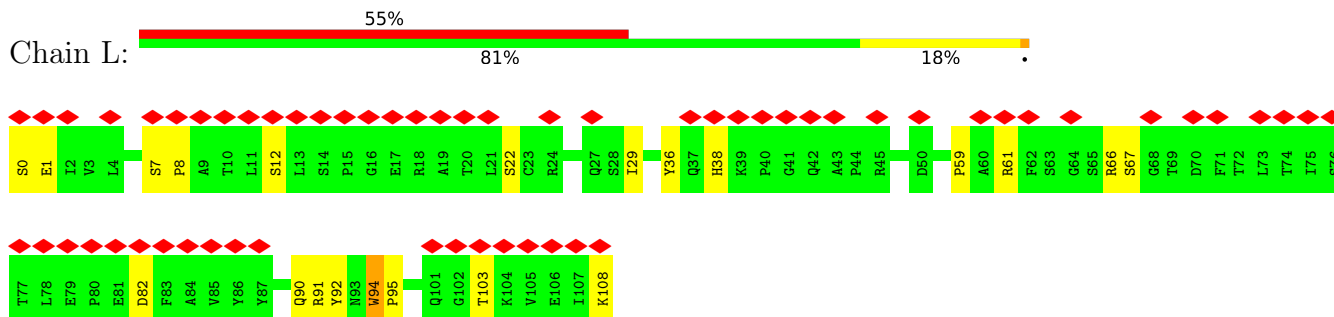
- Molecule 1: C8 scFv heavy chain



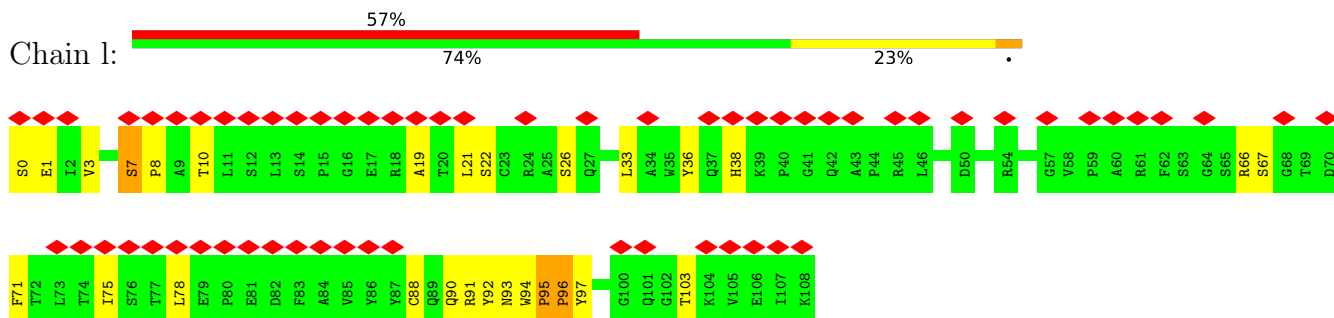
- Molecule 1: C8 scFv heavy chain



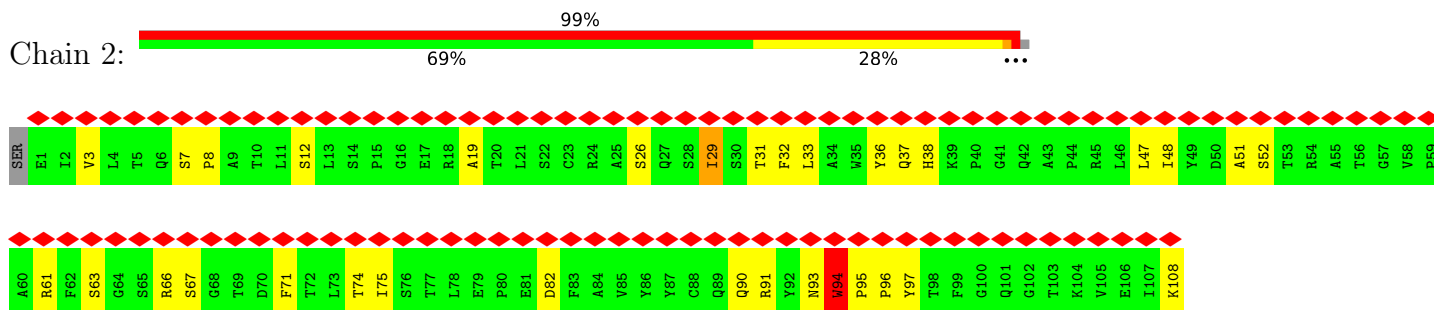
Chain L:



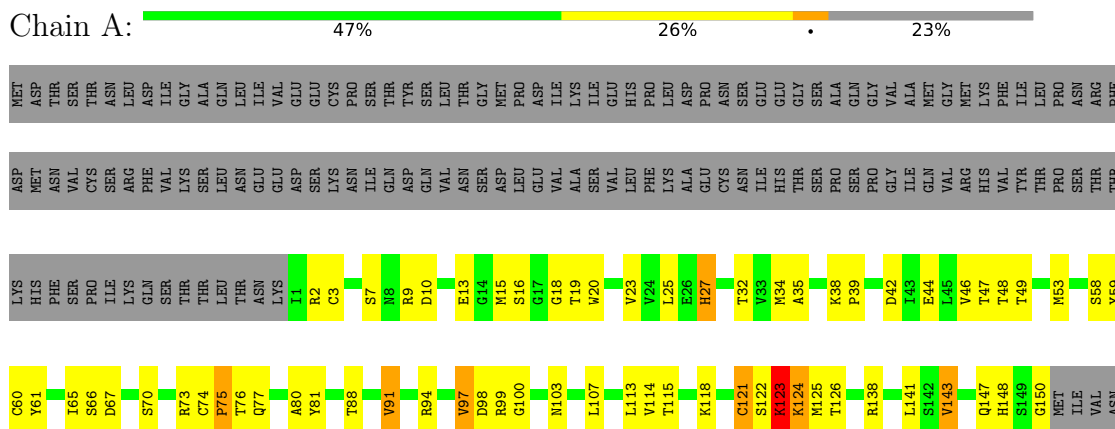
Chain 1:

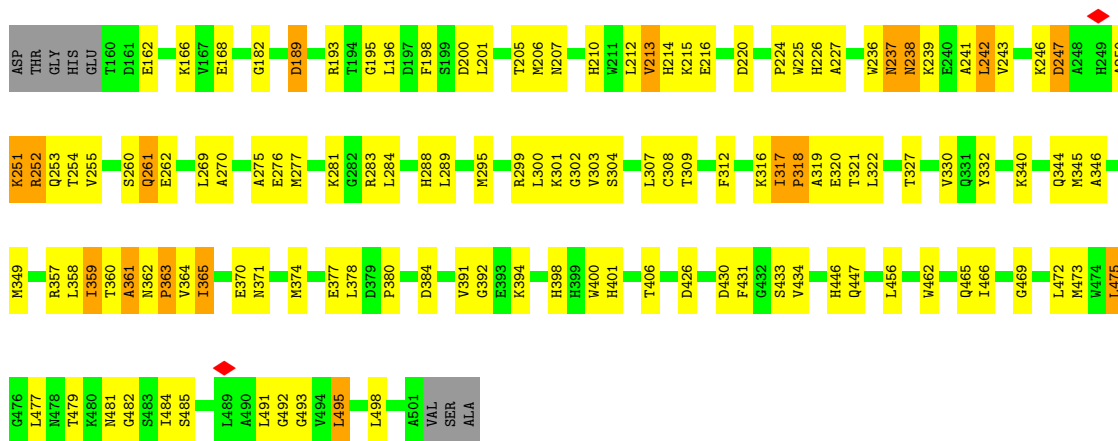


Chain 2:



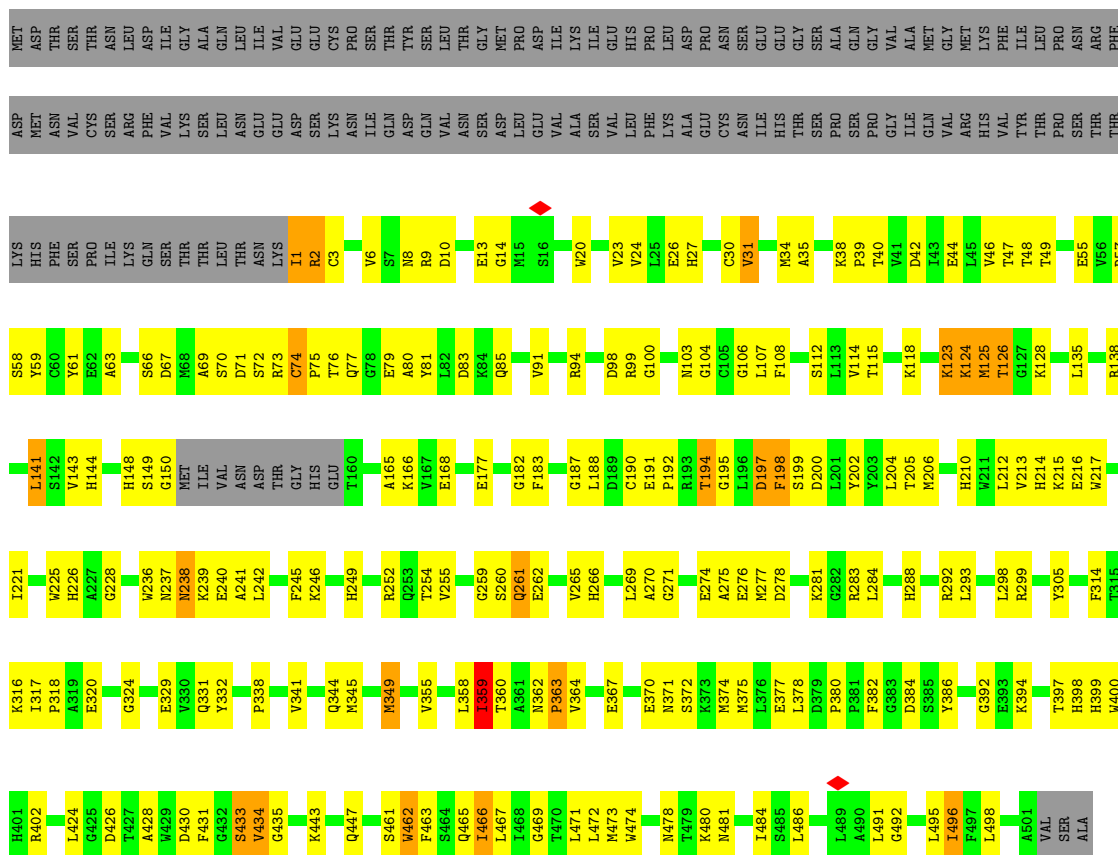
Chain A:





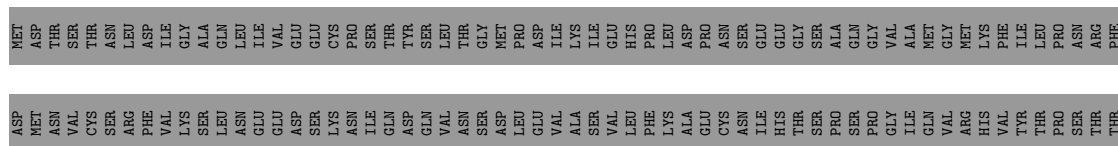
• Molecule 3: Ankyrin repeat family A protein 2,Envelope E protein

Chain B: 43% 30% 23%



• Molecule 3: Ankyrin repeat family A protein 2,Envelope E protein

Chain C: 49% 28% 22%







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

- Molecule 4: Membrane M protein

Chain E: 98%

[illegible]











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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1007280	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	14.196	Depositor
Minimum map value	-6.057	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	265.0, 265.0, 265.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.19	0/957	0.47	1/1298 (0.1%)
1	H	0.15	0/957	0.38	0/1298
1	h	0.14	0/957	0.34	0/1298
2	2	0.22	0/869	0.61	2/1185 (0.2%)
2	L	0.26	0/875	0.46	1/1193 (0.1%)
2	l	0.17	0/875	0.62	3/1193 (0.3%)
3	A	0.56	8/3798 (0.2%)	0.69	10/5138 (0.2%)
3	B	0.60	7/3798 (0.2%)	0.74	14/5138 (0.3%)
3	C	0.50	3/3869 (0.1%)	0.67	7/5236 (0.1%)
4	D	0.32	0/615	0.40	0/838
4	E	0.46	1/615 (0.2%)	0.52	0/838
4	F	0.28	0/615	0.48	0/838
All	All	0.46	19/18800 (0.1%)	0.62	38/25491 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	121	CYS	CA-C	-9.51	1.41	1.52
3	A	243	VAL	C-O	-8.72	1.15	1.24
3	A	243	VAL	CA-CB	-6.44	1.46	1.54
3	B	198	PHE	CA-C	-6.22	1.44	1.52
3	C	126	THR	CA-C	-6.18	1.44	1.52
3	B	197	ASP	C-O	-6.00	1.17	1.24
3	C	193	ARG	CA-C	-5.96	1.45	1.52
3	B	362	ASN	CA-C	-5.93	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	242	LEU	C-O	-5.82	1.16	1.24
3	C	126	THR	C-O	-5.75	1.17	1.23
4	E	25	TYR	C-O	-5.70	1.17	1.24
3	B	2	ARG	CA-C	-5.68	1.45	1.52
3	B	197	ASP	CA-C	-5.64	1.45	1.52
3	A	363	PRO	CA-C	-5.60	1.46	1.52
3	B	124	LYS	C-O	-5.52	1.16	1.23
3	B	126	THR	CA-C	-5.51	1.46	1.52
3	A	121	CYS	C-O	-5.49	1.17	1.24
3	A	243	VAL	CA-C	-5.46	1.45	1.52
3	A	363	PRO	C-O	-5.22	1.17	1.23

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	242	LEU	N-CA-C	-9.79	100.84	113.17
3	B	237	ASN	N-CA-C	9.03	121.20	111.36
2	1	95	PRO	N-CA-C	8.93	121.59	110.70
3	B	433	SER	N-CA-C	8.79	124.32	110.70
3	A	361	ALA	N-CA-C	8.47	120.20	110.97
3	A	251	LYS	N-CA-C	8.35	120.38	111.28
3	B	123	LYS	N-CA-C	8.34	122.90	111.39
3	B	238	ASN	N-CA-C	8.12	119.76	111.07
3	C	239	LYS	N-CA-C	-7.96	103.13	112.92
3	B	359	ILE	O-C-N	-7.93	114.14	121.91
3	C	350	GLN	N-CA-C	7.79	119.56	111.14
3	A	75	PRO	N-CA-C	-7.54	102.88	113.81
2	2	29	ILE	N-CA-C	-7.47	95.40	107.28
3	B	195	GLY	N-CA-C	7.41	121.62	112.73
2	1	95	PRO	CA-C-N	-7.14	110.92	119.84
2	1	95	PRO	C-N-CA	-7.14	110.92	119.84
3	B	195	GLY	O-C-N	-7.09	115.39	122.19
3	A	237	ASN	N-CA-C	6.74	118.63	111.28
3	A	123	LYS	N-CA-C	6.36	120.17	111.39
1	1	120	VAL	N-CA-C	-6.33	101.39	109.80
3	A	241	ALA	N-CA-C	6.31	118.16	111.28
3	C	3	CYS	N-CA-C	6.24	120.92	112.88
3	A	252	ARG	N-CA-C	6.20	118.84	109.23
3	B	74	CYS	CA-C-N	6.11	127.48	119.84
3	B	74	CYS	C-N-CA	6.11	127.48	119.84
3	B	364	VAL	N-CA-C	6.10	116.71	108.17
3	B	194	THR	N-CA-C	5.80	117.68	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	196	LEU	N-CA-C	5.75	119.75	108.18
3	A	362	ASN	N-CA-C	-5.74	97.12	109.81
2	L	94	TRP	N-CA-C	5.57	117.64	110.39
3	C	126	THR	CB-CA-C	-5.56	98.34	109.35
3	B	195	GLY	CA-C-N	-5.51	113.08	122.33
3	B	195	GLY	C-N-CA	-5.51	113.08	122.33
3	B	198	PHE	N-CA-C	-5.42	105.36	112.41
3	A	359	ILE	O-C-N	5.38	126.48	121.96
3	C	349	MET	N-CA-C	5.17	116.92	111.28
3	A	247	ASP	N-CA-C	5.17	117.49	108.76
2	2	94	TRP	N-CA-C	5.01	117.07	110.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	238	ASN	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	933	0	868	66	0
1	H	933	0	868	17	0
1	h	933	0	868	11	0
2	2	846	0	824	55	0
2	L	852	0	831	25	0
2	l	852	0	831	32	0
3	A	3721	0	3682	268	0
3	B	3721	0	3682	286	0
3	C	3790	0	3748	318	0
4	D	600	0	624	10	0
4	E	600	0	624	32	0
4	F	600	0	624	26	0
All	All	18381	0	18074	1039	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 29.

All (1039) 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)
3:A:113:LEU:CD2	3:A:253:GLN:CD	1.79	1.56
3:B:249:HIS:HE1	4:F:16:SER:CB	0.93	1.55
3:C:225:TRP:CH2	3:C:237:ASN:ND2	1.69	1.55
3:A:74:CYS:HB3	3:A:77:GLN:CG	1.34	1.54
3:B:249:HIS:CE1	4:F:16:SER:HB2	1.02	1.53
2:2:29:ILE:HD11	2:2:71:PHE:CE1	1.44	1.52
3:A:113:LEU:CD2	3:A:253:GLN:NE2	1.73	1.50
3:C:316:LYS:HE3	2:2:31:THR:CG2	1.38	1.49
3:A:113:LEU:HD23	3:A:253:GLN:CD	1.05	1.48
3:A:473:MET:CG	3:A:491:LEU:HD13	1.44	1.46
3:A:317:ILE:CG2	3:A:318:PRO:HD3	1.46	1.45
3:C:288:HIS:CE1	3:C:424:LEU:HD22	1.53	1.43
3:B:262:GLU:O	3:B:266:HIS:CD2	1.74	1.39
3:A:113:LEU:HD23	3:A:253:GLN:NE2	1.06	1.36
3:A:98:ASP:HB2	3:A:250:ALA:CB	1.56	1.35
3:B:191:GLU:HB3	3:B:194:THR:CG2	1.56	1.34
3:B:473:MET:HA	3:B:491:LEU:CD1	1.59	1.32
3:A:475:LEU:O	3:A:479:THR:HG23	1.26	1.29
3:A:59:TYR:O	3:A:124:LYS:HB2	1.19	1.27
3:B:249:HIS:CE1	4:F:16:SER:CB	1.78	1.27
3:A:247:ASP:OD1	3:A:252:ARG:O	1.53	1.26
3:C:308:CYS:SG	3:C:339:CYS:CB	2.22	1.26
3:A:225:TRP:CZ2	3:A:237:ASN:ND2	2.01	1.26
3:C:316:LYS:O	3:C:317:ILE:HG13	1.26	1.26
3:B:316:LYS:O	3:B:317:ILE:HG13	1.34	1.25
3:C:262:GLU:O	3:C:266:HIS:CD2	1.90	1.25
3:C:307:LEU:HD12	3:C:340:LYS:O	1.36	1.25
3:A:74:CYS:CB	3:A:77:GLN:HG2	1.66	1.24
3:A:236:TRP:O	3:A:239:LYS:HE3	1.36	1.24
3:C:308:CYS:SG	3:C:339:CYS:SG	1.24	1.24
3:A:113:LEU:HB3	3:A:253:GLN:NE2	1.50	1.24
3:C:316:LYS:CE	2:2:31:THR:HG21	1.69	1.22
3:C:59:TYR:O	3:C:124:LYS:HB2	1.31	1.21
3:C:466:ILE:CG1	3:C:498:LEU:HD13	1.70	1.21
3:C:288:HIS:CE1	3:C:424:LEU:CD2	2.24	1.21
3:C:34:MET:SD	3:C:359:ILE:CD1	2.29	1.20
3:C:225:TRP:CZ2	3:C:237:ASN:ND2	2.09	1.20
3:A:113:LEU:HD23	3:A:253:GLN:CG	1.70	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:113:LEU:CB	3:A:253:GLN:HE22	1.54	1.20
3:C:316:LYS:CE	2:2:31:THR:CG2	2.21	1.19
3:A:113:LEU:CG	3:A:253:GLN:NE2	2.05	1.19
3:C:3:CYS:SG	3:C:30:CYS:SG	1.38	1.19
3:A:318:PRO:HG3	3:A:398:HIS:NE2	1.59	1.18
3:B:191:GLU:CB	3:B:194:THR:CG2	2.22	1.17
3:B:426:ASP:OD2	3:B:447:GLN:HG2	1.42	1.17
4:E:23:ARG:NH1	3:C:241:ALA:HA	1.58	1.17
3:C:60:CYS:SG	3:C:121:CYS:SG	1.18	1.17
3:A:74:CYS:CB	3:A:77:GLN:CG	2.23	1.16
3:B:83:ASP:CG	1:1:65:LYS:NZ	2.02	1.16
3:A:473:MET:HA	3:A:491:LEU:CD1	1.75	1.16
1:1:95:TYR:CE2	1:1:115:GLY:HA3	1.80	1.16
3:B:83:ASP:CG	1:1:65:LYS:HZ3	1.52	1.15
3:C:34:MET:SD	3:C:359:ILE:HD13	1.84	1.15
3:B:426:ASP:OD2	3:B:447:GLN:CG	1.96	1.14
3:A:113:LEU:CB	3:A:253:GLN:NE2	2.09	1.14
2:2:29:ILE:CD1	2:2:71:PHE:CE1	2.31	1.13
3:C:106:GLY:O	3:C:107:LEU:HG	1.47	1.13
3:B:473:MET:CA	3:B:491:LEU:CD1	2.27	1.13
3:C:225:TRP:CZ3	3:C:237:ASN:ND2	2.15	1.13
3:C:307:LEU:HD11	3:C:342:PRO:HD3	1.20	1.13
3:A:307:LEU:HD23	3:A:340:LYS:CB	1.79	1.12
3:B:191:GLU:HB3	3:B:194:THR:HG21	1.21	1.12
3:C:74:CYS:HB2	3:C:77:GLN:HG2	1.19	1.12
3:A:426:ASP:OD2	3:A:447:GLN:HA	1.49	1.12
3:A:98:ASP:CB	3:A:250:ALA:HB1	1.79	1.11
3:B:83:ASP:OD2	1:1:65:LYS:NZ	1.83	1.11
3:B:205:THR:HG22	3:B:210:HIS:ND1	1.65	1.11
3:B:473:MET:CA	3:B:491:LEU:HD13	1.79	1.10
3:B:472:LEU:HB2	3:B:491:LEU:HD21	1.17	1.10
3:C:60:CYS:HB2	3:C:236:TRP:CH2	1.87	1.09
2:1:93:ASN:OD1	3:C:99:ARG:NH1	1.85	1.09
3:B:58:SER:HB3	3:B:126:THR:HG22	1.23	1.09
4:E:23:ARG:HH12	3:C:241:ALA:HA	0.94	1.09
3:C:462:TRP:CZ3	4:F:25:TYR:CD1	2.01	1.09
3:B:239:LYS:O	3:B:240:GLU:CD	1.95	1.09
3:A:473:MET:HA	3:A:491:LEU:HD11	1.25	1.09
3:C:307:LEU:HD11	3:C:342:PRO:CD	1.82	1.09
3:B:58:SER:CB	3:B:126:THR:HG22	1.83	1.07
3:B:191:GLU:CB	3:B:194:THR:HG21	1.83	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:317:ILE:HG22	3:A:318:PRO:CD	1.84	1.07
3:A:307:LEU:HD21	3:A:340:LYS:HD2	1.09	1.06
3:C:205:THR:HG22	3:C:210:HIS:ND1	1.70	1.06
3:A:10:ASP:OD2	3:A:431:PHE:CZ	2.09	1.06
3:A:307:LEU:CD2	3:A:340:LYS:HD2	1.84	1.06
3:B:288:HIS:NE2	3:B:424:LEU:HD22	1.71	1.06
3:A:318:PRO:HG3	3:A:398:HIS:CE1	1.91	1.05
3:A:473:MET:HG2	3:A:491:LEU:HD13	1.16	1.05
3:B:74:CYS:HB3	3:B:75:PRO:HD2	1.33	1.04
3:A:317:ILE:CB	3:A:318:PRO:HD3	1.87	1.04
3:B:1:ILE:HD11	3:B:375:MET:HE2	1.37	1.04
3:C:462:TRP:HA	3:C:498:LEU:HD22	1.38	1.04
3:A:307:LEU:CD2	3:A:340:LYS:HB3	1.88	1.03
3:A:472:LEU:HB2	3:A:491:LEU:HD21	1.39	1.02
3:A:473:MET:HG3	3:A:491:LEU:HD13	1.35	1.02
3:B:24:VAL:CG1	3:B:288:HIS:CE1	2.42	1.02
3:B:61:TYR:CZ	3:B:123:LYS:HB3	1.94	1.02
3:B:239:LYS:O	3:B:240:GLU:CG	2.09	1.01
3:A:98:ASP:CB	3:A:250:ALA:CB	2.38	1.00
2:L:94:TRP:CD1	2:L:95:PRO:HD2	1.95	1.00
3:A:115:THR:HG23	3:A:253:GLN:OE1	1.62	1.00
3:B:24:VAL:HG11	3:B:288:HIS:CE1	1.96	1.00
3:C:373:LYS:HE3	2:2:52:SER:OG	1.62	1.00
3:C:472:LEU:HB2	3:C:491:LEU:HD21	1.39	0.99
3:C:3:CYS:SG	3:C:30:CYS:CB	2.49	0.99
3:B:191:GLU:HB3	3:B:194:THR:HG22	1.40	0.99
3:A:74:CYS:HB3	3:A:77:GLN:HG3	1.42	0.99
3:C:73:ARG:HG3	3:C:77:GLN:HB2	1.45	0.99
3:C:466:ILE:HG13	3:C:498:LEU:CD1	1.93	0.99
3:B:359:ILE:HG21	3:B:377:GLU:HG3	1.43	0.99
2:L:29:ILE:HD13	2:L:90:GLN:CD	1.87	0.99
3:C:60:CYS:HB2	3:C:236:TRP:CZ3	1.98	0.99
3:C:473:MET:N	3:C:491:LEU:HD11	1.77	0.99
3:A:473:MET:CG	3:A:491:LEU:CD1	2.40	0.98
3:A:473:MET:CA	3:A:491:LEU:HD11	1.94	0.98
3:A:426:ASP:OD2	3:A:447:GLN:HG2	1.61	0.98
3:B:249:HIS:CE1	4:F:16:SER:OG	2.16	0.98
2:L:94:TRP:CG	2:L:95:PRO:HD2	1.98	0.98
3:B:83:ASP:OD1	1:1:65:LYS:NZ	1.93	0.97
3:C:74:CYS:HB2	3:C:77:GLN:CG	1.95	0.96
3:C:466:ILE:HG13	3:C:498:LEU:HD13	0.97	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:212:LEU:HD11	3:B:284:LEU:CD1	1.95	0.96
3:C:307:LEU:CD1	3:C:342:PRO:HD3	1.95	0.96
3:A:317:ILE:CG2	3:A:318:PRO:CD	2.42	0.96
3:A:317:ILE:CB	3:A:318:PRO:CD	2.44	0.96
2:I:95:PRO:O	2:I:97:TYR:N	1.99	0.96
3:B:288:HIS:CD2	3:B:424:LEU:HD22	2.00	0.95
3:A:113:LEU:HB3	3:A:253:GLN:HE22	1.02	0.94
3:A:473:MET:CA	3:A:491:LEU:CD1	2.45	0.94
3:C:316:LYS:CE	2:2:31:THR:HG22	1.97	0.94
3:C:462:TRP:CZ3	4:F:25:TYR:HD1	1.17	0.94
2:I:95:PRO:C	2:I:97:TYR:H	1.74	0.94
3:A:113:LEU:CD2	3:A:253:GLN:CG	2.38	0.94
3:A:225:TRP:HZ2	3:A:237:ASN:ND2	1.64	0.94
3:B:473:MET:HA	3:B:491:LEU:HD11	1.50	0.94
3:A:58:SER:HB3	3:A:126:THR:HG22	1.48	0.94
3:A:473:MET:HG2	3:A:491:LEU:CD1	1.95	0.94
3:B:359:ILE:CG2	3:B:377:GLU:HG3	1.98	0.94
3:B:104:GLY:HA2	2:2:32:PHE:CE1	2.01	0.93
3:B:73:ARG:NH1	3:B:81:TYR:HB3	1.82	0.93
3:B:1:ILE:HD11	3:B:375:MET:CE	1.98	0.93
2:2:29:ILE:CD1	2:2:71:PHE:CZ	2.52	0.93
3:A:113:LEU:HD23	3:A:253:GLN:HE21	1.30	0.93
3:A:307:LEU:HD23	3:A:340:LYS:HB3	0.95	0.92
3:C:262:GLU:O	3:C:266:HIS:HD2	1.47	0.92
3:A:317:ILE:HB	3:A:318:PRO:CD	2.00	0.92
3:A:59:TYR:O	3:A:124:LYS:CB	2.15	0.92
3:B:359:ILE:HG22	3:B:378:LEU:HA	1.52	0.92
1:1:95:TYR:HE2	1:1:114:GLN:O	1.50	0.92
3:A:360:THR:HG21	3:A:377:GLU:H	1.35	0.92
3:B:472:LEU:CB	3:B:491:LEU:HD21	2.00	0.91
3:A:357:ARG:NH1	3:A:359:ILE:HD11	1.85	0.91
3:C:61:TYR:CZ	3:C:123:LYS:HE3	2.04	0.91
3:A:317:ILE:HG22	3:A:318:PRO:HD3	0.93	0.91
3:A:479:THR:OG1	3:A:484:ILE:HG22	1.71	0.91
3:C:373:LYS:CE	2:2:52:SER:OG	2.17	0.91
3:A:58:SER:CB	3:A:126:THR:HG22	2.00	0.91
3:B:239:LYS:O	3:B:240:GLU:HG3	1.69	0.91
2:2:29:ILE:HD11	2:2:71:PHE:HE1	1.08	0.90
3:C:89:GLN:C	3:C:239:LYS:NZ	2.30	0.90
3:B:473:MET:CB	3:B:491:LEU:HD13	2.00	0.90
2:2:7:SER:OG	2:2:8:PRO:HD3	1.72	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:262:GLU:O	3:B:266:HIS:HD2	1.28	0.90
3:B:125:MET:HE3	3:B:206:MET:HE3	1.53	0.90
3:C:316:LYS:HE3	2:2:31:THR:HG22	1.55	0.89
3:B:125:MET:HE2	3:B:206:MET:HG2	1.55	0.89
3:A:124:LYS:H	3:A:124:LYS:HD3	1.38	0.89
3:A:98:ASP:HB2	3:A:250:ALA:HB1	0.90	0.89
3:C:60:CYS:SG	3:C:121:CYS:CB	2.60	0.88
1:H:83:MET:HE1	1:H:94:TYR:CE2	2.09	0.88
3:B:205:THR:CG2	3:B:210:HIS:ND1	2.36	0.88
3:C:89:GLN:C	3:C:239:LYS:HZ3	1.82	0.88
1:1:93:VAL:HG11	1:1:95:TYR:OH	1.73	0.88
3:A:205:THR:HG22	3:A:210:HIS:ND1	1.89	0.88
2:1:94:TRP:CD1	2:1:95:PRO:HD2	2.09	0.88
1:1:95:TYR:CD2	1:1:115:GLY:CA	2.57	0.88
3:C:61:TYR:CE1	3:C:123:LYS:HE3	2.09	0.87
3:C:239:LYS:N	3:C:240:GLU:OE1	2.07	0.87
3:C:307:LEU:HD21	3:C:342:PRO:HB3	1.56	0.87
3:B:341:VAL:HB	3:B:363:PRO:O	1.75	0.87
3:A:345:MET:SD	3:A:378:LEU:HD11	2.14	0.87
2:2:29:ILE:HD11	2:2:71:PHE:CZ	2.09	0.87
3:C:473:MET:CA	3:C:491:LEU:HD11	2.03	0.87
2:1:93:ASN:HB2	3:C:105:CYS:SG	2.14	0.87
3:C:349:MET:HE3	3:C:349:MET:HA	1.57	0.86
3:C:58:SER:CB	3:C:126:THR:HG22	2.05	0.86
3:A:307:LEU:HD21	3:A:340:LYS:CD	2.02	0.86
3:A:426:ASP:OD2	3:A:447:GLN:CA	2.24	0.86
3:C:34:MET:SD	3:C:359:ILE:HD11	2.13	0.86
3:B:472:LEU:C	3:B:491:LEU:HD11	2.00	0.86
3:B:212:LEU:HD11	3:B:284:LEU:HD13	1.56	0.85
3:A:236:TRP:O	3:A:239:LYS:CE	2.23	0.85
1:1:95:TYR:CD2	1:1:115:GLY:HA3	2.10	0.85
3:B:61:TYR:OH	3:B:123:LYS:HB3	1.75	0.85
3:B:426:ASP:OD2	3:B:447:GLN:HG3	1.76	0.85
3:C:61:TYR:OH	3:C:123:LYS:HE3	1.76	0.85
1:1:68:PHE:CD2	1:1:81:PHE:CE2	2.63	0.85
3:C:2:ARG:HE	3:C:44:GLU:CB	1.89	0.85
3:C:240:GLU:OE1	3:C:240:GLU:N	2.08	0.84
3:C:58:SER:HB3	3:C:126:THR:HG22	1.58	0.84
3:C:316:LYS:O	3:C:317:ILE:CG1	2.21	0.84
3:C:473:MET:CA	3:C:491:LEU:CD1	2.56	0.84
3:C:473:MET:HB2	3:C:491:LEU:HD13	1.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:462:TRP:CE3	4:F:25:TYR:CD1	2.42	0.83
3:A:212:LEU:HD11	3:A:284:LEU:CD1	2.08	0.83
3:B:473:MET:HB2	3:B:491:LEU:HD13	1.60	0.83
3:C:59:TYR:O	3:C:124:LYS:CB	2.24	0.83
3:A:113:LEU:CD2	3:A:253:GLN:HG3	2.08	0.83
3:B:239:LYS:C	3:B:240:GLU:CD	2.47	0.82
3:A:113:LEU:CG	3:A:253:GLN:CD	2.48	0.82
3:A:469:GLY:O	3:A:491:LEU:HD22	1.78	0.82
3:C:1:ILE:HG22	3:C:142:SER:OG	1.80	0.82
3:C:153:VAL:HG22	1:1:102:ASN:CG	2.03	0.82
3:A:113:LEU:HD21	3:A:253:GLN:CD	2.04	0.82
3:B:288:HIS:CE1	3:B:424:LEU:CD1	2.63	0.82
3:C:349:MET:HA	3:C:349:MET:CE	2.03	0.82
1:1:68:PHE:CD2	1:1:81:PHE:HE2	1.98	0.82
3:B:473:MET:CA	3:B:491:LEU:HD11	2.05	0.82
3:B:24:VAL:HG11	3:B:288:HIS:HE1	1.40	0.81
3:B:288:HIS:NE2	3:B:424:LEU:CD2	2.42	0.81
3:A:113:LEU:CG	3:A:253:GLN:HE22	1.83	0.81
3:A:426:ASP:OD2	3:A:447:GLN:CG	2.28	0.81
1:1:95:TYR:CE2	1:1:115:GLY:CA	2.63	0.81
1:1:93:VAL:HG12	1:1:95:TYR:CE1	2.15	0.80
3:B:469:GLY:O	3:B:491:LEU:HD22	1.81	0.80
2:2:29:ILE:HG13	2:2:71:PHE:HZ	1.45	0.80
3:B:74:CYS:HB3	3:B:75:PRO:CD	2.10	0.80
3:C:2:ARG:HE	3:C:44:GLU:HB3	1.46	0.80
3:C:125:MET:HE2	3:C:206:MET:HG2	1.64	0.80
3:C:205:THR:CG2	3:C:210:HIS:ND1	2.45	0.80
3:B:91:VAL:HG22	3:B:239:LYS:HB3	1.64	0.80
3:B:73:ARG:HA	2:2:93:ASN:ND2	1.96	0.79
2:L:29:ILE:HD13	2:L:90:GLN:NE2	1.97	0.79
3:A:360:THR:CG2	3:A:377:GLU:H	1.95	0.79
3:A:360:THR:HG23	3:A:377:GLU:O	1.83	0.79
3:B:73:ARG:NH2	3:B:79:GLU:O	2.15	0.79
3:B:125:MET:CE	3:B:206:MET:HE3	2.13	0.79
3:B:288:HIS:CE1	3:B:424:LEU:CD2	2.66	0.79
3:B:474:TRP:CZ2	3:B:478:ASN:ND2	2.50	0.79
3:C:288:HIS:NE2	3:C:424:LEU:HD22	1.97	0.79
3:C:2:ARG:HH21	3:C:44:GLU:HB3	1.48	0.79
3:B:191:GLU:HB2	3:B:194:THR:CG2	2.11	0.79
3:C:466:ILE:CG1	3:C:498:LEU:CD1	2.57	0.79
3:A:66:SER:HB3	3:A:118:LYS:HB3	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:74:CYS:CB	3:A:77:GLN:HG3	2.03	0.79
3:B:246:LYS:HG3	3:B:254:THR:OG1	1.82	0.79
3:B:473:MET:HA	3:B:491:LEU:HD13	1.41	0.79
3:C:193:ARG:HG2	3:C:193:ARG:HH11	1.48	0.79
3:C:3:CYS:CB	3:C:30:CYS:SG	2.70	0.78
3:C:91:VAL:HG22	3:C:239:LYS:HB2	1.65	0.78
3:B:472:LEU:HB2	3:B:491:LEU:CD2	2.07	0.78
3:C:469:GLY:HA2	3:C:491:LEU:HD22	1.65	0.78
3:A:473:MET:CB	3:A:491:LEU:HD13	2.13	0.78
3:B:473:MET:N	3:B:491:LEU:HD11	1.97	0.78
4:E:23:ARG:HH22	3:C:241:ALA:HB1	1.48	0.78
3:B:10:ASP:OD2	3:B:431:PHE:CZ	2.37	0.78
3:A:275:ALA:HB2	3:A:284:LEU:CD2	2.14	0.78
3:B:73:ARG:HA	2:2:93:ASN:HD21	1.46	0.78
2:2:94:TRP:CG	2:2:95:PRO:HD2	2.18	0.78
3:C:99:ARG:HA	3:C:103:ASN:HD22	1.49	0.78
3:B:214:HIS:H	4:E:7:HIS:HE1	1.32	0.77
3:C:308:CYS:SG	3:C:339:CYS:HB2	2.23	0.77
3:C:462:TRP:NE1	4:F:25:TYR:OH	2.18	0.77
3:A:307:LEU:CD2	3:A:340:LYS:CD	2.61	0.77
4:E:23:ARG:NH2	3:C:241:ALA:HB1	2.00	0.77
1:1:68:PHE:HD2	1:1:81:PHE:CE2	2.00	0.77
3:B:212:LEU:HD11	3:B:284:LEU:HD11	1.65	0.77
3:C:66:SER:HB3	3:C:118:LYS:HB3	1.67	0.77
3:B:316:LYS:O	3:B:317:ILE:CG1	2.26	0.77
3:C:316:LYS:HE2	2:2:31:THR:HG22	1.65	0.77
1:1:88:PRO:HA	1:1:120:VAL:HG21	1.65	0.77
1:1:93:VAL:CG1	1:1:95:TYR:CZ	2.68	0.77
3:A:475:LEU:O	3:A:479:THR:CG2	2.21	0.76
3:A:345:MET:SD	3:A:378:LEU:CD1	2.73	0.76
3:A:479:THR:OG1	3:A:484:ILE:CG2	2.33	0.76
3:C:224:PRO:HD3	3:C:242:LEU:HD21	1.66	0.76
4:E:23:ARG:HH12	3:C:241:ALA:CA	1.89	0.76
3:B:66:SER:HB3	3:B:118:LYS:HB3	1.68	0.76
3:C:91:VAL:HG23	3:C:239:LYS:HD3	1.68	0.76
3:B:288:HIS:CD2	3:B:424:LEU:CD2	2.69	0.76
3:A:73:ARG:NH1	3:A:80:ALA:HA	2.00	0.75
3:B:24:VAL:CG1	3:B:288:HIS:HE1	1.93	0.75
3:B:262:GLU:HG2	3:B:266:HIS:NE2	2.01	0.75
3:A:98:ASP:H	3:A:250:ALA:CB	1.99	0.75
3:B:345:MET:SD	3:B:378:LEU:HD11	2.27	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:TYR:OH	3:C:123:LYS:CE	2.34	0.75
3:B:305:TYR:HE2	3:B:338:PRO:HB2	1.50	0.75
3:C:473:MET:HA	3:C:491:LEU:CD1	2.16	0.75
3:A:275:ALA:HB2	3:A:284:LEU:HD23	1.67	0.75
3:C:360:THR:OG1	3:C:377:GLU:N	2.18	0.75
3:A:10:ASP:OD2	3:A:431:PHE:CE2	2.39	0.75
3:A:212:LEU:HD11	3:A:284:LEU:HD13	1.68	0.74
3:C:307:LEU:CD1	3:C:340:LYS:O	2.29	0.74
3:B:71:ASP:HA	2:2:94:TRP:CZ2	2.21	0.74
3:B:473:MET:N	3:B:491:LEU:CD1	2.49	0.74
2:2:94:TRP:CD2	2:2:95:PRO:HD2	2.22	0.74
3:C:288:HIS:CE1	3:C:424:LEU:HD21	2.22	0.74
3:B:288:HIS:CE1	3:B:424:LEU:HD11	2.23	0.74
3:A:472:LEU:HB2	3:A:491:LEU:CD2	2.16	0.74
1:1:87:ARG:O	1:1:120:VAL:HG21	1.87	0.74
3:B:345:MET:SD	3:B:378:LEU:CD1	2.76	0.73
1:H:12:VAL:HG11	1:H:86:LEU:HD12	1.70	0.73
3:A:214:HIS:H	4:D:7:HIS:HE1	1.32	0.73
3:B:216:GLU:OE2	4:E:10:ARG:NH2	2.21	0.73
3:C:308:CYS:CB	3:C:339:CYS:HG	1.92	0.73
1:1:93:VAL:HG11	1:1:95:TYR:CZ	2.22	0.73
3:B:73:ARG:CZ	3:B:79:GLU:O	2.36	0.73
3:C:196:LEU:C	3:C:196:LEU:HD12	2.14	0.73
3:A:74:CYS:HB3	3:A:77:GLN:HG2	0.74	0.73
3:C:473:MET:CB	3:C:491:LEU:HD13	2.18	0.73
1:1:68:PHE:HD2	1:1:81:PHE:CZ	2.07	0.73
1:1:68:PHE:CZ	1:1:83:MET:HE3	2.24	0.73
3:A:318:PRO:CG	3:A:398:HIS:CE1	2.70	0.72
2:L:94:TRP:CG	2:L:95:PRO:CD	2.71	0.72
1:H:35:HIS:HD1	1:H:47:TYR:HH	1.36	0.72
3:A:143:VAL:O	3:A:147:GLN:NE2	2.23	0.71
3:A:260:SER:O	3:A:262:GLU:N	2.23	0.71
3:B:59:TYR:O	3:B:124:LYS:HB2	1.90	0.71
3:A:97:VAL:HG22	3:A:250:ALA:O	1.89	0.71
3:C:469:GLY:HA2	3:C:491:LEU:CD2	2.20	0.71
3:A:473:MET:CA	3:A:491:LEU:HD13	2.19	0.71
3:B:249:HIS:CE1	4:F:16:SER:CA	2.72	0.71
3:A:91:VAL:HG13	3:A:239:LYS:O	1.90	0.71
3:A:124:LYS:H	3:A:124:LYS:CD	2.03	0.71
3:C:91:VAL:CG2	3:C:239:LYS:CB	2.68	0.71
2:L:29:ILE:HG21	2:L:90:GLN:HE22	1.55	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:94:TRP:CG	2:l:95:PRO:CD	2.73	0.71
3:C:307:LEU:HD12	3:C:340:LYS:C	2.13	0.71
3:B:61:TYR:CE1	3:B:123:LYS:HB3	2.26	0.70
3:A:357:ARG:HH11	3:A:359:ILE:HD11	1.53	0.70
2:2:29:ILE:HG13	2:2:71:PHE:CZ	2.26	0.70
3:A:124:LYS:HD3	3:A:124:LYS:N	2.04	0.70
3:B:359:ILE:HG22	3:B:378:LEU:CA	2.22	0.70
3:C:332:TYR:O	3:C:371:ASN:HA	1.91	0.70
3:A:39:PRO:HA	3:A:361:ALA:HB2	1.74	0.70
3:C:316:LYS:HE3	2:2:31:THR:HG21	0.73	0.70
1:1:95:TYR:CE2	1:1:114:GLN:O	2.40	0.70
3:C:153:VAL:HG21	1:1:102:ASN:ND2	2.07	0.70
3:A:275:ALA:CB	3:A:284:LEU:HD23	2.22	0.70
3:B:288:HIS:CE1	3:B:424:LEU:HD21	2.26	0.70
3:A:122:SER:HB3	3:A:123:LYS:HE3	1.74	0.70
3:A:465:GLN:HG3	3:A:498:LEU:HD11	1.74	0.69
3:C:70:SER:HB3	3:C:115:THR:HG22	1.74	0.69
3:B:1:ILE:CD1	3:B:375:MET:CE	2.69	0.69
3:C:462:TRP:HA	3:C:498:LEU:CD2	2.18	0.69
3:A:205:THR:CG2	3:A:210:HIS:ND1	2.55	0.69
3:A:309:THR:HG22	3:A:391:VAL:HG21	1.73	0.69
3:C:307:LEU:HD11	3:C:342:PRO:N	2.08	0.69
3:A:200:ASP:HA	3:A:215:LYS:HE2	1.75	0.69
3:A:384:ASP:OD1	3:A:401:HIS:ND1	2.24	0.69
3:C:345:MET:CG	3:C:378:LEU:HD13	2.23	0.69
3:B:275:ALA:HB2	3:B:284:LEU:HD23	1.72	0.69
4:E:23:ARG:NH2	3:C:241:ALA:CB	2.56	0.68
3:A:98:ASP:CB	3:A:250:ALA:HB2	2.23	0.68
3:B:73:ARG:NH1	3:B:81:TYR:CB	2.56	0.68
3:B:249:HIS:HE1	4:F:16:SER:CA	1.96	0.68
3:B:3:CYS:SG	3:B:42:ASP:HB3	2.33	0.68
3:C:1:ILE:CG2	3:C:142:SER:OG	2.41	0.68
3:C:469:GLY:O	3:C:491:LEU:HD22	1.94	0.68
3:C:469:GLY:CA	3:C:491:LEU:HD22	2.24	0.68
3:B:359:ILE:HG23	3:B:377:GLU:O	1.94	0.68
3:B:3:CYS:HB2	3:B:42:ASP:OD2	1.94	0.68
3:C:91:VAL:HG22	3:C:239:LYS:CB	2.23	0.68
3:C:358:LEU:HD23	3:C:360:THR:H	1.57	0.68
3:A:472:LEU:CB	3:A:491:LEU:HD21	2.20	0.67
1:h:101:SER:OG	1:h:103:PHE:O	2.12	0.67
3:C:2:ARG:NH2	3:C:44:GLU:HB3	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:ASP:HB2	1:1:100:TYR:OH	1.95	0.67
3:C:58:SER:HB2	3:C:126:THR:HG22	1.76	0.67
3:A:124:LYS:HG3	3:A:236:TRP:HH2	1.58	0.67
3:A:212:LEU:HD11	3:A:284:LEU:HD11	1.74	0.67
3:B:91:VAL:HG12	3:B:245:PHE:CE2	2.29	0.67
3:B:462:TRP:HA	3:B:498:LEU:HD11	1.77	0.67
3:C:359:ILE:HG23	3:C:377:GLU:HG3	1.76	0.67
3:C:91:VAL:CG2	3:C:239:LYS:CD	2.72	0.67
3:C:473:MET:CB	3:C:491:LEU:CD1	2.73	0.67
3:B:197:ASP:OD1	3:B:199:SER:N	2.18	0.67
3:B:71:ASP:HA	2:2:94:TRP:CE2	2.30	0.67
3:C:481:ASN:OD1	3:C:482:GLY:N	2.26	0.67
3:C:473:MET:HA	3:C:491:LEU:HD11	1.76	0.67
3:A:76:THR:O	3:A:77:GLN:NE2	2.28	0.67
3:A:317:ILE:HB	3:A:318:PRO:HD2	1.77	0.67
3:B:144:HIS:HB3	3:B:360:THR:HG23	1.77	0.67
3:C:153:VAL:CG2	1:1:102:ASN:ND2	2.57	0.67
3:A:15:MET:HE1	3:A:295:MET:HG3	1.77	0.66
3:C:2:ARG:NE	3:C:44:GLU:HB3	2.10	0.66
3:A:74:CYS:SG	3:A:75:PRO:HD2	2.35	0.66
3:A:312:PHE:HD2	3:A:330:VAL:HG11	1.61	0.66
3:C:153:VAL:CG2	1:1:102:ASN:CG	2.69	0.66
3:A:98:ASP:CG	3:A:250:ALA:HB2	2.21	0.66
3:C:360:THR:HG21	3:C:376:LEU:HA	1.76	0.66
3:B:73:ARG:HD2	3:B:79:GLU:O	1.96	0.66
3:C:22:ASP:HB3	3:C:433:SER:HB3	1.77	0.66
3:C:153:VAL:HG13	1:1:102:ASN:OD1	1.96	0.66
3:B:58:SER:HB2	3:B:126:THR:HG22	1.73	0.65
1:1:93:VAL:HG12	1:1:95:TYR:CZ	2.32	0.65
1:1:93:VAL:CG1	1:1:95:TYR:CE1	2.78	0.65
3:C:224:PRO:CD	3:C:242:LEU:HD21	2.25	0.65
2:L:61:ARG:NH1	2:L:82:ASP:OD2	2.29	0.65
3:A:312:PHE:CD2	3:A:330:VAL:HG11	2.32	0.65
3:C:260:SER:O	3:C:262:GLU:N	2.29	0.65
3:C:359:ILE:CG2	3:C:377:GLU:HG3	2.27	0.65
3:B:149:SER:HG	3:C:101:TRP:CD1	2.14	0.64
1:1:121:SER:O	1:1:122:SER:HB2	1.96	0.64
3:A:113:LEU:HD23	3:A:253:GLN:HG3	1.71	0.64
3:C:360:THR:OG1	3:C:377:GLU:O	2.14	0.64
3:C:1:ILE:HD12	3:C:1:ILE:N	2.12	0.64
3:B:191:GLU:OE1	3:B:194:THR:HG21	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:104:GLY:CA	2:2:32:PHE:CE1	2.66	0.64
3:B:430:ASP:OD2	3:B:443:LYS:HE3	1.97	0.64
3:C:462:TRP:O	3:C:466:ILE:HD12	1.96	0.64
2:L:36:TYR:OH	2:L:91:ARG:NH2	2.31	0.64
3:C:460:MET:HG3	3:C:465:GLN:HG3	1.79	0.64
3:A:214:HIS:ND1	3:A:215:LYS:O	2.31	0.64
3:B:316:LYS:C	3:B:317:ILE:HG13	2.17	0.64
3:C:115:THR:OG1	3:C:253:GLN:OE1	2.14	0.64
3:A:345:MET:CG	3:A:378:LEU:HD13	2.28	0.63
3:A:473:MET:N	3:A:491:LEU:HD11	2.13	0.63
3:B:2:ARG:O	3:B:2:ARG:HG3	1.97	0.63
3:B:424:LEU:HB2	3:B:428:ALA:HB2	1.80	0.63
2:2:12:SER:HB3	2:2:108:LYS:HB2	1.81	0.63
3:C:91:VAL:HG22	3:C:239:LYS:HD2	1.80	0.63
3:C:106:GLY:O	3:C:107:LEU:CG	2.36	0.63
3:C:73:ARG:CG	3:C:77:GLN:HB2	2.26	0.63
2:L:94:TRP:CG	2:L:95:PRO:HD2	2.34	0.63
4:E:23:ARG:HH22	3:C:241:ALA:CB	2.11	0.63
3:C:309:THR:HG22	3:C:391:VAL:HG21	1.81	0.63
3:A:58:SER:HB2	3:A:126:THR:HG22	1.79	0.62
3:B:260:SER:O	3:B:262:GLU:N	2.32	0.62
3:C:16:SER:HB2	3:C:434:VAL:HG11	1.82	0.62
3:C:124:LYS:HD3	3:C:236:TRP:CH2	2.34	0.62
2:2:29:ILE:CG1	2:2:71:PHE:CZ	2.81	0.62
3:A:124:LYS:HG3	3:A:236:TRP:CH2	2.34	0.62
3:B:135:LEU:HD22	3:B:198:PHE:CD2	2.33	0.62
4:E:23:ARG:CZ	3:C:241:ALA:HA	2.28	0.62
3:C:19:THR:HG23	3:C:296:ASP:HB3	1.81	0.62
3:A:46:VAL:HG12	3:A:47:THR:HG23	1.81	0.62
3:C:91:VAL:HG23	3:C:239:LYS:CD	2.30	0.62
3:C:91:VAL:HG21	3:C:239:LYS:HB3	1.80	0.62
3:C:288:HIS:ND1	3:C:424:LEU:CD2	2.60	0.62
3:A:312:PHE:HD2	3:A:330:VAL:CG1	2.13	0.62
3:A:115:THR:CG2	3:A:253:GLN:OE1	2.44	0.62
3:B:474:TRP:CH2	3:B:478:ASN:ND2	2.67	0.62
3:C:76:THR:O	3:C:77:GLN:NE2	2.33	0.62
1:1:88:PRO:HA	1:1:120:VAL:CG2	2.30	0.62
2:L:29:ILE:CD1	2:L:90:GLN:CD	2.70	0.61
1:h:6:GLU:H	1:h:114:GLN:HE22	1.46	0.61
3:A:34:MET:HE1	3:A:359:ILE:HG12	1.83	0.61
4:E:27:LYS:HE2	4:F:2:VAL:HG11	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:226:HIS:N	3:B:236:TRP:CZ3	2.68	0.61
3:C:2:ARG:HE	3:C:44:GLU:HB2	1.65	0.61
3:C:34:MET:HE1	3:C:357:ARG:HD2	1.81	0.61
3:C:46:VAL:HG12	3:C:47:THR:HG23	1.81	0.61
3:C:214:HIS:H	4:F:7:HIS:HE1	1.47	0.61
3:A:98:ASP:H	3:A:250:ALA:CA	2.13	0.61
3:B:320:GLU:HB2	3:B:400:TRP:HZ2	1.64	0.61
3:B:358:LEU:HD23	3:B:378:LEU:HB2	1.83	0.61
3:B:481:ASN:H	3:B:484:ILE:HG13	1.65	0.61
3:C:2:ARG:NE	3:C:44:GLU:CB	2.63	0.61
3:C:345:MET:HG3	3:C:378:LEU:HD13	1.81	0.61
3:C:472:LEU:C	3:C:491:LEU:HD11	2.25	0.61
3:A:73:ARG:HG3	3:A:77:GLN:HB2	1.82	0.61
3:B:73:ARG:HD2	3:B:79:GLU:C	2.25	0.61
3:B:472:LEU:HD21	4:F:49:ILE:HG12	1.83	0.61
2:L:7:SER:HG	2:L:22:SER:HG	1.45	0.61
3:A:473:MET:HG3	3:A:491:LEU:CD1	2.21	0.61
3:B:288:HIS:CE1	3:B:424:LEU:HD13	2.35	0.61
3:C:193:ARG:HG2	3:C:193:ARG:NH1	2.14	0.61
3:A:98:ASP:H	3:A:250:ALA:HA	1.65	0.60
3:B:367:GLU:O	3:B:372:SER:OG	2.13	0.60
2:I:94:TRP:C	2:I:96:PRO:HD2	2.26	0.60
3:B:200:ASP:O	3:B:215:LYS:N	2.34	0.60
2:2:36:TYR:OH	2:2:91:ARG:NH2	2.32	0.60
3:B:472:LEU:O	3:B:491:LEU:HD11	2.01	0.60
3:A:16:SER:OG	3:A:434:VAL:CG1	2.50	0.60
3:C:360:THR:HG22	3:C:360:THR:O	2.01	0.60
3:B:465:GLN:HE21	3:B:498:LEU:HD13	1.67	0.60
3:A:80:ALA:O	3:A:94:ARG:NH2	2.35	0.60
2:2:61:ARG:NH1	2:2:82:ASP:OD2	2.33	0.60
3:C:91:VAL:CG2	3:C:239:LYS:HB3	2.30	0.59
1:H:73:ASP:OD2	1:H:76:LYS:NZ	2.34	0.59
1:H:101:SER:OG	1:H:103:PHE:O	2.20	0.59
2:I:94:TRP:CG	2:I:95:PRO:HD3	2.37	0.59
3:A:318:PRO:HG3	3:A:398:HIS:HE2	1.60	0.59
3:A:344:GLN:HE21	3:A:346:ALA:HB2	1.68	0.59
3:C:466:ILE:N	3:C:498:LEU:HD11	2.18	0.59
3:B:239:LYS:C	3:B:240:GLU:OE1	2.46	0.59
1:I:88:PRO:CA	1:I:120:VAL:HG21	2.33	0.59
3:A:216:GLU:OE2	4:D:10:ARG:NH2	2.36	0.59
3:B:262:GLU:O	3:B:266:HIS:NE2	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:138:ARG:HH11	3:A:166:LYS:HD2	1.68	0.58
3:B:430:ASP:OD1	3:B:443:LYS:HD2	2.02	0.58
3:C:359:ILE:O	3:C:359:ILE:HG13	2.01	0.58
3:A:70:SER:HB3	3:A:115:THR:HG22	1.85	0.58
3:A:357:ARG:CZ	3:A:359:ILE:HD11	2.33	0.58
3:B:276:GLU:OE2	3:B:283:ARG:NH2	2.36	0.58
3:C:125:MET:HE3	3:C:206:MET:HE3	1.85	0.58
3:C:345:MET:HE2	3:C:380:PRO:HB3	1.84	0.58
3:B:91:VAL:CG1	3:B:245:PHE:HE2	2.16	0.58
3:B:46:VAL:HG12	3:B:47:THR:HG23	1.85	0.58
2:I:95:PRO:C	2:I:97:TYR:N	2.42	0.58
3:B:73:ARG:HH12	3:B:81:TYR:HB3	1.67	0.58
3:C:24:VAL:HG11	3:C:288:HIS:HE1	1.69	0.58
3:C:473:MET:N	3:C:491:LEU:CD1	2.61	0.58
3:A:91:VAL:CG1	3:A:239:LYS:O	2.51	0.58
3:C:288:HIS:ND1	3:C:424:LEU:HD21	2.18	0.58
3:C:465:GLN:C	3:C:498:LEU:HD11	2.28	0.58
3:A:370:GLU:HG3	3:A:371:ASN:HD22	1.69	0.58
3:B:20:TRP:HB2	3:B:292:ARG:HG2	1.86	0.58
3:C:91:VAL:HG22	3:C:239:LYS:CD	2.34	0.58
3:B:135:LEU:HD22	3:B:198:PHE:HD2	1.68	0.57
3:C:124:LYS:HD3	3:C:236:TRP:HH2	1.67	0.57
3:A:276:GLU:OE2	3:A:283:ARG:NH2	2.37	0.57
3:C:90:TYR:N	3:C:239:LYS:NZ	2.52	0.57
3:A:236:TRP:O	3:A:239:LYS:HG2	2.03	0.57
2:I:36:TYR:OH	2:I:91:ARG:NH2	2.35	0.57
3:C:316:LYS:C	3:C:317:ILE:HG13	2.18	0.57
3:B:138:ARG:HH11	3:B:166:LYS:HD2	1.69	0.57
3:C:465:GLN:HB3	3:C:498:LEU:HD11	1.87	0.57
2:2:48:ILE:HG21	2:2:51:ALA:O	2.03	0.57
1:H:6:GLU:H	1:H:114:GLN:HE22	1.51	0.57
3:A:113:LEU:CD2	3:A:253:GLN:HE21	1.93	0.57
3:A:462:TRP:CD1	3:A:498:LEU:HD23	2.40	0.57
3:C:462:TRP:NE1	4:F:25:TYR:HH	2.01	0.57
3:C:24:VAL:HG11	3:C:288:HIS:CE1	2.40	0.57
3:C:382:PHE:HA	3:C:402:ARG:HB3	1.86	0.57
3:B:212:LEU:HG	3:B:284:LEU:HD21	1.87	0.57
3:B:345:MET:SD	3:B:378:LEU:HD13	2.44	0.57
3:C:345:MET:SD	3:C:378:LEU:HD11	2.45	0.57
3:A:97:VAL:HG13	3:A:250:ALA:O	2.05	0.56
3:A:307:LEU:HD23	3:A:340:LYS:CG	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:10:ASP:OD2	3:A:431:PHE:HZ	1.81	0.56
3:A:193:ARG:HH21	3:B:398:HIS:HE1	1.53	0.56
3:C:3:CYS:SG	3:C:30:CYS:HB2	2.44	0.56
3:B:125:MET:HE1	3:B:265:VAL:HG11	1.87	0.56
3:B:191:GLU:HB2	3:B:194:THR:HG23	1.86	0.56
3:C:345:MET:SD	3:C:378:LEU:CD1	2.93	0.56
2:2:29:ILE:HG13	2:2:29:ILE:O	2.03	0.56
1:H:35:HIS:HB2	1:H:97:VAL:HG22	1.88	0.56
2:L:12:SER:HB3	2:L:108:LYS:HB2	1.88	0.56
3:A:148:HIS:CD2	3:A:150:GLY:H	2.23	0.56
3:B:349:MET:HE1	3:B:397:THR:HG21	1.86	0.56
3:C:35:ALA:HB3	3:C:38:LYS:HB2	1.87	0.56
3:A:236:TRP:C	3:A:239:LYS:HE3	2.26	0.56
3:B:349:MET:HE2	3:B:386:TYR:CG	2.41	0.56
3:C:1:ILE:N	3:C:4:ILE:HG12	2.20	0.56
3:A:121:CYS:SG	3:A:124:LYS:HB3	2.46	0.56
3:B:58:SER:HB3	3:B:126:THR:CG2	2.15	0.56
3:C:34:MET:CE	3:C:359:ILE:CD1	2.83	0.56
3:B:148:HIS:CD2	3:B:150:GLY:H	2.24	0.56
3:C:38:LYS:NZ	3:C:295:MET:O	2.31	0.56
3:C:466:ILE:HG12	3:C:498:LEU:HD13	1.79	0.56
3:A:320:GLU:HB2	3:A:400:TRP:HZ2	1.71	0.56
3:C:99:ARG:HA	3:C:103:ASN:ND2	2.20	0.55
3:C:224:PRO:HD3	3:C:242:LEU:CD2	2.22	0.55
3:B:288:HIS:HE1	3:B:424:LEU:HD11	1.70	0.55
3:B:370:GLU:HG3	3:B:371:ASN:ND2	2.22	0.55
3:C:379:ASP:OD1	3:C:402:ARG:NH2	2.38	0.55
1:h:35:HIS:HB2	1:h:97:VAL:HG22	1.88	0.55
3:A:462:TRP:O	3:A:498:LEU:HD21	2.06	0.55
3:A:99:ARG:HA	3:A:103:ASN:ND2	2.22	0.55
3:C:248:ALA:HB3	3:C:252:ARG:HB2	1.87	0.55
3:B:135:LEU:CD2	3:B:198:PHE:HD2	2.20	0.55
3:A:49:THR:HG22	3:A:283:ARG:HG2	1.89	0.55
3:A:269:LEU:O	4:D:19:TRP:HD1	1.90	0.55
3:B:466:ILE:HG13	3:B:498:LEU:HD23	1.89	0.55
4:E:25:TYR:CD1	4:E:25:TYR:N	2.70	0.55
3:A:113:LEU:HD21	3:A:253:GLN:CG	2.33	0.55
3:B:20:TRP:HA	3:B:293:LEU:O	2.07	0.55
3:C:465:GLN:HB2	3:C:498:LEU:HD21	1.89	0.55
3:A:370:GLU:HG3	3:A:371:ASN:ND2	2.22	0.54
3:B:188:LEU:HD13	3:B:293:LEU:HD23	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:83:MET:HE1	1:H:94:TYR:CD2	2.42	0.54
2:I:93:ASN:OD1	3:C:99:ARG:CZ	2.54	0.54
3:B:359:ILE:HG23	3:B:377:GLU:HG3	1.84	0.54
3:C:349:MET:HE3	3:C:349:MET:CA	2.27	0.54
1:I:39:GLN:HB2	1:I:45:LEU:HD23	1.89	0.54
3:B:138:ARG:NH1	3:B:168:GLU:OE2	2.39	0.54
3:B:246:LYS:HG3	3:B:254:THR:HG1	1.72	0.54
1:I:35:HIS:HB2	1:I:97:VAL:HG22	1.88	0.54
3:C:347:VAL:CG2	3:C:355:VAL:HG21	2.38	0.54
3:B:98:ASP:OD2	3:C:7:SER:OG	2.24	0.54
1:I:95:TYR:CE2	1:I:114:GLN:C	2.85	0.54
3:B:70:SER:HB3	3:B:115:THR:HG22	1.89	0.54
3:B:275:ALA:HB2	3:B:284:LEU:CD2	2.38	0.54
3:C:320:GLU:HB2	3:C:400:TRP:CZ2	2.43	0.54
3:A:61:TYR:O	3:A:261:GLN:HB2	2.07	0.54
3:C:316:LYS:HG3	2:2:31:THR:HB	1.89	0.54
1:H:91:THR:HG23	1:H:119:THR:HA	1.89	0.54
3:B:3:CYS:O	3:B:9:ARG:HD3	2.07	0.54
3:B:91:VAL:HG12	3:B:245:PHE:HE2	1.71	0.54
3:A:475:LEU:C	3:A:479:THR:HG23	2.24	0.54
3:B:465:GLN:NE2	3:B:498:LEU:HD13	2.23	0.54
3:C:125:MET:HG3	3:C:125:MET:O	2.07	0.54
3:B:191:GLU:CB	3:B:194:THR:HG22	2.15	0.53
2:2:7:SER:OG	2:2:8:PRO:CD	2.52	0.53
2:I:94:TRP:CD2	2:I:95:PRO:HD3	2.43	0.53
3:C:60:CYS:CB	3:C:236:TRP:CZ3	2.83	0.53
3:C:80:ALA:O	3:C:94:ARG:NH2	2.41	0.53
2:L:29:ILE:HD13	2:L:90:GLN:OE1	2.06	0.53
3:A:481:ASN:OD1	3:A:482:GLY:N	2.30	0.53
2:I:95:PRO:O	2:I:96:PRO:C	2.51	0.53
3:C:91:VAL:CG2	3:C:239:LYS:HD2	2.37	0.53
3:C:91:VAL:HG12	3:C:245:PHE:CE2	2.44	0.53
3:C:153:VAL:HG22	1:I:102:ASN:CB	2.37	0.53
1:h:91:THR:HG23	1:h:119:THR:HA	1.90	0.53
3:C:155:ASP:H	1:I:100:TYR:HE2	1.53	0.53
2:I:7:SER:OG	2:I:22:SER:OG	2.24	0.53
3:B:202:TYR:CZ	3:B:215:LYS:HG3	2.44	0.53
2:2:94:TRP:CD2	2:2:95:PRO:CD	2.90	0.53
3:A:360:THR:HG21	3:A:377:GLU:N	2.15	0.53
3:C:469:GLY:O	3:C:491:LEU:CD2	2.57	0.53
1:H:68:PHE:CG	1:H:83:MET:HG2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:340:LYS:HA	3:C:364:VAL:HG22	1.91	0.52
1:1:95:TYR:HE2	1:1:114:GLN:C	2.17	0.52
1:H:52:THR:O	1:H:72:ARG:NH1	2.43	0.52
3:B:275:ALA:CB	3:B:284:LEU:HD23	2.40	0.52
3:C:125:MET:CE	3:C:206:MET:HG2	2.39	0.52
3:B:74:CYS:CB	3:B:75:PRO:HD2	2.18	0.52
3:B:125:MET:HE2	3:B:206:MET:CG	2.35	0.52
3:C:91:VAL:CG2	3:C:239:LYS:HD3	2.35	0.52
3:A:113:LEU:HB3	3:A:253:GLN:HE21	1.60	0.52
2:2:94:TRP:CG	2:2:95:PRO:CD	2.92	0.52
3:A:195:GLY:O	3:A:288:HIS:ND1	2.42	0.52
1:1:88:PRO:HA	1:1:120:VAL:CB	2.40	0.52
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.91	0.52
3:B:433:SER:O	3:B:434:VAL:C	2.52	0.52
3:C:3:CYS:HA	3:C:6:VAL:HG23	1.90	0.52
3:C:89:GLN:CA	3:C:239:LYS:NZ	2.72	0.52
3:C:469:GLY:C	3:C:491:LEU:HD22	2.35	0.52
3:A:307:LEU:CD2	3:A:340:LYS:CG	2.87	0.52
3:A:345:MET:SD	3:A:378:LEU:HD13	2.50	0.52
3:B:359:ILE:CG2	3:B:377:GLU:C	2.83	0.52
3:B:462:TRP:CD1	3:B:498:LEU:HD11	2.44	0.52
3:C:2:ARG:CZ	3:C:44:GLU:HB3	2.40	0.52
3:C:248:ALA:O	3:C:250:ALA:N	2.41	0.52
3:A:35:ALA:HB3	3:A:38:LYS:HB2	1.92	0.52
3:A:251:LYS:HG3	3:A:252:ARG:HG3	1.92	0.52
3:B:99:ARG:HA	3:B:103:ASN:ND2	2.24	0.52
3:C:197:ASP:O	3:C:199:SER:N	2.39	0.52
1:1:34:MET:HB3	1:1:79:LEU:HD22	1.92	0.52
1:1:36:TRP:CD1	1:1:81:PHE:CD1	2.98	0.52
1:1:95:TYR:CD2	1:1:115:GLY:N	2.78	0.52
1:h:83:MET:HG3	1:h:83:MET:O	2.10	0.52
3:B:76:THR:O	3:B:77:GLN:NE2	2.43	0.52
3:A:316:LYS:O	3:A:316:LYS:HG2	2.10	0.51
4:D:11:LYS:NZ	4:D:13:GLN:OE1	2.42	0.51
2:l:92:TYR:CZ	3:C:105:CYS:SG	3.03	0.51
3:B:26:GLU:OE1	4:E:15:ARG:NH1	2.43	0.51
3:B:318:PRO:HG2	3:B:398:HIS:CG	2.44	0.51
3:A:98:ASP:CG	3:A:250:ALA:CB	2.83	0.51
3:C:1:ILE:N	3:C:1:ILE:CD1	2.73	0.51
3:C:230:ASP:OD1	3:C:230:ASP:N	2.43	0.51
3:C:317:ILE:HG23	3:C:318:PRO:HD2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:238:ASN:CA	3:C:240:GLU:OE1	2.58	0.51
3:C:262:GLU:HG2	3:C:266:HIS:NE2	2.26	0.51
3:B:241:ALA:HB1	4:E:1:ALA:HB2	1.93	0.51
4:E:51:TRP:HA	4:E:60:LYS:HD2	1.92	0.51
1:h:39:GLN:HE22	2:l:38:HIS:HE1	1.58	0.51
3:B:177:GLU:HG2	3:B:187:GLY:HA2	1.93	0.51
4:E:49:ILE:HG12	3:C:472:LEU:HD21	1.92	0.51
3:B:13:GLU:OE1	3:B:14:GLY:N	2.44	0.51
3:C:466:ILE:N	3:C:498:LEU:CD1	2.73	0.51
2:L:94:TRP:CD2	2:L:95:PRO:HD2	2.45	0.51
3:C:61:TYR:O	3:C:261:GLN:HB2	2.11	0.51
3:C:370:GLU:HG3	3:C:371:ASN:ND2	2.26	0.51
1:H:11:LEU:HD11	1:H:121:SER:HA	1.93	0.50
3:B:40:THR:HG21	3:B:359:ILE:HD11	1.93	0.50
3:C:276:GLU:OE2	3:C:283:ARG:NH2	2.44	0.50
3:C:317:ILE:CG2	3:C:318:PRO:HD2	2.41	0.50
3:A:138:ARG:NH1	3:A:168:GLU:OE2	2.44	0.50
2:2:29:ILE:HD12	2:2:71:PHE:CZ	2.45	0.50
2:2:94:TRP:CD1	2:2:95:PRO:HD2	2.46	0.50
3:C:153:VAL:O	1:1:102:ASN:OD1	2.29	0.50
3:C:153:VAL:HG11	1:1:102:ASN:HD21	1.74	0.50
3:C:194:THR:O	3:C:194:THR:OG1	2.27	0.50
3:C:216:GLU:OE2	4:F:10:ARG:NH2	2.45	0.50
3:C:331:GLN:HA	3:C:372:SER:O	2.11	0.50
4:D:51:TRP:HA	4:D:60:LYS:HD2	1.93	0.50
3:B:35:ALA:HB3	3:B:38:LYS:HB2	1.92	0.50
3:B:359:ILE:CG2	3:B:377:GLU:O	2.59	0.50
3:C:308:CYS:HB3	3:C:332:TYR:CZ	2.45	0.50
2:2:29:ILE:CD1	2:2:71:PHE:HE1	1.98	0.50
3:A:74:CYS:O	3:A:75:PRO:C	2.54	0.50
3:A:472:LEU:C	3:A:491:LEU:HD11	2.37	0.50
2:l:93:ASN:CB	3:C:105:CYS:SG	2.95	0.50
3:B:345:MET:CG	3:B:378:LEU:HD13	2.42	0.50
3:B:72:SER:HA	3:B:112:SER:O	2.12	0.50
3:B:100:GLY:HA3	3:B:107:LEU:O	2.12	0.50
3:B:269:LEU:O	4:E:19:TRP:HD1	1.95	0.50
3:B:332:TYR:O	3:B:371:ASN:HA	2.12	0.50
1:1:35:HIS:ND1	1:1:47:TYR:OH	2.33	0.50
3:A:193:ARG:HH21	3:B:398:HIS:CE1	2.29	0.49
3:B:182:GLY:O	3:B:299:ARG:NH1	2.45	0.49
3:A:98:ASP:N	3:A:250:ALA:CB	2.74	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:59:TYR:CD1	3:B:225:TRP:HB3	2.47	0.49
3:C:465:GLN:CB	3:C:498:LEU:HD21	2.42	0.49
3:A:358:LEU:HD21	3:A:360:THR:OG1	2.13	0.49
3:C:378:LEU:C	3:C:378:LEU:HD12	2.37	0.49
1:1:91:THR:HG23	1:1:119:THR:HA	1.93	0.49
3:B:474:TRP:CE2	3:B:478:ASN:ND2	2.79	0.49
1:1:39:GLN:HE22	2:2:38:HIS:HE1	1.61	0.49
3:B:74:CYS:SG	2:2:93:ASN:HB2	2.53	0.49
3:B:344:GLN:HA	3:B:358:LEU:HD11	1.95	0.49
3:C:214:HIS:ND1	3:C:215:LYS:O	2.29	0.49
1:1:14:PRO:HD3	1:1:121:SER:OG	2.13	0.49
3:B:91:VAL:HG12	3:B:245:PHE:CZ	2.48	0.49
3:B:266:HIS:CD2	3:C:259:GLY:H	2.31	0.49
3:C:466:ILE:HG12	3:C:498:LEU:CD1	2.41	0.49
2:2:94:TRP:HA	2:2:94:TRP:CE3	2.47	0.49
3:C:238:ASN:C	3:C:240:GLU:OE1	2.56	0.49
4:F:3:THR:OG1	4:F:4:LEU:N	2.46	0.49
3:B:55:GLU:HA	3:B:128:LYS:HG2	1.95	0.48
4:E:24:GLU:HA	4:E:27:LYS:HE3	1.93	0.48
3:C:462:TRP:CD1	4:F:25:TYR:HH	2.31	0.48
1:1:36:TRP:CD1	1:1:81:PHE:HD1	2.30	0.48
1:1:83:MET:O	1:1:83:MET:HG3	2.12	0.48
3:A:73:ARG:NH1	3:A:81:TYR:H	2.11	0.48
3:A:182:GLY:O	3:A:299:ARG:NH1	2.46	0.48
3:B:370:GLU:HG3	3:B:371:ASN:HD22	1.78	0.48
3:B:462:TRP:O	3:B:498:LEU:HD21	2.13	0.48
3:C:70:SER:HA	3:C:114:VAL:O	2.13	0.48
3:B:125:MET:O	3:B:125:MET:HG3	2.13	0.48
2:L:7:SER:OG	2:L:8:PRO:HD3	2.14	0.48
3:A:307:LEU:HD23	3:A:340:LYS:CD	2.40	0.48
3:B:473:MET:N	3:B:491:LEU:HD13	2.24	0.48
3:C:208:ASN:N	3:C:208:ASN:OD1	2.46	0.48
1:h:73:ASP:OD2	1:h:76:LYS:NZ	2.46	0.48
1:1:73:ASP:OD2	1:1:76:LYS:NZ	2.45	0.48
3:B:288:HIS:ND1	3:B:424:LEU:HD21	2.29	0.48
3:C:91:VAL:CG2	3:C:239:LYS:HB2	2.32	0.48
1:1:67:ARG:NH1	1:1:87:ARG:HG3	2.29	0.48
3:A:15:MET:HG3	3:A:18:GLY:H	1.79	0.48
3:A:113:LEU:HG	3:A:253:GLN:CD	2.33	0.48
3:C:270:ALA:H	4:F:7:HIS:HB3	1.78	0.48
3:A:13:GLU:OE1	3:A:357:ARG:NH2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:16:SER:OG	3:A:434:VAL:HG13	2.14	0.48
3:B:73:ARG:CD	3:B:79:GLU:O	2.62	0.48
3:B:345:MET:HE2	3:B:380:PRO:HB3	1.95	0.48
3:C:307:LEU:HD21	3:C:342:PRO:CB	2.35	0.48
3:C:317:ILE:CG2	3:C:318:PRO:CD	2.92	0.48
3:C:38:LYS:NZ	3:C:296:ASP:HA	2.29	0.47
3:A:59:TYR:CD2	3:A:125:MET:HE3	2.49	0.47
3:A:67:ASP:OD1	3:A:67:ASP:N	2.47	0.47
3:C:277:MET:HG3	3:C:281:LYS:O	2.13	0.47
3:C:317:ILE:HG22	3:C:318:PRO:N	2.29	0.47
3:A:100:GLY:HA3	3:A:107:LEU:O	2.14	0.47
3:A:430:ASP:HA	3:A:433:SER:HB2	1.96	0.47
2:I:92:TYR:CE1	3:C:105:CYS:SG	3.07	0.47
3:C:215:LYS:C	3:C:217:TRP:H	2.22	0.47
3:C:225:TRP:CE2	3:C:237:ASN:ND2	2.74	0.47
3:B:91:VAL:CG1	3:B:245:PHE:CE2	2.93	0.47
3:A:113:LEU:HG	3:A:253:GLN:OE1	2.14	0.47
3:A:319:ALA:HB3	3:A:327:THR:OG1	2.14	0.47
3:A:374:MET:HE2	3:A:374:MET:HB2	1.71	0.47
4:E:52:LEU:HB2	3:C:475:LEU:HD21	1.96	0.47
3:C:201:LEU:HB3	3:C:212:LEU:HD22	1.96	0.47
1:I:119:THR:HG22	1:I:120:VAL:O	2.15	0.47
3:A:345:MET:HG3	3:A:378:LEU:HD13	1.97	0.47
2:I:94:TRP:O	2:I:96:PRO:HD2	2.14	0.47
3:B:259:GLY:H	3:C:266:HIS:CD2	2.32	0.47
3:B:473:MET:HA	3:B:491:LEU:HD12	1.78	0.47
3:C:342:PRO:HG3	3:C:391:VAL:HG23	1.97	0.47
2:2:19:ALA:HB3	2:2:75:ILE:HB	1.97	0.47
1:h:12:VAL:HG11	1:h:86:LEU:HD12	1.95	0.47
4:E:24:GLU:O	4:E:27:LYS:HB3	2.15	0.47
3:C:307:LEU:CD1	3:C:340:LYS:C	2.84	0.47
3:C:373:LYS:NZ	2:2:52:SER:OG	2.47	0.47
3:B:49:THR:HG22	3:B:283:ARG:HG2	1.96	0.47
4:F:10:ARG:HA	4:F:10:ARG:HD3	1.71	0.47
3:A:34:MET:CE	3:A:359:ILE:HG12	2.45	0.46
3:B:6:VAL:HG12	3:B:8:ASN:H	1.79	0.46
3:B:61:TYR:O	3:B:261:GLN:HB2	2.15	0.46
3:B:378:LEU:HD12	3:B:378:LEU:C	2.40	0.46
3:C:141:LEU:C	3:C:141:LEU:HD12	2.40	0.46
3:C:180:LEU:HB2	3:C:183:PHE:HB2	1.95	0.46
1:H:91:THR:HA	1:H:118:VAL:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:29:ILE:HG21	2:L:90:GLN:NE2	2.27	0.46
3:B:125:MET:CE	3:B:206:MET:CE	2.91	0.46
3:B:270:ALA:H	4:E:7:HIS:HB3	1.79	0.46
3:C:24:VAL:CG1	3:C:288:HIS:CE1	2.98	0.46
4:D:3:THR:OG1	4:D:4:LEU:N	2.47	0.46
3:B:24:VAL:HG13	3:B:288:HIS:CE1	2.40	0.46
3:B:462:TRP:HA	3:B:498:LEU:CD1	2.45	0.46
3:A:97:VAL:HA	3:A:250:ALA:HA	1.97	0.46
4:E:53:LEU:HD11	3:C:471:LEU:HD11	1.96	0.46
3:C:202:TYR:CE2	3:C:215:LYS:HG2	2.50	0.46
3:C:462:TRP:O	3:C:466:ILE:CD1	2.63	0.46
2:2:63:SER:OG	2:2:74:THR:HB	2.16	0.46
3:A:88:THR:HG23	3:C:88:THR:HG23	1.96	0.46
3:C:226:HIS:CG	3:C:227:ALA:H	2.33	0.46
1:1:68:PHE:CD2	1:1:81:PHE:CZ	2.96	0.46
2:1:66:ARG:HG3	2:1:71:PHE:CE2	2.51	0.46
3:C:193:ARG:NH1	3:C:193:ARG:CG	2.72	0.46
1:H:105:TYR:CG	2:L:95:PRO:HG3	2.51	0.46
3:B:70:SER:HA	3:B:114:VAL:O	2.16	0.46
3:B:73:ARG:HH11	3:B:81:TYR:HB3	1.71	0.46
3:C:224:PRO:CD	3:C:242:LEU:CD2	2.78	0.46
3:A:469:GLY:O	3:A:491:LEU:CD2	2.59	0.46
3:B:63:ALA:HB2	3:B:242:LEU:HD23	1.97	0.46
3:C:125:MET:CE	3:C:206:MET:HE3	2.46	0.46
3:C:1:ILE:H2	3:C:4:ILE:HG12	1.81	0.46
3:C:89:GLN:CA	3:C:239:LYS:HZ1	2.29	0.46
2:L:90:GLN:HE21	2:L:92:TYR:HB2	1.81	0.46
3:A:226:HIS:CG	3:A:227:ALA:H	2.34	0.46
3:A:479:THR:HG1	3:A:484:ILE:HG22	1.79	0.46
3:B:358:LEU:CD2	3:B:378:LEU:HD22	2.46	0.46
3:C:240:GLU:N	3:C:240:GLU:CD	2.74	0.45
3:C:262:GLU:O	3:C:262:GLU:HG2	2.16	0.45
3:A:378:LEU:C	3:A:378:LEU:HD12	2.42	0.45
3:B:226:HIS:N	3:B:236:TRP:CE3	2.84	0.45
3:C:7:SER:HB2	3:C:322:LEU:HD22	1.98	0.45
3:C:224:PRO:HB3	3:C:238:ASN:O	2.16	0.45
3:A:3:CYS:O	3:A:9:ARG:HD3	2.17	0.45
3:A:60:CYS:HA	3:A:124:LYS:CB	2.46	0.45
3:A:345:MET:HE2	3:A:380:PRO:HB3	1.99	0.45
3:B:80:ALA:HB3	3:B:114:VAL:HG23	1.97	0.45
3:A:27:HIS:NE2	3:A:48:THR:HG23	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:73:ARG:CA	2:2:93:ASN:HD21	2.23	0.45
3:C:138:ARG:HH11	3:C:166:LYS:HD2	1.82	0.45
3:A:19:THR:HB	3:A:20:TRP:HD1	1.82	0.45
3:A:224:PRO:HA	3:A:238:ASN:HB2	1.98	0.45
3:A:275:ALA:CB	3:A:284:LEU:CD2	2.88	0.45
3:B:66:SER:OG	3:B:67:ASP:N	2.47	0.45
3:B:217:TRP:NE1	4:E:5:PRO:O	2.50	0.45
3:B:495:LEU:HD23	3:B:495:LEU:HA	1.77	0.45
3:C:238:ASN:HA	3:C:240:GLU:OE1	2.16	0.45
3:A:246:LYS:HG3	3:A:254:THR:OG1	2.17	0.45
3:A:363:PRO:HB3	3:A:374:MET:HE1	1.99	0.45
3:B:69:ALA:HA	1:1:57:SER:OG	2.16	0.45
3:B:288:HIS:CG	3:B:424:LEU:HD21	2.52	0.45
3:A:302:GLY:HA3	3:A:364:VAL:HG21	1.98	0.45
3:A:307:LEU:CD2	3:A:340:LYS:CB	2.68	0.45
3:A:359:ILE:HG22	3:A:359:ILE:O	2.17	0.45
3:B:13:GLU:HA	3:B:34:MET:HG3	1.99	0.45
3:B:48:THR:OG1	3:B:284:LEU:HB2	2.17	0.45
4:E:26:THR:O	4:E:30:ILE:HB	2.16	0.45
3:C:349:MET:O	3:C:352:LEU:HD21	2.16	0.45
1:1:67:ARG:HH11	1:1:87:ARG:HG3	1.81	0.45
2:L:0:SER:OG	2:L:1:GLU:N	2.48	0.45
3:A:2:ARG:NH1	3:A:44:GLU:OE1	2.47	0.45
3:A:201:LEU:HA	3:A:213:VAL:O	2.17	0.45
3:A:358:LEU:CD2	3:A:360:THR:OG1	2.65	0.45
3:A:495:LEU:HD13	3:A:495:LEU:HA	1.77	0.45
3:B:226:HIS:H	3:B:236:TRP:HZ3	1.65	0.45
3:B:331:GLN:HA	3:B:372:SER:O	2.16	0.45
3:B:467:LEU:HD13	4:E:69:LEU:HD21	1.99	0.45
3:C:345:MET:SD	3:C:387:ILE:HG12	2.57	0.45
2:L:59:PRO:HB2	2:L:61:ARG:HD3	1.99	0.44
3:A:262:GLU:O	3:A:262:GLU:HG2	2.16	0.44
3:B:252:ARG:HA	1:1:104:TYR:OH	2.16	0.44
3:C:71:ASP:O	3:C:113:LEU:HD12	2.18	0.44
3:C:212:LEU:HD11	3:C:284:LEU:HD13	1.99	0.44
3:A:74:CYS:HB2	3:A:77:GLN:HG3	1.92	0.44
3:B:246:LYS:CG	3:B:254:THR:OG1	2.60	0.44
3:B:278:ASP:OD1	3:B:278:ASP:N	2.46	0.44
3:B:314:PHE:CE2	3:B:398:HIS:HB2	2.53	0.44
3:B:345:MET:HB2	3:B:355:VAL:O	2.16	0.44
3:A:10:ASP:CG	3:A:431:PHE:CZ	2.92	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:ILE:O	3:C:2:ARG:HB3	2.18	0.44
3:C:420:ARG:HG3	3:C:424:LEU:HD12	1.99	0.44
3:C:262:GLU:O	3:C:266:HIS:NE2	2.42	0.44
1:1:105:TYR:HB2	2:2:95:PRO:HG3	2.00	0.44
2:2:3:VAL:HG22	2:2:26:SER:HB3	1.99	0.44
3:A:260:SER:C	3:A:262:GLU:H	2.25	0.44
4:E:69:LEU:HD23	4:F:70:ILE:HD13	1.99	0.44
1:1:49:SER:CB	1:1:81:PHE:HE1	2.30	0.44
2:2:66:ARG:HG3	2:2:71:PHE:CE2	2.52	0.44
1:H:39:GLN:HE22	2:L:38:HIS:HE1	1.66	0.44
3:B:85:GLN:HE22	3:B:94:ARG:NH1	2.15	0.44
3:A:98:ASP:CA	3:A:250:ALA:HB1	2.44	0.44
3:B:30:CYS:HB3	3:B:44:GLU:HG3	2.00	0.44
3:B:205:THR:CG2	3:B:210:HIS:CE1	3.00	0.44
3:B:433:SER:C	3:B:435:GLY:N	2.76	0.44
3:A:25:LEU:N	3:A:289:LEU:O	2.44	0.43
2:l:3:VAL:HG22	2:l:26:SER:HB3	2.00	0.43
3:B:71:ASP:OD1	3:B:72:SER:N	2.51	0.43
1:h:39:GLN:HB2	1:h:45:LEU:HD23	1.99	0.43
3:A:7:SER:HB2	3:A:322:LEU:HD22	1.99	0.43
3:A:300:LEU:HA	3:A:300:LEU:HD23	1.85	0.43
2:L:29:ILE:CD1	2:L:90:GLN:OE1	2.66	0.43
2:L:90:GLN:HE21	2:L:92:TYR:N	2.16	0.43
3:A:70:SER:HA	3:A:114:VAL:O	2.18	0.43
3:A:426:ASP:OD2	3:A:447:GLN:CB	2.66	0.43
3:B:426:ASP:CG	3:B:447:GLN:HG3	2.41	0.43
3:C:1:ILE:CD1	3:C:1:ILE:H3	2.30	0.43
3:C:6:VAL:HG21	3:C:30:CYS:SG	2.59	0.43
2:2:95:PRO:O	2:2:97:TYR:N	2.51	0.43
3:A:98:ASP:H	3:A:250:ALA:HB1	1.80	0.43
3:A:277:MET:HG3	3:A:281:LYS:O	2.18	0.43
3:A:309:THR:O	3:A:309:THR:OG1	2.30	0.43
3:B:471:LEU:HD11	4:F:53:LEU:HD11	2.00	0.43
3:C:59:TYR:CE1	3:C:225:TRP:HB3	2.53	0.43
3:C:204:LEU:O	3:C:210:HIS:HA	2.19	0.43
3:A:270:ALA:H	4:D:7:HIS:HB3	1.82	0.43
3:B:492:GLY:O	3:B:496:ILE:HG22	2.18	0.43
3:A:392:GLY:C	3:A:394:LYS:H	2.26	0.43
2:l:33:LEU:HD11	2:l:88:CYS:HB2	2.00	0.43
3:B:465:GLN:HG3	3:B:498:LEU:HD22	2.01	0.43
3:C:153:VAL:CG1	1:1:102:ASN:ND2	2.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:33:LEU:HD23	2:2:90:GLN:OE1	2.19	0.43
3:A:74:CYS:C	3:A:76:THR:N	2.71	0.43
2:l:21:LEU:HD23	2:l:103:THR:HB	2.01	0.43
1:H:35:HIS:ND1	1:H:47:TYR:OH	2.28	0.43
3:A:189:ASP:OD1	3:A:189:ASP:N	2.47	0.43
3:B:316:LYS:NZ	3:B:329:GLU:OE1	2.52	0.43
1:1:87:ARG:C	1:1:120:VAL:HG21	2.42	0.43
2:2:37:GLN:HB2	2:2:47:LEU:HD11	2.01	0.43
3:A:162:GLU:OE2	3:A:301:LYS:NZ	2.46	0.43
3:A:332:TYR:O	3:A:371:ASN:HA	2.18	0.43
3:A:472:LEU:C	3:A:491:LEU:HD21	2.44	0.43
3:C:263:GLY:HA2	3:C:266:HIS:HD2	1.84	0.43
3:C:269:LEU:O	4:F:19:TRP:HD1	2.01	0.43
1:1:36:TRP:CE2	1:1:81:PHE:HB2	2.54	0.43
3:B:27:HIS:NE2	3:B:48:THR:HG23	2.34	0.42
3:B:204:LEU:O	3:B:210:HIS:HA	2.19	0.42
3:B:277:MET:HG3	3:B:281:LYS:O	2.19	0.42
3:B:480:LYS:HA	3:B:484:ILE:HD11	2.01	0.42
3:C:200:ASP:HA	3:C:215:LYS:HD2	2.01	0.42
3:C:302:GLY:HA3	3:C:364:VAL:HG21	2.01	0.42
4:F:53:LEU:O	4:F:60:LYS:HG2	2.19	0.42
3:A:123:LYS:HE2	3:A:123:LYS:HB3	1.75	0.42
3:A:242:LEU:HD12	3:A:242:LEU:HA	1.72	0.42
3:A:275:ALA:HB2	3:A:284:LEU:HD21	1.99	0.42
3:B:99:ARG:HG3	3:B:103:ASN:HD22	1.84	0.42
3:B:498:LEU:HD12	3:B:498:LEU:HA	1.51	0.42
3:C:495:LEU:HA	3:C:495:LEU:HD12	1.81	0.42
3:A:308:CYS:SG	3:A:365:ILE:HD11	2.59	0.42
3:A:349:MET:HE2	3:A:349:MET:HB2	1.79	0.42
3:A:359:ILE:O	3:A:360:THR:HG23	2.19	0.42
3:A:484:ILE:HG13	3:A:485:SER:H	1.84	0.42
3:B:384:ASP:HB3	3:B:399:HIS:HE1	1.84	0.42
3:C:200:ASP:O	3:C:215:LYS:HG3	2.19	0.42
4:F:45:ALA:O	4:F:49:ILE:HG13	2.19	0.42
3:A:3:CYS:HB2	3:A:42:ASP:OD2	2.19	0.42
3:A:303:VAL:O	3:A:304:SER:OG	2.31	0.42
3:A:473:MET:N	3:A:491:LEU:CD1	2.78	0.42
3:C:161:ASP:OD2	3:C:164:ARG:NH1	2.53	0.42
2:L:94:TRP:CD2	2:L:95:PRO:CD	3.01	0.42
3:C:59:TYR:CD1	3:C:225:TRP:HB3	2.55	0.42
3:B:59:TYR:CE1	3:B:225:TRP:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:225:TRP:C	3:B:236:TRP:CE3	2.97	0.42
3:C:2:ARG:NH2	3:C:44:GLU:CB	2.59	0.42
2:2:29:ILE:CG1	2:2:71:PHE:CE1	3.00	0.42
2:2:66:ARG:HG2	2:2:67:SER:N	2.35	0.42
3:B:61:TYR:CZ	3:B:123:LYS:CB	2.85	0.42
3:B:238:ASN:ND2	3:B:240:GLU:O	2.53	0.42
1:h:105:TYR:CG	2:l:95:PRO:HG3	2.54	0.42
2:l:7:SER:OG	2:l:8:PRO:HD3	2.19	0.42
3:B:392:GLY:C	3:B:394:LYS:H	2.28	0.42
3:C:34:MET:CE	3:C:359:ILE:HD13	2.49	0.42
3:A:98:ASP:N	3:A:250:ALA:HB1	2.35	0.42
3:A:462:TRP:CZ3	4:D:25:TYR:HB3	2.55	0.42
2:l:19:ALA:HB3	2:l:75:ILE:HB	2.01	0.42
3:B:57:ARG:H	3:B:228:GLY:H	1.68	0.42
3:B:61:TYR:OH	3:B:123:LYS:HD3	2.20	0.42
4:E:39:ASN:ND2	4:F:10:ARG:HH11	2.17	0.42
1:1:49:SER:HB3	1:1:81:PHE:HE1	1.84	0.42
3:A:477:LEU:HA	3:A:477:LEU:HD12	1.86	0.41
3:B:6:VAL:HG21	3:B:30:CYS:SG	2.60	0.41
3:B:262:GLU:O	3:B:262:GLU:HG2	2.20	0.41
3:B:359:ILE:O	3:B:360:THR:C	2.61	0.41
3:C:317:ILE:HG23	3:C:318:PRO:CD	2.50	0.41
1:h:2:VAL:HA	1:h:25:SER:O	2.19	0.41
3:B:67:ASP:N	3:B:67:ASP:OD1	2.52	0.41
3:C:491:LEU:O	3:C:492:GLY:C	2.62	0.41
3:C:196:LEU:O	3:C:196:LEU:CG	2.68	0.41
3:C:370:GLU:HG3	3:C:371:ASN:HD22	1.86	0.41
3:C:485:SER:O	3:C:486:LEU:C	2.64	0.41
3:A:426:ASP:OD1	3:A:446:HIS:CG	2.73	0.41
3:A:433:SER:O	3:A:434:VAL:C	2.64	0.41
4:D:10:ARG:HA	4:D:10:ARG:HD3	1.87	0.41
3:B:1:ILE:CD1	3:B:1:ILE:N	2.82	0.41
3:B:190:CYS:O	3:B:192:PRO:HD3	2.21	0.41
3:B:374:MET:HB2	3:B:374:MET:HE3	1.80	0.41
2:2:29:ILE:CG1	2:2:71:PHE:HZ	2.18	0.41
3:A:206:MET:HE2	3:A:206:MET:HB3	1.87	0.41
3:A:492:GLY:O	3:A:493:GLY:C	2.62	0.41
4:D:68:LEU:HD23	4:D:68:LEU:HA	1.86	0.41
1:1:19:ARG:HH21	1:1:80:TYR:HE2	1.69	0.41
4:E:66:MET:HB3	4:F:66:MET:HE2	2.03	0.41
3:C:133:GLU:HA	3:C:171:PRO:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:374:MET:HE3	3:C:374:MET:HB2	1.89	0.41
3:A:53:MET:HE3	3:A:53:MET:HB2	1.99	0.41
3:A:74:CYS:SG	3:A:77:GLN:HG2	2.58	0.41
3:A:212:LEU:HG	3:A:284:LEU:HD21	2.02	0.41
3:C:473:MET:HB2	3:C:491:LEU:CD1	2.35	0.41
3:A:236:TRP:O	3:A:239:LYS:CG	2.69	0.41
3:A:320:GLU:HG2	3:A:321:THR:O	2.20	0.41
2:l:78:LEU:HD23	2:l:78:LEU:HA	1.93	0.41
3:B:106:GLY:O	3:B:107:LEU:HG	2.20	0.41
3:B:215:LYS:HB3	3:B:215:LYS:HE2	1.84	0.41
3:B:271:GLY:HA2	4:E:18:THR:HB	2.02	0.41
3:B:359:ILE:H	3:B:378:LEU:HA	1.85	0.41
3:A:462:TRP:NE1	3:A:498:LEU:HD23	2.36	0.41
2:l:8:PRO:C	2:l:10:THR:H	2.29	0.41
2:l:66:ARG:HG2	2:l:67:SER:N	2.36	0.41
3:B:2:ARG:HH11	3:B:2:ARG:HD2	1.73	0.41
3:B:72:SER:OG	2:2:94:TRP:CZ3	2.73	0.41
3:B:288:HIS:HE1	3:B:424:LEU:CD1	2.23	0.41
3:B:316:LYS:HD2	3:C:101:TRP:CZ2	2.55	0.41
3:B:324:GLY:HA3	3:B:402:ARG:HH11	1.85	0.41
3:B:461:SER:O	3:B:463:PHE:N	2.52	0.41
4:E:3:THR:OG1	4:E:4:LEU:N	2.53	0.41
4:E:67:ILE:HA	4:E:70:ILE:HG22	2.03	0.41
3:C:34:MET:CE	3:C:359:ILE:HD12	2.50	0.41
3:C:153:VAL:HG11	1:1:102:ASN:ND2	2.36	0.41
3:C:476:GLY:O	3:C:484:ILE:HG23	2.21	0.41
3:B:382:PHE:HA	3:B:402:ARG:HB3	2.01	0.41
3:C:480:LYS:HA	3:C:484:ILE:HD11	2.02	0.41
1:1:103:PHE:O	1:1:104:TYR:C	2.64	0.41
3:A:196:LEU:HB3	3:A:198:PHE:CE1	2.55	0.40
2:l:0:SER:OG	2:l:1:GLU:N	2.53	0.40
3:B:39:PRO:HG3	3:B:183:PHE:HD2	1.84	0.40
3:B:108:PHE:HB2	3:C:320:GLU:O	2.21	0.40
3:B:141:LEU:HD11	3:B:165:ALA:HB3	2.02	0.40
3:B:341:VAL:CB	3:B:363:PRO:O	2.60	0.40
3:C:473:MET:HA	3:C:491:LEU:HD12	2.01	0.40
3:A:207:ASN:OD1	3:A:207:ASN:N	2.51	0.40
3:B:74:CYS:CB	3:B:75:PRO:CD	2.82	0.40
3:B:298:LEU:HD23	3:B:298:LEU:HA	1.89	0.40
4:E:53:LEU:O	4:E:60:LYS:HG2	2.21	0.40
3:C:333:ALA:HA	3:C:371:ASN:OD1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:8:PRO:O	2:L:103:THR:OG1	2.35	0.40
2:L:66:ARG:HG2	2:L:67:SER:N	2.37	0.40
3:A:97:VAL:HG21	3:A:113:LEU:HD22	2.03	0.40
3:A:308:CYS:HB3	3:A:332:TYR:CZ	2.56	0.40
3:B:212:LEU:HG	3:B:284:LEU:CD2	2.51	0.40
3:C:9:ARG:HH22	3:C:377:GLU:CD	2.30	0.40
3:C:38:LYS:HZ3	3:C:296:ASP:HA	1.85	0.40
3:C:320:GLU:HB2	3:C:400:TRP:HZ2	1.82	0.40
3:A:73:ARG:CZ	3:A:80:ALA:HA	2.51	0.40
3:A:99:ARG:HA	3:A:103:ASN:HD22	1.85	0.40
3:A:247:ASP:OD1	3:A:253:GLN:HA	2.21	0.40
3:A:462:TRP:CE2	3:A:498:LEU:HD23	2.56	0.40
3:B:73:ARG:NE	3:B:79:GLU:O	2.53	0.40
3:C:190:CYS:O	3:C:192:PRO:HD3	2.22	0.40
2:l:94:TRP:CE2	3:C:71:ASP:HA	2.56	0.40
3:B:10:ASP:OD1	3:B:31:VAL:HG22	2.22	0.40
3:C:90:TYR:N	3:C:239:LYS:HZ2	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	119/122 (98%)	116 (98%)	3 (2%)	0	100	100
1	H	119/122 (98%)	118 (99%)	1 (1%)	0	100	100
1	h	119/122 (98%)	118 (99%)	1 (1%)	0	100	100
2	2	106/109 (97%)	99 (93%)	6 (6%)	1 (1%)	14	47
2	L	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
2	l	107/109 (98%)	96 (90%)	10 (9%)	1 (1%)	14	47
3	A	488/639 (76%)	435 (89%)	50 (10%)	3 (1%)	21	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	488/639 (76%)	433 (89%)	51 (10%)	4 (1%)	16	50
3	C	499/639 (78%)	441 (88%)	57 (11%)	1 (0%)	43	73
4	D	73/3423 (2%)	66 (90%)	7 (10%)	0	100	100
4	E	73/3423 (2%)	66 (90%)	7 (10%)	0	100	100
4	F	73/3423 (2%)	65 (89%)	8 (11%)	0	100	100
All	All	2371/12879 (18%)	2153 (91%)	208 (9%)	10 (0%)	31	62

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	317	ILE
3	A	261	GLN
3	A	318	PRO
3	C	261	GLN
2	1	96	PRO
3	B	261	GLN
2	2	96	PRO
3	B	462	TRP
3	B	363	PRO
3	B	434	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	100/101 (99%)	99 (99%)	1 (1%)	68	80
1	H	100/101 (99%)	98 (98%)	2 (2%)	48	72
1	h	100/101 (99%)	99 (99%)	1 (1%)	68	80
2	2	92/93 (99%)	91 (99%)	1 (1%)	65	79
2	L	93/93 (100%)	93 (100%)	0	100	100
2	l	93/93 (100%)	91 (98%)	2 (2%)	45	71
3	A	400/534 (75%)	380 (95%)	20 (5%)	22	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	400/534 (75%)	385 (96%)	15 (4%)	29	62
3	C	408/534 (76%)	399 (98%)	9 (2%)	45	71
4	D	64/2832 (2%)	63 (98%)	1 (2%)	55	75
4	E	64/2832 (2%)	62 (97%)	2 (3%)	35	66
4	F	64/2832 (2%)	64 (100%)	0	100	100
All	All	1978/10680 (18%)	1924 (97%)	54 (3%)	40	68

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	6	GLU
1	H	97	VAL
3	A	23	VAL
3	A	27	HIS
3	A	32	THR
3	A	65	ILE
3	A	91	VAL
3	A	97	VAL
3	A	123	LYS
3	A	124	LYS
3	A	141	LEU
3	A	143	VAL
3	A	189	ASP
3	A	213	VAL
3	A	220	ASP
3	A	255	VAL
3	A	365	ILE
3	A	406	THR
3	A	456	LEU
3	A	466	ILE
3	A	475	LEU
3	A	495	LEU
4	D	25	TYR
1	h	97	VAL
2	l	7	SER
2	l	90	GLN
3	B	1	ILE
3	B	23	VAL
3	B	31	VAL
3	B	125	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	141	LEU
3	B	143	VAL
3	B	213	VAL
3	B	221	ILE
3	B	255	VAL
3	B	274	GLU
3	B	349	MET
3	B	359	ILE
3	B	466	ILE
3	B	486	LEU
3	B	496	ILE
4	E	25	TYR
4	E	68	LEU
3	C	23	VAL
3	C	97	VAL
3	C	193	ARG
3	C	208	ASN
3	C	213	VAL
3	C	255	VAL
3	C	284	LEU
3	C	396	ILE
3	C	406	THR
1	1	97	VAL
2	2	94	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
2	L	42	GLN
2	L	90	GLN
3	A	77	GLN
3	A	103	ASN
3	A	148	HIS
3	A	219	HIS
3	A	331	GLN
3	A	344	GLN
3	A	371	ASN
3	A	399	HIS
4	D	7	HIS
1	h	39	GLN
2	l	42	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	77	GLN
3	B	85	GLN
3	B	103	ASN
3	B	148	HIS
3	B	163	ASN
3	B	238	ASN
3	B	249	HIS
3	B	266	HIS
3	B	288	HIS
3	B	371	ASN
3	B	398	HIS
4	E	7	HIS
3	C	103	ASN
3	C	219	HIS
3	C	266	HIS
3	C	288	HIS
3	C	323	HIS
3	C	331	GLN
3	C	344	GLN
3	C	350	GLN
3	C	371	ASN
3	C	401	HIS
3	C	447	GLN
3	C	478	ASN
4	F	7	HIS
4	F	34	ASN
1	1	39	GLN
1	1	102	ASN
2	2	42	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

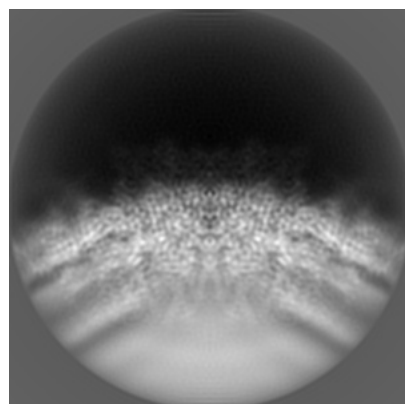
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27055. These allow visual inspection of the internal detail of the map and identification of artifacts.

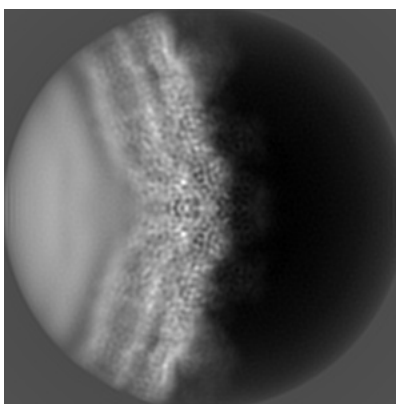
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

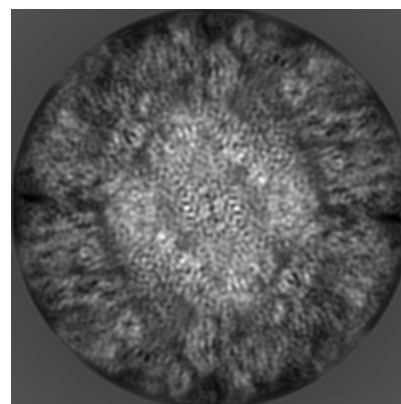
6.1.1 Primary map



X

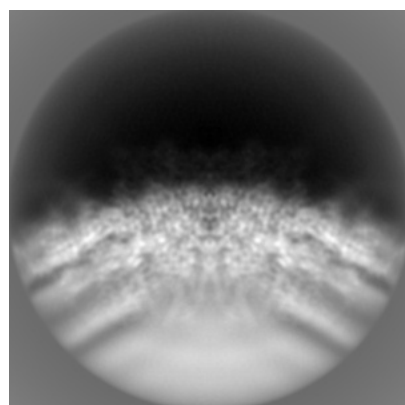


Y

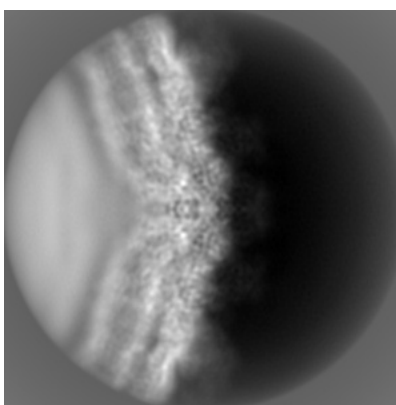


Z

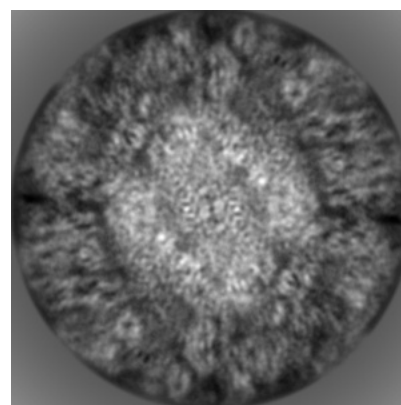
6.1.2 Raw map



X



Y

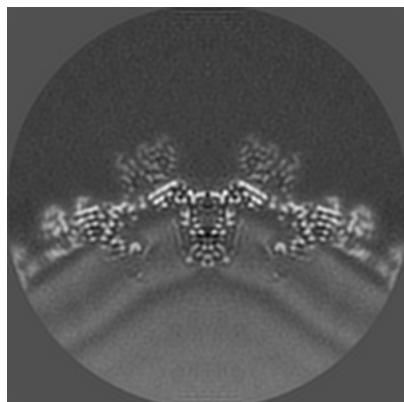


Z

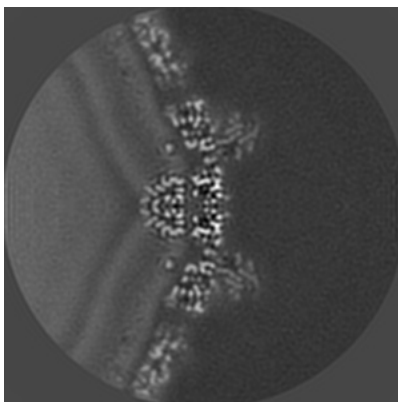
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

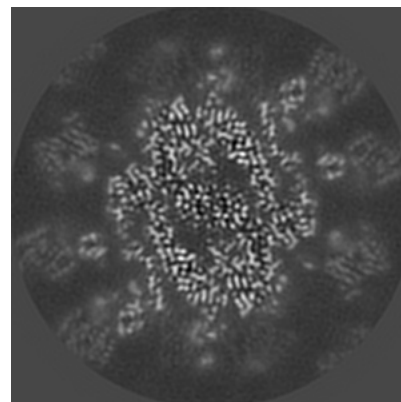
6.2.1 Primary map



X Index: 125

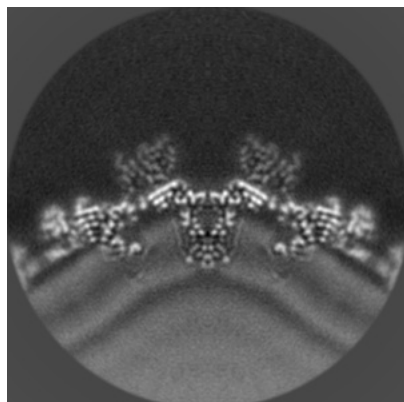


Y Index: 125

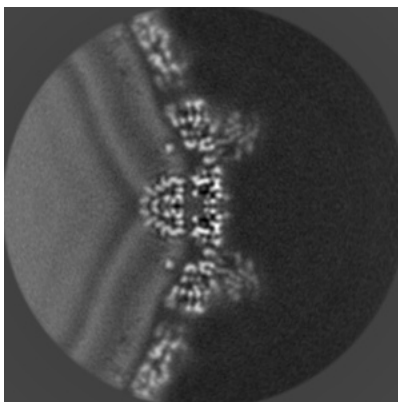


Z Index: 125

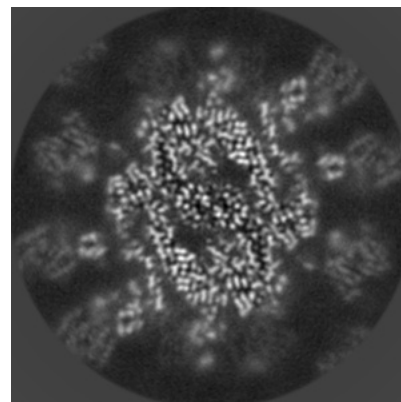
6.2.2 Raw map



X Index: 125



Y Index: 125

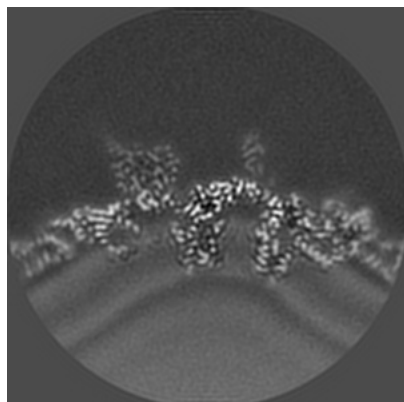


Z Index: 125

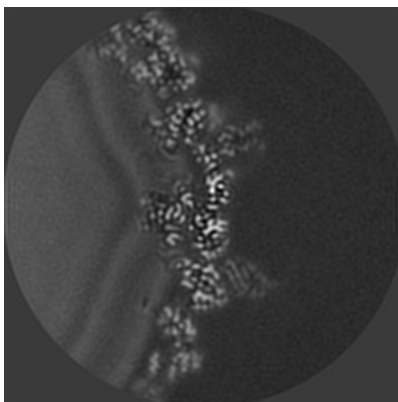
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

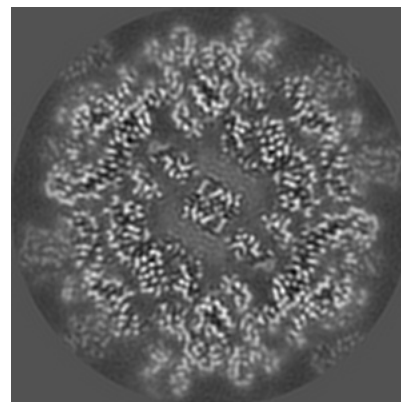
6.3.1 Primary map



X Index: 133

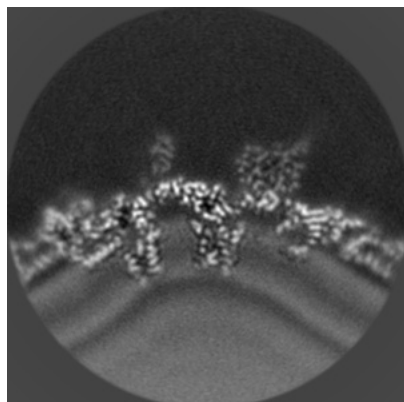


Y Index: 134

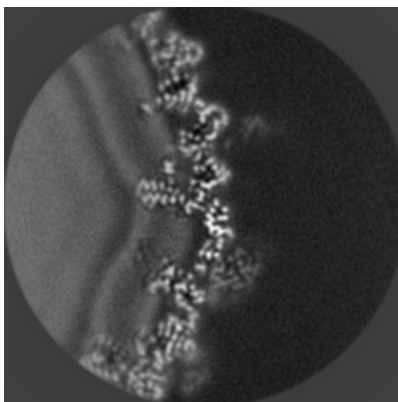


Z Index: 112

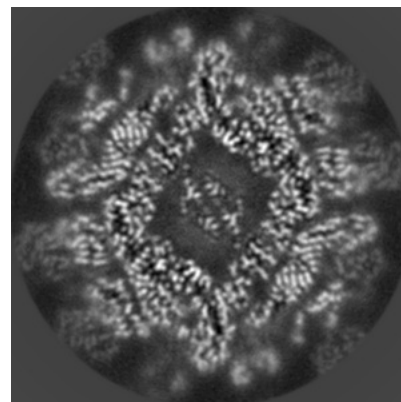
6.3.2 Raw map



X Index: 117



Y Index: 112

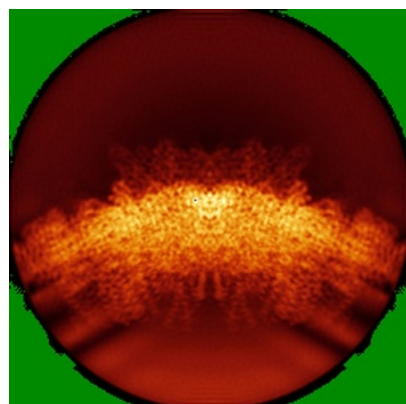


Z Index: 116

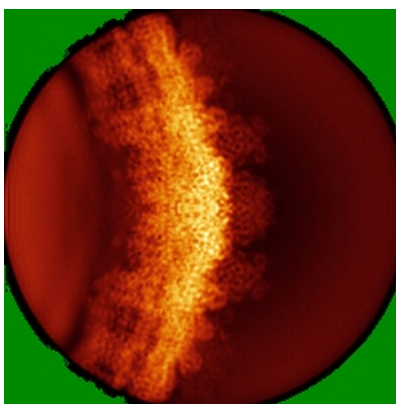
The images above show the largest variance slices of the map in three orthogonal directions.

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

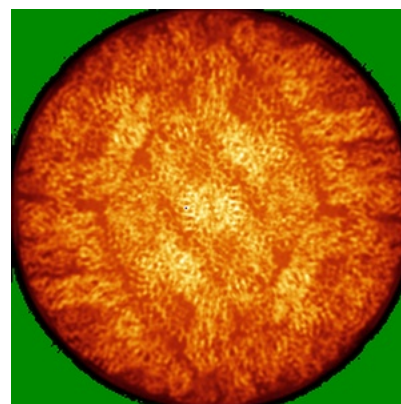
6.4.1 Primary map



X

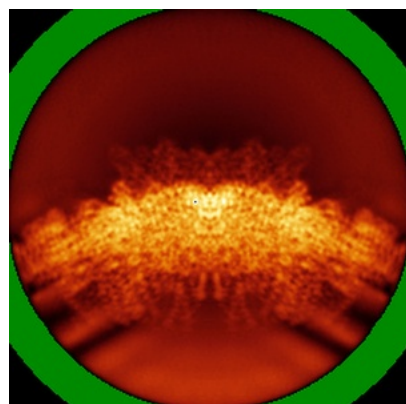


Y

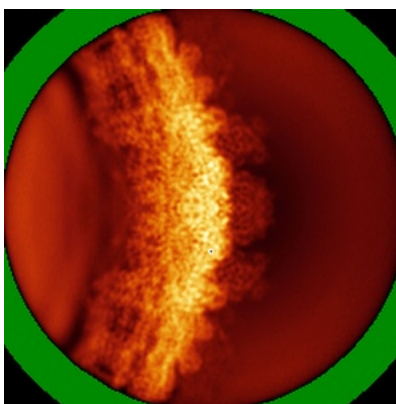


Z

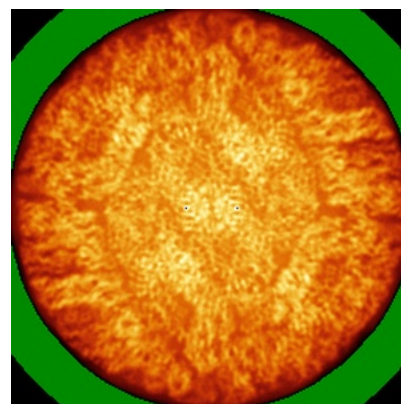
6.4.2 Raw map



X



Y

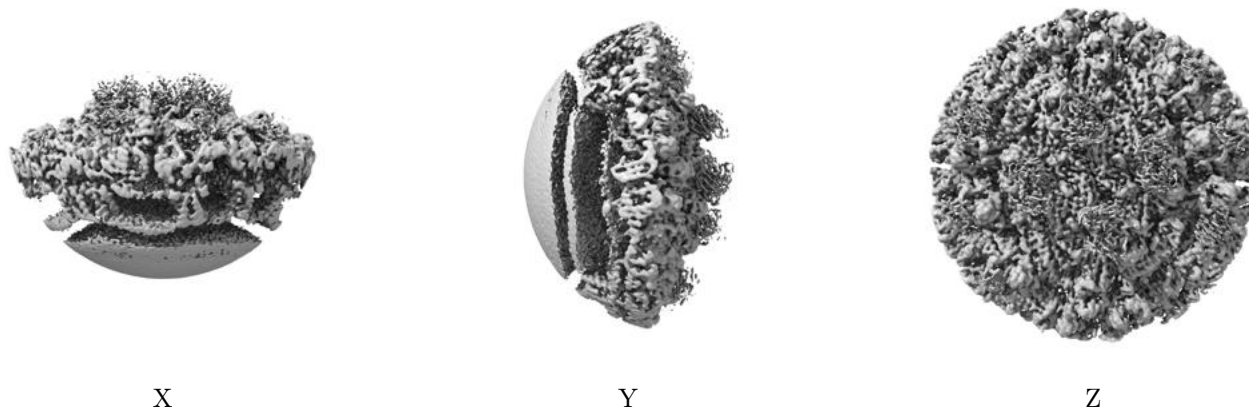


Z

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 1.5. 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.

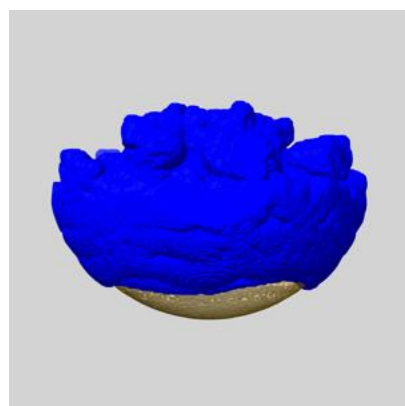
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

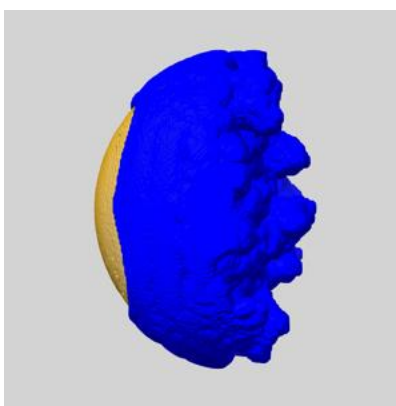
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

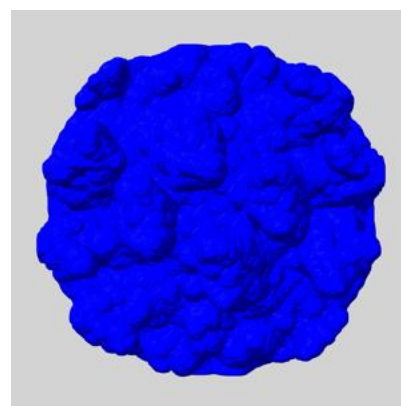
6.6.1 emd_27055_msk_1.map [i](#)



X



Y

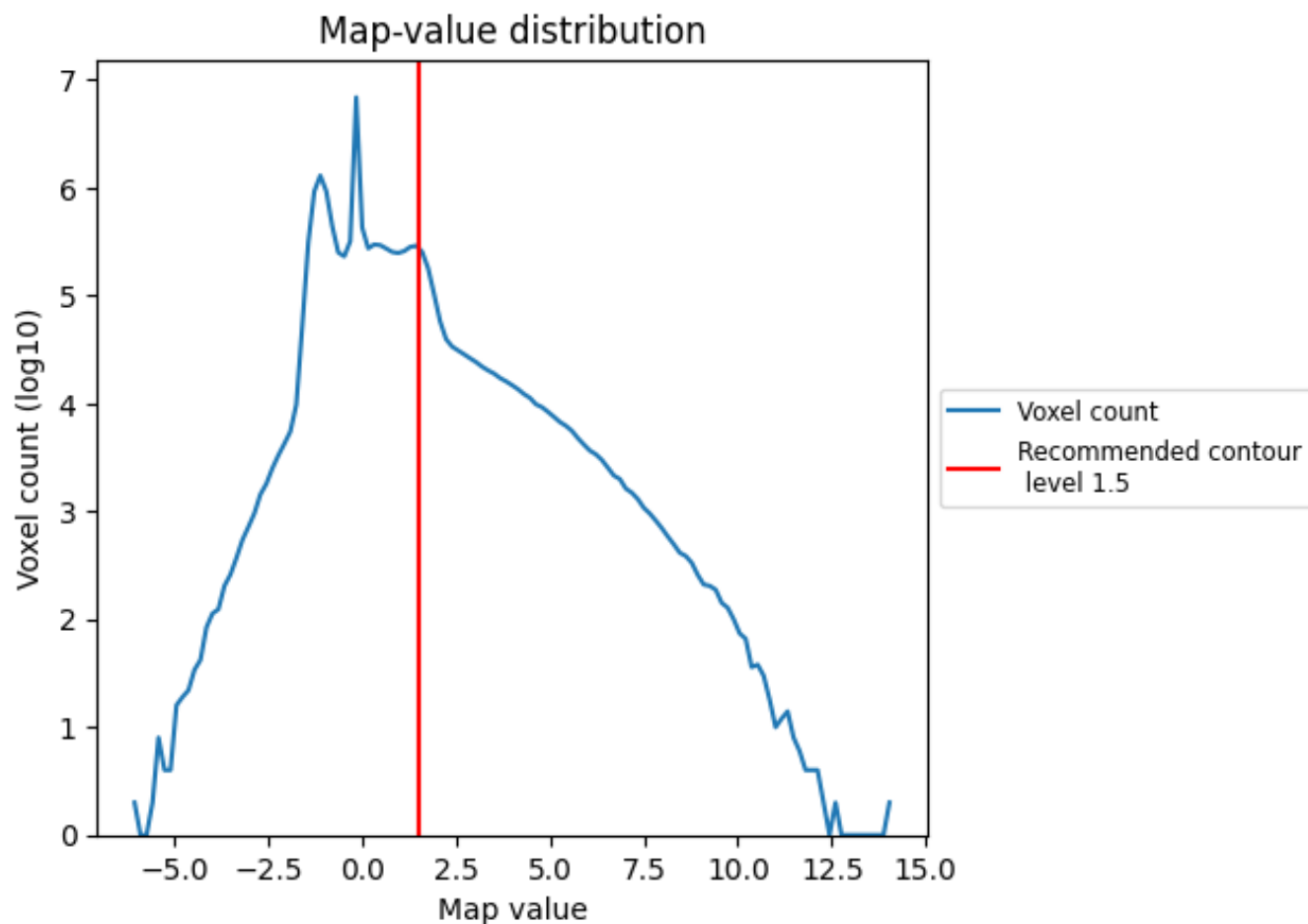


Z

7 Map analysis [i](#)

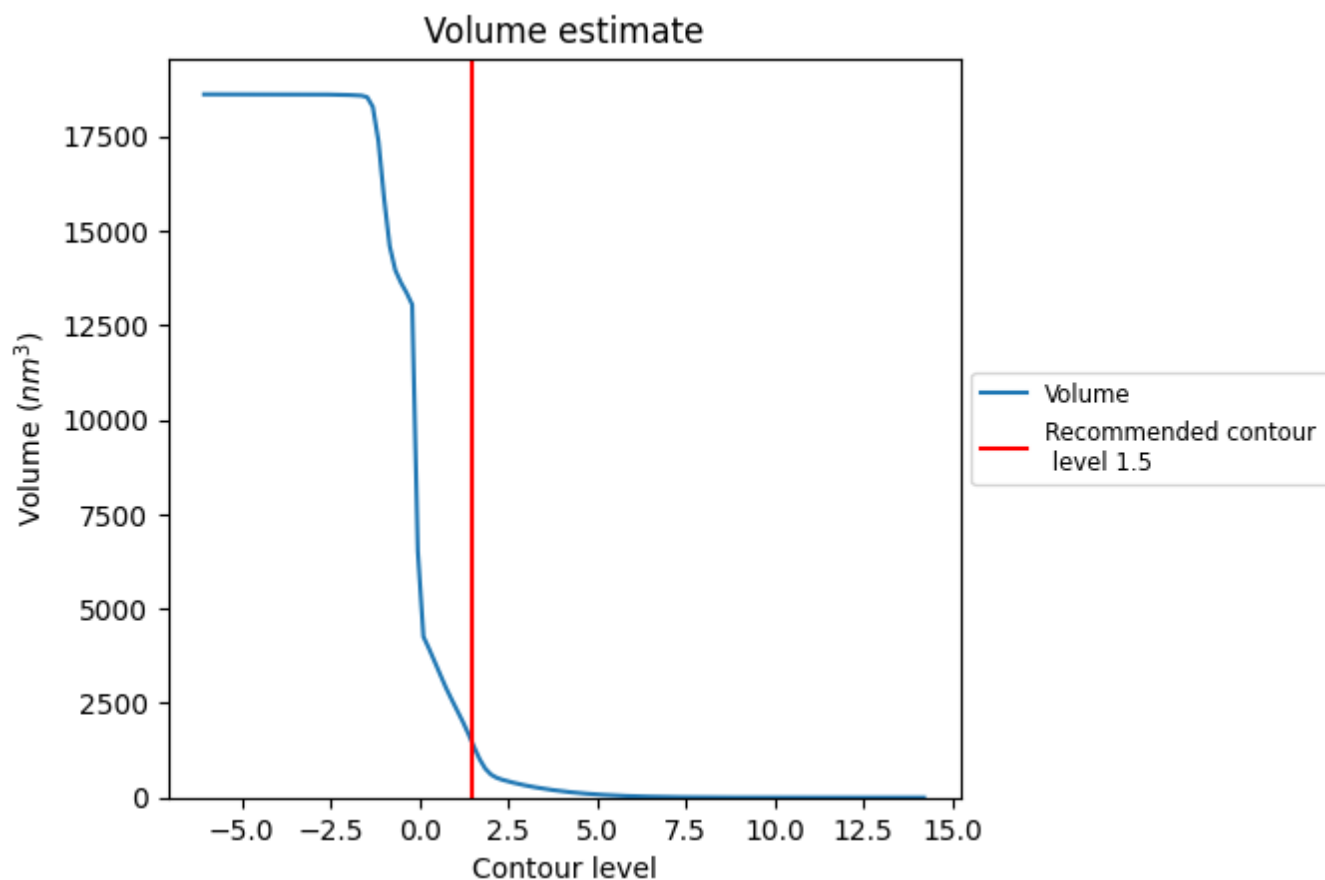
This section contains the results of statistical analysis of the map.

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.

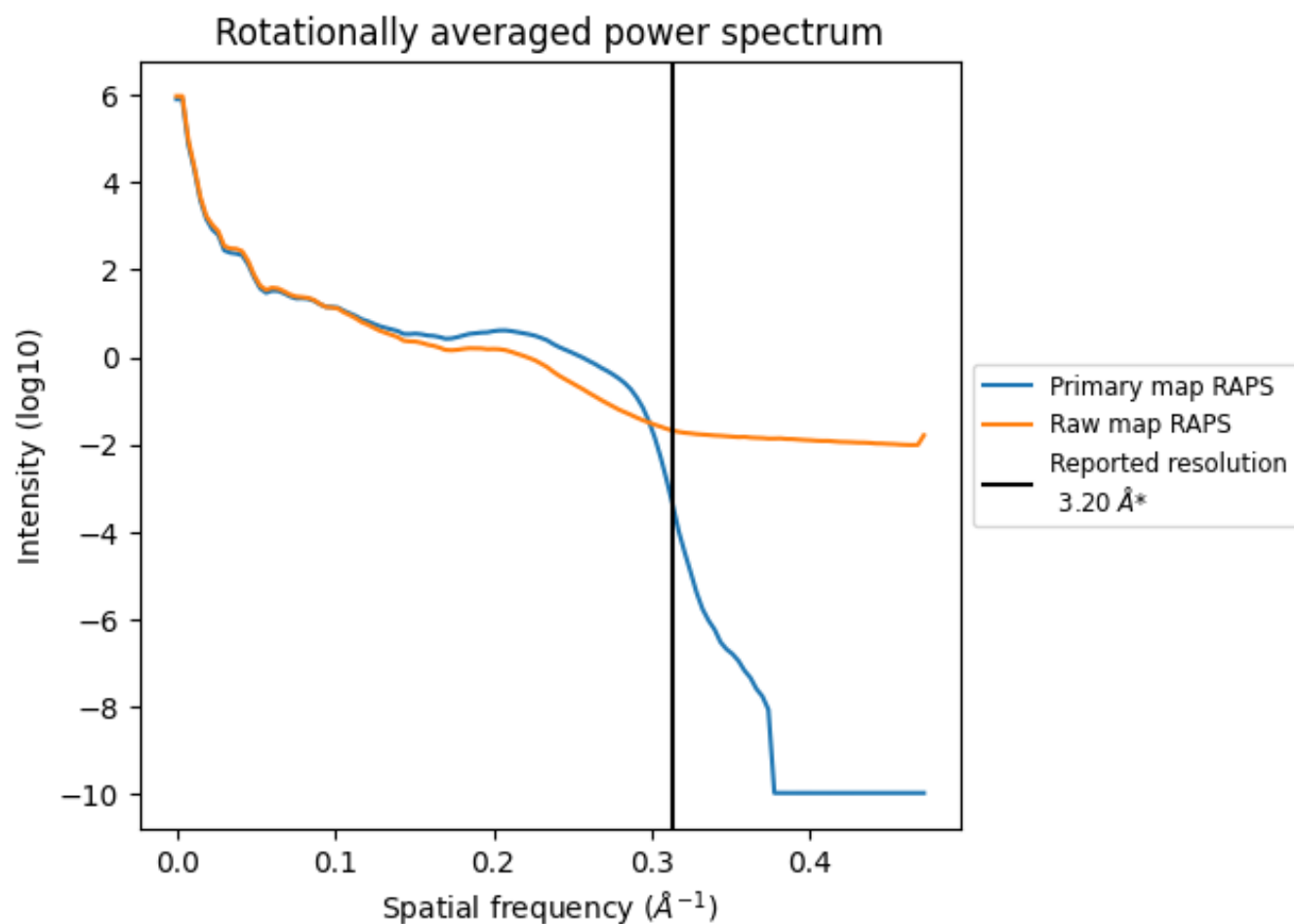
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1420 nm³; this corresponds to an approximate mass of 1283 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 ⓘ

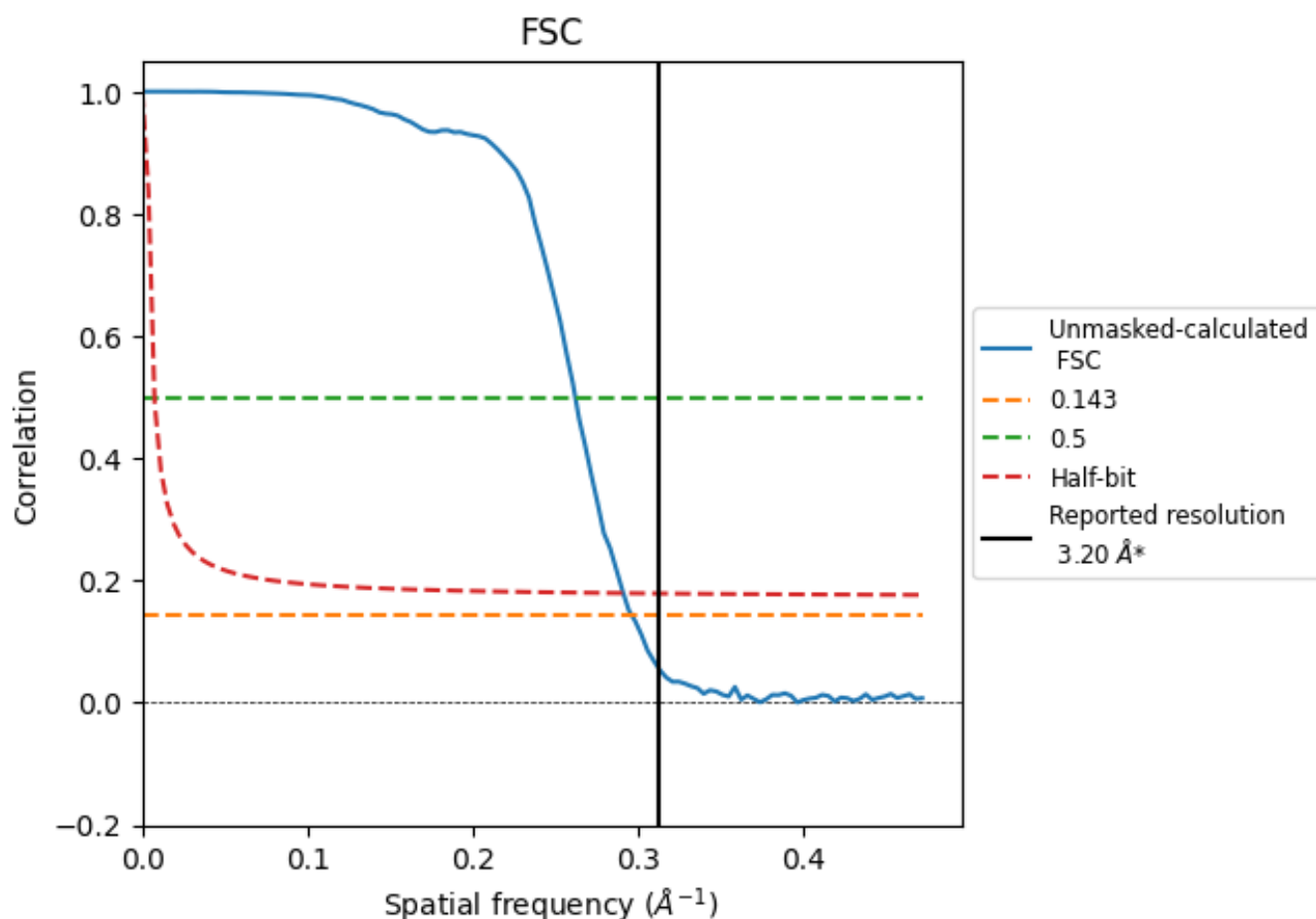


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

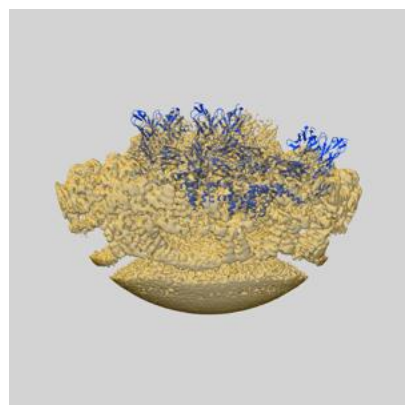
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	3.82	3.44

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

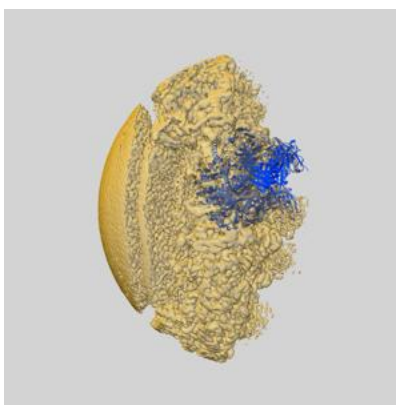
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27055 and PDB model 8CXG. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

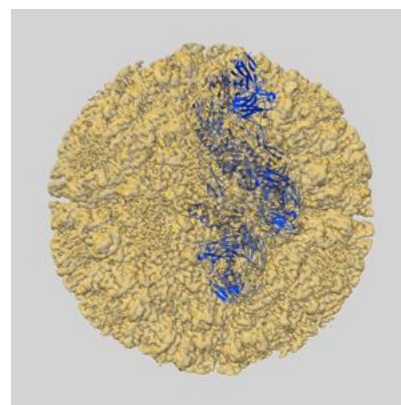
9.1 Map-model overlay [i](#)



X



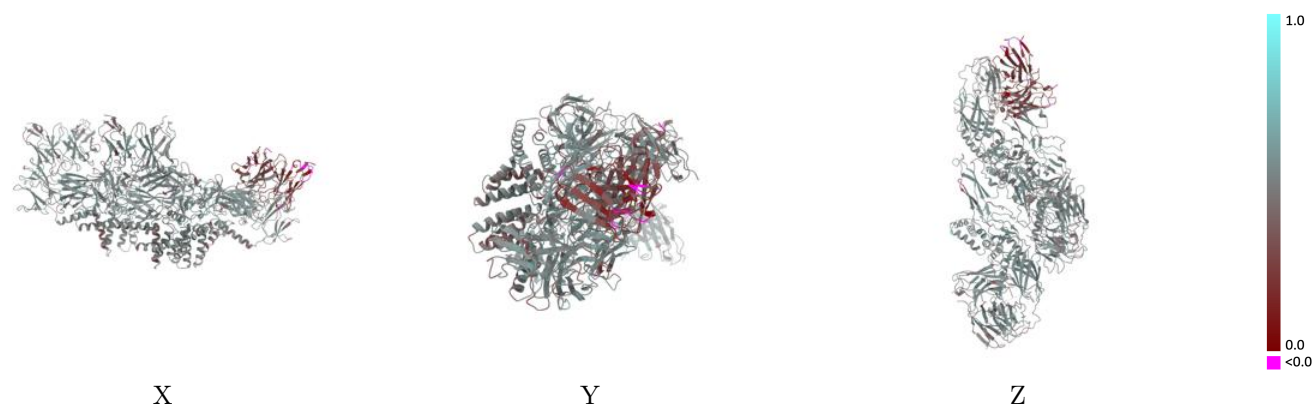
Y



Z

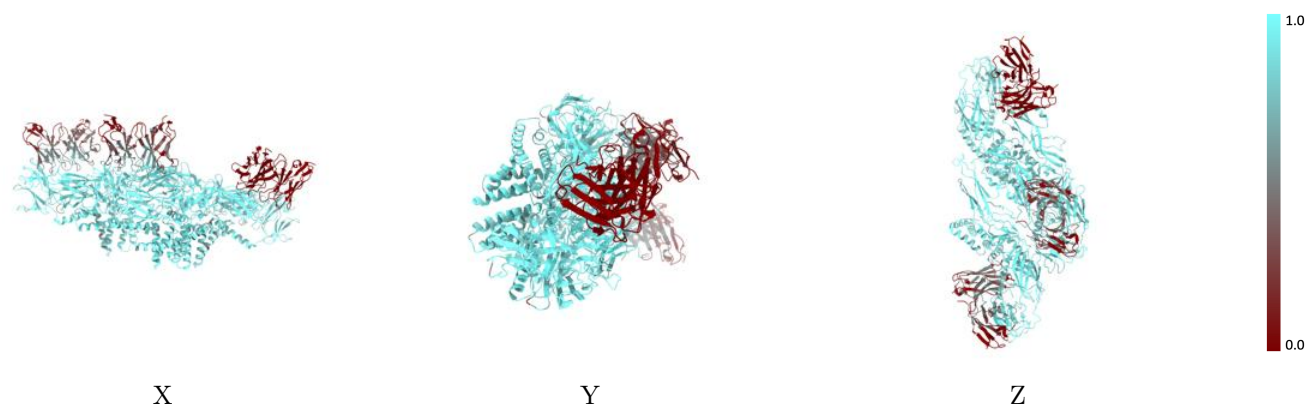
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



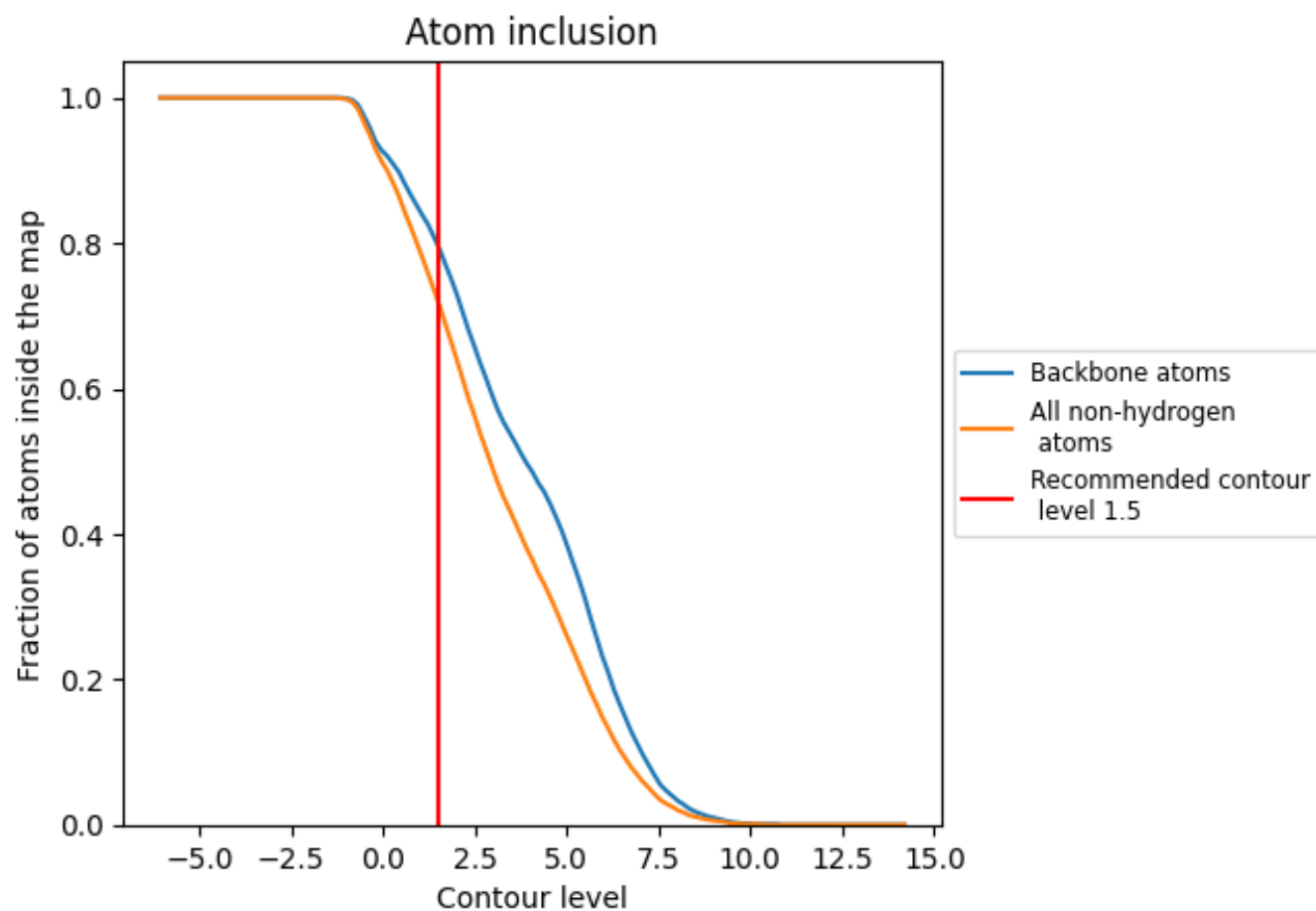
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7190	0.4850
1	0.0030	0.3020
2	0.0000	0.2290
A	0.9140	0.5140
B	0.9080	0.5030
C	0.9090	0.5040
D	0.9210	0.5430
E	0.9180	0.5310
F	0.9110	0.5120
H	0.4120	0.5090
L	0.3250	0.4950
h	0.3920	0.5030
l	0.3390	0.4970

1.0

0.0

<0.0