



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 05:27 AM UTC

PDB ID : 9CJL / pdb_00009cjl
EMDB ID : EMD-45635
Title : Molecular basis of TMED9 dodecamer
Authors : Le, X.; Xiong, P.
Deposited on : 2024-07-06
Resolution : 5.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

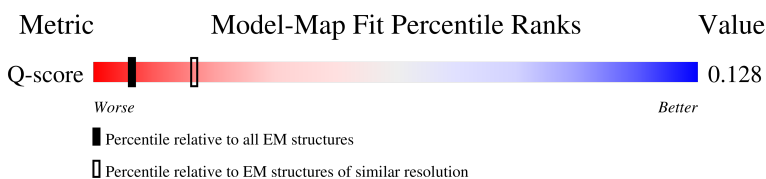
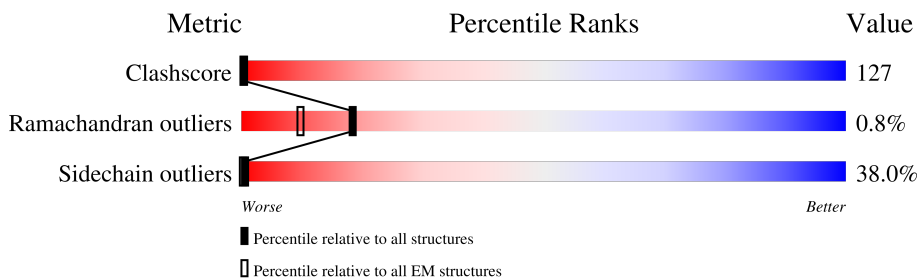
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.50 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.



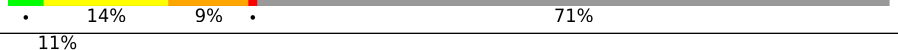
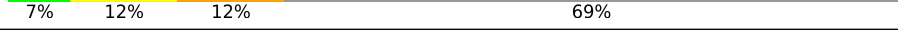
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	520 (5.00 - 6.00)

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	235	17% 6% 17% 11% 65%
1	B	235	10% 5% 16% 13% 65%
1	C	235	10% 8% 11% 15% 65%
1	D	235	17% 14% 69%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	235	
1	F	235	
1	G	235	
1	H	235	
1	I	235	
1	J	235	
1	K	235	
1	L	235	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	9ED	B	301	-	-	X	-
2	9ED	H	301	-	-	X	-

2 Entry composition [i](#)

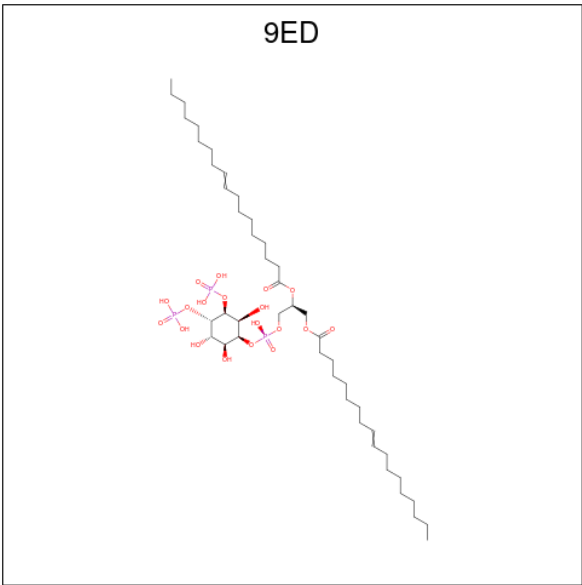
There are 2 unique types of molecules in this entry. The entry contains 7985 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

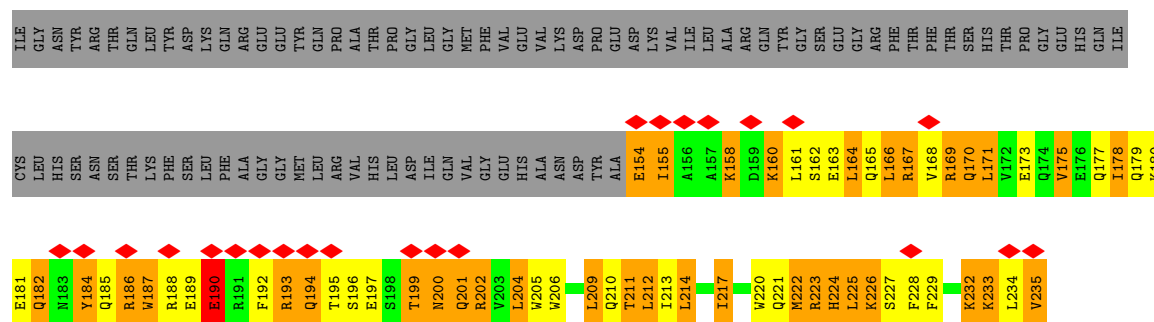
- Molecule 1 is a protein called Transmembrane emp24 domain-containing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	82	Total	C	N	O	S	0	0
			709	453	131	124	1		
1	B	82	Total	C	N	O	S	0	0
			709	453	131	124	1		
1	C	82	Total	C	N	O	S	0	0
			709	453	131	124	1		
1	D	74	Total	C	N	O	S	0	0
			648	414	121	112	1		
1	E	74	Total	C	N	O	S	0	0
			648	414	121	112	1		
1	F	74	Total	C	N	O	S	0	0
			648	414	121	112	1		
1	G	74	Total	C	N	O	S	0	0
			648	414	121	112	1		
1	H	74	Total	C	N	O	S	0	0
			648	414	121	112	1		
1	I	74	Total	C	N	O	S	0	0
			648	414	121	112	1		
1	J	69	Total	C	N	O	S	0	0
			607	386	115	105	1		
1	K	67	Total	C	N	O	S	0	0
			593	378	113	101	1		
1	L	74	Total	C	N	O	S	0	0
			648	414	121	112	1		

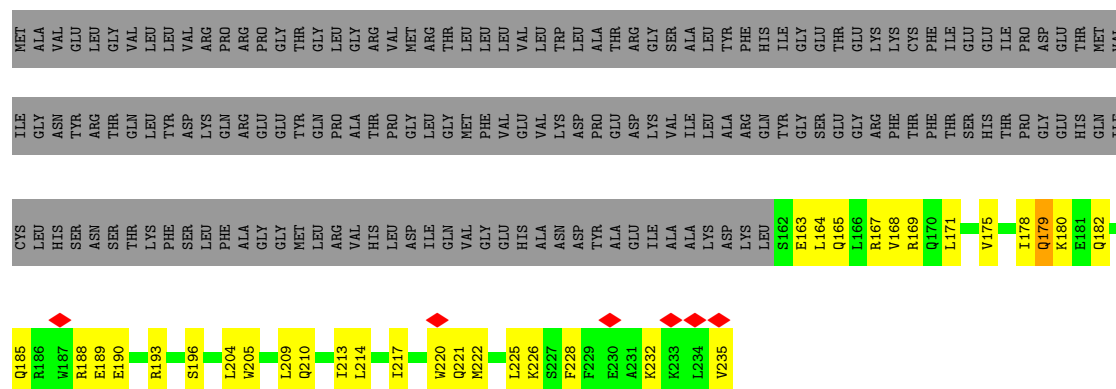
- Molecule 2 is [(2R)-2-[(E)-octadec-9-enoyl]oxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] (E)-octadec-9-enoate (CCD ID: 9ED) (formula: C₄₅H₈₅O₁₉P₃) (labeled as "Ligand of Interest" by depositor).



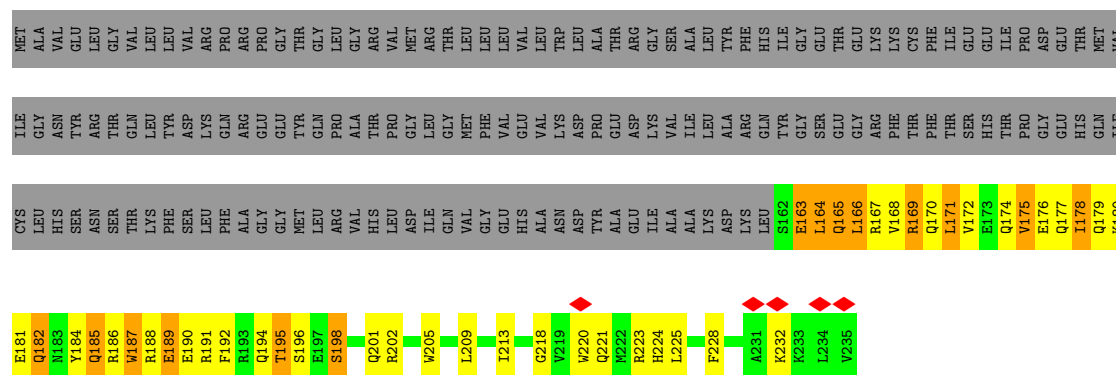
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	B	1	61	43	16	2	0
2	H	1	61	43	16	2	0



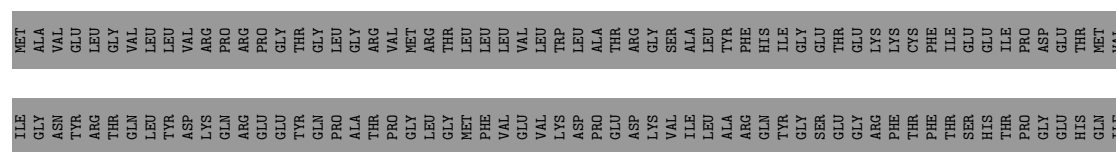
• Molecule 1: Transmembrane emp24 domain-containing protein 9

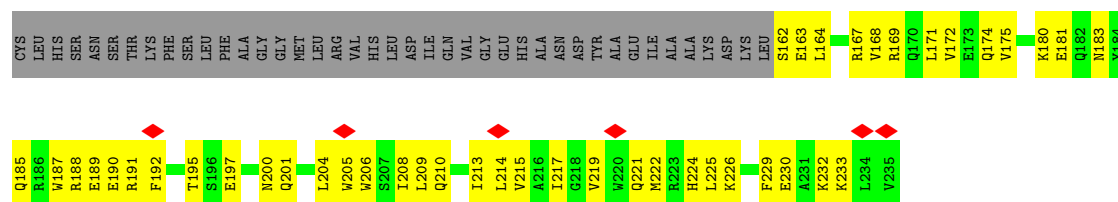


• Molecule 1: Transmembrane emp24 domain-containing protein 9

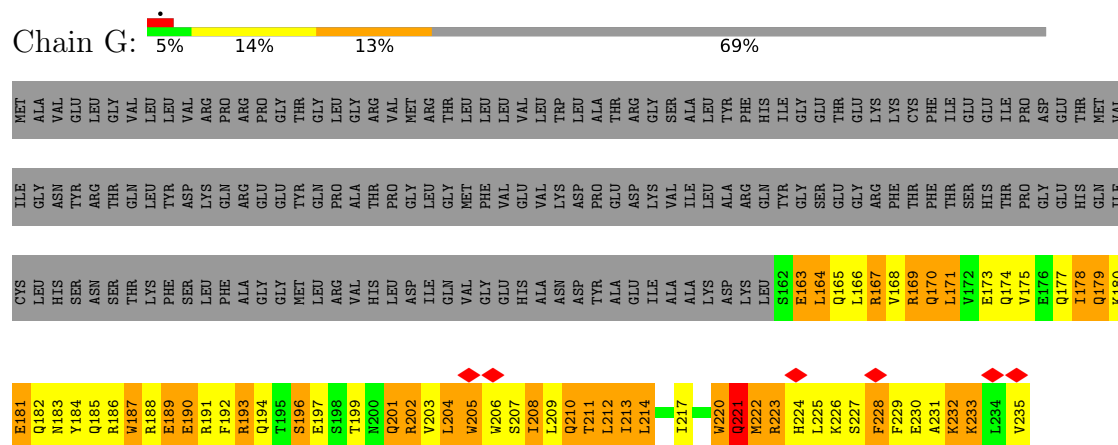


• Molecule 1: Transmembrane emp24 domain-containing protein 9

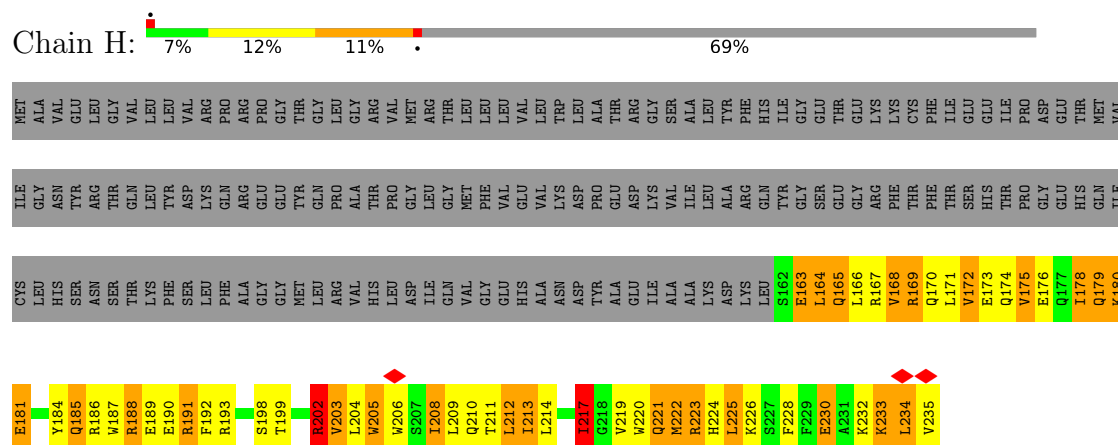




• Molecule 1: Transmembrane emp24 domain-containing protein 9



• Molecule 1: Transmembrane emp24 domain-containing protein 9



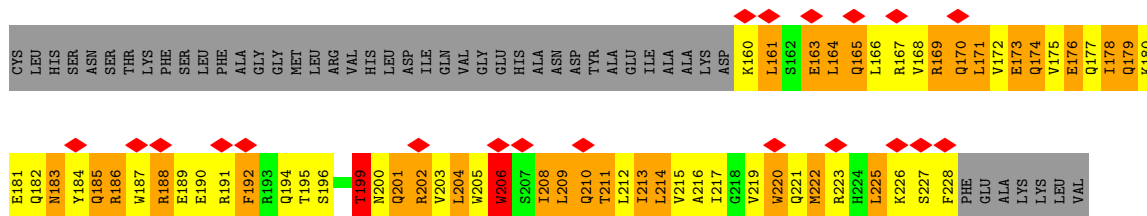
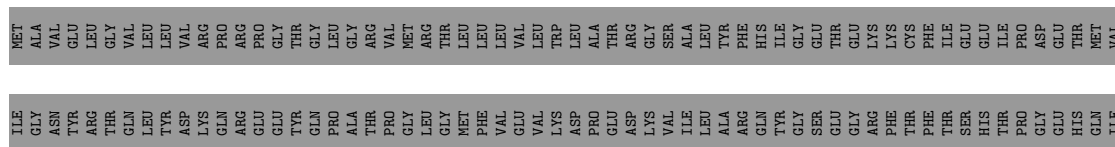
• Molecule 1: Transmembrane emp24 domain-containing protein 9





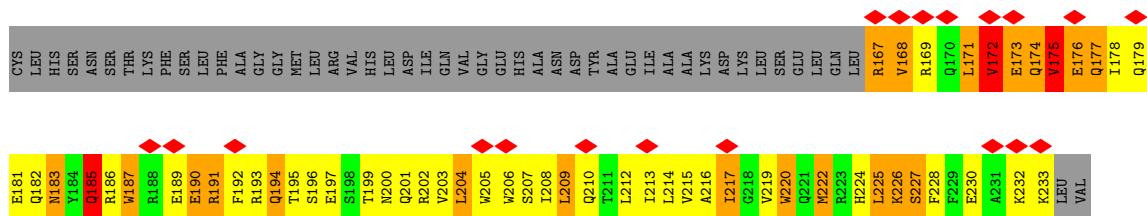
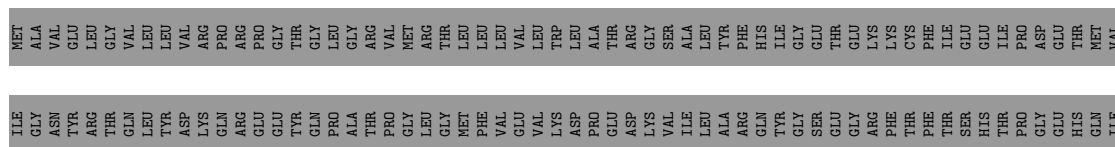
- Molecule 1: Transmembrane emp24 domain-containing protein 9

Chain J: 9% 13% 12% 71%



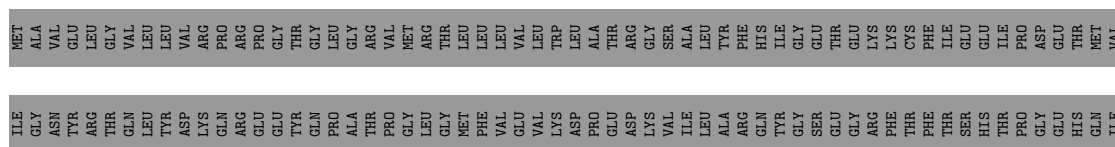
- Molecule 1: Transmembrane emp24 domain-containing protein 9

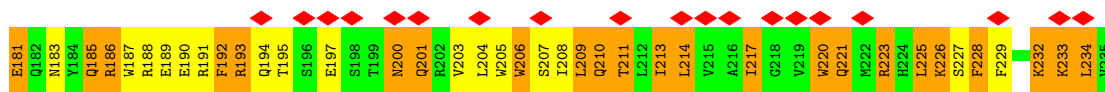
Chain K: 8% 14% 9% 71%



- Molecule 1: Transmembrane emp24 domain-containing protein 9

Chain L: 11% 7% 12% 12% 69%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198652	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 ($e^-/\text{\AA}^2$)	43.2	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	264.0, 264.0, 264.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9ED

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	0.56	0/721	1.04	2/969 (0.2%)
1	B	0.77	1/721 (0.1%)	1.21	7/969 (0.7%)
1	C	0.51	0/721	1.00	1/969 (0.1%)
1	D	0.18	0/660	0.43	0/888
1	E	0.51	0/660	0.92	1/888 (0.1%)
1	F	0.19	0/660	0.47	0/888
1	G	0.59	0/660	1.21	2/888 (0.2%)
1	H	0.49	0/660	1.10	1/888 (0.1%)
1	I	0.18	0/660	0.40	0/888
1	J	0.94	4/618 (0.6%)	1.39	6/832 (0.7%)
1	K	0.53	0/605	1.20	6/813 (0.7%)
1	L	0.48	0/660	1.06	2/888 (0.2%)
All	All	0.54	5/8006 (0.1%)	1.00	28/10768 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	202	ARG	N-CA	7.24	1.55	1.46
1	J	196	SER	C-O	7.24	1.32	1.24
1	J	199	THR	C-O	6.42	1.31	1.24
1	J	192	PHE	C-O	5.71	1.30	1.24
1	B	183	ASN	CA-C	5.02	1.59	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	202	ARG	N-CA-C	-12.63	96.15	111.69
1	G	179	GLN	N-CA-C	7.46	119.31	111.03
1	J	183	ASN	CB-CA-C	-7.27	99.36	110.92
1	B	175	VAL	N-CA-C	7.20	117.33	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	TRP	N-CA-C	-7.11	103.47	111.14
1	A	212	LEU	N-CA-C	-7.01	104.87	113.50
1	H	217	ILE	N-CA-CB	6.91	118.64	110.55
1	B	183	ASN	N-CA-C	6.84	125.36	110.80
1	J	206	TRP	N-CA-C	-6.70	103.90	111.07
1	B	208	ILE	CB-CA-C	-6.58	103.42	112.04
1	B	230	GLU	N-CA-C	-6.50	105.22	113.02
1	L	225	LEU	N-CA-C	-6.34	104.45	111.36
1	L	211	THR	N-CA-C	5.98	120.58	113.16
1	K	185	GLN	N-CA-C	-5.76	104.91	111.07
1	K	209	LEU	N-CA-C	-5.70	104.97	111.07
1	G	221	GLN	N-CA-C	-5.50	105.18	111.07
1	J	201	GLN	N-CA-C	5.46	117.66	111.11
1	B	182	GLN	O-C-N	-5.46	116.34	122.12
1	C	190	GLU	CB-CA-C	-5.40	110.33	116.54
1	J	220	TRP	N-CA-C	5.25	119.74	113.23
1	K	172	VAL	CB-CA-C	-5.15	105.38	111.97
1	B	168	VAL	N-CA-CB	5.14	117.53	110.54
1	J	204	LEU	N-CA-C	-5.13	105.58	111.07
1	K	187	TRP	N-CA-C	-5.12	105.59	111.07
1	K	175	VAL	N-CA-CB	5.03	117.38	110.54
1	B	189	GLU	N-CA-C	-5.03	105.69	111.07
1	E	178	ILE	N-CA-C	-5.02	105.50	110.62
1	K	172	VAL	N-CA-CB	5.02	116.42	110.55

There are no chirality outliers.

There are no planarity outliers.

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	709	0	726	259	0
1	B	709	0	727	294	0
1	C	709	0	728	198	0
1	D	648	0	660	181	0
1	E	648	0	660	224	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	648	0	660	144	0
1	G	648	0	660	340	0
1	H	648	0	660	358	0
1	I	648	0	660	161	0
1	J	607	0	618	406	0
1	K	593	0	594	289	0
1	L	648	0	659	213	0
2	B	61	0	0	58	0
2	H	61	0	0	34	0
All	All	7985	0	8012	2026	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 127.

All (2026) 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:G:225:LEU:HB3	1:G:229:PHE:CZ	1.22	1.67
1:A:220:TRP:CZ3	1:J:216:ALA:HB2	1.17	1.66
1:A:205:TRP:HH2	1:J:205:TRP:CD1	1.09	1.64
1:H:168:VAL:CG1	1:I:167:ARG:HH11	1.06	1.64
1:A:205:TRP:CH2	1:J:205:TRP:HD1	1.08	1.62
1:B:216:ALA:HA	2:B:301:9ED:C40	1.15	1.59
1:B:172:VAL:HG13	1:C:171:LEU:CD1	1.17	1.59
1:G:225:LEU:HB3	1:G:229:PHE:CE2	1.37	1.59
1:C:184:TYR:CD2	1:F:187:TRP:CH2	1.90	1.58
1:A:205:TRP:CH2	1:J:205:TRP:CD1	1.85	1.58
1:J:206:TRP:CZ2	1:K:212:LEU:CD2	1.83	1.56
1:J:206:TRP:CZ2	1:K:212:LEU:HD23	1.05	1.56
1:B:212:LEU:HD23	2:B:301:9ED:C53	1.34	1.56
1:J:206:TRP:HZ2	1:K:212:LEU:CD2	1.14	1.53
1:B:188:ARG:CZ	1:J:186:ARG:CD	1.84	1.52
1:J:191:ARG:CZ	1:K:193:ARG:HB3	1.36	1.52
1:K:216:ALA:HB1	1:L:220:TRP:CZ2	1.40	1.51
2:H:301:9ED:C6	1:I:213:ILE:HG21	1.40	1.50
1:A:171:LEU:CD2	1:C:169:ARG:HH22	1.21	1.49
1:A:210:GLN:NE2	1:F:208:ILE:HD11	1.22	1.49
1:E:184:TYR:CE1	1:G:186:ARG:HD3	1.48	1.48
1:D:189:GLU:CB	1:H:187:TRP:HH2	1.20	1.48
1:J:167:ARG:NH2	1:K:168:VAL:CG1	1.76	1.47
1:J:167:ARG:HH21	1:K:168:VAL:CG1	1.25	1.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ARG:NH2	1:F:189:GLU:HA	1.27	1.47
1:K:176:GLU:CG	1:L:178:ILE:CD1	1.91	1.46
1:J:187:TRP:CB	1:J:191:ARG:HH12	1.24	1.46
1:K:176:GLU:HG3	1:L:178:ILE:CD1	1.40	1.45
1:J:187:TRP:HB3	1:J:191:ARG:NH1	1.14	1.44
1:K:187:TRP:N	1:L:188:ARG:NH2	1.64	1.44
1:B:188:ARG:CZ	1:J:186:ARG:HD3	0.98	1.44
1:G:175:VAL:HG21	1:H:170:GLN:NE2	1.14	1.44
1:A:201:GLN:NE2	1:J:194:GLN:HG2	1.32	1.43
1:B:215:VAL:HG21	2:B:301:9ED:C63	1.45	1.43
1:K:173:GLU:OE2	1:L:174:GLN:CA	1.65	1.43
1:G:225:LEU:CB	1:G:229:PHE:CZ	1.96	1.43
1:A:171:LEU:CD2	1:C:169:ARG:NH2	1.75	1.43
1:A:171:LEU:O	1:A:175:VAL:CG2	1.67	1.43
1:B:172:VAL:CG1	1:C:171:LEU:HD11	1.46	1.43
1:B:200:ASN:OD1	1:F:200:ASN:CB	1.64	1.43
1:J:167:ARG:NH2	1:K:168:VAL:HG13	1.20	1.42
1:J:184:TYR:HA	1:K:193:ARG:NH2	1.18	1.42
1:H:168:VAL:CG1	1:I:167:ARG:HD3	1.47	1.41
1:E:187:TRP:NE1	1:E:191:ARG:NE	1.68	1.41
1:G:225:LEU:HD12	1:G:229:PHE:CZ	1.55	1.40
1:E:187:TRP:NE1	1:E:191:ARG:HE	0.93	1.39
1:E:187:TRP:CD1	1:E:191:ARG:HE	1.38	1.39
1:A:171:LEU:HD23	1:C:169:ARG:NH2	1.10	1.38
1:B:184:TYR:CZ	1:J:182:GLN:HB2	1.57	1.38
1:H:168:VAL:CG1	1:I:167:ARG:NH1	1.81	1.38
1:G:175:VAL:CG2	1:H:170:GLN:HE22	1.34	1.38
1:B:215:VAL:HG11	2:B:301:9ED:C63	1.54	1.38
1:C:229:PHE:HE1	1:G:232:LYS:CE	1.36	1.36
1:B:230:GLU:O	1:B:234:LEU:HD22	1.21	1.36
1:D:189:GLU:CB	1:H:187:TRP:CH2	2.08	1.35
1:H:188:ARG:CB	1:I:188:ARG:HH22	1.38	1.35
1:G:225:LEU:HD12	1:G:229:PHE:CE1	1.60	1.35
1:G:210:GLN:HE22	1:H:209:LEU:CD2	1.40	1.35
1:J:167:ARG:NH1	1:K:171:LEU:CD2	1.89	1.35
1:B:215:VAL:HB	2:B:301:9ED:C51	1.55	1.34
1:C:184:TYR:CD2	1:F:187:TRP:CZ3	2.15	1.34
1:J:173:GLU:HB3	1:K:179:GLN:CD	1.51	1.34
1:B:216:ALA:CA	2:B:301:9ED:C40	2.06	1.34
1:H:172:VAL:O	1:H:175:VAL:HG13	1.25	1.34
1:D:189:GLU:HB3	1:H:187:TRP:CH2	1.63	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:GLN:O	1:J:177:GLN:HG2	1.29	1.32
1:D:168:VAL:HB	1:E:167:ARG:CD	1.59	1.32
1:G:165:GLN:O	1:G:168:VAL:HG22	1.30	1.32
1:H:188:ARG:HB2	1:I:188:ARG:NH2	1.43	1.32
1:B:188:ARG:NH2	1:J:186:ARG:HD3	1.43	1.32
1:D:225:LEU:CB	1:E:228:PHE:HZ	1.43	1.32
1:H:171:LEU:HD22	1:I:171:LEU:CD1	1.59	1.32
1:K:202:ARG:O	1:K:205:TRP:CB	1.77	1.32
1:B:181:GLU:O	1:B:185:GLN:CG	1.76	1.31
1:H:172:VAL:O	1:H:175:VAL:CG1	1.77	1.31
1:J:210:GLN:O	1:J:214:LEU:HG	1.26	1.31
1:G:225:LEU:CD1	1:G:229:PHE:CZ	2.13	1.31
1:J:206:TRP:CE3	1:K:215:VAL:HG21	1.66	1.31
1:G:168:VAL:HB	1:H:167:ARG:CD	1.61	1.30
1:C:229:PHE:CD2	1:G:228:PHE:CE1	2.02	1.30
1:A:202:ARG:O	1:A:206:TRP:N	1.65	1.30
1:D:188:ARG:NH1	1:E:188:ARG:HH21	1.29	1.30
1:J:210:GLN:HA	1:J:213:ILE:CD1	1.59	1.30
1:J:210:GLN:CA	1:J:213:ILE:CD1	2.09	1.30
1:A:197:GLU:OE2	1:J:194:GLN:HG3	1.14	1.29
1:J:170:GLN:CD	1:K:175:VAL:HB	1.53	1.29
1:B:184:TYR:OH	1:J:182:GLN:CB	1.80	1.29
1:E:188:ARG:NH1	1:F:185:GLN:HG2	1.45	1.29
1:A:203:VAL:HG11	1:B:199:THR:CG2	1.63	1.28
1:B:212:LEU:CD2	2:B:301:9ED:C53	2.11	1.28
1:H:168:VAL:HG11	1:I:167:ARG:CD	1.64	1.28
1:H:198:SER:O	1:H:202:ARG:CG	1.81	1.28
1:A:220:TRP:CZ3	1:J:216:ALA:CB	2.13	1.28
1:D:188:ARG:NH2	1:F:192:PHE:HD2	1.31	1.28
1:G:192:PHE:CZ	1:I:192:PHE:CD1	2.20	1.28
1:J:184:TYR:HB2	1:K:189:GLU:CB	1.62	1.28
1:K:176:GLU:CG	1:L:178:ILE:HD12	1.52	1.28
1:A:171:LEU:CG	1:C:169:ARG:HH22	1.46	1.27
1:B:172:VAL:CG1	1:C:171:LEU:CD1	2.06	1.27
1:G:225:LEU:CD1	1:G:229:PHE:CE1	2.15	1.27
1:J:173:GLU:HB3	1:K:179:GLN:OE1	1.20	1.27
1:E:165:GLN:O	1:E:168:VAL:HG12	1.33	1.27
1:D:179:GLN:OE1	1:H:176:GLU:HG3	1.30	1.27
1:K:187:TRP:HA	1:L:188:ARG:NH1	1.48	1.27
1:K:216:ALA:HB1	1:L:220:TRP:CH2	1.70	1.26
1:C:184:TYR:CE2	1:F:187:TRP:CH2	2.21	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:168:VAL:O	1:H:171:LEU:HG	1.27	1.25
1:A:220:TRP:CH2	1:J:212:LEU:O	1.89	1.25
1:B:215:VAL:CG2	2:B:301:9ED:C63	2.13	1.25
1:B:220:TRP:HB2	2:B:301:9ED:C31	1.66	1.25
1:E:165:GLN:HA	1:F:167:ARG:NH1	1.48	1.25
1:G:171:LEU:CD1	1:H:171:LEU:HB3	1.67	1.25
1:J:191:ARG:HH12	1:K:193:ARG:CD	1.49	1.24
1:A:204:LEU:HD11	1:L:206:TRP:CD1	1.71	1.24
1:C:184:TYR:CE2	1:F:187:TRP:HH2	1.55	1.24
1:K:227:SER:O	1:K:230:GLU:HG2	1.32	1.24
1:B:184:TYR:OH	1:J:182:GLN:C	1.80	1.23
1:B:165:GLN:NE2	1:C:161:LEU:HD22	1.51	1.23
1:G:221:GLN:HB3	1:H:220:TRP:NE1	1.54	1.23
1:G:192:PHE:CZ	1:I:192:PHE:HD1	1.56	1.23
1:H:171:LEU:CD2	1:I:171:LEU:HD12	1.67	1.22
1:K:169:ARG:CD	1:L:167:ARG:O	1.86	1.22
1:K:173:GLU:OE2	1:L:174:GLN:HA	1.08	1.22
1:H:188:ARG:CB	1:I:188:ARG:NH2	1.98	1.22
1:H:198:SER:O	1:H:202:ARG:HG2	1.12	1.22
1:K:202:ARG:O	1:K:205:TRP:HB3	1.04	1.22
1:K:216:ALA:CB	1:L:220:TRP:CZ2	2.21	1.22
1:H:208:ILE:HG21	2:H:301:9ED:C56	1.69	1.22
1:E:184:TYR:HE1	1:G:186:ARG:CD	1.54	1.21
1:J:167:ARG:HH11	1:K:171:LEU:CD2	1.49	1.21
1:D:225:LEU:CB	1:E:228:PHE:CZ	2.24	1.21
1:K:200:ASN:O	1:K:203:VAL:HG12	1.36	1.20
1:B:188:ARG:NE	1:J:186:ARG:HD3	1.53	1.20
1:F:183:ASN:OD1	1:F:187:TRP:CE2	1.94	1.20
1:B:172:VAL:O	1:B:176:GLU:OE1	1.55	1.20
1:B:215:VAL:CG1	2:B:301:9ED:C63	2.19	1.20
1:J:173:GLU:CB	1:K:179:GLN:OE1	1.89	1.19
1:A:171:LEU:O	1:A:175:VAL:HG23	1.07	1.19
1:J:191:ARG:NH2	1:K:193:ARG:HB3	1.55	1.19
1:A:209:LEU:HD23	1:J:205:TRP:CD2	1.78	1.19
1:D:164:LEU:HB3	1:E:167:ARG:HH22	1.08	1.18
1:D:168:VAL:CB	1:E:167:ARG:CD	2.20	1.18
1:K:187:TRP:CA	1:L:188:ARG:NH2	2.07	1.18
1:H:174:GLN:HE22	1:I:178:ILE:CD1	1.57	1.18
1:J:184:TYR:CA	1:K:193:ARG:NH2	2.05	1.18
1:C:229:PHE:CE1	1:G:232:LYS:CE	2.25	1.17
1:J:167:ARG:NH1	1:K:171:LEU:HD23	1.49	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ARG:HH21	1:F:189:GLU:CA	1.57	1.17
1:J:209:LEU:C	1:J:213:ILE:HD11	1.69	1.17
1:A:171:LEU:HD13	1:A:174:GLN:OE1	1.43	1.17
1:B:184:TYR:CE1	1:B:188:ARG:NH1	2.13	1.17
1:J:170:GLN:CG	1:K:175:VAL:HB	1.73	1.17
1:B:229:PHE:CE1	1:E:232:LYS:HD2	1.79	1.16
1:J:174:GLN:C	1:J:177:GLN:HG2	1.71	1.16
1:B:184:TYR:OH	1:J:182:GLN:HB2	1.37	1.16
1:J:191:ARG:CZ	1:K:193:ARG:CB	2.22	1.16
1:B:222:MET:CB	1:D:220:TRP:HH2	1.59	1.15
1:D:225:LEU:HD11	1:D:226:LYS:NZ	1.61	1.15
1:G:164:LEU:CD2	1:H:164:LEU:HD22	1.77	1.15
1:J:166:LEU:CD1	1:L:171:LEU:HD21	1.75	1.15
1:C:188:ARG:O	1:F:191:ARG:CZ	1.95	1.15
1:G:210:GLN:HE22	1:H:209:LEU:HD21	1.07	1.15
1:J:184:TYR:CD1	1:K:189:GLU:HG3	1.81	1.14
1:L:210:GLN:HE22	1:L:214:LEU:HD22	0.99	1.14
1:J:167:ARG:CG	1:K:172:VAL:HG22	1.77	1.14
1:G:204:LEU:CD2	1:H:202:ARG:NH2	2.11	1.14
1:H:168:VAL:HG12	1:I:167:ARG:NH1	1.45	1.13
1:J:166:LEU:HB3	1:L:174:GLN:HE22	1.01	1.13
1:D:165:GLN:O	1:D:168:VAL:HG12	1.48	1.13
1:E:188:ARG:HH12	1:F:185:GLN:CG	1.60	1.13
1:E:166:LEU:HD23	1:H:166:LEU:HD13	1.16	1.13
1:B:215:VAL:CB	2:B:301:9ED:C63	2.26	1.13
1:G:232:LYS:HG3	1:H:228:PHE:CZ	1.83	1.12
1:B:181:GLU:O	1:B:185:GLN:CD	1.92	1.12
1:H:205:TRP:HB3	2:H:301:9ED:C58	1.79	1.12
1:B:216:ALA:O	2:B:301:9ED:O22	1.68	1.11
1:C:229:PHE:HE1	1:G:232:LYS:HE2	1.09	1.11
1:B:222:MET:CG	1:D:220:TRP:CH2	2.34	1.11
1:G:164:LEU:HD22	1:H:164:LEU:HD22	1.17	1.11
1:J:166:LEU:HD13	1:L:171:LEU:HD21	1.32	1.11
1:B:181:GLU:O	1:B:185:GLN:HG2	1.47	1.10
1:C:224:HIS:HB3	1:I:222:MET:CE	1.80	1.10
1:C:229:PHE:CE1	1:G:232:LYS:CD	2.34	1.10
1:D:225:LEU:HB3	1:E:228:PHE:CZ	1.86	1.10
1:G:174:GLN:HE21	1:I:178:ILE:CD1	1.63	1.10
1:J:166:LEU:CB	1:L:174:GLN:HE22	1.64	1.10
1:J:209:LEU:O	1:J:213:ILE:CD1	1.98	1.10
1:K:169:ARG:HD3	1:L:167:ARG:O	1.49	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:168:VAL:CG1	1:H:167:ARG:HD2	1.81	1.10
1:J:210:GLN:CA	1:J:213:ILE:HD11	1.78	1.10
2:H:301:9ED:C3	1:I:217:ILE:CD1	2.30	1.10
1:A:210:GLN:NE2	1:F:208:ILE:CD1	2.15	1.09
1:J:181:GLU:O	1:J:184:TYR:CD2	1.66	1.09
1:A:205:TRP:CZ3	1:J:205:TRP:CD1	2.39	1.09
1:B:232:LYS:HB3	1:E:232:LYS:NZ	1.68	1.09
1:D:225:LEU:HB3	1:E:228:PHE:HZ	0.94	1.09
1:G:208:ILE:O	1:G:212:LEU:HG	1.52	1.09
1:J:167:ARG:HG2	1:K:172:VAL:HG22	1.12	1.09
1:E:202:ARG:HH22	1:G:204:LEU:HD12	0.96	1.09
1:K:222:MET:HA	1:K:222:MET:HE3	1.28	1.09
1:C:188:ARG:HB3	1:F:191:ARG:HD2	1.23	1.08
1:B:210:GLN:HA	1:B:213:ILE:HD12	1.30	1.08
1:B:222:MET:CG	1:D:220:TRP:HH2	1.67	1.08
1:B:222:MET:HG3	1:D:220:TRP:CH2	1.87	1.08
1:J:184:TYR:HB2	1:K:189:GLU:HB3	1.12	1.08
1:K:176:GLU:OE1	1:L:177:GLN:O	1.65	1.08
1:A:197:GLU:HG2	1:A:201:GLN:HE22	0.98	1.08
1:A:224:HIS:HE1	1:B:223:ARG:NH1	1.52	1.08
1:G:225:LEU:CG	1:G:229:PHE:CZ	2.35	1.08
2:H:301:9ED:C4	1:I:213:ILE:CG2	2.31	1.08
1:D:168:VAL:CG2	1:E:167:ARG:HD3	1.81	1.08
1:H:168:VAL:HG12	1:I:167:ARG:HH11	0.91	1.08
1:B:172:VAL:HG13	1:C:171:LEU:HD12	1.25	1.08
1:G:174:GLN:HE21	1:I:178:ILE:HD12	1.19	1.07
1:J:210:GLN:C	1:J:213:ILE:CD1	2.26	1.07
1:D:188:ARG:NH2	1:F:192:PHE:CD2	2.18	1.07
1:J:210:GLN:HA	1:J:213:ILE:HD13	1.14	1.07
1:A:203:VAL:HG11	1:B:199:THR:HG21	1.28	1.07
1:A:204:LEU:HB3	1:J:202:ARG:HH21	1.08	1.07
1:G:174:GLN:NE2	1:I:178:ILE:CD1	2.17	1.07
1:E:187:TRP:HE1	1:E:191:ARG:NE	1.35	1.07
1:B:230:GLU:O	1:B:234:LEU:CD2	2.03	1.07
1:D:225:LEU:HB2	1:E:228:PHE:CZ	1.88	1.06
1:J:163:GLU:HB2	1:L:171:LEU:CD1	1.84	1.06
1:K:176:GLU:OE1	1:L:177:GLN:C	1.98	1.06
1:K:187:TRP:CA	1:L:188:ARG:HH12	1.67	1.06
1:J:191:ARG:NH1	1:K:193:ARG:CG	2.18	1.06
1:K:226:LYS:HD2	1:L:228:PHE:CZ	1.89	1.06
1:D:188:ARG:NH2	1:F:189:GLU:CA	2.17	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:ARG:HH22	1:H:170:GLN:CB	1.68	1.06
1:A:201:GLN:NE2	1:J:194:GLN:CG	2.19	1.06
1:A:205:TRP:CZ3	1:J:205:TRP:HB2	1.90	1.06
1:D:168:VAL:CG2	1:E:167:ARG:CD	2.32	1.06
1:G:232:LYS:HZ2	1:G:232:LYS:HA	1.17	1.06
1:H:168:VAL:HG11	1:I:167:ARG:NH1	1.57	1.06
1:J:163:GLU:CB	1:L:171:LEU:HD12	1.85	1.06
1:J:167:ARG:HA	1:K:172:VAL:HG13	1.35	1.06
1:J:174:GLN:O	1:J:177:GLN:CG	2.03	1.06
1:K:202:ARG:HG2	1:L:205:TRP:HE1	1.19	1.06
1:A:209:LEU:HD21	1:J:205:TRP:CH2	1.89	1.06
1:B:220:TRP:CB	2:B:301:9ED:C31	2.33	1.06
1:E:187:TRP:CD1	1:E:191:ARG:NE	2.07	1.06
1:J:167:ARG:NH1	1:K:171:LEU:HD21	1.61	1.06
1:K:176:GLU:HG2	1:L:178:ILE:CD1	1.70	1.06
1:H:199:THR:HA	1:H:202:ARG:HG3	1.35	1.05
1:E:169:ARG:HH22	1:H:170:GLN:HB2	1.17	1.05
1:A:213:ILE:O	1:A:217:ILE:CD1	2.05	1.05
1:G:164:LEU:CD2	1:H:164:LEU:CD2	2.33	1.05
1:G:210:GLN:NE2	1:H:209:LEU:CD2	2.19	1.05
1:A:201:GLN:HE21	1:J:194:GLN:CG	1.70	1.05
1:B:200:ASN:CG	1:F:200:ASN:HB3	1.81	1.05
1:B:229:PHE:HE2	1:D:232:LYS:HD3	1.19	1.05
1:G:164:LEU:HD22	1:H:164:LEU:CD2	1.86	1.05
1:G:178:ILE:HG21	1:I:178:ILE:HD13	1.38	1.05
2:H:301:9ED:C3	1:I:217:ILE:HD13	1.85	1.05
1:E:184:TYR:CE1	1:G:186:ARG:CD	2.35	1.04
2:H:301:9ED:C6	1:I:213:ILE:CG2	2.34	1.04
1:G:225:LEU:CG	1:G:229:PHE:HZ	1.66	1.04
1:K:169:ARG:HD2	1:L:167:ARG:O	1.56	1.04
1:A:171:LEU:HD12	1:A:175:VAL:HG22	1.39	1.04
1:E:188:ARG:HH12	1:F:185:GLN:HG2	0.89	1.04
1:B:172:VAL:O	1:B:176:GLU:CD	2.01	1.04
1:D:225:LEU:CD1	1:D:226:LYS:NZ	2.19	1.04
1:H:174:GLN:HE22	1:I:178:ILE:HD11	1.13	1.04
2:H:301:9ED:C50	1:I:217:ILE:HG12	1.88	1.04
1:J:206:TRP:HE3	1:K:215:VAL:HG21	0.90	1.04
1:D:168:VAL:CB	1:E:167:ARG:HD2	1.87	1.03
1:H:168:VAL:HA	1:H:171:LEU:CD2	1.87	1.03
1:J:177:GLN:HG3	1:J:178:ILE:HD13	1.36	1.03
1:C:155:ILE:HD13	1:C:155:ILE:H	1.21	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:GLN:NE2	1:G:206:TRP:CZ2	2.25	1.03
1:J:167:ARG:HG2	1:K:172:VAL:CG2	1.89	1.03
1:D:189:GLU:HB2	1:H:187:TRP:CH2	1.87	1.03
1:G:221:GLN:HB3	1:H:220:TRP:HE1	1.07	1.03
1:B:229:PHE:HE1	1:E:232:LYS:HD2	1.11	1.03
1:C:229:PHE:CE1	1:G:232:LYS:HE2	1.88	1.03
1:D:188:ARG:CZ	1:E:188:ARG:HH21	1.71	1.03
1:G:168:VAL:HB	1:H:167:ARG:HD3	1.06	1.03
1:G:207:SER:HA	1:H:206:TRP:NE1	1.74	1.03
1:J:211:THR:O	1:J:215:VAL:HG23	1.57	1.03
1:K:169:ARG:HD2	1:L:167:ARG:C	1.82	1.03
1:C:224:HIS:HB3	1:I:222:MET:HE1	1.38	1.02
1:K:226:LYS:HD2	1:L:228:PHE:HZ	1.20	1.02
1:D:179:GLN:OE1	1:H:176:GLU:CG	2.07	1.02
1:D:225:LEU:HD11	1:D:226:LYS:HZ3	0.92	1.02
1:G:165:GLN:O	1:G:168:VAL:CG2	2.07	1.02
1:J:166:LEU:HB3	1:L:174:GLN:NE2	1.74	1.02
1:J:184:TYR:CG	1:K:189:GLU:HG3	1.95	1.02
1:K:187:TRP:HB2	1:L:188:ARG:NH2	1.75	1.02
1:G:175:VAL:CG2	1:H:170:GLN:NE2	2.04	1.02
1:A:202:ARG:O	1:A:206:TRP:HB2	1.57	1.01
1:D:189:GLU:HB3	1:H:187:TRP:HH2	0.86	1.01
1:G:168:VAL:CB	1:H:167:ARG:CD	2.37	1.01
2:H:301:9ED:C49	1:I:217:ILE:HG12	1.89	1.01
1:K:187:TRP:CB	1:L:188:ARG:NH2	2.23	1.01
1:B:184:TYR:CZ	1:J:182:GLN:CB	2.38	1.01
1:B:184:TYR:OH	1:J:183:ASN:N	1.94	1.01
1:C:188:ARG:O	1:F:191:ARG:NH2	1.92	1.01
1:C:210:GLN:NE2	1:G:206:TRP:CH2	2.28	1.01
1:H:188:ARG:HE	1:I:188:ARG:NH2	1.58	1.01
1:A:203:VAL:O	1:A:207:SER:CB	2.08	1.00
1:G:171:LEU:HD11	1:H:171:LEU:HB3	1.36	1.00
1:G:193:ARG:HA	1:H:191:ARG:NH2	1.74	1.00
1:B:229:PHE:CE2	1:D:232:LYS:HD3	1.96	1.00
1:G:192:PHE:CE2	1:H:191:ARG:CZ	2.44	1.00
1:H:199:THR:O	1:H:203:VAL:HG22	1.59	1.00
1:J:167:ARG:HH11	1:K:171:LEU:HD21	0.87	1.00
1:J:209:LEU:O	1:J:213:ILE:HD11	1.58	1.00
1:J:210:GLN:HG2	1:J:214:LEU:CD2	1.90	1.00
1:B:232:LYS:CB	1:E:232:LYS:NZ	2.25	1.00
1:E:165:GLN:O	1:E:168:VAL:CG1	2.09	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:LYS:HG3	1:H:228:PHE:CE1	1.96	1.00
2:H:301:9ED:C50	1:I:217:ILE:CD1	2.39	1.00
1:J:210:GLN:O	1:J:213:ILE:CD1	2.09	1.00
1:D:168:VAL:HB	1:E:167:ARG:HD3	1.42	1.00
1:K:187:TRP:HA	1:L:188:ARG:HH12	0.87	1.00
1:A:204:LEU:CB	1:J:202:ARG:HH21	1.75	1.00
1:B:184:TYR:OH	1:J:182:GLN:CA	2.10	1.00
1:J:173:GLU:HB3	1:K:179:GLN:NE2	1.77	1.00
1:A:197:GLU:OE2	1:J:194:GLN:CG	2.09	0.99
1:A:220:TRP:CE3	1:J:216:ALA:HB2	1.97	0.99
1:E:169:ARG:NH2	1:H:170:GLN:HG3	1.77	0.99
1:G:221:GLN:HG2	1:H:220:TRP:CD1	1.97	0.99
1:H:172:VAL:HA	1:H:175:VAL:CG1	1.92	0.99
1:J:206:TRP:CE2	1:K:212:LEU:HD23	1.96	0.99
1:J:210:GLN:N	1:J:213:ILE:HD11	1.76	0.99
1:J:199:THR:HG23	1:K:204:LEU:HD23	1.45	0.99
1:B:215:VAL:CB	2:B:301:9ED:C51	2.39	0.98
1:G:207:SER:HB2	1:H:206:TRP:CD1	1.98	0.98
1:A:222:MET:HE2	1:A:222:MET:HA	1.41	0.98
1:G:168:VAL:CB	1:H:167:ARG:HD3	1.93	0.98
1:H:219:VAL:CG2	2:H:301:9ED:O22	2.11	0.98
1:K:173:GLU:CG	1:L:177:GLN:OE1	2.11	0.98
1:B:222:MET:CB	1:D:220:TRP:CH2	2.47	0.98
1:J:210:GLN:O	1:J:213:ILE:HD12	1.62	0.98
1:B:165:GLN:NE2	1:C:161:LEU:CD2	2.25	0.98
1:B:184:TYR:HH	1:J:183:ASN:N	1.62	0.98
1:K:169:ARG:HH11	1:L:167:ARG:HB3	1.23	0.98
1:A:209:LEU:HD23	1:J:205:TRP:CE3	1.97	0.98
1:B:172:VAL:HG11	1:C:171:LEU:HD11	1.41	0.98
1:G:232:LYS:CG	1:H:228:PHE:CZ	2.46	0.98
1:C:184:TYR:CD2	1:F:187:TRP:HH2	1.48	0.98
1:E:169:ARG:HH22	1:H:170:GLN:CG	1.76	0.98
1:D:188:ARG:NH1	1:E:188:ARG:NH2	2.12	0.97
1:J:181:GLU:HB3	1:J:184:TYR:OH	1.58	0.97
1:J:184:TYR:HA	1:K:193:ARG:HH22	1.22	0.97
1:A:197:GLU:CG	1:A:201:GLN:HE22	1.76	0.97
1:G:192:PHE:CE1	1:I:192:PHE:CD1	2.51	0.97
1:A:204:LEU:HB3	1:J:202:ARG:NH2	1.80	0.97
1:D:168:VAL:HG23	1:E:167:ARG:CD	1.94	0.97
1:D:178:ILE:HD13	1:E:178:ILE:HD11	1.46	0.97
1:E:165:GLN:CA	1:F:167:ARG:HH12	1.76	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:PHE:CE2	1:I:222:MET:HE1	2.00	0.97
1:A:213:ILE:O	1:A:217:ILE:HD11	1.65	0.97
1:B:208:ILE:HG22	2:B:301:9ED:C4	1.95	0.96
1:D:168:VAL:HB	1:E:167:ARG:NE	1.79	0.96
1:K:200:ASN:O	1:K:203:VAL:CG1	2.12	0.96
1:A:226:LYS:HZ2	1:L:225:LEU:CD2	1.77	0.96
1:B:172:VAL:O	1:B:175:VAL:HG23	1.65	0.96
1:J:210:GLN:CA	1:J:213:ILE:HD13	1.83	0.96
1:K:173:GLU:HG3	1:L:177:GLN:NE2	1.80	0.96
1:A:202:ARG:C	1:A:206:TRP:HB2	1.89	0.96
1:C:229:PHE:HD2	1:G:228:PHE:HE1	1.06	0.96
1:H:172:VAL:C	1:H:175:VAL:HG12	1.91	0.96
1:H:214:LEU:HD12	1:I:214:LEU:HD23	1.47	0.96
1:C:167:ARG:HH11	1:C:167:ARG:HB2	1.26	0.96
1:A:204:LEU:HD11	1:L:206:TRP:HD1	1.31	0.95
1:B:184:TYR:HH	1:J:182:GLN:CA	1.78	0.95
1:J:191:ARG:HH12	1:K:193:ARG:HD2	0.81	0.95
1:B:184:TYR:HH	1:J:182:GLN:C	1.68	0.95
1:C:188:ARG:HB3	1:F:191:ARG:CD	1.95	0.95
1:J:181:GLU:O	1:J:184:TYR:CG	2.18	0.95
1:E:202:ARG:NH2	1:G:204:LEU:HD12	1.80	0.95
1:G:171:LEU:HD12	1:H:171:LEU:HB3	1.48	0.95
1:C:201:GLN:O	1:C:205:TRP:CB	2.15	0.95
1:A:197:GLU:HG2	1:A:201:GLN:NE2	1.81	0.95
1:G:225:LEU:CB	1:G:229:PHE:CE2	2.32	0.95
1:G:211:THR:CG2	1:H:209:LEU:HD11	1.97	0.94
1:K:187:TRP:CA	1:L:188:ARG:NH1	2.26	0.94
1:L:210:GLN:NE2	1:L:214:LEU:HD22	1.81	0.94
1:B:172:VAL:O	1:B:175:VAL:CG2	2.15	0.94
1:D:210:GLN:O	1:D:213:ILE:HG12	1.67	0.94
1:D:225:LEU:CD1	1:D:226:LYS:HZ3	1.77	0.94
1:H:172:VAL:O	1:H:175:VAL:HG12	1.66	0.94
1:J:210:GLN:O	1:J:214:LEU:CG	2.16	0.94
1:A:201:GLN:HE22	1:J:194:GLN:HG2	1.25	0.94
1:A:214:LEU:HD22	1:A:214:LEU:H	1.30	0.94
1:B:172:VAL:HG13	1:C:171:LEU:HD11	1.01	0.94
1:H:188:ARG:HB3	1:I:188:ARG:NH2	1.81	0.94
1:A:201:GLN:HE21	1:J:194:GLN:HG2	1.15	0.94
1:C:229:PHE:CE1	1:G:232:LYS:HD3	2.03	0.94
1:D:178:ILE:HD13	1:E:174:GLN:HE21	1.33	0.94
1:D:204:LEU:HD13	1:H:205:TRP:CZ2	2.01	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:186:ARG:HA	1:L:186:ARG:CZ	1.96	0.94
1:L:232:LYS:HZ2	1:L:232:LYS:HA	1.32	0.94
1:H:169:ARG:HA	1:H:169:ARG:HE	1.31	0.93
1:B:216:ALA:HB1	2:B:301:9ED:C37	1.97	0.93
1:G:225:LEU:CD1	1:G:229:PHE:HE1	1.75	0.93
1:D:164:LEU:HB3	1:E:167:ARG:NH2	1.83	0.93
1:G:225:LEU:HD13	1:G:229:PHE:CE1	2.01	0.93
1:K:176:GLU:HG2	1:L:178:ILE:HD12	0.93	0.93
1:H:172:VAL:C	1:H:175:VAL:CG1	2.42	0.93
1:A:171:LEU:HD12	1:A:175:VAL:CG2	1.99	0.93
1:A:204:LEU:CD1	1:L:206:TRP:CD1	2.52	0.93
1:C:188:ARG:CB	1:F:191:ARG:HD2	1.98	0.93
1:D:196:SER:HG	1:E:195:THR:HG1	1.09	0.93
1:C:184:TYR:CG	1:F:187:TRP:CZ3	2.57	0.93
1:G:232:LYS:NZ	1:G:235:VAL:HG21	1.83	0.93
1:B:215:VAL:HG11	2:B:301:9ED:C62	1.99	0.93
1:C:229:PHE:CD2	1:G:228:PHE:HE1	1.66	0.93
1:D:165:GLN:O	1:D:168:VAL:CG1	2.17	0.93
1:D:189:GLU:OE2	1:E:188:ARG:HG2	1.69	0.93
1:J:210:GLN:HG2	1:J:214:LEU:HD23	1.48	0.93
1:K:173:GLU:HG3	1:L:177:GLN:CD	1.92	0.93
1:C:184:TYR:CE2	1:F:187:TRP:CZ3	2.51	0.92
1:G:210:GLN:OE1	1:H:206:TRP:NE1	2.01	0.92
1:J:167:ARG:HH22	1:K:168:VAL:HG13	1.27	0.92
1:J:174:GLN:HA	1:J:177:GLN:CD	1.94	0.92
1:E:223:ARG:NE	2:H:301:9ED:O12	2.03	0.92
1:B:216:ALA:O	2:B:301:9ED:C35	2.16	0.92
1:C:210:GLN:HE22	1:G:206:TRP:HZ2	1.07	0.92
1:G:232:LYS:HA	1:G:232:LYS:NZ	1.85	0.92
1:H:202:ARG:HB3	1:H:202:ARG:CZ	2.00	0.92
1:J:210:GLN:C	1:J:213:ILE:HD12	1.92	0.92
1:D:168:VAL:CB	1:E:167:ARG:HD3	1.91	0.92
1:G:210:GLN:HE22	1:H:209:LEU:HD22	1.31	0.92
1:B:220:TRP:HB2	2:B:301:9ED:C35	2.00	0.92
1:G:187:TRP:HE1	1:G:191:ARG:HD2	1.32	0.92
1:K:227:SER:O	1:K:230:GLU:CG	2.17	0.92
1:B:172:VAL:HG13	1:C:171:LEU:HD13	1.48	0.92
1:J:184:TYR:CB	1:K:189:GLU:CB	2.47	0.92
1:J:206:TRP:CE3	1:K:215:VAL:CG2	2.52	0.92
1:E:165:GLN:HA	1:F:167:ARG:HH12	1.23	0.91
1:J:191:ARG:NH1	1:K:193:ARG:CD	2.18	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ASN:OD1	1:F:200:ASN:HB3	0.74	0.91
1:C:228:PHE:CZ	1:I:222:MET:HE1	2.06	0.91
1:K:173:GLU:OE2	1:L:174:GLN:N	2.02	0.91
1:K:183:ASN:O	1:L:188:ARG:NH2	2.03	0.91
1:J:206:TRP:CZ2	1:K:212:LEU:HD22	1.97	0.91
1:D:189:GLU:C	1:H:187:TRP:CH2	2.49	0.91
1:J:166:LEU:HD13	1:L:171:LEU:CD2	2.00	0.91
1:A:205:TRP:CZ3	1:J:205:TRP:CG	2.59	0.91
1:B:188:ARG:NH2	1:J:186:ARG:CD	2.15	0.91
1:B:188:ARG:NH2	1:J:186:ARG:CG	2.34	0.91
1:G:178:ILE:HG21	1:H:174:GLN:NE2	1.85	0.91
1:A:205:TRP:HZ3	1:J:205:TRP:CB	1.82	0.91
1:H:168:VAL:HG11	1:I:167:ARG:HD3	1.06	0.91
1:J:174:GLN:HA	1:J:177:GLN:CG	2.01	0.91
2:H:301:9ED:C50	1:I:217:ILE:CG1	2.49	0.91
1:G:221:GLN:CB	1:H:220:TRP:HE1	1.84	0.91
1:J:167:ARG:HD2	1:K:168:VAL:HG12	1.51	0.91
1:K:216:ALA:HB1	1:L:220:TRP:HZ2	1.23	0.91
1:A:220:TRP:HH2	1:J:212:LEU:O	1.30	0.90
1:J:206:TRP:CH2	1:K:212:LEU:HA	2.05	0.90
1:A:221:GLN:OE1	1:B:220:TRP:CH2	2.24	0.90
1:A:224:HIS:CE1	1:B:223:ARG:NH1	2.39	0.90
1:J:184:TYR:HA	1:K:193:ARG:HH21	1.28	0.90
1:J:213:ILE:HD12	1:J:213:ILE:H	1.34	0.90
1:B:210:GLN:HA	1:B:213:ILE:CD1	2.00	0.90
2:H:301:9ED:C5	1:I:213:ILE:HG21	1.99	0.90
1:G:221:GLN:CB	1:H:220:TRP:NE1	2.34	0.90
1:J:176:GLU:OE1	1:J:179:GLN:NE2	2.04	0.90
1:B:210:GLN:CA	1:B:213:ILE:HD12	2.01	0.90
1:B:219:VAL:HB	2:B:301:9ED:C39	2.02	0.90
1:H:174:GLN:NE2	1:I:178:ILE:CD1	2.34	0.90
2:H:301:9ED:C3	1:I:217:ILE:HD11	1.99	0.90
1:B:184:TYR:CE1	1:J:182:GLN:OE1	2.25	0.90
1:E:165:GLN:CA	1:F:167:ARG:NH1	2.32	0.90
1:K:169:ARG:CD	1:L:167:ARG:C	2.43	0.90
1:A:205:TRP:CD1	1:J:201:GLN:HB3	2.07	0.90
1:A:226:LYS:HZ2	1:L:225:LEU:HD23	1.36	0.90
1:A:171:LEU:CD2	1:C:169:ARG:CZ	2.49	0.90
1:E:180:LYS:NZ	1:G:182:GLN:HB3	1.87	0.90
1:G:178:ILE:HG22	1:I:178:ILE:HG21	1.52	0.90
1:K:203:VAL:O	1:K:207:SER:N	2.04	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LYS:NZ	1:A:180:LYS:HB2	1.87	0.89
1:B:232:LYS:HB3	1:E:232:LYS:HZ3	1.34	0.89
1:D:225:LEU:HB2	1:E:228:PHE:CE1	2.07	0.89
1:A:171:LEU:O	1:A:175:VAL:HG22	1.73	0.89
1:A:204:LEU:HG	1:J:202:ARG:HH22	1.34	0.89
1:A:154:GLU:HB3	1:A:155:ILE:HD12	1.52	0.89
1:A:213:ILE:O	1:A:217:ILE:HD12	1.73	0.89
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.36	0.89
1:B:184:TYR:CE1	1:B:188:ARG:CZ	2.54	0.89
1:C:184:TYR:HD2	1:F:187:TRP:CH2	1.66	0.89
1:H:168:VAL:HG11	1:I:167:ARG:CZ	2.01	0.89
1:J:167:ARG:HH21	1:K:168:VAL:HG11	1.36	0.89
1:K:187:TRP:CA	1:L:188:ARG:CZ	2.49	0.89
1:A:209:LEU:HD23	1:J:205:TRP:CE2	2.06	0.89
1:B:220:TRP:HB2	2:B:301:9ED:O22	1.72	0.89
1:G:174:GLN:NE2	1:I:178:ILE:HD12	1.83	0.89
1:J:205:TRP:HA	1:J:208:ILE:HG13	1.52	0.89
1:D:189:GLU:C	1:H:187:TRP:CZ2	2.51	0.89
1:G:214:LEU:HA	1:G:217:ILE:HD12	1.53	0.89
1:J:167:ARG:NH2	1:K:168:VAL:HG12	1.85	0.89
1:A:205:TRP:CZ3	1:J:205:TRP:CB	2.55	0.89
1:H:171:LEU:HD12	1:H:172:VAL:N	1.88	0.89
1:J:206:TRP:HZ2	1:K:212:LEU:HD22	1.29	0.89
1:H:172:VAL:HA	1:H:175:VAL:HG12	1.52	0.89
1:J:174:GLN:CA	1:J:177:GLN:HG2	2.03	0.89
1:K:176:GLU:HG3	1:L:178:ILE:HD13	0.90	0.89
1:B:216:ALA:O	2:B:301:9ED:C37	2.21	0.89
1:B:222:MET:HB3	1:D:220:TRP:HH2	1.36	0.89
1:B:165:GLN:HE22	1:C:161:LEU:CD2	1.85	0.88
1:C:188:ARG:HD2	1:F:191:ARG:HD2	1.54	0.88
1:A:201:GLN:HE21	1:J:194:GLN:CB	1.87	0.88
1:A:209:LEU:CD2	1:J:205:TRP:CZ3	2.56	0.88
1:A:179:GLN:OE1	1:B:175:VAL:HG13	1.72	0.88
1:C:154:GLU:HB3	1:C:155:ILE:HD13	1.54	0.88
1:C:193:ARG:HG3	1:C:193:ARG:HH21	1.39	0.88
1:H:172:VAL:CA	1:H:175:VAL:HG12	2.03	0.88
1:K:173:GLU:HG3	1:L:177:GLN:OE1	1.71	0.88
1:B:188:ARG:NH2	1:J:186:ARG:HG3	1.88	0.88
1:A:226:LYS:NZ	1:L:225:LEU:CD2	2.37	0.88
1:E:169:ARG:NH2	1:H:170:GLN:HB2	1.87	0.88
1:H:168:VAL:O	1:H:171:LEU:CG	2.18	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:TRP:HZ3	1:J:216:ALA:CB	1.66	0.87
1:B:208:ILE:CG2	2:B:301:9ED:C4	2.52	0.87
1:D:168:VAL:HG23	1:E:167:ARG:HD2	1.55	0.87
1:B:226:LYS:O	1:B:226:LYS:NZ	2.07	0.87
1:E:186:ARG:NH1	1:E:186:ARG:HA	1.87	0.87
1:G:207:SER:HB2	1:H:206:TRP:HD1	1.39	0.87
2:H:301:9ED:C50	1:I:217:ILE:HD13	2.04	0.87
1:J:170:GLN:OE1	1:K:175:VAL:HB	1.71	0.87
1:A:210:GLN:HE22	1:F:208:ILE:HD11	1.06	0.87
1:C:169:ARG:HH11	1:C:169:ARG:HG3	1.40	0.87
1:G:171:LEU:HD12	1:I:171:LEU:HD11	1.57	0.87
1:A:188:ARG:NH2	1:A:188:ARG:HB3	1.87	0.87
1:D:204:LEU:HD13	1:H:205:TRP:HZ2	1.34	0.87
1:K:222:MET:HA	1:K:222:MET:CE	2.04	0.87
1:E:188:ARG:NH1	1:F:185:GLN:CG	2.29	0.87
1:B:212:LEU:HD23	2:B:301:9ED:C49	2.05	0.87
1:E:192:PHE:CG	1:F:192:PHE:CE1	2.63	0.87
1:J:165:GLN:NE2	1:J:165:GLN:HA	1.88	0.87
1:J:167:ARG:HH21	1:K:168:VAL:HG12	1.32	0.87
2:H:301:9ED:C4	1:I:213:ILE:HG21	2.02	0.87
1:G:169:ARG:NE	1:G:169:ARG:HA	1.89	0.87
1:G:221:GLN:HE21	1:H:221:GLN:HE22	1.23	0.87
1:A:220:TRP:CD2	2:B:301:9ED:O09	2.27	0.87
1:G:204:LEU:CD2	1:H:202:ARG:HH21	1.87	0.87
1:B:188:ARG:NH1	1:J:186:ARG:CD	2.36	0.86
1:F:183:ASN:OD1	1:F:187:TRP:CZ2	2.27	0.86
1:H:174:GLN:NE2	1:I:178:ILE:HD11	1.90	0.86
1:A:203:VAL:O	1:A:207:SER:N	2.07	0.86
1:A:224:HIS:HE1	1:B:223:ARG:HH12	1.15	0.86
1:J:170:GLN:CD	1:K:175:VAL:CB	2.46	0.86
1:B:208:ILE:O	2:B:301:9ED:C4	2.22	0.86
1:J:163:GLU:HA	1:J:166:LEU:HD12	1.56	0.86
1:J:206:TRP:CZ3	1:K:212:LEU:HA	2.11	0.86
1:A:205:TRP:HB2	1:J:202:ARG:HG3	1.57	0.86
1:D:193:ARG:NH1	1:H:190:GLU:OE1	2.08	0.86
1:B:233:LYS:O	1:B:233:LYS:NZ	2.08	0.86
1:C:166:LEU:HD22	1:C:166:LEU:O	1.76	0.86
1:H:169:ARG:HA	1:H:169:ARG:NE	1.89	0.86
1:J:163:GLU:HB2	1:L:171:LEU:HD12	0.94	0.86
1:A:204:LEU:HG	1:J:202:ARG:NH2	1.90	0.86
1:G:232:LYS:HZ1	1:G:235:VAL:HG21	1.40	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:ILE:HG13	1:I:178:ILE:HG12	1.57	0.86
1:E:165:GLN:CB	1:F:167:ARG:HH12	1.89	0.86
1:H:188:ARG:HB2	1:I:188:ARG:HH22	0.70	0.86
1:C:233:LYS:O	1:C:233:LYS:NZ	2.08	0.85
1:G:204:LEU:HD21	1:H:202:ARG:NH2	1.91	0.85
1:J:180:LYS:HB3	1:K:186:ARG:HD3	1.56	0.85
1:J:206:TRP:CH2	1:K:212:LEU:CD2	2.58	0.85
1:C:210:GLN:HA	1:C:213:ILE:HD12	1.57	0.85
1:K:176:GLU:CG	1:L:178:ILE:HD13	1.80	0.85
1:A:171:LEU:HD23	1:C:169:ARG:HH21	1.38	0.85
1:H:168:VAL:HG13	1:I:167:ARG:HD3	1.53	0.85
1:C:158:LYS:HA	1:C:161:LEU:HD12	1.57	0.85
1:A:197:GLU:CD	1:J:194:GLN:HG3	2.02	0.85
1:J:166:LEU:HD12	1:L:171:LEU:HD11	1.59	0.85
1:A:220:TRP:CZ2	1:J:212:LEU:O	2.29	0.85
1:G:168:VAL:CG1	1:H:167:ARG:CD	2.54	0.85
1:K:210:GLN:HA	1:K:213:ILE:HD12	1.57	0.85
1:L:201:GLN:HA	1:L:201:GLN:NE2	1.92	0.85
1:D:178:ILE:CD1	1:E:178:ILE:HD11	2.06	0.85
1:H:225:LEU:HD13	1:I:225:LEU:HD13	1.56	0.85
1:B:184:TYR:CZ	1:B:188:ARG:CZ	2.60	0.85
1:H:172:VAL:CA	1:H:175:VAL:CG1	2.55	0.85
1:A:209:LEU:HD13	1:A:209:LEU:C	2.01	0.85
1:E:174:GLN:O	1:E:178:ILE:HG12	1.76	0.85
1:B:216:ALA:O	2:B:301:9ED:C39	2.24	0.84
1:C:224:HIS:CB	1:I:222:MET:HE2	2.07	0.84
1:H:168:VAL:HA	1:H:171:LEU:HD23	1.59	0.84
1:L:163:GLU:HG3	1:L:167:ARG:HH12	1.42	0.84
1:B:232:LYS:CB	1:E:232:LYS:HZ1	1.86	0.84
1:B:220:TRP:CG	2:B:301:9ED:C31	2.60	0.84
1:D:210:GLN:HA	1:D:213:ILE:HG12	1.59	0.84
1:G:225:LEU:HD12	1:G:229:PHE:HZ	1.27	0.84
1:H:205:TRP:CB	2:H:301:9ED:C58	2.54	0.84
1:A:209:LEU:CD2	1:J:205:TRP:CE3	2.60	0.84
1:H:225:LEU:CD1	1:I:225:LEU:HD13	2.08	0.84
1:J:206:TRP:CH2	1:K:212:LEU:HD23	2.07	0.84
1:D:188:ARG:CZ	1:F:189:GLU:HA	2.06	0.84
1:G:207:SER:HA	1:H:206:TRP:HE1	1.38	0.84
1:J:167:ARG:HA	1:K:172:VAL:CG1	2.08	0.84
1:A:171:LEU:CD1	1:A:175:VAL:HG22	2.06	0.84
1:A:226:LYS:CD	1:L:225:LEU:HD22	2.07	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ARG:HH11	1:C:167:ARG:CB	1.90	0.84
1:C:201:GLN:O	1:C:205:TRP:HB3	1.77	0.84
1:E:169:ARG:HH22	1:H:170:GLN:HG3	1.36	0.84
1:L:210:GLN:HA	1:L:210:GLN:HE21	1.43	0.84
1:G:196:SER:OG	1:H:191:ARG:NH2	2.10	0.84
1:A:203:VAL:HG11	1:B:199:THR:HG23	1.58	0.84
1:G:210:GLN:NE2	1:H:209:LEU:HD21	1.86	0.84
1:J:170:GLN:HG2	1:K:175:VAL:HB	1.57	0.84
1:J:191:ARG:HD3	1:K:196:SER:HB3	1.59	0.84
1:A:202:ARG:O	1:A:206:TRP:CB	2.25	0.84
1:A:220:TRP:CZ2	1:J:212:LEU:C	2.56	0.84
1:H:199:THR:CA	1:H:202:ARG:HG3	2.08	0.84
1:B:220:TRP:CB	2:B:301:9ED:O22	2.26	0.83
1:E:202:ARG:HH22	1:G:204:LEU:CD1	1.88	0.83
1:K:169:ARG:NH1	1:L:167:ARG:HB3	1.94	0.83
1:B:184:TYR:OH	1:B:188:ARG:NH2	2.10	0.83
1:B:219:VAL:HB	2:B:301:9ED:C40	2.07	0.83
1:J:170:GLN:OE1	1:K:175:VAL:CG1	2.26	0.83
1:B:164:LEU:O	1:B:164:LEU:HD22	1.77	0.83
1:B:215:VAL:HG21	2:B:301:9ED:C57	2.07	0.83
1:C:221:GLN:NE2	1:I:222:MET:SD	2.51	0.83
1:B:188:ARG:CZ	1:J:186:ARG:HD2	2.05	0.83
2:H:301:9ED:C4	1:I:213:ILE:HG22	2.08	0.83
1:K:173:GLU:HG3	1:L:177:GLN:HE22	1.41	0.83
1:B:181:GLU:O	1:B:185:GLN:NE2	2.11	0.83
1:C:184:TYR:CD2	1:F:187:TRP:HZ3	1.97	0.83
1:C:200:ASN:O	1:C:202:ARG:N	2.11	0.83
1:D:165:GLN:C	1:D:168:VAL:HG12	2.03	0.83
1:H:233:LYS:O	1:H:233:LYS:HD3	1.78	0.83
1:A:155:ILE:HD12	1:A:155:ILE:H	1.42	0.83
1:H:219:VAL:HG22	2:H:301:9ED:O22	1.77	0.83
1:J:170:GLN:CG	1:K:175:VAL:CB	2.56	0.83
1:B:184:TYR:HH	1:J:182:GLN:HB2	1.35	0.83
1:J:166:LEU:HD11	1:L:171:LEU:HD21	1.60	0.83
1:D:225:LEU:CD1	1:D:226:LYS:HZ2	1.89	0.83
1:J:186:ARG:HB3	1:J:186:ARG:CZ	2.08	0.83
1:A:205:TRP:HZ3	1:J:205:TRP:CG	1.96	0.83
1:G:178:ILE:HG21	1:H:174:GLN:HE21	1.40	0.82
1:H:208:ILE:HD12	2:H:301:9ED:C56	2.08	0.82
1:G:168:VAL:HG11	1:H:167:ARG:HD2	1.61	0.82
1:G:232:LYS:NZ	1:G:235:VAL:CG2	2.40	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:186:ARG:NE	1:H:186:ARG:HA	1.94	0.82
1:J:167:ARG:CD	1:K:168:VAL:HG12	2.09	0.82
1:J:180:LYS:HB3	1:K:186:ARG:CD	2.09	0.82
1:L:232:LYS:HA	1:L:232:LYS:NZ	1.94	0.82
1:H:210:GLN:HA	1:H:213:ILE:HD13	1.61	0.82
1:J:166:LEU:CD1	1:L:171:LEU:CD2	2.55	0.82
2:B:301:9ED:C49	1:D:213:ILE:HG21	2.10	0.82
1:A:209:LEU:HD21	1:J:205:TRP:CZ3	2.15	0.82
1:B:184:TYR:HE1	1:B:188:ARG:NH1	1.77	0.82
1:C:224:HIS:CB	1:I:222:MET:CE	2.57	0.82
1:A:214:LEU:HA	1:A:217:ILE:HD12	1.60	0.82
1:K:186:ARG:NH1	1:L:188:ARG:HD2	1.94	0.82
1:G:192:PHE:HE2	1:H:191:ARG:CZ	1.93	0.81
1:B:158:LYS:HB2	1:B:158:LYS:HZ2	1.43	0.81
1:G:225:LEU:O	1:G:229:PHE:CG	2.32	0.81
1:H:174:GLN:HE22	1:I:178:ILE:HD13	1.44	0.81
1:H:233:LYS:HA	1:H:233:LYS:CE	2.06	0.81
1:A:226:LYS:NZ	1:L:225:LEU:HD23	1.95	0.81
1:E:168:VAL:HG11	1:F:167:ARG:CZ	2.10	0.81
1:J:210:GLN:HA	1:J:213:ILE:HD11	1.47	0.81
1:L:234:LEU:O	1:L:234:LEU:HD22	1.78	0.81
1:B:210:GLN:O	1:B:213:ILE:HB	1.79	0.81
1:D:210:GLN:C	1:D:213:ILE:HG12	2.06	0.81
1:H:168:VAL:CG1	1:I:167:ARG:CD	2.34	0.81
1:D:193:ARG:CZ	1:H:190:GLU:OE1	2.28	0.81
1:A:209:LEU:CD2	1:J:205:TRP:CH2	2.64	0.81
1:H:233:LYS:HA	1:H:233:LYS:HZ2	1.45	0.81
1:I:202:ARG:HE	1:I:206:TRP:HE1	1.26	0.81
1:A:203:VAL:CG1	1:B:199:THR:HG21	2.11	0.81
1:G:164:LEU:HD21	1:H:164:LEU:CG	2.06	0.81
1:H:219:VAL:HG21	2:H:301:9ED:O22	1.78	0.81
1:J:191:ARG:NH1	1:K:193:ARG:HG2	1.96	0.81
1:C:188:ARG:HD2	1:F:191:ARG:CD	2.10	0.81
1:G:211:THR:HG22	1:H:209:LEU:HD11	1.61	0.81
1:D:164:LEU:HD23	1:E:163:GLU:OE1	1.79	0.81
1:K:179:GLN:CD	1:L:181:GLU:HG3	2.06	0.81
1:G:192:PHE:CD2	1:H:191:ARG:NH2	2.49	0.80
1:G:232:LYS:CD	1:H:228:PHE:HZ	1.92	0.80
1:J:170:GLN:OE1	1:K:175:VAL:CB	2.28	0.80
1:B:173:GLU:O	1:B:176:GLU:HG2	1.81	0.80
1:A:224:HIS:CE1	1:B:223:ARG:HH12	1.97	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:GLN:HB2	1:F:167:ARG:HH12	1.44	0.80
1:E:166:LEU:HD12	1:E:166:LEU:O	1.80	0.80
1:J:167:ARG:CG	1:K:172:VAL:CG2	2.56	0.80
1:E:192:PHE:CZ	1:F:192:PHE:HA	2.17	0.80
1:J:174:GLN:HA	1:J:177:GLN:HG2	1.62	0.80
1:J:177:GLN:OE1	1:K:179:GLN:HA	1.82	0.80
1:J:209:LEU:O	1:J:213:ILE:HD12	1.79	0.80
1:A:203:VAL:O	1:A:207:SER:OG	1.99	0.80
1:D:164:LEU:CB	1:E:167:ARG:HH22	1.92	0.80
1:D:188:ARG:HH11	1:E:188:ARG:HH21	1.29	0.80
1:A:205:TRP:HB2	1:J:202:ARG:CG	2.10	0.80
1:B:184:TYR:CE1	1:J:182:GLN:HB2	2.17	0.80
1:G:204:LEU:HD22	1:H:202:ARG:NH2	1.94	0.80
1:H:172:VAL:HA	1:H:175:VAL:HG11	1.64	0.80
1:L:232:LYS:HA	1:L:232:LYS:CE	2.11	0.80
1:A:222:MET:HE2	1:A:222:MET:CA	2.12	0.79
1:B:172:VAL:C	1:B:176:GLU:OE1	2.24	0.79
1:D:168:VAL:CG2	1:E:167:ARG:HD2	2.02	0.79
1:F:183:ASN:ND2	1:F:187:TRP:CZ2	2.50	0.79
1:A:205:TRP:NE1	1:J:201:GLN:HB3	1.96	0.79
1:C:221:GLN:HE21	1:I:222:MET:HB2	1.48	0.79
1:C:228:PHE:CZ	1:I:222:MET:CE	2.65	0.79
1:D:189:GLU:HB2	1:H:187:TRP:CZ3	2.17	0.79
1:G:174:GLN:NE2	1:I:178:ILE:HD13	1.96	0.79
1:D:164:LEU:HG	1:E:164:LEU:HB3	1.65	0.79
1:D:210:GLN:O	1:D:213:ILE:CG1	2.29	0.79
1:J:187:TRP:CB	1:J:191:ARG:NH1	2.04	0.79
1:L:163:GLU:HG3	1:L:167:ARG:NH1	1.98	0.79
1:A:167:ARG:HG2	1:A:167:ARG:HH11	1.47	0.79
1:B:175:VAL:HA	1:B:178:ILE:HD12	1.65	0.79
1:G:169:ARG:HA	1:G:169:ARG:HE	1.46	0.79
1:H:168:VAL:CG1	1:I:167:ARG:CZ	2.60	0.78
1:H:168:VAL:HG11	1:I:167:ARG:HH11	0.96	0.78
1:C:188:ARG:CD	1:F:191:ARG:HD2	2.12	0.78
1:E:165:GLN:C	1:E:168:VAL:HG12	2.06	0.78
1:C:224:HIS:HB3	1:I:222:MET:HE2	1.65	0.78
1:F:183:ASN:ND2	1:F:187:TRP:CH2	2.51	0.78
1:G:214:LEU:HG	1:H:213:ILE:HB	1.64	0.78
1:K:202:ARG:HG2	1:L:205:TRP:NE1	1.97	0.78
1:C:201:GLN:O	1:C:205:TRP:HB2	1.81	0.78
1:H:165:GLN:NE2	1:H:165:GLN:O	2.16	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:VAL:HG11	1:I:203:VAL:HG12	1.65	0.78
1:J:187:TRP:HB3	1:J:191:ARG:CZ	2.08	0.78
1:A:180:LYS:HB2	1:A:180:LYS:HZ2	1.45	0.78
1:E:192:PHE:HB2	1:F:192:PHE:CE1	2.18	0.78
1:D:188:ARG:HE	1:F:189:GLU:HG3	1.46	0.78
1:C:210:GLN:CD	1:G:206:TRP:CH2	2.60	0.78
1:J:180:LYS:HB3	1:K:186:ARG:NE	1.98	0.78
1:D:171:LEU:HD11	1:E:171:LEU:HB3	1.64	0.78
1:G:186:ARG:HA	1:G:186:ARG:HH11	1.47	0.78
1:G:232:LYS:CG	1:H:228:PHE:HZ	1.96	0.78
1:B:200:ASN:OD1	1:F:200:ASN:C	2.27	0.78
1:C:164:LEU:HD12	1:C:164:LEU:O	1.82	0.78
1:E:166:LEU:CD2	1:H:166:LEU:HD13	2.06	0.77
1:G:221:GLN:NE2	1:H:221:GLN:HE22	1.82	0.77
1:G:225:LEU:CD1	1:G:229:PHE:HZ	1.69	0.77
1:C:210:GLN:NE2	1:G:206:TRP:HH2	1.81	0.77
1:J:211:THR:HA	1:J:214:LEU:CD2	2.15	0.77
1:H:174:GLN:NE2	1:I:178:ILE:HD13	1.99	0.77
1:J:184:TYR:CA	1:K:193:ARG:HH22	1.83	0.77
1:A:226:LYS:HD2	1:L:225:LEU:HD22	1.64	0.77
1:B:232:LYS:HB3	1:E:232:LYS:HZ1	1.41	0.77
1:C:229:PHE:HE1	1:G:232:LYS:NZ	1.82	0.77
1:E:187:TRP:HE1	1:E:191:ARG:CD	1.98	0.77
1:G:165:GLN:C	1:G:168:VAL:HG22	2.08	0.77
1:H:199:THR:O	1:H:203:VAL:CG2	2.32	0.77
1:B:216:ALA:C	2:B:301:9ED:C37	2.57	0.77
1:C:188:ARG:HD3	1:F:187:TRP:HB3	1.66	0.77
1:D:188:ARG:CZ	1:E:188:ARG:NH2	2.45	0.77
1:H:198:SER:O	1:H:202:ARG:HG3	1.82	0.77
1:B:230:GLU:OE1	1:B:230:GLU:HA	1.83	0.77
1:A:224:HIS:CE1	1:B:223:ARG:CZ	2.68	0.77
1:E:189:GLU:OE2	1:F:188:ARG:NH1	2.18	0.77
1:A:160:LYS:C	1:A:160:LYS:HZ2	1.92	0.77
1:D:168:VAL:CA	1:E:167:ARG:HD2	2.14	0.77
1:E:176:GLU:O	1:E:179:GLN:HB3	1.84	0.77
1:A:171:LEU:CD1	1:A:174:GLN:OE1	2.29	0.77
1:B:193:ARG:HD2	1:F:197:GLU:CD	2.09	0.77
1:C:234:LEU:O	1:C:234:LEU:HD23	1.85	0.77
1:K:227:SER:C	1:K:230:GLU:HG2	2.09	0.77
1:A:203:VAL:O	1:A:207:SER:HB3	1.83	0.77
1:E:186:ARG:HA	1:E:186:ARG:CZ	2.14	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:PHE:CE1	1:I:192:PHE:HD1	1.93	0.77
1:B:200:ASN:OD1	1:F:200:ASN:CA	2.33	0.76
1:D:210:GLN:CA	1:D:213:ILE:HG12	2.15	0.76
1:E:169:ARG:NH2	1:H:170:GLN:CG	2.39	0.76
1:K:216:ALA:CB	1:L:220:TRP:CH2	2.60	0.76
1:A:221:GLN:C	1:A:221:GLN:HE21	1.93	0.76
1:B:172:VAL:O	1:B:176:GLU:OE2	2.03	0.76
1:G:171:LEU:HD21	1:H:170:GLN:OE1	1.85	0.76
1:K:187:TRP:HA	1:L:188:ARG:CZ	2.11	0.76
1:A:210:GLN:CD	1:F:208:ILE:HD11	2.10	0.76
1:B:184:TYR:CE1	1:J:182:GLN:CB	2.67	0.76
1:G:232:LYS:CE	1:G:232:LYS:HA	2.15	0.76
1:H:163:GLU:HA	1:H:166:LEU:HD12	1.65	0.76
1:B:188:ARG:NH1	1:J:186:ARG:HD2	1.98	0.76
1:H:210:GLN:HE21	1:I:214:LEU:HD21	1.49	0.76
1:J:184:TYR:CB	1:K:193:ARG:HH22	1.97	0.76
1:L:210:GLN:NE2	1:L:210:GLN:HA	2.00	0.76
1:A:171:LEU:HG	1:C:169:ARG:HH22	1.48	0.76
1:A:213:ILE:HG12	1:A:214:LEU:HD13	1.66	0.76
1:E:184:TYR:HD1	1:E:187:TRP:CE3	2.03	0.76
1:J:180:LYS:C	1:K:186:ARG:HD3	2.10	0.76
1:J:210:GLN:HG2	1:J:214:LEU:HD21	1.67	0.76
1:B:226:LYS:C	1:B:226:LYS:HD3	2.11	0.76
1:D:189:GLU:CA	1:H:187:TRP:HH2	1.98	0.76
1:D:171:LEU:HD11	1:E:171:LEU:CB	2.16	0.76
1:D:175:VAL:HG22	1:E:174:GLN:HG3	1.67	0.76
1:K:200:ASN:C	1:K:203:VAL:HG12	2.11	0.76
1:G:192:PHE:CE1	1:I:192:PHE:HB3	2.19	0.76
1:J:170:GLN:HG2	1:K:175:VAL:CG2	2.16	0.76
1:A:226:LYS:HZ2	1:L:225:LEU:HA	1.49	0.76
1:J:166:LEU:CD1	1:L:171:LEU:HD11	2.16	0.76
1:J:184:TYR:CD1	1:K:189:GLU:CG	2.65	0.76
1:G:203:VAL:CG1	1:H:202:ARG:NH2	2.49	0.76
1:H:185:GLN:HE22	1:I:184:TYR:HB3	1.48	0.76
1:A:220:TRP:CG	2:B:301:9ED:O09	2.39	0.75
1:E:184:TYR:HE1	1:G:186:ARG:HD3	0.68	0.75
1:E:184:TYR:CD1	1:E:187:TRP:CZ3	2.74	0.75
1:G:203:VAL:HG12	1:H:202:ARG:NH2	2.01	0.75
1:J:210:GLN:O	1:J:213:ILE:HD13	1.85	0.75
1:J:220:TRP:CG	1:J:223:ARG:HD2	2.13	0.75
1:B:220:TRP:HB2	2:B:301:9ED:O20	1.85	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:HD13	1:A:209:LEU:O	1.86	0.75
1:H:168:VAL:C	1:H:171:LEU:HG	2.10	0.75
1:H:168:VAL:HG11	1:I:167:ARG:NE	2.00	0.75
1:B:181:GLU:C	1:B:185:GLN:NE2	2.44	0.75
1:D:188:ARG:HH21	1:F:189:GLU:HA	0.69	0.75
1:E:192:PHE:HB2	1:F:192:PHE:CZ	2.20	0.75
1:B:184:TYR:HH	1:J:182:GLN:CB	1.81	0.75
1:D:178:ILE:HD13	1:E:174:GLN:NE2	2.02	0.75
1:A:224:HIS:CE1	1:B:223:ARG:NH2	2.55	0.75
1:G:208:ILE:HG23	1:G:212:LEU:HD11	1.68	0.75
1:E:184:TYR:CD1	1:E:187:TRP:CE3	2.75	0.74
1:K:187:TRP:HB2	1:L:188:ARG:CZ	2.17	0.74
1:A:214:LEU:HD22	1:A:214:LEU:N	2.02	0.74
1:B:176:GLU:CD	1:B:176:GLU:H	1.95	0.74
1:K:173:GLU:CD	1:L:177:GLN:OE1	2.29	0.74
1:J:163:GLU:HA	1:L:171:LEU:HD11	1.70	0.74
1:B:210:GLN:CB	1:B:213:ILE:HD12	2.17	0.74
1:G:186:ARG:NH1	1:G:186:ARG:O	2.20	0.74
1:H:181:GLU:HA	1:H:184:TYR:HD2	1.53	0.74
1:H:210:GLN:NE2	1:I:214:LEU:HD21	2.03	0.74
1:H:233:LYS:HA	1:H:233:LYS:NZ	2.02	0.74
1:B:204:LEU:HD23	1:B:204:LEU:C	2.12	0.74
1:B:214:LEU:HD11	1:F:214:LEU:HB3	1.68	0.74
1:E:168:VAL:HA	1:E:171:LEU:HD23	1.70	0.74
1:G:207:SER:CB	1:H:206:TRP:CD1	2.69	0.74
1:G:232:LYS:N	1:G:232:LYS:HD2	2.01	0.74
1:J:173:GLU:HG3	1:L:181:GLU:OE2	1.88	0.74
1:G:171:LEU:CD1	1:I:171:LEU:HD11	2.17	0.74
1:J:184:TYR:HB2	1:K:189:GLU:HB2	1.65	0.74
1:J:191:ARG:NH2	1:K:193:ARG:CB	2.45	0.74
1:G:193:ARG:HA	1:H:191:ARG:HH21	1.49	0.73
1:E:187:TRP:CD1	1:E:191:ARG:CD	2.70	0.73
1:H:168:VAL:HA	1:H:171:LEU:HD21	1.68	0.73
1:B:202:ARG:O	1:B:206:TRP:HD1	1.72	0.73
1:B:232:LYS:HB2	1:E:232:LYS:NZ	2.02	0.73
1:E:166:LEU:HD23	1:H:166:LEU:CD1	2.08	0.73
1:L:163:GLU:OE2	1:L:167:ARG:CZ	2.37	0.73
1:A:205:TRP:CD1	1:J:201:GLN:CB	2.71	0.73
1:B:233:LYS:HG3	1:B:234:LEU:HD13	1.70	0.73
1:A:205:TRP:CE2	1:J:201:GLN:HB3	2.23	0.73
1:G:192:PHE:CZ	1:I:192:PHE:CE1	2.77	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:221:GLN:HE21	1:H:221:GLN:NE2	1.86	0.73
1:B:214:LEU:HB2	1:F:215:VAL:HG22	1.69	0.73
1:J:178:ILE:HD13	1:J:178:ILE:N	2.03	0.73
1:A:202:ARG:O	1:A:206:TRP:CA	2.35	0.73
1:L:163:GLU:CG	1:L:167:ARG:HH12	2.01	0.73
1:B:215:VAL:CG1	2:B:301:9ED:C62	2.61	0.73
1:G:168:VAL:HG12	1:H:167:ARG:HD2	1.69	0.73
1:J:202:ARG:HD2	1:K:204:LEU:HD11	1.69	0.73
1:J:161:LEU:HD12	1:J:161:LEU:N	2.04	0.73
1:B:202:ARG:O	1:B:202:ARG:HD2	1.88	0.73
1:E:187:TRP:NE1	1:E:191:ARG:CD	2.51	0.73
1:A:226:LYS:NZ	1:L:225:LEU:HD22	2.02	0.72
1:C:211:THR:OG1	1:G:206:TRP:CZ3	2.39	0.72
1:E:209:LEU:O	1:E:213:ILE:HG12	1.89	0.72
1:H:180:LYS:O	1:H:184:TYR:CD2	2.42	0.72
1:H:208:ILE:HG21	2:H:301:9ED:C61	2.18	0.72
1:G:214:LEU:HD22	1:G:214:LEU:C	2.15	0.72
1:B:215:VAL:HG21	2:B:301:9ED:C53	2.18	0.72
1:E:192:PHE:CD2	1:F:192:PHE:CE1	2.77	0.72
1:H:171:LEU:CD2	1:I:171:LEU:CD1	2.44	0.72
1:K:174:GLN:O	1:K:174:GLN:NE2	2.22	0.72
1:A:221:GLN:OE1	1:B:220:TRP:HH2	1.70	0.72
1:H:168:VAL:CB	1:I:167:ARG:HD3	2.19	0.72
1:J:173:GLU:HB2	1:K:179:GLN:OE1	1.89	0.72
1:K:176:GLU:OE1	1:L:178:ILE:HA	1.89	0.72
1:L:163:GLU:OE2	1:L:167:ARG:NH1	2.22	0.72
1:C:166:LEU:HD22	1:C:166:LEU:C	2.14	0.72
1:D:222:MET:O	1:D:225:LEU:HG	1.88	0.72
1:E:166:LEU:HD12	1:E:166:LEU:C	2.15	0.72
1:H:188:ARG:HB3	1:I:188:ARG:HH21	1.52	0.72
1:J:180:LYS:CB	1:K:186:ARG:HD3	2.19	0.72
1:D:204:LEU:CD1	1:H:205:TRP:CH2	2.73	0.72
1:B:188:ARG:HH22	1:J:186:ARG:HG3	1.52	0.72
1:G:181:GLU:HA	1:G:184:TYR:HD2	1.55	0.72
1:K:173:GLU:OE2	1:L:174:GLN:CB	2.37	0.72
1:K:176:GLU:OE2	1:K:180:LYS:HE3	1.90	0.72
1:B:226:LYS:HE3	1:B:230:GLU:HG2	1.70	0.72
1:G:210:GLN:NE2	1:H:209:LEU:HD22	1.95	0.72
1:H:168:VAL:CG2	1:I:167:ARG:HD3	2.20	0.72
1:G:233:LYS:HA	1:G:233:LYS:CE	2.19	0.71
1:D:168:VAL:HA	1:E:167:ARG:HD2	1.69	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:LEU:HD23	1:G:212:LEU:N	2.04	0.71
1:H:214:LEU:HD23	1:H:214:LEU:C	2.14	0.71
1:C:169:ARG:HG3	1:C:169:ARG:NH1	1.98	0.71
1:C:185:GLN:CG	1:C:188:ARG:NH1	2.52	0.71
1:E:180:LYS:HZ3	1:G:182:GLN:HB3	1.53	0.71
1:J:186:ARG:HB3	1:J:186:ARG:NH2	2.05	0.71
1:A:204:LEU:CB	1:J:202:ARG:NH2	2.45	0.71
1:E:192:PHE:CB	1:F:192:PHE:CE1	2.73	0.71
1:H:171:LEU:HD22	1:I:171:LEU:HD12	0.79	0.71
1:H:223:ARG:NH1	1:H:223:ARG:O	2.24	0.71
1:C:228:PHE:CE2	1:I:222:MET:CE	2.73	0.71
1:D:204:LEU:CD1	1:H:205:TRP:CZ2	2.73	0.71
1:K:212:LEU:HD13	1:L:217:ILE:HD11	1.72	0.71
1:A:171:LEU:CG	1:C:169:ARG:NH2	2.28	0.71
1:A:188:ARG:HB3	1:A:188:ARG:HH21	1.54	0.71
1:D:164:LEU:CB	1:E:167:ARG:NH2	2.53	0.71
1:H:202:ARG:HB3	1:H:202:ARG:NH1	2.06	0.71
1:L:163:GLU:CG	1:L:167:ARG:NH1	2.53	0.71
1:G:233:LYS:N	1:G:233:LYS:HD2	2.04	0.71
1:C:210:GLN:NE2	1:G:206:TRP:HZ2	1.75	0.70
1:D:190:GLU:HA	1:H:187:TRP:CZ2	2.26	0.70
1:K:167:ARG:HD3	1:K:168:VAL:H	1.56	0.70
1:K:220:TRP:CE3	1:K:220:TRP:HA	2.24	0.70
1:A:197:GLU:HB2	1:B:192:PHE:CE2	2.25	0.70
1:B:206:TRP:HA	1:B:209:LEU:HD12	1.73	0.70
1:J:173:GLU:HG3	1:L:181:GLU:CD	2.16	0.70
1:A:203:VAL:CG1	1:B:199:THR:CG2	2.57	0.70
1:D:189:GLU:CD	1:E:188:ARG:HG2	2.16	0.70
1:G:221:GLN:HG2	1:H:220:TRP:HD1	1.52	0.70
1:C:171:LEU:N	1:C:171:LEU:HD23	2.06	0.70
1:B:184:TYR:CD1	1:J:182:GLN:OE1	2.44	0.70
1:A:223:ARG:HH12	1:J:217:ILE:HD13	1.56	0.70
1:E:184:TYR:HD1	1:E:187:TRP:HE3	1.36	0.70
1:G:211:THR:CG2	1:H:209:LEU:CD1	2.69	0.70
1:H:198:SER:C	1:H:202:ARG:CG	2.64	0.70
1:J:191:ARG:NH1	1:K:193:ARG:CB	2.46	0.70
1:B:220:TRP:N	2:B:301:9ED:O22	2.24	0.70
1:G:178:ILE:HG12	1:H:174:GLN:HE21	1.55	0.70
1:A:209:LEU:CD2	1:J:205:TRP:CE2	2.75	0.70
1:B:222:MET:SD	1:D:220:TRP:CZ2	2.84	0.70
1:B:191:ARG:HD2	1:B:191:ARG:C	2.16	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:GLU:N	1:H:187:TRP:CZ2	2.60	0.70
1:A:220:TRP:HZ3	1:J:216:ALA:HB2	0.88	0.69
1:C:164:LEU:HD12	1:C:164:LEU:C	2.17	0.69
1:E:180:LYS:HZ3	1:G:182:GLN:CB	2.04	0.69
1:A:204:LEU:CG	1:J:202:ARG:NH2	2.55	0.69
1:A:209:LEU:CD2	1:J:205:TRP:CZ2	2.76	0.69
1:A:220:TRP:HZ2	1:J:212:LEU:C	2.00	0.69
1:B:208:ILE:HD13	1:B:208:ILE:N	2.06	0.69
1:C:185:GLN:HG2	1:C:188:ARG:NH1	2.07	0.69
1:A:197:GLU:HB2	1:B:192:PHE:HE2	1.57	0.69
1:A:209:LEU:HD21	1:J:205:TRP:CZ2	2.26	0.69
1:C:229:PHE:CE1	1:G:232:LYS:NZ	2.58	0.69
1:D:188:ARG:CZ	1:F:192:PHE:CD2	2.76	0.69
1:J:170:GLN:OE1	1:K:175:VAL:HG12	1.90	0.69
1:L:232:LYS:N	1:L:232:LYS:HD2	2.06	0.69
1:G:163:GLU:OE1	1:G:163:GLU:N	2.18	0.69
1:G:202:ARG:HH11	1:G:202:ARG:HA	1.58	0.69
1:B:202:ARG:HD2	1:B:202:ARG:C	2.18	0.69
1:B:215:VAL:CG1	2:B:301:9ED:C51	2.71	0.69
1:G:232:LYS:HZ2	1:G:235:VAL:CG2	2.04	0.69
1:B:229:PHE:HE1	1:E:232:LYS:CD	1.98	0.69
1:G:164:LEU:C	1:G:164:LEU:HD12	2.18	0.69
1:K:176:GLU:OE1	1:L:178:ILE:CA	2.41	0.69
1:D:190:GLU:N	1:H:187:TRP:CH2	2.61	0.69
1:F:183:ASN:CG	1:F:187:TRP:CZ2	2.71	0.69
1:G:178:ILE:CG2	1:H:174:GLN:HE21	2.05	0.69
1:J:187:TRP:CD1	1:K:193:ARG:NE	2.54	0.69
1:K:187:TRP:N	1:L:188:ARG:CZ	2.53	0.69
1:A:155:ILE:HA	1:A:158:LYS:HD2	1.75	0.69
1:D:178:ILE:CD1	1:E:174:GLN:HG2	2.23	0.69
1:E:221:GLN:HA	1:E:224:HIS:CD2	2.28	0.69
1:G:164:LEU:HD21	1:H:164:LEU:HD22	1.73	0.69
1:J:191:ARG:NH1	1:K:193:ARG:HB3	2.00	0.69
1:K:171:LEU:C	1:K:171:LEU:HD12	2.17	0.69
1:A:210:GLN:HE22	1:F:208:ILE:CD1	1.94	0.68
1:G:208:ILE:HD13	1:G:212:LEU:HD21	1.76	0.68
1:D:209:LEU:O	1:D:213:ILE:HG23	1.92	0.68
1:J:174:GLN:CA	1:J:177:GLN:CD	2.66	0.68
1:L:163:GLU:OE2	1:L:167:ARG:HG3	1.93	0.68
1:G:164:LEU:HD12	1:G:164:LEU:O	1.92	0.68
1:G:201:GLN:OE1	1:G:201:GLN:HA	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:VAL:CG2	1:I:233:LYS:HE2	2.23	0.68
1:K:176:GLU:CD	1:L:177:GLN:C	2.61	0.68
1:G:207:SER:O	1:G:210:GLN:HB3	1.94	0.68
1:J:180:LYS:HB3	1:K:186:ARG:HE	1.57	0.68
1:J:184:TYR:CB	1:K:189:GLU:HB2	2.21	0.68
1:J:220:TRP:HB2	1:J:223:ARG:HD2	1.74	0.68
1:J:213:ILE:HD12	1:J:213:ILE:N	2.07	0.68
1:A:197:GLU:CG	1:J:194:GLN:HG2	2.23	0.68
1:B:154:GLU:HB3	1:B:155:ILE:HD12	1.76	0.68
1:B:155:ILE:HD12	1:B:155:ILE:N	2.07	0.68
1:A:221:GLN:OE1	1:B:220:TRP:CZ3	2.47	0.68
1:G:168:VAL:HB	1:H:167:ARG:NE	2.08	0.68
1:J:180:LYS:CA	1:K:186:ARG:HD3	2.23	0.68
1:J:210:GLN:C	1:J:214:LEU:HG	2.16	0.68
1:A:171:LEU:HD21	1:C:169:ARG:CZ	2.24	0.68
1:B:216:ALA:C	2:B:301:9ED:C40	2.66	0.68
1:C:232:LYS:HA	1:C:235:VAL:HB	1.75	0.68
1:C:235:VAL:HG21	1:I:233:LYS:HE2	1.74	0.68
1:K:169:ARG:NH1	1:L:167:ARG:CB	2.57	0.68
1:L:193:ARG:HH11	1:L:193:ARG:HG3	1.58	0.68
1:J:173:GLU:CB	1:K:179:GLN:CD	2.46	0.67
1:L:171:LEU:C	1:L:171:LEU:HD23	2.18	0.67
1:A:215:VAL:HG21	1:L:214:LEU:CD2	2.24	0.67
1:C:170:GLN:HG3	1:C:171:LEU:HD23	1.76	0.67
1:E:175:VAL:HB	1:F:174:GLN:OE1	1.95	0.67
1:A:179:GLN:OE1	1:B:175:VAL:CG1	2.42	0.67
1:B:191:ARG:HG2	1:B:191:ARG:HH11	1.58	0.67
1:B:165:GLN:HE22	1:C:161:LEU:HD21	1.59	0.67
1:B:173:GLU:O	1:B:176:GLU:CG	2.37	0.67
1:G:221:GLN:CG	1:H:220:TRP:CD1	2.76	0.67
1:B:172:VAL:O	1:B:175:VAL:HG22	1.93	0.67
1:C:232:LYS:HE3	1:I:233:LYS:HD3	1.75	0.67
1:D:188:ARG:HH22	1:F:192:PHE:HD2	0.70	0.67
1:J:177:GLN:HG3	1:J:178:ILE:CD1	2.21	0.67
1:B:184:TYR:CZ	1:B:188:ARG:NH2	2.63	0.67
1:B:216:ALA:CB	2:B:301:9ED:C37	2.72	0.67
1:E:192:PHE:CD2	1:F:192:PHE:CD1	2.82	0.67
1:A:221:GLN:CD	1:B:220:TRP:CH2	2.73	0.67
1:H:233:LYS:HZ2	1:H:233:LYS:CA	2.07	0.67
1:L:217:ILE:HD13	1:L:217:ILE:N	2.10	0.67
1:B:210:GLN:HA	1:B:213:ILE:CG1	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:214:LEU:HD22	1:G:214:LEU:O	1.95	0.67
1:G:231:ALA:O	1:G:235:VAL:HG22	1.95	0.67
1:B:212:LEU:HD22	2:B:301:9ED:C53	2.23	0.67
1:G:189:GLU:HA	1:G:189:GLU:OE2	1.91	0.67
1:A:220:TRP:HZ2	1:J:212:LEU:HB3	1.59	0.66
1:B:188:ARG:HH21	1:J:183:ASN:HA	1.60	0.66
1:G:174:GLN:HE22	1:H:174:GLN:NE2	1.93	0.66
1:K:185:GLN:HA	1:K:185:GLN:NE2	2.09	0.66
1:C:210:GLN:OE1	1:G:206:TRP:CH2	2.48	0.66
1:A:160:LYS:O	1:A:160:LYS:NZ	2.21	0.66
1:C:210:GLN:CD	1:G:206:TRP:CZ2	2.74	0.66
1:E:188:ARG:HH12	1:F:185:GLN:CD	2.02	0.66
1:A:197:GLU:CG	1:J:194:GLN:CG	2.74	0.66
1:H:219:VAL:HG21	2:H:301:9ED:C35	2.25	0.66
1:J:167:ARG:CA	1:K:172:VAL:HG13	2.21	0.66
1:J:170:GLN:HG2	1:K:175:VAL:CB	2.20	0.66
1:B:184:TYR:CE2	1:J:179:GLN:O	2.48	0.66
1:B:222:MET:HB3	1:D:220:TRP:CH2	2.21	0.66
1:C:185:GLN:HG3	1:C:188:ARG:HH12	1.59	0.66
1:D:164:LEU:CG	1:E:164:LEU:HB3	2.22	0.66
1:J:174:GLN:HB2	1:J:177:GLN:NE2	2.10	0.66
1:B:229:PHE:HE2	1:D:232:LYS:CD	2.04	0.66
1:J:166:LEU:CB	1:L:174:GLN:NE2	2.41	0.66
1:J:199:THR:HG23	1:K:204:LEU:CD2	2.24	0.66
1:J:209:LEU:HD13	1:J:212:LEU:HD12	1.78	0.66
1:D:165:GLN:OE1	1:D:168:VAL:HG11	1.96	0.66
1:G:232:LYS:HD3	1:H:228:PHE:HZ	1.59	0.66
1:H:169:ARG:NH2	1:I:167:ARG:HH22	1.92	0.66
1:J:191:ARG:NH1	1:K:193:ARG:HD2	1.58	0.66
1:L:188:ARG:HD3	1:L:191:ARG:HD2	1.75	0.66
1:D:210:GLN:HA	1:D:213:ILE:CG1	2.25	0.66
1:G:192:PHE:CE2	1:H:191:ARG:NH1	2.63	0.66
1:J:168:VAL:HA	1:J:171:LEU:HD22	1.77	0.66
1:D:171:LEU:CD1	1:E:171:LEU:HB3	2.26	0.66
1:G:178:ILE:CG1	1:H:174:GLN:HE21	2.08	0.66
1:A:171:LEU:HG	1:C:169:ARG:NH2	2.06	0.65
1:B:188:ARG:NE	1:J:186:ARG:CD	2.30	0.65
1:J:206:TRP:HE3	1:K:215:VAL:CG2	1.85	0.65
1:D:213:ILE:HG13	1:D:214:LEU:HD12	1.78	0.65
1:K:171:LEU:HD12	1:K:171:LEU:O	1.96	0.65
1:C:185:GLN:CG	1:C:188:ARG:HH12	2.10	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:LYS:HZ3	1:G:183:ASN:N	1.94	0.65
1:J:211:THR:HA	1:J:214:LEU:HD21	1.76	0.65
1:L:178:ILE:HD13	1:L:178:ILE:N	2.10	0.65
1:A:210:GLN:OE1	1:B:210:GLN:HG2	1.97	0.65
1:G:203:VAL:HG12	1:H:202:ARG:HH22	1.62	0.65
1:G:204:LEU:HD23	1:H:202:ARG:HH21	1.61	0.65
1:D:196:SER:OG	1:E:195:THR:OG1	2.02	0.65
1:K:202:ARG:O	1:K:205:TRP:HB2	1.89	0.65
1:K:216:ALA:CB	1:L:220:TRP:HZ2	1.88	0.65
1:L:169:ARG:NH1	1:L:169:ARG:HG2	2.10	0.65
1:D:168:VAL:HG21	1:E:167:ARG:HD3	1.75	0.65
1:G:178:ILE:CG2	1:I:178:ILE:HG21	2.26	0.65
1:G:192:PHE:CD2	1:H:191:ARG:CZ	2.80	0.65
1:A:212:LEU:HB3	1:J:209:LEU:HD21	1.77	0.65
1:B:226:LYS:HG2	1:D:228:PHE:HE1	1.62	0.65
1:J:177:GLN:HB3	1:K:179:GLN:HG3	1.78	0.65
1:K:226:LYS:HD2	1:L:228:PHE:CE1	2.32	0.65
1:G:210:GLN:OE1	1:H:206:TRP:CE2	2.50	0.65
1:L:233:LYS:N	1:L:233:LYS:HE2	2.12	0.65
1:F:183:ASN:OD1	1:F:187:TRP:NE1	2.29	0.64
1:G:178:ILE:CG2	1:I:178:ILE:HD13	2.21	0.64
1:H:176:GLU:HA	1:H:176:GLU:OE1	1.97	0.64
1:B:181:GLU:O	1:B:185:GLN:HG3	1.89	0.64
1:E:168:VAL:HB	1:F:167:ARG:HD3	1.80	0.64
1:G:174:GLN:HE21	1:I:178:ILE:HD13	1.51	0.64
1:K:169:ARG:CD	1:L:171:LEU:HB2	2.28	0.64
1:A:209:LEU:C	1:A:209:LEU:CD1	2.70	0.64
1:E:174:GLN:NE2	1:E:178:ILE:HD11	2.12	0.64
1:H:178:ILE:HG13	1:I:178:ILE:CG1	2.28	0.64
1:E:202:ARG:HH21	1:E:205:TRP:HZ2	1.45	0.64
1:G:163:GLU:H	1:G:163:GLU:CD	2.04	0.64
1:H:175:VAL:HG23	1:I:174:GLN:NE2	2.12	0.64
1:J:188:ARG:HG3	1:J:188:ARG:NH1	2.13	0.64
2:H:301:9ED:C3	1:I:213:ILE:CG2	2.75	0.64
1:B:184:TYR:OH	1:J:182:GLN:HB3	1.92	0.64
1:G:180:LYS:O	1:G:184:TYR:CD2	2.51	0.64
1:J:199:THR:CG2	1:K:204:LEU:HD23	2.26	0.64
1:A:171:LEU:C	1:A:175:VAL:HG23	2.12	0.64
1:B:167:ARG:HB2	1:B:167:ARG:HH11	1.62	0.64
1:D:225:LEU:HD12	1:D:226:LYS:N	2.13	0.64
1:H:181:GLU:HA	1:H:184:TYR:CD2	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:169:ARG:NE	1:L:168:VAL:HA	2.13	0.64
1:C:211:THR:HG1	1:G:206:TRP:HZ3	1.34	0.64
1:J:166:LEU:HD12	1:L:171:LEU:CD1	2.27	0.64
1:B:214:LEU:HD12	1:F:215:VAL:HG22	1.79	0.63
1:H:210:GLN:HE21	1:I:214:LEU:CD2	2.11	0.63
1:J:187:TRP:C	1:J:191:ARG:NH1	2.56	0.63
1:C:178:ILE:HD13	1:C:178:ILE:N	2.13	0.63
1:D:189:GLU:CA	1:H:187:TRP:CH2	2.78	0.63
1:H:189:GLU:HB2	1:I:188:ARG:NH1	2.13	0.63
1:K:169:ARG:HD3	1:L:171:LEU:H	1.62	0.63
1:B:164:LEU:HD22	1:B:164:LEU:C	2.22	0.63
1:B:228:PHE:CE2	1:F:229:PHE:CD1	2.76	0.63
1:C:228:PHE:HZ	1:I:222:MET:CE	2.11	0.63
1:G:170:GLN:NE2	1:G:170:GLN:O	2.31	0.63
1:K:172:VAL:HB	1:L:174:GLN:HG3	1.80	0.63
1:L:186:ARG:HA	1:L:186:ARG:NH1	2.12	0.63
1:D:188:ARG:HD3	1:E:188:ARG:NH2	2.13	0.63
1:C:155:ILE:H	1:C:155:ILE:CD1	1.98	0.63
1:G:181:GLU:HA	1:G:184:TYR:CD2	2.32	0.63
1:J:161:LEU:HD12	1:J:161:LEU:H	1.63	0.63
1:K:203:VAL:O	1:K:207:SER:HB3	1.99	0.63
1:A:226:LYS:NZ	1:L:225:LEU:HA	2.14	0.63
1:D:178:ILE:HD11	1:E:174:GLN:HG2	1.81	0.63
1:A:224:HIS:CE1	1:B:223:ARG:HH22	2.16	0.62
1:A:165:GLN:HE22	1:A:169:ARG:HH21	1.44	0.62
1:D:214:LEU:HD13	1:E:213:ILE:HD12	1.82	0.62
1:G:225:LEU:C	1:G:229:PHE:CD2	2.77	0.62
1:K:187:TRP:CB	1:L:188:ARG:NH1	2.61	0.62
1:C:188:ARG:CG	1:F:191:ARG:HD2	2.29	0.62
1:H:205:TRP:HE3	2:H:301:9ED:C58	2.12	0.62
1:K:169:ARG:HA	1:K:172:VAL:HG23	1.81	0.62
1:B:215:VAL:CB	2:B:301:9ED:C62	2.77	0.62
1:H:203:VAL:CG1	1:I:203:VAL:HG12	2.29	0.62
1:B:158:LYS:HZ2	1:B:158:LYS:CB	2.13	0.62
1:B:203:VAL:O	1:B:203:VAL:HG12	2.00	0.62
1:G:232:LYS:CD	1:H:228:PHE:CZ	2.79	0.62
1:K:179:GLN:NE2	1:L:181:GLU:HG3	2.14	0.62
1:K:187:TRP:CB	1:L:188:ARG:CZ	2.73	0.62
1:B:222:MET:SD	1:D:220:TRP:CH2	2.93	0.62
1:E:184:TYR:CD1	1:E:187:TRP:HZ3	2.16	0.62
1:H:180:LYS:O	1:H:184:TYR:HD2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:301:9ED:C49	1:I:217:ILE:CG1	2.74	0.62
1:A:193:ARG:HD3	1:B:189:GLU:HB2	1.81	0.62
1:L:169:ARG:HG2	1:L:169:ARG:HH11	1.64	0.62
1:L:193:ARG:CZ	1:L:193:ARG:HB2	2.29	0.62
1:C:228:PHE:HZ	1:I:222:MET:HE3	1.65	0.62
1:F:213:ILE:HG23	1:F:217:ILE:HD13	1.82	0.62
1:J:167:ARG:CZ	1:K:171:LEU:HD23	2.26	0.62
1:A:215:VAL:HG21	1:L:214:LEU:HD21	1.81	0.61
1:J:199:THR:HA	1:K:204:LEU:HD21	1.81	0.61
1:K:187:TRP:CB	1:L:188:ARG:HH12	2.11	0.61
1:K:217:ILE:HD13	1:K:217:ILE:N	2.14	0.61
1:F:188:ARG:CZ	1:F:191:ARG:NH1	2.64	0.61
1:H:198:SER:C	1:H:202:ARG:HG3	2.23	0.61
1:J:166:LEU:CD1	1:L:171:LEU:CG	2.78	0.61
1:A:226:LYS:HE3	1:L:229:PHE:CE1	2.35	0.61
1:D:210:GLN:HA	1:D:213:ILE:CD1	2.30	0.61
1:H:230:GLU:HA	1:H:230:GLU:OE2	1.99	0.61
1:J:188:ARG:HH11	1:J:188:ARG:CG	2.14	0.61
1:J:220:TRP:CB	1:J:223:ARG:HD2	2.30	0.61
1:A:214:LEU:HD12	1:B:213:ILE:HD13	1.83	0.61
1:B:235:VAL:HG23	1:B:235:VAL:O	2.01	0.61
1:B:191:ARG:HH11	1:B:191:ARG:CG	2.13	0.61
1:G:225:LEU:CA	1:G:229:PHE:CZ	2.79	0.61
1:L:193:ARG:HH11	1:L:193:ARG:CG	2.14	0.61
1:A:223:ARG:HG3	1:A:223:ARG:NH1	2.11	0.61
1:C:217:ILE:HD13	1:C:217:ILE:N	2.15	0.61
1:J:213:ILE:CD1	1:J:213:ILE:H	1.99	0.61
1:K:176:GLU:OE1	1:L:178:ILE:N	2.32	0.61
1:E:168:VAL:CB	1:F:167:ARG:HD3	2.30	0.61
1:K:220:TRP:HA	1:K:220:TRP:HE3	1.66	0.60
1:E:192:PHE:CE2	1:F:192:PHE:HA	2.36	0.60
1:G:232:LYS:HZ2	1:G:235:VAL:HG22	1.64	0.60
1:I:180:LYS:HA	1:I:180:LYS:HE3	1.83	0.60
1:L:211:THR:O	1:L:211:THR:HG22	2.01	0.60
1:B:202:ARG:O	1:B:206:TRP:CD1	2.53	0.60
1:D:221:GLN:HB2	1:E:220:TRP:CZ3	2.37	0.60
1:G:186:ARG:HH22	1:G:190:GLU:HG2	1.67	0.60
1:B:168:VAL:HA	1:B:171:LEU:HG	1.82	0.60
1:E:175:VAL:O	1:E:178:ILE:HB	2.01	0.60
1:J:173:GLU:HB3	1:K:179:GLN:HE22	1.64	0.60
1:J:202:ARG:NH1	1:K:204:LEU:HD12	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:LEU:HD13	1:C:167:ARG:HH12	1.67	0.60
1:F:180:LYS:HA	1:F:180:LYS:HE3	1.83	0.60
1:K:194:GLN:HA	1:K:194:GLN:NE2	2.14	0.60
1:J:173:GLU:HA	1:J:173:GLU:OE2	2.01	0.60
1:A:221:GLN:O	1:A:221:GLN:NE2	2.25	0.60
1:B:184:TYR:CE1	1:J:182:GLN:HB3	2.36	0.60
1:B:208:ILE:HG23	2:B:301:9ED:C4	2.32	0.60
1:G:164:LEU:HD21	1:H:164:LEU:CD2	2.21	0.60
1:J:167:ARG:CZ	1:K:168:VAL:CG1	2.73	0.60
1:J:191:ARG:NE	1:K:193:ARG:HB3	2.10	0.60
1:A:234:LEU:HD23	1:A:234:LEU:N	2.15	0.60
1:B:184:TYR:HE1	1:B:188:ARG:HH12	1.50	0.60
1:D:214:LEU:HD11	1:E:213:ILE:HG23	1.84	0.60
1:E:184:TYR:CZ	1:G:186:ARG:HD3	2.28	0.60
1:G:225:LEU:HD11	1:H:224:HIS:HB2	1.84	0.60
1:H:175:VAL:HG23	1:I:174:GLN:HE21	1.65	0.60
1:D:171:LEU:CD1	1:E:171:LEU:CB	2.78	0.60
1:B:179:GLN:HA	1:B:179:GLN:HE21	1.67	0.60
1:E:180:LYS:NZ	1:G:183:ASN:N	2.49	0.60
1:G:221:GLN:HG2	1:H:220:TRP:NE1	2.15	0.60
1:K:227:SER:HA	1:K:230:GLU:OE2	2.01	0.60
1:G:205:TRP:HE3	1:G:209:LEU:HD11	1.67	0.59
1:J:187:TRP:C	1:J:191:ARG:HH11	2.09	0.59
1:K:186:ARG:HH12	1:L:188:ARG:HD2	1.64	0.59
1:L:171:LEU:O	1:L:174:GLN:OE1	2.20	0.59
1:C:184:TYR:CG	1:F:187:TRP:HZ3	2.11	0.59
1:G:167:ARG:HD2	1:G:167:ARG:C	2.27	0.59
1:J:178:ILE:HG22	1:J:182:GLN:HE21	1.68	0.59
1:J:184:TYR:HB2	1:K:189:GLU:CG	2.31	0.59
1:A:171:LEU:C	1:A:175:VAL:CG2	2.68	0.59
1:C:210:GLN:OE1	1:G:206:TRP:CZ2	2.55	0.59
1:J:206:TRP:CH2	1:K:212:LEU:CA	2.84	0.59
1:A:205:TRP:HA	1:A:208:ILE:HB	1.85	0.59
1:B:232:LYS:CB	1:E:232:LYS:HZ3	2.03	0.59
1:G:206:TRP:HA	1:G:209:LEU:HD12	1.83	0.59
1:A:202:ARG:HB3	1:A:206:TRP:CD1	2.37	0.59
1:A:161:LEU:C	1:A:161:LEU:HD12	2.27	0.59
1:C:187:TRP:C	1:C:189:GLU:H	2.08	0.59
1:E:220:TRP:HE1	1:E:223:ARG:HH21	1.50	0.59
1:G:178:ILE:HD13	1:H:178:ILE:HG12	1.84	0.59
1:A:221:GLN:CD	1:B:220:TRP:HH2	2.10	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:187:TRP:CD1	1:K:193:ARG:CZ	2.86	0.59
1:A:171:LEU:HG	1:C:169:ARG:HH12	1.67	0.59
1:E:168:VAL:HG21	1:F:167:ARG:CD	2.33	0.59
1:J:206:TRP:CZ3	1:K:215:VAL:HG21	2.33	0.59
1:C:185:GLN:HG3	1:C:188:ARG:NH1	2.17	0.59
1:C:188:ARG:HB3	1:F:191:ARG:NE	2.18	0.59
1:H:168:VAL:HG21	1:I:167:ARG:CD	2.32	0.59
1:K:222:MET:N	1:K:222:MET:SD	2.75	0.59
1:J:210:GLN:CG	1:J:214:LEU:HD23	2.26	0.59
1:G:232:LYS:HZ1	1:G:235:VAL:CG2	2.11	0.58
1:H:185:GLN:HA	1:H:188:ARG:HD3	1.85	0.58
1:H:225:LEU:HB2	1:I:225:LEU:HD11	1.83	0.58
1:L:169:ARG:HH11	1:L:169:ARG:CG	2.14	0.58
2:B:301:9ED:C57	1:D:213:ILE:HG22	2.33	0.58
1:G:221:GLN:NE2	1:H:221:GLN:NE2	2.47	0.58
1:B:216:ALA:O	2:B:301:9ED:C40	2.51	0.58
1:C:199:THR:C	1:C:201:GLN:H	2.11	0.58
1:C:229:PHE:CZ	1:G:231:ALA:HB1	2.39	0.58
1:G:188:ARG:NH2	1:H:188:ARG:HD2	2.19	0.58
1:J:170:GLN:CG	1:K:175:VAL:CG2	2.80	0.58
1:J:222:MET:HA	1:J:225:LEU:HD22	1.85	0.58
1:K:227:SER:HA	1:K:230:GLU:CD	2.28	0.58
1:A:177:GLN:HA	1:A:177:GLN:HE21	1.69	0.58
1:C:221:GLN:NE2	1:I:222:MET:HB2	2.17	0.58
1:G:186:ARG:HH22	1:G:190:GLU:CG	2.17	0.58
1:G:192:PHE:HZ	1:I:192:PHE:HD1	1.40	0.58
1:J:188:ARG:HD3	1:K:189:GLU:OE1	2.03	0.58
1:H:234:LEU:HD13	1:H:234:LEU:N	2.17	0.58
1:J:173:GLU:CB	1:K:179:GLN:NE2	2.61	0.58
1:J:210:GLN:C	1:J:213:ILE:HD13	2.12	0.58
1:A:203:VAL:O	1:A:207:SER:CA	2.52	0.58
1:A:204:LEU:O	1:A:207:SER:OG	2.20	0.58
1:A:234:LEU:CD1	1:J:227:SER:HB2	2.32	0.58
1:G:168:VAL:HG23	1:G:169:ARG:N	2.17	0.58
1:G:225:LEU:C	1:G:229:PHE:CE2	2.81	0.58
1:A:178:ILE:HG21	1:C:175:VAL:HG11	1.85	0.58
1:F:187:TRP:O	1:F:190:GLU:HG3	2.03	0.58
1:G:192:PHE:CE2	1:I:192:PHE:CE1	2.92	0.58
1:H:225:LEU:HD12	1:I:225:LEU:HD13	1.86	0.58
1:J:163:GLU:HA	1:L:171:LEU:CD1	2.32	0.58
1:K:176:GLU:CG	1:L:178:ILE:HD11	2.20	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:HD3	1:F:233:LYS:HB2	1.85	0.58
1:C:229:PHE:CD1	1:G:232:LYS:HD3	2.39	0.58
1:H:168:VAL:HG22	1:H:171:LEU:HD21	1.84	0.58
1:G:204:LEU:HD23	1:G:204:LEU:N	2.18	0.58
1:H:178:ILE:HD13	1:H:181:GLU:HG3	1.85	0.58
1:F:168:VAL:HG12	1:F:169:ARG:HH11	1.69	0.57
1:H:210:GLN:NE2	1:I:214:LEU:CD2	2.67	0.57
1:H:233:LYS:HD3	1:H:233:LYS:C	2.25	0.57
1:J:188:ARG:HG3	1:J:188:ARG:HH11	1.67	0.57
1:C:193:ARG:HH21	1:C:193:ARG:CG	2.14	0.57
1:C:212:LEU:HD13	1:C:212:LEU:N	2.18	0.57
1:D:190:GLU:CA	1:H:187:TRP:CZ2	2.86	0.57
1:G:211:THR:HG21	1:H:209:LEU:HD11	1.85	0.57
1:H:179:GLN:OE1	1:H:179:GLN:HA	2.05	0.57
1:D:189:GLU:O	1:H:187:TRP:HZ2	1.87	0.57
1:A:223:ARG:HH21	1:J:220:TRP:HB3	1.69	0.57
1:G:167:ARG:NH2	1:G:168:VAL:HG12	2.18	0.57
1:C:225:LEU:O	1:C:225:LEU:HD22	2.05	0.57
1:E:189:GLU:HG2	1:F:188:ARG:NH1	2.19	0.57
1:G:221:GLN:CG	1:H:220:TRP:NE1	2.67	0.57
1:B:188:ARG:NH2	1:J:182:GLN:C	2.61	0.57
1:C:193:ARG:HG3	1:C:193:ARG:NH2	2.12	0.57
1:J:184:TYR:CB	1:K:193:ARG:NH2	2.61	0.57
1:B:222:MET:SD	1:D:220:TRP:HZ2	2.26	0.57
1:G:177:GLN:HE22	1:I:178:ILE:HG22	1.70	0.57
1:G:188:ARG:NH1	1:I:192:PHE:CE2	2.70	0.57
1:J:181:GLU:HB3	1:J:184:TYR:HH	1.60	0.57
1:A:205:TRP:CG	1:J:201:GLN:HB3	2.40	0.57
1:B:216:ALA:CA	2:B:301:9ED:C37	2.82	0.57
1:D:164:LEU:O	1:E:167:ARG:NH2	2.38	0.57
1:G:204:LEU:HD21	1:H:202:ARG:CZ	2.34	0.57
1:G:233:LYS:HA	1:G:233:LYS:NZ	2.20	0.57
1:E:164:LEU:HD13	1:F:164:LEU:HD13	1.87	0.57
1:D:193:ARG:NH2	1:H:190:GLU:OE1	2.38	0.56
1:G:232:LYS:HD3	1:H:228:PHE:CZ	2.40	0.56
1:J:211:THR:N	1:J:214:LEU:HD21	2.20	0.56
1:H:208:ILE:CG2	2:H:301:9ED:C61	2.83	0.56
2:H:301:9ED:C3	1:I:213:ILE:HG23	2.34	0.56
1:D:163:GLU:OE1	1:D:164:LEU:CD1	2.54	0.56
1:G:188:ARG:HH22	1:H:188:ARG:NE	2.03	0.56
1:L:171:LEU:O	1:L:174:GLN:HB3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:VAL:HG13	1:L:179:GLN:HE21	1.71	0.56
1:A:205:TRP:HB2	1:J:202:ARG:HG2	1.86	0.56
1:D:163:GLU:HG2	1:D:164:LEU:HD12	1.87	0.56
1:G:225:LEU:O	1:G:229:PHE:CD2	2.59	0.56
1:H:214:LEU:HD12	1:I:214:LEU:CD2	2.30	0.56
1:I:226:LYS:O	1:I:230:GLU:HG2	2.05	0.56
1:A:224:HIS:ND1	1:B:224:HIS:HE1	2.04	0.56
1:D:165:GLN:HA	1:D:168:VAL:HG12	1.88	0.56
1:L:163:GLU:OE1	1:L:163:GLU:HA	2.05	0.56
1:G:191:ARG:HA	1:G:194:GLN:HE21	1.71	0.56
1:K:216:ALA:HB2	1:L:220:TRP:CZ2	2.35	0.56
1:L:234:LEU:HD22	1:L:234:LEU:C	2.30	0.56
1:G:174:GLN:HG3	1:I:175:VAL:HG22	1.88	0.56
1:G:232:LYS:HZ2	1:G:232:LYS:CA	2.05	0.56
1:I:187:TRP:O	1:I:191:ARG:HG3	2.05	0.56
1:J:210:GLN:CG	1:J:214:LEU:CD2	2.77	0.56
1:H:164:LEU:HD23	1:I:164:LEU:HD11	1.88	0.55
1:H:205:TRP:CE3	2:H:301:9ED:C58	2.89	0.55
1:A:171:LEU:CG	1:C:169:ARG:HH12	2.19	0.55
1:G:193:ARG:HA	1:H:191:ARG:HH22	1.65	0.55
1:G:203:VAL:HG11	1:H:202:ARG:NH2	2.20	0.55
1:B:155:ILE:HD12	1:B:155:ILE:H	1.71	0.55
1:C:210:GLN:HG3	1:I:211:THR:HG21	1.88	0.55
1:K:227:SER:HB3	1:K:230:GLU:OE2	2.06	0.55
1:D:165:GLN:CA	1:D:168:VAL:HG12	2.36	0.55
1:A:171:LEU:HG	1:C:169:ARG:NH1	2.21	0.55
1:C:169:ARG:HH11	1:C:169:ARG:CG	2.13	0.55
1:G:167:ARG:HH22	1:H:167:ARG:HB2	1.72	0.55
1:G:171:LEU:HD12	1:H:171:LEU:CB	2.28	0.55
1:B:212:LEU:HD23	2:B:301:9ED:C50	2.36	0.55
1:G:225:LEU:HD13	1:G:229:PHE:HE1	1.50	0.55
1:H:222:MET:HE2	1:H:226:LYS:HG3	1.88	0.55
1:B:179:GLN:HG3	1:B:180:LYS:HE3	1.88	0.55
1:E:176:GLU:O	1:E:179:GLN:CB	2.55	0.55
1:L:200:ASN:OD1	1:L:200:ASN:N	2.35	0.55
1:F:226:LYS:O	1:F:230:GLU:HG2	2.07	0.55
1:G:220:TRP:CD1	1:G:220:TRP:C	2.84	0.55
1:J:174:GLN:HB2	1:J:177:GLN:CD	2.32	0.55
1:K:185:GLN:HA	1:K:185:GLN:HE21	1.72	0.55
1:K:187:TRP:CD1	1:L:191:ARG:HE	2.25	0.55
1:L:170:GLN:OE1	1:L:170:GLN:HA	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:HG21	1:B:199:THR:HG21	1.88	0.55
1:G:232:LYS:CE	1:G:232:LYS:CA	2.85	0.55
1:H:192:PHE:CD1	1:H:192:PHE:C	2.85	0.55
1:A:171:LEU:HD21	1:C:169:ARG:NH1	2.22	0.54
1:E:168:VAL:CG2	1:F:167:ARG:HD3	2.37	0.54
1:E:184:TYR:CE1	1:G:186:ARG:NE	2.76	0.54
1:G:225:LEU:O	1:G:229:PHE:CD1	2.60	0.54
1:K:187:TRP:HD1	1:L:191:ARG:NE	2.05	0.54
1:D:221:GLN:HB2	1:E:220:TRP:HZ3	1.72	0.54
1:G:178:ILE:HG22	1:I:178:ILE:CG2	2.29	0.54
1:J:211:THR:CA	1:J:214:LEU:HD21	2.37	0.54
1:A:188:ARG:O	1:A:192:PHE:CD2	2.60	0.54
1:B:214:LEU:HD12	1:F:215:VAL:CG2	2.36	0.54
1:C:160:LYS:O	1:C:160:LYS:HE2	2.07	0.54
1:E:187:TRP:CD1	1:E:187:TRP:C	2.85	0.54
1:J:171:LEU:HD13	1:J:171:LEU:N	2.23	0.54
1:L:163:GLU:CD	1:L:167:ARG:NH1	2.66	0.54
1:B:215:VAL:HB	2:B:301:9ED:C62	2.28	0.54
1:H:209:LEU:HD23	1:H:209:LEU:C	2.31	0.54
1:L:179:GLN:OE1	1:L:179:GLN:HA	2.06	0.54
1:B:166:LEU:CD1	1:B:169:ARG:HD2	2.36	0.54
1:A:220:TRP:HZ3	1:J:216:ALA:CA	2.19	0.54
1:B:184:TYR:HH	1:J:183:ASN:H	1.50	0.54
1:G:187:TRP:CD1	1:G:187:TRP:C	2.85	0.54
1:G:210:GLN:CD	1:H:209:LEU:HD22	2.33	0.54
1:G:217:ILE:HA	1:G:220:TRP:CE3	2.42	0.54
1:C:235:VAL:HG21	1:I:233:LYS:CE	2.36	0.54
1:G:180:LYS:O	1:G:184:TYR:HD2	1.91	0.54
1:J:170:GLN:HG2	1:K:175:VAL:HG23	1.90	0.54
1:A:210:GLN:CD	1:F:208:ILE:CD1	2.74	0.54
1:B:188:ARG:HH22	1:J:182:GLN:C	2.15	0.54
1:D:190:GLU:HA	1:H:187:TRP:CE2	2.43	0.54
1:E:168:VAL:HG21	1:F:167:ARG:HD3	1.89	0.54
1:G:174:GLN:NE2	1:H:174:GLN:NE2	2.55	0.54
1:J:191:ARG:HE	1:K:197:GLU:CD	2.15	0.54
1:J:192:PHE:C	1:J:192:PHE:CD1	2.85	0.54
1:B:188:ARG:CD	1:J:186:ARG:HD3	2.34	0.54
1:D:163:GLU:OE1	1:D:164:LEU:HD13	2.07	0.54
1:G:192:PHE:HE1	1:I:192:PHE:HB3	1.72	0.54
1:J:163:GLU:CA	1:L:171:LEU:HD11	2.37	0.54
1:J:186:ARG:CG	1:J:186:ARG:HH21	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:192:PHE:CD1	1:L:192:PHE:C	2.85	0.54
1:J:169:ARG:CB	1:J:169:ARG:CZ	2.86	0.53
1:C:210:GLN:CD	1:G:206:TRP:HH2	2.08	0.53
1:C:229:PHE:HD2	1:G:228:PHE:CE1	1.77	0.53
1:G:221:GLN:HB3	1:H:220:TRP:CE2	2.37	0.53
1:A:222:MET:CA	1:A:222:MET:CE	2.86	0.53
1:A:223:ARG:HH11	1:A:223:ARG:CG	2.13	0.53
1:B:202:ARG:HH22	1:B:206:TRP:HB2	1.72	0.53
1:D:175:VAL:HA	1:D:178:ILE:HG12	1.91	0.53
1:G:221:GLN:HE22	1:H:217:ILE:HG22	1.73	0.53
1:J:163:GLU:CA	1:L:171:LEU:CD1	2.87	0.53
1:A:197:GLU:HG2	1:J:194:GLN:HG2	1.88	0.53
1:C:209:LEU:HG	1:C:213:ILE:HD11	1.91	0.53
1:D:164:LEU:C	1:E:167:ARG:NH2	2.66	0.53
1:E:223:ARG:CD	2:H:301:9ED:O12	2.56	0.53
1:J:167:ARG:CD	1:K:172:VAL:HG22	2.36	0.53
1:B:202:ARG:NH2	1:B:206:TRP:HB2	2.24	0.53
1:D:189:GLU:O	1:H:187:TRP:CZ2	2.61	0.53
1:E:221:GLN:HA	1:E:224:HIS:NE2	2.23	0.53
1:A:202:ARG:HA	1:A:205:TRP:CD1	2.44	0.53
1:C:214:LEU:HD11	1:I:211:THR:HG23	1.91	0.53
1:J:170:GLN:NE2	1:K:176:GLU:HA	2.22	0.53
1:L:221:GLN:OE1	1:L:225:LEU:HG	2.08	0.53
1:E:165:GLN:HA	1:F:167:ARG:HH11	1.60	0.53
1:A:161:LEU:HD12	1:A:161:LEU:O	2.08	0.53
1:H:219:VAL:CG2	2:H:301:9ED:C35	2.86	0.53
1:D:204:LEU:HB3	1:E:202:ARG:NH1	2.24	0.52
1:G:187:TRP:HE1	1:G:191:ARG:CD	2.13	0.52
1:L:185:GLN:HG2	1:L:186:ARG:HE	1.75	0.52
1:A:167:ARG:HH12	1:A:171:LEU:HD23	1.73	0.52
1:D:164:LEU:CD2	1:E:163:GLU:OE1	2.56	0.52
1:G:186:ARG:HA	1:G:186:ARG:NH1	2.19	0.52
1:G:188:ARG:NH1	1:I:192:PHE:CD2	2.77	0.52
1:J:174:GLN:CA	1:J:177:GLN:CG	2.69	0.52
1:A:201:GLN:HE21	1:J:194:GLN:CA	2.22	0.52
1:H:225:LEU:HD23	1:H:226:LYS:HG2	1.91	0.52
1:J:180:LYS:HD2	1:K:186:ARG:NE	2.24	0.52
1:A:204:LEU:HD11	1:L:206:TRP:CG	2.39	0.52
1:B:203:VAL:HB	1:F:204:LEU:HD11	1.91	0.52
1:F:162:SER:OG	1:F:163:GLU:N	2.41	0.52
1:G:178:ILE:HD11	1:H:174:GLN:HG2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:PHE:CE2	1:I:192:PHE:CD1	2.93	0.52
1:G:193:ARG:CA	1:H:191:ARG:HH21	2.19	0.52
1:H:225:LEU:CD1	1:I:225:LEU:CD1	2.84	0.52
1:J:171:LEU:HD12	1:J:174:GLN:HE22	1.75	0.52
1:L:209:LEU:O	1:L:213:ILE:HD13	2.09	0.52
1:A:167:ARG:HH11	1:A:167:ARG:CG	2.15	0.52
1:A:215:VAL:HG21	1:L:214:LEU:HD23	1.92	0.52
1:B:179:GLN:HE21	1:B:179:GLN:CA	2.21	0.52
1:C:212:LEU:N	1:C:212:LEU:CD1	2.73	0.52
1:G:231:ALA:O	1:G:235:VAL:HG13	2.10	0.52
1:G:233:LYS:N	1:G:233:LYS:CD	2.73	0.52
1:H:188:ARG:HH21	1:I:188:ARG:CZ	2.22	0.52
1:J:202:ARG:HD2	1:K:204:LEU:CD1	2.36	0.52
1:J:210:GLN:C	1:J:214:LEU:CG	2.81	0.52
1:A:160:LYS:HE3	1:A:161:LEU:HA	1.91	0.52
1:D:188:ARG:NH1	1:F:192:PHE:CD2	2.76	0.52
1:G:233:LYS:HA	1:G:233:LYS:HE3	1.91	0.52
1:G:233:LYS:CE	1:G:233:LYS:CA	2.86	0.52
1:I:202:ARG:HE	1:I:206:TRP:NE1	2.03	0.52
1:K:203:VAL:C	1:K:205:TRP:N	2.67	0.52
1:E:168:VAL:HG11	1:F:167:ARG:NH1	2.25	0.52
1:G:187:TRP:HZ2	1:G:191:ARG:NH1	2.08	0.52
1:G:204:LEU:CD2	1:G:204:LEU:N	2.73	0.52
1:G:207:SER:HA	1:H:206:TRP:CD1	2.42	0.52
1:J:186:ARG:NH2	1:J:186:ARG:CB	2.73	0.52
1:A:171:LEU:O	1:A:171:LEU:HD12	2.10	0.52
1:A:233:LYS:NZ	1:L:229:PHE:CG	2.78	0.52
1:A:177:GLN:CA	1:A:177:GLN:NE2	2.73	0.52
1:B:165:GLN:HA	1:B:168:VAL:HG13	1.90	0.52
1:B:167:ARG:CB	1:B:167:ARG:NH1	2.73	0.52
1:D:193:ARG:NH2	1:H:190:GLU:CD	2.68	0.52
1:B:179:GLN:CA	1:B:179:GLN:NE2	2.73	0.52
1:D:204:LEU:CD1	1:H:205:TRP:HH2	2.21	0.52
1:E:220:TRP:NE1	1:E:223:ARG:HH21	2.07	0.52
1:A:171:LEU:CD2	1:C:169:ARG:NH1	2.73	0.51
1:A:186:ARG:HH12	1:A:190:GLU:HB2	1.75	0.51
1:H:171:LEU:HD12	1:H:171:LEU:C	2.34	0.51
1:L:171:LEU:HD23	1:L:171:LEU:O	2.10	0.51
1:A:167:ARG:NH1	1:C:169:ARG:HH21	2.07	0.51
1:A:204:LEU:C	1:A:207:SER:OG	2.53	0.51
1:B:158:LYS:CB	1:B:158:LYS:NZ	2.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:9ED:O06	2:B:301:9ED:O13	2.28	0.51
1:C:187:TRP:C	1:C:187:TRP:CE3	2.88	0.51
1:E:180:LYS:HZ2	1:G:182:GLN:HB3	1.73	0.51
1:H:178:ILE:HA	1:H:181:GLU:HG2	1.93	0.51
1:J:174:GLN:O	1:J:177:GLN:HG3	2.05	0.51
1:A:220:TRP:CZ2	1:J:212:LEU:HB3	2.45	0.51
1:B:216:ALA:C	2:B:301:9ED:C35	2.82	0.51
1:H:233:LYS:HA	1:H:233:LYS:HE3	1.90	0.51
1:J:206:TRP:CH2	1:K:212:LEU:CB	2.93	0.51
1:J:220:TRP:CG	1:J:220:TRP:O	2.62	0.51
1:G:174:GLN:HE22	1:I:178:ILE:CD1	2.16	0.51
2:H:301:9ED:O06	2:H:301:9ED:O13	2.28	0.51
1:J:166:LEU:HA	1:J:169:ARG:HH12	1.75	0.51
1:K:169:ARG:HD3	1:L:171:LEU:HB2	1.93	0.51
1:B:164:LEU:C	1:B:164:LEU:HD13	2.36	0.51
1:H:168:VAL:CG2	1:I:167:ARG:CD	2.86	0.51
1:H:199:THR:HA	1:H:202:ARG:CG	2.24	0.51
1:J:176:GLU:HA	1:J:176:GLU:OE2	2.08	0.51
1:A:204:LEU:HA	1:A:207:SER:OG	2.11	0.51
1:A:221:GLN:NE2	1:A:221:GLN:CA	2.73	0.51
1:K:185:GLN:NE2	1:K:185:GLN:CA	2.73	0.51
1:K:212:LEU:HD21	1:L:213:ILE:HG13	1.92	0.51
1:A:171:LEU:CB	1:C:169:ARG:HH22	2.19	0.51
1:A:185:GLN:O	1:A:185:GLN:HG2	2.10	0.51
1:D:188:ARG:NH1	1:F:192:PHE:CE2	2.73	0.51
1:G:188:ARG:HE	1:I:185:GLN:NE2	2.09	0.51
1:J:191:ARG:CZ	1:K:193:ARG:HD2	2.29	0.51
1:B:167:ARG:HH11	1:B:167:ARG:CB	2.23	0.51
1:C:221:GLN:NE2	1:I:222:MET:CB	2.74	0.51
1:G:196:SER:CB	1:H:191:ARG:HH12	2.23	0.51
1:J:206:TRP:CH2	1:K:212:LEU:HD22	2.39	0.51
1:A:188:ARG:HB3	1:A:188:ARG:CZ	2.40	0.51
1:B:193:ARG:HG3	1:F:197:GLU:HG3	1.91	0.51
1:H:212:LEU:HD13	1:H:212:LEU:N	2.25	0.51
1:L:178:ILE:CD1	1:L:178:ILE:N	2.74	0.51
1:B:184:TYR:CZ	1:J:182:GLN:HB3	2.42	0.50
1:D:220:TRP:CE3	1:D:221:GLN:HG2	2.46	0.50
1:G:193:ARG:CA	1:H:191:ARG:NH2	2.61	0.50
1:H:233:LYS:NZ	1:H:233:LYS:CB	2.73	0.50
1:J:166:LEU:CD1	1:L:171:LEU:CD1	2.84	0.50
1:J:180:LYS:O	1:K:186:ARG:HD3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:186:ARG:HA	1:L:186:ARG:NE	2.26	0.50
1:B:204:LEU:HD23	1:B:204:LEU:O	2.11	0.50
1:B:232:LYS:HZ3	1:F:232:LYS:HG2	1.77	0.50
1:D:165:GLN:OE1	1:D:168:VAL:CG1	2.58	0.50
1:K:169:ARG:HD2	1:L:167:ARG:CA	2.41	0.50
1:A:226:LYS:HG3	1:L:229:PHE:CE1	2.46	0.50
1:G:186:ARG:NH1	1:G:186:ARG:CA	2.74	0.50
1:J:192:PHE:C	1:J:192:PHE:HD1	2.20	0.50
1:J:206:TRP:HZ3	1:K:215:VAL:HB	1.77	0.50
1:L:221:GLN:O	1:L:225:LEU:HG	2.11	0.50
1:A:226:LYS:HG3	1:L:229:PHE:CZ	2.47	0.50
1:D:225:LEU:HD13	1:D:226:LYS:HZ2	1.71	0.50
1:H:186:ARG:HA	1:H:186:ARG:HE	1.73	0.50
1:H:202:ARG:NH1	1:H:202:ARG:CB	2.73	0.50
1:H:234:LEU:N	1:H:234:LEU:CD1	2.74	0.50
1:K:190:GLU:HB2	1:K:193:ARG:NH1	2.26	0.50
1:L:187:TRP:HB3	1:L:191:ARG:HH12	1.76	0.50
2:B:301:9ED:C49	1:D:213:ILE:CG2	2.83	0.50
1:G:178:ILE:CD1	1:H:174:GLN:HG2	2.42	0.50
1:A:215:VAL:HG11	1:L:214:LEU:HG	1.94	0.50
1:B:229:PHE:CE2	1:D:232:LYS:CD	2.83	0.50
1:H:169:ARG:HH21	1:I:167:ARG:HH22	1.58	0.50
1:K:167:ARG:CD	1:K:167:ARG:N	2.73	0.50
1:L:193:ARG:CG	1:L:193:ARG:NH1	2.73	0.50
1:G:187:TRP:NE1	1:G:191:ARG:HD2	2.15	0.50
1:G:188:ARG:HH22	1:H:188:ARG:HD2	1.77	0.50
1:J:187:TRP:CE3	1:J:191:ARG:NH2	2.80	0.50
1:K:187:TRP:CH2	1:K:191:ARG:HD2	2.47	0.50
1:A:221:GLN:HE21	1:A:221:GLN:CA	2.25	0.50
1:H:180:LYS:C	1:H:184:TYR:CD2	2.90	0.50
1:J:225:LEU:HD12	1:J:228:PHE:CE2	2.46	0.50
1:A:167:ARG:HG2	1:A:167:ARG:NH1	2.22	0.50
1:B:233:LYS:C	1:B:233:LYS:CD	2.85	0.50
1:J:177:GLN:OE1	1:K:179:GLN:CA	2.55	0.50
1:K:167:ARG:HD2	1:L:167:ARG:HE	1.77	0.50
1:L:166:LEU:HD23	1:L:166:LEU:C	2.36	0.50
1:B:214:LEU:CD1	1:F:214:LEU:HB3	2.41	0.49
1:C:225:LEU:HD22	1:C:225:LEU:C	2.36	0.49
1:C:229:PHE:HZ	1:G:231:ALA:HB1	1.77	0.49
1:G:165:GLN:OE1	1:G:168:VAL:CG2	2.60	0.49
1:J:184:TYR:CG	1:K:189:GLU:CG	2.82	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HG	1:C:169:ARG:CZ	2.42	0.49
1:B:229:PHE:HD1	1:F:229:PHE:HE2	1.60	0.49
1:E:192:PHE:CG	1:F:192:PHE:CD1	3.00	0.49
1:E:201:GLN:HB3	1:E:205:TRP:CZ3	2.46	0.49
1:B:215:VAL:HG13	1:D:217:ILE:HD11	1.94	0.49
1:D:204:LEU:HB3	1:E:202:ARG:HH11	1.76	0.49
1:D:220:TRP:HE3	1:D:221:GLN:HG2	1.77	0.49
1:E:188:ARG:NH1	1:F:185:GLN:HE21	2.11	0.49
1:J:167:ARG:CZ	1:K:168:VAL:HG12	2.38	0.49
1:J:184:TYR:CD1	1:J:185:GLN:N	2.81	0.49
1:B:187:TRP:CD1	1:B:190:GLU:OE1	2.64	0.49
1:C:160:LYS:C	1:C:160:LYS:CD	2.85	0.49
1:C:204:LEU:C	1:C:204:LEU:CD2	2.86	0.49
1:F:201:GLN:HE22	1:F:205:TRP:HE3	1.59	0.49
1:G:164:LEU:HD21	1:H:164:LEU:CB	2.42	0.49
1:H:203:VAL:HG11	1:I:203:VAL:CG1	2.39	0.49
1:L:234:LEU:C	1:L:234:LEU:HD13	2.37	0.49
1:A:205:TRP:CD2	1:J:201:GLN:HB3	2.48	0.49
1:B:165:GLN:CD	1:C:161:LEU:HD22	2.31	0.49
1:J:167:ARG:HH12	1:K:171:LEU:HD23	1.65	0.49
1:C:184:TYR:HE2	1:F:187:TRP:HH2	1.43	0.49
1:E:192:PHE:HZ	1:F:195:THR:HB	1.78	0.49
1:K:187:TRP:CD1	1:L:191:ARG:NE	2.81	0.49
1:L:210:GLN:NE2	1:L:210:GLN:CA	2.73	0.49
1:L:226:LYS:N	1:L:226:LYS:CD	2.75	0.49
1:B:216:ALA:CB	2:B:301:9ED:C40	2.89	0.49
1:K:169:ARG:HG2	1:L:171:LEU:HB2	1.94	0.49
1:L:171:LEU:CD2	1:L:171:LEU:C	2.86	0.49
1:B:219:VAL:HG13	1:D:220:TRP:CZ2	2.48	0.49
1:C:164:LEU:C	1:C:164:LEU:CD1	2.86	0.49
1:J:214:LEU:HD12	1:J:215:VAL:H	1.78	0.49
1:A:177:GLN:HA	1:A:177:GLN:NE2	2.27	0.49
1:A:222:MET:C	1:A:222:MET:SD	2.96	0.49
1:B:191:ARG:CG	1:B:191:ARG:NH1	2.73	0.49
1:C:193:ARG:CG	1:C:193:ARG:NH2	2.73	0.49
1:E:166:LEU:C	1:E:166:LEU:CD1	2.85	0.49
1:G:188:ARG:HH22	1:H:188:ARG:CD	2.26	0.49
1:J:166:LEU:HA	1:J:169:ARG:NH1	2.28	0.49
1:A:167:ARG:CG	1:A:167:ARG:NH1	2.73	0.48
1:B:202:ARG:CZ	1:B:203:VAL:HG22	2.43	0.48
1:E:174:GLN:HE21	1:E:178:ILE:HD11	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:221:GLN:CG	1:H:220:TRP:HE1	2.25	0.48
1:J:166:LEU:HB2	1:L:174:GLN:HE22	1.66	0.48
1:J:206:TRP:CZ3	1:K:215:VAL:CG2	2.94	0.48
1:K:190:GLU:HA	1:K:193:ARG:CZ	2.43	0.48
1:E:225:LEU:HD12	1:F:225:LEU:HD22	1.95	0.48
1:F:168:VAL:HG12	1:F:169:ARG:NH1	2.27	0.48
1:G:196:SER:HB3	1:H:191:ARG:HH12	1.78	0.48
1:J:173:GLU:CB	1:K:179:GLN:HE22	2.25	0.48
1:J:174:GLN:CB	1:J:177:GLN:NE2	2.75	0.48
1:C:224:HIS:HB2	1:I:222:MET:HE2	1.91	0.48
1:J:184:TYR:CA	1:K:193:ARG:HH21	1.97	0.48
1:J:187:TRP:CA	1:J:191:ARG:NH1	2.74	0.48
1:A:221:GLN:NE2	1:A:221:GLN:HA	2.27	0.48
1:D:205:TRP:HE1	1:D:209:LEU:HD11	1.79	0.48
1:A:220:TRP:CE2	2:B:301:9ED:O09	2.64	0.48
1:A:223:ARG:HH12	1:J:217:ILE:HA	1.77	0.48
1:B:171:LEU:HA	1:B:174:GLN:NE2	2.28	0.48
1:C:185:GLN:HB2	1:C:186:ARG:HE	1.77	0.48
1:E:187:TRP:HZ2	1:H:187:TRP:CZ3	2.32	0.48
1:G:186:ARG:HH11	1:G:186:ARG:CA	2.22	0.48
1:G:214:LEU:C	1:G:214:LEU:CD2	2.85	0.48
1:H:180:LYS:C	1:H:184:TYR:HD2	2.22	0.48
1:A:188:ARG:CZ	1:A:188:ARG:CB	2.91	0.48
1:D:217:ILE:O	1:D:221:GLN:HG3	2.13	0.48
1:E:188:ARG:NH1	1:F:185:GLN:NE2	2.62	0.48
1:G:181:GLU:CA	1:G:184:TYR:HD2	2.24	0.48
1:G:192:PHE:CE1	1:I:192:PHE:CG	3.02	0.48
1:H:225:LEU:HB2	1:I:225:LEU:CD1	2.43	0.48
1:J:186:ARG:HH21	1:J:186:ARG:HG2	1.78	0.48
1:L:163:GLU:HG3	1:L:167:ARG:CZ	2.43	0.48
1:B:193:ARG:HD2	1:F:197:GLU:OE2	2.14	0.48
1:C:160:LYS:HE2	1:C:164:LEU:HB2	1.96	0.48
1:D:164:LEU:CA	1:E:167:ARG:NH2	2.77	0.48
1:D:210:GLN:O	1:D:213:ILE:HG13	2.12	0.48
1:E:180:LYS:NZ	1:G:179:GLN:O	2.46	0.48
1:G:178:ILE:HG12	1:H:174:GLN:CG	2.44	0.48
1:J:171:LEU:HA	1:J:174:GLN:NE2	2.28	0.48
1:J:211:THR:O	1:J:215:VAL:CG2	2.46	0.48
1:A:186:ARG:HG2	1:A:186:ARG:HH11	1.79	0.48
1:A:206:TRP:HA	1:A:206:TRP:CE3	2.49	0.48
1:E:163:GLU:CD	1:E:163:GLU:H	2.20	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:LEU:HD13	1:H:171:LEU:HD23	1.96	0.48
1:B:226:LYS:C	1:B:226:LYS:CD	2.84	0.48
1:C:164:LEU:HA	1:C:167:ARG:NH1	2.28	0.48
1:D:204:LEU:HD11	1:H:205:TRP:HH2	1.78	0.48
1:E:180:LYS:NZ	1:G:182:GLN:CB	2.64	0.48
1:B:222:MET:SD	1:B:223:ARG:N	2.87	0.47
1:C:232:LYS:CE	1:I:233:LYS:HD3	2.44	0.47
1:G:204:LEU:HD22	1:H:202:ARG:HH22	1.77	0.47
1:H:188:ARG:HE	1:I:188:ARG:CZ	2.24	0.47
1:L:166:LEU:HG	1:L:170:GLN:HE21	1.79	0.47
1:L:214:LEU:HD12	1:L:214:LEU:HA	1.75	0.47
1:C:229:PHE:CZ	1:G:231:ALA:CB	2.96	0.47
1:C:232:LYS:HE2	1:C:232:LYS:HB3	1.66	0.47
1:E:168:VAL:HG21	1:F:167:ARG:HG2	1.96	0.47
1:G:186:ARG:NH1	1:G:186:ARG:C	2.72	0.47
1:J:166:LEU:HB2	1:L:174:GLN:NE2	2.26	0.47
1:J:183:ASN:O	1:J:187:TRP:CD1	2.67	0.47
1:D:185:GLN:O	1:D:189:GLU:HG2	2.14	0.47
1:G:210:GLN:HG3	1:H:206:TRP:CZ2	2.49	0.47
1:B:155:ILE:HA	1:B:158:LYS:NZ	2.28	0.47
1:C:221:GLN:HE21	1:I:222:MET:CB	2.24	0.47
1:D:213:ILE:HG13	1:D:214:LEU:N	2.28	0.47
1:G:180:LYS:C	1:G:184:TYR:CD2	2.92	0.47
1:G:182:GLN:OE1	1:G:182:GLN:HA	2.14	0.47
1:J:174:GLN:CB	1:J:177:GLN:CD	2.88	0.47
1:L:204:LEU:O	1:L:204:LEU:HD23	2.14	0.47
1:A:161:LEU:HD13	1:C:158:LYS:HD2	1.97	0.47
1:A:226:LYS:CE	1:L:225:LEU:HD22	2.44	0.47
1:I:201:GLN:HE22	1:I:205:TRP:HE3	1.61	0.47
1:K:209:LEU:HA	1:K:212:LEU:HD12	1.95	0.47
1:C:212:LEU:HD13	1:C:212:LEU:H	1.80	0.47
1:F:183:ASN:OD1	1:F:187:TRP:CD2	2.62	0.47
1:G:187:TRP:HZ2	1:G:191:ARG:HH11	1.63	0.47
1:B:228:PHE:CD1	1:B:228:PHE:C	2.90	0.47
1:C:190:GLU:HA	1:C:190:GLU:OE2	2.13	0.47
1:E:180:LYS:NZ	1:G:183:ASN:H	2.12	0.47
1:G:192:PHE:HE2	1:H:191:ARG:NE	2.13	0.47
1:G:212:LEU:HD23	1:G:212:LEU:H	1.76	0.47
1:H:185:GLN:HA	1:H:188:ARG:CD	2.45	0.47
1:J:184:TYR:CB	1:K:189:GLU:CG	2.92	0.47
1:K:174:GLN:NE2	1:K:174:GLN:C	2.73	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:TRP:C	1:C:189:GLU:N	2.71	0.47
1:K:185:GLN:OE1	1:K:189:GLU:HG2	2.15	0.47
1:G:181:GLU:C	1:G:181:GLU:CD	2.83	0.47
1:I:226:LYS:HD2	1:I:226:LYS:C	2.40	0.47
1:J:199:THR:CG2	1:K:204:LEU:CD2	2.90	0.47
1:A:186:ARG:C	1:A:186:ARG:NH1	2.73	0.47
1:B:205:TRP:CZ3	1:B:208:ILE:HB	2.50	0.47
1:E:165:GLN:CA	1:E:168:VAL:HG12	2.44	0.47
1:E:168:VAL:HG13	1:E:169:ARG:N	2.28	0.47
1:G:167:ARG:NH1	1:G:168:VAL:HA	2.30	0.47
1:H:210:GLN:HE21	1:I:214:LEU:CG	2.27	0.47
1:H:221:GLN:HA	1:H:224:HIS:NE2	2.30	0.47
1:H:228:PHE:O	1:H:228:PHE:HD1	1.97	0.47
1:I:162:SER:OG	1:I:163:GLU:N	2.48	0.47
1:K:183:ASN:ND2	1:K:183:ASN:C	2.73	0.47
1:A:158:LYS:HE3	1:A:158:LYS:HB3	1.61	0.46
1:C:184:TYR:CE2	1:F:187:TRP:HZ3	2.17	0.46
1:E:218:GLY:HA2	1:E:221:GLN:NE2	2.30	0.46
1:I:184:TYR:O	1:I:188:ARG:HB2	2.15	0.46
1:J:163:GLU:CB	1:L:171:LEU:CD1	2.65	0.46
1:K:225:LEU:HA	1:K:228:PHE:CD2	2.50	0.46
1:E:163:GLU:CD	1:E:163:GLU:N	2.73	0.46
1:E:232:LYS:HB3	1:F:232:LYS:NZ	2.30	0.46
1:F:209:LEU:O	1:F:213:ILE:HG12	2.15	0.46
1:G:164:LEU:HD21	1:H:164:LEU:HB2	1.96	0.46
1:G:170:GLN:NE2	1:G:170:GLN:C	2.73	0.46
1:G:182:GLN:NE2	1:H:181:GLU:HB3	2.30	0.46
1:L:206:TRP:C	1:L:206:TRP:CE3	2.93	0.46
1:C:167:ARG:HH11	1:C:167:ARG:CG	2.27	0.46
1:C:211:THR:OG1	1:G:206:TRP:HZ3	1.89	0.46
1:D:178:ILE:CD1	1:E:174:GLN:CG	2.92	0.46
1:D:193:ARG:CZ	1:H:190:GLU:CD	2.87	0.46
1:G:169:ARG:O	1:G:169:ARG:HD3	2.15	0.46
1:H:225:LEU:HD12	1:I:225:LEU:CD1	2.45	0.46
1:A:166:LEU:HD13	1:A:169:ARG:HD2	1.97	0.46
1:C:155:ILE:HD13	1:C:155:ILE:N	2.06	0.46
1:D:225:LEU:HD12	1:D:225:LEU:C	2.41	0.46
1:E:198:SER:O	1:E:202:ARG:HB3	2.15	0.46
1:G:202:ARG:HA	1:G:202:ARG:NH1	2.26	0.46
1:H:165:GLN:NE2	1:H:165:GLN:C	2.73	0.46
1:J:169:ARG:NH1	1:J:169:ARG:HB2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLU:CD	1:J:194:GLN:CG	2.76	0.46
1:C:225:LEU:HA	1:C:228:PHE:CD2	2.51	0.46
1:F:169:ARG:HH12	1:F:172:VAL:HG21	1.80	0.46
1:K:169:ARG:HE	1:L:168:VAL:HA	1.80	0.46
1:A:223:ARG:NH1	1:A:223:ARG:CG	2.73	0.46
1:B:166:LEU:HD12	1:B:169:ARG:HD2	1.97	0.46
1:D:226:LYS:HD3	1:D:226:LYS:HA	1.77	0.46
1:G:221:GLN:NE2	1:H:217:ILE:HG22	2.29	0.46
1:I:188:ARG:HA	1:I:191:ARG:HG3	1.98	0.46
1:A:186:ARG:CZ	1:A:186:ARG:HB3	2.46	0.46
1:A:193:ARG:HD3	1:B:189:GLU:CG	2.45	0.46
1:E:186:ARG:N	1:E:186:ARG:HD2	2.30	0.46
1:H:223:ARG:NH1	1:H:223:ARG:C	2.73	0.46
1:I:221:GLN:O	1:I:225:LEU:HD23	2.16	0.46
1:J:180:LYS:O	1:J:184:TYR:HD2	1.98	0.46
1:J:210:GLN:C	1:J:214:LEU:CD2	2.89	0.46
1:J:211:THR:CA	1:J:214:LEU:CG	2.69	0.46
1:J:183:ASN:O	1:J:187:TRP:HD1	1.98	0.46
1:J:210:GLN:C	1:J:214:LEU:HD21	2.40	0.46
1:J:221:GLN:HE22	1:K:226:LYS:HG3	1.81	0.46
1:L:226:LYS:HA	1:L:226:LYS:HD2	1.74	0.46
1:A:197:GLU:HG3	1:J:194:GLN:CG	2.44	0.46
1:B:203:VAL:HB	1:F:204:LEU:CD1	2.46	0.46
1:B:214:LEU:HA	1:B:217:ILE:HD12	1.98	0.46
1:C:225:LEU:HA	1:C:225:LEU:HD23	1.77	0.46
1:F:188:ARG:NH1	1:F:191:ARG:NH1	2.63	0.46
1:G:164:LEU:HD13	1:H:164:LEU:HD21	1.34	0.46
1:F:226:LYS:HD2	1:F:226:LYS:C	2.40	0.45
1:G:223:ARG:NH2	1:G:226:LYS:HB3	2.31	0.45
1:C:222:MET:SD	1:C:222:MET:C	2.99	0.45
1:D:165:GLN:HA	1:D:168:VAL:CG1	2.46	0.45
1:E:188:ARG:HH12	1:F:185:GLN:NE2	2.14	0.45
1:E:198:SER:O	1:E:202:ARG:CB	2.64	0.45
1:F:188:ARG:HE	1:F:188:ARG:HB2	1.59	0.45
1:G:163:GLU:N	1:G:163:GLU:CD	2.73	0.45
1:G:213:ILE:HD12	1:G:213:ILE:HA	1.76	0.45
1:J:167:ARG:HG2	1:K:172:VAL:CG1	2.46	0.45
1:B:234:LEU:HD13	1:B:234:LEU:N	2.31	0.45
1:E:165:GLN:HA	1:E:168:VAL:HG12	1.99	0.45
1:G:177:GLN:HE22	1:I:178:ILE:CG2	2.28	0.45
1:G:180:LYS:C	1:G:184:TYR:HD2	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:GLN:OE1	1:H:209:LEU:HD22	2.16	0.45
1:I:188:ARG:HD2	1:I:191:ARG:HD3	1.99	0.45
1:K:227:SER:CA	1:K:230:GLU:HG2	2.47	0.45
1:D:185:GLN:HG2	1:F:185:GLN:HE21	1.80	0.45
1:E:180:LYS:HZ3	1:G:182:GLN:C	2.24	0.45
1:H:212:LEU:N	1:H:212:LEU:CD1	2.79	0.45
1:J:211:THR:HA	1:J:214:LEU:CG	2.07	0.45
1:A:177:GLN:C	1:A:177:GLN:CD	2.85	0.45
1:A:212:LEU:HD23	1:J:209:LEU:HD23	1.99	0.45
1:B:205:TRP:CE3	1:B:205:TRP:O	2.70	0.45
1:E:187:TRP:HD1	1:E:191:ARG:HG3	1.81	0.45
1:K:173:GLU:OE2	1:L:174:GLN:HB2	2.15	0.45
1:C:187:TRP:HZ3	1:F:188:ARG:NH2	2.14	0.45
1:G:208:ILE:HG23	1:G:212:LEU:CD1	2.43	0.45
1:D:171:LEU:CD1	1:E:171:LEU:HB2	2.47	0.45
1:D:214:LEU:CD1	1:E:213:ILE:HD12	2.46	0.45
1:B:222:MET:HB2	1:D:220:TRP:CH2	2.46	0.45
1:B:224:HIS:HB3	1:F:222:MET:HE1	1.99	0.45
1:G:175:VAL:HG21	1:H:170:GLN:HE22	0.49	0.45
1:G:207:SER:CA	1:H:206:TRP:CD1	3.00	0.45
1:J:167:ARG:HG2	1:K:172:VAL:CB	2.43	0.45
1:C:187:TRP:CE3	1:C:187:TRP:O	2.70	0.45
1:C:226:LYS:HA	1:G:228:PHE:CE1	2.52	0.45
1:H:217:ILE:HG22	1:H:221:GLN:HE22	1.82	0.45
1:J:187:TRP:HB3	1:J:191:ARG:HH12	0.41	0.45
1:K:226:LYS:NZ	1:L:228:PHE:HE1	2.15	0.45
1:A:197:GLU:HG3	1:J:194:GLN:HG2	1.97	0.45
1:A:223:ARG:NH1	1:J:217:ILE:HD13	2.29	0.45
1:A:226:LYS:HZ3	1:L:225:LEU:CD2	2.29	0.45
1:E:189:GLU:C	1:E:189:GLU:CD	2.85	0.45
1:H:178:ILE:HD13	1:H:181:GLU:CG	2.47	0.45
1:J:166:LEU:HD12	1:L:171:LEU:CG	2.47	0.45
1:K:179:GLN:NE2	1:L:181:GLU:CG	2.79	0.45
1:B:228:PHE:CD1	1:B:228:PHE:O	2.70	0.44
1:C:223:ARG:C	1:C:223:ARG:CD	2.90	0.44
1:D:182:GLN:NE2	1:H:180:LYS:HG2	2.32	0.44
1:H:189:GLU:C	1:H:189:GLU:CD	2.85	0.44
1:J:222:MET:SD	1:J:222:MET:N	2.90	0.44
1:K:203:VAL:C	1:K:205:TRP:H	2.24	0.44
1:A:201:GLN:HE21	1:J:194:GLN:HA	1.83	0.44
1:B:191:ARG:HH22	1:J:190:GLU:CD	2.25	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:HA	2:B:301:9ED:C53	2.48	0.44
1:C:194:GLN:HE21	1:C:194:GLN:HB3	1.51	0.44
1:D:167:ARG:HD2	1:F:168:VAL:HG22	2.00	0.44
1:E:180:LYS:HE2	1:G:183:ASN:CA	2.47	0.44
1:E:185:GLN:NE2	1:F:181:GLU:HG3	2.32	0.44
1:J:180:LYS:HD2	1:K:186:ARG:CZ	2.48	0.44
1:K:173:GLU:CG	1:L:177:GLN:CD	2.71	0.44
1:K:185:GLN:OE1	1:K:189:GLU:OE2	2.36	0.44
1:K:190:GLU:C	1:K:190:GLU:CD	2.85	0.44
1:A:202:ARG:HB3	1:A:206:TRP:HD1	1.81	0.44
1:C:184:TYR:HD1	1:C:184:TYR:HA	1.68	0.44
1:C:186:ARG:HA	1:C:186:ARG:HD3	1.76	0.44
1:H:181:GLU:CA	1:H:184:TYR:HD2	2.28	0.44
1:A:224:HIS:ND1	1:B:224:HIS:CE1	2.85	0.44
1:C:179:GLN:OE1	1:C:179:GLN:N	2.51	0.44
1:D:225:LEU:CA	1:E:228:PHE:CZ	2.97	0.44
1:E:164:LEU:HA	1:E:167:ARG:CZ	2.48	0.44
1:K:169:ARG:CG	1:L:171:LEU:HB2	2.47	0.44
1:K:189:GLU:HA	1:K:192:PHE:CD2	2.53	0.44
1:G:170:GLN:C	1:G:170:GLN:CD	2.86	0.44
1:G:192:PHE:CE1	1:I:192:PHE:CB	2.95	0.44
1:H:202:ARG:HA	1:H:202:ARG:HH11	1.82	0.44
1:H:223:ARG:C	1:H:223:ARG:CZ	2.90	0.44
1:B:226:LYS:HA	1:D:228:PHE:CZ	2.53	0.44
1:E:192:PHE:CE2	1:F:192:PHE:CA	2.99	0.44
1:B:202:ARG:C	1:B:202:ARG:CD	2.85	0.44
1:G:208:ILE:HD12	1:G:212:LEU:HD11	1.98	0.44
1:H:165:GLN:HE21	1:H:165:GLN:HA	1.83	0.44
1:L:180:LYS:HA	1:L:183:ASN:ND2	2.32	0.44
1:B:171:LEU:HA	1:B:174:GLN:HE21	1.83	0.44
1:B:181:GLU:C	1:B:185:GLN:HE21	2.23	0.44
1:C:186:ARG:CD	1:C:186:ARG:N	2.81	0.44
1:G:174:GLN:HE22	1:H:174:GLN:CD	2.25	0.44
1:G:180:LYS:HA	1:G:183:ASN:ND2	2.32	0.44
1:G:192:PHE:HD2	1:H:191:ARG:NH2	2.12	0.44
1:G:228:PHE:CD2	1:H:228:PHE:HE2	2.36	0.44
1:J:167:ARG:HG2	1:K:172:VAL:HG13	1.99	0.44
1:J:170:GLN:CD	1:J:170:GLN:C	2.85	0.44
1:B:179:GLN:C	1:B:179:GLN:CD	2.85	0.44
1:B:220:TRP:CA	2:B:301:9ED:O22	2.66	0.44
1:C:170:GLN:C	1:C:170:GLN:CD	2.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:ARG:NH2	1:F:188:ARG:O	2.50	0.44
1:E:166:LEU:CD1	1:E:169:ARG:HD3	2.48	0.44
1:G:207:SER:CA	1:H:206:TRP:NE1	2.63	0.44
1:H:188:ARG:C	1:I:188:ARG:HH22	2.26	0.44
1:I:168:VAL:HG12	1:I:169:ARG:NH1	2.33	0.44
1:K:194:GLN:C	1:K:194:GLN:CD	2.86	0.44
1:A:204:LEU:CA	1:A:207:SER:OG	2.66	0.43
1:B:232:LYS:NZ	1:F:232:LYS:HG2	2.32	0.43
1:B:233:LYS:HE3	1:B:234:LEU:HD12	2.00	0.43
1:E:174:GLN:NE2	1:E:178:ILE:CD1	2.81	0.43
1:G:169:ARG:HH21	1:H:167:ARG:HH12	1.64	0.43
1:G:185:GLN:C	1:G:185:GLN:CD	2.86	0.43
1:H:186:ARG:HH21	1:H:189:GLU:HB2	1.83	0.43
1:K:227:SER:HA	1:K:230:GLU:HG2	2.00	0.43
1:E:186:ARG:HH12	1:E:189:GLU:HB2	1.82	0.43
1:G:222:MET:HE1	1:G:229:PHE:HE2	1.83	0.43
1:J:184:TYR:HA	1:K:193:ARG:CZ	2.21	0.43
1:C:166:LEU:C	1:C:166:LEU:CD2	2.86	0.43
1:D:185:GLN:HG2	1:E:188:ARG:NH1	2.33	0.43
1:E:168:VAL:HG21	1:F:167:ARG:CG	2.48	0.43
1:K:204:LEU:HD22	1:K:204:LEU:HA	1.78	0.43
1:A:161:LEU:HD22	1:C:158:LYS:HD2	1.99	0.43
1:B:162:SER:HA	1:B:165:GLN:CD	2.43	0.43
1:E:168:VAL:HG11	1:F:167:ARG:NE	2.34	0.43
1:J:195:THR:HG21	1:K:200:ASN:CB	2.49	0.43
1:C:194:GLN:OE1	1:E:201:GLN:NE2	2.51	0.43
1:I:209:LEU:O	1:I:213:ILE:HG12	2.18	0.43
1:B:214:LEU:HB2	1:F:215:VAL:CG2	2.42	0.43
1:F:221:GLN:HA	1:F:224:HIS:HB2	2.00	0.43
1:G:168:VAL:CG2	1:G:169:ARG:N	2.81	0.43
1:G:222:MET:O	1:G:222:MET:HE3	2.18	0.43
1:C:194:GLN:CD	1:E:201:GLN:NE2	2.77	0.43
1:C:202:ARG:HD3	1:C:202:ARG:HA	1.60	0.43
1:D:164:LEU:HD11	1:E:164:LEU:HD22	1.95	0.43
1:E:181:GLU:HA	1:E:184:TYR:HD2	1.83	0.43
1:H:171:LEU:CG	1:I:171:LEU:HD12	2.41	0.43
1:H:233:LYS:NZ	1:H:233:LYS:CA	2.73	0.43
1:L:163:GLU:CD	1:L:163:GLU:C	2.86	0.43
1:L:232:LYS:HZ2	1:L:232:LYS:CA	2.17	0.43
1:E:166:LEU:HD21	1:H:166:LEU:HB3	2.01	0.43
1:E:192:PHE:CE2	1:F:192:PHE:N	2.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:233:LYS:HZ2	1:H:233:LYS:CB	2.31	0.43
1:A:233:LYS:HD3	1:L:233:LYS:HE3	2.01	0.43
1:B:172:VAL:CG1	1:C:171:LEU:HD12	2.13	0.43
1:B:233:LYS:O	1:B:233:LYS:HD2	2.19	0.43
1:C:188:ARG:HD2	1:F:191:ARG:CG	2.49	0.43
1:D:178:ILE:HD13	1:E:174:GLN:CG	2.49	0.43
1:G:190:GLU:HA	1:G:193:ARG:NE	2.33	0.43
1:G:206:TRP:NE1	1:H:206:TRP:CH2	2.85	0.43
1:K:185:GLN:C	1:K:185:GLN:CD	2.86	0.43
1:A:193:ARG:HD3	1:B:189:GLU:CB	2.47	0.43
1:B:172:VAL:C	1:B:175:VAL:HG22	2.44	0.43
1:E:187:TRP:HB2	1:G:193:ARG:HH22	1.84	0.43
1:J:188:ARG:NE	1:K:189:GLU:OE1	2.51	0.43
1:K:212:LEU:HD11	1:L:213:ILE:HB	2.00	0.43
1:A:197:GLU:OE2	1:J:190:GLU:O	2.36	0.42
1:B:204:LEU:C	1:B:204:LEU:CD2	2.85	0.42
1:C:187:TRP:C	1:C:187:TRP:HE3	2.27	0.42
1:C:221:GLN:CD	1:C:221:GLN:C	2.85	0.42
1:D:189:GLU:OE2	1:E:188:ARG:CG	2.56	0.42
1:K:226:LYS:NZ	1:L:228:PHE:CE1	2.81	0.42
1:E:181:GLU:HA	1:E:184:TYR:CD2	2.54	0.42
1:L:170:GLN:N	1:L:170:GLN:CD	2.76	0.42
1:L:223:ARG:C	1:L:223:ARG:HD2	2.41	0.42
1:A:180:LYS:HZ2	1:A:180:LYS:CB	2.25	0.42
1:F:163:GLU:OE1	1:F:167:ARG:NE	2.53	0.42
1:H:189:GLU:HB2	1:I:188:ARG:HH12	1.81	0.42
1:J:186:ARG:CG	1:J:186:ARG:NH2	2.79	0.42
1:K:167:ARG:HD3	1:K:168:VAL:HG23	2.01	0.42
1:L:186:ARG:HH22	1:L:189:GLU:HB2	1.83	0.42
1:B:188:ARG:CD	1:J:186:ARG:HE	2.32	0.42
1:C:222:MET:SD	1:C:223:ARG:N	2.92	0.42
1:F:219:VAL:O	1:F:222:MET:HB3	2.19	0.42
1:J:164:LEU:HD13	1:J:164:LEU:HA	1.81	0.42
1:D:189:GLU:OE1	1:E:191:ARG:HD2	2.20	0.42
1:H:178:ILE:CG1	1:I:178:ILE:HG12	2.39	0.42
1:K:200:ASN:CA	1:K:203:VAL:HG12	2.50	0.42
1:B:191:ARG:C	1:B:191:ARG:CD	2.86	0.42
1:H:210:GLN:C	1:H:210:GLN:CD	2.87	0.42
1:H:214:LEU:C	1:H:214:LEU:CD2	2.85	0.42
1:I:217:ILE:O	1:I:221:GLN:HG2	2.19	0.42
1:J:188:ARG:CD	1:K:189:GLU:OE1	2.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:186:ARG:NE	1:L:186:ARG:CA	2.83	0.42
1:L:233:LYS:N	1:L:233:LYS:CE	2.81	0.42
1:A:220:TRP:HZ2	1:J:212:LEU:CB	2.29	0.42
1:G:233:LYS:HA	1:G:233:LYS:HZ1	1.84	0.42
1:K:216:ALA:CA	1:L:220:TRP:HZ2	2.31	0.42
1:A:205:TRP:O	1:A:205:TRP:CE3	2.72	0.42
1:B:188:ARG:HH21	1:J:183:ASN:CA	2.32	0.42
1:B:202:ARG:NH2	1:B:206:TRP:CB	2.83	0.42
1:D:214:LEU:HD21	1:E:213:ILE:HG23	2.02	0.42
1:G:212:LEU:H	1:G:212:LEU:CD2	2.32	0.42
1:H:169:ARG:HH21	1:I:167:ARG:HH12	1.66	0.42
1:H:199:THR:N	1:H:202:ARG:HG3	2.35	0.42
1:L:179:GLN:N	1:L:179:GLN:CD	2.76	0.42
1:B:229:PHE:CZ	1:D:232:LYS:HD3	2.49	0.42
1:B:232:LYS:HZ3	1:F:232:LYS:C	2.28	0.42
1:C:178:ILE:HA	1:C:181:GLU:CD	2.45	0.42
1:C:229:PHE:CD1	1:G:232:LYS:HE2	2.48	0.42
1:E:184:TYR:CD1	1:E:187:TRP:HE3	2.21	0.42
1:J:170:GLN:CD	1:K:175:VAL:C	2.88	0.42
1:G:196:SER:OG	1:H:191:ARG:CZ	2.68	0.42
1:G:214:LEU:HG	1:H:213:ILE:CB	2.43	0.42
1:H:188:ARG:C	1:I:188:ARG:NH2	2.77	0.42
1:J:205:TRP:CE3	1:J:208:ILE:HB	2.55	0.42
1:B:205:TRP:CE3	1:B:208:ILE:HB	2.54	0.41
1:B:208:ILE:N	1:B:208:ILE:CD1	2.72	0.41
1:D:178:ILE:CD1	1:E:178:ILE:CD1	2.88	0.41
1:G:221:GLN:CB	1:H:220:TRP:CD1	3.03	0.41
1:K:174:GLN:NE2	1:K:174:GLN:CA	2.82	0.41
1:K:177:GLN:OE1	1:K:177:GLN:HA	2.11	0.41
1:B:214:LEU:CD1	1:F:214:LEU:CB	2.99	0.41
1:G:193:ARG:HE	1:G:193:ARG:HB3	1.43	0.41
1:A:171:LEU:CG	1:C:169:ARG:NH1	2.80	0.41
1:A:232:LYS:HA	1:A:235:VAL:HG22	2.01	0.41
1:C:211:THR:HG23	1:G:206:TRP:CH2	2.55	0.41
1:G:168:VAL:CB	1:H:167:ARG:NE	2.77	0.41
1:H:221:GLN:HA	1:H:224:HIS:CD2	2.55	0.41
1:K:200:ASN:HA	1:K:203:VAL:HG12	2.02	0.41
1:K:205:TRP:HE3	1:K:206:TRP:N	2.19	0.41
1:B:232:LYS:HB2	1:E:232:LYS:HZ1	1.70	0.41
2:B:301:9ED:O06	2:B:301:9ED:P02	2.79	0.41
1:D:169:ARG:NE	1:D:169:ARG:HA	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:LYS:HA	1:D:235:VAL:HG22	2.01	0.41
1:G:202:ARG:HA	1:G:202:ARG:HD3	1.37	0.41
1:G:205:TRP:CE3	1:G:209:LEU:HD11	2.52	0.41
1:H:168:VAL:HA	1:H:171:LEU:CG	2.46	0.41
1:H:220:TRP:HD1	1:H:221:GLN:OE1	2.04	0.41
2:H:301:9ED:O06	2:H:301:9ED:P02	2.79	0.41
1:K:176:GLU:HG3	1:L:178:ILE:N	2.36	0.41
1:A:226:LYS:HZ2	1:L:225:LEU:CA	2.24	0.41
1:B:188:ARG:NE	1:J:186:ARG:NE	2.68	0.41
1:E:182:GLN:NE2	1:E:186:ARG:HD3	2.36	0.41
1:E:205:TRP:CE2	1:G:208:ILE:HG13	2.55	0.41
1:H:163:GLU:HA	1:H:166:LEU:CD1	2.45	0.41
1:J:177:GLN:HG3	1:J:178:ILE:N	2.35	0.41
1:L:178:ILE:HD13	1:L:178:ILE:H	1.83	0.41
1:L:223:ARG:C	1:L:223:ARG:CD	2.93	0.41
1:C:155:ILE:CD1	1:C:155:ILE:N	2.74	0.41
1:D:180:LYS:HD2	1:D:180:LYS:C	2.45	0.41
1:E:169:ARG:NH2	1:H:170:GLN:CB	2.50	0.41
1:H:168:VAL:HG21	1:I:167:ARG:HD2	2.02	0.41
1:H:222:MET:HE2	1:H:223:ARG:HA	2.03	0.41
1:J:167:ARG:HH12	1:K:171:LEU:CD2	2.15	0.41
1:G:165:GLN:CA	1:G:168:VAL:HG22	2.51	0.41
1:G:204:LEU:HD23	1:G:204:LEU:H	1.84	0.41
1:H:168:VAL:HG21	1:I:167:ARG:HD3	1.94	0.41
1:H:230:GLU:N	1:H:230:GLU:CD	2.78	0.41
1:J:171:LEU:N	1:J:171:LEU:CD1	2.83	0.41
1:A:222:MET:SD	1:A:222:MET:O	2.79	0.41
1:D:178:ILE:HD12	1:E:178:ILE:HD11	1.96	0.41
1:F:206:TRP:O	1:F:210:GLN:HG2	2.21	0.41
1:H:171:LEU:CD1	1:H:172:VAL:HG12	2.51	0.41
1:H:212:LEU:HD13	1:H:212:LEU:H	1.86	0.41
1:I:169:ARG:HA	1:I:169:ARG:NE	2.36	0.41
1:J:177:GLN:HE21	1:J:178:ILE:HD11	1.86	0.41
1:A:208:ILE:HA	1:A:208:ILE:HD13	1.75	0.41
1:F:171:LEU:O	1:F:175:VAL:HG23	2.21	0.41
1:H:221:GLN:HA	1:H:221:GLN:OE1	2.21	0.41
1:J:205:TRP:CE2	1:J:208:ILE:HD12	2.56	0.41
1:J:221:GLN:HE21	1:K:226:LYS:HB2	1.85	0.41
1:K:172:VAL:HG11	1:L:174:GLN:HE21	1.86	0.41
1:A:216:ALA:O	1:A:220:TRP:CD1	2.74	0.41
1:A:220:TRP:CE3	1:J:216:ALA:CB	2.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ILE:HA	1:B:181:GLU:CD	2.46	0.41
1:C:188:ARG:HB3	1:F:191:ARG:CZ	2.51	0.41
1:C:235:VAL:HG22	1:I:233:LYS:HE2	2.02	0.41
1:E:168:VAL:CA	1:E:171:LEU:HD23	2.46	0.41
1:E:168:VAL:HG23	1:E:171:LEU:HD23	2.03	0.41
1:G:223:ARG:HH21	1:G:226:LYS:HB3	1.85	0.41
1:J:191:ARG:CD	1:K:196:SER:HB3	2.41	0.41
1:J:195:THR:HG21	1:K:200:ASN:HB3	2.02	0.41
1:B:191:ARG:HD2	1:B:191:ARG:O	2.21	0.40
1:B:214:LEU:HA	1:B:217:ILE:CD1	2.50	0.40
1:C:182:GLN:N	1:C:182:GLN:OE1	2.53	0.40
1:J:184:TYR:HB3	1:K:189:GLU:HB2	2.01	0.40
1:L:223:ARG:HD2	1:L:223:ARG:HA	1.62	0.40
1:B:173:GLU:N	1:B:173:GLU:OE2	2.54	0.40
1:H:202:ARG:CZ	1:H:202:ARG:CB	2.85	0.40
1:J:177:GLN:HB2	1:K:182:GLN:HB2	2.03	0.40
1:K:195:THR:O	1:K:199:THR:OG1	2.29	0.40
1:A:221:GLN:NE2	1:A:224:HIS:HB3	2.36	0.40
1:C:167:ARG:NH1	1:C:167:ARG:CG	2.82	0.40
1:H:202:ARG:HB2	1:H:203:VAL:H	1.64	0.40
1:J:190:GLU:HB3	1:J:194:GLN:NE2	2.37	0.40
1:K:227:SER:CA	1:K:230:GLU:OE2	2.68	0.40
1:A:193:ARG:HD3	1:B:189:GLU:CD	2.47	0.40
1:B:165:GLN:CD	1:C:161:LEU:CD2	2.91	0.40
1:C:222:MET:HG2	1:G:224:HIS:CD2	2.56	0.40
1:D:188:ARG:HE	1:F:189:GLU:CG	2.26	0.40
1:E:175:VAL:CB	1:F:174:GLN:OE1	2.68	0.40
1:G:178:ILE:HG12	1:H:174:GLN:NE2	2.29	0.40
1:A:204:LEU:HA	1:A:204:LEU:HD12	1.65	0.40
1:B:216:ALA:CA	2:B:301:9ED:C39	2.91	0.40
1:E:192:PHE:HE2	1:F:192:PHE:N	2.18	0.40
1:E:218:GLY:O	1:E:221:GLN:HG2	2.22	0.40
1:H:178:ILE:HD13	1:H:178:ILE:HA	1.74	0.40
1:J:165:GLN:HA	1:J:165:GLN:HE21	1.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	80/235 (34%)	78 (98%)	1 (1%)	1 (1%)	9	41
1	B	80/235 (34%)	77 (96%)	1 (1%)	2 (2%)	4	25
1	C	80/235 (34%)	70 (88%)	8 (10%)	2 (2%)	4	25
1	D	72/235 (31%)	72 (100%)	0	0	100	100
1	E	72/235 (31%)	71 (99%)	1 (1%)	0	100	100
1	F	72/235 (31%)	72 (100%)	0	0	100	100
1	G	72/235 (31%)	68 (94%)	3 (4%)	1 (1%)	9	39
1	H	72/235 (31%)	69 (96%)	2 (3%)	1 (1%)	9	39
1	I	72/235 (31%)	72 (100%)	0	0	100	100
1	J	67/235 (28%)	67 (100%)	0	0	100	100
1	K	65/235 (28%)	62 (95%)	3 (5%)	0	100	100
1	L	72/235 (31%)	71 (99%)	1 (1%)	0	100	100
All	All	876/2820 (31%)	849 (97%)	20 (2%)	7 (1%)	18	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ILE
1	C	201	GLN
1	B	183	ASN
1	H	202	ARG
1	B	205	TRP
1	C	200	ASN
1	G	210	GLN

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	77/207 (37%)	32 (42%)	45 (58%)	0	0
1	B	77/207 (37%)	38 (49%)	39 (51%)	0	0
1	C	77/207 (37%)	28 (36%)	49 (64%)	0	0
1	D	71/207 (34%)	70 (99%)	1 (1%)	59	72
1	E	71/207 (34%)	52 (73%)	19 (27%)	0	3
1	F	71/207 (34%)	71 (100%)	0	100	100
1	G	71/207 (34%)	36 (51%)	35 (49%)	0	0
1	H	71/207 (34%)	37 (52%)	34 (48%)	0	0
1	I	71/207 (34%)	71 (100%)	0	100	100
1	J	67/207 (32%)	33 (49%)	34 (51%)	0	0
1	K	64/207 (31%)	34 (53%)	30 (47%)	0	0
1	L	71/207 (34%)	31 (44%)	40 (56%)	0	0
All	All	859/2484 (35%)	533 (62%)	326 (38%)	0	1

All (326) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	LYS
1	A	159	ASP
1	A	160	LYS
1	A	161	LEU
1	A	163	GLU
1	A	164	LEU
1	A	166	LEU
1	A	167	ARG
1	A	169	ARG
1	A	170	GLN
1	A	171	LEU
1	A	172	VAL
1	A	173	GLU
1	A	175	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	176	GLU
1	A	177	GLN
1	A	178	ILE
1	A	180	LYS
1	A	181	GLU
1	A	184	TYR
1	A	185	GLN
1	A	188	ARG
1	A	189	GLU
1	A	194	GLN
1	A	195	THR
1	A	196	SER
1	A	199	THR
1	A	204	LEU
1	A	205	TRP
1	A	206	TRP
1	A	208	ILE
1	A	209	LEU
1	A	211	THR
1	A	212	LEU
1	A	213	ILE
1	A	214	LEU
1	A	215	VAL
1	A	221	GLN
1	A	222	MET
1	A	223	ARG
1	A	225	LEU
1	A	229	PHE
1	A	230	GLU
1	A	232	LYS
1	A	234	LEU
1	B	155	ILE
1	B	158	LYS
1	B	160	LYS
1	B	161	LEU
1	B	163	GLU
1	B	164	LEU
1	B	166	LEU
1	B	168	VAL
1	B	170	GLN
1	B	173	GLU
1	B	175	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	176	GLU
1	B	177	GLN
1	B	178	ILE
1	B	179	GLN
1	B	180	LYS
1	B	184	TYR
1	B	185	GLN
1	B	186	ARG
1	B	191	ARG
1	B	192	PHE
1	B	196	SER
1	B	197	GLU
1	B	202	ARG
1	B	204	LEU
1	B	210	GLN
1	B	214	LEU
1	B	215	VAL
1	B	217	ILE
1	B	221	GLN
1	B	222	MET
1	B	224	HIS
1	B	225	LEU
1	B	226	LYS
1	B	230	GLU
1	B	232	LYS
1	B	233	LYS
1	B	234	LEU
1	B	235	VAL
1	C	154	GLU
1	C	155	ILE
1	C	158	LYS
1	C	160	LYS
1	C	162	SER
1	C	163	GLU
1	C	164	LEU
1	C	165	GLN
1	C	166	LEU
1	C	167	ARG
1	C	168	VAL
1	C	169	ARG
1	C	170	GLN
1	C	171	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	173	GLU
1	C	175	VAL
1	C	177	GLN
1	C	178	ILE
1	C	180	LYS
1	C	182	GLN
1	C	184	TYR
1	C	186	ARG
1	C	187	TRP
1	C	190	GLU
1	C	192	PHE
1	C	193	ARG
1	C	194	GLN
1	C	195	THR
1	C	196	SER
1	C	197	GLU
1	C	199	THR
1	C	202	ARG
1	C	204	LEU
1	C	206	TRP
1	C	209	LEU
1	C	211	THR
1	C	212	LEU
1	C	214	LEU
1	C	217	ILE
1	C	220	TRP
1	C	222	MET
1	C	223	ARG
1	C	224	HIS
1	C	225	LEU
1	C	226	LYS
1	C	227	SER
1	C	232	LYS
1	C	233	LYS
1	C	235	VAL
1	D	179	GLN
1	E	163	GLU
1	E	164	LEU
1	E	165	GLN
1	E	166	LEU
1	E	169	ARG
1	E	170	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	171	LEU
1	E	172	VAL
1	E	175	VAL
1	E	177	GLN
1	E	182	GLN
1	E	185	GLN
1	E	187	TRP
1	E	189	GLU
1	E	190	GLU
1	E	194	GLN
1	E	195	THR
1	E	196	SER
1	E	198	SER
1	G	163	GLU
1	G	164	LEU
1	G	166	LEU
1	G	167	ARG
1	G	169	ARG
1	G	170	GLN
1	G	171	LEU
1	G	173	GLU
1	G	178	ILE
1	G	181	GLU
1	G	187	TRP
1	G	189	GLU
1	G	190	GLU
1	G	193	ARG
1	G	196	SER
1	G	197	GLU
1	G	199	THR
1	G	201	GLN
1	G	202	ARG
1	G	204	LEU
1	G	205	TRP
1	G	208	ILE
1	G	211	THR
1	G	212	LEU
1	G	213	ILE
1	G	214	LEU
1	G	220	TRP
1	G	221	GLN
1	G	222	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	223	ARG
1	G	227	SER
1	G	228	PHE
1	G	230	GLU
1	G	232	LYS
1	G	233	LYS
1	H	163	GLU
1	H	164	LEU
1	H	165	GLN
1	H	168	VAL
1	H	169	ARG
1	H	172	VAL
1	H	173	GLU
1	H	175	VAL
1	H	178	ILE
1	H	179	GLN
1	H	180	LYS
1	H	181	GLU
1	H	185	GLN
1	H	188	ARG
1	H	191	ARG
1	H	193	ARG
1	H	202	ARG
1	H	203	VAL
1	H	204	LEU
1	H	205	TRP
1	H	208	ILE
1	H	211	THR
1	H	212	LEU
1	H	213	ILE
1	H	217	ILE
1	H	221	GLN
1	H	222	MET
1	H	223	ARG
1	H	225	LEU
1	H	230	GLU
1	H	232	LYS
1	H	233	LYS
1	H	234	LEU
1	H	235	VAL
1	J	160	LYS
1	J	161	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	163	GLU
1	J	164	LEU
1	J	165	GLN
1	J	169	ARG
1	J	170	GLN
1	J	171	LEU
1	J	172	VAL
1	J	173	GLU
1	J	174	GLN
1	J	175	VAL
1	J	176	GLU
1	J	178	ILE
1	J	179	GLN
1	J	185	GLN
1	J	186	ARG
1	J	188	ARG
1	J	189	GLU
1	J	199	THR
1	J	200	ASN
1	J	203	VAL
1	J	204	LEU
1	J	206	TRP
1	J	208	ILE
1	J	209	LEU
1	J	210	GLN
1	J	211	THR
1	J	213	ILE
1	J	214	LEU
1	J	219	VAL
1	J	222	MET
1	J	225	LEU
1	J	226	LYS
1	K	167	ARG
1	K	168	VAL
1	K	171	LEU
1	K	172	VAL
1	K	173	GLU
1	K	174	GLN
1	K	175	VAL
1	K	176	GLU
1	K	177	GLN
1	K	178	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	181	GLU
1	K	183	ASN
1	K	185	GLN
1	K	190	GLU
1	K	191	ARG
1	K	194	GLN
1	K	201	GLN
1	K	204	LEU
1	K	208	ILE
1	K	214	LEU
1	K	217	ILE
1	K	219	VAL
1	K	220	TRP
1	K	222	MET
1	K	224	HIS
1	K	225	LEU
1	K	226	LYS
1	K	227	SER
1	K	232	LYS
1	K	233	LYS
1	L	162	SER
1	L	163	GLU
1	L	164	LEU
1	L	165	GLN
1	L	169	ARG
1	L	170	GLN
1	L	172	VAL
1	L	174	GLN
1	L	176	GLU
1	L	178	ILE
1	L	179	GLN
1	L	181	GLU
1	L	185	GLN
1	L	186	ARG
1	L	190	GLU
1	L	192	PHE
1	L	193	ARG
1	L	194	GLN
1	L	195	THR
1	L	197	GLU
1	L	200	ASN
1	L	201	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	203	VAL
1	L	206	TRP
1	L	207	SER
1	L	208	ILE
1	L	209	LEU
1	L	210	GLN
1	L	213	ILE
1	L	214	LEU
1	L	217	ILE
1	L	220	TRP
1	L	221	GLN
1	L	223	ARG
1	L	226	LYS
1	L	227	SER
1	L	228	PHE
1	L	232	LYS
1	L	233	LYS
1	L	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	185	GLN
1	A	201	GLN
1	A	221	GLN
1	A	224	HIS
1	B	165	GLN
1	B	170	GLN
1	B	174	GLN
1	B	177	GLN
1	B	179	GLN
1	B	183	ASN
1	B	185	GLN
1	B	210	GLN
1	B	224	HIS
1	C	183	ASN
1	C	194	GLN
1	C	210	GLN
1	D	182	GLN
1	E	165	GLN
1	E	174	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	185	GLN
1	E	201	GLN
1	F	177	GLN
1	F	185	GLN
1	G	170	GLN
1	G	174	GLN
1	G	177	GLN
1	G	185	GLN
1	G	194	GLN
1	G	200	ASN
1	G	210	GLN
1	G	221	GLN
1	H	165	GLN
1	H	170	GLN
1	H	174	GLN
1	H	177	GLN
1	H	185	GLN
1	H	210	GLN
1	I	170	GLN
1	I	174	GLN
1	I	221	GLN
1	J	165	GLN
1	J	174	GLN
1	J	179	GLN
1	J	182	GLN
1	J	194	GLN
1	J	200	ASN
1	J	221	GLN
1	K	174	GLN
1	K	185	GLN
1	K	194	GLN
1	K	201	GLN
1	L	170	GLN
1	L	174	GLN
1	L	179	GLN
1	L	183	ASN
1	L	194	GLN
1	L	210	GLN

5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	9ED	H	301	-	61,61,67	1.62	11 (18%)	73,76,85	2.28	13 (17%)
2	9ED	B	301	-	61,61,67	1.62	10 (16%)	73,76,85	2.28	13 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9ED	H	301	-	-	28/57/81/88	0/1/1/1
2	9ED	B	301	-	-	27/57/81/88	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	9ED	C63-C62	4.27	1.56	1.31
2	H	301	9ED	C63-C62	4.27	1.55	1.31
2	B	301	9ED	C61-C60	4.18	1.55	1.31
2	H	301	9ED	C61-C60	4.17	1.55	1.31
2	B	301	9ED	P02-O05	3.78	1.66	1.59
2	H	301	9ED	P02-O05	3.76	1.66	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	9ED	P01-O04	3.47	1.69	1.59
2	H	301	9ED	P01-O04	3.46	1.69	1.59
2	H	301	9ED	C43-C41	-3.33	1.35	1.51
2	B	301	9ED	C43-C41	-3.30	1.35	1.51
2	B	301	9ED	O19-C32	3.14	1.43	1.34
2	H	301	9ED	O19-C32	3.13	1.43	1.34
2	H	301	9ED	O20-C35	3.13	1.42	1.33
2	B	301	9ED	O20-C35	3.11	1.42	1.33
2	B	301	9ED	C24-C23	2.60	1.59	1.52
2	H	301	9ED	C24-C23	2.58	1.59	1.52
2	B	301	9ED	P01-O10	2.13	1.67	1.59
2	H	301	9ED	P01-O10	2.12	1.67	1.59
2	H	301	9ED	C33-C32	2.04	1.56	1.50
2	B	301	9ED	C33-C32	2.03	1.56	1.50
2	H	301	9ED	C27-C28	2.01	1.57	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	9ED	C47-C52-C56	-7.44	78.11	113.86
2	B	301	9ED	C47-C52-C56	-7.44	78.11	113.86
2	B	301	9ED	O07-C26-C25	-7.10	91.75	109.94
2	H	301	9ED	O07-C26-C25	-7.08	91.78	109.94
2	B	301	9ED	O07-C26-C23	-7.01	91.97	109.94
2	H	301	9ED	O07-C26-C23	-7.01	91.98	109.94
2	H	301	9ED	C28-C27-C24	-6.38	99.63	110.83
2	B	301	9ED	C28-C27-C24	-6.38	99.64	110.83
2	H	301	9ED	C26-C23-C24	-5.65	103.02	110.86
2	B	301	9ED	C26-C23-C24	-5.65	103.02	110.86
2	B	301	9ED	C36-C34-C33	5.29	132.57	113.13
2	H	301	9ED	C36-C34-C33	5.28	132.54	113.13
2	H	301	9ED	O04-C25-C28	4.00	117.20	108.73
2	B	301	9ED	O04-C25-C28	4.00	117.19	108.73
2	B	301	9ED	O08-C27-C28	3.94	119.67	110.38
2	H	301	9ED	O08-C27-C28	3.94	119.67	110.38
2	B	301	9ED	C25-C26-C23	3.77	116.75	109.11
2	H	301	9ED	C25-C26-C23	3.77	116.75	109.11
2	B	301	9ED	O19-C32-C33	3.60	119.27	111.48
2	H	301	9ED	O19-C32-C33	3.59	119.24	111.48
2	B	301	9ED	C43-C41-C38	3.28	130.95	114.37
2	H	301	9ED	C43-C41-C38	3.28	130.95	114.37
2	H	301	9ED	O20-C35-C37	2.69	120.04	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	9ED	O20-C35-C37	2.69	120.03	111.83
2	B	301	9ED	C52-C47-C48	2.31	126.05	114.37
2	H	301	9ED	C52-C47-C48	2.31	126.03	114.37

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	9ED	C29-O10-P01-O04
2	B	301	9ED	C29-O10-P01-O11
2	B	301	9ED	C24-C23-O05-P02
2	B	301	9ED	C26-C23-O05-P02
2	H	301	9ED	C29-O10-P01-O04
2	H	301	9ED	C29-O10-P01-O11
2	H	301	9ED	C24-C23-O05-P02
2	H	301	9ED	C26-C23-O05-P02
2	B	301	9ED	C38-C41-C43-C46
2	B	301	9ED	O21-C32-O19-C30
2	H	301	9ED	C38-C41-C43-C46
2	B	301	9ED	C33-C32-O19-C30
2	H	301	9ED	C33-C32-O19-C30
2	H	301	9ED	O21-C32-O19-C30
2	B	301	9ED	C35-C37-C39-C40
2	H	301	9ED	C35-C37-C39-C40
2	B	301	9ED	C53-C49-C50-C3
2	H	301	9ED	C53-C49-C50-C3
2	B	301	9ED	C49-C53-C57-C63
2	H	301	9ED	C49-C53-C57-C63
2	H	301	9ED	C52-C47-C48-C54
2	B	301	9ED	C52-C47-C48-C54
2	B	301	9ED	C44-C45-C51-C62
2	H	301	9ED	C44-C45-C51-C62
2	B	301	9ED	C51-C62-C63-C57
2	H	301	9ED	C51-C62-C63-C57
2	B	301	9ED	C36-C38-C41-C43
2	H	301	9ED	C36-C38-C41-C43
2	H	301	9ED	C37-C39-C40-C42
2	B	301	9ED	C37-C39-C40-C42
2	H	301	9ED	C50-C3-C4-C5
2	B	301	9ED	C41-C43-C46-C60
2	H	301	9ED	C41-C43-C46-C60
2	B	301	9ED	C47-C48-C54-C58

Continued on next page...

Continued from previous page...

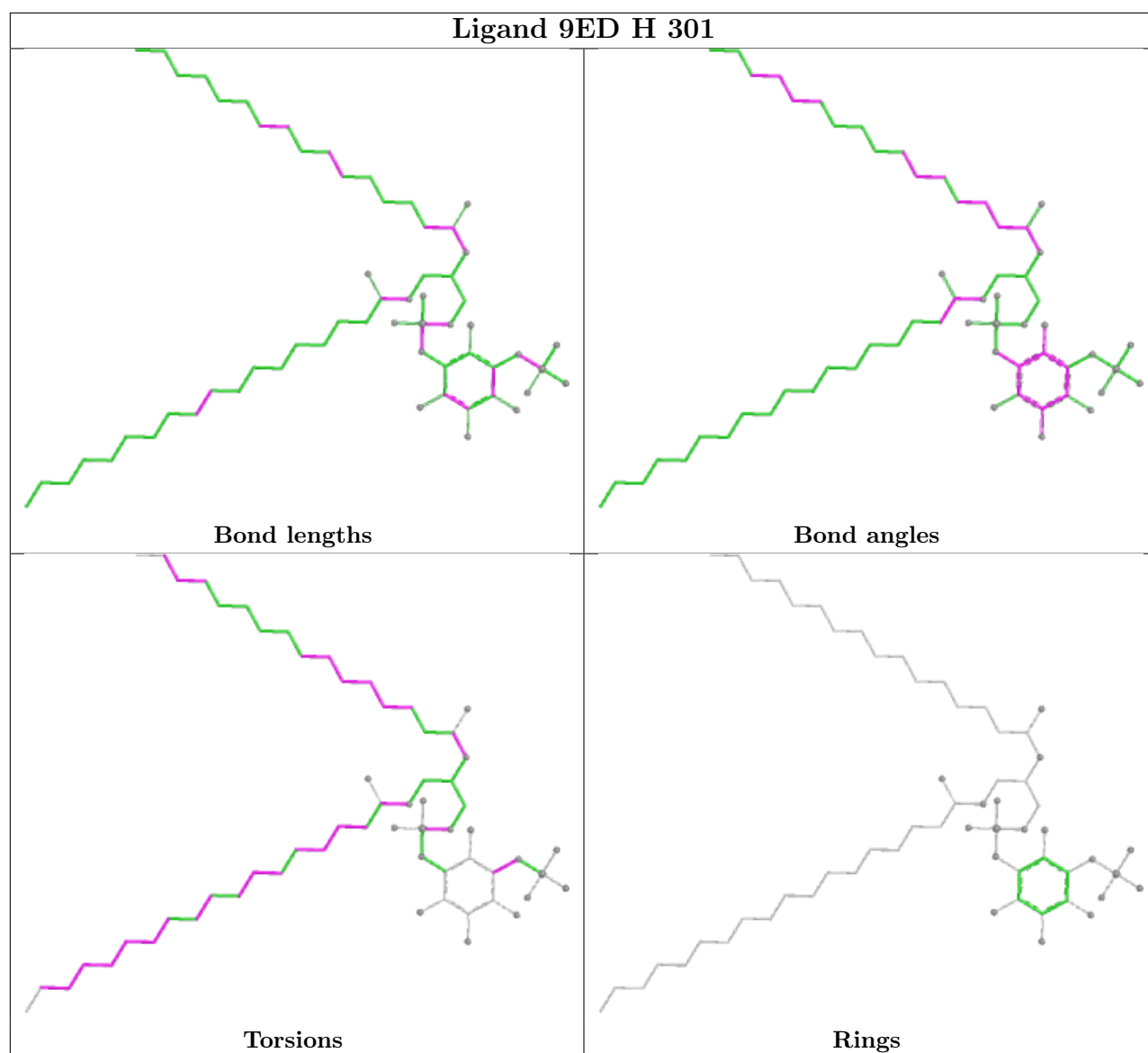
Mol	Chain	Res	Type	Atoms
2	B	301	9ED	C39-C40-C42-C44
2	H	301	9ED	C39-C40-C42-C44
2	H	301	9ED	C4-C3-C50-C49
2	B	301	9ED	C48-C54-C58-C1
2	B	301	9ED	C42-C44-C45-C51
2	H	301	9ED	C42-C44-C45-C51
2	H	301	9ED	C3-C4-C5-C6
2	H	301	9ED	C47-C48-C54-C58
2	B	301	9ED	C29-O10-P01-O16
2	H	301	9ED	C29-O10-P01-O16
2	B	301	9ED	C37-C35-O20-C31
2	H	301	9ED	C37-C35-O20-C31
2	B	301	9ED	O22-C35-O20-C31
2	H	301	9ED	O22-C35-O20-C31
2	B	301	9ED	C4-C3-C50-C49
2	B	301	9ED	C50-C49-C53-C57
2	H	301	9ED	C50-C49-C53-C57
2	H	301	9ED	C34-C36-C38-C41
2	B	301	9ED	C34-C36-C38-C41
2	H	301	9ED	C33-C34-C36-C38
2	B	301	9ED	C33-C34-C36-C38

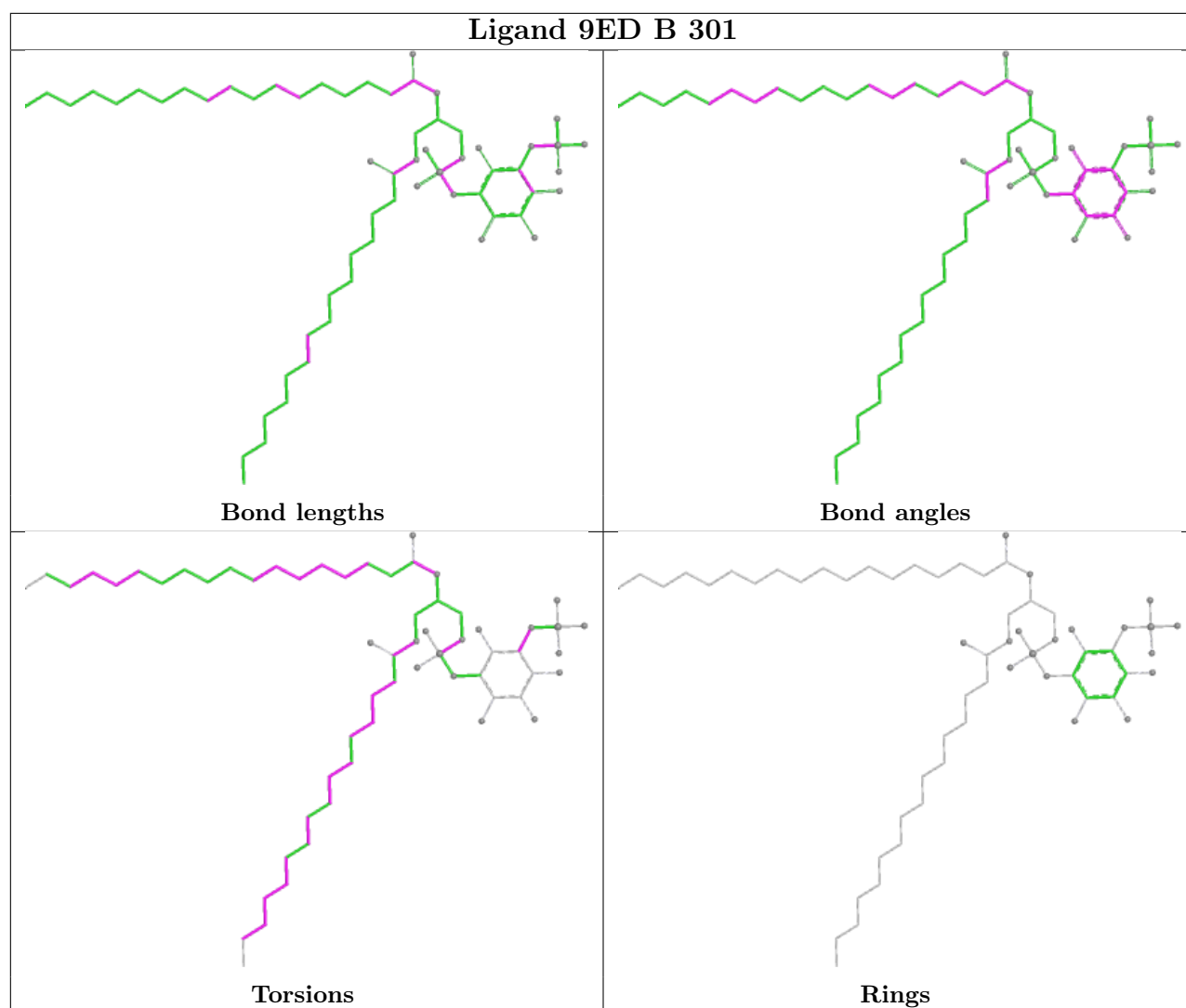
There are no ring outliers.

2 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	9ED	34	0
2	B	301	9ED	58	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

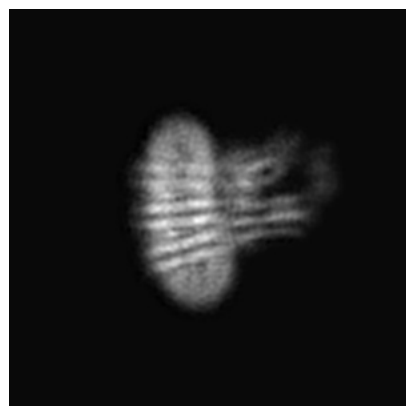
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45635. These allow visual inspection of the internal detail of the map and identification of artifacts.

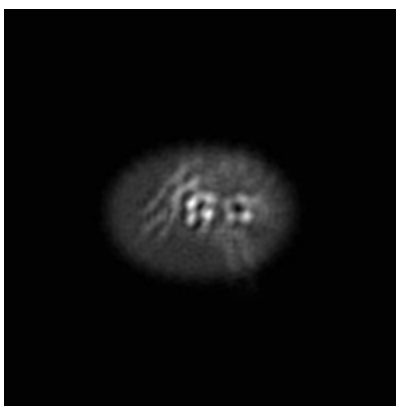
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

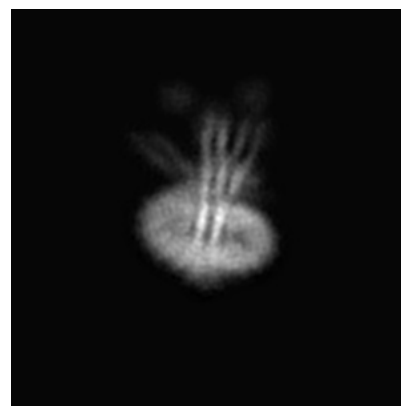
6.1.1 Primary map



X

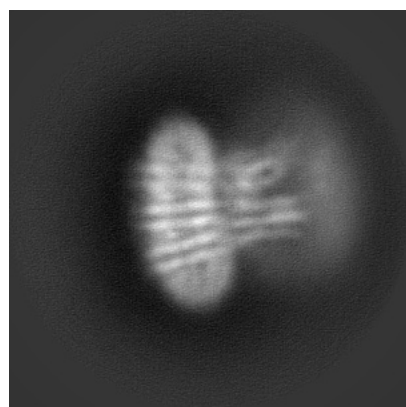


Y

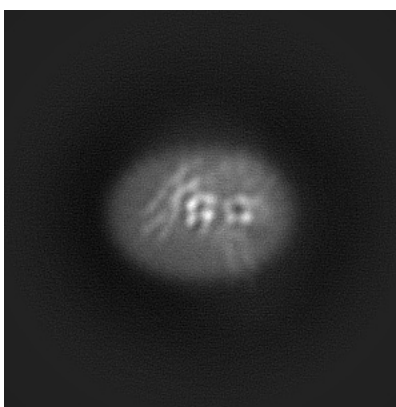


Z

6.1.2 Raw map



X



Y

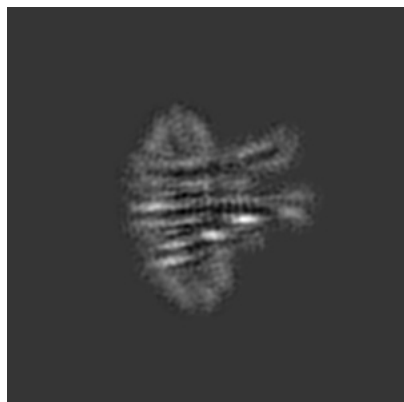


Z

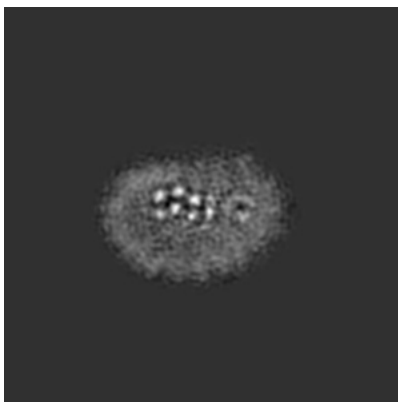
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

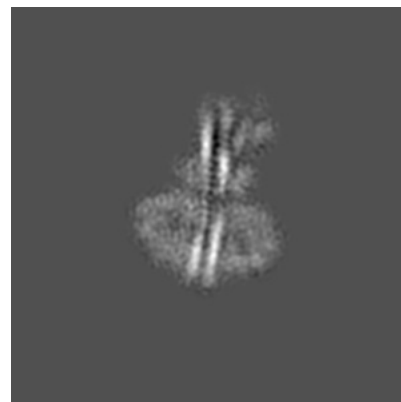
6.2.1 Primary map



X Index: 160

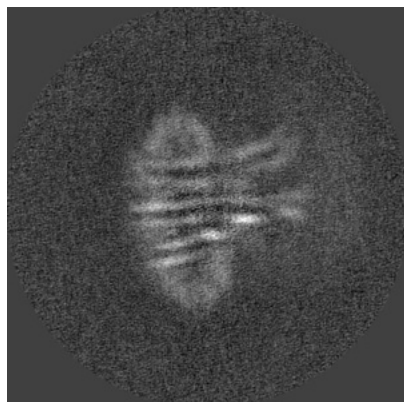


Y Index: 160

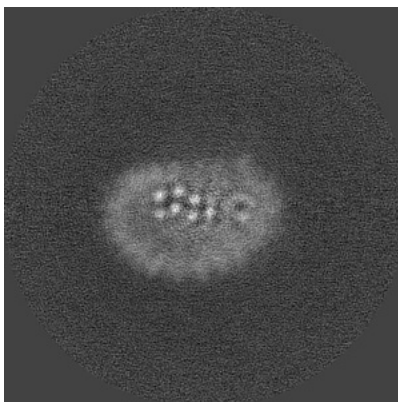


Z Index: 160

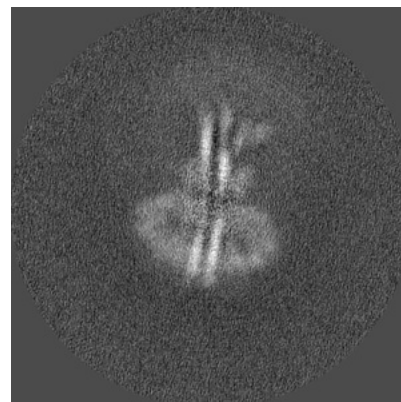
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

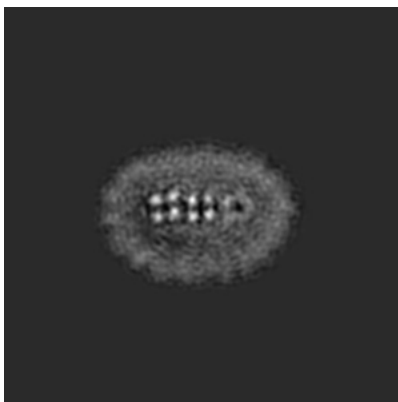
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

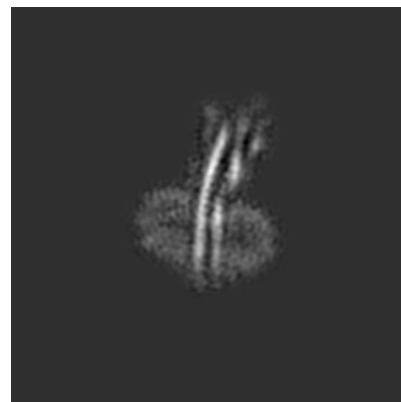
6.3.1 Primary map



X Index: 166

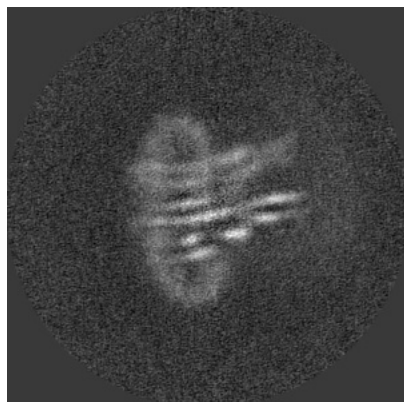


Y Index: 151

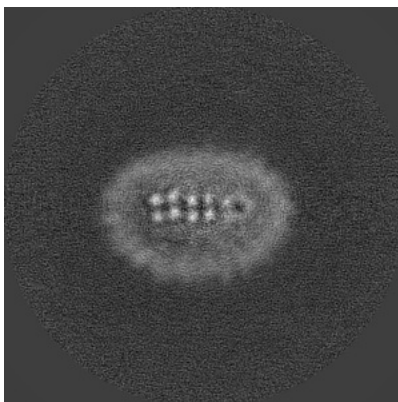


Z Index: 150

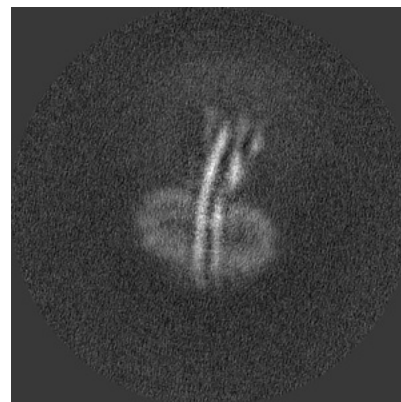
6.3.2 Raw map



X Index: 166



Y Index: 151



Z Index: 150

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

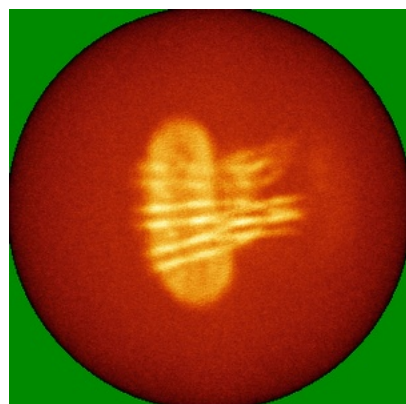


Y

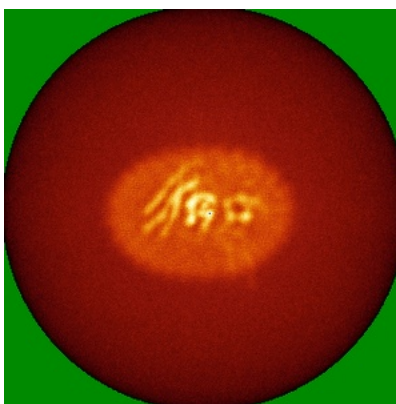


Z

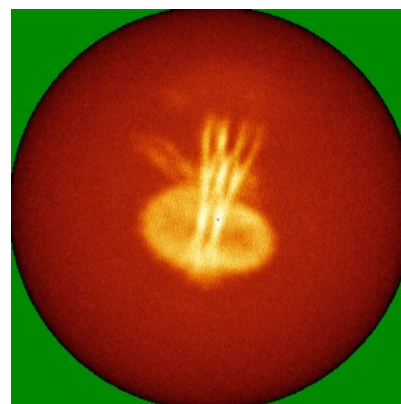
6.4.2 Raw map



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.

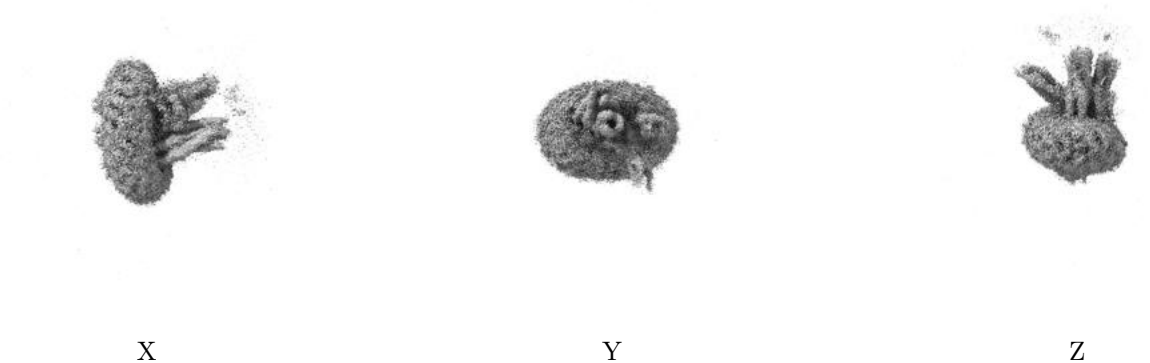
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

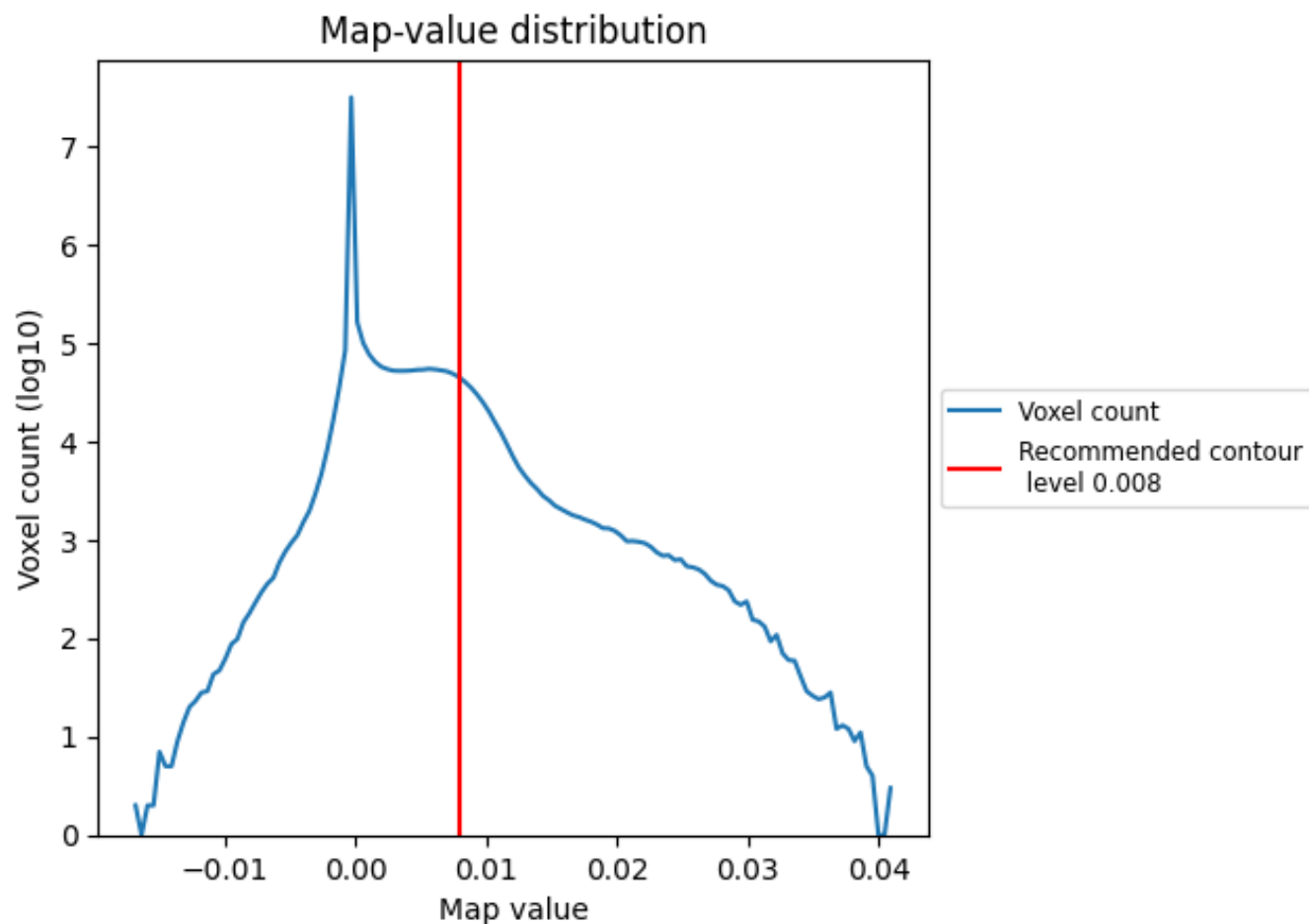
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

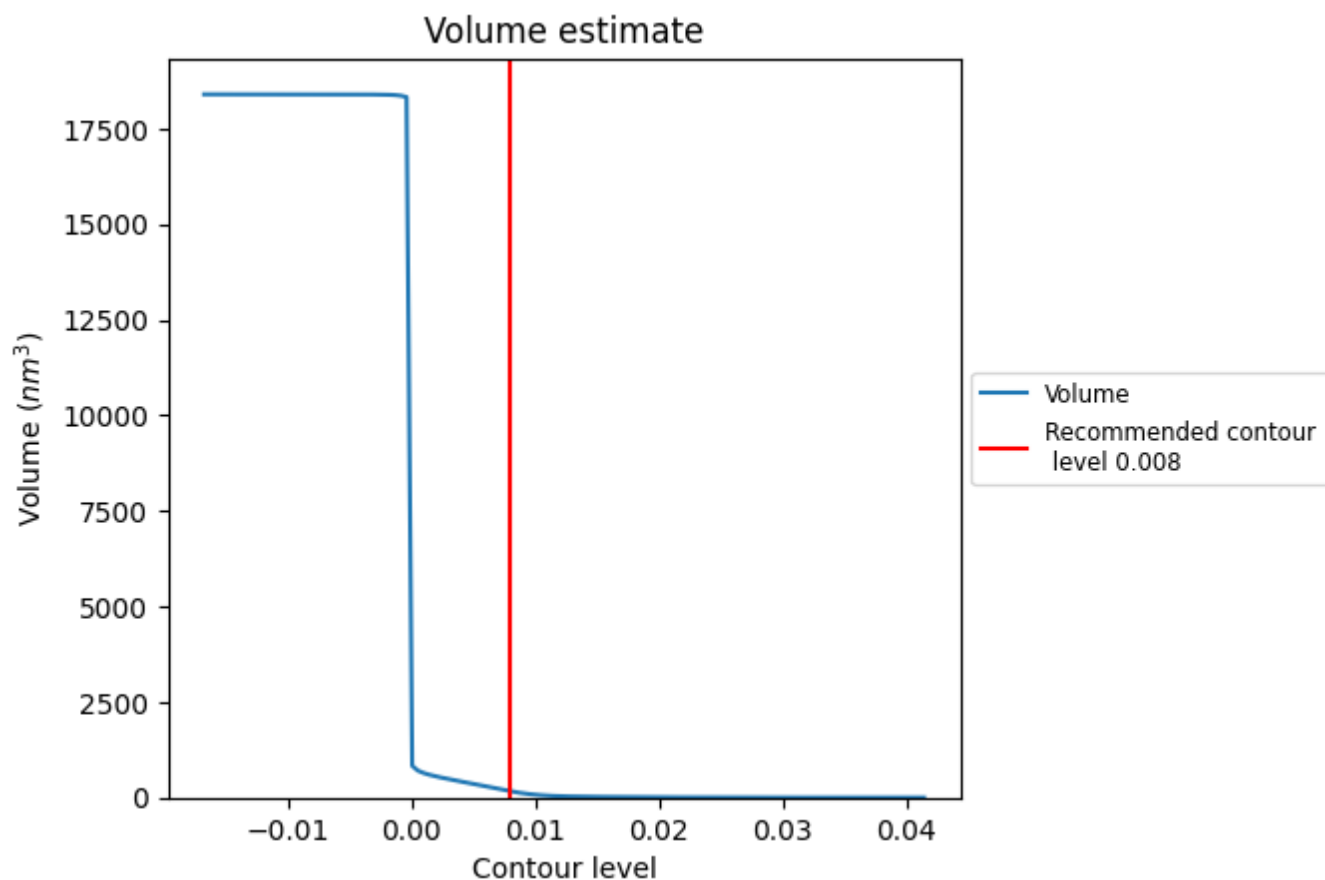
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

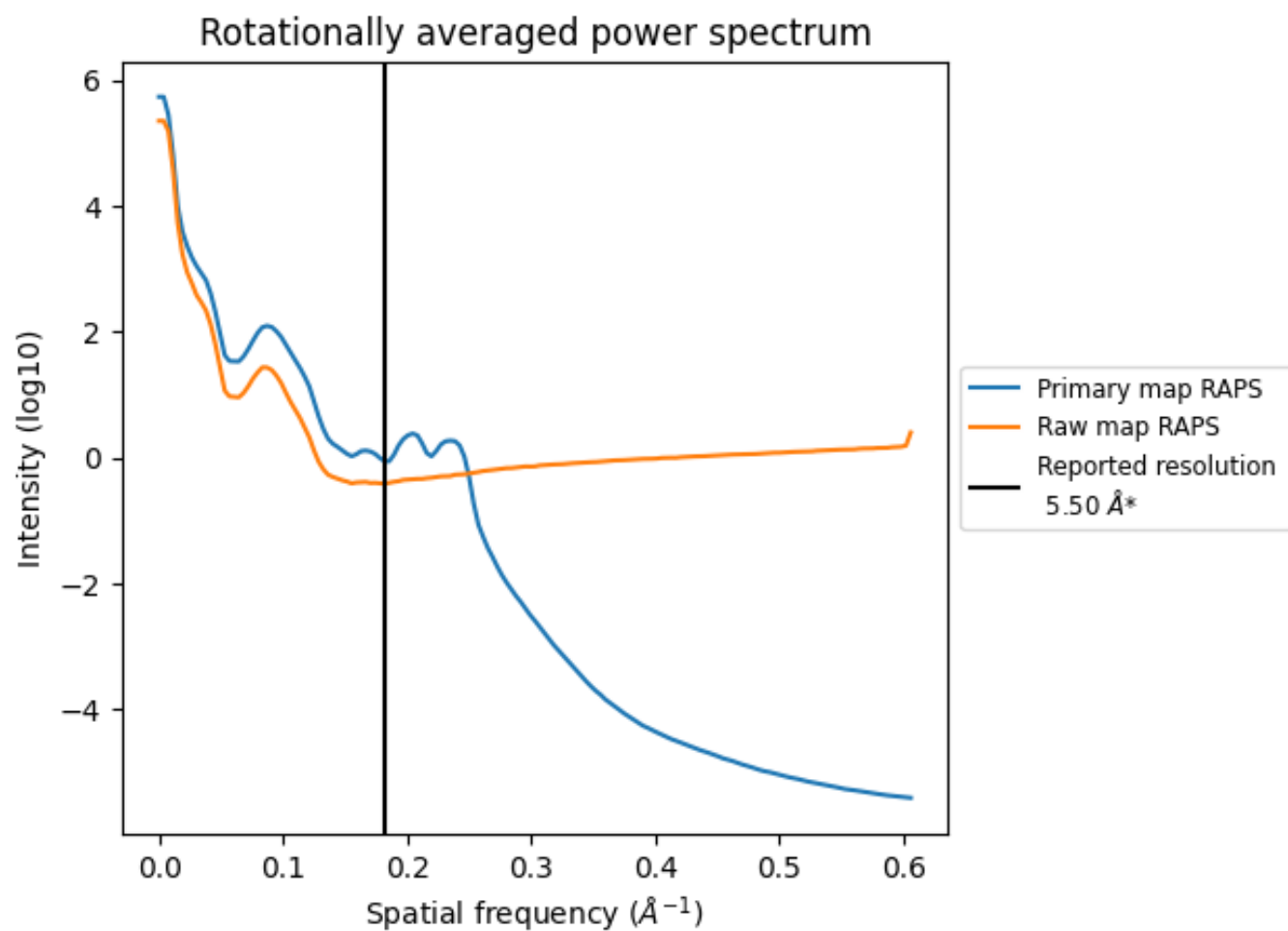
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 162 nm³; this corresponds to an approximate mass of 147 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 ⓘ

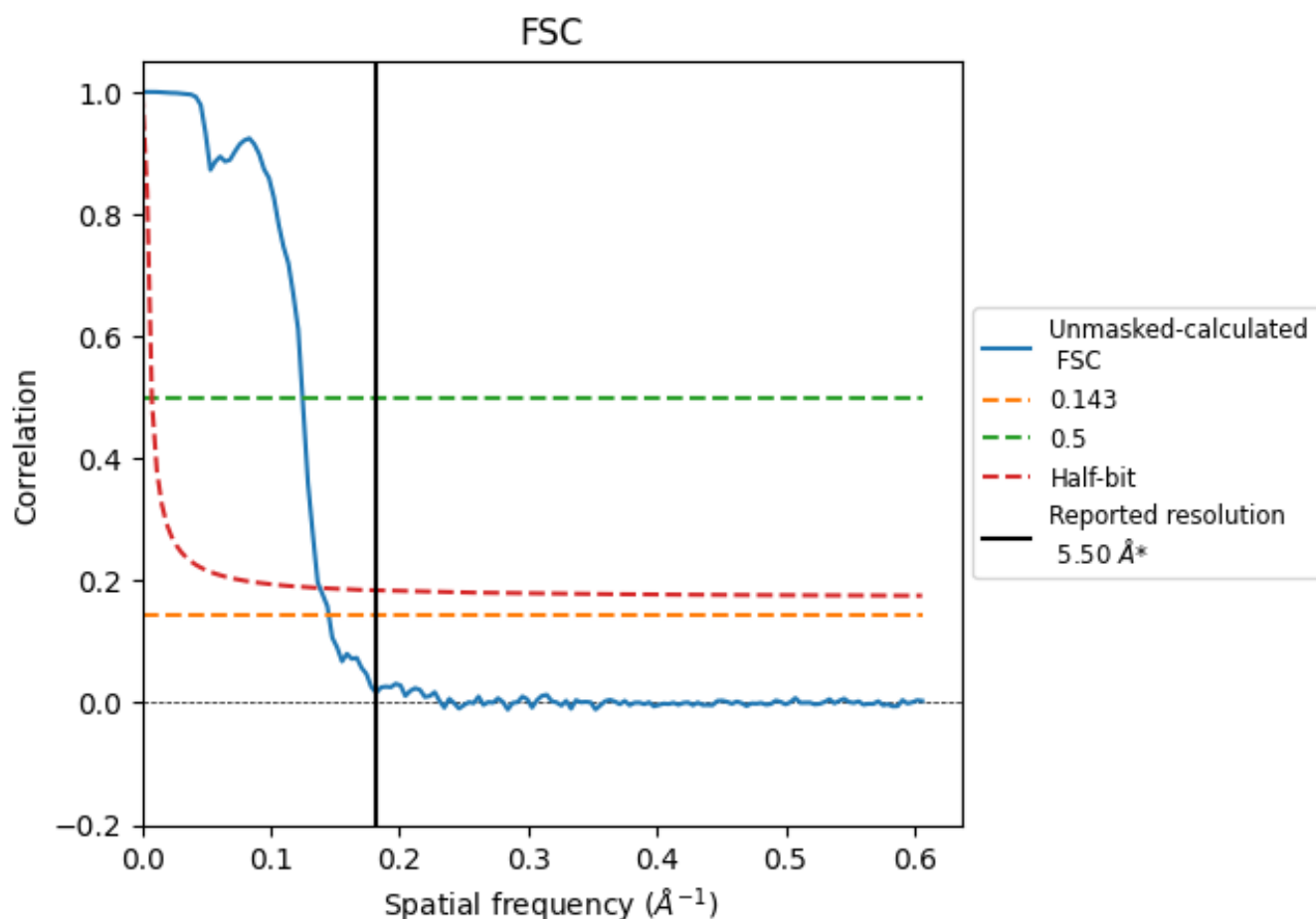


*Reported resolution corresponds to spatial frequency of 0.182 Å⁻¹

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 0.182 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

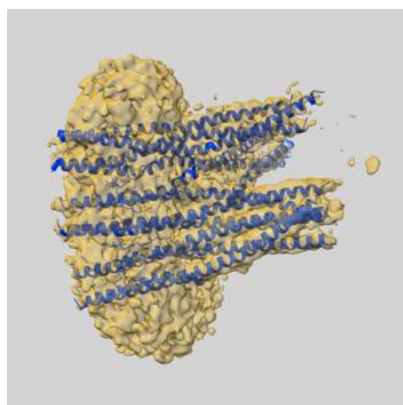
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.90	8.03	7.24

*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 6.90 differs from the reported value 5.5 by more than 10 %

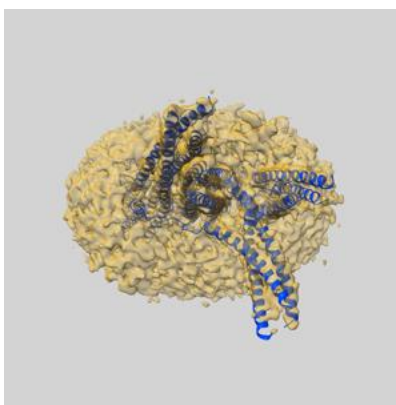
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45635 and PDB model 9CJL. Per-residue inclusion information can be found in section [3](#) on page [6](#).

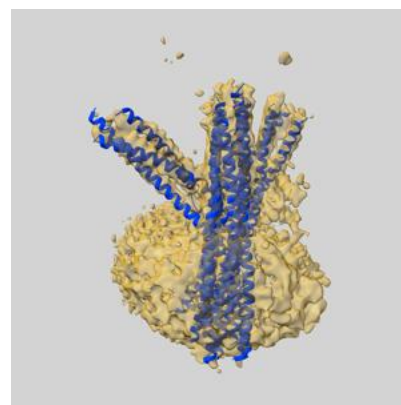
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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](#)



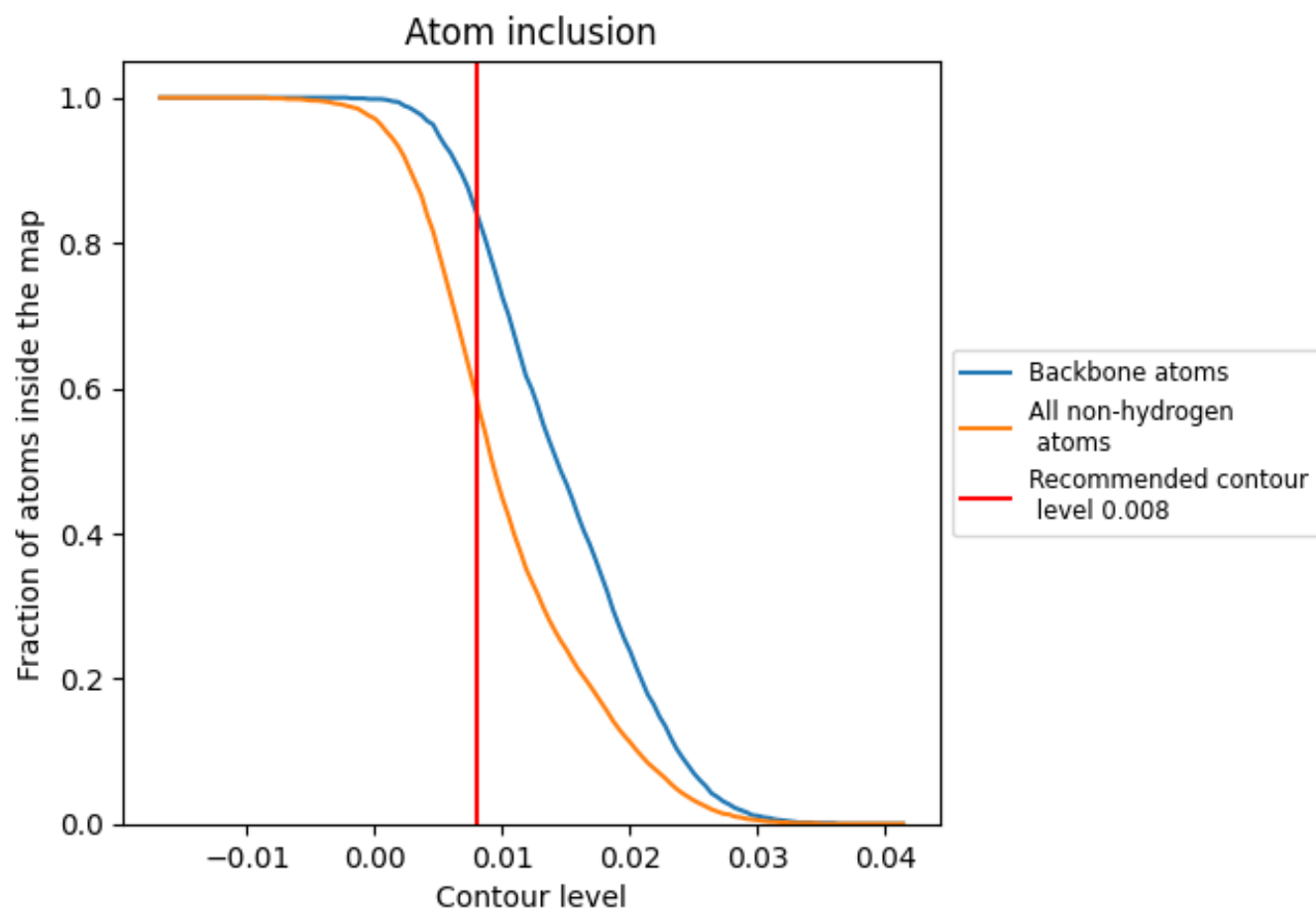
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 59% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5860	0.1280
A	0.4260	0.0950
B	0.5300	0.1240
C	0.5700	0.1890
D	0.6510	0.1300
E	0.6490	0.1240
F	0.6300	0.1020
G	0.6670	0.1740
H	0.6550	0.1450
I	0.5820	0.1160
J	0.6040	0.1260
K	0.5610	0.1170
L	0.5230	0.0910

1.0

0.0

<0.0