



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:36 AM UTC

PDB ID : 7YOX / pdb_00007yox
EMDB ID : EMD-33989
Title : Cryo-EM structure of the N-terminal domain of hMCM8/9 and HROB
Authors : Zheng, J.F.; Weng, Z.F.; Liu, Y.F.
Deposited on : 2022-08-02
Resolution : 3.95 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

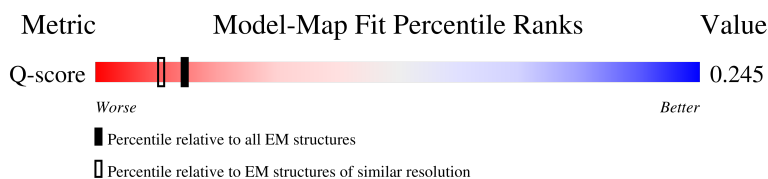
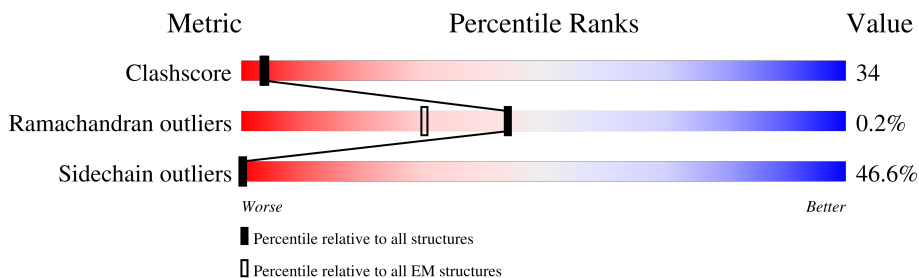
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.95 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	7707 (3.45 - 4.45)

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	316	
1	C	316	
1	F	316	
2	B	276	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	276	35% 45% 20%
2	E	276	34% 51% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13878 atoms, of which 0 are hydrogens and 0 are deuteriums.

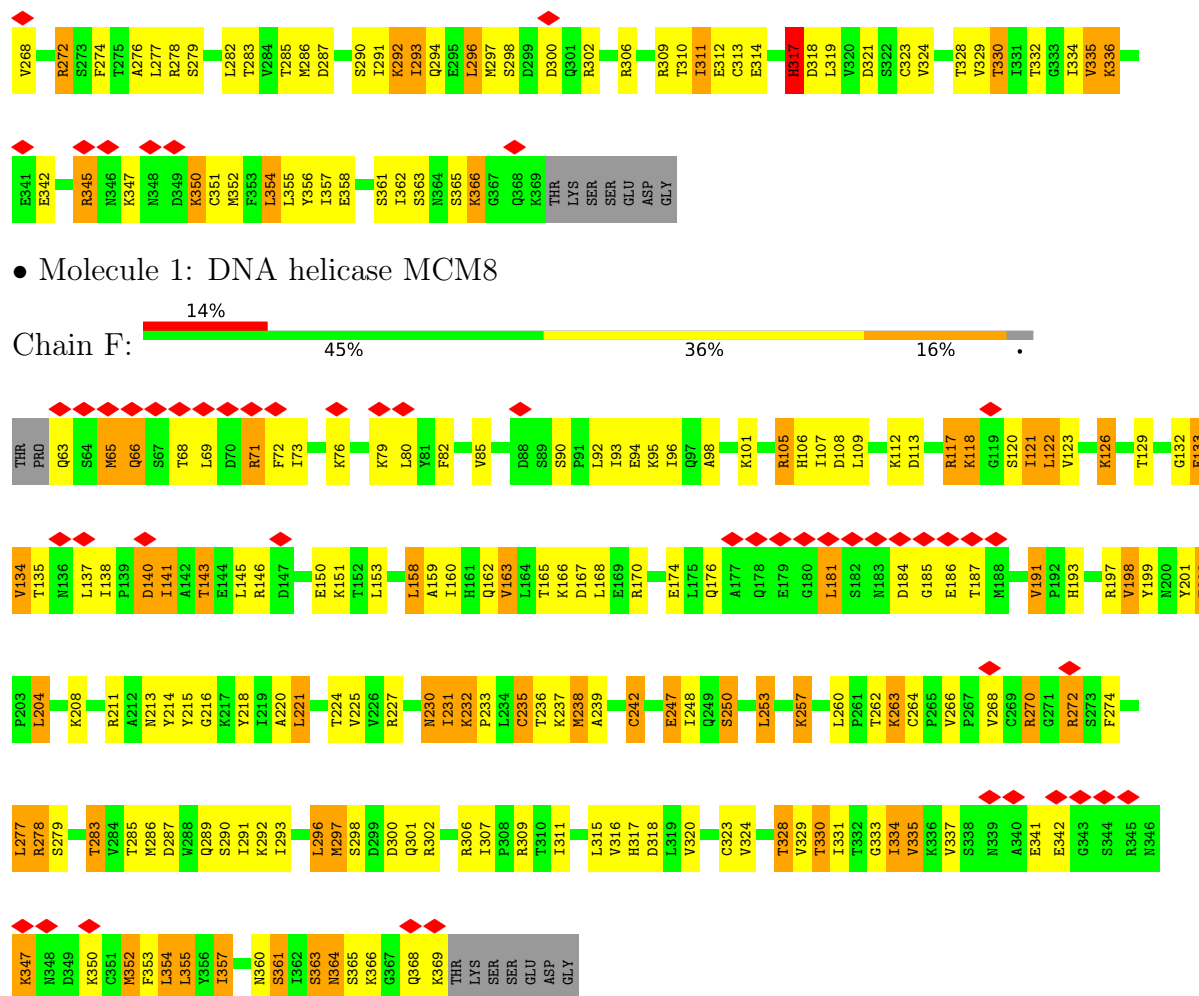
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA helicase MCM8.

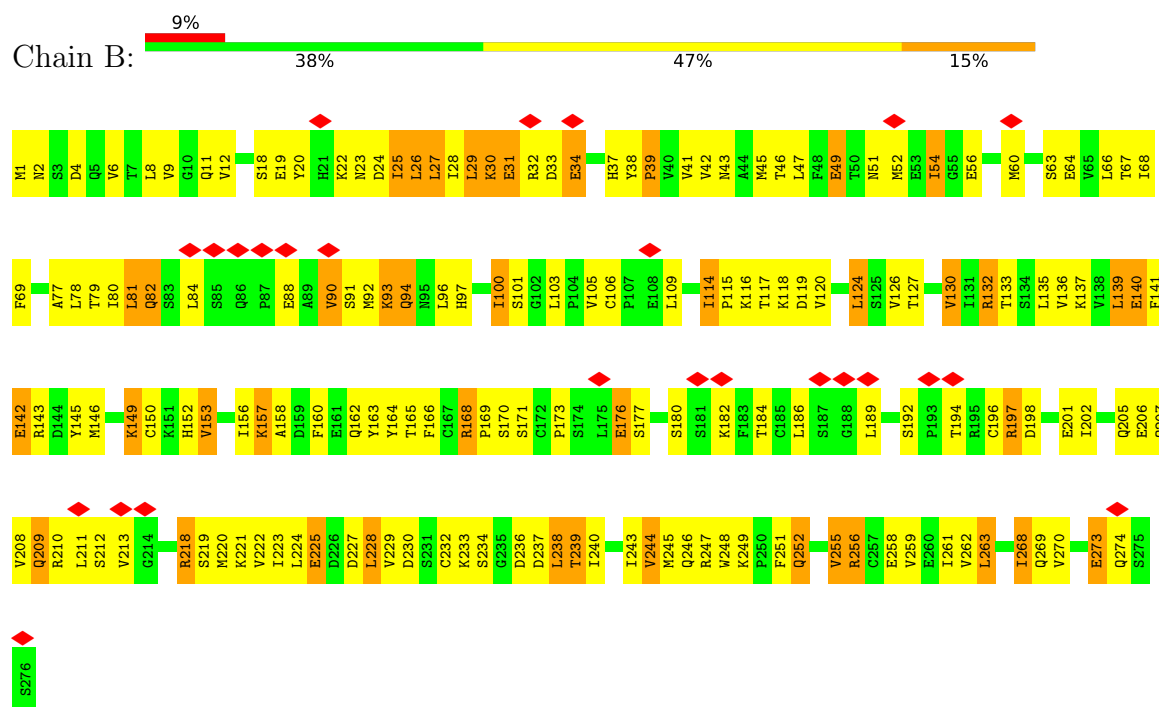
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	307	Total	C	N	O	S	0	0
			2420	1525	414	465	16		
1	C	307	Total	C	N	O	S	0	0
			2420	1525	414	465	16		
1	F	307	Total	C	N	O	S	0	0
			2420	1525	414	465	16		

- Molecule 2 is a protein called DNA helicase MCM9.

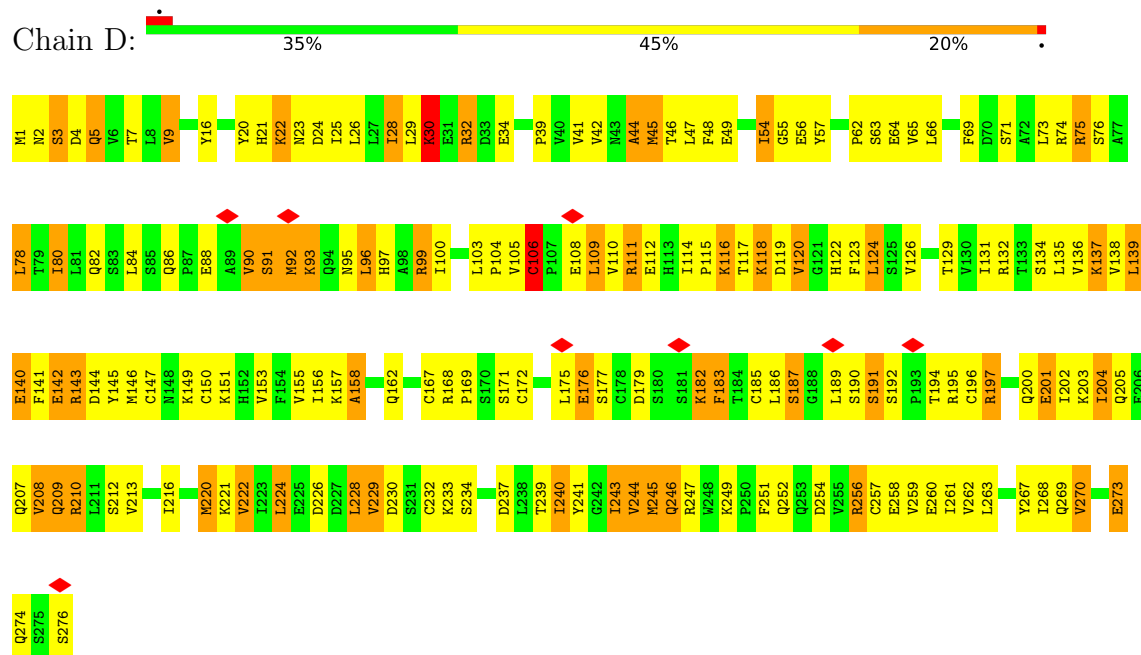
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	276	Total	C	N	O	S	0	0
			2206	1390	371	427	18		
2	D	276	Total	C	N	O	S	0	0
			2206	1390	371	427	18		
2	E	276	Total	C	N	O	S	0	0
			2206	1390	371	427	18		



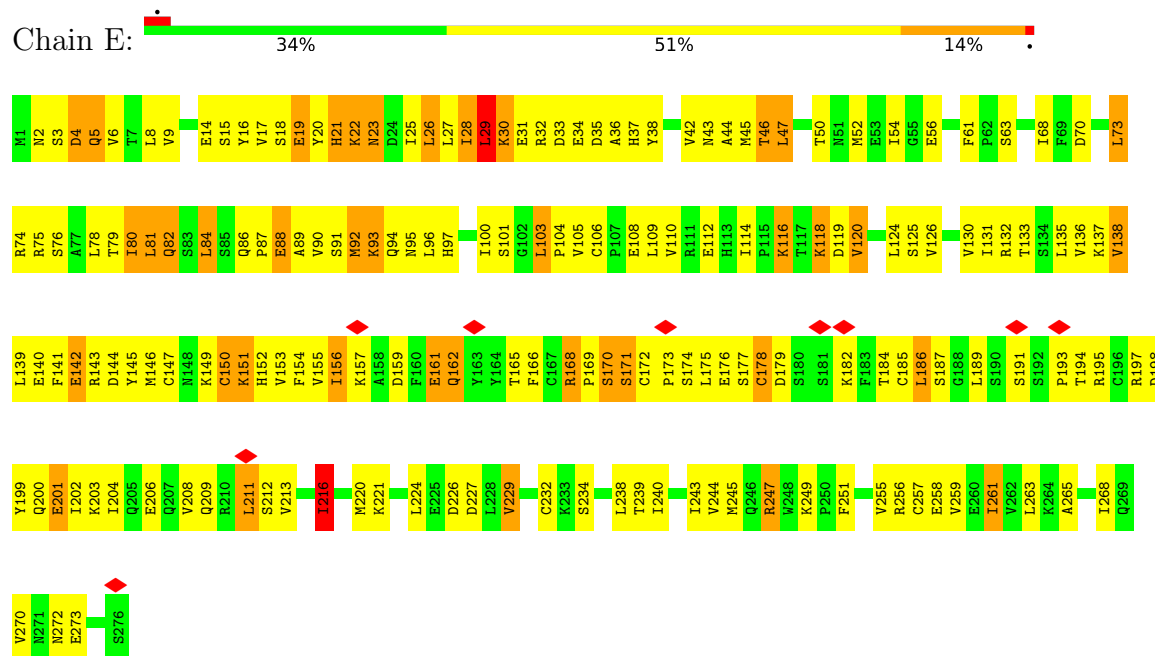
• Molecule 2: DNA helicase MCM9



• Molecule 2: DNA helicase MCM9



• Molecule 2: DNA helicase MCM9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95257	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.361	Depositor
Minimum map value	-0.166	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	211.712, 211.712, 211.712	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.827, 0.827, 0.827	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.49	0/2465	0.93	7/3334 (0.2%)
1	C	0.48	0/2465	0.94	8/3334 (0.2%)
1	F	0.48	0/2465	0.94	5/3334 (0.1%)
2	B	0.47	0/2246	0.94	1/3037 (0.0%)
2	D	0.47	0/2246	0.97	5/3037 (0.2%)
2	E	0.45	0/2246	0.97	6/3037 (0.2%)
All	All	0.47	0/14133	0.95	32/19113 (0.2%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	162	GLN	N-CA-C	-10.10	98.92	112.26
2	D	106	CYS	N-CA-C	-7.52	101.45	108.22
1	C	132	GLY	N-CA-C	6.72	120.80	112.73
2	B	20	TYR	N-CA-C	6.67	118.63	111.36
1	A	93	ILE	N-CA-C	6.41	117.15	110.62
1	F	202	GLU	N-CA-C	6.28	122.07	113.16
2	E	265	ALA	N-CA-C	6.25	118.81	109.25
1	C	251	PHE	CA-C-N	-6.25	113.34	119.90
1	C	251	PHE	C-N-CA	-6.25	113.34	119.90
1	A	202	GLU	CA-C-N	-6.06	113.53	119.90
1	A	202	GLU	C-N-CA	-6.06	113.53	119.90
1	C	317	HIS	CB-CA-C	-6.05	109.61	116.63
2	D	44	ALA	N-CA-C	5.98	117.88	111.36
2	E	216	ILE	N-CA-C	5.86	115.40	108.96
2	D	30	LYS	N-CA-C	5.85	117.66	111.28
1	A	76	LYS	N-CA-C	5.81	117.70	111.36
1	F	132	GLY	N-CA-C	5.55	119.40	112.73
1	F	90	SER	N-CA-C	5.53	116.66	109.64
2	E	255	VAL	N-CA-C	-5.47	100.30	108.46
2	E	29	LEU	N-CA-C	-5.44	105.43	111.36
2	D	158	ALA	N-CA-C	-5.43	102.00	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	TYR	CA-C-N	-5.29	116.24	123.12
1	A	356	TYR	C-N-CA	-5.29	116.24	123.12
2	E	4	ASP	N-CA-C	-5.28	105.52	111.28
1	F	317	HIS	CB-CA-C	-5.20	110.60	116.63
1	F	185	GLY	N-CA-C	-5.16	104.39	111.76
1	C	317	HIS	N-CA-C	5.15	116.78	108.08
2	E	247	ARG	N-CA-C	-5.11	100.57	108.90
1	A	317	HIS	CB-CA-C	-5.09	110.72	116.63
1	C	202	GLU	CA-C-N	-5.09	114.67	119.76
1	C	202	GLU	C-N-CA	-5.09	114.67	119.76
1	C	119	GLY	N-CA-C	-5.03	108.31	115.30

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	2420	0	2425	128	0
1	C	2420	0	2425	150	0
1	F	2420	0	2422	119	0
2	B	2206	0	2195	123	0
2	D	2206	0	2192	150	0
2	E	2206	0	2188	283	0
All	All	13878	0	13847	933	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 34.

All (933) 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:E:29:LEU:HD21	2:E:30:LYS:CE	1.21	1.66
2:E:154:PHE:CD1	2:E:173:PRO:CD	1.86	1.59
1:A:315:LEU:HD11	1:A:319:LEU:CD1	1.35	1.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:TRP:HH2	1:F:235:CYS:SG	1.27	1.56
2:E:29:LEU:CD2	2:E:30:LYS:CE	1.84	1.54
1:A:331:ILE:CD1	1:A:362:ILE:HG23	1.10	1.54
2:E:154:PHE:HB3	2:E:173:PRO:CG	1.40	1.51
2:E:27:LEU:HA	2:E:30:LYS:CG	1.37	1.51
2:D:54:ILE:HD12	2:D:55:GLY:N	1.19	1.50
1:A:331:ILE:HD11	1:A:362:ILE:CG2	1.41	1.47
2:E:30:LYS:NZ	2:E:89:ALA:HB1	1.27	1.45
2:E:133:THR:HG23	2:E:202:ILE:CG2	1.47	1.45
2:E:154:PHE:CB	2:E:173:PRO:HG3	1.47	1.42
1:C:151:LYS:NZ	1:C:152:THR:HG22	1.21	1.41
1:A:315:LEU:HD12	1:A:319:LEU:CB	1.48	1.40
2:E:29:LEU:CD2	2:E:30:LYS:HE2	1.39	1.40
2:E:154:PHE:CD1	2:E:173:PRO:CG	2.05	1.39
1:C:314:GLU:HG3	1:C:356:TYR:CE2	1.58	1.38
1:C:293:ILE:CD1	1:C:311:ILE:O	1.71	1.36
2:E:22:LYS:HA	2:E:25:ILE:CD1	1.57	1.34
1:A:315:LEU:CD1	1:A:319:LEU:HB3	1.58	1.32
2:E:154:PHE:CB	2:E:173:PRO:CG	2.06	1.32
1:A:315:LEU:CD1	1:A:319:LEU:CD1	2.10	1.30
1:C:293:ILE:CD1	1:C:293:ILE:H	1.29	1.29
2:B:248:TRP:CH2	1:F:235:CYS:SG	2.09	1.28
2:E:154:PHE:CG	2:E:173:PRO:CG	2.15	1.28
2:D:129:THR:HG22	2:D:237:ASP:OD1	1.13	1.28
1:F:66:GLN:OE1	1:F:72:PHE:CB	1.81	1.27
2:E:29:LEU:CG	2:E:30:LYS:HE2	1.65	1.26
2:E:82:GLN:OE1	2:E:82:GLN:N	1.67	1.26
2:E:154:PHE:CG	2:E:173:PRO:HG3	1.69	1.26
1:F:66:GLN:OE1	1:F:72:PHE:HB3	1.10	1.26
1:F:199:TYR:HB3	1:F:361:SER:OG	1.35	1.26
2:E:18:SER:C	2:E:22:LYS:HZ2	1.45	1.25
2:E:118:LYS:CD	2:E:118:LYS:C	2.07	1.25
2:B:9:VAL:CG1	2:B:54:ILE:HD11	1.66	1.25
2:B:46:THR:O	2:B:49:GLU:HG3	1.37	1.25
1:F:198:VAL:HG23	1:F:360:ASN:OD1	1.09	1.25
1:C:104:THR:O	1:C:107:ILE:CG1	1.86	1.22
2:E:22:LYS:HA	2:E:25:ILE:CG1	1.69	1.22
2:E:81:LEU:O	2:E:84:LEU:HD21	1.36	1.22
2:D:129:THR:CG2	2:D:207:GLN:HG3	1.70	1.21
2:E:154:PHE:CD1	2:E:173:PRO:HD3	1.55	1.21
1:A:98:ALA:HB2	1:A:137:LEU:CD2	1.70	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:CD1	1:A:319:LEU:HD12	1.67	1.19
2:B:77:ALA:O	2:B:81:LEU:HD23	1.40	1.19
1:C:161:HIS:O	1:C:165:THR:HG22	1.43	1.18
2:E:118:LYS:O	2:E:118:LYS:HD3	1.41	1.18
1:C:104:THR:O	1:C:107:ILE:HG13	1.41	1.17
2:E:154:PHE:CE1	2:E:173:PRO:HD3	1.77	1.17
2:E:84:LEU:CB	2:E:90:VAL:HG11	1.75	1.17
1:C:293:ILE:HD11	1:C:311:ILE:O	1.35	1.16
2:D:144:ASP:HB3	2:D:187:SER:HB3	1.20	1.16
1:A:352:MET:SD	2:B:139:LEU:HD21	1.86	1.16
1:A:331:ILE:CD1	1:A:362:ILE:CG2	2.06	1.15
1:C:161:HIS:O	1:C:165:THR:CG2	1.95	1.15
2:E:30:LYS:HZ1	2:E:89:ALA:CB	1.60	1.15
2:E:43:ASN:HB3	2:E:46:THR:OG1	1.43	1.15
2:D:129:THR:CG2	2:D:237:ASP:OD1	1.94	1.15
1:C:109:LEU:H	1:C:109:LEU:HD23	1.05	1.15
1:F:198:VAL:CG2	1:F:360:ASN:OD1	1.93	1.14
1:A:98:ALA:CB	1:A:137:LEU:HD23	1.77	1.14
2:E:29:LEU:CG	2:E:30:LYS:CE	2.22	1.13
2:E:29:LEU:HD23	2:E:30:LYS:H	0.99	1.13
2:D:29:LEU:HD23	2:D:93:LYS:HG2	1.31	1.13
2:B:238:LEU:N	2:B:238:LEU:HD13	1.61	1.12
2:E:211:LEU:HD13	2:E:211:LEU:N	1.64	1.12
2:B:153:VAL:HG11	2:B:173:PRO:HB2	1.30	1.12
1:C:151:LYS:NZ	1:C:152:THR:CG2	2.13	1.12
1:C:293:ILE:HD12	1:C:293:ILE:N	1.61	1.12
2:E:22:LYS:HA	2:E:25:ILE:HD11	1.28	1.11
2:E:29:LEU:CD2	2:E:30:LYS:HE3	1.63	1.11
2:E:97:HIS:CE1	2:E:197:ARG:HH22	1.69	1.11
1:A:149:PRO:HB2	1:A:334:ILE:HG21	1.24	1.10
2:E:36:ALA:O	2:E:93:LYS:HD2	1.47	1.10
2:E:118:LYS:C	2:E:118:LYS:HD2	1.72	1.10
1:F:238:MET:HE1	1:F:278:ARG:HA	1.26	1.10
1:C:293:ILE:CD1	1:C:293:ILE:N	1.94	1.10
2:E:18:SER:C	2:E:22:LYS:NZ	2.07	1.10
2:E:133:THR:HG23	2:E:202:ILE:HG21	1.29	1.10
2:D:54:ILE:CD1	2:D:55:GLY:N	2.14	1.09
1:C:336:LYS:HB2	1:C:336:LYS:NZ	1.44	1.09
2:E:133:THR:HG23	2:E:202:ILE:HG22	1.14	1.09
2:E:80:ILE:HD13	2:E:80:ILE:H	1.03	1.09
2:E:27:LEU:HA	2:E:30:LYS:HG2	1.25	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:LEU:CA	2:E:30:LYS:HG3	1.81	1.08
1:F:302:ARG:NH2	1:F:306:ARG:O	1.84	1.08
2:E:76:SER:O	2:E:80:ILE:CD1	2.01	1.08
2:E:80:ILE:HD13	2:E:80:ILE:N	1.64	1.08
2:E:211:LEU:H	2:E:211:LEU:CD1	1.65	1.08
2:E:76:SER:O	2:E:80:ILE:HD13	1.51	1.08
1:C:293:ILE:HD13	1:C:311:ILE:O	1.52	1.08
2:D:28:ILE:HD13	2:D:29:LEU:N	1.67	1.08
2:E:27:LEU:CA	2:E:30:LYS:CG	2.32	1.07
2:D:54:ILE:HD12	2:D:54:ILE:C	1.77	1.07
2:E:154:PHE:CD1	2:E:173:PRO:HG2	1.89	1.07
2:B:31:GLU:O	2:B:93:LYS:NZ	1.85	1.07
2:E:82:GLN:H	2:E:82:GLN:CD	1.54	1.07
1:C:70:ASP:HA	1:C:76:LYS:HZ3	1.19	1.07
2:D:144:ASP:HB3	2:D:187:SER:CB	1.84	1.06
2:E:22:LYS:CA	2:E:25:ILE:HG12	1.84	1.06
1:A:149:PRO:HB2	1:A:334:ILE:CG2	1.83	1.06
2:E:29:LEU:HD23	2:E:30:LYS:N	1.69	1.06
2:E:30:LYS:NZ	2:E:89:ALA:CB	2.16	1.06
2:E:23:ASN:HA	2:E:26:LEU:CD1	1.86	1.06
2:E:79:THR:O	2:E:82:GLN:CG	2.04	1.06
2:E:118:LYS:CD	2:E:118:LYS:O	2.03	1.05
2:D:140:GLU:HA	2:D:196:CYS:HA	1.37	1.05
2:E:20:TYR:O	2:E:23:ASN:ND2	1.90	1.05
1:A:331:ILE:HD13	1:A:362:ILE:HG23	1.37	1.05
2:E:21:HIS:O	2:E:25:ILE:HG12	1.55	1.05
2:E:84:LEU:HB3	2:E:90:VAL:HG11	1.36	1.05
2:E:79:THR:O	2:E:82:GLN:HG2	1.54	1.04
2:D:202:ILE:HG12	2:D:224:LEU:HD11	1.38	1.04
1:F:218:TYR:CE2	1:F:333:GLY:HA2	1.93	1.04
2:D:5:GLN:OE1	2:D:5:GLN:HA	1.55	1.04
2:D:3:SER:O	2:D:7:THR:HG23	1.59	1.03
2:E:29:LEU:HG	2:E:30:LYS:HE2	1.38	1.03
2:E:23:ASN:CA	2:E:26:LEU:CD1	2.38	1.02
1:A:71:ARG:HH12	1:A:169:GLU:HG2	1.21	1.02
2:E:84:LEU:HD13	2:E:90:VAL:HG21	1.39	1.02
1:A:315:LEU:HD11	1:A:319:LEU:HD13	1.06	1.02
2:E:211:LEU:HD13	2:E:211:LEU:H	0.88	1.02
2:B:9:VAL:HG13	2:B:54:ILE:HD11	1.37	1.01
2:B:238:LEU:N	2:B:238:LEU:CD1	2.23	1.00
1:C:293:ILE:H	1:C:293:ILE:HD13	0.89	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:LEU:HD22	2:B:29:LEU:HD23	1.42	1.00
2:D:202:ILE:O	2:D:222:VAL:HG23	1.62	1.00
2:E:154:PHE:HB3	2:E:173:PRO:HG2	1.34	1.00
2:E:154:PHE:CB	2:E:173:PRO:HG2	1.89	1.00
2:B:232:CYS:SG	2:B:238:LEU:HD21	2.02	1.00
1:C:151:LYS:HZ1	1:C:152:THR:HG22	1.19	1.00
1:C:222:ARG:HG3	1:C:222:ARG:NH1	1.61	1.00
2:B:228:LEU:HB3	2:B:268:ILE:HG13	1.43	0.99
1:C:222:ARG:HH11	1:C:222:ARG:CG	1.73	0.99
2:E:133:THR:CG2	2:E:202:ILE:HG22	1.91	0.99
2:E:211:LEU:N	2:E:211:LEU:CD1	2.21	0.99
1:A:315:LEU:HD11	1:A:319:LEU:HD12	1.21	0.99
2:E:22:LYS:HA	2:E:25:ILE:HG12	1.40	0.99
2:B:236:ASP:O	2:B:238:LEU:HD11	1.63	0.99
1:C:109:LEU:HD23	1:C:109:LEU:N	1.71	0.98
2:D:129:THR:HG23	2:D:207:GLN:HG3	1.00	0.98
1:A:322:SER:HB3	1:A:362:ILE:HD12	1.44	0.98
2:E:84:LEU:CB	2:E:90:VAL:CG1	2.42	0.98
2:E:79:THR:O	2:E:82:GLN:CD	1.93	0.98
2:E:84:LEU:HB3	2:E:90:VAL:CG1	1.93	0.98
2:E:21:HIS:O	2:E:25:ILE:N	1.94	0.97
2:E:133:THR:CG2	2:E:202:ILE:CG2	2.42	0.97
2:E:81:LEU:O	2:E:84:LEU:CD2	2.11	0.97
2:B:224:LEU:HD22	2:B:268:ILE:HD11	1.46	0.97
2:E:80:ILE:CD1	2:E:80:ILE:N	2.22	0.97
1:C:222:ARG:HG3	1:C:222:ARG:HH11	0.81	0.97
2:E:23:ASN:CA	2:E:26:LEU:HD11	1.90	0.97
2:B:9:VAL:HG13	2:B:54:ILE:CD1	1.94	0.96
1:A:149:PRO:CB	1:A:334:ILE:CG2	2.44	0.96
2:E:27:LEU:HA	2:E:30:LYS:HG3	0.98	0.96
2:D:147:CYS:CB	2:D:150:CYS:SG	2.54	0.96
1:F:334:ILE:HD12	1:F:335:VAL:N	1.79	0.96
1:C:70:ASP:HA	1:C:76:LYS:NZ	1.81	0.96
2:D:115:PRO:HD2	2:D:220:MET:HE1	1.46	0.96
2:B:236:ASP:O	2:B:238:LEU:CD1	2.13	0.96
1:C:314:GLU:CG	1:C:356:TYR:CE2	2.49	0.95
2:D:129:THR:HG23	2:D:207:GLN:CG	1.95	0.95
1:C:151:LYS:HZ3	1:C:152:THR:CG2	1.73	0.95
2:D:115:PRO:HD2	2:D:220:MET:CE	1.96	0.95
2:E:27:LEU:HD23	2:E:30:LYS:HG3	1.47	0.95
2:E:84:LEU:HD13	2:E:90:VAL:CG2	1.96	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:ILE:CD1	2:D:54:ILE:C	2.38	0.95
1:C:64:SER:O	1:C:65:MET:HB2	1.66	0.94
2:E:154:PHE:CD1	2:E:173:PRO:HD2	2.01	0.94
2:B:116:LYS:HE2	1:F:231:ILE:HD13	1.49	0.94
1:F:66:GLN:CD	1:F:72:PHE:HB3	1.92	0.94
2:E:18:SER:O	2:E:22:LYS:NZ	1.98	0.94
2:E:23:ASN:HA	2:E:26:LEU:HD11	1.43	0.94
2:E:23:ASN:HD22	2:E:23:ASN:H	1.06	0.94
2:E:118:LYS:C	2:E:118:LYS:HD3	1.80	0.94
1:C:109:LEU:N	1:C:109:LEU:CD2	2.31	0.93
1:A:322:SER:CB	1:A:362:ILE:HD12	1.97	0.93
2:B:12:VAL:HG11	2:B:51:ASN:HB2	1.50	0.93
1:F:302:ARG:HH21	1:F:306:ARG:C	1.76	0.93
2:B:218:ARG:NH1	1:F:230:ASN:HA	1.83	0.93
2:E:29:LEU:HD21	2:E:30:LYS:CD	1.99	0.92
2:D:129:THR:HG22	2:D:237:ASP:CG	1.92	0.92
2:E:154:PHE:HD1	2:E:173:PRO:CD	1.70	0.92
1:C:313:CYS:SG	1:C:357:ILE:HG23	2.09	0.92
2:D:141:PHE:O	2:D:157:LYS:HG3	1.70	0.92
1:C:141:ILE:O	1:C:144:GLU:HG2	1.70	0.91
1:C:293:ILE:N	1:C:293:ILE:HD13	1.71	0.91
2:E:80:ILE:H	2:E:80:ILE:CD1	1.82	0.91
2:B:9:VAL:HG11	2:B:54:ILE:HD11	1.50	0.91
1:C:148:ALA:HB1	1:C:151:LYS:CG	1.99	0.91
1:C:109:LEU:H	1:C:109:LEU:CD2	1.83	0.91
2:E:29:LEU:HD23	2:E:30:LYS:HE2	1.49	0.91
1:A:149:PRO:CB	1:A:334:ILE:HG21	1.99	0.91
2:D:71:SER:O	2:D:75:ARG:HG3	1.69	0.90
2:E:22:LYS:CA	2:E:25:ILE:CG1	2.46	0.90
1:A:80:LEU:HD11	1:A:237:LYS:HE3	1.53	0.90
1:C:73:ILE:O	1:C:76:LYS:NZ	2.05	0.90
1:C:111:ASP:O	1:C:115:ILE:HG13	1.72	0.90
1:C:148:ALA:HB3	1:C:151:LYS:HD3	1.54	0.89
1:F:159:ALA:O	1:F:163:VAL:HG23	1.71	0.89
1:C:336:LYS:HB2	1:C:336:LYS:HZ2	1.11	0.89
2:B:9:VAL:CG1	2:B:54:ILE:CD1	2.50	0.89
2:B:142:GLU:OE2	2:B:157:LYS:NZ	2.06	0.89
2:D:54:ILE:HD12	2:D:55:GLY:H	1.31	0.89
1:F:199:TYR:CB	1:F:361:SER:OG	2.19	0.89
2:B:43:ASN:HD21	2:B:45:MET:HG3	1.38	0.89
1:C:148:ALA:O	1:C:152:THR:HG23	1.73	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:LEU:CD2	2:B:268:ILE:HD11	2.03	0.88
1:C:151:LYS:HZ1	1:C:152:THR:CG2	1.82	0.88
2:E:29:LEU:HD23	2:E:30:LYS:HG2	1.52	0.88
2:E:30:LYS:HE2	2:E:89:ALA:O	1.73	0.88
2:B:9:VAL:HG13	2:B:54:ILE:CG1	2.04	0.88
1:A:98:ALA:HB2	1:A:137:LEU:HD23	0.88	0.88
2:D:147:CYS:HB2	2:D:150:CYS:SG	2.14	0.88
2:E:81:LEU:N	2:E:82:GLN:OE1	2.06	0.88
2:D:139:LEU:O	2:D:197:ARG:N	2.06	0.87
2:B:79:THR:O	2:B:82:GLN:HG2	1.73	0.87
2:B:143:ARG:HD2	2:B:166:PHE:CG	2.10	0.87
2:E:44:ALA:HA	2:E:47:LEU:HD23	1.57	0.87
1:C:336:LYS:NZ	1:C:336:LYS:CB	2.37	0.87
2:D:202:ILE:CG1	2:D:224:LEU:HD11	2.04	0.87
1:C:314:GLU:HG3	1:C:356:TYR:HE2	1.00	0.86
1:C:336:LYS:HZ2	1:C:336:LYS:CB	1.88	0.86
2:E:29:LEU:HG	2:E:30:LYS:CE	1.98	0.86
1:F:198:VAL:O	1:F:361:SER:HB3	1.75	0.86
2:B:26:LEU:HD22	2:B:29:LEU:CD2	2.04	0.86
2:B:238:LEU:HD13	2:B:238:LEU:H	1.39	0.86
2:B:223:ILE:HG22	2:B:225:GLU:OE2	1.76	0.86
1:C:148:ALA:HB1	1:C:151:LYS:HG2	1.55	0.85
2:E:84:LEU:CG	2:E:90:VAL:HG11	2.06	0.85
2:E:17:VAL:O	2:E:21:HIS:ND1	1.79	0.85
2:E:27:LEU:HD23	2:E:30:LYS:CG	2.06	0.85
2:D:54:ILE:HD12	2:D:55:GLY:CA	2.07	0.85
2:E:23:ASN:C	2:E:26:LEU:CD1	2.49	0.85
1:F:238:MET:HE1	1:F:278:ARG:CA	2.07	0.85
2:E:118:LYS:HD2	2:E:119:ASP:N	1.93	0.84
1:A:331:ILE:HD12	1:A:362:ILE:HG23	1.55	0.84
2:B:43:ASN:HD21	2:B:45:MET:CG	1.89	0.84
2:E:26:LEU:HD12	2:E:26:LEU:H	1.40	0.84
2:E:154:PHE:CE1	2:E:173:PRO:CD	2.45	0.84
1:C:108:ASP:OD1	1:C:108:ASP:N	2.06	0.83
2:E:29:LEU:HD21	2:E:30:LYS:HE3	0.84	0.83
1:C:104:THR:O	1:C:107:ILE:HG12	1.77	0.83
2:E:19:GLU:HA	2:E:22:LYS:HZ3	1.43	0.83
2:E:110:VAL:HG22	2:E:125:SER:HB3	1.60	0.83
1:F:238:MET:CE	1:F:278:ARG:HA	2.06	0.83
2:E:97:HIS:CE1	2:E:197:ARG:NH2	2.47	0.82
1:A:347:LYS:HD3	1:A:347:LYS:C	2.05	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:309:ARG:H	1:F:309:ARG:HD2	1.44	0.82
1:C:112:LYS:HA	1:C:164:LEU:HD21	1.60	0.81
2:E:22:LYS:CA	2:E:25:ILE:HD11	2.09	0.81
1:A:342:GLU:OE2	1:A:351:CYS:HA	1.79	0.81
1:C:161:HIS:HD2	1:C:191:VAL:HG23	1.46	0.81
1:F:198:VAL:C	1:F:361:SER:HB3	2.05	0.81
2:B:46:THR:O	2:B:49:GLU:CG	2.26	0.81
2:E:25:ILE:HB	2:E:80:ILE:HG21	1.61	0.81
2:E:27:LEU:CA	2:E:30:LYS:HG2	2.01	0.80
2:D:29:LEU:HD23	2:D:93:LYS:CG	2.10	0.80
2:E:19:GLU:HA	2:E:22:LYS:NZ	1.96	0.80
2:B:2:ASN:O	2:B:6:VAL:HG23	1.80	0.80
2:E:2:ASN:OD1	2:E:3:SER:N	2.15	0.80
2:D:129:THR:CG2	2:D:207:GLN:CG	2.57	0.80
2:D:244:VAL:HG21	2:D:261:ILE:CG2	2.11	0.80
1:A:315:LEU:CD1	1:A:319:LEU:HD13	1.96	0.80
1:F:221:LEU:HD23	1:F:357:ILE:HD13	1.63	0.80
2:E:25:ILE:HG21	2:E:80:ILE:HG13	1.63	0.79
2:E:154:PHE:HD1	2:E:173:PRO:HG2	1.35	0.79
1:A:331:ILE:HD12	1:A:362:ILE:HA	1.62	0.79
2:E:26:LEU:O	2:E:27:LEU:HB2	1.82	0.79
1:C:314:GLU:OE2	1:C:356:TYR:CD2	2.36	0.79
2:E:29:LEU:CD2	2:E:30:LYS:HG2	2.13	0.79
2:D:147:CYS:HB3	2:D:150:CYS:SG	2.23	0.79
2:E:30:LYS:HZ3	2:E:89:ALA:HB1	1.47	0.78
2:D:244:VAL:CG2	2:D:261:ILE:CG2	2.61	0.78
2:D:24:ASP:O	2:D:28:ILE:HG22	1.84	0.78
2:E:43:ASN:CB	2:E:46:THR:OG1	2.28	0.78
1:C:148:ALA:O	1:C:152:THR:CG2	2.32	0.78
2:E:19:GLU:N	2:E:22:LYS:NZ	2.32	0.78
2:E:145:TYR:CE2	2:E:156:ILE:HG12	2.18	0.78
2:E:36:ALA:O	2:E:93:LYS:CD	2.32	0.77
1:F:121:ILE:HG21	1:F:160:ILE:HG12	1.66	0.77
1:A:352:MET:SD	2:B:139:LEU:CD2	2.71	0.77
1:C:314:GLU:OE2	1:C:356:TYR:HD2	1.67	0.77
2:E:16:TYR:CE2	2:E:20:TYR:HE2	2.04	0.76
2:D:29:LEU:O	2:D:93:LYS:CE	2.34	0.76
1:C:336:LYS:HB2	1:C:336:LYS:HZ1	1.48	0.76
2:D:71:SER:O	2:D:75:ARG:CG	2.33	0.76
1:C:161:HIS:CD2	1:C:191:VAL:HG23	2.21	0.76
2:D:24:ASP:O	2:D:28:ILE:CG2	2.34	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:21:HIS:C	2:E:25:ILE:HG12	2.11	0.75
2:D:91:SER:HB2	2:D:93:LYS:NZ	2.02	0.75
2:D:140:GLU:CA	2:D:196:CYS:HA	2.16	0.75
1:C:161:HIS:O	1:C:165:THR:HG23	1.85	0.75
2:E:154:PHE:HB3	2:E:173:PRO:CB	2.17	0.75
2:D:5:GLN:OE1	2:D:5:GLN:CA	2.32	0.74
2:E:23:ASN:HA	2:E:26:LEU:HD13	1.67	0.74
1:F:232:LYS:HB3	1:F:232:LYS:NZ	2.02	0.74
2:E:20:TYR:C	2:E:23:ASN:HD21	1.96	0.74
1:F:96:ILE:HD13	1:F:158:LEU:CD2	2.18	0.74
2:E:21:HIS:O	2:E:25:ILE:CG1	2.35	0.74
2:E:22:LYS:C	2:E:25:ILE:HG12	2.13	0.74
2:D:91:SER:CB	2:D:93:LYS:HZ1	2.00	0.74
2:E:23:ASN:C	2:E:26:LEU:HD12	2.12	0.74
2:B:31:GLU:C	2:B:93:LYS:HZ1	1.92	0.74
1:A:317:HIS:O	1:A:320:VAL:HG22	1.89	0.73
2:E:145:TYR:CE2	2:E:156:ILE:CG1	2.72	0.73
2:E:154:PHE:HD1	2:E:173:PRO:CG	1.74	0.73
1:F:334:ILE:HD12	1:F:334:ILE:C	2.13	0.73
2:B:140:GLU:HA	2:B:196:CYS:HA	1.71	0.72
1:C:314:GLU:HG3	1:C:356:TYR:CD2	2.22	0.72
1:A:315:LEU:CD1	1:A:319:LEU:CB	2.36	0.72
2:B:237:ASP:C	2:B:238:LEU:CD1	2.62	0.72
2:E:17:VAL:HG13	2:E:21:HIS:HD1	1.54	0.72
1:C:312:GLU:HB3	1:C:356:TYR:CE1	2.23	0.72
2:E:23:ASN:O	2:E:26:LEU:CD1	2.37	0.72
2:B:153:VAL:HG11	2:B:173:PRO:CB	2.15	0.72
1:A:322:SER:HB3	1:A:362:ILE:CD1	2.19	0.72
1:A:315:LEU:HD13	1:A:319:LEU:HD12	1.67	0.71
2:E:76:SER:O	2:E:80:ILE:HD11	1.90	0.71
1:F:201:TYR:HB3	1:F:220:ALA:HB2	1.72	0.71
2:D:28:ILE:HD13	2:D:28:ILE:C	2.15	0.71
1:F:221:LEU:HD23	1:F:357:ILE:CD1	2.21	0.71
2:E:79:THR:C	2:E:82:GLN:OE1	2.18	0.71
1:C:104:THR:HA	1:C:107:ILE:HG12	1.71	0.71
1:C:112:LYS:CA	1:C:164:LEU:HD21	2.21	0.71
2:D:29:LEU:O	2:D:93:LYS:HE3	1.91	0.71
2:D:244:VAL:CG2	2:D:261:ILE:HG23	2.21	0.71
1:F:302:ARG:NH2	1:F:306:ARG:N	2.38	0.71
2:E:154:PHE:HB3	2:E:173:PRO:HG3	1.11	0.71
1:C:148:ALA:CB	1:C:151:LYS:CG	2.69	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LYS:CB	1:C:164:LEU:HD21	2.21	0.70
1:C:148:ALA:CB	1:C:151:LYS:HD3	2.21	0.70
1:C:151:LYS:HE2	1:C:152:THR:N	2.06	0.70
2:E:23:ASN:HD22	2:E:23:ASN:N	1.84	0.70
2:E:84:LEU:HD13	2:E:90:VAL:HG11	1.73	0.70
2:D:74:ARG:HE	2:D:96:LEU:HB2	1.55	0.70
2:B:46:THR:HA	2:B:49:GLU:HG2	1.74	0.70
2:D:29:LEU:CD2	2:D:93:LYS:HG2	2.17	0.70
2:E:84:LEU:HD13	2:E:90:VAL:CG1	2.22	0.70
2:E:84:LEU:CD1	2:E:90:VAL:HG11	2.22	0.70
2:B:92:MET:O	2:B:92:MET:SD	2.50	0.70
2:E:84:LEU:HB2	2:E:90:VAL:CG1	2.22	0.70
2:B:116:LYS:CE	1:F:231:ILE:HD13	2.21	0.70
2:E:19:GLU:CA	2:E:22:LYS:NZ	2.54	0.69
1:F:309:ARG:H	1:F:309:ARG:CD	2.04	0.69
2:B:237:ASP:C	2:B:238:LEU:HD13	2.17	0.69
2:D:202:ILE:O	2:D:222:VAL:CG2	2.39	0.69
2:E:27:LEU:CD2	2:E:30:LYS:HG3	2.20	0.69
2:D:120:VAL:HG23	2:D:244:VAL:HG22	1.74	0.69
1:F:66:GLN:OE1	1:F:72:PHE:HB2	1.87	0.69
1:C:112:LYS:HG2	1:C:164:LEU:HD22	1.74	0.69
1:A:98:ALA:HA	1:A:101:LYS:NZ	2.08	0.69
2:B:64:GLU:O	2:B:67:THR:OG1	2.11	0.69
1:C:112:LYS:CG	1:C:164:LEU:CD2	2.70	0.69
1:A:201:TYR:HB3	1:A:220:ALA:HB2	1.75	0.69
2:B:130:VAL:HG11	2:B:232:CYS:SG	2.33	0.69
1:C:69:LEU:C	1:C:76:LYS:HZ1	2.00	0.68
1:A:149:PRO:CB	1:A:334:ILE:HG23	2.23	0.68
1:C:254:PRO:HB2	1:C:255:ASP:OD1	1.93	0.68
1:A:331:ILE:HD11	1:A:362:ILE:CB	2.21	0.68
2:B:120:VAL:HA	2:B:244:VAL:HB	1.75	0.68
1:A:315:LEU:CD1	1:A:319:LEU:CG	2.71	0.68
2:E:6:VAL:O	2:E:9:VAL:HB	1.93	0.68
2:D:45:MET:HA	2:D:104:PRO:HG3	1.74	0.68
2:E:84:LEU:CD1	2:E:90:VAL:HG21	2.21	0.68
2:B:248:TRP:CZ3	1:F:235:CYS:SG	2.84	0.68
1:F:150:GLU:HG2	1:F:151:LYS:N	2.08	0.67
1:A:323:CYS:SG	1:A:329:VAL:HG11	2.34	0.67
2:E:79:THR:OG1	2:E:80:ILE:CD1	2.42	0.67
2:E:30:LYS:HZ3	2:E:89:ALA:CB	2.02	0.67
1:C:125:PHE:HE1	1:C:142:ALA:HB2	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:18:SER:C	2:E:22:LYS:HZ1	2.02	0.67
2:E:30:LYS:HZ3	2:E:89:ALA:CA	2.07	0.67
2:B:79:THR:HA	2:B:82:GLN:CD	2.20	0.67
1:A:257:LYS:HA	2:E:256:ARG:HA	1.75	0.66
2:B:77:ALA:C	2:B:81:LEU:HD23	2.20	0.66
2:B:224:LEU:CD2	2:B:268:ILE:CD1	2.72	0.66
2:E:28:ILE:HD12	2:E:93:LYS:HE2	1.77	0.66
2:E:154:PHE:CG	2:E:173:PRO:HG2	2.11	0.66
1:C:151:LYS:HZ3	1:C:152:THR:HG22	0.85	0.66
2:B:224:LEU:HD22	2:B:268:ILE:CD1	2.23	0.66
2:E:22:LYS:O	2:E:25:ILE:HG13	1.95	0.66
1:F:306:ARG:O	1:F:306:ARG:HD2	1.96	0.66
2:D:202:ILE:HB	2:D:222:VAL:HG23	1.78	0.66
1:A:331:ILE:HD11	1:A:362:ILE:HG23	0.67	0.66
2:E:43:ASN:OD1	2:E:101:SER:O	2.14	0.66
2:E:154:PHE:CG	2:E:173:PRO:HD3	2.26	0.66
1:A:78:TRP:HB2	1:A:158:LEU:HD11	1.77	0.66
2:D:115:PRO:CD	2:D:220:MET:HE1	2.24	0.66
2:E:29:LEU:CD2	2:E:30:LYS:N	2.56	0.66
2:E:86:GLN:HB3	2:E:88:GLU:OE2	1.95	0.66
2:B:115:PRO:HG3	2:B:124:LEU:HD22	1.78	0.65
2:E:145:TYR:HE2	2:E:156:ILE:CG1	2.08	0.65
1:F:309:ARG:HD2	1:F:309:ARG:N	2.10	0.65
2:E:27:LEU:HD23	2:E:30:LYS:CB	2.25	0.65
1:F:302:ARG:NH2	1:F:306:ARG:H	1.93	0.65
2:D:91:SER:CB	2:D:93:LYS:NZ	2.59	0.65
2:D:157:LYS:HG2	2:D:158:ALA:O	1.96	0.65
2:E:19:GLU:N	2:E:22:LYS:HZ2	1.92	0.65
1:F:218:TYR:CE2	1:F:333:GLY:CA	2.75	0.65
1:A:146:ARG:O	1:A:217:LYS:HB3	1.96	0.65
2:B:223:ILE:CG2	2:B:225:GLU:OE2	2.45	0.65
2:D:91:SER:O	2:D:93:LYS:HE2	1.97	0.65
2:D:204:ILE:HD12	2:D:220:MET:HG3	1.78	0.65
2:B:77:ALA:O	2:B:81:LEU:CD2	2.32	0.65
1:F:239:ALA:HA	1:F:250:SER:HA	1.79	0.65
2:B:9:VAL:HG13	2:B:54:ILE:HG12	1.79	0.65
2:B:236:ASP:C	2:B:238:LEU:CD1	2.70	0.65
1:A:286:MET:SD	1:A:287:ASP:N	2.70	0.65
2:E:22:LYS:CA	2:E:25:ILE:CD1	2.54	0.65
2:B:153:VAL:CG1	2:B:173:PRO:HB2	2.19	0.64
2:B:238:LEU:HB3	2:B:270:VAL:HA	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ARG:NH1	1:C:222:ARG:CG	2.42	0.64
2:E:44:ALA:HB3	2:E:103:LEU:HA	1.79	0.64
1:A:315:LEU:HD12	1:A:319:LEU:HB3	0.72	0.64
2:E:21:HIS:O	2:E:25:ILE:HG23	1.97	0.64
1:A:211:ARG:H	1:A:214:TYR:HB2	1.63	0.64
2:B:79:THR:HA	2:B:82:GLN:CG	2.27	0.64
2:E:161:GLU:HG3	2:E:165:THR:HG23	1.80	0.64
2:E:87:PRO:O	2:E:90:VAL:HG22	1.98	0.63
2:E:79:THR:O	2:E:82:GLN:OE1	2.13	0.63
1:C:104:THR:O	1:C:107:ILE:CD1	2.46	0.63
2:E:79:THR:OG1	2:E:80:ILE:HD13	1.98	0.63
1:F:238:MET:HE2	1:F:283:THR:CG2	2.29	0.63
1:C:313:CYS:SG	1:C:357:ILE:CG2	2.85	0.63
2:B:64:GLU:O	2:B:68:ILE:HG13	1.98	0.63
2:E:172:CYS:SG	2:E:173:PRO:HD2	2.38	0.62
2:D:116:LYS:HB3	2:D:118:LYS:HG3	1.81	0.62
2:B:47:LEU:HD21	2:B:69:PHE:CZ	2.35	0.62
2:D:202:ILE:HB	2:D:222:VAL:CG2	2.28	0.62
1:C:125:PHE:CE1	1:C:142:ALA:HB2	2.33	0.62
2:E:133:THR:CG2	2:E:202:ILE:HG21	2.19	0.62
2:D:22:LYS:HG2	2:D:80:ILE:HD11	1.82	0.62
2:B:12:VAL:HG11	2:B:51:ASN:CB	2.28	0.62
2:B:46:THR:C	2:B:49:GLU:HG3	2.22	0.62
1:A:80:LEU:CD1	1:A:237:LYS:HE3	2.27	0.62
1:C:292:LYS:C	1:C:293:ILE:HD12	2.25	0.62
2:D:200:GLN:HB2	2:D:229:VAL:HB	1.82	0.61
1:A:149:PRO:CG	1:A:334:ILE:CG2	2.78	0.61
1:A:102:PHE:C	1:A:102:PHE:CD2	2.78	0.61
1:A:146:ARG:O	1:A:217:LYS:CB	2.48	0.61
1:C:104:THR:CA	1:C:107:ILE:HG12	2.31	0.61
1:F:221:LEU:CD2	1:F:357:ILE:CD1	2.78	0.61
2:D:202:ILE:C	2:D:222:VAL:HG23	2.24	0.61
2:E:23:ASN:ND2	2:E:23:ASN:H	1.83	0.61
2:E:23:ASN:O	2:E:26:LEU:HD12	1.99	0.61
2:B:43:ASN:ND2	2:B:45:MET:CG	2.62	0.61
1:F:198:VAL:O	1:F:361:SER:CB	2.48	0.61
1:C:148:ALA:HB3	1:C:151:LYS:CD	2.28	0.60
2:B:143:ARG:HD2	2:B:166:PHE:CB	2.30	0.60
2:D:138:VAL:HB	1:F:353:PHE:HB2	1.82	0.60
2:E:44:ALA:HA	2:E:47:LEU:CD2	2.31	0.60
2:B:43:ASN:ND2	2:B:45:MET:HG3	2.11	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:LYS:CG	1:C:164:LEU:HD21	2.31	0.60
1:C:150:GLU:CD	1:C:150:GLU:H	2.09	0.60
2:B:237:ASP:C	2:B:238:LEU:HD12	2.25	0.60
1:A:146:ARG:O	1:A:217:LYS:HA	2.01	0.60
2:E:23:ASN:O	2:E:26:LEU:HD13	2.01	0.60
2:E:29:LEU:HD13	2:E:90:VAL:CG1	2.31	0.60
1:A:311:ILE:HG22	1:A:356:TYR:HA	1.84	0.60
1:A:328:THR:H	1:A:368:GLN:HE22	1.47	0.60
1:F:66:GLN:CD	1:F:72:PHE:CB	2.65	0.60
1:F:247:GLU:C	1:F:247:GLU:OE2	2.43	0.60
2:D:9:VAL:CG2	2:D:54:ILE:HB	2.31	0.60
2:D:28:ILE:HD13	2:D:29:LEU:H	1.65	0.60
2:E:29:LEU:CD1	2:E:30:LYS:CE	2.79	0.60
2:E:110:VAL:HG22	2:E:125:SER:CB	2.30	0.59
1:F:221:LEU:CD2	1:F:357:ILE:HD12	2.32	0.59
1:A:78:TRP:HZ2	1:A:85:VAL:HA	1.68	0.59
1:A:131:GLY:O	1:A:135:THR:HG23	2.02	0.59
1:F:242:CYS:HB2	1:F:264:CYS:SG	2.42	0.59
2:D:91:SER:HB2	2:D:93:LYS:HZ3	1.65	0.59
2:E:29:LEU:HD23	2:E:30:LYS:CG	2.31	0.59
2:E:154:PHE:CG	2:E:173:PRO:CD	2.61	0.59
2:D:139:LEU:N	2:D:196:CYS:SG	2.76	0.59
1:A:342:GLU:OE2	1:A:342:GLU:HA	2.02	0.59
2:D:62:PRO:HG2	2:D:122:HIS:HA	1.85	0.59
1:C:151:LYS:HZ1	1:C:152:THR:CB	2.16	0.59
1:F:159:ALA:O	1:F:163:VAL:CG2	2.49	0.59
1:A:71:ARG:HH12	1:A:169:GLU:CG	2.07	0.59
2:E:29:LEU:CD2	2:E:30:LYS:CG	2.80	0.59
2:E:22:LYS:O	2:E:25:ILE:CG1	2.51	0.58
1:F:122:LEU:HA	1:F:197:ARG:HB2	1.85	0.58
2:B:127:THR:HA	2:B:239:THR:HA	1.85	0.58
2:D:221:LYS:HB2	2:D:262:VAL:HG22	1.85	0.58
2:E:25:ILE:CB	2:E:80:ILE:HG21	2.31	0.58
1:F:242:CYS:CB	1:F:264:CYS:SG	2.91	0.58
2:E:27:LEU:C	2:E:30:LYS:HG2	2.29	0.58
2:D:140:GLU:HA	2:D:195:ARG:O	2.03	0.58
2:E:156:ILE:O	2:E:156:ILE:HG13	2.03	0.58
1:A:74:PRO:HB2	1:A:162:GLN:HG3	1.85	0.58
2:B:79:THR:C	2:B:82:GLN:HG2	2.27	0.58
1:C:226:VAL:CG2	1:C:227:ARG:N	2.66	0.58
2:E:16:TYR:CE2	2:E:20:TYR:CE2	2.89	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:MET:HB2	1:F:253:LEU:HD21	1.86	0.58
1:A:319:LEU:O	1:A:322:SER:HB2	2.04	0.57
1:C:104:THR:C	1:C:107:ILE:HG12	2.29	0.57
2:E:16:TYR:O	2:E:19:GLU:OE2	2.22	0.57
1:F:218:TYR:CZ	1:F:333:GLY:HA2	2.40	0.57
2:D:144:ASP:CB	2:D:187:SER:CB	2.73	0.57
2:E:226:ASP:O	2:E:229:VAL:HG13	2.05	0.57
2:D:44:ALA:O	2:D:48:PHE:CD1	2.57	0.57
2:E:29:LEU:CG	2:E:30:LYS:HE3	2.15	0.57
2:B:176:GLU:O	2:B:176:GLU:HG2	2.04	0.57
1:F:306:ARG:HD3	1:F:309:ARG:HH12	1.68	0.57
2:B:256:ARG:HA	1:F:257:LYS:HA	1.86	0.57
2:E:31:GLU:HG2	2:E:38:TYR:HE1	1.69	0.57
2:D:191:SER:HA	2:D:195:ARG:HH21	1.70	0.56
1:C:255:ASP:OD1	1:C:257:LYS:HE3	2.05	0.56
2:D:202:ILE:HG13	2:D:224:LEU:HD21	1.87	0.56
2:E:19:GLU:CA	2:E:22:LYS:HZ3	2.16	0.56
1:C:151:LYS:CE	1:C:152:THR:HG22	2.26	0.56
1:C:249:GLN:HG2	1:C:265:PRO:HD3	1.88	0.56
1:C:314:GLU:HB2	1:C:358:GLU:HG2	1.87	0.56
2:D:111:ARG:HH21	2:D:116:LYS:H	1.52	0.56
2:E:17:VAL:O	2:E:21:HIS:CG	2.56	0.56
2:E:22:LYS:C	2:E:25:ILE:CG1	2.76	0.56
2:D:204:ILE:CD1	2:D:220:MET:HG3	2.35	0.56
2:D:200:GLN:HB3	2:D:224:LEU:HD12	1.87	0.56
2:D:241:TYR:HB2	2:D:267:TYR:HB3	1.87	0.56
2:E:29:LEU:HG	2:E:30:LYS:NZ	2.21	0.56
2:E:29:LEU:CD1	2:E:30:LYS:HE3	2.34	0.56
1:C:148:ALA:CB	1:C:151:LYS:CD	2.84	0.56
2:E:30:LYS:NZ	2:E:89:ALA:CA	2.68	0.56
1:F:302:ARG:NH2	1:F:306:ARG:C	2.47	0.56
2:E:84:LEU:HD12	2:E:87:PRO:HA	1.88	0.56
1:A:347:LYS:HD3	1:A:348:ASN:N	2.21	0.56
1:C:70:ASP:CA	1:C:76:LYS:NZ	2.65	0.55
1:C:213:ASN:HA	2:E:193:PRO:HB3	1.88	0.55
1:F:329:VAL:HG22	1:F:364:ASN:HB3	1.87	0.55
1:C:226:VAL:HG13	1:C:292:LYS:O	2.06	0.55
2:D:9:VAL:HG23	2:D:54:ILE:HB	1.88	0.55
1:A:98:ALA:HA	1:A:101:LYS:HZ3	1.71	0.55
2:E:29:LEU:HD11	2:E:30:LYS:HE3	1.87	0.55
1:A:149:PRO:CG	1:A:334:ILE:HG21	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:140:GLU:HA	2:D:196:CYS:CA	2.25	0.55
1:F:238:MET:CE	1:F:283:THR:OG1	2.54	0.55
2:B:141:PHE:HB2	2:B:197:ARG:HB2	1.87	0.55
2:B:232:CYS:SG	2:B:238:LEU:CD2	2.87	0.55
1:C:176:GLN:O	1:C:179:GLU:O	2.25	0.55
2:B:26:LEU:HA	2:B:29:LEU:HD23	1.89	0.55
2:D:29:LEU:O	2:D:93:LYS:HE2	2.07	0.54
2:E:20:TYR:C	2:E:23:ASN:ND2	2.62	0.54
2:E:27:LEU:CB	2:E:30:LYS:HG3	2.36	0.54
2:E:197:ARG:NH2	2:E:226:ASP:HB3	2.23	0.54
1:A:288:TRP:HE1	1:A:314:GLU:HG3	1.72	0.54
1:C:104:THR:C	1:C:107:ILE:CG1	2.75	0.54
2:D:117:THR:HG22	2:D:261:ILE:HD11	1.89	0.54
1:F:238:MET:HE2	1:F:283:THR:HG21	1.90	0.54
1:A:149:PRO:HB2	1:A:334:ILE:HG23	1.77	0.54
1:A:149:PRO:CD	1:A:216:GLY:O	2.56	0.54
2:B:133:THR:HG23	2:B:202:ILE:HG22	1.90	0.54
2:E:78:LEU:HA	2:E:81:LEU:HD23	1.90	0.54
2:E:145:TYR:HE2	2:E:156:ILE:H	1.56	0.54
2:D:200:GLN:CB	2:D:224:LEU:HD12	2.37	0.53
1:C:161:HIS:HD2	1:C:191:VAL:CG2	2.19	0.53
2:D:106:CYS:HB2	2:D:109:LEU:HB2	1.89	0.53
1:F:215:TYR:CD1	1:F:216:GLY:N	2.77	0.53
2:E:16:TYR:HB2	2:E:50:THR:HG21	1.90	0.53
2:E:145:TYR:CE2	2:E:156:ILE:HG13	2.43	0.53
1:A:131:GLY:O	1:A:135:THR:CG2	2.56	0.53
1:F:198:VAL:C	1:F:361:SER:CB	2.79	0.53
2:B:218:ARG:CZ	1:F:230:ASN:HA	2.39	0.53
1:C:257:LYS:HA	2:D:256:ARG:HA	1.91	0.53
2:E:29:LEU:C	2:E:89:ALA:O	2.50	0.53
2:E:97:HIS:HE1	2:E:197:ARG:NH2	2.06	0.53
2:E:43:ASN:O	2:E:46:THR:OG1	2.27	0.53
1:A:133:GLU:HG2	1:A:134:VAL:N	2.24	0.52
2:E:9:VAL:HG22	2:E:54:ILE:HG22	1.90	0.52
1:C:75:TYR:HB3	1:C:162:GLN:HG2	1.90	0.52
2:E:81:LEU:C	2:E:82:GLN:OE1	2.47	0.52
2:E:133:THR:HA	2:E:202:ILE:HG22	1.90	0.52
1:A:350:LYS:HG3	2:B:165:THR:HG21	1.92	0.52
1:C:239:ALA:HB2	1:C:282:LEU:HB2	1.92	0.52
1:F:238:MET:HE2	1:F:283:THR:OG1	2.09	0.52
2:B:27:LEU:HA	2:B:30:LYS:HZ1	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:LYS:HB3	1:F:232:LYS:HZ3	1.72	0.52
1:C:144:GLU:HG3	1:C:145:LEU:N	2.24	0.52
1:A:328:THR:N	1:A:368:GLN:HE22	2.07	0.51
2:B:224:LEU:HD21	2:B:268:ILE:CD1	2.39	0.51
2:E:21:HIS:HB2	2:E:25:ILE:HG23	1.91	0.51
1:F:302:ARG:CZ	1:F:306:ARG:O	2.56	0.51
2:B:149:LYS:H	2:B:180:SER:HB3	1.75	0.51
2:B:270:VAL:HB	2:B:273:GLU:HB3	1.93	0.51
1:C:207:LEU:HB3	1:C:309:ARG:HB2	1.93	0.51
2:D:138:VAL:C	2:D:196:CYS:SG	2.93	0.51
2:D:202:ILE:CB	2:D:222:VAL:HG23	2.40	0.51
2:D:244:VAL:CG2	2:D:261:ILE:HG22	2.40	0.51
2:E:29:LEU:CD2	2:E:30:LYS:CD	2.74	0.51
1:A:319:LEU:CD1	1:A:359:ALA:O	2.59	0.51
1:C:145:LEU:HA	1:C:152:THR:HG21	1.93	0.51
2:B:106:CYS:HB2	2:B:109:LEU:HB2	1.93	0.51
2:D:115:PRO:HB3	2:D:124:LEU:HD21	1.93	0.51
1:A:93:ILE:HA	1:A:96:ILE:HG23	1.93	0.51
2:B:9:VAL:HG11	2:B:54:ILE:CD1	2.32	0.51
1:C:69:LEU:HD23	1:C:76:LYS:CE	2.40	0.51
1:F:306:ARG:HD3	1:F:309:ARG:NH1	2.26	0.51
2:E:30:LYS:HE2	2:E:30:LYS:N	2.26	0.51
2:E:118:LYS:HD2	2:E:119:ASP:CA	2.40	0.51
2:E:76:SER:O	2:E:79:THR:OG1	2.25	0.51
2:E:80:ILE:C	2:E:82:GLN:OE1	2.53	0.51
2:E:120:VAL:HG23	2:E:261:ILE:HG23	1.93	0.51
2:E:172:CYS:H	2:E:178:CYS:H	1.58	0.51
2:B:238:LEU:HB3	2:B:270:VAL:HG22	1.93	0.50
2:D:16:TYR:HE2	2:D:42:VAL:HG13	1.76	0.50
1:C:238:MET:HE2	1:C:276:ALA:HB1	1.92	0.50
1:C:241:LEU:HD12	1:C:248:ILE:HG12	1.93	0.50
1:F:211:ARG:H	1:F:214:TYR:HB2	1.77	0.50
1:A:329:VAL:HG12	1:A:364:ASN:HA	1.92	0.50
2:E:29:LEU:HD11	2:E:30:LYS:CE	2.41	0.50
1:A:331:ILE:HD11	1:A:362:ILE:HG12	1.94	0.50
2:B:160:PHE:HA	2:B:164:TYR:HA	1.92	0.50
2:B:27:LEU:HA	2:B:30:LYS:NZ	2.27	0.50
2:E:152:HIS:ND1	2:E:174:SER:HB3	2.26	0.50
1:A:331:ILE:CD1	1:A:362:ILE:CB	2.84	0.50
1:C:151:LYS:HE2	1:C:151:LYS:C	2.37	0.50
2:D:25:ILE:HA	2:D:28:ILE:HG23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:244:VAL:HG23	2:D:261:ILE:HG22	1.92	0.50
1:F:334:ILE:CD1	1:F:335:VAL:O	2.60	0.50
2:E:19:GLU:CA	2:E:22:LYS:HZ2	2.20	0.50
2:E:27:LEU:O	2:E:31:GLU:N	2.40	0.50
2:E:154:PHE:HD1	2:E:173:PRO:HD2	1.56	0.50
1:A:237:LYS:HG2	1:A:250:SER:HB2	1.93	0.49
1:C:148:ALA:HB1	1:C:151:LYS:HG3	1.86	0.49
1:C:278:ARG:HG3	1:C:283:THR:HG21	1.94	0.49
2:D:244:VAL:HG23	2:D:261:ILE:CG2	2.43	0.49
2:E:27:LEU:CG	2:E:30:LYS:HG3	2.42	0.49
1:A:339:ASN:OD1	1:A:342:GLU:HG2	2.13	0.49
1:C:175:LEU:O	1:C:179:GLU:OE2	2.30	0.49
2:D:28:ILE:C	2:D:28:ILE:CD1	2.82	0.49
1:F:232:LYS:HB3	1:F:232:LYS:HZ2	1.77	0.49
2:E:21:HIS:O	2:E:25:ILE:CB	2.61	0.49
1:F:181:LEU:HB3	1:F:184:ASP:H	1.77	0.49
2:D:245:MET:HE2	2:D:245:MET:HB3	1.70	0.49
2:E:84:LEU:HB3	2:E:90:VAL:HG12	1.89	0.49
1:F:96:ILE:HD13	1:F:158:LEU:HD22	1.91	0.49
2:B:43:ASN:ND2	2:B:45:MET:HG2	2.28	0.48
2:E:211:LEU:N	2:E:211:LEU:HD12	2.20	0.48
2:B:34:GLU:HB2	2:B:94:GLN:HG2	1.95	0.48
1:C:249:GLN:HB3	1:C:265:PRO:HB3	1.95	0.48
2:D:24:ASP:O	2:D:28:ILE:HG23	2.11	0.48
1:F:215:TYR:HB2	1:F:355:LEU:HD11	1.95	0.48
1:A:319:LEU:HD12	1:A:359:ALA:O	2.12	0.48
2:B:46:THR:HA	2:B:49:GLU:CG	2.42	0.48
1:A:75:TYR:HD1	1:A:162:GLN:HB2	1.78	0.48
1:A:207:LEU:HD21	1:A:221:LEU:HD22	1.96	0.48
1:C:292:LYS:HG2	1:C:310:THR:HB	1.94	0.48
2:E:92:MET:O	2:E:92:MET:HG2	2.12	0.48
1:A:331:ILE:HD11	1:A:362:ILE:CG1	2.43	0.48
1:C:64:SER:O	1:C:65:MET:CB	2.45	0.48
2:E:22:LYS:N	2:E:25:ILE:HG12	2.27	0.48
1:A:333:GLY:HA3	1:A:358:GLU:O	2.13	0.48
2:D:142:GLU:HA	2:D:157:LYS:HA	1.95	0.48
2:D:256:ARG:HE	2:D:256:ARG:HB2	1.48	0.48
1:C:69:LEU:HD23	1:C:76:LYS:HE2	1.95	0.48
1:F:165:THR:HG22	1:F:191:VAL:HG21	1.95	0.48
1:C:98:ALA:HB2	1:C:137:LEU:HD23	1.96	0.48
1:C:101:LYS:HA	1:C:101:LYS:HD3	1.52	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:16:TYR:C	2:E:16:TYR:CD2	2.92	0.48
1:F:199:TYR:CA	1:F:361:SER:OG	2.61	0.48
2:B:43:ASN:HD21	2:B:45:MET:HG2	1.77	0.48
2:D:109:LEU:HD12	2:D:109:LEU:HA	1.77	0.48
1:A:339:ASN:ND2	1:A:342:GLU:OE1	2.47	0.47
2:D:32:ARG:HE	2:D:32:ARG:HB2	1.58	0.47
2:E:79:THR:HG1	2:E:80:ILE:HD13	1.79	0.47
2:E:81:LEU:CA	2:E:82:GLN:OE1	2.62	0.47
2:E:142:GLU:HB2	2:E:195:ARG:HH21	1.79	0.47
2:E:247:ARG:HD2	2:E:247:ARG:HA	1.64	0.47
1:C:255:ASP:OD1	1:C:255:ASP:N	2.47	0.47
2:E:144:ASP:HB3	2:E:186:LEU:H	1.79	0.47
1:F:302:ARG:HH22	1:F:306:ARG:N	2.12	0.47
1:A:239:ALA:H	1:A:283:THR:HB	1.78	0.47
2:E:29:LEU:CD2	2:E:29:LEU:N	2.76	0.47
1:F:65:MET:H	1:F:65:MET:HG3	1.42	0.47
1:F:330:THR:HG22	1:F:363:SER:OG	2.14	0.47
1:A:138:ILE:HG21	1:A:144:GLU:HG2	1.96	0.47
1:A:331:ILE:HD12	1:A:331:ILE:HA	1.69	0.47
1:F:352:MET:HE3	1:F:352:MET:HB3	1.71	0.47
2:D:129:THR:CB	2:D:237:ASP:OD1	2.60	0.47
2:E:118:LYS:HD2	2:E:119:ASP:HA	1.97	0.47
2:D:244:VAL:HG21	2:D:261:ILE:HG23	1.89	0.47
2:E:34:GLU:O	2:E:93:LYS:HD3	2.15	0.47
1:F:296:LEU:HD23	1:F:296:LEU:HA	1.67	0.47
2:E:92:MET:N	2:E:92:MET:HE3	2.30	0.47
1:A:323:CYS:SG	1:A:329:VAL:CG1	3.03	0.47
1:A:348:ASN:HB2	2:B:168:ARG:HB3	1.96	0.47
2:E:172:CYS:SG	2:E:173:PRO:CD	3.02	0.47
2:E:216:ILE:H	2:E:216:ILE:HG12	1.37	0.47
1:A:181:LEU:H	1:A:181:LEU:HG	1.49	0.46
1:C:163:VAL:HG12	1:C:164:LEU:N	2.30	0.46
2:B:25:ILE:HG12	2:B:80:ILE:HG13	1.97	0.46
2:B:259:VAL:HB	1:F:233:PRO:O	2.15	0.46
2:E:16:TYR:O	2:E:16:TYR:CD2	2.67	0.46
1:C:149:PRO:HB3	1:C:218:TYR:HB2	1.96	0.46
1:C:345:ARG:HD2	1:C:345:ARG:HA	1.37	0.46
2:E:201:GLU:OE1	2:E:221:LYS:HE3	2.16	0.46
2:B:236:ASP:O	2:B:238:LEU:HD13	2.06	0.46
2:E:25:ILE:HG21	2:E:80:ILE:CG1	2.39	0.46
2:E:29:LEU:HD21	2:E:30:LYS:CG	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:PRO:HG3	2:D:124:LEU:HD11	1.97	0.46
2:E:21:HIS:C	2:E:25:ILE:HG23	2.41	0.46
2:D:269:GLN:HE22	2:D:274:GLN:HB3	1.80	0.46
1:F:150:GLU:CG	1:F:151:LYS:N	2.77	0.46
1:C:98:ALA:HB1	1:C:134:VAL:HA	1.98	0.46
2:E:22:LYS:CB	2:E:25:ILE:HD11	2.45	0.46
2:E:30:LYS:HZ1	2:E:89:ALA:HB1	0.66	0.46
2:B:91:SER:OG	2:B:93:LYS:CE	2.64	0.46
1:C:232:LYS:HB3	1:C:232:LYS:HE2	1.54	0.46
1:F:224:THR:HA	1:F:328:THR:HA	1.97	0.46
1:A:333:GLY:HA3	1:A:359:ALA:HA	1.97	0.45
1:C:173:ALA:HA	1:C:176:GLN:HE21	1.81	0.45
2:D:2:ASN:ND2	2:D:4:ASP:HB3	2.31	0.45
2:E:21:HIS:O	2:E:25:ILE:CG2	2.64	0.45
2:E:138:VAL:HA	2:E:198:ASP:HA	1.97	0.45
2:E:145:TYR:OH	2:E:156:ILE:HG13	2.16	0.45
1:A:331:ILE:O	1:A:331:ILE:HG22	2.16	0.45
1:C:208:LYS:H	1:C:208:LYS:HG3	1.53	0.45
2:B:37:HIS:HB3	2:B:97:HIS:HE1	1.81	0.45
2:B:91:SER:OG	2:B:93:LYS:NZ	2.49	0.45
1:C:107:ILE:HG13	1:C:107:ILE:H	1.41	0.45
2:D:240:ILE:H	2:D:240:ILE:HG12	1.65	0.45
1:A:317:HIS:HB3	1:A:318:ASP:H	1.58	0.45
2:B:143:ARG:HD2	2:B:166:PHE:CD1	2.50	0.45
1:C:188:MET:HE2	1:C:188:MET:HB2	1.64	0.45
1:A:166:LYS:HD3	1:A:166:LYS:HA	1.51	0.45
2:E:23:ASN:ND2	2:E:23:ASN:N	2.49	0.45
1:A:345:ARG:HD2	1:A:345:ARG:HA	1.42	0.45
2:B:26:LEU:HD22	2:B:26:LEU:HA	1.74	0.45
2:D:21:HIS:CE1	2:D:42:VAL:HA	2.51	0.45
2:E:168:ARG:NH2	2:E:170:SER:HA	2.32	0.45
2:E:171:SER:HB2	2:E:177:SER:HA	1.99	0.45
1:F:105:ARG:HE	1:F:105:ARG:HB3	1.48	0.45
1:C:163:VAL:CG1	1:C:164:LEU:N	2.78	0.45
1:F:264:CYS:HA	1:F:274:PHE:HZ	1.82	0.45
2:B:81:LEU:HA	2:B:90:VAL:HG11	1.98	0.45
1:F:297:MET:HG3	1:F:302:ARG:HB3	1.98	0.45
1:A:126:LYS:H	1:A:126:LYS:HG3	1.37	0.45
1:A:146:ARG:O	1:A:217:LYS:CA	2.64	0.45
1:F:247:GLU:OE2	1:F:247:GLU:O	2.35	0.45
1:F:302:ARG:HH21	1:F:306:ARG:CA	2.28	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LYS:C	1:A:347:LYS:CD	2.78	0.44
1:C:226:VAL:HG22	1:C:227:ARG:N	2.31	0.44
1:F:352:MET:H	1:F:352:MET:HG2	1.67	0.44
2:D:204:ILE:H	2:D:204:ILE:HG13	1.74	0.44
2:E:20:TYR:CA	2:E:23:ASN:HD21	2.30	0.44
2:E:141:PHE:HB2	2:E:197:ARG:HB2	1.98	0.44
2:E:147:CYS:HB3	2:E:150:CYS:HB3	1.99	0.44
1:F:105:ARG:HH12	1:F:133:GLU:H	1.66	0.44
1:A:111:ASP:HB3	1:A:114:GLU:HB2	2.00	0.44
1:A:133:GLU:CG	1:A:134:VAL:N	2.80	0.44
1:A:151:LYS:HA	1:A:151:LYS:HD3	1.62	0.44
2:E:93:LYS:HE2	2:E:93:LYS:HB2	1.79	0.44
1:F:98:ALA:HB1	1:F:134:VAL:HA	1.99	0.44
1:F:272:ARG:CD	1:F:272:ARG:N	2.80	0.44
1:A:96:ILE:HG22	1:A:155:CYS:HB2	1.98	0.44
1:A:206:GLN:HG2	1:A:209:ASN:HB2	2.00	0.44
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.61	0.44
1:C:144:GLU:CG	1:C:145:LEU:N	2.80	0.44
1:F:270:ARG:HE	1:F:270:ARG:HB2	1.57	0.44
2:B:38:TYR:HA	2:B:39:PRO:HD3	1.79	0.44
1:C:354:LEU:HD13	1:C:354:LEU:HA	1.85	0.44
2:D:28:ILE:HG13	2:D:96:LEU:HD11	1.98	0.44
2:E:116:LYS:HA	2:E:116:LYS:HD3	1.42	0.44
2:B:51:ASN:HB3	2:B:54:ILE:HB	1.99	0.44
2:B:103:LEU:HD22	2:B:109:LEU:HD13	2.00	0.44
1:F:302:ARG:HH21	1:F:306:ARG:N	2.14	0.44
2:D:134:SER:HB3	2:D:201:GLU:H	1.81	0.44
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.39	0.44
1:A:366:LYS:H	1:A:366:LYS:HG2	1.50	0.44
2:D:54:ILE:CD1	2:D:55:GLY:CA	2.85	0.44
1:F:277:LEU:HD13	1:F:277:LEU:HA	1.80	0.44
1:F:334:ILE:HD11	1:F:335:VAL:O	2.18	0.44
1:F:347:LYS:H	1:F:347:LYS:HG2	1.62	0.44
1:A:71:ARG:HA	1:A:71:ARG:HD2	1.36	0.43
2:B:153:VAL:HG21	2:B:173:PRO:HG2	2.00	0.43
1:C:65:MET:HE3	1:C:65:MET:HB3	1.72	0.43
1:C:104:THR:O	1:C:107:ILE:HD11	2.18	0.43
2:D:246:GLN:H	2:D:246:GLN:HG3	1.42	0.43
2:E:5:GLN:H	2:E:5:GLN:HG2	1.40	0.43
1:F:126:LYS:HD2	1:F:126:LYS:HA	1.60	0.43
1:A:149:PRO:HB3	1:A:334:ILE:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:ARG:HE	2:B:132:ARG:HB2	1.63	0.43
2:B:143:ARG:CZ	2:B:166:PHE:HB2	2.47	0.43
2:B:149:LYS:HB2	2:B:180:SER:HB3	1.99	0.43
1:C:211:ARG:HA	1:C:211:ARG:HD3	1.50	0.43
2:D:5:GLN:NE2	2:D:57:TYR:OH	2.51	0.43
2:D:44:ALA:O	2:D:48:PHE:HD1	1.98	0.43
2:E:270:VAL:HB	2:E:273:GLU:HB2	1.99	0.43
1:F:141:ILE:H	1:F:141:ILE:HG12	1.31	0.43
1:A:101:LYS:HB2	1:A:101:LYS:HE2	1.35	0.43
2:E:118:LYS:O	2:E:118:LYS:HD2	1.91	0.43
2:B:222:VAL:HG22	2:B:263:LEU:HB3	2.01	0.43
2:D:39:PRO:HB3	2:D:99:ARG:HD2	1.99	0.43
2:D:112:GLU:HB3	2:D:210:ARG:HG3	2.01	0.43
2:D:137:LYS:HB2	2:D:137:LYS:HE2	1.35	0.43
2:E:73:LEU:HD13	2:E:73:LEU:HA	1.87	0.43
2:E:78:LEU:HD23	2:E:81:LEU:CD2	2.49	0.43
1:F:129:THR:HG22	1:F:141:ILE:HG13	2.01	0.43
1:C:317:HIS:HB3	1:C:318:ASP:H	1.58	0.43
2:D:115:PRO:CD	2:D:220:MET:CE	2.84	0.43
2:E:25:ILE:CG2	2:E:80:ILE:HG21	2.49	0.43
2:E:139:LEU:HD12	2:E:139:LEU:HA	1.71	0.43
2:D:30:LYS:HD3	2:D:90:VAL:HG13	2.01	0.43
2:D:139:LEU:HD13	1:F:350:LYS:HE2	2.00	0.43
2:E:26:LEU:CD1	2:E:26:LEU:H	2.12	0.43
1:A:156:MET:HE2	1:A:156:MET:HB2	1.87	0.43
1:A:309:ARG:HE	1:A:309:ARG:HB2	1.71	0.43
1:C:112:LYS:HG2	1:C:164:LEU:CD2	2.34	0.43
1:C:215:TYR:HA	1:C:335:VAL:HB	2.00	0.43
1:F:330:THR:HG22	1:F:330:THR:O	2.18	0.43
1:A:71:ARG:NH1	1:A:169:GLU:HG2	2.07	0.43
2:B:139:LEU:HD13	2:B:139:LEU:HA	1.78	0.43
1:C:111:ASP:HB3	1:C:114:GLU:HB2	2.00	0.43
1:F:297:MET:HB3	1:F:297:MET:HE3	1.76	0.43
1:A:286:MET:SD	1:A:287:ASP:OD2	2.76	0.43
1:C:207:LEU:HD13	1:C:207:LEU:HA	1.60	0.43
1:F:66:GLN:HB3	1:F:72:PHE:HB2	2.00	0.43
1:A:301:GLN:HE21	1:A:301:GLN:HB3	1.51	0.42
1:A:366:LYS:HA	1:A:369:LYS:HE2	2.01	0.42
2:B:206:GLU:HA	2:B:210:ARG:HH21	1.84	0.42
1:C:222:ARG:HG2	1:C:330:THR:HG23	2.00	0.42
2:D:182:LYS:HE2	2:D:182:LYS:HB2	1.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:LEU:HD13	1:F:204:LEU:HA	1.86	0.42
2:B:158:ALA:HA	2:B:166:PHE:HB3	2.01	0.42
1:C:314:GLU:CG	1:C:356:TYR:CD2	2.95	0.42
1:C:350:LYS:HB2	2:E:166:PHE:H	1.84	0.42
2:D:208:VAL:CG1	2:D:209:GLN:N	2.82	0.42
1:C:121:ILE:HG21	1:C:160:ILE:HG13	2.01	0.42
2:E:29:LEU:HD23	2:E:29:LEU:N	2.35	0.42
2:E:84:LEU:CD2	2:E:90:VAL:HG11	2.47	0.42
1:F:263:LYS:HG3	1:F:270:ARG:HB3	2.01	0.42
1:A:339:ASN:HD21	1:A:342:GLU:CD	2.26	0.42
2:B:218:ARG:HA	2:B:218:ARG:HD3	1.74	0.42
1:C:107:ILE:HG22	1:C:167:ASP:OD2	2.19	0.42
1:C:217:LYS:HZ2	1:C:217:LYS:HG2	1.66	0.42
1:C:222:ARG:HD2	1:C:296:LEU:CD1	2.49	0.42
2:D:45:MET:HE2	2:D:45:MET:HB2	1.90	0.42
2:D:224:LEU:HB3	2:D:228:LEU:HB3	2.01	0.42
2:D:9:VAL:HG23	2:D:54:ILE:CB	2.49	0.42
2:D:28:ILE:CD1	2:D:29:LEU:HG	2.49	0.42
2:E:47:LEU:HD12	2:E:54:ILE:HG13	2.02	0.42
1:F:96:ILE:HG21	1:F:158:LEU:HD23	2.00	0.42
1:F:105:ARG:HH22	1:F:133:GLU:HB2	1.85	0.42
1:F:118:LYS:HZ2	1:F:118:LYS:HG2	1.75	0.42
1:A:118:LYS:HB2	1:A:318:ASP:HB3	2.00	0.42
1:A:315:LEU:HD13	1:A:315:LEU:HA	1.73	0.42
1:C:272:ARG:H	1:C:272:ARG:HG2	1.42	0.42
2:D:103:LEU:HD11	2:D:123:PHE:HD2	1.84	0.42
1:C:207:LEU:HD13	1:C:221:LEU:HD11	2.00	0.42
2:D:92:MET:HE3	2:D:92:MET:HB3	1.76	0.42
2:D:145:TYR:HD2	2:D:156:ILE:HB	1.84	0.42
2:B:261:ILE:HD12	2:B:261:ILE:HA	1.83	0.42
1:C:166:LYS:HD2	1:C:166:LYS:HA	1.36	0.42
2:E:43:ASN:HB3	2:E:46:THR:CB	2.42	0.42
1:F:96:ILE:CG2	1:F:158:LEU:HD23	2.50	0.42
1:A:369:LYS:HE2	1:A:369:LYS:HB2	1.85	0.42
1:C:314:GLU:CD	1:C:356:TYR:CD2	2.98	0.42
2:D:140:GLU:HB3	2:D:195:ARG:C	2.45	0.42
2:B:209:GLN:H	2:B:209:GLN:HG3	1.62	0.42
1:C:118:LYS:HB2	1:C:118:LYS:HE2	1.72	0.42
2:D:186:LEU:HD12	2:D:186:LEU:HA	1.80	0.42
2:E:154:PHE:CE1	2:E:173:PRO:HD2	2.41	0.42
1:A:205:THR:CG2	1:A:219:ILE:HB	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ASP:HB3	1:A:368:GLN:OE1	2.20	0.41
2:D:29:LEU:HA	2:D:93:LYS:HE2	2.02	0.41
2:D:210:ARG:HA	2:D:210:ARG:HH11	1.84	0.41
2:B:100:ILE:HD13	2:B:100:ILE:HA	1.74	0.41
2:B:114:ILE:HG12	2:B:206:GLU:HG2	2.01	0.41
2:D:2:ASN:HD21	2:D:4:ASP:HB3	1.85	0.41
2:D:243:ILE:H	2:D:243:ILE:HG13	1.60	0.41
2:D:270:VAL:HB	2:D:273:GLU:HB2	2.01	0.41
2:E:26:LEU:HD12	2:E:26:LEU:N	2.21	0.41
1:A:224:THR:HA	1:A:328:THR:HA	2.02	0.41
1:A:248:ILE:H	1:A:248:ILE:HG13	1.48	0.41
2:B:28:ILE:HD13	2:B:28:ILE:HA	1.86	0.41
2:B:130:VAL:CG1	2:B:232:CYS:SG	3.05	0.41
1:C:79:LYS:HD3	1:C:79:LYS:HA	1.82	0.41
1:F:117:ARG:HE	1:F:118:LYS:HG3	1.86	0.41
2:B:252:GLN:HB3	2:B:255:VAL:HG23	2.02	0.41
1:C:234:LEU:HD23	1:C:234:LEU:HA	1.66	0.41
1:C:240:PHE:HB3	1:C:274:PHE:HD2	1.85	0.41
2:D:16:TYR:CE2	2:D:42:VAL:HG13	2.54	0.41
2:D:176:GLU:H	2:D:176:GLU:HG3	1.42	0.41
1:C:107:ILE:CG2	1:C:167:ASP:OD2	2.69	0.41
2:E:84:LEU:HB2	2:E:90:VAL:HG13	1.97	0.41
2:E:161:GLU:O	2:E:162:GLN:C	2.59	0.41
2:D:78:LEU:HD13	2:D:78:LEU:HA	1.82	0.41
2:D:140:GLU:H	2:D:140:GLU:HG3	1.55	0.41
2:E:103:LEU:HG	2:E:104:PRO:N	2.34	0.41
1:F:71:ARG:HA	1:F:71:ARG:HD2	1.69	0.41
2:D:22:LYS:HB2	2:D:22:LYS:HE2	1.72	0.41
2:D:93:LYS:HA	2:D:93:LYS:HD3	1.83	0.41
2:E:161:GLU:HB2	2:E:165:THR:CG2	2.51	0.41
1:F:96:ILE:CD1	1:F:158:LEU:CD2	2.94	0.41
1:A:153:LEU:HD21	1:A:360:ASN:HD21	1.85	0.41
1:A:217:LYS:HE2	1:A:217:LYS:HB2	1.84	0.41
1:A:328:THR:HG22	1:A:368:GLN:NE2	2.36	0.41
2:B:248:TRP:CH2	1:F:238:MET:HE3	2.56	0.41
2:B:256:ARG:HE	2:B:256:ARG:HB3	1.78	0.41
1:C:240:PHE:HB3	1:C:274:PHE:CD2	2.55	0.41
1:C:366:LYS:HZ3	1:C:366:LYS:HG3	1.67	0.41
2:D:115:PRO:HD2	2:D:220:MET:SD	2.61	0.41
2:D:143:ARG:O	2:D:156:ILE:O	2.39	0.41
2:E:152:HIS:CE1	2:E:174:SER:HB3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:162:GLN:HE21	2:E:162:GLN:HB3	1.76	0.41
2:E:197:ARG:HB3	2:E:226:ASP:OD1	2.21	0.41
1:F:96:ILE:CD1	1:F:158:LEU:HD22	2.51	0.41
1:A:291:ILE:HG23	1:A:315:LEU:HD23	2.03	0.41
2:D:71:SER:O	2:D:75:ARG:HG2	2.18	0.41
2:D:141:PHE:CD1	2:D:197:ARG:HB3	2.56	0.41
1:F:231:ILE:H	1:F:231:ILE:HG13	1.53	0.41
2:D:9:VAL:HG22	2:D:54:ILE:HB	2.01	0.40
2:D:145:TYR:HB3	2:D:183:PHE:HE2	1.86	0.40
1:C:208:LYS:HB2	1:C:208:LYS:HE2	1.19	0.40
2:D:116:LYS:HA	2:D:116:LYS:HD3	1.35	0.40
1:A:314:GLU:HB2	1:A:356:TYR:HE1	1.86	0.40
2:D:103:LEU:H	2:D:241:TYR:HE2	1.68	0.40
2:E:86:GLN:HB2	2:E:89:ALA:HB3	2.02	0.40
2:E:97:HIS:HE2	2:E:197:ARG:HH22	1.63	0.40
2:E:151:LYS:HB2	2:E:151:LYS:HE2	1.28	0.40
2:E:161:GLU:CG	2:E:165:THR:HG23	2.50	0.40
1:A:125:PHE:HD2	1:A:202:GLU:HG3	1.86	0.40
1:A:331:ILE:HD12	1:A:362:ILE:CA	2.43	0.40
2:B:31:GLU:C	2:B:93:LYS:NZ	2.63	0.40
1:C:112:LYS:HZ3	1:C:112:LYS:HG3	1.68	0.40
2:D:29:LEU:HA	2:D:93:LYS:CE	2.52	0.40
1:F:354:LEU:HD13	1:F:354:LEU:HA	1.71	0.40
2:E:37:HIS:HD2	2:E:95:ASN:HB2	1.85	0.40
2:E:168:ARG:HA	2:E:169:PRO:HD3	1.94	0.40
1:F:122:LEU:H	1:F:122:LEU:HG	1.57	0.40
1:F:140:ASP:HB2	1:F:143:THR:HB	2.03	0.40
1:F:311:ILE:HD13	1:F:311:ILE:HA	1.97	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	305/316 (96%)	301 (99%)	4 (1%)	0	100	100
1	C	305/316 (96%)	300 (98%)	5 (2%)	0	100	100
1	F	305/316 (96%)	304 (100%)	1 (0%)	0	100	100
2	B	274/276 (99%)	268 (98%)	4 (2%)	2 (1%)	18	53
2	D	274/276 (99%)	271 (99%)	2 (1%)	1 (0%)	30	65
2	E	274/276 (99%)	272 (99%)	2 (1%)	0	100	100
All	All	1737/1776 (98%)	1716 (99%)	18 (1%)	3 (0%)	44	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	169	PRO
2	B	39	PRO
2	B	169	PRO

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	272/280 (97%)	150 (55%)	122 (45%)	0	0
1	C	272/280 (97%)	143 (53%)	129 (47%)	0	0
1	F	272/280 (97%)	144 (53%)	128 (47%)	0	0
2	B	259/259 (100%)	144 (56%)	115 (44%)	0	0
2	D	259/259 (100%)	131 (51%)	128 (49%)	0	0
2	E	259/259 (100%)	138 (53%)	121 (47%)	0	0
All	All	1593/1617 (98%)	850 (53%)	743 (47%)	0	0

All (743) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	64	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	71	ARG
1	A	75	TYR
1	A	76	LYS
1	A	78	TRP
1	A	79	LYS
1	A	83	SER
1	A	92	LEU
1	A	93	ILE
1	A	96	ILE
1	A	97	GLN
1	A	101	LYS
1	A	107	ILE
1	A	108	ASP
1	A	109	LEU
1	A	112	LYS
1	A	114	GLU
1	A	117	ARG
1	A	121	ILE
1	A	123	VAL
1	A	126	LYS
1	A	127	GLU
1	A	130	GLU
1	A	135	THR
1	A	137	LEU
1	A	138	ILE
1	A	141	ILE
1	A	145	LEU
1	A	151	LYS
1	A	153	LEU
1	A	155	CYS
1	A	158	LEU
1	A	160	ILE
1	A	166	LYS
1	A	169	GLU
1	A	170	ARG
1	A	175	LEU
1	A	178	GLN
1	A	179	GLU
1	A	181	LEU
1	A	182	SER
1	A	188	MET
1	A	189	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	190	ASN
1	A	191	VAL
1	A	195	HIS
1	A	198	VAL
1	A	202	GLU
1	A	204	LEU
1	A	205	THR
1	A	208	LYS
1	A	222	ARG
1	A	225	VAL
1	A	226	VAL
1	A	227	ARG
1	A	229	SER
1	A	231	ILE
1	A	232	LYS
1	A	235	CYS
1	A	236	THR
1	A	237	LYS
1	A	245	CYS
1	A	247	GLU
1	A	248	ILE
1	A	253	LEU
1	A	257	LYS
1	A	260	LEU
1	A	263	LYS
1	A	266	VAL
1	A	268	VAL
1	A	272	ARG
1	A	278	ARG
1	A	282	LEU
1	A	283	THR
1	A	285	THR
1	A	286	MET
1	A	287	ASP
1	A	289	GLN
1	A	290	SER
1	A	291	ILE
1	A	292	LYS
1	A	293	ILE
1	A	294	GLN
1	A	296	LEU
1	A	297	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	298	SER
1	A	300	ASP
1	A	301	GLN
1	A	303	GLU
1	A	306	ARG
1	A	307	ILE
1	A	309	ARG
1	A	311	ILE
1	A	314	GLU
1	A	315	LEU
1	A	316	VAL
1	A	317	HIS
1	A	319	LEU
1	A	321	ASP
1	A	322	SER
1	A	324	VAL
1	A	328	THR
1	A	329	VAL
1	A	331	ILE
1	A	334	ILE
1	A	335	VAL
1	A	336	LYS
1	A	337	VAL
1	A	341	GLU
1	A	345	ARG
1	A	346	ASN
1	A	350	LYS
1	A	351	CYS
1	A	352	MET
1	A	353	PHE
1	A	354	LEU
1	A	357	ILE
1	A	361	SER
1	A	363	SER
1	A	366	LYS
1	A	369	LYS
2	B	1	MET
2	B	4	ASP
2	B	8	LEU
2	B	11	GLN
2	B	18	SER
2	B	19	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	22	LYS
2	B	23	ASN
2	B	24	ASP
2	B	25	ILE
2	B	26	LEU
2	B	27	LEU
2	B	29	LEU
2	B	30	LYS
2	B	31	GLU
2	B	32	ARG
2	B	33	ASP
2	B	34	GLU
2	B	41	VAL
2	B	42	VAL
2	B	49	GLU
2	B	52	MET
2	B	54	ILE
2	B	56	GLU
2	B	60	MET
2	B	63	SER
2	B	66	LEU
2	B	78	LEU
2	B	81	LEU
2	B	82	GLN
2	B	84	LEU
2	B	88	GLU
2	B	90	VAL
2	B	93	LYS
2	B	94	GLN
2	B	96	LEU
2	B	100	ILE
2	B	101	SER
2	B	105	VAL
2	B	114	ILE
2	B	117	THR
2	B	118	LYS
2	B	119	ASP
2	B	124	LEU
2	B	126	VAL
2	B	130	VAL
2	B	132	ARG
2	B	135	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	136	VAL
2	B	137	LYS
2	B	139	LEU
2	B	140	GLU
2	B	142	GLU
2	B	145	TYR
2	B	146	MET
2	B	149	LYS
2	B	150	CYS
2	B	152	HIS
2	B	153	VAL
2	B	156	ILE
2	B	157	LYS
2	B	162	GLN
2	B	163	TYR
2	B	168	ARG
2	B	170	SER
2	B	171	SER
2	B	176	GLU
2	B	177	SER
2	B	182	LYS
2	B	184	THR
2	B	186	LEU
2	B	189	LEU
2	B	192	SER
2	B	194	THR
2	B	197	ARG
2	B	198	ASP
2	B	201	GLU
2	B	205	GLN
2	B	207	GLN
2	B	208	VAL
2	B	209	GLN
2	B	211	LEU
2	B	212	SER
2	B	213	VAL
2	B	218	ARG
2	B	219	SER
2	B	220	MET
2	B	221	LYS
2	B	225	GLU
2	B	227	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	228	LEU
2	B	229	VAL
2	B	230	ASP
2	B	233	LYS
2	B	234	SER
2	B	238	LEU
2	B	239	THR
2	B	240	ILE
2	B	243	ILE
2	B	244	VAL
2	B	245	MET
2	B	246	GLN
2	B	247	ARG
2	B	249	LYS
2	B	251	PHE
2	B	252	GLN
2	B	255	VAL
2	B	256	ARG
2	B	258	GLU
2	B	262	VAL
2	B	263	LEU
2	B	268	ILE
2	B	269	GLN
2	B	273	GLU
2	B	274	GLN
1	C	63	GLN
1	C	65	MET
1	C	69	LEU
1	C	71	ARG
1	C	72	PHE
1	C	76	LYS
1	C	79	LYS
1	C	80	LEU
1	C	84	GLU
1	C	85	VAL
1	C	92	LEU
1	C	93	ILE
1	C	94	GLU
1	C	96	ILE
1	C	100	GLU
1	C	101	LYS
1	C	106	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	107	ILE
1	C	108	ASP
1	C	109	LEU
1	C	112	LYS
1	C	113	ASP
1	C	118	LYS
1	C	120	SER
1	C	122	LEU
1	C	123	VAL
1	C	126	LYS
1	C	134	VAL
1	C	137	LEU
1	C	138	ILE
1	C	141	ILE
1	C	145	LEU
1	C	151	LYS
1	C	152	THR
1	C	153	LEU
1	C	156	MET
1	C	160	ILE
1	C	162	GLN
1	C	163	VAL
1	C	164	LEU
1	C	165	THR
1	C	166	LYS
1	C	169	GLU
1	C	170	ARG
1	C	174	GLU
1	C	176	GLN
1	C	179	GLU
1	C	184	ASP
1	C	186	GLU
1	C	187	THR
1	C	188	MET
1	C	189	VAL
1	C	191	VAL
1	C	193	HIS
1	C	194	ILE
1	C	198	VAL
1	C	204	LEU
1	C	207	LEU
1	C	208	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	210	VAL
1	C	211	ARG
1	C	213	ASN
1	C	215	TYR
1	C	217	LYS
1	C	219	ILE
1	C	222	ARG
1	C	224	THR
1	C	226	VAL
1	C	227	ARG
1	C	229	SER
1	C	230	ASN
1	C	232	LYS
1	C	234	LEU
1	C	235	CYS
1	C	236	THR
1	C	237	LYS
1	C	245	CYS
1	C	247	GLU
1	C	248	ILE
1	C	249	GLN
1	C	253	LEU
1	C	255	ASP
1	C	257	LYS
1	C	264	CYS
1	C	266	VAL
1	C	268	VAL
1	C	272	ARG
1	C	277	LEU
1	C	279	SER
1	C	285	THR
1	C	286	MET
1	C	287	ASP
1	C	290	SER
1	C	291	ILE
1	C	292	LYS
1	C	293	ILE
1	C	294	GLN
1	C	296	LEU
1	C	297	MET
1	C	298	SER
1	C	300	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	302	ARG
1	C	306	ARG
1	C	311	ILE
1	C	317	HIS
1	C	319	LEU
1	C	321	ASP
1	C	323	CYS
1	C	324	VAL
1	C	328	THR
1	C	329	VAL
1	C	330	THR
1	C	332	THR
1	C	334	ILE
1	C	335	VAL
1	C	336	LYS
1	C	342	GLU
1	C	345	ARG
1	C	347	LYS
1	C	350	LYS
1	C	351	CYS
1	C	352	MET
1	C	354	LEU
1	C	355	LEU
1	C	361	SER
1	C	362	ILE
1	C	363	SER
1	C	365	SER
1	C	366	LYS
2	D	1	MET
2	D	3	SER
2	D	5	GLN
2	D	9	VAL
2	D	20	TYR
2	D	22	LYS
2	D	23	ASN
2	D	26	LEU
2	D	28	ILE
2	D	30	LYS
2	D	32	ARG
2	D	34	GLU
2	D	41	VAL
2	D	45	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	46	THR
2	D	47	LEU
2	D	49	GLU
2	D	54	ILE
2	D	56	GLU
2	D	63	SER
2	D	64	GLU
2	D	65	VAL
2	D	66	LEU
2	D	69	PHE
2	D	73	LEU
2	D	75	ARG
2	D	76	SER
2	D	78	LEU
2	D	80	ILE
2	D	82	GLN
2	D	84	LEU
2	D	86	GLN
2	D	88	GLU
2	D	90	VAL
2	D	91	SER
2	D	92	MET
2	D	93	LYS
2	D	95	ASN
2	D	96	LEU
2	D	97	HIS
2	D	99	ARG
2	D	100	ILE
2	D	105	VAL
2	D	106	CYS
2	D	108	GLU
2	D	109	LEU
2	D	110	VAL
2	D	111	ARG
2	D	114	ILE
2	D	116	LYS
2	D	118	LYS
2	D	119	ASP
2	D	120	VAL
2	D	124	LEU
2	D	126	VAL
2	D	131	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	132	ARG
2	D	135	LEU
2	D	136	VAL
2	D	137	LYS
2	D	139	LEU
2	D	140	GLU
2	D	142	GLU
2	D	143	ARG
2	D	146	MET
2	D	149	LYS
2	D	151	LYS
2	D	153	VAL
2	D	155	VAL
2	D	167	CYS
2	D	168	ARG
2	D	171	SER
2	D	172	CYS
2	D	175	LEU
2	D	176	GLU
2	D	177	SER
2	D	179	ASP
2	D	182	LYS
2	D	183	PHE
2	D	185	CYS
2	D	187	SER
2	D	189	LEU
2	D	190	SER
2	D	191	SER
2	D	192	SER
2	D	194	THR
2	D	197	ARG
2	D	201	GLU
2	D	203	LYS
2	D	204	ILE
2	D	205	GLN
2	D	208	VAL
2	D	209	GLN
2	D	210	ARG
2	D	212	SER
2	D	213	VAL
2	D	216	ILE
2	D	220	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	222	VAL
2	D	224	LEU
2	D	226	ASP
2	D	228	LEU
2	D	229	VAL
2	D	230	ASP
2	D	232	CYS
2	D	233	LYS
2	D	234	SER
2	D	239	THR
2	D	240	ILE
2	D	243	ILE
2	D	244	VAL
2	D	245	MET
2	D	246	GLN
2	D	247	ARG
2	D	249	LYS
2	D	251	PHE
2	D	252	GLN
2	D	254	ASP
2	D	256	ARG
2	D	257	CYS
2	D	258	GLU
2	D	259	VAL
2	D	260	GLU
2	D	263	LEU
2	D	268	ILE
2	D	270	VAL
2	D	273	GLU
2	D	276	SER
2	E	4	ASP
2	E	5	GLN
2	E	8	LEU
2	E	14	GLU
2	E	15	SER
2	E	19	GLU
2	E	21	HIS
2	E	22	LYS
2	E	23	ASN
2	E	26	LEU
2	E	28	ILE
2	E	29	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	30	LYS
2	E	32	ARG
2	E	33	ASP
2	E	35	ASP
2	E	42	VAL
2	E	45	MET
2	E	46	THR
2	E	47	LEU
2	E	52	MET
2	E	56	GLU
2	E	61	PHE
2	E	63	SER
2	E	68	ILE
2	E	70	ASP
2	E	73	LEU
2	E	74	ARG
2	E	75	ARG
2	E	80	ILE
2	E	81	LEU
2	E	82	GLN
2	E	84	LEU
2	E	88	GLU
2	E	91	SER
2	E	92	MET
2	E	93	LYS
2	E	94	GLN
2	E	96	LEU
2	E	100	ILE
2	E	103	LEU
2	E	105	VAL
2	E	106	CYS
2	E	108	GLU
2	E	109	LEU
2	E	112	GLU
2	E	114	ILE
2	E	116	LYS
2	E	118	LYS
2	E	120	VAL
2	E	124	LEU
2	E	126	VAL
2	E	130	VAL
2	E	131	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	132	ARG
2	E	135	LEU
2	E	136	VAL
2	E	137	LYS
2	E	138	VAL
2	E	140	GLU
2	E	142	GLU
2	E	143	ARG
2	E	146	MET
2	E	149	LYS
2	E	150	CYS
2	E	151	LYS
2	E	153	VAL
2	E	155	VAL
2	E	156	ILE
2	E	157	LYS
2	E	159	ASP
2	E	161	GLU
2	E	162	GLN
2	E	168	ARG
2	E	170	SER
2	E	171	SER
2	E	175	LEU
2	E	176	GLU
2	E	178	CYS
2	E	179	ASP
2	E	182	LYS
2	E	184	THR
2	E	185	CYS
2	E	186	LEU
2	E	187	SER
2	E	189	LEU
2	E	191	SER
2	E	194	THR
2	E	199	TYR
2	E	200	GLN
2	E	201	GLU
2	E	203	LYS
2	E	204	ILE
2	E	206	GLU
2	E	208	VAL
2	E	209	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	211	LEU
2	E	212	SER
2	E	213	VAL
2	E	216	ILE
2	E	220	MET
2	E	224	LEU
2	E	227	ASP
2	E	229	VAL
2	E	232	CYS
2	E	234	SER
2	E	238	LEU
2	E	239	THR
2	E	240	ILE
2	E	243	ILE
2	E	244	VAL
2	E	245	MET
2	E	249	LYS
2	E	251	PHE
2	E	257	CYS
2	E	258	GLU
2	E	259	VAL
2	E	261	ILE
2	E	263	LEU
2	E	268	ILE
2	E	272	ASN
1	F	63	GLN
1	F	65	MET
1	F	66	GLN
1	F	68	THR
1	F	69	LEU
1	F	71	ARG
1	F	73	ILE
1	F	76	LYS
1	F	79	LYS
1	F	80	LEU
1	F	82	PHE
1	F	85	VAL
1	F	92	LEU
1	F	93	ILE
1	F	94	GLU
1	F	95	LYS
1	F	101	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	105	ARG
1	F	106	HIS
1	F	107	ILE
1	F	108	ASP
1	F	109	LEU
1	F	112	LYS
1	F	113	ASP
1	F	117	ARG
1	F	118	LYS
1	F	120	SER
1	F	121	ILE
1	F	122	LEU
1	F	123	VAL
1	F	126	LYS
1	F	133	GLU
1	F	134	VAL
1	F	135	THR
1	F	137	LEU
1	F	138	ILE
1	F	140	ASP
1	F	141	ILE
1	F	143	THR
1	F	145	LEU
1	F	146	ARG
1	F	153	LEU
1	F	158	LEU
1	F	162	GLN
1	F	163	VAL
1	F	166	LYS
1	F	167	ASP
1	F	168	LEU
1	F	170	ARG
1	F	174	GLU
1	F	176	GLN
1	F	181	LEU
1	F	186	GLU
1	F	187	THR
1	F	191	VAL
1	F	193	HIS
1	F	198	VAL
1	F	202	GLU
1	F	204	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	208	LYS
1	F	213	ASN
1	F	221	LEU
1	F	225	VAL
1	F	227	ARG
1	F	230	ASN
1	F	231	ILE
1	F	232	LYS
1	F	235	CYS
1	F	236	THR
1	F	237	LYS
1	F	238	MET
1	F	242	CYS
1	F	247	GLU
1	F	248	ILE
1	F	250	SER
1	F	253	LEU
1	F	257	LYS
1	F	260	LEU
1	F	262	THR
1	F	263	LYS
1	F	266	VAL
1	F	268	VAL
1	F	270	ARG
1	F	272	ARG
1	F	277	LEU
1	F	278	ARG
1	F	279	SER
1	F	283	THR
1	F	285	THR
1	F	286	MET
1	F	287	ASP
1	F	289	GLN
1	F	290	SER
1	F	291	ILE
1	F	292	LYS
1	F	293	ILE
1	F	296	LEU
1	F	297	MET
1	F	298	SER
1	F	300	ASP
1	F	301	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	307	ILE
1	F	315	LEU
1	F	316	VAL
1	F	318	ASP
1	F	320	VAL
1	F	323	CYS
1	F	324	VAL
1	F	328	THR
1	F	330	THR
1	F	331	ILE
1	F	334	ILE
1	F	335	VAL
1	F	337	VAL
1	F	341	GLU
1	F	342	GLU
1	F	347	LYS
1	F	352	MET
1	F	354	LEU
1	F	355	LEU
1	F	357	ILE
1	F	361	SER
1	F	363	SER
1	F	364	ASN
1	F	365	SER
1	F	366	LYS
1	F	368	GLN
1	F	369	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	106	HIS
1	A	176	GLN
1	A	183	ASN
1	A	190	ASN
1	A	193	HIS
1	A	289	GLN
1	A	317	HIS
1	A	346	ASN
1	A	360	ASN
1	A	368	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	5	GLN
2	B	59	ASN
2	B	82	GLN
2	B	94	GLN
2	B	97	HIS
2	B	162	GLN
2	B	205	GLN
2	B	207	GLN
2	B	269	GLN
2	B	271	ASN
1	C	66	GLN
1	C	106	HIS
1	C	136	ASN
1	C	161	HIS
1	C	162	GLN
1	C	176	GLN
1	C	190	ASN
1	C	195	HIS
1	C	200	ASN
1	C	206	GLN
1	C	289	GLN
1	C	360	ASN
2	D	2	ASN
2	D	21	HIS
2	D	23	ASN
2	D	37	HIS
2	D	82	GLN
2	D	95	ASN
2	D	252	GLN
2	D	269	GLN
2	D	271	ASN
2	E	23	ASN
2	E	37	HIS
2	E	59	ASN
2	E	86	GLN
2	E	94	GLN
2	E	97	HIS
2	E	162	GLN
2	E	266	ASN
2	E	269	GLN
1	F	136	ASN
1	F	176	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

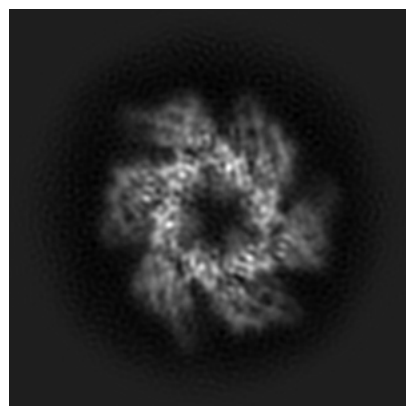
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33989. These allow visual inspection of the internal detail of the map and identification of artifacts.

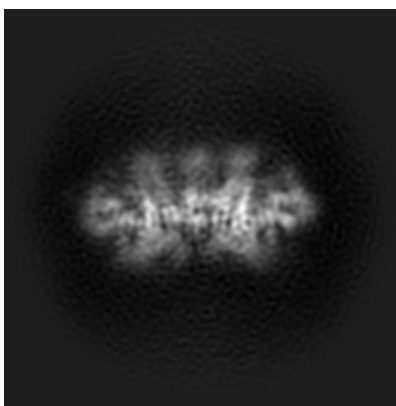
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

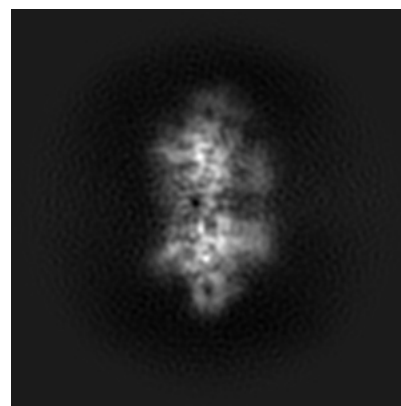
6.1.1 Primary map



X

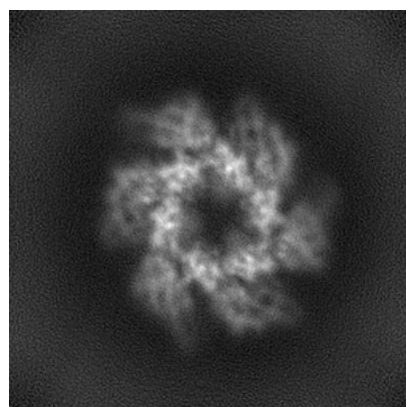


Y

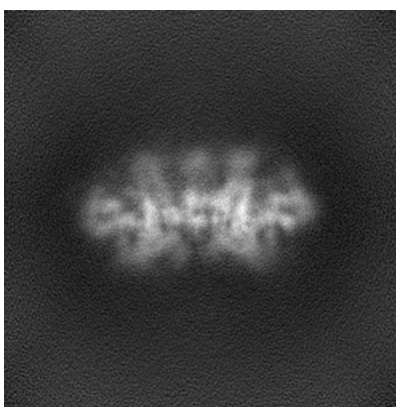


Z

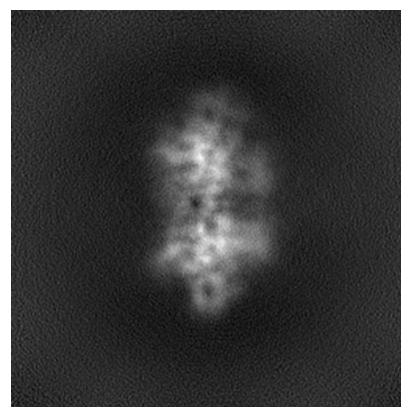
6.1.2 Raw map



X



Y

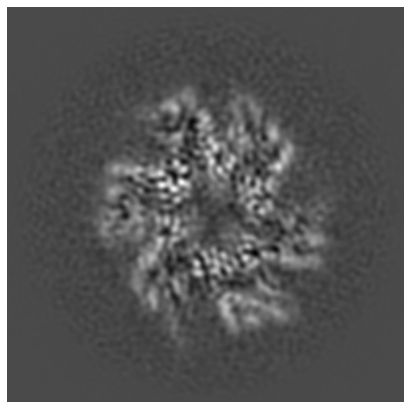


Z

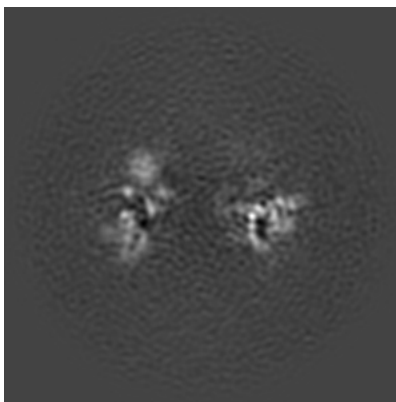
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

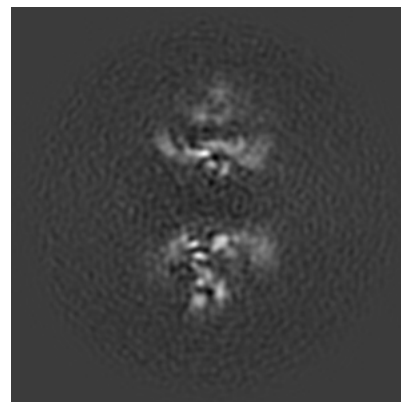
6.2.1 Primary map



X Index: 128

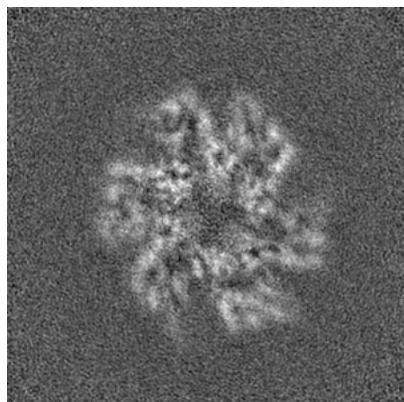


Y Index: 128

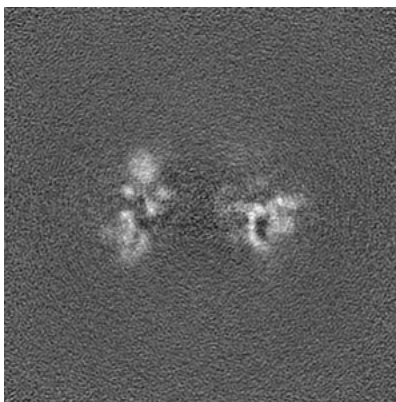


Z Index: 128

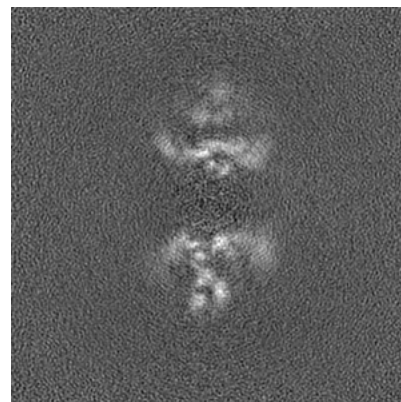
6.2.2 Raw map



X Index: 128



Y Index: 128

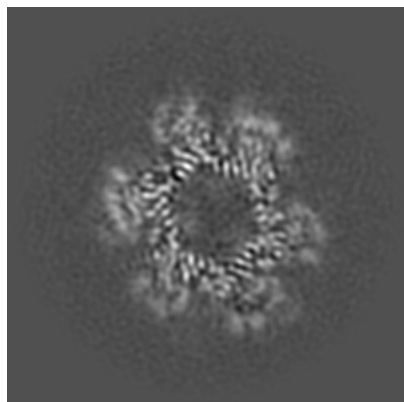


Z Index: 128

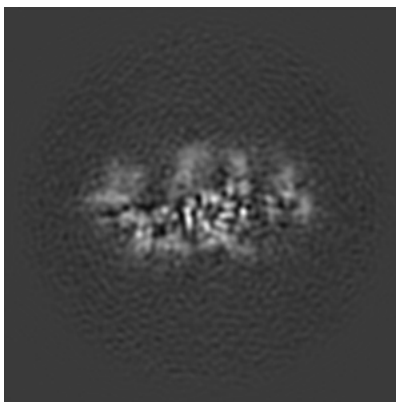
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

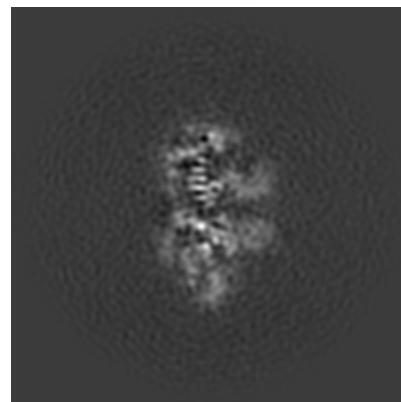
6.3.1 Primary map



X Index: 121

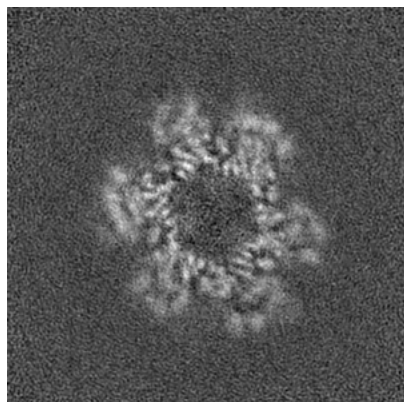


Y Index: 103

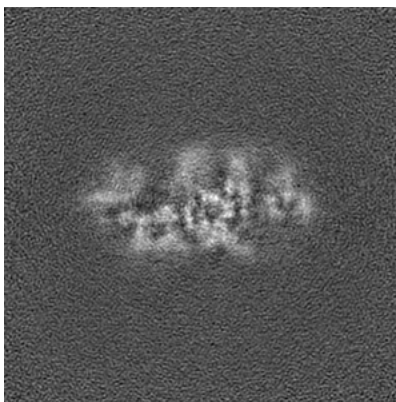


Z Index: 153

6.3.2 Raw map



X Index: 121



Y Index: 104

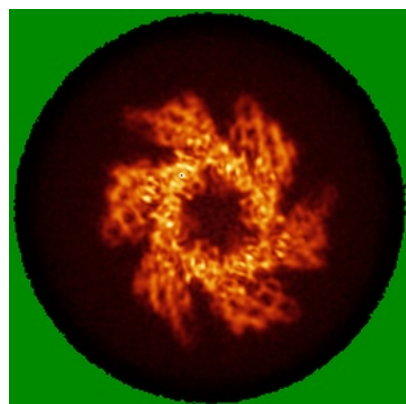


Z Index: 152

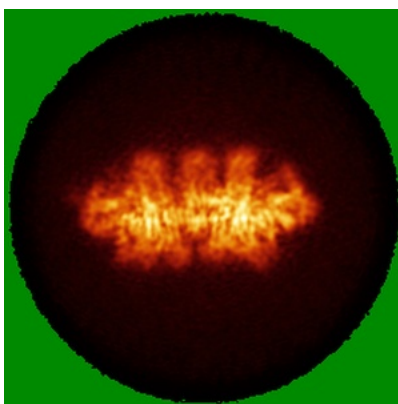
The images above show the largest variance slices of the map in three orthogonal directions.

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

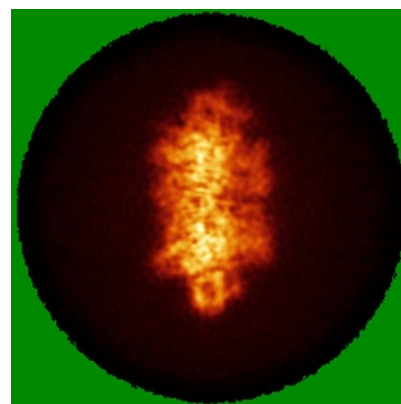
6.4.1 Primary map



X

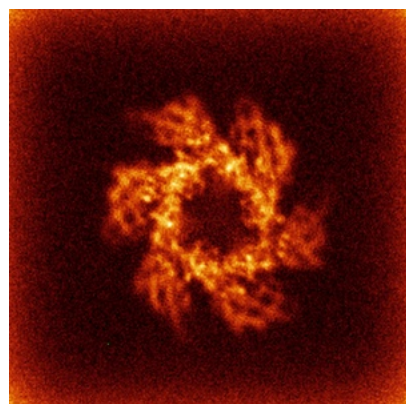


Y

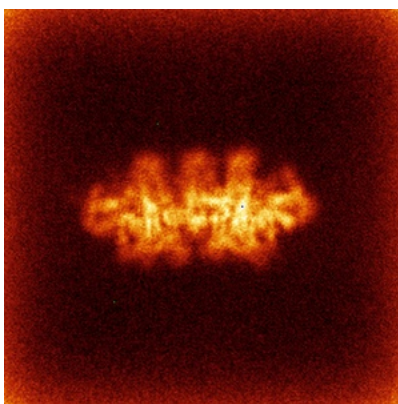


Z

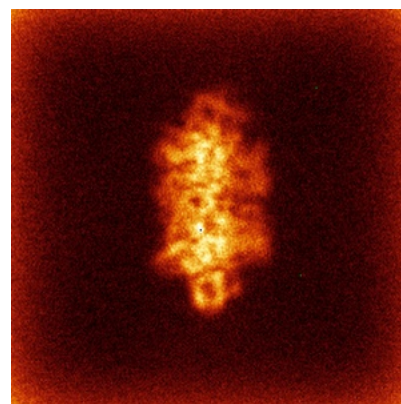
6.4.2 Raw map



X



Y

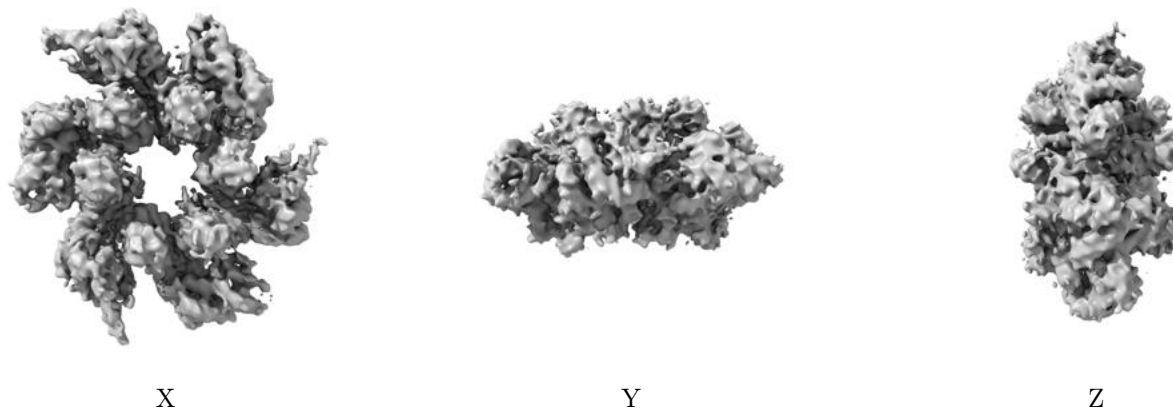


Z

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

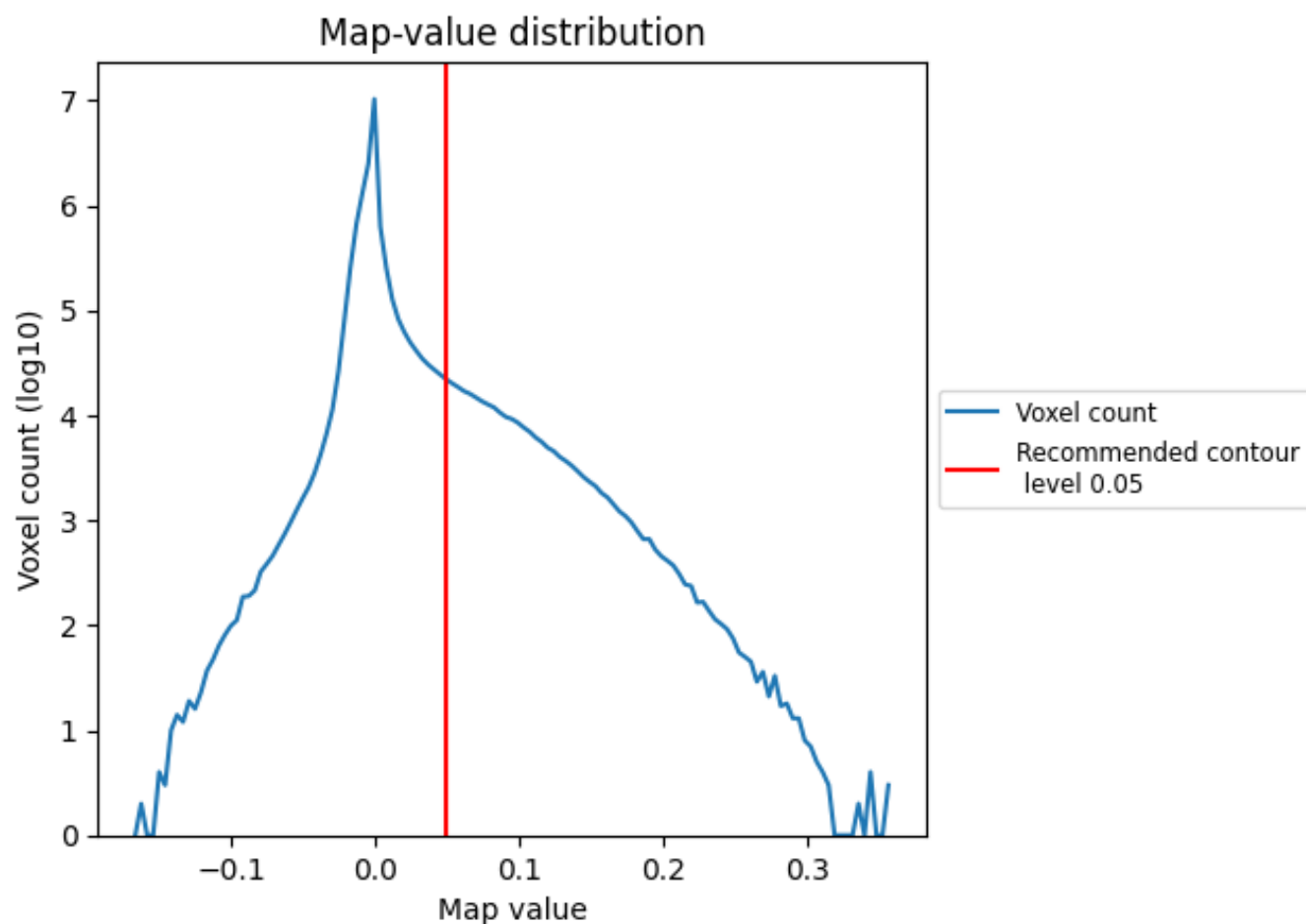
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

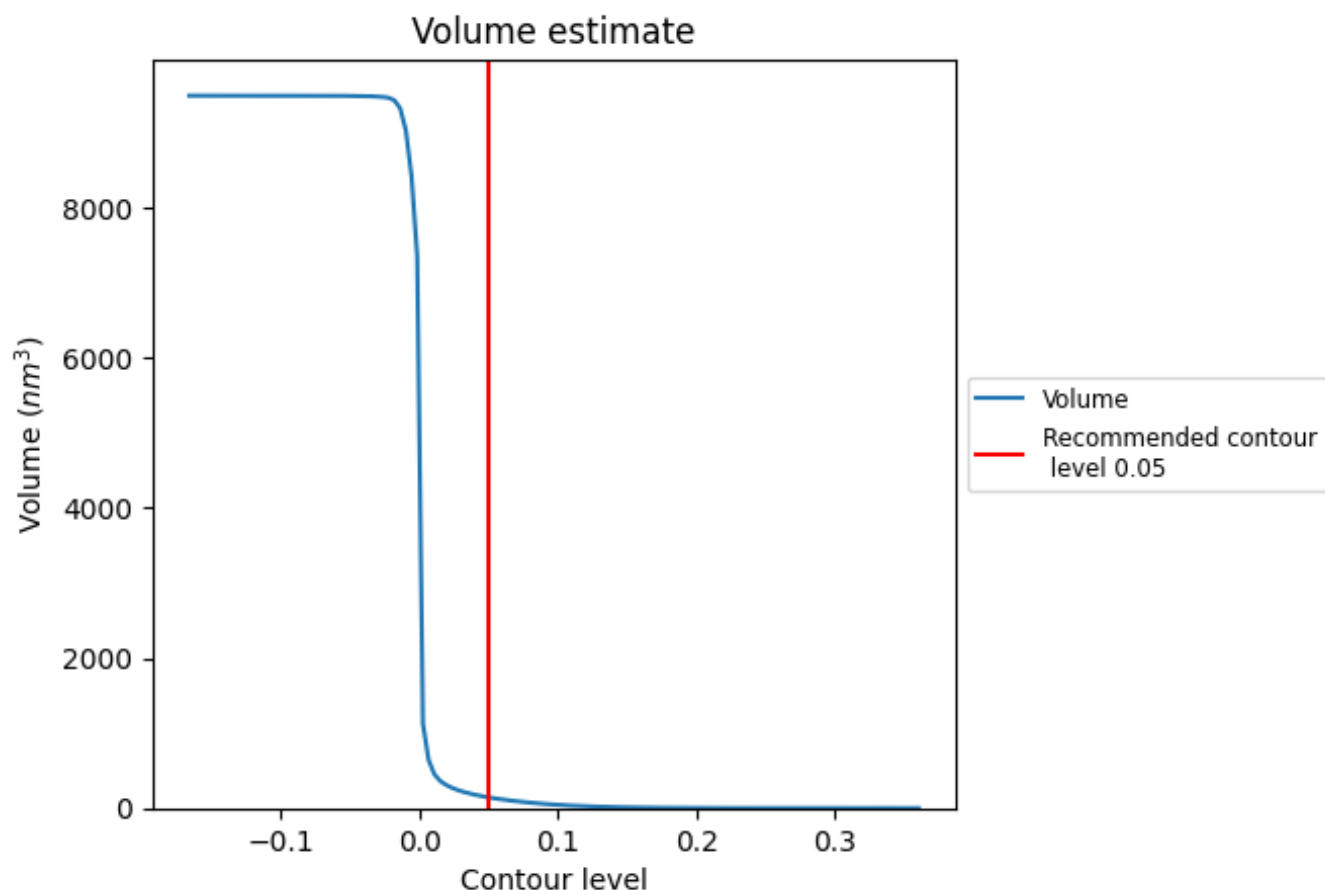
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

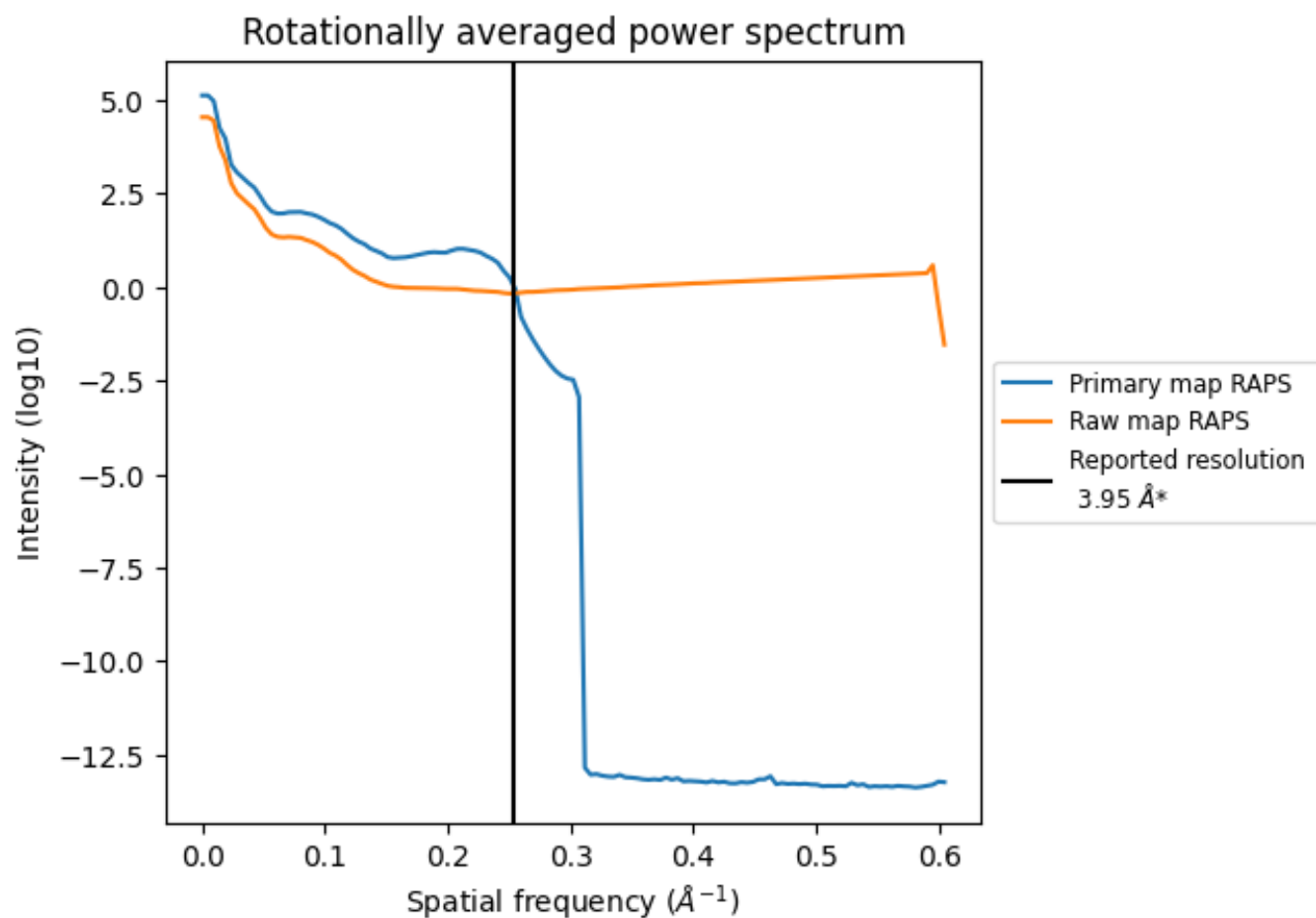
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm^3 ; this corresponds to an approximate mass of 130 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 ⓘ

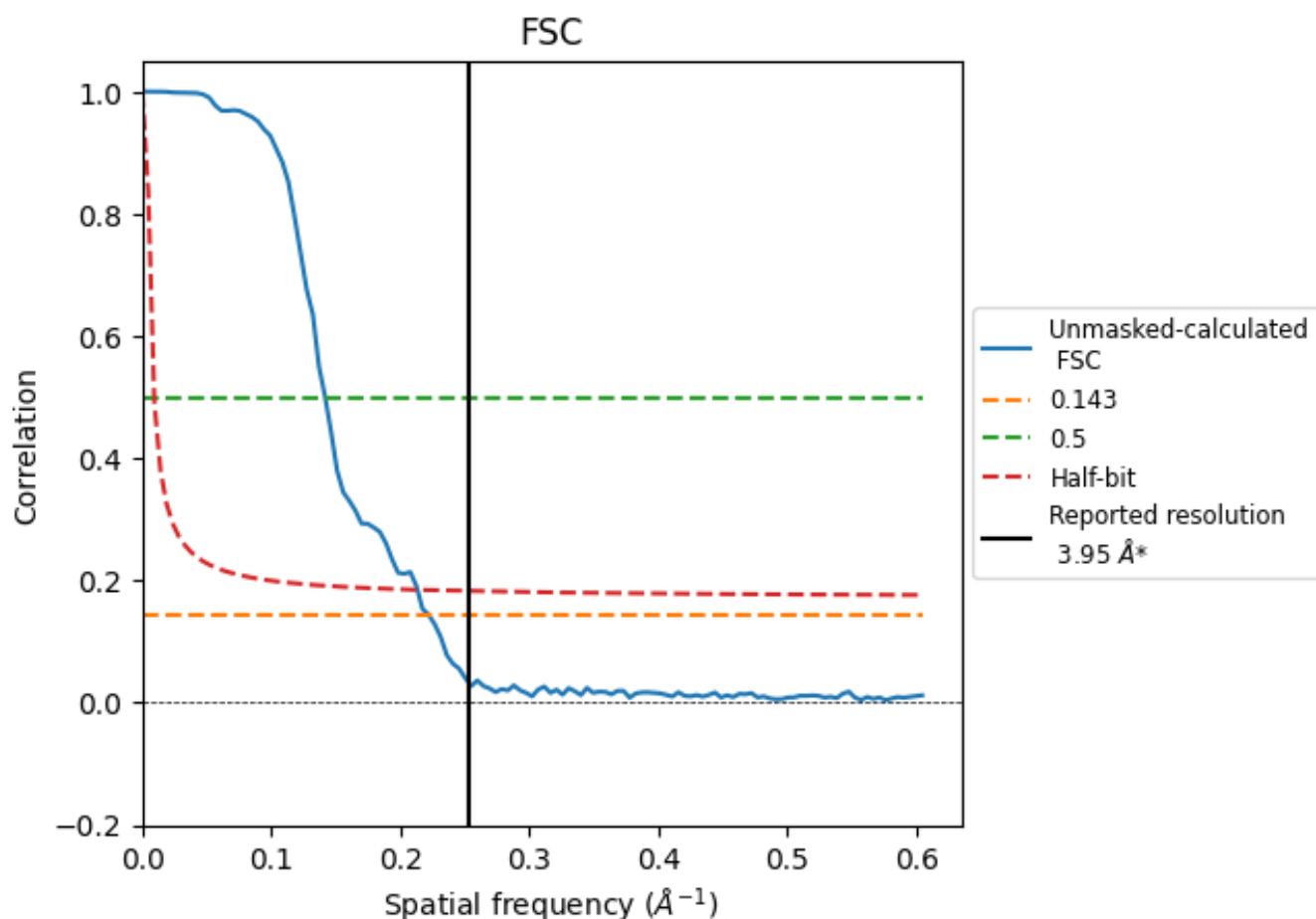


*Reported resolution corresponds to spatial frequency of 0.253 Å⁻¹

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 0.253 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.95	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.50	7.05	4.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.50 differs from the reported value 3.95 by more than 10 %

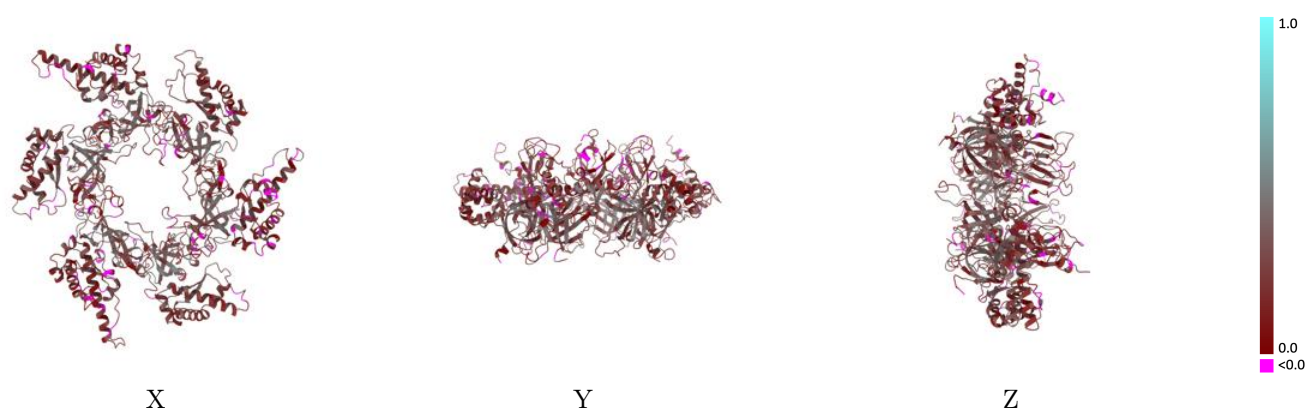
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-33989 and PDB model 7YOX. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)

This section was not generated.

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

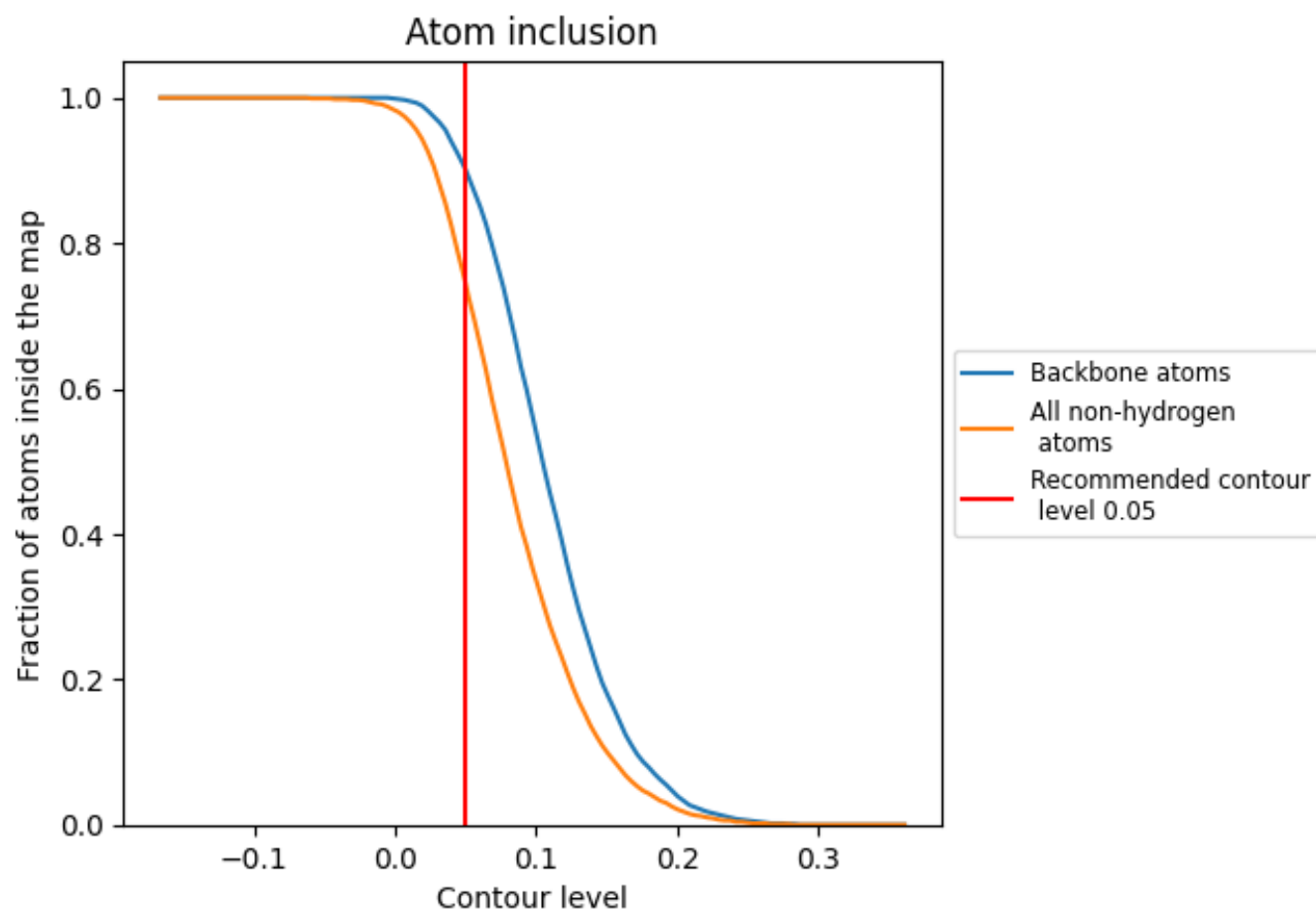


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 74% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.2450
A	0.6610	0.2230
B	0.7460	0.2580
C	0.7500	0.2460
D	0.8130	0.2590
E	0.8090	0.2540
F	0.6950	0.2320

1.0

0.0

<0.0