



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:08 PM UTC

PDB ID : 5HI9 / pdb_00005hi9
EMDB ID : EMD-6580
Title : Structure of the full-length TRPV2 channel by cryo-electron microscopy
Authors : Huynh, K.W.; Cohen, M.R.; Jiansen, J.; Samanta, A.; Lodowski, D.T.; Zhou, Z.H.; Moiseenkova-Bell, V.Y.
Deposited on : 2016-01-11
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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

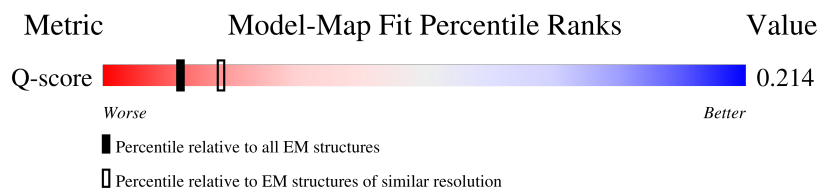
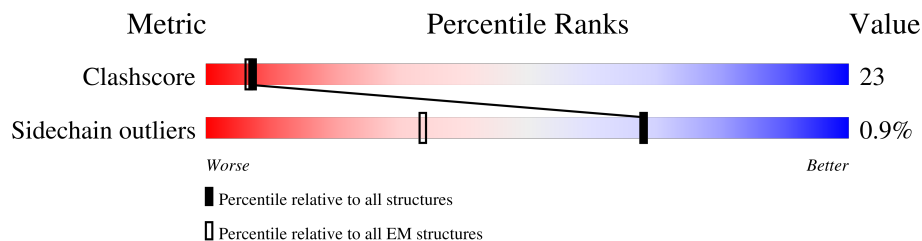
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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

Mol	Chain	Length	Quality of chain
1	A	770	9% 57% 18% • • 22%
1	B	770	9% 57% 18% • • 22%
1	C	770	9% 58% 17% • • 22%
1	D	770	9% 58% 17% • • 22%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19636 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 Transient Receptor Potential Cation Channel Subfamily V Member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	602	Total	C	N	O	S	0	0
			4909	3207	825	849	28		
1	B	602	Total	C	N	O	S	0	0
			4909	3207	825	849	28		
1	C	602	Total	C	N	O	S	0	0
			4909	3207	825	849	28		
1	D	602	Total	C	N	O	S	0	0
			4909	3207	825	849	28		

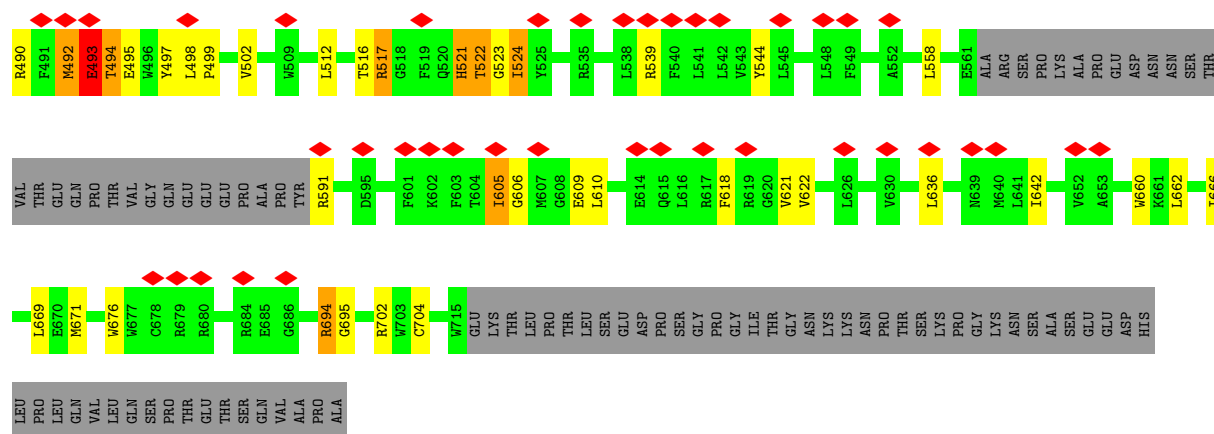
There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	PRO	LEU	conflict	UNP Q9WUD2
A	762	THR	-	expression tag	UNP Q9WUD2
A	763	GLU	-	expression tag	UNP Q9WUD2
A	764	THR	-	expression tag	UNP Q9WUD2
A	765	SER	-	expression tag	UNP Q9WUD2
A	766	GLN	-	expression tag	UNP Q9WUD2
A	767	VAL	-	expression tag	UNP Q9WUD2
A	768	ALA	-	expression tag	UNP Q9WUD2
A	769	PRO	-	expression tag	UNP Q9WUD2
A	770	ALA	-	expression tag	UNP Q9WUD2
B	151	PRO	LEU	conflict	UNP Q9WUD2
B	762	THR	-	expression tag	UNP Q9WUD2
B	763	GLU	-	expression tag	UNP Q9WUD2
B	764	THR	-	expression tag	UNP Q9WUD2
B	765	SER	-	expression tag	UNP Q9WUD2
B	766	GLN	-	expression tag	UNP Q9WUD2
B	767	VAL	-	expression tag	UNP Q9WUD2
B	768	ALA	-	expression tag	UNP Q9WUD2
B	769	PRO	-	expression tag	UNP Q9WUD2
B	770	ALA	-	expression tag	UNP Q9WUD2
C	151	PRO	LEU	conflict	UNP Q9WUD2

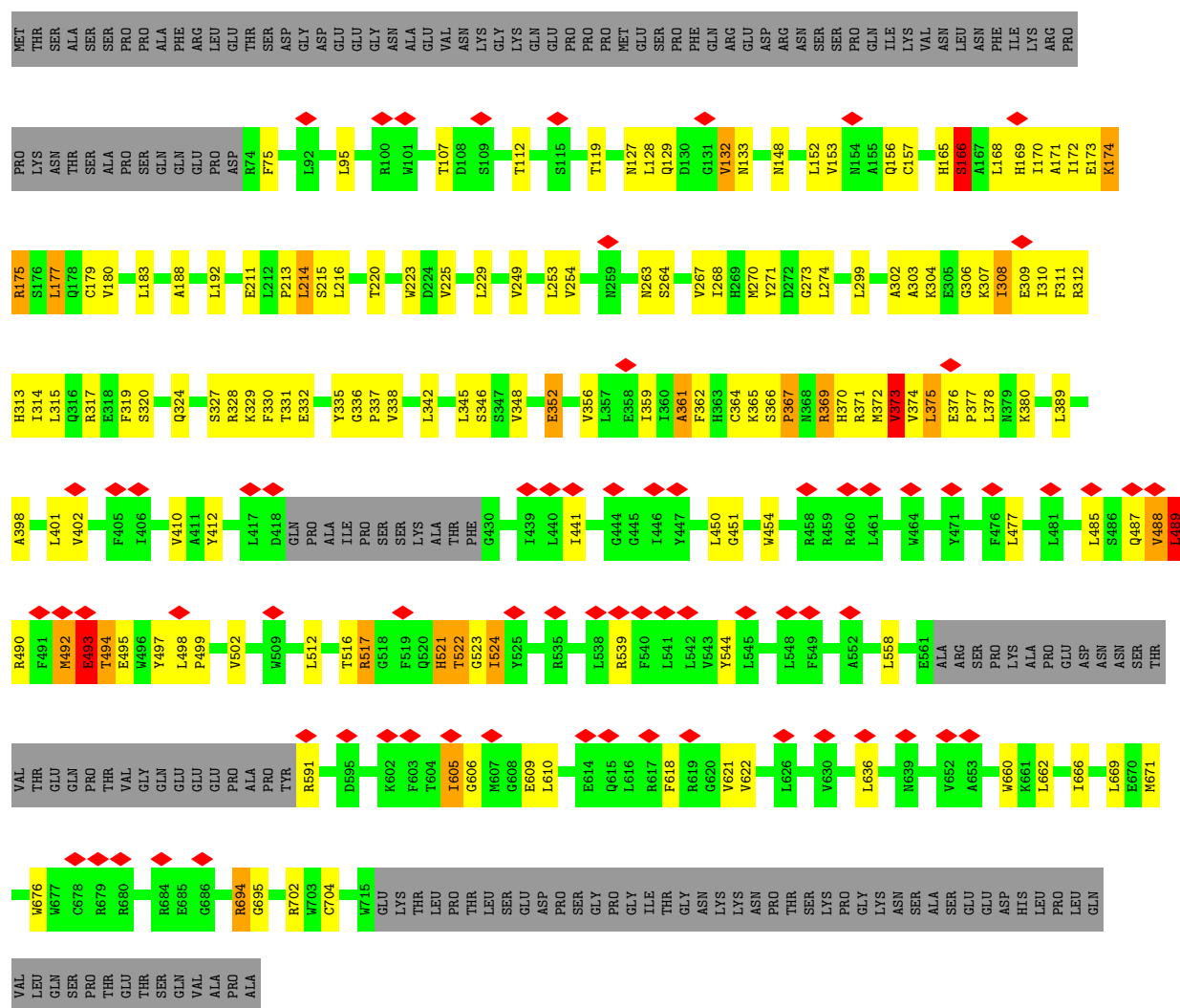
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	762	THR	-	expression tag	UNP Q9WUD2
C	763	GLU	-	expression tag	UNP Q9WUD2
C	764	THR	-	expression tag	UNP Q9WUD2
C	765	SER	-	expression tag	UNP Q9WUD2
C	766	GLN	-	expression tag	UNP Q9WUD2
C	767	VAL	-	expression tag	UNP Q9WUD2
C	768	ALA	-	expression tag	UNP Q9WUD2
C	769	PRO	-	expression tag	UNP Q9WUD2
C	770	ALA	-	expression tag	UNP Q9WUD2
D	151	PRO	LEU	conflict	UNP Q9WUD2
D	762	THR	-	expression tag	UNP Q9WUD2
D	763	GLU	-	expression tag	UNP Q9WUD2
D	764	THR	-	expression tag	UNP Q9WUD2
D	765	SER	-	expression tag	UNP Q9WUD2
D	766	GLN	-	expression tag	UNP Q9WUD2
D	767	VAL	-	expression tag	UNP Q9WUD2
D	768	ALA	-	expression tag	UNP Q9WUD2
D	769	PRO	-	expression tag	UNP Q9WUD2
D	770	ALA	-	expression tag	UNP Q9WUD2



• Molecule 1: Transient Receptor Potential Cation Channel Subfamily V Member 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	42550	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	21	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.017	Depositor
Map size ($\text{\AA}$)	247.68, 247.68, 247.68	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.29, 1.29, 1.29	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/5031	1.01	18/6822 (0.3%)
1	B	0.61	0/5031	1.01	18/6822 (0.3%)
1	C	0.61	0/5031	1.01	18/6822 (0.3%)
1	D	0.61	0/5031	1.01	18/6822 (0.3%)
All	All	0.61	0/20124	1.01	72/27288 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
1	B	0	16
1	C	0	16
1	D	0	16
All	All	0	64

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	ILE	N-CA-C	14.80	125.67	110.72
1	D	308	ILE	N-CA-C	14.80	125.67	110.72
1	C	308	ILE	N-CA-C	14.80	125.66	110.72
1	B	308	ILE	N-CA-C	14.78	125.65	110.72
1	B	307	LYS	CB-CA-C	12.77	130.32	109.89
1	D	307	LYS	CB-CA-C	12.76	130.30	109.89
1	A	307	LYS	CB-CA-C	12.76	130.30	109.89
1	C	307	LYS	CB-CA-C	12.74	130.27	109.89
1	B	524	ILE	N-CA-C	-12.25	95.77	111.09
1	C	524	ILE	N-CA-C	-12.24	95.79	111.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	524	ILE	N-CA-C	-12.22	95.81	111.09
1	D	524	ILE	N-CA-C	-12.22	95.81	111.09
1	C	494	THR	N-CA-C	11.78	129.13	110.17
1	B	494	THR	N-CA-C	11.75	129.09	110.17
1	A	494	THR	N-CA-C	11.74	129.08	110.17
1	D	494	THR	N-CA-C	11.72	129.04	110.17
1	D	307	LYS	N-CA-C	-10.50	94.21	109.96
1	D	346	SER	N-CA-C	10.50	122.68	111.03
1	A	346	SER	N-CA-C	10.48	122.67	111.03
1	C	346	SER	N-CA-C	10.48	122.66	111.03
1	A	307	LYS	N-CA-C	-10.47	94.25	109.96
1	B	346	SER	N-CA-C	10.47	122.65	111.03
1	B	307	LYS	N-CA-C	-10.46	94.27	109.96
1	C	307	LYS	N-CA-C	-10.46	94.27	109.96
1	C	361	ALA	N-CA-C	9.00	120.86	111.14
1	A	361	ALA	N-CA-C	9.00	120.86	111.14
1	D	361	ALA	N-CA-C	8.99	120.84	111.14
1	B	361	ALA	N-CA-C	8.98	120.84	111.14
1	C	517	ARG	N-CA-C	8.62	124.11	111.02
1	D	517	ARG	N-CA-C	8.59	124.08	111.02
1	A	517	ARG	N-CA-C	8.59	124.08	111.02
1	B	517	ARG	N-CA-C	8.58	124.07	111.02
1	B	335	TYR	N-CA-C	8.32	123.17	111.52
1	D	335	TYR	N-CA-C	8.32	123.17	111.52
1	A	335	TYR	N-CA-C	8.31	123.16	111.52
1	C	335	TYR	N-CA-C	8.30	123.14	111.52
1	B	132	VAL	CB-CA-C	-8.29	100.96	110.41
1	A	132	VAL	CB-CA-C	-8.28	100.97	110.41
1	C	132	VAL	CB-CA-C	-8.27	100.98	110.41
1	D	132	VAL	CB-CA-C	-8.27	100.98	110.41
1	C	166	SER	N-CA-C	8.16	122.94	111.52
1	A	166	SER	N-CA-C	8.13	122.91	111.52
1	D	166	SER	N-CA-C	8.11	122.88	111.52
1	B	166	SER	N-CA-C	8.11	122.87	111.52
1	D	605	ILE	N-CA-C	8.02	118.12	110.42
1	B	605	ILE	N-CA-C	8.00	118.10	110.42
1	A	605	ILE	N-CA-C	7.98	118.08	110.42
1	C	605	ILE	N-CA-C	7.96	118.06	110.42
1	B	493	GLU	N-CA-C	7.71	127.21	110.80
1	A	493	GLU	N-CA-C	7.70	127.20	110.80
1	C	493	GLU	N-CA-C	7.70	127.20	110.80
1	D	493	GLU	N-CA-C	7.69	127.19	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	522	THR	N-CA-C	-7.53	103.05	111.71
1	A	522	THR	N-CA-C	-7.53	103.06	111.71
1	C	522	THR	N-CA-C	-7.51	103.08	111.71
1	B	522	THR	N-CA-C	-7.50	103.08	111.71
1	A	493	GLU	CB-CA-C	-6.88	96.72	110.42
1	C	493	GLU	CB-CA-C	-6.88	96.72	110.42
1	B	493	GLU	CB-CA-C	-6.86	96.76	110.42
1	D	493	GLU	CB-CA-C	-6.86	96.77	110.42
1	C	489	LEU	N-CA-C	6.24	117.88	111.14
1	A	489	LEU	N-CA-C	6.22	117.86	111.14
1	B	489	LEU	N-CA-C	6.21	117.85	111.14
1	D	489	LEU	N-CA-C	6.21	117.84	111.14
1	B	373	VAL	N-CA-C	5.47	119.70	112.04
1	A	373	VAL	N-CA-C	5.46	119.68	112.04
1	D	373	VAL	N-CA-C	5.45	119.67	112.04
1	C	373	VAL	N-CA-C	5.44	119.65	112.04
1	C	211	GLU	N-CA-C	5.18	118.73	111.90
1	B	211	GLU	N-CA-C	5.17	118.73	111.90
1	A	211	GLU	N-CA-C	5.17	118.72	111.90
1	D	211	GLU	N-CA-C	5.17	118.72	111.90

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	SER	Peptide
1	A	174	LYS	Peptide
1	A	175	ARG	Peptide
1	A	177	LEU	Peptide
1	A	308	ILE	Peptide
1	A	309	GLU	Peptide
1	A	336	GLY	Peptide
1	A	352	GLU	Peptide
1	A	367	PRO	Peptide
1	A	369	ARG	Peptide
1	A	375	LEU	Peptide
1	A	488	VAL	Peptide
1	A	489	LEU	Peptide
1	A	492	MET	Peptide
1	A	493	GLU	Peptide
1	A	521	HIS	Peptide
1	B	166	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	174	LYS	Peptide
1	B	175	ARG	Peptide
1	B	177	LEU	Peptide
1	B	308	ILE	Peptide
1	B	309	GLU	Peptide
1	B	336	GLY	Peptide
1	B	352	GLU	Peptide
1	B	367	PRO	Peptide
1	B	369	ARG	Peptide
1	B	375	LEU	Peptide
1	B	488	VAL	Peptide
1	B	489	LEU	Peptide
1	B	492	MET	Peptide
1	B	493	GLU	Peptide
1	B	521	HIS	Peptide
1	C	166	SER	Peptide
1	C	174	LYS	Peptide
1	C	175	ARG	Peptide
1	C	177	LEU	Peptide
1	C	308	ILE	Peptide
1	C	309	GLU	Peptide
1	C	336	GLY	Peptide
1	C	352	GLU	Peptide
1	C	367	PRO	Peptide
1	C	369	ARG	Peptide
1	C	375	LEU	Peptide
1	C	488	VAL	Peptide
1	C	489	LEU	Peptide
1	C	492	MET	Peptide
1	C	493	GLU	Peptide
1	C	521	HIS	Peptide
1	D	166	SER	Peptide
1	D	174	LYS	Peptide
1	D	175	ARG	Peptide
1	D	177	LEU	Peptide
1	D	308	ILE	Peptide
1	D	309	GLU	Peptide
1	D	336	GLY	Peptide
1	D	352	GLU	Peptide
1	D	367	PRO	Peptide
1	D	369	ARG	Peptide
1	D	375	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	488	VAL	Peptide
1	D	489	LEU	Peptide
1	D	492	MET	Peptide
1	D	493	GLU	Peptide
1	D	521	HIS	Peptide

5.2 Too-close contacts [i](#)

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	4909	0	4965	237	0
1	B	4909	0	4965	248	0
1	C	4909	0	4965	243	0
1	D	4909	0	4965	237	0
All	All	19636	0	19860	927	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 23.

All (927) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TRP:HE3	1:A:270:MET:SD	1.54	1.30
1:D:223:TRP:HE3	1:D:270:MET:SD	1.54	1.30
1:B:223:TRP:HE3	1:B:270:MET:SD	1.54	1.28
1:C:223:TRP:HE3	1:C:270:MET:SD	1.54	1.28
1:A:223:TRP:CE3	1:A:270:MET:SD	2.34	1.20
1:B:223:TRP:CE3	1:B:270:MET:SD	2.34	1.20
1:D:223:TRP:CE3	1:D:270:MET:SD	2.34	1.20
1:C:223:TRP:CE3	1:C:270:MET:SD	2.34	1.19
1:B:168:LEU:HD13	1:B:183:LEU:HD22	1.20	1.14
1:C:168:LEU:HD13	1:C:183:LEU:HD22	1.20	1.12
1:D:361:ALA:HB1	1:D:669:LEU:HD11	1.20	1.11
1:A:361:ALA:HB1	1:A:669:LEU:HD11	1.20	1.11
1:D:168:LEU:HD13	1:D:183:LEU:HD22	1.20	1.11
1:A:168:LEU:HD13	1:A:183:LEU:HD22	1.20	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ALA:HB1	1:C:669:LEU:HD11	1.20	1.07
1:B:361:ALA:HB1	1:B:669:LEU:HD11	1.19	1.06
1:B:694:ARG:NH1	1:B:695:GLY:N	2.03	1.06
1:A:263:ASN:O	1:A:267:VAL:HG23	1.55	1.06
1:C:694:ARG:NH1	1:C:695:GLY:N	2.03	1.06
1:D:694:ARG:NH1	1:D:695:GLY:N	2.03	1.06
1:A:169:HIS:CE1	1:A:192:LEU:HD12	1.91	1.05
1:D:169:HIS:CE1	1:D:192:LEU:HD12	1.91	1.05
1:A:441:ILE:HG22	1:A:487:GLN:NE2	1.71	1.05
1:D:441:ILE:HG22	1:D:487:GLN:NE2	1.71	1.05
1:A:694:ARG:NH1	1:A:695:GLY:N	2.03	1.04
1:B:441:ILE:HG22	1:B:487:GLN:NE2	1.71	1.04
1:C:263:ASN:O	1:C:267:VAL:HG23	1.55	1.04
1:D:263:ASN:O	1:D:267:VAL:HG23	1.55	1.04
1:B:169:HIS:CE1	1:B:192:LEU:HD12	1.91	1.04
1:C:169:HIS:CE1	1:C:192:LEU:HD12	1.91	1.04
1:C:169:HIS:HE1	1:C:192:LEU:HD12	1.23	1.04
1:C:441:ILE:HG22	1:C:487:GLN:NE2	1.71	1.04
1:B:263:ASN:O	1:B:267:VAL:HG23	1.55	1.03
1:C:264:SER:O	1:C:268:ILE:HG13	1.59	1.03
1:A:169:HIS:HE1	1:A:192:LEU:HD12	1.23	1.02
1:A:694:ARG:NH1	1:A:695:GLY:CA	2.23	1.02
1:B:694:ARG:NH1	1:B:695:GLY:CA	2.23	1.02
1:B:264:SER:O	1:B:268:ILE:HG13	1.59	1.02
1:B:317:ARG:HD2	1:B:319:PHE:CE2	1.95	1.02
1:C:694:ARG:NH1	1:C:695:GLY:CA	2.23	1.02
1:D:694:ARG:NH1	1:D:695:GLY:CA	2.23	1.02
1:D:264:SER:O	1:D:268:ILE:HG13	1.59	1.01
1:D:317:ARG:HD2	1:D:319:PHE:CE2	1.95	1.01
1:A:317:ARG:HD2	1:A:319:PHE:CE2	1.95	1.01
1:A:502:VAL:HG21	1:B:558:LEU:HD21	1.43	1.01
1:A:264:SER:O	1:A:268:ILE:HG13	1.59	1.00
1:C:317:ARG:HD2	1:C:319:PHE:CE2	1.95	1.00
1:A:165:HIS:HB2	1:A:170:ILE:HD11	1.43	1.00
1:C:165:HIS:HB2	1:C:170:ILE:HD11	1.43	0.99
1:D:169:HIS:HE1	1:D:192:LEU:HD12	1.23	0.99
1:D:165:HIS:HB2	1:D:170:ILE:HD11	1.42	0.99
1:B:165:HIS:HB2	1:B:170:ILE:HD11	1.43	0.98
1:B:169:HIS:HE1	1:B:192:LEU:HD12	1.23	0.96
1:C:299:LEU:HD11	1:C:314:ILE:HG13	1.47	0.96
1:D:299:LEU:HD11	1:D:314:ILE:HG13	1.47	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LEU:O	1:A:489:LEU:HD13	1.67	0.95
1:B:299:LEU:HD11	1:B:314:ILE:HG13	1.47	0.95
1:B:485:LEU:O	1:B:489:LEU:HD13	1.67	0.95
1:D:485:LEU:O	1:D:489:LEU:HD13	1.67	0.94
1:A:299:LEU:HD11	1:A:314:ILE:HG13	1.47	0.94
1:C:485:LEU:O	1:C:489:LEU:HD13	1.67	0.94
1:A:317:ARG:HD2	1:A:319:PHE:HE2	1.31	0.94
1:C:317:ARG:HD2	1:C:319:PHE:HE2	1.31	0.92
1:B:317:ARG:HD2	1:B:319:PHE:HE2	1.31	0.92
1:B:168:LEU:HD22	1:B:183:LEU:HD23	1.54	0.89
1:D:168:LEU:CD1	1:D:183:LEU:HD22	2.03	0.89
1:A:168:LEU:HD22	1:A:183:LEU:HD23	1.54	0.89
1:D:317:ARG:HD2	1:D:319:PHE:HE2	1.31	0.89
1:A:694:ARG:HH11	1:A:695:GLY:N	1.70	0.89
1:B:317:ARG:NH1	1:B:330:PHE:CE1	2.41	0.89
1:C:694:ARG:HH11	1:C:695:GLY:N	1.70	0.89
1:A:168:LEU:CD1	1:A:183:LEU:HD22	2.03	0.88
1:B:168:LEU:CD1	1:B:183:LEU:HD22	2.03	0.88
1:D:317:ARG:NH1	1:D:330:PHE:CE1	2.42	0.88
1:C:317:ARG:NH1	1:C:330:PHE:CE1	2.41	0.88
1:C:168:LEU:HD22	1:C:183:LEU:HD23	1.54	0.88
1:D:694:ARG:HH12	1:D:695:GLY:HA3	1.38	0.88
1:A:317:ARG:NH1	1:A:330:PHE:CE1	2.41	0.88
1:C:168:LEU:CD1	1:C:183:LEU:HD22	2.03	0.87
1:D:168:LEU:HD22	1:D:183:LEU:HD23	1.54	0.87
1:B:157:CYS:HB2	1:B:165:HIS:CD2	2.10	0.87
1:A:157:CYS:HB2	1:A:165:HIS:CD2	2.10	0.86
1:C:694:ARG:HH12	1:C:695:GLY:HA3	1.38	0.86
1:A:558:LEU:HD21	1:D:502:VAL:HG21	1.58	0.86
1:A:223:TRP:HB2	1:A:270:MET:HE1	1.58	0.86
1:A:694:ARG:HH12	1:A:695:GLY:HA3	1.38	0.86
1:B:223:TRP:HB2	1:B:270:MET:HE1	1.57	0.86
1:B:694:ARG:HH11	1:B:695:GLY:N	1.70	0.86
1:B:694:ARG:HH12	1:B:695:GLY:HA3	1.38	0.86
1:A:310:ILE:HD12	1:A:311:PHE:N	1.92	0.85
1:B:310:ILE:HD12	1:B:311:PHE:N	1.92	0.85
1:C:157:CYS:HB2	1:C:165:HIS:CD2	2.11	0.85
1:D:694:ARG:HH11	1:D:695:GLY:N	1.70	0.85
1:D:157:CYS:HB2	1:D:165:HIS:CD2	2.10	0.85
1:B:618:PHE:O	1:B:621:VAL:HG22	1.78	0.84
1:C:310:ILE:HD12	1:C:311:PHE:N	1.92	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:618:PHE:O	1:D:621:VAL:HG22	1.77	0.84
1:D:441:ILE:HG22	1:D:487:GLN:HE22	1.42	0.84
1:A:618:PHE:O	1:A:621:VAL:HG22	1.78	0.84
1:D:223:TRP:HB2	1:D:270:MET:HE1	1.57	0.84
1:C:223:TRP:HB2	1:C:270:MET:HE1	1.57	0.84
1:D:310:ILE:HD12	1:D:311:PHE:N	1.92	0.84
1:A:441:ILE:HG22	1:A:487:GLN:HE22	1.42	0.83
1:C:328:ARG:NE	1:C:702:ARG:HD3	1.93	0.83
1:B:169:HIS:CD2	1:B:213:PRO:HG3	2.13	0.83
1:B:328:ARG:NE	1:B:702:ARG:HD3	1.93	0.83
1:C:169:HIS:CD2	1:C:213:PRO:HG3	2.14	0.83
1:B:441:ILE:HG22	1:B:487:GLN:HE22	1.42	0.83
1:A:169:HIS:CD2	1:A:213:PRO:HG3	2.14	0.83
1:A:502:VAL:CG2	1:B:558:LEU:HD21	2.08	0.83
1:B:342:LEU:HD21	1:B:704:CYS:HB3	1.60	0.83
1:C:618:PHE:O	1:C:621:VAL:HG22	1.78	0.83
1:A:342:LEU:HD21	1:A:704:CYS:HB3	1.60	0.82
1:A:328:ARG:NE	1:A:702:ARG:HD3	1.93	0.82
1:A:558:LEU:HD21	1:D:502:VAL:CG2	2.09	0.82
1:A:539:ARG:HD2	1:D:522:THR:OG1	1.80	0.82
1:C:342:LEU:HD21	1:C:704:CYS:HB3	1.60	0.82
1:C:441:ILE:HG22	1:C:487:GLN:HE22	1.42	0.82
1:C:502:VAL:HG21	1:D:558:LEU:HD21	1.60	0.82
1:D:328:ARG:NE	1:D:702:ARG:HD3	1.93	0.82
1:B:311:PHE:O	1:B:314:ILE:HG22	1.80	0.82
1:D:311:PHE:O	1:D:314:ILE:HG22	1.80	0.81
1:A:311:PHE:O	1:A:314:ILE:HG22	1.80	0.81
1:B:168:LEU:HD22	1:B:183:LEU:CD2	2.11	0.81
1:D:169:HIS:CD2	1:D:213:PRO:HG3	2.14	0.81
1:A:168:LEU:HD22	1:A:183:LEU:CD2	2.11	0.81
1:C:168:LEU:HD22	1:C:183:LEU:CD2	2.11	0.81
1:D:342:LEU:HD21	1:D:704:CYS:HB3	1.60	0.81
1:C:311:PHE:O	1:C:314:ILE:HG22	1.80	0.80
1:A:270:MET:O	1:A:274:LEU:HD23	1.82	0.80
1:D:168:LEU:HD22	1:D:183:LEU:CD2	2.11	0.80
1:D:312:ARG:HB2	1:D:375:LEU:HD11	1.64	0.80
1:A:312:ARG:HB2	1:A:375:LEU:HD11	1.64	0.79
1:A:169:HIS:HE1	1:A:192:LEU:CD1	1.96	0.79
1:C:312:ARG:HB2	1:C:375:LEU:HD11	1.64	0.79
1:B:270:MET:O	1:B:274:LEU:HD23	1.82	0.78
1:D:270:MET:O	1:D:274:LEU:HD23	1.82	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TRP:HE3	1:A:270:MET:CE	1.96	0.78
1:B:223:TRP:HE3	1:B:270:MET:CE	1.96	0.78
1:B:169:HIS:HE1	1:B:192:LEU:CD1	1.96	0.78
1:B:223:TRP:CB	1:B:270:MET:HE1	2.14	0.78
1:C:502:VAL:CG2	1:D:558:LEU:HD21	2.13	0.78
1:B:502:VAL:HG21	1:C:558:LEU:HD21	1.66	0.78
1:C:694:ARG:HH12	1:C:695:GLY:CA	1.93	0.78
1:D:169:HIS:HE1	1:D:192:LEU:CD1	1.96	0.78
1:D:223:TRP:HE3	1:D:270:MET:CE	1.96	0.78
1:C:223:TRP:HE3	1:C:270:MET:CE	1.96	0.78
1:A:223:TRP:CB	1:A:270:MET:HE1	2.14	0.77
1:D:170:ILE:O	1:D:173:GLU:HB3	1.84	0.77
1:B:312:ARG:HB2	1:B:375:LEU:HD11	1.64	0.77
1:D:361:ALA:HB1	1:D:669:LEU:CD1	2.10	0.77
1:B:172:ILE:O	1:B:175:ARG:HB2	1.85	0.77
1:B:694:ARG:HH12	1:B:695:GLY:CA	1.93	0.77
1:C:522:THR:OG1	1:D:539:ARG:HD2	1.84	0.77
1:A:694:ARG:HH12	1:A:695:GLY:CA	1.93	0.77
1:C:270:MET:O	1:C:274:LEU:HD23	1.82	0.77
1:A:361:ALA:HB1	1:A:669:LEU:CD1	2.10	0.77
1:C:172:ILE:O	1:C:175:ARG:HB2	1.85	0.77
1:A:172:ILE:O	1:A:175:ARG:HB2	1.85	0.77
1:B:502:VAL:CG2	1:C:558:LEU:HD21	2.15	0.77
1:C:170:ILE:O	1:C:173:GLU:HB3	1.84	0.77
1:C:223:TRP:CB	1:C:270:MET:HE1	2.14	0.77
1:D:172:ILE:O	1:D:175:ARG:HB2	1.85	0.77
1:B:366:SER:OG	1:B:369:ARG:HG3	1.85	0.77
1:D:223:TRP:CB	1:D:270:MET:HE1	2.14	0.76
1:A:170:ILE:O	1:A:173:GLU:HB3	1.84	0.76
1:B:170:ILE:O	1:B:173:GLU:HB3	1.84	0.76
1:A:324:GLN:NE2	1:A:327:SER:HB2	2.01	0.76
1:B:324:GLN:NE2	1:B:327:SER:HB2	2.01	0.76
1:C:362:PHE:CE2	1:C:669:LEU:HD13	2.21	0.76
1:D:317:ARG:CD	1:D:319:PHE:HE2	1.99	0.76
1:A:366:SER:OG	1:A:369:ARG:HG3	1.85	0.76
1:A:362:PHE:CE2	1:A:669:LEU:HD13	2.21	0.76
1:C:169:HIS:HE1	1:C:192:LEU:CD1	1.96	0.76
1:B:317:ARG:CD	1:B:319:PHE:HE2	1.99	0.76
1:D:362:PHE:CE2	1:D:669:LEU:HD13	2.21	0.76
1:A:317:ARG:CD	1:A:319:PHE:HE2	1.99	0.76
1:C:366:SER:OG	1:C:369:ARG:HG3	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:PHE:CE2	1:B:669:LEU:HD13	2.21	0.75
1:D:324:GLN:NE2	1:D:327:SER:HB2	2.01	0.75
1:D:361:ALA:CB	1:D:669:LEU:HD21	2.17	0.75
1:C:310:ILE:HD12	1:C:311:PHE:CA	2.17	0.75
1:C:361:ALA:CB	1:C:669:LEU:HD21	2.17	0.75
1:D:310:ILE:HD12	1:D:311:PHE:CA	2.17	0.75
1:D:366:SER:OG	1:D:369:ARG:HG3	1.85	0.75
1:C:324:GLN:NE2	1:C:327:SER:HB2	2.01	0.75
1:C:371:ARG:O	1:C:374:VAL:HG22	1.87	0.75
1:D:371:ARG:O	1:D:374:VAL:HG22	1.87	0.75
1:A:361:ALA:CB	1:A:669:LEU:HD21	2.17	0.75
1:C:317:ARG:CD	1:C:319:PHE:HE2	1.99	0.75
1:B:310:ILE:HD12	1:B:311:PHE:CA	2.17	0.75
1:A:299:LEU:HD11	1:A:314:ILE:CG1	2.17	0.75
1:B:299:LEU:HD11	1:B:314:ILE:CG1	2.17	0.75
1:D:694:ARG:HH12	1:D:695:GLY:CA	1.93	0.75
1:C:299:LEU:HD11	1:C:314:ILE:CG1	2.17	0.74
1:D:299:LEU:HD11	1:D:314:ILE:CG1	2.17	0.74
1:D:328:ARG:CD	1:D:702:ARG:HD3	2.17	0.74
1:A:310:ILE:HD12	1:A:311:PHE:CA	2.17	0.74
1:C:328:ARG:CD	1:C:702:ARG:HD3	2.17	0.74
1:D:317:ARG:NH1	1:D:330:PHE:HE1	1.85	0.74
1:B:371:ARG:O	1:B:374:VAL:HG22	1.87	0.74
1:A:522:THR:OG1	1:B:539:ARG:HD2	1.87	0.74
1:B:361:ALA:CB	1:B:669:LEU:HD21	2.17	0.73
1:B:268:ILE:HG23	1:B:313:HIS:CD2	2.23	0.73
1:B:328:ARG:CD	1:B:702:ARG:HD3	2.17	0.73
1:B:621:VAL:HG23	1:B:622:VAL:H	1.54	0.73
1:A:328:ARG:CD	1:A:702:ARG:HD3	2.17	0.73
1:A:621:VAL:HG23	1:A:622:VAL:H	1.54	0.73
1:A:317:ARG:NH1	1:A:330:PHE:HE1	1.85	0.72
1:A:371:ARG:O	1:A:374:VAL:HG22	1.87	0.72
1:C:303:ALA:HA	1:C:372:MET:HE1	1.72	0.72
1:C:317:ARG:NH1	1:C:330:PHE:HE1	1.85	0.72
1:C:268:ILE:HG23	1:C:313:HIS:CD2	2.23	0.72
1:C:621:VAL:HG23	1:C:622:VAL:H	1.54	0.72
1:A:268:ILE:HG23	1:A:313:HIS:CD2	2.23	0.72
1:D:621:VAL:HG23	1:D:622:VAL:H	1.54	0.72
1:B:317:ARG:NH1	1:B:330:PHE:HE1	1.85	0.72
1:D:303:ALA:HA	1:D:372:MET:HE1	1.71	0.72
1:D:268:ILE:HG23	1:D:313:HIS:CD2	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ALA:HA	1:B:372:MET:HE1	1.72	0.72
1:D:177:LEU:HD13	1:D:225:VAL:HG12	1.72	0.72
1:A:303:ALA:HA	1:A:372:MET:HE1	1.71	0.71
1:B:177:LEU:HD13	1:B:225:VAL:HG12	1.72	0.71
1:C:177:LEU:HD13	1:C:225:VAL:HG12	1.72	0.70
1:A:177:LEU:HD13	1:A:225:VAL:HG12	1.71	0.70
1:B:165:HIS:HB2	1:B:170:ILE:CD1	2.22	0.70
1:A:223:TRP:CZ3	1:A:270:MET:SD	2.85	0.69
1:B:223:TRP:CZ3	1:B:270:MET:SD	2.85	0.69
1:D:361:ALA:CB	1:D:669:LEU:HD11	2.12	0.69
1:B:522:THR:OG1	1:C:539:ARG:HD2	1.92	0.69
1:C:223:TRP:CZ3	1:C:270:MET:SD	2.85	0.69
1:A:361:ALA:CB	1:A:669:LEU:HD11	2.12	0.69
1:D:223:TRP:CZ3	1:D:270:MET:SD	2.85	0.69
1:C:165:HIS:HB2	1:C:170:ILE:CD1	2.21	0.69
1:A:329:LYS:HB3	1:A:331:THR:OG1	1.93	0.68
1:D:310:ILE:HD12	1:D:311:PHE:HA	1.76	0.68
1:A:621:VAL:HG23	1:A:622:VAL:N	2.09	0.68
1:B:361:ALA:HB1	1:B:669:LEU:CD1	2.10	0.68
1:C:361:ALA:HB1	1:C:669:LEU:CD1	2.10	0.68
1:C:329:LYS:HB3	1:C:331:THR:OG1	1.93	0.68
1:D:165:HIS:HB2	1:D:170:ILE:CD1	2.21	0.68
1:A:223:TRP:HB2	1:A:270:MET:CE	2.24	0.68
1:D:621:VAL:HG23	1:D:622:VAL:N	2.09	0.68
1:B:361:ALA:CB	1:B:669:LEU:HD11	2.12	0.67
1:D:324:GLN:CD	1:D:327:SER:HB2	2.19	0.67
1:B:329:LYS:HB3	1:B:331:THR:OG1	1.93	0.67
1:A:310:ILE:HD12	1:A:311:PHE:HA	1.76	0.67
1:C:310:ILE:HD12	1:C:311:PHE:HA	1.76	0.67
1:D:329:LYS:HB3	1:D:331:THR:OG1	1.93	0.67
1:C:621:VAL:HG23	1:C:622:VAL:N	2.09	0.67
1:B:223:TRP:HB2	1:B:270:MET:CE	2.24	0.67
1:C:223:TRP:HB2	1:C:270:MET:CE	2.24	0.67
1:B:328:ARG:HD2	1:B:702:ARG:CG	2.25	0.67
1:C:324:GLN:CD	1:C:327:SER:HB2	2.19	0.67
1:D:223:TRP:HB2	1:D:270:MET:CE	2.24	0.67
1:B:310:ILE:HD12	1:B:311:PHE:HA	1.76	0.66
1:A:489:LEU:N	1:A:489:LEU:HD12	2.11	0.66
1:B:324:GLN:CD	1:B:327:SER:HB2	2.19	0.66
1:D:214:LEU:HD23	1:D:229:LEU:HD11	1.78	0.66
1:D:489:LEU:HD12	1:D:489:LEU:N	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HD2	1:A:702:ARG:CG	2.25	0.66
1:B:165:HIS:CB	1:B:170:ILE:HD11	2.23	0.66
1:C:489:LEU:N	1:C:489:LEU:HD12	2.11	0.66
1:C:214:LEU:HD23	1:C:229:LEU:HD11	1.78	0.66
1:A:214:LEU:HD23	1:A:229:LEU:HD11	1.78	0.66
1:A:591:ARG:N	1:D:412:TYR:HH	1.93	0.66
1:B:328:ARG:HG2	1:B:694:ARG:HH22	1.61	0.66
1:B:621:VAL:HG23	1:B:622:VAL:N	2.09	0.66
1:B:214:LEU:HD23	1:B:229:LEU:HD11	1.78	0.66
1:B:342:LEU:HD21	1:B:704:CYS:CB	2.26	0.66
1:B:489:LEU:HD12	1:B:489:LEU:N	2.11	0.66
1:D:342:LEU:HD21	1:D:704:CYS:CB	2.26	0.66
1:A:177:LEU:CD1	1:A:225:VAL:HG12	2.26	0.66
1:A:324:GLN:CD	1:A:327:SER:HB2	2.19	0.66
1:C:177:LEU:CD1	1:C:225:VAL:HG12	2.26	0.66
1:C:328:ARG:HD2	1:C:702:ARG:CG	2.25	0.66
1:A:342:LEU:HD21	1:A:704:CYS:CB	2.26	0.65
1:C:328:ARG:HG2	1:C:694:ARG:HH22	1.61	0.65
1:A:328:ARG:HG2	1:A:694:ARG:HH22	1.61	0.65
1:B:177:LEU:CD1	1:B:225:VAL:HG12	2.26	0.65
1:D:165:HIS:CB	1:D:170:ILE:HD11	2.22	0.65
1:C:165:HIS:CB	1:C:170:ILE:HD11	2.23	0.65
1:D:328:ARG:HD2	1:D:702:ARG:CG	2.25	0.65
1:D:177:LEU:CD1	1:D:225:VAL:HG12	2.26	0.65
1:A:165:HIS:HB2	1:A:170:ILE:CD1	2.21	0.65
1:A:223:TRP:CA	1:A:270:MET:HE1	2.27	0.65
1:C:361:ALA:CB	1:C:669:LEU:HD11	2.12	0.65
1:D:610:LEU:O	1:D:610:LEU:HD23	1.97	0.65
1:C:342:LEU:HD21	1:C:704:CYS:CB	2.26	0.65
1:B:223:TRP:CA	1:B:270:MET:HE1	2.27	0.64
1:B:223:TRP:CH2	1:B:273:GLY:HA3	2.33	0.64
1:C:223:TRP:CA	1:C:270:MET:HE1	2.27	0.64
1:C:610:LEU:HD23	1:C:610:LEU:O	1.97	0.64
1:A:223:TRP:HZ3	1:A:274:LEU:HD22	1.63	0.64
1:A:610:LEU:O	1:A:610:LEU:HD23	1.97	0.64
1:D:223:TRP:HZ3	1:D:274:LEU:HD22	1.63	0.64
1:B:389:LEU:HD22	1:B:671:MET:HB3	1.79	0.64
1:C:487:GLN:O	1:C:490:ARG:HG2	1.98	0.64
1:D:223:TRP:CH2	1:D:273:GLY:HA3	2.33	0.64
1:D:223:TRP:CA	1:D:270:MET:HE1	2.27	0.64
1:B:128:LEU:HD21	1:B:174:LYS:HG3	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:LEU:HD23	1:B:610:LEU:O	1.97	0.64
1:C:223:TRP:CH2	1:C:273:GLY:HA3	2.33	0.64
1:D:328:ARG:HG2	1:D:694:ARG:HH22	1.61	0.64
1:A:165:HIS:CB	1:A:170:ILE:HD11	2.23	0.64
1:D:168:LEU:HD11	1:D:180:VAL:HA	1.80	0.64
1:D:487:GLN:O	1:D:490:ARG:HG2	1.98	0.64
1:C:168:LEU:HD11	1:C:180:VAL:HA	1.80	0.63
1:A:487:GLN:O	1:A:490:ARG:HG2	1.98	0.63
1:B:694:ARG:HH11	1:B:695:GLY:H	1.46	0.63
1:B:270:MET:O	1:B:274:LEU:CD2	2.47	0.63
1:B:487:GLN:O	1:B:490:ARG:HG2	1.98	0.63
1:A:666:ILE:O	1:A:669:LEU:HG	1.99	0.63
1:C:128:LEU:HD21	1:C:174:LYS:HG3	1.80	0.63
1:A:389:LEU:HD22	1:A:671:MET:HB3	1.79	0.63
1:A:694:ARG:HH11	1:A:695:GLY:H	1.46	0.63
1:C:223:TRP:HZ3	1:C:274:LEU:HD22	1.63	0.63
1:D:270:MET:O	1:D:274:LEU:CD2	2.47	0.63
1:A:168:LEU:HD11	1:A:180:VAL:HA	1.80	0.63
1:A:223:TRP:CH2	1:A:273:GLY:HA3	2.32	0.63
1:C:666:ILE:O	1:C:669:LEU:HG	1.99	0.63
1:D:329:LYS:O	1:D:330:PHE:HB2	1.99	0.62
1:B:329:LYS:O	1:B:330:PHE:HB2	1.99	0.62
1:B:522:THR:O	1:B:524:ILE:N	2.32	0.62
1:C:694:ARG:HH11	1:C:695:GLY:H	1.46	0.62
1:D:522:THR:O	1:D:524:ILE:N	2.33	0.62
1:A:128:LEU:HD21	1:A:174:LYS:HG3	1.80	0.62
1:A:270:MET:O	1:A:274:LEU:CD2	2.47	0.62
1:B:223:TRP:HZ3	1:B:274:LEU:HD22	1.63	0.62
1:C:389:LEU:HD22	1:C:671:MET:HB3	1.79	0.62
1:D:389:LEU:HD22	1:D:671:MET:HB3	1.79	0.62
1:A:317:ARG:HD2	1:A:319:PHE:CZ	2.34	0.62
1:A:522:THR:O	1:A:524:ILE:N	2.32	0.62
1:B:666:ILE:O	1:B:669:LEU:HG	1.99	0.62
1:C:522:THR:O	1:C:524:ILE:N	2.33	0.62
1:B:168:LEU:HD11	1:B:180:VAL:HA	1.80	0.62
1:D:317:ARG:HD2	1:D:319:PHE:CZ	2.34	0.62
1:D:666:ILE:O	1:D:669:LEU:HG	1.99	0.62
1:C:270:MET:O	1:C:274:LEU:CD2	2.47	0.62
1:C:329:LYS:O	1:C:330:PHE:HB2	1.99	0.62
1:A:329:LYS:O	1:A:330:PHE:HB2	1.99	0.62
1:B:337:PRO:HB3	1:C:173:GLU:OE2	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:LEU:HD21	1:D:174:LYS:HG3	1.80	0.61
1:C:156:GLN:HG2	1:C:166:SER:OG	2.00	0.61
1:B:312:ARG:CB	1:B:375:LEU:HD11	2.30	0.61
1:B:317:ARG:HD2	1:B:319:PHE:CZ	2.34	0.61
1:C:317:ARG:HD2	1:C:319:PHE:CZ	2.34	0.61
1:A:488:VAL:O	1:A:488:VAL:HG12	2.01	0.61
1:D:694:ARG:HH11	1:D:695:GLY:H	1.46	0.61
1:A:329:LYS:HB2	1:A:331:THR:H	1.65	0.61
1:B:502:VAL:HG21	1:C:558:LEU:HD11	1.82	0.61
1:D:156:GLN:HG2	1:D:166:SER:OG	2.00	0.61
1:D:488:VAL:HG12	1:D:488:VAL:O	2.01	0.61
1:B:156:GLN:HG2	1:B:166:SER:OG	2.00	0.61
1:C:157:CYS:CB	1:C:165:HIS:CD2	2.84	0.61
1:D:312:ARG:CB	1:D:375:LEU:HD11	2.30	0.61
1:A:312:ARG:CB	1:A:375:LEU:HD11	2.30	0.60
1:A:516:THR:O	1:A:516:THR:HG23	2.01	0.60
1:A:156:GLN:HG2	1:A:166:SER:OG	2.00	0.60
1:B:329:LYS:HB2	1:B:331:THR:H	1.65	0.60
1:B:370:HIS:HA	1:B:662:LEU:HD21	1.83	0.60
1:D:516:THR:HG23	1:D:516:THR:O	2.01	0.60
1:B:310:ILE:HD12	1:B:310:ILE:C	2.27	0.60
1:B:170:ILE:O	1:B:173:GLU:CB	2.49	0.60
1:C:170:ILE:O	1:C:173:GLU:CB	2.49	0.60
1:C:329:LYS:HB2	1:C:331:THR:H	1.65	0.60
1:D:171:ALA:O	1:D:174:LYS:N	2.35	0.60
1:A:157:CYS:CB	1:A:165:HIS:CD2	2.84	0.60
1:C:370:HIS:HA	1:C:662:LEU:HD21	1.83	0.60
1:A:370:HIS:HA	1:A:662:LEU:HD21	1.83	0.60
1:C:412:TYR:HH	1:D:591:ARG:N	2.00	0.60
1:C:488:VAL:HG12	1:C:488:VAL:O	2.01	0.60
1:C:516:THR:HG23	1:C:516:THR:O	2.01	0.60
1:A:171:ALA:O	1:A:174:LYS:N	2.35	0.59
1:C:310:ILE:HD12	1:C:310:ILE:C	2.27	0.59
1:D:310:ILE:HD12	1:D:310:ILE:C	2.27	0.59
1:A:310:ILE:HD12	1:A:310:ILE:C	2.27	0.59
1:C:312:ARG:CB	1:C:375:LEU:HD11	2.30	0.59
1:D:329:LYS:HB2	1:D:331:THR:H	1.65	0.59
1:B:348:VAL:HG23	1:B:356:VAL:HG22	1.84	0.59
1:B:516:THR:HG23	1:B:516:THR:O	2.01	0.59
1:C:171:ALA:O	1:C:174:LYS:N	2.35	0.59
1:A:170:ILE:O	1:A:173:GLU:CB	2.49	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:VAL:HG23	1:A:356:VAL:HG22	1.84	0.59
1:B:171:ALA:O	1:B:174:LYS:N	2.35	0.59
1:C:348:VAL:HG23	1:C:356:VAL:HG22	1.84	0.59
1:D:170:ILE:O	1:D:173:GLU:CB	2.49	0.59
1:D:370:HIS:HA	1:D:662:LEU:HD21	1.83	0.59
1:B:172:ILE:HG13	1:B:180:VAL:HG21	1.85	0.59
1:C:312:ARG:HA	1:C:375:LEU:CD1	2.33	0.59
1:A:166:SER:O	1:A:168:LEU:N	2.36	0.59
1:A:489:LEU:HG	1:A:494:THR:HB	1.85	0.59
1:B:312:ARG:HA	1:B:375:LEU:HD13	1.85	0.59
1:B:488:VAL:HG12	1:B:488:VAL:O	2.01	0.59
1:B:489:LEU:HG	1:B:494:THR:HB	1.85	0.59
1:D:366:SER:CB	1:D:369:ARG:HG3	2.33	0.59
1:A:312:ARG:HA	1:A:375:LEU:HD13	1.85	0.58
1:B:166:SER:O	1:B:168:LEU:N	2.36	0.58
1:C:166:SER:O	1:C:168:LEU:N	2.36	0.58
1:B:412:TYR:HH	1:C:591:ARG:N	2.01	0.58
1:B:694:ARG:H	1:B:694:ARG:HD3	1.68	0.58
1:D:166:SER:O	1:D:168:LEU:N	2.36	0.58
1:A:694:ARG:H	1:A:694:ARG:HD3	1.68	0.58
1:C:172:ILE:HG13	1:C:180:VAL:HG21	1.85	0.58
1:D:348:VAL:HG23	1:D:356:VAL:HG22	1.84	0.58
1:D:157:CYS:CB	1:D:165:HIS:CD2	2.84	0.58
1:A:172:ILE:HG13	1:A:180:VAL:HG21	1.85	0.58
1:B:609:GLU:O	1:B:610:LEU:HB3	2.04	0.58
1:C:441:ILE:CG2	1:C:487:GLN:HE22	2.15	0.58
1:D:168:LEU:O	1:D:172:ILE:HD12	2.04	0.58
1:D:694:ARG:H	1:D:694:ARG:HD3	1.68	0.58
1:A:312:ARG:HA	1:A:375:LEU:CD1	2.33	0.58
1:D:312:ARG:HA	1:D:375:LEU:HD13	1.85	0.58
1:D:312:ARG:HA	1:D:375:LEU:CD1	2.33	0.58
1:A:168:LEU:O	1:A:172:ILE:HD12	2.04	0.58
1:C:312:ARG:HA	1:C:375:LEU:HD13	1.85	0.58
1:C:489:LEU:HG	1:C:494:THR:HB	1.85	0.58
1:C:361:ALA:HB2	1:C:669:LEU:HD21	1.85	0.58
1:C:366:SER:CB	1:C:369:ARG:HG3	2.33	0.58
1:C:609:GLU:O	1:C:610:LEU:HB3	2.04	0.58
1:D:361:ALA:HB2	1:D:669:LEU:HD21	1.85	0.58
1:B:223:TRP:HH2	1:B:273:GLY:C	2.12	0.57
1:B:312:ARG:HA	1:B:375:LEU:CD1	2.33	0.57
1:D:489:LEU:HG	1:D:494:THR:HB	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ARG:HD2	1:B:702:ARG:HG3	1.86	0.57
1:C:223:TRP:HH2	1:C:273:GLY:C	2.12	0.57
1:B:157:CYS:CB	1:B:165:HIS:CD2	2.84	0.57
1:B:361:ALA:HB2	1:B:669:LEU:HD21	1.85	0.57
1:C:328:ARG:HD2	1:C:702:ARG:HG3	1.86	0.57
1:D:172:ILE:HG13	1:D:180:VAL:HG21	1.85	0.57
1:A:361:ALA:HB2	1:A:669:LEU:HD21	1.85	0.57
1:C:168:LEU:O	1:C:172:ILE:HD12	2.04	0.57
1:B:168:LEU:O	1:B:172:ILE:HD12	2.04	0.57
1:B:441:ILE:CG2	1:B:487:GLN:HE22	2.15	0.57
1:A:223:TRP:HH2	1:A:273:GLY:C	2.12	0.57
1:A:366:SER:CB	1:A:369:ARG:HG3	2.33	0.57
1:D:268:ILE:CG2	1:D:313:HIS:NE2	2.67	0.57
1:D:328:ARG:HD2	1:D:702:ARG:HG3	1.86	0.57
1:A:223:TRP:CE3	1:A:270:MET:CE	2.83	0.57
1:C:169:HIS:CE1	1:C:192:LEU:CD1	2.77	0.57
1:C:312:ARG:HD2	1:C:375:LEU:HD21	1.87	0.57
1:B:312:ARG:HD2	1:B:375:LEU:HD21	1.87	0.57
1:C:268:ILE:CG2	1:C:313:HIS:NE2	2.67	0.57
1:C:694:ARG:H	1:C:694:ARG:HD3	1.68	0.57
1:B:366:SER:CB	1:B:369:ARG:HG3	2.33	0.57
1:C:157:CYS:HB2	1:C:165:HIS:HD2	1.67	0.57
1:D:223:TRP:CE3	1:D:270:MET:CE	2.83	0.57
1:A:268:ILE:CG2	1:A:313:HIS:NE2	2.67	0.56
1:D:157:CYS:HB2	1:D:165:HIS:HD2	1.67	0.56
1:A:312:ARG:HD2	1:A:375:LEU:HD21	1.87	0.56
1:A:328:ARG:HD2	1:A:702:ARG:HG3	1.86	0.56
1:A:494:THR:HG22	1:A:495:GLU:N	2.20	0.56
1:A:521:HIS:O	1:A:522:THR:C	2.48	0.56
1:A:539:ARG:CD	1:D:522:THR:OG1	2.52	0.56
1:A:609:GLU:O	1:A:610:LEU:HB3	2.04	0.56
1:B:268:ILE:CG2	1:B:313:HIS:NE2	2.67	0.56
1:D:328:ARG:HD2	1:D:702:ARG:CD	2.36	0.56
1:C:370:HIS:O	1:C:373:VAL:HG22	2.06	0.56
1:D:312:ARG:HD2	1:D:375:LEU:HD21	1.87	0.56
1:A:441:ILE:CG2	1:A:487:GLN:HE22	2.15	0.56
1:B:337:PRO:CA	1:C:173:GLU:OE2	2.54	0.56
1:C:328:ARG:HD2	1:C:702:ARG:CD	2.36	0.56
1:D:223:TRP:HH2	1:D:273:GLY:C	2.12	0.56
1:D:609:GLU:O	1:D:610:LEU:HB3	2.04	0.56
1:B:370:HIS:O	1:B:373:VAL:HG22	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ASN:O	1:C:267:VAL:CG2	2.44	0.56
1:D:268:ILE:HG21	1:D:313:HIS:CE1	2.41	0.56
1:D:370:HIS:O	1:D:373:VAL:HG22	2.06	0.56
1:B:521:HIS:O	1:B:522:THR:C	2.48	0.56
1:A:328:ARG:HD2	1:A:702:ARG:CD	2.36	0.56
1:C:489:LEU:HB3	1:C:494:THR:O	2.06	0.56
1:D:489:LEU:HB3	1:D:494:THR:O	2.06	0.56
1:A:370:HIS:O	1:A:373:VAL:HG22	2.06	0.56
1:B:328:ARG:HD2	1:B:702:ARG:CD	2.36	0.56
1:D:315:LEU:HD21	1:D:377:PRO:HG2	1.88	0.56
1:D:441:ILE:CG2	1:D:487:GLN:HE22	2.15	0.56
1:B:268:ILE:HG21	1:B:313:HIS:CE1	2.41	0.55
1:C:157:CYS:CB	1:C:165:HIS:HD2	2.19	0.55
1:D:521:HIS:O	1:D:522:THR:C	2.48	0.55
1:A:558:LEU:HD11	1:D:502:VAL:HG21	1.88	0.55
1:D:494:THR:HG22	1:D:495:GLU:N	2.20	0.55
1:A:268:ILE:HG21	1:A:313:HIS:CE1	2.41	0.55
1:B:315:LEU:HD21	1:B:377:PRO:HG2	1.88	0.55
1:A:694:ARG:NH1	1:A:695:GLY:H	1.99	0.55
1:C:315:LEU:HD21	1:C:377:PRO:HG2	1.88	0.55
1:C:328:ARG:HD2	1:C:702:ARG:HD3	1.88	0.55
1:C:494:THR:HG22	1:C:495:GLU:N	2.20	0.55
1:C:521:HIS:O	1:C:522:THR:C	2.48	0.55
1:A:270:MET:HG3	1:A:274:LEU:CD2	2.37	0.55
1:B:263:ASN:O	1:B:267:VAL:CG2	2.44	0.55
1:C:312:ARG:HG3	1:C:375:LEU:HD22	1.89	0.55
1:A:312:ARG:HG3	1:A:375:LEU:HD22	1.89	0.55
1:B:270:MET:HG3	1:B:274:LEU:CD2	2.37	0.55
1:B:494:THR:HG22	1:B:495:GLU:N	2.20	0.55
1:B:694:ARG:HD3	1:B:694:ARG:N	2.22	0.55
1:A:315:LEU:HD21	1:A:377:PRO:HG2	1.88	0.55
1:A:489:LEU:HB3	1:A:494:THR:O	2.06	0.55
1:D:270:MET:HG3	1:D:274:LEU:CD2	2.37	0.55
1:A:179:CYS:O	1:A:183:LEU:HD13	2.07	0.55
1:B:179:CYS:O	1:B:183:LEU:HD13	2.07	0.55
1:B:268:ILE:HG23	1:B:313:HIS:NE2	2.22	0.55
1:C:694:ARG:HD3	1:C:694:ARG:N	2.22	0.55
1:A:412:TYR:HH	1:B:591:ARG:N	2.05	0.54
1:B:157:CYS:CB	1:B:165:HIS:HD2	2.19	0.54
1:C:172:ILE:HG22	1:C:220:THR:HG21	1.89	0.54
1:C:270:MET:HG3	1:C:274:LEU:CD2	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:LEU:HB3	1:B:494:THR:O	2.06	0.54
1:B:521:HIS:O	1:B:523:GLY:N	2.41	0.54
1:A:521:HIS:O	1:A:523:GLY:N	2.41	0.54
1:A:694:ARG:HD3	1:A:694:ARG:N	2.22	0.54
1:D:175:ARG:HD2	1:D:220:THR:HB	1.89	0.54
1:D:521:HIS:O	1:D:523:GLY:N	2.41	0.54
1:B:328:ARG:HD2	1:B:702:ARG:HD3	1.88	0.54
1:D:328:ARG:HD2	1:D:702:ARG:HD3	1.88	0.54
1:A:175:ARG:HD2	1:A:220:THR:HB	1.89	0.54
1:D:179:CYS:O	1:D:183:LEU:HD13	2.07	0.54
1:D:694:ARG:NH1	1:D:695:GLY:H	1.99	0.54
1:C:175:ARG:HD2	1:C:220:THR:HB	1.89	0.54
1:C:268:ILE:HG21	1:C:313:HIS:CE1	2.41	0.54
1:D:268:ILE:HG23	1:D:313:HIS:NE2	2.22	0.54
1:D:694:ARG:HD3	1:D:694:ARG:N	2.22	0.54
1:B:175:ARG:HD2	1:B:220:THR:HB	1.89	0.54
1:B:312:ARG:HG3	1:B:375:LEU:HD22	1.89	0.54
1:D:312:ARG:HG3	1:D:375:LEU:HD22	1.89	0.54
1:A:172:ILE:HG22	1:A:220:THR:HG21	1.89	0.54
1:C:268:ILE:HG23	1:C:313:HIS:NE2	2.22	0.54
1:B:223:TRP:CE3	1:B:270:MET:CE	2.83	0.54
1:C:522:THR:C	1:C:524:ILE:H	2.16	0.54
1:D:157:CYS:CB	1:D:165:HIS:HD2	2.19	0.54
1:D:172:ILE:HG22	1:D:220:THR:HG21	1.89	0.54
1:A:342:LEU:CD2	1:A:704:CYS:HB3	2.36	0.53
1:C:494:THR:CG2	1:C:495:GLU:H	2.21	0.53
1:C:521:HIS:O	1:C:523:GLY:N	2.41	0.53
1:D:522:THR:C	1:D:524:ILE:H	2.16	0.53
1:A:268:ILE:CG2	1:A:313:HIS:CE1	2.92	0.53
1:A:494:THR:CG2	1:A:495:GLU:H	2.21	0.53
1:B:268:ILE:CG2	1:B:313:HIS:CE1	2.92	0.53
1:A:157:CYS:CB	1:A:165:HIS:HD2	2.19	0.53
1:D:299:LEU:CD1	1:D:314:ILE:CG1	2.85	0.53
1:B:299:LEU:CD1	1:B:314:ILE:HG13	2.31	0.53
1:C:179:CYS:O	1:C:183:LEU:HD13	2.07	0.53
1:A:398:ALA:O	1:A:402:VAL:HG22	2.09	0.53
1:A:263:ASN:O	1:A:267:VAL:CG2	2.45	0.52
1:A:299:LEU:CD1	1:A:314:ILE:CG1	2.85	0.52
1:B:172:ILE:HG22	1:B:220:THR:HG21	1.89	0.52
1:B:694:ARG:NH1	1:B:695:GLY:H	1.99	0.52
1:C:268:ILE:CG2	1:C:313:HIS:CE1	2.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:494:THR:CG2	1:D:495:GLU:H	2.21	0.52
1:A:522:THR:C	1:A:524:ILE:H	2.16	0.52
1:C:299:LEU:CD1	1:C:314:ILE:CG1	2.85	0.52
1:D:268:ILE:CG2	1:D:313:HIS:CE1	2.92	0.52
1:A:268:ILE:HG23	1:A:313:HIS:NE2	2.22	0.52
1:B:494:THR:CG2	1:B:495:GLU:H	2.21	0.52
1:B:398:ALA:O	1:B:402:VAL:HG22	2.09	0.52
1:C:253:LEU:HD12	1:C:267:VAL:HG13	1.91	0.52
1:C:328:ARG:HG2	1:C:694:ARG:NH2	2.25	0.52
1:A:489:LEU:N	1:A:489:LEU:CD1	2.73	0.52
1:C:175:ARG:O	1:C:175:ARG:HG2	2.10	0.52
1:D:489:LEU:N	1:D:489:LEU:CD1	2.73	0.52
1:B:328:ARG:HG2	1:B:694:ARG:NH2	2.25	0.52
1:B:342:LEU:CD2	1:B:704:CYS:HB3	2.36	0.52
1:B:522:THR:C	1:B:524:ILE:H	2.16	0.52
1:C:398:ALA:O	1:C:402:VAL:HG22	2.09	0.52
1:D:75:PHE:CE2	1:D:95:LEU:HD11	2.45	0.52
1:D:329:LYS:CB	1:D:331:THR:H	2.23	0.52
1:A:328:ARG:O	1:A:330:PHE:N	2.42	0.52
1:B:175:ARG:O	1:B:175:ARG:HG2	2.10	0.52
1:B:215:SER:HA	1:B:249:VAL:HG23	1.92	0.52
1:C:215:SER:HA	1:C:249:VAL:HG23	1.92	0.52
1:A:215:SER:HA	1:A:249:VAL:HG23	1.92	0.51
1:A:253:LEU:HD12	1:A:267:VAL:HG13	1.91	0.51
1:B:157:CYS:HB2	1:B:165:HIS:HD2	1.67	0.51
1:C:223:TRP:CE3	1:C:270:MET:CE	2.83	0.51
1:D:253:LEU:HD12	1:D:267:VAL:HG13	1.91	0.51
1:D:328:ARG:O	1:D:330:PHE:N	2.42	0.51
1:A:370:HIS:CB	1:A:662:LEU:HD21	2.40	0.51
1:D:370:HIS:CB	1:D:662:LEU:HD21	2.40	0.51
1:B:489:LEU:N	1:B:489:LEU:CD1	2.73	0.51
1:C:694:ARG:NH1	1:C:695:GLY:H	1.99	0.51
1:D:215:SER:HA	1:D:249:VAL:HG23	1.92	0.51
1:A:75:PHE:CE2	1:A:95:LEU:HD11	2.45	0.51
1:A:328:ARG:HG2	1:A:694:ARG:NH2	2.25	0.51
1:C:312:ARG:HG3	1:C:375:LEU:HD13	1.93	0.51
1:D:398:ALA:O	1:D:402:VAL:HG22	2.09	0.51
1:D:517:ARG:O	1:D:660:TRP:NE1	2.31	0.51
1:A:175:ARG:HG2	1:A:175:ARG:O	2.10	0.51
1:A:268:ILE:CG2	1:A:313:HIS:CD2	2.94	0.51
1:A:312:ARG:HG3	1:A:375:LEU:HD13	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:LYS:CB	1:C:331:THR:H	2.23	0.51
1:C:370:HIS:CB	1:C:662:LEU:HD21	2.40	0.51
1:A:522:THR:OG1	1:B:539:ARG:CD	2.58	0.51
1:C:489:LEU:N	1:C:489:LEU:CD1	2.73	0.51
1:D:175:ARG:O	1:D:175:ARG:HG2	2.10	0.51
1:B:370:HIS:CB	1:B:662:LEU:HD21	2.40	0.51
1:C:75:PHE:CE2	1:C:95:LEU:HD11	2.45	0.51
1:A:175:ARG:CD	1:A:220:THR:HB	2.41	0.51
1:B:253:LEU:HD12	1:B:267:VAL:HG13	1.91	0.51
1:D:175:ARG:CD	1:D:220:THR:HB	2.41	0.51
1:B:75:PHE:CE2	1:B:95:LEU:HD11	2.45	0.50
1:B:299:LEU:CD1	1:B:314:ILE:CG1	2.85	0.50
1:A:328:ARG:HD2	1:A:702:ARG:HD3	1.88	0.50
1:B:223:TRP:HA	1:B:270:MET:HE1	1.94	0.50
1:B:268:ILE:CG2	1:B:313:HIS:CD2	2.94	0.50
1:B:312:ARG:HG3	1:B:375:LEU:HD13	1.93	0.50
1:C:494:THR:CG2	1:C:495:GLU:N	2.75	0.50
1:A:329:LYS:CB	1:A:331:THR:H	2.23	0.50
1:B:329:LYS:CB	1:B:331:THR:H	2.23	0.50
1:C:268:ILE:CG2	1:C:313:HIS:CD2	2.94	0.50
1:D:312:ARG:HG3	1:D:375:LEU:HD13	1.93	0.50
1:A:223:TRP:HA	1:A:270:MET:HE1	1.94	0.50
1:B:337:PRO:CB	1:C:173:GLU:OE2	2.59	0.50
1:D:223:TRP:HA	1:D:270:MET:HE1	1.94	0.50
1:D:494:THR:CG2	1:D:495:GLU:N	2.75	0.50
1:A:644:LEU:HD12	1:B:638:LEU:HD11	1.93	0.50
1:A:401:LEU:HG	1:A:512:LEU:HD13	1.94	0.50
1:B:175:ARG:CD	1:B:220:THR:HB	2.41	0.50
1:B:303:ALA:HA	1:B:372:MET:CE	2.40	0.50
1:C:522:THR:OG1	1:D:539:ARG:CD	2.57	0.50
1:B:401:LEU:HG	1:B:512:LEU:HD13	1.94	0.50
1:C:401:LEU:HG	1:C:512:LEU:HD13	1.94	0.50
1:A:303:ALA:HA	1:A:372:MET:CE	2.40	0.50
1:B:489:LEU:CD1	1:B:489:LEU:H	2.25	0.50
1:B:494:THR:CG2	1:B:495:GLU:N	2.75	0.50
1:C:75:PHE:CZ	1:C:95:LEU:HD11	2.47	0.50
1:C:175:ARG:CD	1:C:220:THR:HB	2.41	0.50
1:B:522:THR:C	1:B:524:ILE:N	2.70	0.50
1:C:517:ARG:O	1:C:660:TRP:NE1	2.31	0.50
1:D:303:ALA:HA	1:D:372:MET:CE	2.40	0.50
1:D:401:LEU:HG	1:D:512:LEU:HD13	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:ARG:O	1:A:660:TRP:NE1	2.31	0.49
1:C:502:VAL:HG21	1:D:558:LEU:HD11	1.94	0.49
1:D:254:VAL:HG21	1:D:302:ALA:HA	1.94	0.49
1:B:517:ARG:O	1:B:660:TRP:NE1	2.31	0.49
1:C:489:LEU:CD1	1:C:489:LEU:H	2.25	0.49
1:D:75:PHE:CZ	1:D:95:LEU:HD11	2.47	0.49
1:A:299:LEU:CD1	1:A:314:ILE:HG13	2.31	0.49
1:D:342:LEU:CD2	1:D:704:CYS:HB3	2.36	0.49
1:B:75:PHE:CZ	1:B:95:LEU:HD11	2.47	0.49
1:D:306:GLY:HA2	1:D:372:MET:SD	2.53	0.49
1:D:328:ARG:HG2	1:D:694:ARG:NH2	2.25	0.49
1:A:254:VAL:HG21	1:A:302:ALA:HA	1.95	0.49
1:C:129:GLN:HA	1:C:129:GLN:NE2	2.28	0.49
1:D:489:LEU:CD1	1:D:489:LEU:H	2.25	0.49
1:A:312:ARG:CB	1:A:375:LEU:CD1	2.91	0.49
1:C:328:ARG:O	1:C:330:PHE:N	2.42	0.49
1:D:263:ASN:O	1:D:267:VAL:CG2	2.44	0.49
1:D:268:ILE:CG2	1:D:313:HIS:CD2	2.94	0.49
1:A:75:PHE:CZ	1:A:95:LEU:HD11	2.47	0.49
1:C:306:GLY:HA2	1:C:372:MET:SD	2.53	0.49
1:C:362:PHE:CZ	1:C:669:LEU:HD13	2.48	0.49
1:A:494:THR:CG2	1:A:495:GLU:N	2.75	0.49
1:B:270:MET:SD	1:B:274:LEU:HD21	2.53	0.49
1:B:328:ARG:O	1:B:330:PHE:N	2.42	0.49
1:B:362:PHE:CZ	1:B:669:LEU:HD13	2.48	0.49
1:B:522:THR:HG23	1:C:539:ARG:NH2	2.28	0.49
1:C:254:VAL:HG21	1:C:302:ALA:HA	1.95	0.49
1:C:303:ALA:HA	1:C:372:MET:CE	2.40	0.49
1:C:312:ARG:CB	1:C:375:LEU:CD1	2.91	0.49
1:D:312:ARG:CB	1:D:375:LEU:CD1	2.91	0.49
1:D:362:PHE:CZ	1:D:669:LEU:HD13	2.48	0.49
1:A:441:ILE:HG22	1:A:487:GLN:HE21	1.70	0.49
1:B:172:ILE:O	1:B:175:ARG:CB	2.60	0.49
1:D:129:GLN:HA	1:D:129:GLN:NE2	2.28	0.49
1:D:270:MET:SD	1:D:274:LEU:HD21	2.53	0.49
1:D:329:LYS:O	1:D:330:PHE:CB	2.61	0.49
1:A:315:LEU:CD2	1:A:377:PRO:HG2	2.43	0.48
1:B:129:GLN:NE2	1:B:129:GLN:HA	2.28	0.48
1:B:169:HIS:CE1	1:B:192:LEU:CD1	2.77	0.48
1:B:315:LEU:CD2	1:B:377:PRO:HG2	2.43	0.48
1:B:522:THR:OG1	1:C:539:ARG:CD	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:TRP:HA	1:C:270:MET:HE1	1.94	0.48
1:C:270:MET:SD	1:C:274:LEU:HD21	2.53	0.48
1:C:270:MET:HG3	1:C:274:LEU:HD21	1.96	0.48
1:C:315:LEU:CD2	1:C:377:PRO:HG2	2.44	0.48
1:D:172:ILE:O	1:D:175:ARG:CB	2.60	0.48
1:A:129:GLN:NE2	1:A:129:GLN:HA	2.28	0.48
1:D:315:LEU:CD2	1:D:377:PRO:HG2	2.43	0.48
1:A:362:PHE:CZ	1:A:669:LEU:HD13	2.48	0.48
1:A:157:CYS:HB2	1:A:165:HIS:HD2	1.67	0.48
1:A:216:LEU:O	1:A:220:THR:HG23	2.14	0.48
1:A:306:GLY:HA2	1:A:372:MET:SD	2.53	0.48
1:A:522:THR:C	1:A:524:ILE:N	2.70	0.48
1:B:254:VAL:HG21	1:B:302:ALA:HA	1.95	0.48
1:B:312:ARG:CB	1:B:375:LEU:CD1	2.91	0.48
1:D:169:HIS:CE1	1:D:192:LEU:CD1	2.77	0.48
1:D:216:LEU:O	1:D:220:THR:HG23	2.14	0.48
1:A:489:LEU:CD1	1:A:489:LEU:H	2.25	0.48
1:B:306:GLY:HA2	1:B:372:MET:SD	2.53	0.48
1:B:441:ILE:HG22	1:B:487:GLN:HE21	1.70	0.48
1:C:329:LYS:O	1:C:330:PHE:CB	2.61	0.48
1:A:270:MET:SD	1:A:274:LEU:HD21	2.53	0.48
1:A:320:SER:HB3	1:A:329:LYS:HG2	1.95	0.48
1:B:320:SER:HB3	1:B:329:LYS:HG2	1.95	0.48
1:C:320:SER:HB3	1:C:329:LYS:HG2	1.95	0.48
1:D:320:SER:HB3	1:D:329:LYS:HG2	1.95	0.48
1:D:370:HIS:CA	1:D:662:LEU:HD21	2.44	0.48
1:C:216:LEU:O	1:C:220:THR:HG23	2.14	0.48
1:B:216:LEU:O	1:B:220:THR:HG23	2.14	0.47
1:C:129:GLN:HB3	1:C:132:VAL:O	2.14	0.47
1:C:376:GLU:O	1:C:380:LYS:HG2	2.14	0.47
1:D:129:GLN:HB3	1:D:132:VAL:O	2.14	0.47
1:D:376:GLU:O	1:D:380:LYS:HG2	2.14	0.47
1:A:329:LYS:O	1:A:330:PHE:CB	2.61	0.47
1:A:621:VAL:CG2	1:A:622:VAL:H	2.24	0.47
1:B:370:HIS:CA	1:B:662:LEU:HD21	2.44	0.47
1:B:312:ARG:HG3	1:B:375:LEU:CD2	2.44	0.47
1:C:410:VAL:HG21	1:C:441:ILE:HD11	1.96	0.47
1:D:270:MET:HG3	1:D:274:LEU:HD21	1.95	0.47
1:D:376:GLU:N	1:D:377:PRO:CD	2.78	0.47
1:D:410:VAL:HG21	1:D:441:ILE:HD11	1.97	0.47
1:A:312:ARG:HG3	1:A:375:LEU:CD2	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLU:O	1:A:380:LYS:HG2	2.14	0.47
1:A:410:VAL:HG21	1:A:441:ILE:HD11	1.96	0.47
1:B:376:GLU:N	1:B:377:PRO:CD	2.77	0.47
1:B:410:VAL:HG21	1:B:441:ILE:HD11	1.96	0.47
1:B:621:VAL:CG2	1:B:622:VAL:N	2.78	0.47
1:C:342:LEU:CD2	1:C:704:CYS:HB3	2.36	0.47
1:B:129:GLN:HB3	1:B:132:VAL:O	2.14	0.47
1:B:376:GLU:O	1:B:380:LYS:HG2	2.14	0.47
1:C:370:HIS:CA	1:C:662:LEU:HD21	2.44	0.47
1:A:621:VAL:CG2	1:A:622:VAL:N	2.78	0.47
1:B:270:MET:HG3	1:B:274:LEU:HD21	1.95	0.47
1:A:129:GLN:HB3	1:A:132:VAL:O	2.14	0.47
1:A:270:MET:HG3	1:A:274:LEU:HD21	1.95	0.47
1:B:494:THR:HG22	1:B:495:GLU:H	1.80	0.47
1:C:494:THR:HG22	1:C:495:GLU:H	1.80	0.47
1:D:299:LEU:CD1	1:D:314:ILE:HG13	2.31	0.47
1:A:605:ILE:N	1:A:606:GLY:HA2	2.30	0.47
1:D:605:ILE:N	1:D:606:GLY:HA2	2.30	0.47
1:A:376:GLU:N	1:A:377:PRO:CD	2.78	0.47
1:C:376:GLU:N	1:C:377:PRO:CD	2.78	0.46
1:B:605:ILE:N	1:B:606:GLY:HA2	2.30	0.46
1:C:312:ARG:HG3	1:C:375:LEU:CD2	2.44	0.46
1:D:312:ARG:HG3	1:D:375:LEU:CD2	2.44	0.46
1:A:494:THR:HG22	1:A:495:GLU:H	1.80	0.46
1:B:489:LEU:HD12	1:B:489:LEU:H	1.79	0.46
1:A:370:HIS:CA	1:A:662:LEU:HD21	2.44	0.46
1:C:605:ILE:N	1:C:606:GLY:HA2	2.30	0.46
1:D:494:THR:HG22	1:D:495:GLU:H	1.80	0.46
1:B:112:THR:HG22	1:B:119:THR:HG22	1.98	0.46
1:B:621:VAL:CG2	1:B:622:VAL:H	2.24	0.46
1:D:327:SER:O	1:D:328:ARG:HB2	2.16	0.46
1:D:522:THR:C	1:D:524:ILE:N	2.70	0.45
1:D:621:VAL:CG2	1:D:622:VAL:N	2.78	0.45
1:A:223:TRP:HH2	1:A:273:GLY:HA3	1.79	0.45
1:A:539:ARG:NH2	1:D:522:THR:HG23	2.32	0.45
1:C:522:THR:C	1:C:524:ILE:N	2.70	0.45
1:A:112:THR:HG22	1:A:119:THR:HG22	1.98	0.45
1:B:327:SER:O	1:B:328:ARG:HB2	2.16	0.45
1:A:327:SER:O	1:A:328:ARG:HB2	2.16	0.45
1:C:337:PRO:HB3	1:D:173:GLU:OE2	2.16	0.45
1:C:441:ILE:HG22	1:C:487:GLN:HE21	1.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:621:VAL:CG2	1:C:622:VAL:H	2.24	0.45
1:D:487:GLN:OE1	1:D:490:ARG:NE	2.48	0.45
1:A:489:LEU:HD12	1:A:489:LEU:H	1.79	0.45
1:C:172:ILE:O	1:C:175:ARG:CB	2.60	0.45
1:C:112:THR:HG22	1:C:119:THR:HG22	1.98	0.45
1:C:310:ILE:CD1	1:C:311:PHE:N	2.73	0.45
1:D:544:TYR:HB2	1:D:636:LEU:HD11	1.99	0.45
1:A:373:VAL:HB	1:A:378:LEU:HD12	1.99	0.45
1:C:312:ARG:HG3	1:C:375:LEU:CD1	2.47	0.45
1:A:492:MET:O	1:A:493:GLU:HB2	2.17	0.44
1:A:544:TYR:HB2	1:A:636:LEU:HD11	1.99	0.44
1:B:223:TRP:O	1:B:223:TRP:CD1	2.70	0.44
1:C:127:ASN:HD22	1:C:133:ASN:ND2	2.16	0.44
1:C:223:TRP:O	1:C:223:TRP:CG	2.70	0.44
1:D:492:MET:O	1:D:493:GLU:HB2	2.18	0.44
1:B:544:TYR:HB2	1:B:636:LEU:HD11	1.99	0.44
1:D:223:TRP:HH2	1:D:273:GLY:HA3	1.79	0.44
1:D:223:TRP:O	1:D:223:TRP:CD1	2.70	0.44
1:D:223:TRP:O	1:D:223:TRP:CG	2.71	0.44
1:A:223:TRP:CD1	1:A:223:TRP:O	2.70	0.44
1:A:312:ARG:HG3	1:A:375:LEU:CD1	2.47	0.44
1:C:223:TRP:O	1:C:223:TRP:CD1	2.70	0.44
1:A:607:MET:HG2	1:B:607:MET:HE1	1.99	0.44
1:B:487:GLN:OE1	1:B:490:ARG:NE	2.48	0.44
1:C:327:SER:O	1:C:328:ARG:HB2	2.16	0.44
1:D:112:THR:HG22	1:D:119:THR:HG22	1.98	0.44
1:D:373:VAL:HB	1:D:378:LEU:HD12	1.99	0.44
1:A:315:LEU:HD21	1:A:377:PRO:CG	2.48	0.44
1:B:223:TRP:HH2	1:B:273:GLY:HA3	1.79	0.44
1:D:621:VAL:CG2	1:D:622:VAL:H	2.24	0.44
1:B:315:LEU:HD21	1:B:377:PRO:CG	2.48	0.44
1:C:373:VAL:HB	1:C:378:LEU:HD12	1.99	0.44
1:B:127:ASN:HD22	1:B:133:ASN:ND2	2.16	0.44
1:C:492:MET:O	1:C:493:GLU:HB2	2.17	0.44
1:C:544:TYR:HB2	1:C:636:LEU:HD11	1.99	0.44
1:A:331:THR:O	1:A:332:GLU:HG2	2.18	0.44
1:B:329:LYS:O	1:B:330:PHE:CB	2.61	0.44
1:C:401:LEU:HD12	1:C:512:LEU:HD22	2.00	0.44
1:D:127:ASN:HD22	1:D:133:ASN:ND2	2.15	0.44
1:B:223:TRP:O	1:B:223:TRP:CG	2.70	0.43
1:B:352:GLU:OE1	1:B:352:GLU:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:LEU:HD12	1:B:512:LEU:HD22	2.00	0.43
1:D:312:ARG:HG3	1:D:375:LEU:CD1	2.47	0.43
1:D:331:THR:O	1:D:332:GLU:HG2	2.18	0.43
1:B:312:ARG:HG3	1:B:375:LEU:CD1	2.47	0.43
1:B:492:MET:O	1:B:493:GLU:HB2	2.18	0.43
1:A:223:TRP:O	1:A:223:TRP:CG	2.70	0.43
1:C:223:TRP:HH2	1:C:273:GLY:HA3	1.79	0.43
1:D:401:LEU:HD12	1:D:512:LEU:HD22	2.00	0.43
1:D:662:LEU:O	1:D:666:ILE:N	2.45	0.43
1:A:352:GLU:HA	1:A:352:GLU:OE1	2.18	0.43
1:A:401:LEU:HD12	1:A:512:LEU:HD22	2.00	0.43
1:A:497:TYR:CD2	1:A:498:LEU:N	2.87	0.43
1:D:497:TYR:CD2	1:D:498:LEU:N	2.87	0.43
1:B:497:TYR:CD2	1:B:498:LEU:N	2.87	0.43
1:C:489:LEU:HD12	1:C:489:LEU:H	1.79	0.43
1:D:352:GLU:OE1	1:D:352:GLU:HA	2.19	0.43
1:A:332:GLU:OE1	1:A:342:LEU:HD22	2.19	0.43
1:B:373:VAL:HB	1:B:378:LEU:HD12	1.99	0.43
1:C:497:TYR:CD2	1:C:498:LEU:N	2.87	0.43
1:B:129:GLN:HA	1:B:129:GLN:HE21	1.84	0.43
1:B:329:LYS:HB2	1:B:331:THR:O	2.19	0.43
1:C:299:LEU:CD1	1:C:314:ILE:HG13	2.31	0.43
1:C:331:THR:O	1:C:332:GLU:HG2	2.18	0.43
1:A:127:ASN:HD22	1:A:133:ASN:ND2	2.15	0.43
1:A:487:GLN:OE1	1:A:490:ARG:NE	2.47	0.43
1:C:153:VAL:HG22	1:C:188:ALA:HB2	2.01	0.43
1:C:352:GLU:HA	1:C:352:GLU:OE1	2.18	0.43
1:D:410:VAL:HG11	1:D:441:ILE:HD11	2.01	0.43
1:C:314:ILE:HG23	1:C:315:LEU:N	2.34	0.42
1:C:337:PRO:HG2	1:C:338:VAL:H	1.84	0.42
1:C:522:THR:HG23	1:D:539:ARG:NH2	2.34	0.42
1:A:157:CYS:HB2	1:A:165:HIS:NE2	2.33	0.42
1:A:271:TYR:CD1	1:A:271:TYR:C	2.98	0.42
1:B:337:PRO:HG2	1:B:338:VAL:H	1.84	0.42
1:B:454:TRP:CE2	1:B:676:TRP:HB2	2.55	0.42
1:C:621:VAL:CG2	1:C:622:VAL:N	2.78	0.42
1:D:153:VAL:HG22	1:D:188:ALA:HB2	2.01	0.42
1:D:332:GLU:OE1	1:D:342:LEU:HD22	2.19	0.42
1:D:314:ILE:HG23	1:D:315:LEU:N	2.34	0.42
1:D:454:TRP:CE2	1:D:676:TRP:HB2	2.55	0.42
1:A:172:ILE:O	1:A:175:ARG:CB	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PRO:HG2	1:A:338:VAL:H	1.84	0.42
1:A:410:VAL:HG11	1:A:441:ILE:HD11	2.01	0.42
1:B:331:THR:O	1:B:332:GLU:HG2	2.18	0.42
1:C:662:LEU:O	1:C:666:ILE:N	2.45	0.42
1:D:304:LYS:HA	1:D:359:ILE:HD13	2.01	0.42
1:A:173:GLU:OE2	1:D:337:PRO:HB3	2.20	0.42
1:B:223:TRP:HH2	1:B:273:GLY:CA	2.33	0.42
1:C:223:TRP:HH2	1:C:273:GLY:CA	2.33	0.42
1:D:337:PRO:HG2	1:D:338:VAL:H	1.84	0.42
1:D:498:LEU:N	1:D:499:PRO:CD	2.83	0.42
1:A:153:VAL:HG22	1:A:188:ALA:HB2	2.01	0.42
1:A:329:LYS:HB2	1:A:331:THR:O	2.19	0.42
1:B:107:THR:HG23	1:B:148:ASN:HD21	1.85	0.42
1:B:153:VAL:HG22	1:B:188:ALA:HB2	2.01	0.42
1:A:337:PRO:HB3	1:B:173:GLU:OE2	2.19	0.42
1:B:332:GLU:OE1	1:B:342:LEU:HD22	2.19	0.42
1:C:129:GLN:HA	1:C:129:GLN:HE21	1.84	0.42
1:C:315:LEU:HD21	1:C:377:PRO:CG	2.48	0.42
1:C:329:LYS:HB2	1:C:331:THR:O	2.19	0.42
1:C:454:TRP:CE2	1:C:676:TRP:HB2	2.55	0.42
1:D:345:LEU:CD2	1:D:348:VAL:HG12	2.50	0.42
1:A:107:THR:HG23	1:A:148:ASN:HD21	1.85	0.42
1:A:441:ILE:CG2	1:A:487:GLN:NE2	2.62	0.42
1:A:454:TRP:CE2	1:A:676:TRP:HB2	2.55	0.42
1:A:498:LEU:N	1:A:499:PRO:CD	2.83	0.42
1:B:271:TYR:CD1	1:B:271:TYR:C	2.98	0.42
1:B:410:VAL:HG11	1:B:441:ILE:HD11	2.01	0.42
1:D:315:LEU:HD21	1:D:377:PRO:CG	2.48	0.42
1:B:337:PRO:HB3	1:C:173:GLU:CD	2.44	0.42
1:A:223:TRP:HH2	1:A:273:GLY:CA	2.33	0.41
1:A:345:LEU:CD2	1:A:348:VAL:HG12	2.50	0.41
1:B:644:LEU:HD11	1:C:642:ILE:HG13	2.01	0.41
1:C:332:GLU:OE1	1:C:342:LEU:HD22	2.19	0.41
1:D:310:ILE:CD1	1:D:311:PHE:N	2.73	0.41
1:D:329:LYS:HB2	1:D:331:THR:O	2.19	0.41
1:D:489:LEU:HD12	1:D:489:LEU:H	1.79	0.41
1:B:331:THR:O	1:B:332:GLU:CG	2.68	0.41
1:B:345:LEU:CD2	1:B:348:VAL:HG12	2.50	0.41
1:C:271:TYR:CD1	1:C:271:TYR:C	2.98	0.41
1:C:331:THR:O	1:C:332:GLU:CG	2.69	0.41
1:D:271:TYR:CD1	1:D:271:TYR:C	2.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:THR:O	1:D:332:GLU:CG	2.69	0.41
1:B:498:LEU:N	1:B:499:PRO:CD	2.83	0.41
1:C:498:LEU:N	1:C:499:PRO:CD	2.83	0.41
1:D:157:CYS:HB2	1:D:165:HIS:NE2	2.33	0.41
1:A:304:LYS:HA	1:A:359:ILE:HD13	2.01	0.41
1:A:314:ILE:HG23	1:A:315:LEU:N	2.34	0.41
1:C:107:THR:HG23	1:C:148:ASN:HD21	1.85	0.41
1:D:223:TRP:HH2	1:D:273:GLY:CA	2.33	0.41
1:C:410:VAL:HG11	1:C:441:ILE:HD11	2.01	0.41
1:A:331:THR:O	1:A:332:GLU:CG	2.68	0.41
1:B:304:LYS:HA	1:B:359:ILE:HD13	2.01	0.41
1:B:365:LYS:O	1:B:367:PRO:HD3	2.21	0.41
1:A:365:LYS:O	1:A:367:PRO:HD3	2.21	0.41
1:B:157:CYS:HB2	1:B:165:HIS:NE2	2.33	0.41
1:C:157:CYS:HB2	1:C:165:HIS:NE2	2.33	0.41
1:C:304:LYS:HA	1:C:359:ILE:HD13	2.01	0.41
1:C:365:LYS:O	1:C:367:PRO:HD3	2.21	0.41
1:D:107:THR:HG23	1:D:148:ASN:HD21	1.85	0.41
1:A:168:LEU:CG	1:A:183:LEU:HD22	2.50	0.41
1:A:247:ASN:HB3	1:A:251:HIS:HB2	2.03	0.41
1:B:270:MET:HG3	1:B:274:LEU:HD23	2.03	0.41
1:B:299:LEU:CD1	1:B:314:ILE:HG12	2.51	0.41
1:B:314:ILE:HG23	1:B:315:LEU:N	2.34	0.41
1:B:337:PRO:HA	1:C:173:GLU:OE2	2.21	0.41
1:D:129:GLN:HA	1:D:129:GLN:HE21	1.84	0.41
1:D:450:LEU:HD12	1:D:451:GLY:N	2.36	0.41
1:B:310:ILE:CD1	1:B:311:PHE:N	2.73	0.41
1:B:324:GLN:HG2	1:B:327:SER:CB	2.51	0.41
1:C:299:LEU:CD1	1:C:314:ILE:HG12	2.51	0.41
1:C:345:LEU:CD2	1:C:348:VAL:HG12	2.50	0.41
1:D:168:LEU:CD2	1:D:183:LEU:CD2	2.93	0.41
1:C:317:ARG:CG	1:C:319:PHE:HE2	2.34	0.40
1:C:694:ARG:NH1	1:C:695:GLY:HA2	2.29	0.40
1:A:129:GLN:HA	1:A:129:GLN:HE21	1.84	0.40
1:A:450:LEU:HD12	1:A:451:GLY:N	2.36	0.40
1:A:502:VAL:HG21	1:B:558:LEU:CD2	2.33	0.40
1:B:168:LEU:CG	1:B:183:LEU:HD22	2.50	0.40
1:B:629:TYR:HA	1:B:632:LEU:HG	2.04	0.40
1:C:247:ASN:HB3	1:C:251:HIS:HB2	2.03	0.40
1:D:331:THR:C	1:D:332:GLU:HG3	2.46	0.40
1:D:364:CYS:SG	1:D:369:ARG:NH2	2.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:LYS:O	1:D:367:PRO:HD3	2.21	0.40
1:A:270:MET:HG3	1:A:274:LEU:HD23	2.03	0.40
1:B:168:LEU:HD22	1:B:183:LEU:HD22	2.01	0.40
1:B:331:THR:C	1:B:332:GLU:HG3	2.46	0.40
1:A:629:TYR:HA	1:A:632:LEU:HG	2.04	0.40
1:B:168:LEU:CD2	1:B:183:LEU:CD2	2.93	0.40
1:B:247:ASN:HB3	1:B:251:HIS:HB2	2.03	0.40
1:B:364:CYS:SG	1:B:369:ARG:NH2	2.94	0.40
1:C:168:LEU:CG	1:C:183:LEU:HD22	2.50	0.40
1:C:314:ILE:HD12	1:C:317:ARG:CZ	2.52	0.40
1:D:441:ILE:HG22	1:D:487:GLN:HE21	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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	535/683 (78%)	530 (99%)	5 (1%)	70	76
1	B	535/683 (78%)	530 (99%)	5 (1%)	70	76
1	C	535/683 (78%)	530 (99%)	5 (1%)	70	76
1	D	535/683 (78%)	530 (99%)	5 (1%)	70	76
All	All	2140/2732 (78%)	2120 (99%)	20 (1%)	68	76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	LEU
1	A	214	LEU
1	A	373	VAL
1	A	477	LEU
1	A	694	ARG
1	B	152	LEU
1	B	214	LEU
1	B	373	VAL
1	B	477	LEU
1	B	694	ARG
1	C	152	LEU
1	C	214	LEU
1	C	373	VAL
1	C	477	LEU
1	C	694	ARG
1	D	152	LEU
1	D	214	LEU
1	D	373	VAL
1	D	477	LEU
1	D	694	ARG

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	127	ASN
1	A	129	GLN
1	A	141	GLN
1	A	165	HIS
1	A	169	HIS
1	A	222	GLN
1	A	235	GLN
1	A	251	HIS
1	A	324	GLN
1	A	363	HIS
1	A	383	GLN
1	A	396	ASN
1	A	521	HIS
1	A	673	ASN
1	B	127	ASN
1	B	129	GLN
1	B	141	GLN
1	B	165	HIS
1	B	169	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	222	GLN
1	B	235	GLN
1	B	251	HIS
1	B	294	GLN
1	B	324	GLN
1	B	363	HIS
1	B	383	GLN
1	B	396	ASN
1	B	673	ASN
1	C	127	ASN
1	C	129	GLN
1	C	165	HIS
1	C	169	HIS
1	C	222	GLN
1	C	235	GLN
1	C	251	HIS
1	C	294	GLN
1	C	324	GLN
1	C	363	HIS
1	C	383	GLN
1	C	396	ASN
1	C	521	HIS
1	C	673	ASN
1	D	127	ASN
1	D	129	GLN
1	D	165	HIS
1	D	169	HIS
1	D	222	GLN
1	D	235	GLN
1	D	251	HIS
1	D	383	GLN
1	D	396	ASN
1	D	521	HIS
1	D	673	ASN

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 [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.

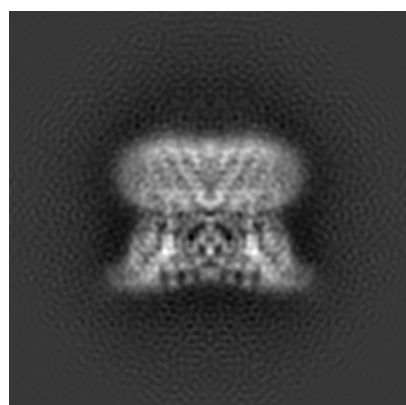
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6580. These allow visual inspection of the internal detail of the map and identification of artifacts.

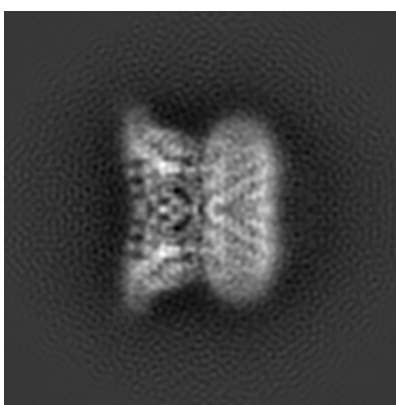
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

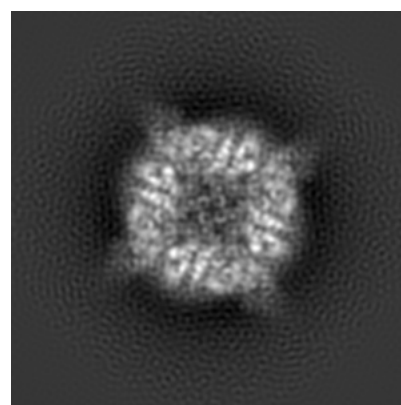
6.1.1 Primary map



X



Y

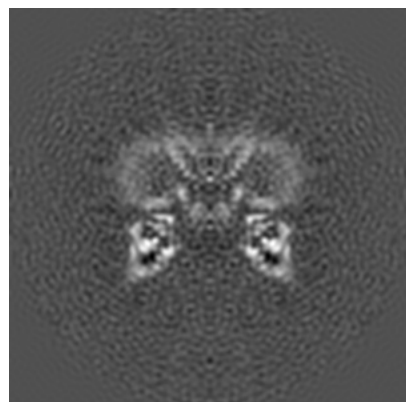


Z

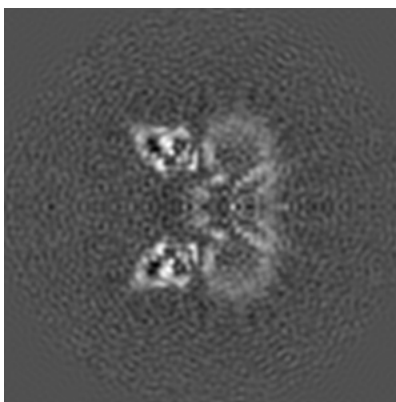
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

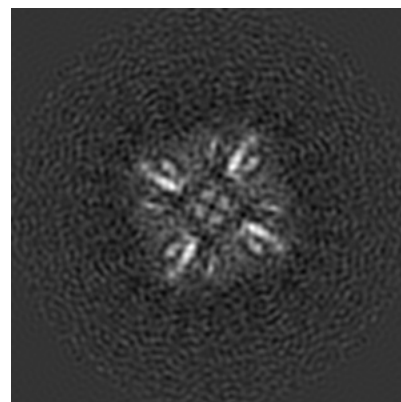
6.2.1 Primary map



X Index: 96



Y Index: 96

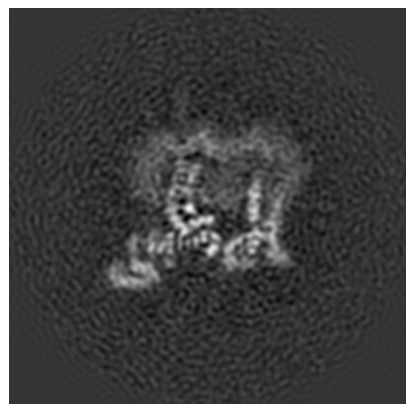


Z Index: 96

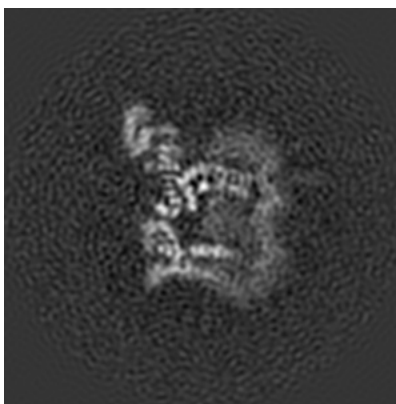
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

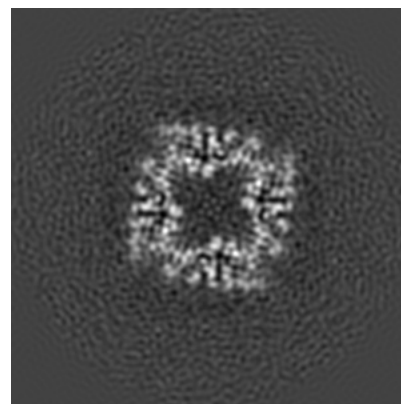
6.3.1 Primary map



X Index: 115



Y Index: 115

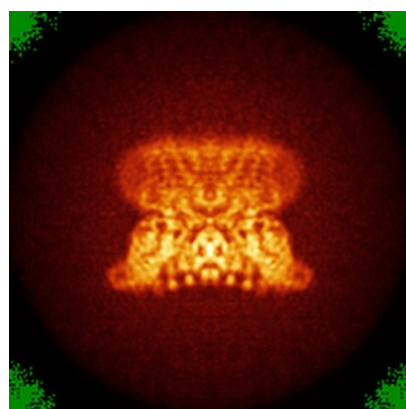


Z Index: 76

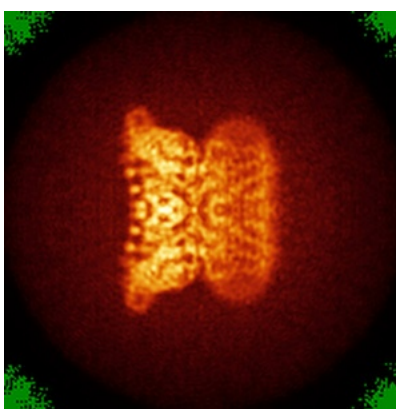
The images above show the largest variance slices of the map in three orthogonal directions.

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

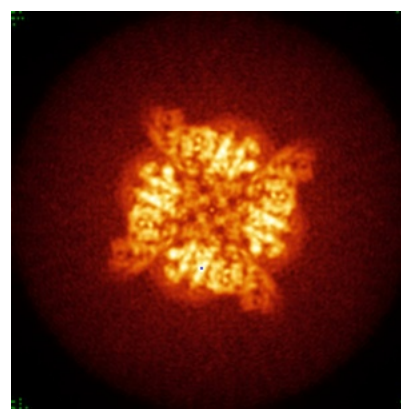
6.4.1 Primary map



X



Y

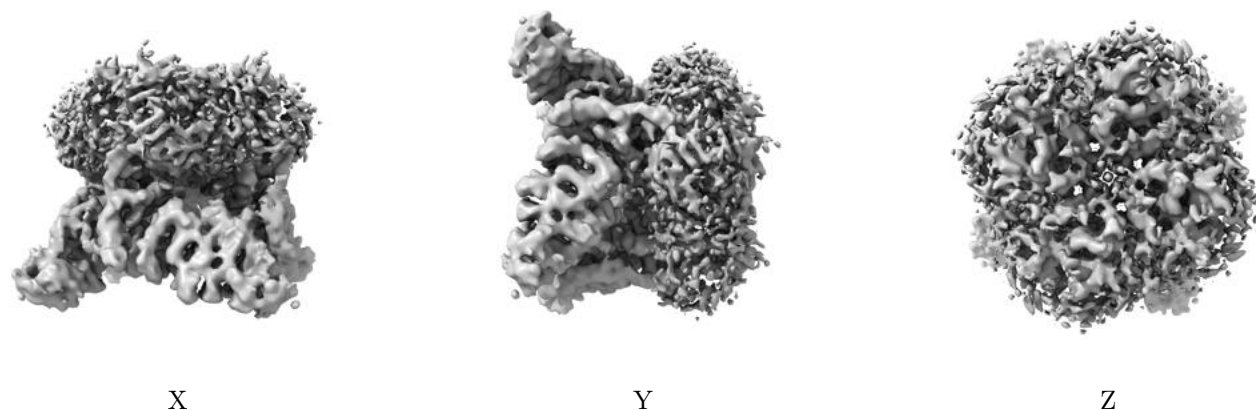


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

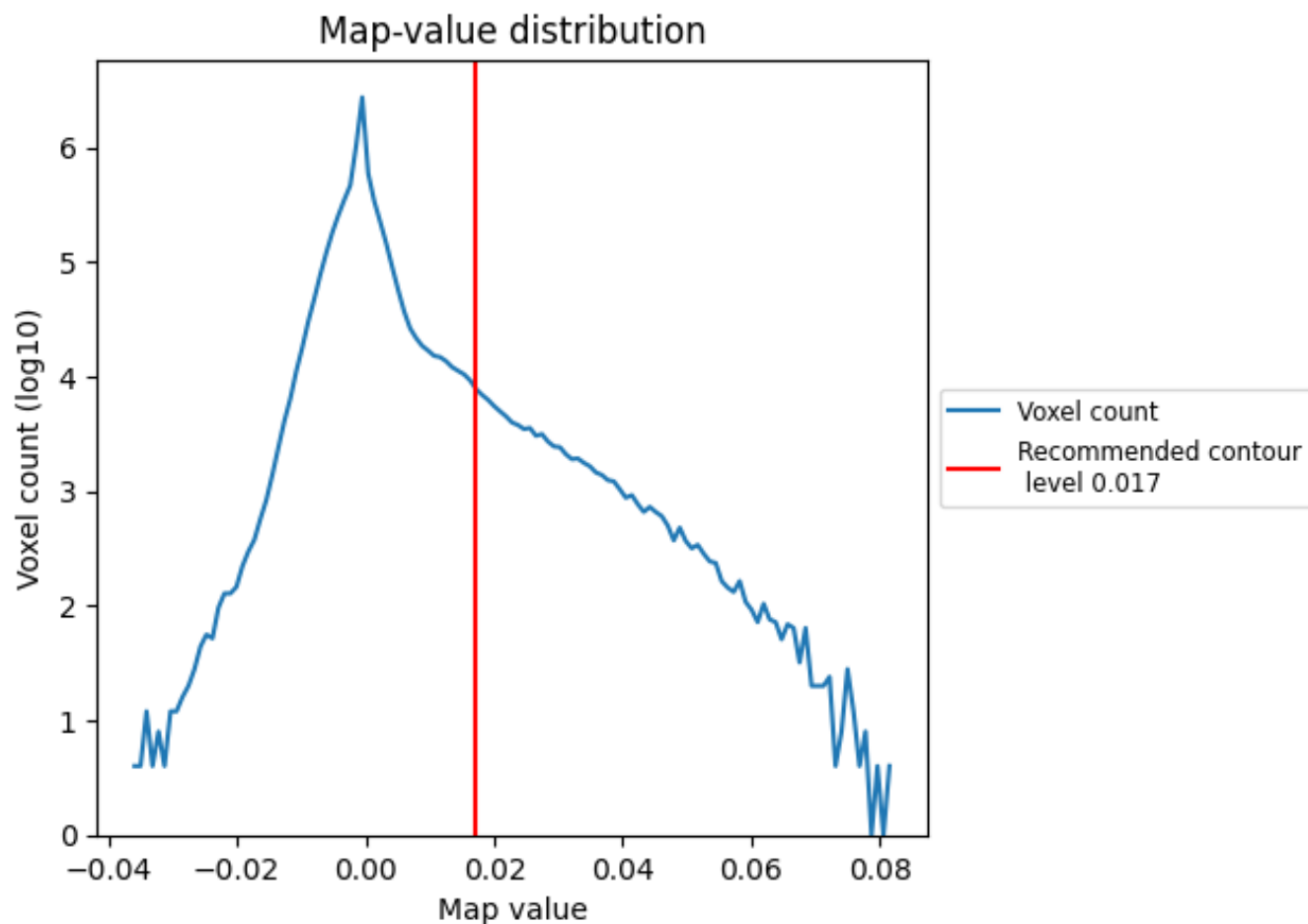
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

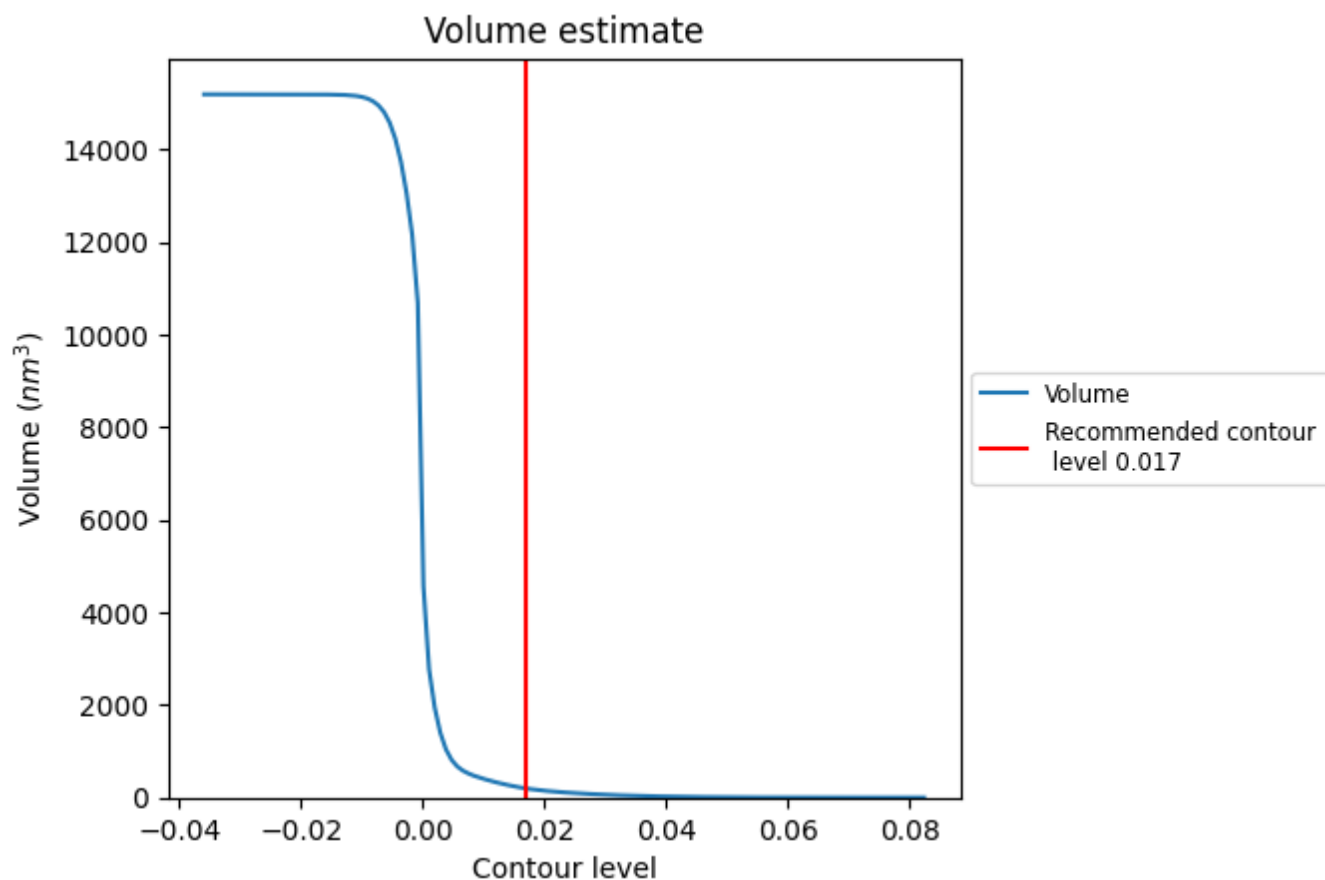
This section contains the results of statistical analysis of the map.

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.

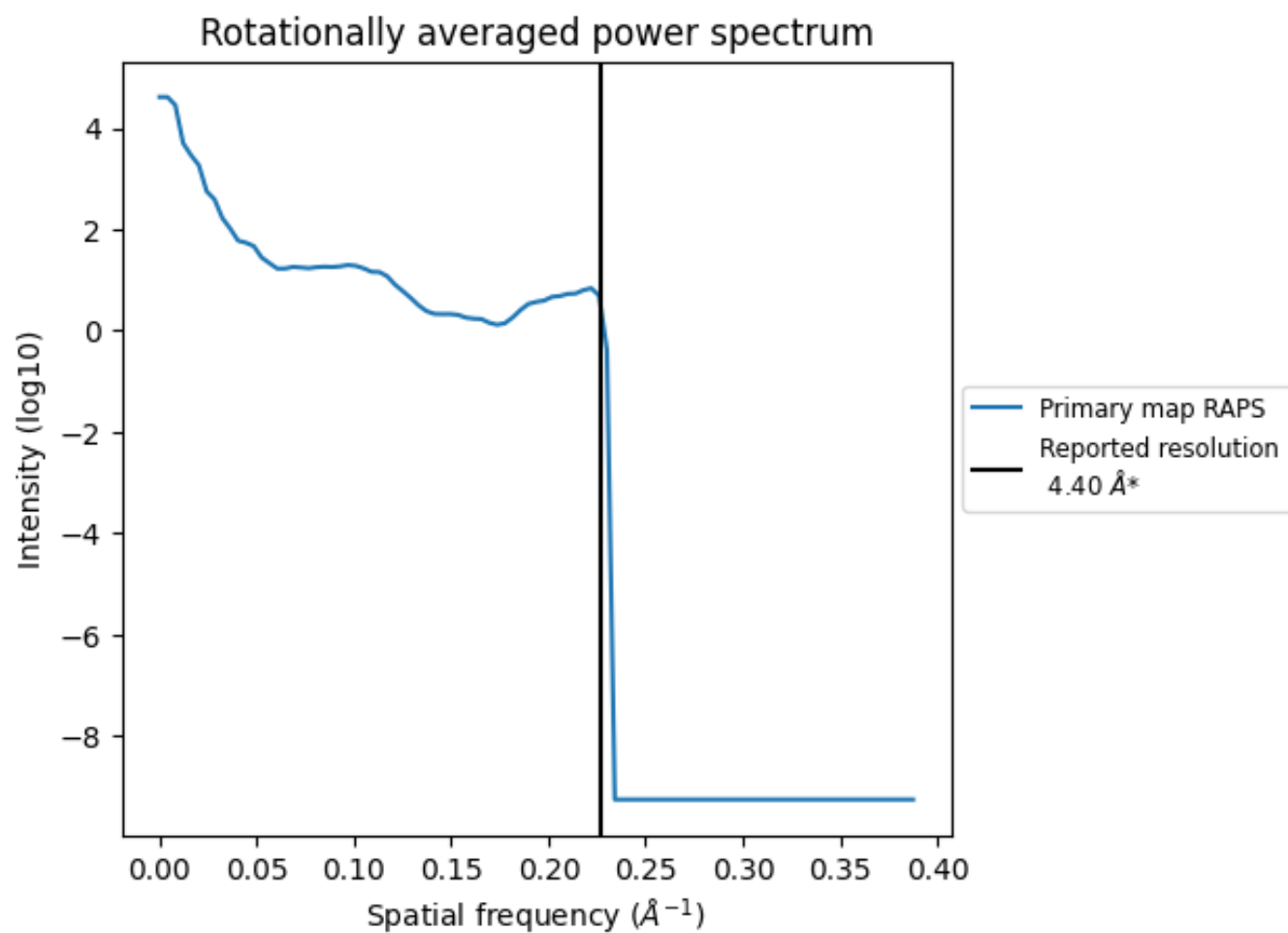
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 198 nm³; this corresponds to an approximate mass of 179 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 ⓘ

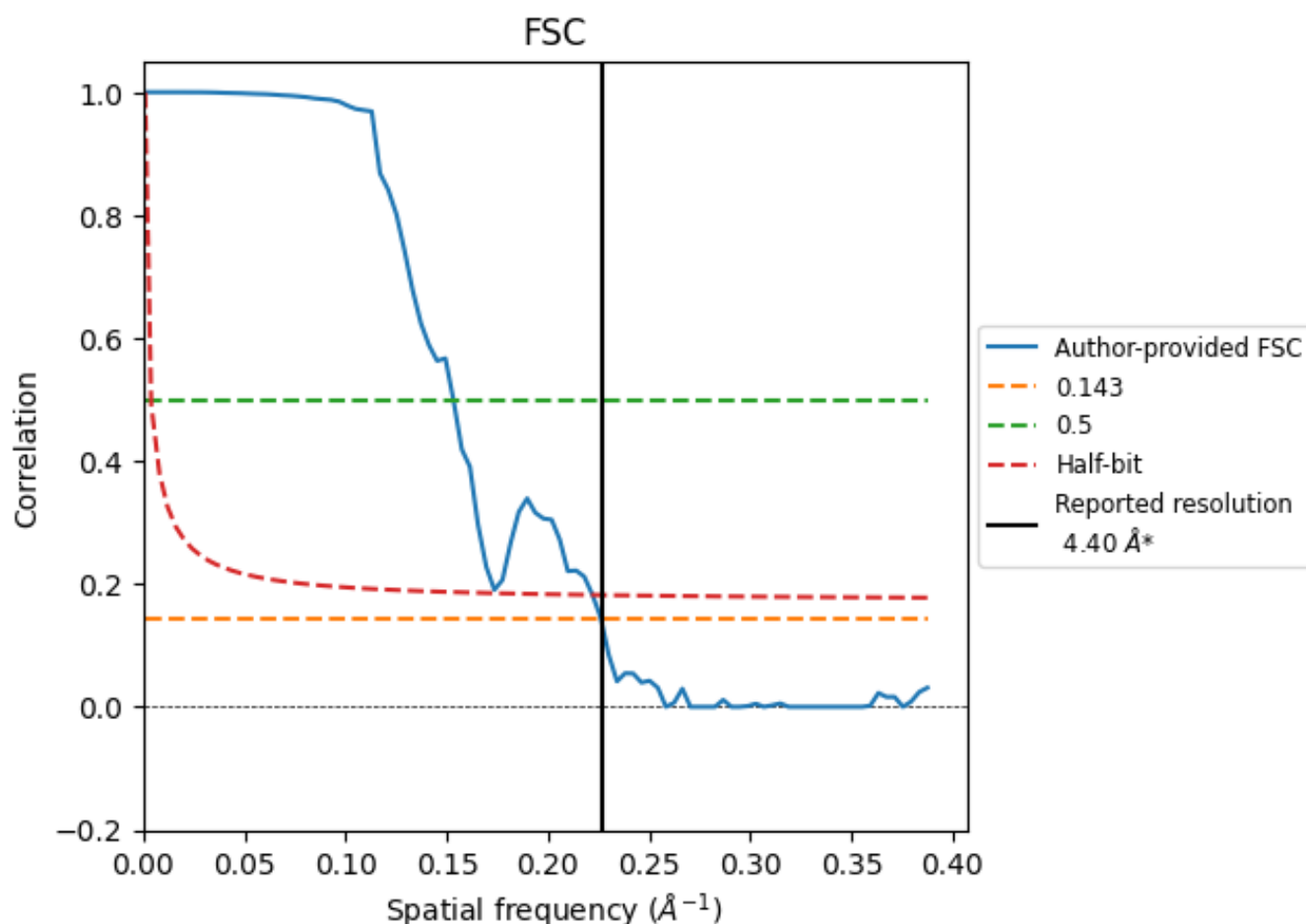


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

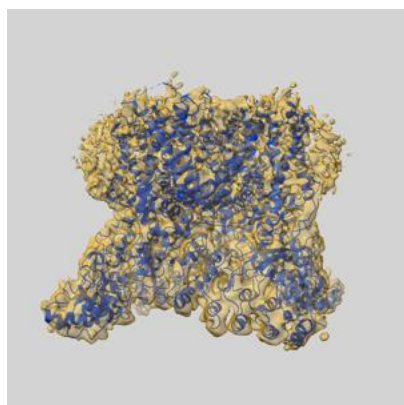
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.42	6.52	4.50
Unmasked-calculated*	-	-	-

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

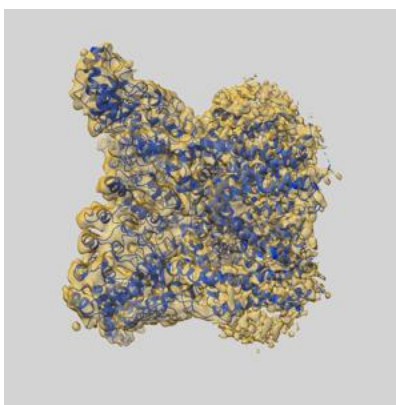
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6580 and PDB model 5HI9. Per-residue inclusion information can be found in section 3 on page 5.

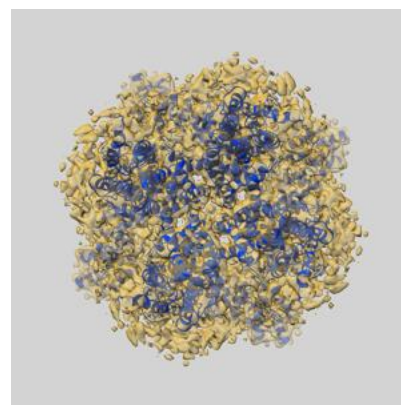
9.1 Map-model overlay [i](#)



X



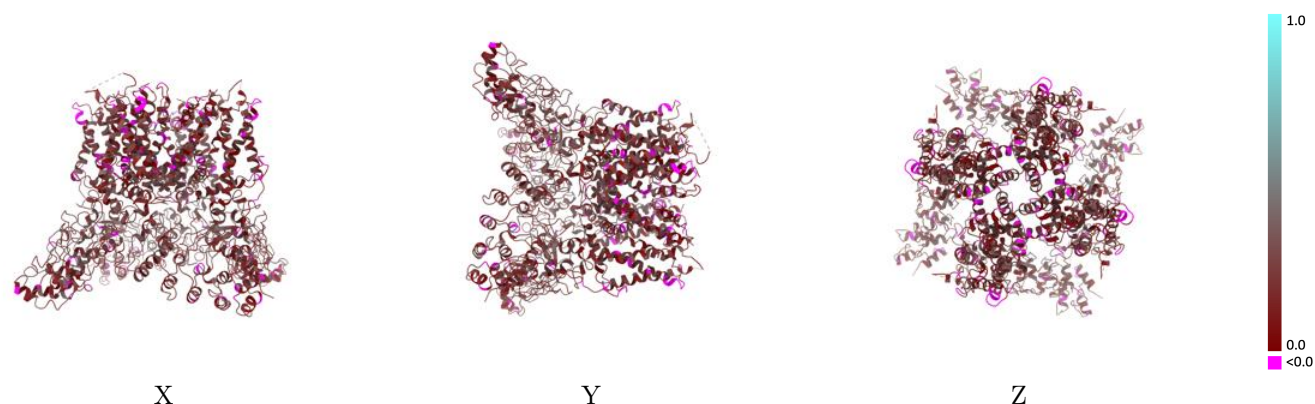
Y



Z

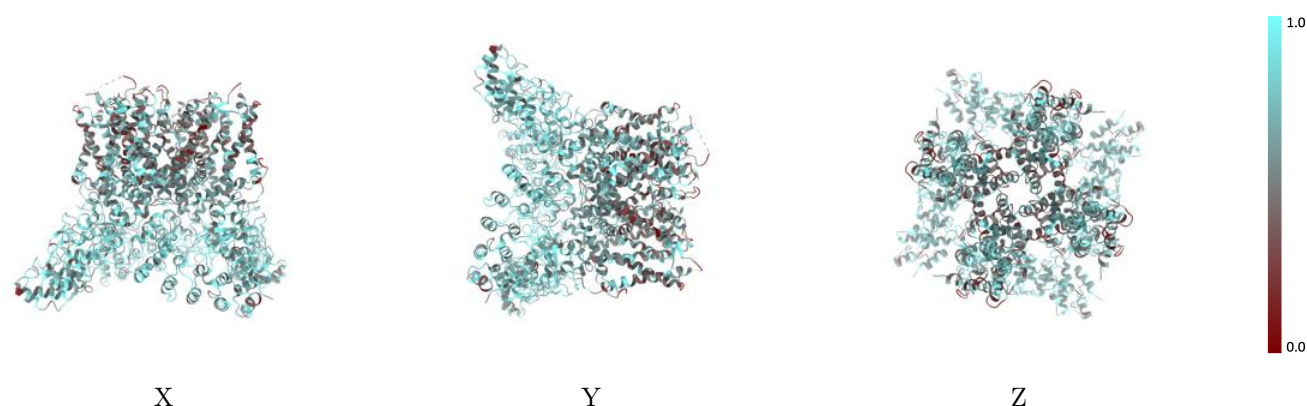
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



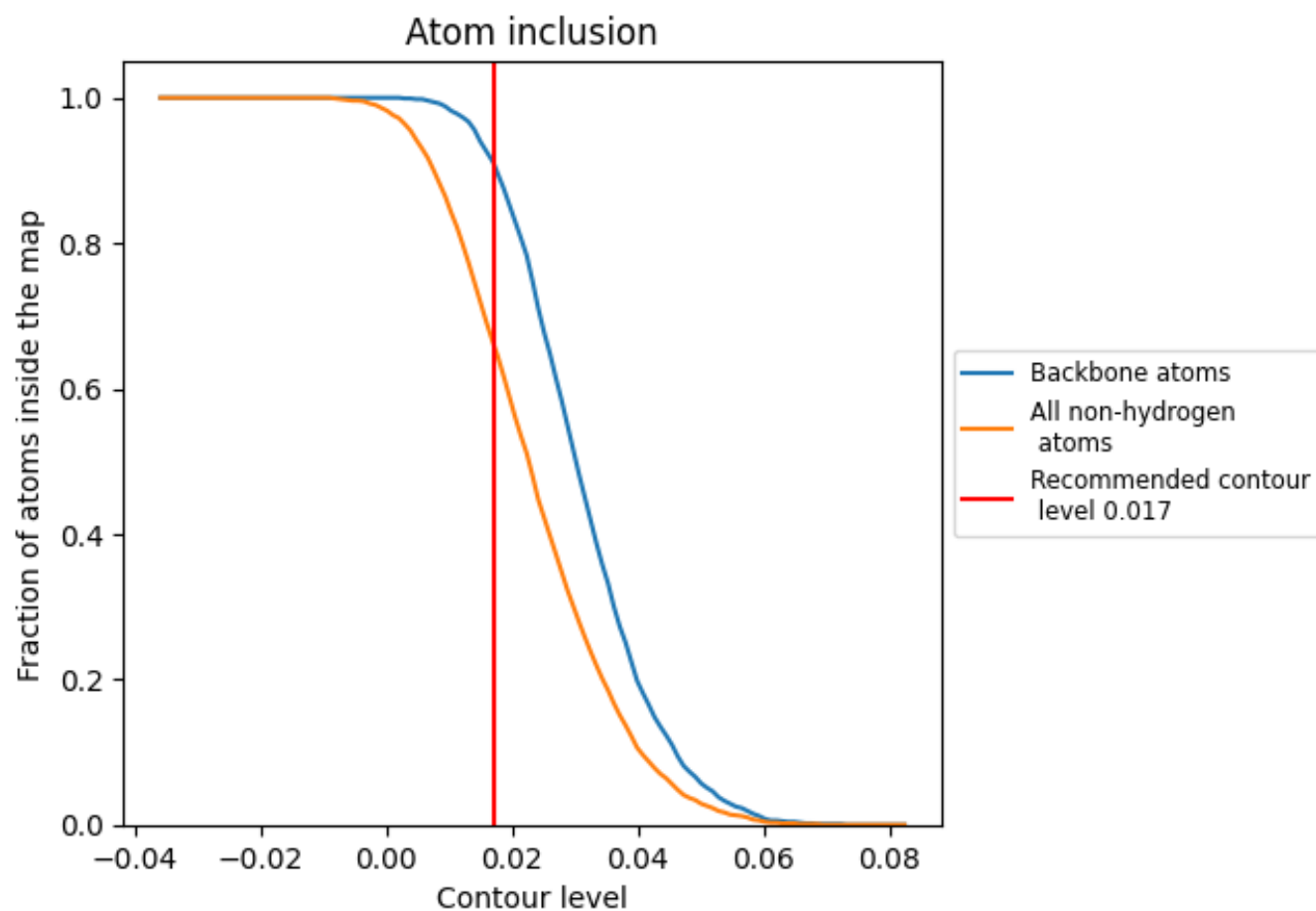
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 66% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6620	0.2140
A	0.6630	0.2130
B	0.6630	0.2150
C	0.6600	0.2130
D	0.6610	0.2130

