



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:48 AM UTC

PDB ID : 5Y81 / pdb_00005y81
EMDB ID : EMD-6816
Title : NuA4 TEEAA sub-complex
Authors : Wang, X.; Cai, G.
Deposited on : 2017-08-18
Resolution : 4.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

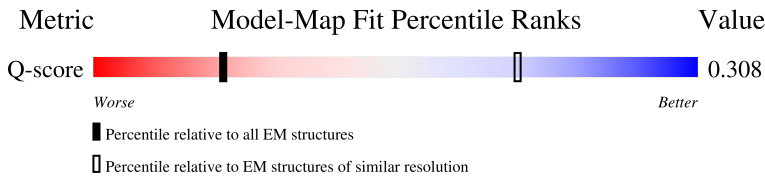
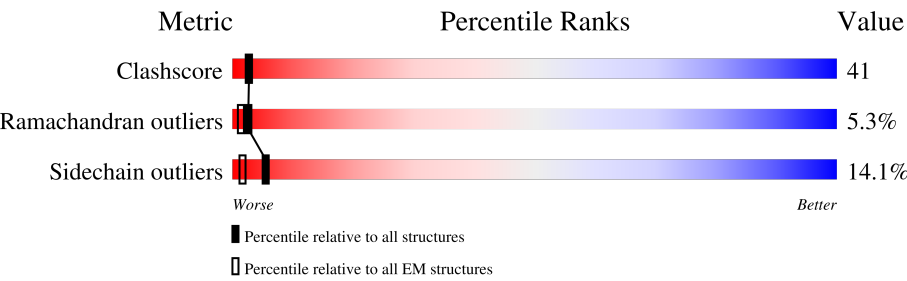
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.70 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	1989 (4.20 - 5.20)

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	B	1115	45%32%10%12%
2	C	336	25%10%6%58%
3	D	500	56%16%28%
4	H	279	40%15%45%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	A	2627	58%16%24%
6	F	490	5%41%42%14%
7	G	375	9%38%53%6%
8	E	41	5%24%73%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 25723 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 Transcription-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	981	Total	C	N	O	S	0	0
			5937	3675	1116	1136	10		

- Molecule 2 is a protein called Chromatin modification-related protein EAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	140	Total	C	N	O	S	0	0
			800	489	156	154	1		

- Molecule 3 is a protein called Eaf1-disorder domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	360	Total	C	N	O	0	0
			1800	1080	360	360		

- Molecule 4 is a protein called Chromatin modification-related protein EAF5.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	154	Total	C	N	O	0	0
			764	456	154	154		

- Molecule 5 is a protein called Transcription-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	A	2007	Total	C	N	O	0	0
			10017	5997	2008	2012		

- Molecule 6 is a protein called Actin-related protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	421	Total	C	N	O	S	1	0
			3334	2121	553	648	12		

There is a discrepancy between the modelled and reference sequences:

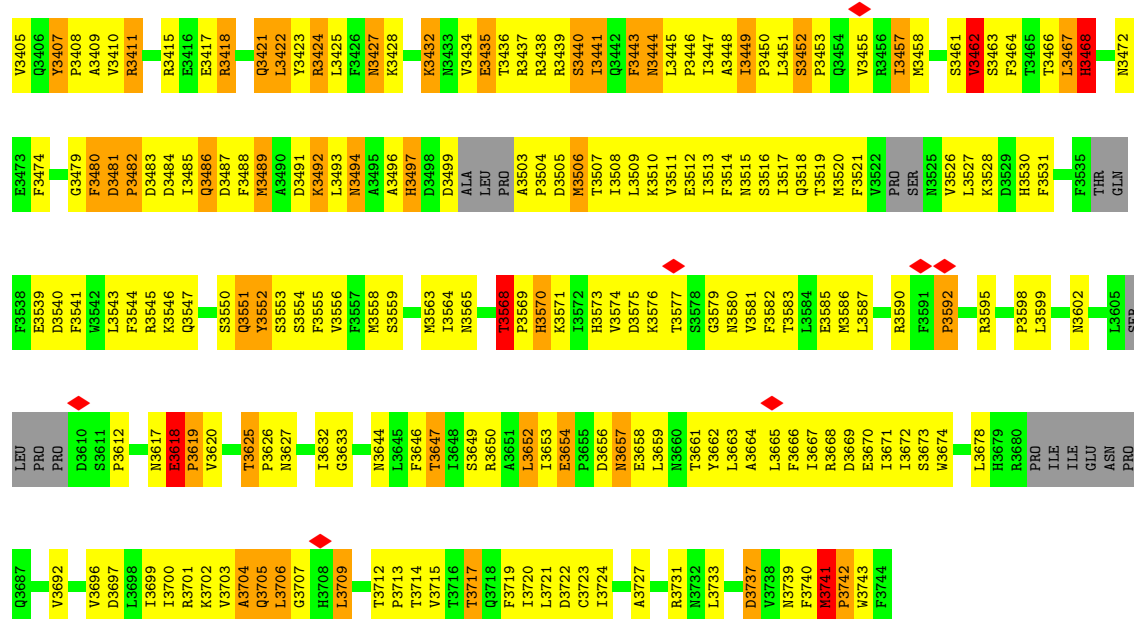
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	PRO	-	expression tag	UNP P80428

- Molecule 7 is a protein called Actin.

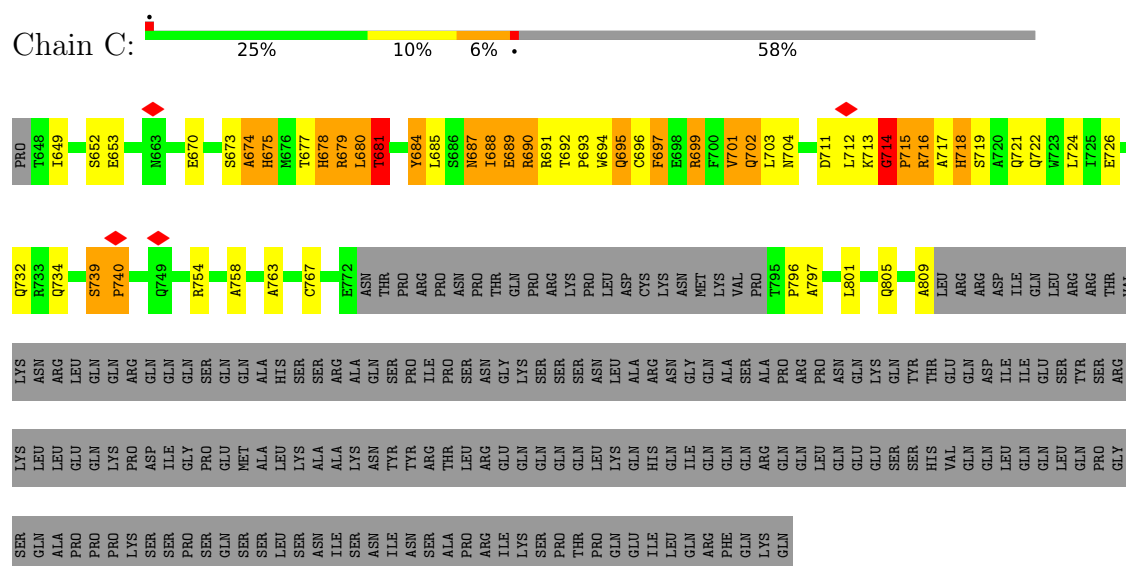
Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	351	Total	C	N	O	S	0	0
			2729	1735	458	519	17		

- Molecule 8 is a protein called Chromatin modification-related protein EAF1.

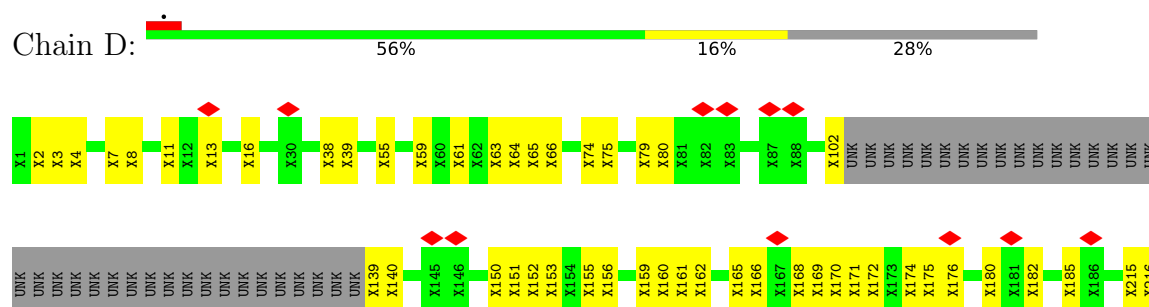
Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	41	Total	C	N	O	S	0	0
			342	222	56	61	3		

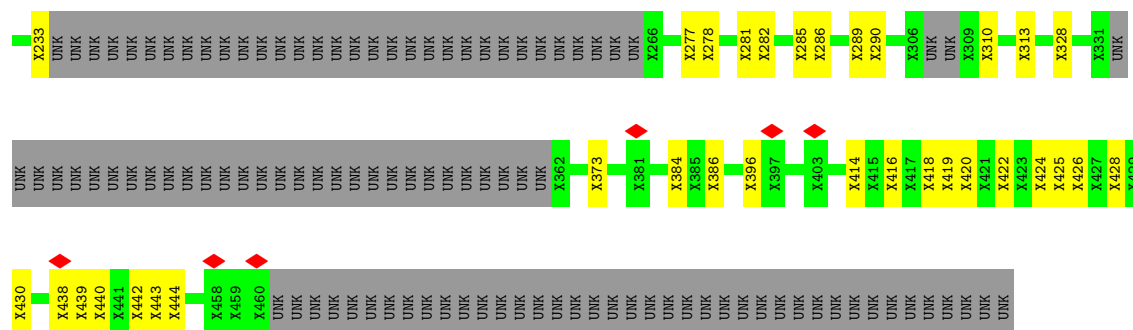


• Molecule 2: Chromatin modification-related protein EAF1

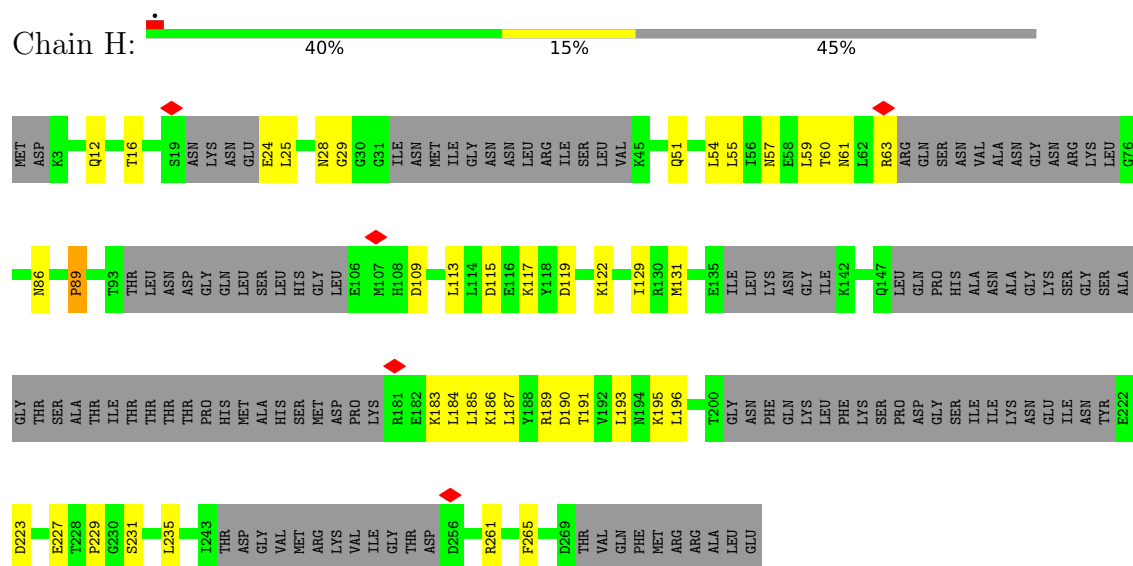


• Molecule 3: Eaf1-disorder domain

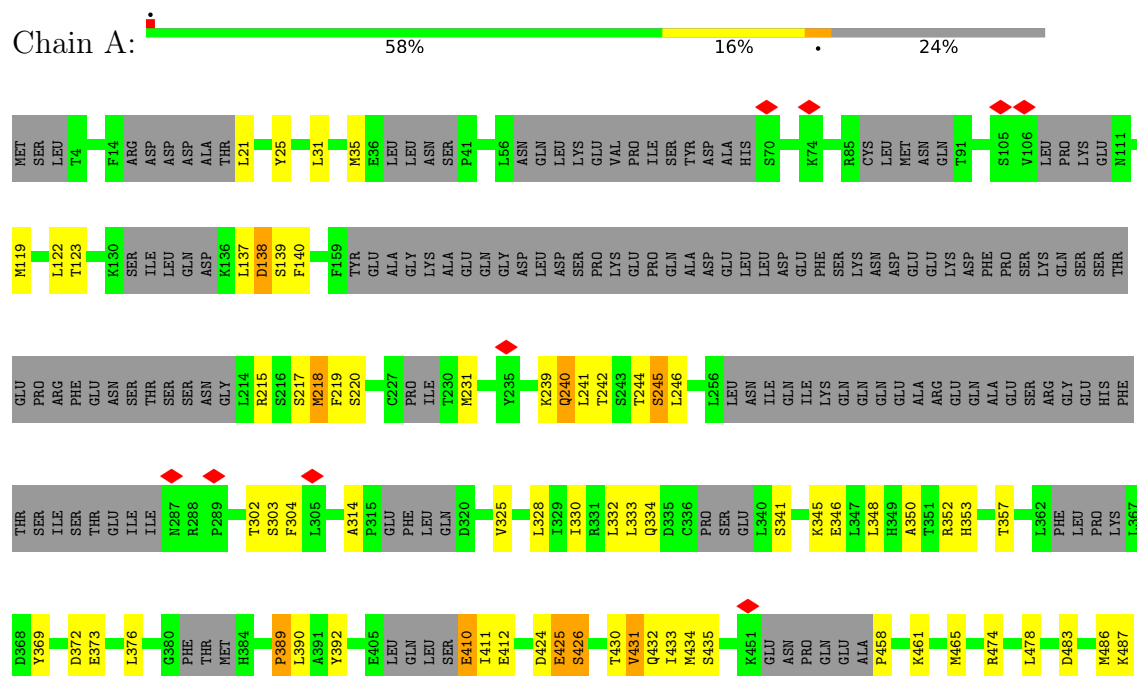




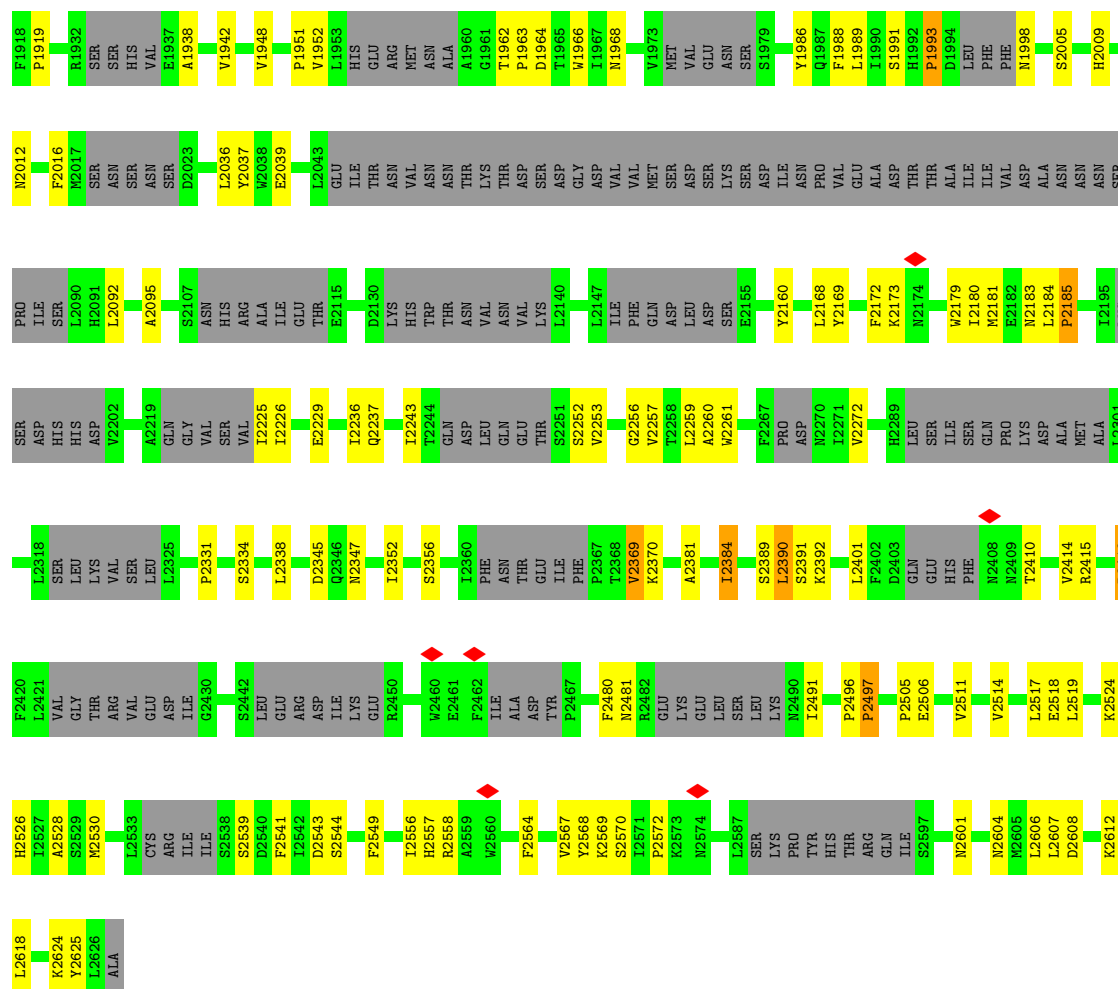
• Molecule 4: Chromatin modification-related protein EAF5



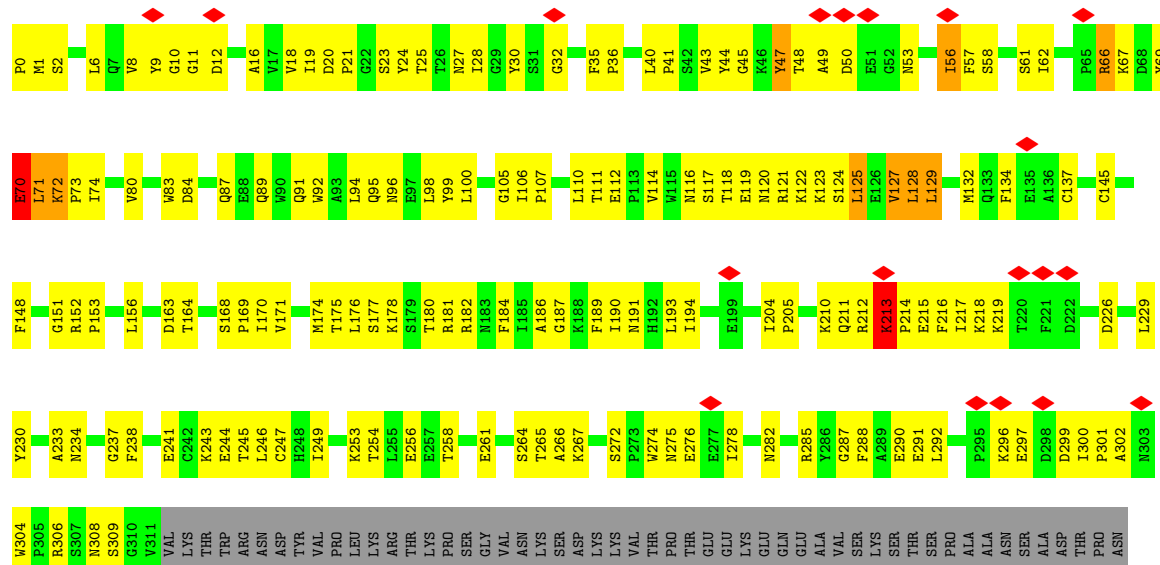
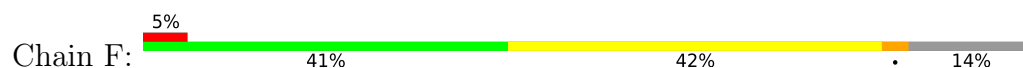
• Molecule 5: Transcription-associated protein 1

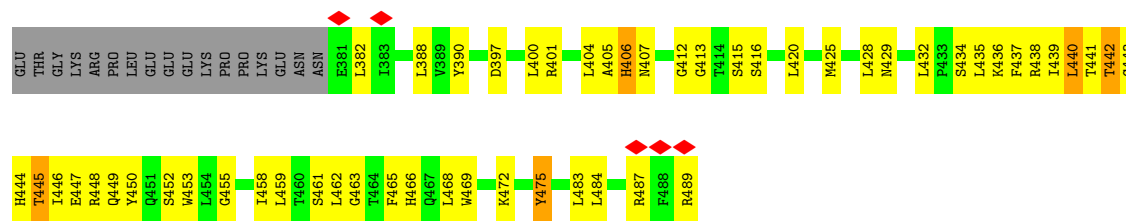




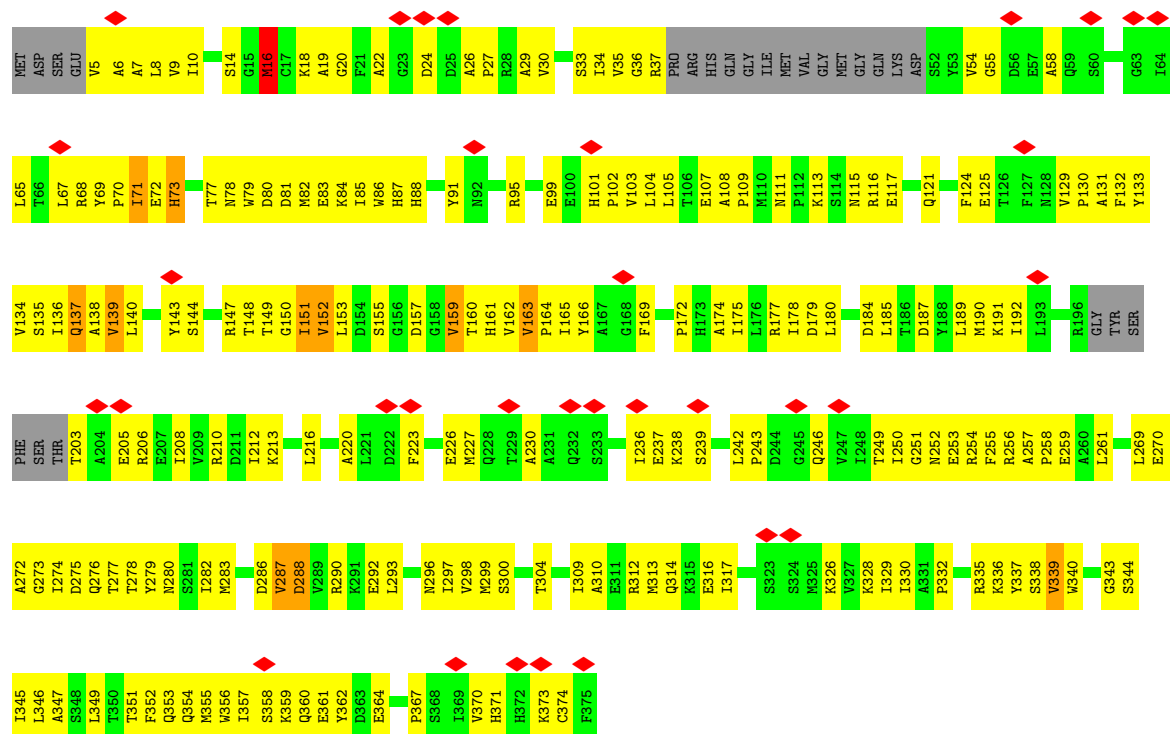


• Molecule 6: Actin-related protein 4





• Molecule 7: Actin



• Molecule 8: Chromatin modification-related protein EAF1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63197	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.132	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0225	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	B	0.45	0/5992	1.03	34/8237 (0.4%)
2	C	0.36	0/805	1.01	5/1110 (0.5%)
4	H	0.34	0/755	0.69	2/1039 (0.2%)
5	A	0.42	1/9944 (0.0%)	0.95	56/13772 (0.4%)
6	F	0.38	1/3406 (0.0%)	0.68	1/4618 (0.0%)
7	G	0.35	0/2787	0.69	1/3776 (0.0%)
8	E	0.43	0/351	0.74	0/473
All	All	0.41	2/24040 (0.0%)	0.90	99/33025 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	410	GLU	C-N	16.37	1.55	1.33
6	F	475	TYR	C-O	-6.00	1.17	1.24

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1919	PRO	N-CA-CB	12.12	110.93	102.81
2	C	714	GLY	CA-C-N	11.74	134.52	119.84
2	C	714	GLY	C-N-CA	11.74	134.52	119.84
1	B	3618	GLU	CA-C-N	-11.64	105.29	119.84
1	B	3618	GLU	C-N-CA	-11.64	105.29	119.84
1	B	3497	HIS	N-CA-C	-11.62	98.69	111.36
1	B	3163	TYR	CA-C-N	11.02	133.61	119.84
1	B	3163	TYR	C-N-CA	11.02	133.61	119.84
5	A	962	PRO	CA-C-N	10.39	132.83	119.84
5	A	962	PRO	C-N-CA	10.39	132.83	119.84
5	A	914	ASP	CA-C-N	-8.95	108.65	119.84
5	A	914	ASP	C-N-CA	-8.95	108.65	119.84
1	B	3452	SER	CA-C-N	8.68	130.69	119.84
1	B	3452	SER	C-N-CA	8.68	130.69	119.84
1	B	3741	MET	CA-C-N	8.31	130.23	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3741	MET	C-N-CA	8.31	130.23	119.84
1	B	3568	THR	CA-C-N	8.23	127.87	119.56
1	B	3568	THR	C-N-CA	8.23	127.87	119.56
1	B	2786	VAL	CA-C-N	8.15	130.02	119.84
1	B	2786	VAL	C-N-CA	8.15	130.02	119.84
1	B	2905	ARG	N-CA-C	-7.93	98.75	111.04
5	A	2618	LEU	CA-C-N	7.67	128.28	120.38
5	A	2618	LEU	C-N-CA	7.67	128.28	120.38
5	A	777	PRO	N-CA-CB	7.50	111.12	103.25
5	A	891	PRO	N-CA-CB	7.43	111.05	103.25
5	A	2496	PRO	N-CA-CB	7.36	110.22	103.08
1	B	3129	PRO	N-CA-CB	7.33	111.08	103.38
4	H	89	PRO	N-CA-CB	7.25	110.86	103.25
5	A	1993	PRO	N-CA-CB	7.21	110.18	103.41
5	A	707	PRO	N-CA-CB	7.17	110.78	103.25
5	A	2497	PRO	N-CA-CB	7.15	110.75	103.25
5	A	786	PRO	N-CA-CB	7.12	110.72	103.25
5	A	573	PRO	N-CA-CB	7.09	110.69	103.25
5	A	1474	PRO	N-CA-CB	6.96	110.66	103.00
1	B	2921	PRO	N-CA-CB	6.94	110.11	103.52
2	C	681	THR	N-CA-C	-6.79	103.81	111.14
5	A	2331	PRO	N-CA-CB	6.76	110.34	103.25
2	C	796	PRO	N-CA-CB	6.74	110.33	103.25
5	A	1336	PRO	N-CA-CB	6.65	110.32	103.00
5	A	833	PRO	N-CA-CB	6.64	110.23	103.25
5	A	877	PRO	N-CA-CB	6.62	110.10	103.48
2	C	740	PRO	N-CA-CB	6.61	110.19	103.25
5	A	1951	PRO	N-CA-CB	6.60	110.18	103.25
5	A	882	PRO	N-CA-CB	6.57	110.26	103.23
5	A	874	PRO	N-CA-CB	6.46	110.03	103.25
5	A	575	PRO	N-CA-CB	6.43	110.49	103.23
1	B	2910	GLN	N-CA-C	-6.39	104.23	111.07
5	A	458	PRO	N-CA-CB	6.39	110.03	103.00
5	A	1321	PRO	N-CA-CB	6.39	109.96	103.25
5	A	1563	PRO	N-CA-CB	6.38	110.02	103.00
5	A	579	PRO	N-CA-CB	6.36	110.43	103.30
5	A	852	PRO	N-CA-CB	6.33	109.90	103.25
5	A	805	PRO	N-CA-CB	6.32	109.88	103.25
5	A	1548	PRO	N-CA-CB	6.23	110.12	103.52
5	A	1453	PRO	N-CA-CB	6.22	109.92	103.15
5	A	1632	GLU	CB-CA-C	-6.20	109.41	116.54
5	A	1963	PRO	N-CA-CB	6.17	110.29	103.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3564	ILE	N-CA-C	-6.16	104.99	113.00
4	H	229	PRO	N-CA-CB	6.14	109.84	103.15
5	A	2185	PRO	N-CA-CB	6.11	110.05	103.33
5	A	866	PRO	N-CA-CB	6.08	109.63	103.25
1	B	2638	ASN	N-CA-C	-6.07	104.58	111.07
1	B	3359	LEU	N-CA-C	-6.03	104.28	111.69
5	A	1742	PRO	N-CA-CB	6.00	109.88	103.52
1	B	3506	MET	CA-C-N	5.99	128.62	120.54
1	B	3506	MET	C-N-CA	5.99	128.62	120.54
5	A	1252	ALA	CA-C-N	5.96	125.97	119.89
5	A	1252	ALA	C-N-CA	5.96	125.97	119.89
1	B	3654	GLU	CA-C-N	5.95	126.29	119.92
1	B	3654	GLU	C-N-CA	5.95	126.29	119.92
5	A	568	PRO	N-CA-CB	5.94	109.49	103.25
5	A	2505	PRO	N-CA-CB	5.94	109.48	103.25
5	A	215	ARG	CB-CA-C	-5.91	109.75	116.54
5	A	961	LYS	CA-C-N	5.86	126.42	120.38
5	A	961	LYS	C-N-CA	5.86	126.42	120.38
1	B	3288	LEU	CB-CA-C	-5.85	109.82	116.54
5	A	1300	ASN	CA-C-N	5.84	127.14	119.84
5	A	1300	ASN	C-N-CA	5.84	127.14	119.84
1	B	3468	HIS	N-CA-C	5.75	119.11	111.75
5	A	994	THR	CA-C-N	5.64	126.89	119.84
5	A	994	THR	C-N-CA	5.64	126.89	119.84
1	B	2943	ILE	N-CA-C	-5.59	105.05	110.42
1	B	3551	GLN	O-C-N	-5.55	114.81	122.30
5	A	1156	TYR	CB-CA-C	-5.55	110.16	116.54
1	B	3705	GLN	N-CA-C	-5.49	105.37	111.36
1	B	3551	GLN	CA-C-N	5.48	132.01	121.54
1	B	3551	GLN	C-N-CA	5.48	132.01	121.54
1	B	2648	SER	N-CA-C	5.32	117.16	110.24
5	A	1345	LEU	CA-C-N	5.29	126.45	119.84
5	A	1345	LEU	C-N-CA	5.29	126.45	119.84
1	B	3060	TRP	N-CA-C	-5.28	105.21	110.97
5	A	1368	LEU	CB-CA-C	-5.28	110.47	116.54
5	A	2272	VAL	CB-CA-C	-5.26	108.70	113.70
6	F	215	GLU	CB-CA-C	-5.25	110.50	116.54
5	A	969	LYS	N-CA-C	-5.13	105.33	111.03
1	B	2667	VAL	N-CA-C	-5.10	105.53	110.42
7	G	339	VAL	N-CA-C	-5.08	105.55	110.42
5	A	2160	TYR	N-CA-C	-5.07	105.76	111.28
5	A	325	VAL	CB-CA-C	-5.01	108.94	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5937	0	4061	734	0
2	C	800	0	481	67	0
3	D	1800	0	405	60	0
4	H	764	0	309	25	0
5	A	10017	0	4245	338	0
6	F	3334	0	3292	267	0
7	G	2729	0	2697	248	0
8	E	342	0	331	41	0
All	All	25723	0	15821	1712	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 41.

All (1712) 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:B:3106:TRP:CZ3	1:B:3668:ARG:HD2	1.26	1.69
7:G:163:VAL:CG2	7:G:175:ILE:HG12	1.24	1.67
7:G:163:VAL:HG22	7:G:175:ILE:CG1	1.28	1.64
7:G:163:VAL:CG2	7:G:175:ILE:CG1	1.76	1.59
1:B:3139:GLN:CB	1:B:3418:ARG:HH21	1.07	1.58
7:G:163:VAL:CG2	7:G:175:ILE:CD1	1.81	1.57
1:B:3236:ARG:HG3	1:B:3338:CYS:CB	1.30	1.54
1:B:3474:PHE:CE2	1:B:3526:VAL:HG21	1.38	1.53
1:B:3427:ASN:CB	1:B:3443:PHE:HE1	1.17	1.53
1:B:3106:TRP:CH2	1:B:3668:ARG:HD2	1.39	1.52
1:B:3171:LEU:HD23	1:B:3172:ARG:N	1.22	1.52
1:B:3474:PHE:CE2	1:B:3526:VAL:CG2	1.90	1.51
5:A:2243:ILE:HA	5:A:2252:SER:CB	1.39	1.51
1:B:3427:ASN:HB2	1:B:3443:PHE:CE1	1.47	1.49
1:B:3625:THR:CB	1:B:3727:ALA:HB1	1.39	1.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3403:PHE:CB	1:B:3457:ILE:HB	1.42	1.47
1:B:3043:PHE:CB	1:B:3060:TRP:NE1	1.77	1.47
1:B:3106:TRP:CH2	1:B:3668:ARG:CD	1.98	1.47
1:B:3106:TRP:HH2	1:B:3668:ARG:CG	1.24	1.46
1:B:3731:ARG:NH2	2:C:694:TRP:CD1	1.82	1.46
1:B:2828:TRP:CB	1:B:2842:LEU:HD21	1.45	1.45
1:B:2828:TRP:CB	1:B:2842:LEU:CD2	1.97	1.42
1:B:3427:ASN:CB	1:B:3443:PHE:CE1	2.01	1.41
1:B:3139:GLN:CB	1:B:3418:ARG:NH2	1.83	1.39
1:B:3043:PHE:CB	1:B:3060:TRP:HE1	1.33	1.38
1:B:2633:TRP:CB	5:A:2624:LYS:CB	1.99	1.38
1:B:3731:ARG:NH2	2:C:694:TRP:HD1	1.08	1.38
1:B:3731:ARG:HH21	2:C:694:TRP:CD1	1.38	1.38
1:B:3253:LEU:CD2	1:B:3314:LEU:CB	2.00	1.37
1:B:3450:PRO:C	1:B:3451:LEU:HD12	1.49	1.35
1:B:3731:ARG:HD2	2:C:694:TRP:NE1	1.39	1.34
2:C:721:GLN:O	2:C:724:LEU:CB	1.75	1.34
1:B:3244:ASP:HA	1:B:3247:ARG:CD	1.57	1.33
1:B:3367:HIS:HE1	5:A:912:TYR:O	1.08	1.32
1:B:3568:THR:HB	1:B:3569:PRO:CD	1.56	1.32
1:B:3705:GLN:CB	1:B:3709:LEU:HA	1.61	1.31
1:B:3106:TRP:CH2	1:B:3668:ARG:CG	2.09	1.30
1:B:3427:ASN:CA	1:B:3443:PHE:CE1	2.11	1.30
1:B:3667:ILE:CD1	1:B:3692:VAL:CB	2.12	1.28
6:F:442:THR:CG2	6:F:448:ARG:HE	1.45	1.27
1:B:3424:ARG:NH1	1:B:3447:ILE:HA	1.50	1.26
1:B:3719:PHE:HA	1:B:3722:ASP:OD2	1.34	1.25
5:A:333:LEU:CB	5:A:376:LEU:CB	2.14	1.25
3:D:418:UNK:CB	6:F:441:THR:H	1.50	1.23
5:A:1093:LYS:O	5:A:1095:LEU:N	1.71	1.22
6:F:87:GLN:CG	6:F:132:MET:HE2	1.68	1.22
5:A:430:THR:O	5:A:432:GLN:N	1.73	1.21
5:A:2243:ILE:CB	5:A:2252:SER:C	2.14	1.21
1:B:3427:ASN:CA	1:B:3443:PHE:HE1	1.45	1.21
1:B:3374:PHE:CB	1:B:3392:MET:CB	2.17	1.21
1:B:3100:LEU:HD13	1:B:3101:LEU:N	1.56	1.21
6:F:444:HIS:O	6:F:446:ILE:N	1.70	1.21
1:B:3474:PHE:CD2	1:B:3526:VAL:HG11	1.74	1.20
7:G:163:VAL:HG21	7:G:175:ILE:CD1	1.50	1.20
1:B:3163:TYR:CB	1:B:3167:LEU:CD2	2.21	1.19
6:F:87:GLN:O	6:F:132:MET:HE1	1.43	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1372:GLU:O	5:A:1375:PHE:N	1.76	1.18
5:A:1043:LEU:O	5:A:1046:ALA:HB3	1.43	1.18
1:B:3450:PRO:O	1:B:3451:LEU:CD1	1.91	1.17
6:F:213:LYS:HB3	6:F:214:PRO:CD	1.70	1.17
1:B:3568:THR:HB	1:B:3569:PRO:HD2	1.18	1.17
5:A:1363:LEU:O	5:A:1364:PRO:CB	1.85	1.16
1:B:3474:PHE:CE2	1:B:3526:VAL:HG22	1.76	1.16
6:F:62:ILE:O	6:F:71:LEU:HD21	1.45	1.16
1:B:3528:LYS:CB	1:B:3632:ILE:O	1.93	1.16
1:B:3236:ARG:CG	1:B:3338:CYS:CB	2.24	1.15
1:B:3427:ASN:HA	1:B:3443:PHE:CE1	1.78	1.15
1:B:3740:PHE:C	1:B:3742:PRO:HD3	1.68	1.15
5:A:1091:SER:CB	5:A:1099:ALA:HA	1.76	1.15
1:B:3360:LEU:CB	1:B:3424:ARG:HH21	1.57	1.14
1:B:3099:GLU:HB2	1:B:3425:LEU:HD11	1.16	1.14
1:B:3106:TRP:CH2	1:B:3668:ARG:CB	2.29	1.14
1:B:3496:ALA:HB1	2:C:684:TYR:CE1	1.83	1.14
1:B:3106:TRP:HH2	1:B:3668:ARG:CD	1.43	1.14
1:B:3367:HIS:CE1	5:A:912:TYR:O	1.99	1.14
5:A:1091:SER:CA	5:A:1099:ALA:HB2	1.77	1.13
1:B:3450:PRO:O	1:B:3451:LEU:HD12	0.95	1.13
1:B:3068:LEU:HD23	1:B:3081:ALA:CB	1.76	1.13
1:B:3625:THR:CB	1:B:3727:ALA:CB	2.26	1.12
5:A:2243:ILE:CA	5:A:2252:SER:CB	2.26	1.12
5:A:137:LEU:O	5:A:139:SER:N	1.82	1.12
5:A:631:VAL:CB	5:A:1587:GLN:CB	2.26	1.12
1:B:2690:ILE:HA	1:B:3715:VAL:CB	1.80	1.11
6:F:213:LYS:HB3	6:F:214:PRO:HD2	1.24	1.11
1:B:3360:LEU:CB	1:B:3424:ARG:NH2	2.13	1.11
1:B:2647:THR:CB	1:B:2651:ASN:OD1	1.99	1.10
1:B:2659:GLU:HG3	1:B:2681:ARG:CB	1.80	1.10
1:B:3171:LEU:CD2	1:B:3172:ARG:N	2.12	1.10
1:B:3106:TRP:HB2	1:B:3665:LEU:HD13	1.16	1.10
1:B:3244:ASP:HA	1:B:3247:ARG:HD3	1.17	1.10
1:B:3253:LEU:HD21	1:B:3314:LEU:CB	1.76	1.09
1:B:3450:PRO:C	1:B:3451:LEU:CD1	2.24	1.09
5:A:239:LYS:O	5:A:241:LEU:N	1.83	1.09
1:B:3053:LEU:CB	1:B:3056:ALA:HB2	1.82	1.09
1:B:3496:ALA:HB1	2:C:684:TYR:HE1	0.98	1.09
1:B:3106:TRP:CZ3	1:B:3668:ARG:CD	2.21	1.09
1:B:3489:MET:HE2	1:B:3511:VAL:HG23	1.27	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:87:GLN:HG2	6:F:132:MET:HE2	1.24	1.08
1:B:3116:MET:O	1:B:3119:ASN:N	1.86	1.08
1:B:3427:ASN:HA	1:B:3443:PHE:CZ	1.87	1.08
6:F:442:THR:HG21	6:F:448:ARG:HE	1.07	1.08
1:B:3568:THR:CB	1:B:3569:PRO:CD	2.28	1.08
5:A:1292:ILE:O	5:A:1294:CYS:N	1.86	1.08
7:G:138:ALA:CB	7:G:165:ILE:HD11	1.83	1.08
7:G:163:VAL:HG22	7:G:175:ILE:CD1	1.58	1.07
1:B:3407:TYR:H	1:B:3408:PRO:CD	1.69	1.06
5:A:1091:SER:CB	5:A:1099:ALA:CB	2.33	1.06
1:B:3068:LEU:HB2	1:B:3078:ALA:CB	1.86	1.06
1:B:3106:TRP:HH2	1:B:3668:ARG:HG3	1.17	1.06
1:B:3163:TYR:CB	1:B:3167:LEU:HD23	1.82	1.06
2:C:673:SER:HA	2:C:681:THR:HG21	1.36	1.06
7:G:163:VAL:HG21	7:G:175:ILE:HD13	1.08	1.06
1:B:2828:TRP:CB	1:B:2842:LEU:HD23	1.78	1.05
1:B:3068:LEU:HD23	1:B:3081:ALA:HB3	1.33	1.05
1:B:2638:ASN:O	1:B:2642:SER:N	1.89	1.05
1:B:3068:LEU:HB2	1:B:3078:ALA:HB1	1.33	1.05
1:B:3474:PHE:CD2	1:B:3526:VAL:HG21	1.91	1.05
1:B:3705:GLN:CB	1:B:3709:LEU:CA	2.33	1.05
1:B:2670:GLN:CA	1:B:2837:PRO:HG3	1.85	1.05
1:B:3163:TYR:CB	1:B:3167:LEU:HD22	1.86	1.05
1:B:3068:LEU:CD2	1:B:3081:ALA:HB3	1.86	1.05
5:A:1859:LEU:O	5:A:1861:ARG:N	1.89	1.05
7:G:163:VAL:HG23	7:G:175:ILE:HG12	1.11	1.05
1:B:3377:THR:CB	1:B:3390:ARG:O	2.05	1.04
1:B:3618:GLU:O	1:B:3619:PRO:C	1.96	1.04
1:B:3407:TYR:H	1:B:3408:PRO:HD2	1.22	1.04
5:A:1091:SER:HA	5:A:1099:ALA:HB2	1.37	1.04
1:B:3043:PHE:CB	1:B:3060:TRP:CD1	2.40	1.03
5:A:1097:ASP:O	5:A:1099:ALA:N	1.91	1.03
1:B:3618:GLU:O	1:B:3620:VAL:N	1.90	1.03
1:B:3244:ASP:HA	1:B:3247:ARG:HD2	1.37	1.03
5:A:1152:ALA:O	5:A:1154:SER:N	1.91	1.03
5:A:2243:ILE:CB	5:A:2253:VAL:N	2.19	1.03
1:B:3403:PHE:CB	1:B:3457:ILE:CB	2.36	1.02
5:A:1292:ILE:C	5:A:1294:CYS:H	1.68	1.02
1:B:3719:PHE:O	1:B:3722:ASP:HB2	1.58	1.02
5:A:424:ASP:O	5:A:426:SER:N	1.91	1.02
1:B:3404:ALA:H	1:B:3457:ILE:HG22	1.22	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1441:LEU:O	5:A:1445:PHE:N	1.93	1.01
1:B:3171:LEU:O	1:B:3174:THR:N	1.93	1.01
1:B:3085:TYR:C	1:B:3104:ILE:CD1	2.34	1.01
7:G:163:VAL:HG23	7:G:175:ILE:CG1	1.69	1.01
1:B:3427:ASN:HB2	1:B:3443:PHE:CD1	1.95	1.01
3:D:79:UNK:O	3:D:80:UNK:O	1.77	1.01
7:G:163:VAL:CG2	7:G:175:ILE:HD11	1.87	1.01
5:A:1091:SER:CB	5:A:1099:ALA:CA	2.39	1.00
1:B:2670:GLN:N	1:B:2837:PRO:HG3	1.76	1.00
1:B:2638:ASN:O	1:B:2642:SER:HB3	1.62	1.00
5:A:1043:LEU:O	5:A:1046:ALA:CB	2.10	0.99
2:C:715:PRO:O	2:C:717:ALA:N	1.96	0.99
1:B:3099:GLU:CB	1:B:3425:LEU:HD11	1.91	0.99
2:C:713:LYS:O	2:C:714:GLY:O	1.79	0.99
1:B:3703:VAL:O	1:B:3704:ALA:O	1.80	0.99
1:B:3427:ASN:CA	1:B:3443:PHE:CZ	2.45	0.99
6:F:87:GLN:O	6:F:132:MET:CE	2.11	0.98
1:B:3474:PHE:CD2	1:B:3526:VAL:CG1	2.46	0.98
1:B:3649:SER:OG	1:B:3705:GLN:HA	1.63	0.98
6:F:442:THR:HG21	6:F:448:ARG:NE	1.77	0.98
1:B:3244:ASP:CA	1:B:3247:ARG:HD3	1.93	0.97
1:B:3424:ARG:HH12	1:B:3447:ILE:HA	1.07	0.97
1:B:3741:MET:N	1:B:3742:PRO:CD	2.26	0.97
1:B:3106:TRP:HB2	1:B:3665:LEU:CD1	1.93	0.97
6:F:71:LEU:HD11	6:F:229:LEU:HD13	1.45	0.97
6:F:66:ARG:HB3	6:F:66:ARG:NH1	1.79	0.97
5:A:1372:GLU:O	5:A:1374:LEU:N	1.97	0.97
5:A:1157:ILE:O	5:A:1159:GLU:N	1.95	0.97
1:B:2659:GLU:CG	1:B:2681:ARG:CB	2.42	0.97
1:B:3411:ARG:O	1:B:3415:ARG:N	1.97	0.96
5:A:1227:SER:O	5:A:1231:LYS:CB	2.12	0.96
6:F:91:GLN:HB2	6:F:132:MET:CE	1.95	0.96
5:A:1300:ASN:O	5:A:1302:LYS:N	1.98	0.96
6:F:211:GLN:OE1	6:F:217:ILE:HD12	1.65	0.96
1:B:3391:LEU:O	1:B:3402:SER:CB	2.14	0.95
3:D:418:UNK:CB	6:F:441:THR:N	2.28	0.95
1:B:3424:ARG:NE	1:B:3445:LEU:CB	2.29	0.95
1:B:3649:SER:CB	1:B:3705:GLN:HA	1.96	0.95
1:B:3740:PHE:C	1:B:3742:PRO:CD	2.39	0.95
1:B:3492:LYS:HA	1:B:3492:LYS:HE3	1.48	0.95
5:A:516:GLU:O	5:A:518:MET:N	2.00	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3422:LEU:HD22	1:B:3422:LEU:H	1.27	0.94
6:F:442:THR:CG2	6:F:448:ARG:NE	2.30	0.94
1:B:2822:GLN:O	1:B:2825:LEU:N	1.99	0.94
1:B:3106:TRP:CH2	1:B:3668:ARG:HB3	1.99	0.94
1:B:3253:LEU:HD23	1:B:3314:LEU:CB	1.97	0.94
1:B:3085:TYR:C	1:B:3104:ILE:HD11	1.92	0.94
1:B:3668:ARG:HE	1:B:3672:ILE:HD13	1.32	0.94
1:B:3171:LEU:HD23	1:B:3172:ARG:CA	1.98	0.94
1:B:3247:ARG:HH21	1:B:3247:ARG:HG3	1.33	0.94
1:B:3171:LEU:CD2	1:B:3172:ARG:H	1.76	0.94
2:C:722:GLN:C	2:C:724:LEU:H	1.72	0.94
1:B:3649:SER:HB2	1:B:3704:ALA:O	1.68	0.93
1:B:3053:LEU:CB	1:B:3056:ALA:CB	2.45	0.93
8:E:391:ILE:HA	8:E:394:TYR:HB2	1.48	0.93
7:G:138:ALA:HB1	7:G:165:ILE:HD11	1.47	0.92
1:B:3740:PHE:CB	1:B:3742:PRO:HD3	1.98	0.92
6:F:129:LEU:H	6:F:129:LEU:HD22	1.32	0.92
1:B:2817:CYS:CB	1:B:2852:PHE:CZ	2.52	0.92
1:B:3474:PHE:CG	1:B:3526:VAL:HG11	2.04	0.92
1:B:3667:ILE:HD12	1:B:3692:VAL:CB	1.98	0.92
1:B:3644:ASN:HA	1:B:3647:THR:OG1	1.69	0.92
6:F:213:LYS:CB	6:F:214:PRO:CD	2.47	0.92
1:B:3244:ASP:O	1:B:3247:ARG:HG2	1.69	0.92
1:B:3424:ARG:HE	1:B:3445:LEU:CB	1.83	0.92
5:A:244:THR:O	5:A:245:SER:O	1.88	0.92
7:G:139:VAL:HG13	7:G:165:ILE:HG21	1.50	0.92
1:B:2690:ILE:CA	1:B:3715:VAL:CB	2.47	0.91
6:F:91:GLN:HB2	6:F:132:MET:HE1	1.51	0.91
1:B:3244:ASP:CA	1:B:3247:ARG:CD	2.46	0.91
1:B:3667:ILE:HD13	1:B:3692:VAL:CB	1.99	0.91
7:G:286:ASP:HB3	7:G:288:ASP:OD1	1.71	0.91
1:B:3731:ARG:CD	2:C:694:TRP:HE1	1.82	0.91
5:A:239:LYS:C	5:A:241:LEU:H	1.78	0.91
4:H:51:GLN:O	4:H:55:LEU:N	2.04	0.91
7:G:163:VAL:HG22	7:G:175:ILE:HD11	1.49	0.91
1:B:2961:ASP:C	1:B:2963:CYS:H	1.78	0.91
5:A:1091:SER:CA	5:A:1099:ALA:CB	2.48	0.91
1:B:3055:LYS:O	1:B:3059:GLN:N	2.03	0.90
1:B:2640:LEU:HD21	1:B:2662:LEU:CB	2.02	0.90
1:B:3219:TYR:N	1:B:3220:PRO:HD3	1.87	0.90
1:B:3731:ARG:CD	2:C:694:TRP:NE1	2.33	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1506:LEU:O	5:A:1508:GLU:N	2.04	0.90
1:B:2638:ASN:O	1:B:2642:SER:CB	2.20	0.90
1:B:3253:LEU:HD22	1:B:3314:LEU:CB	2.00	0.90
1:B:3618:GLU:CB	1:B:3620:VAL:O	2.20	0.89
1:B:3062:PHE:HZ	1:B:3657:ASN:C	1.79	0.89
1:B:3106:TRP:HZ3	1:B:3668:ARG:HD2	1.13	0.89
5:A:1069:LYS:O	5:A:1072:TYR:N	2.05	0.89
1:B:3703:VAL:O	1:B:3704:ALA:C	2.14	0.89
1:B:3568:THR:HG22	1:B:3569:PRO:HD3	1.55	0.89
5:A:511:ASP:O	5:A:515:GLU:CB	2.20	0.89
1:B:3106:TRP:CH2	1:B:3668:ARG:NH2	2.39	0.88
1:B:3107:LEU:HA	1:B:3110:ILE:HD12	1.54	0.88
1:B:3731:ARG:CZ	2:C:694:TRP:HD1	1.85	0.88
5:A:914:ASP:O	5:A:915:PRO:C	2.13	0.88
1:B:3407:TYR:N	1:B:3408:PRO:CD	2.34	0.88
7:G:151:ILE:HG23	7:G:297:ILE:HA	1.54	0.88
1:B:3568:THR:CB	1:B:3569:PRO:HD3	2.03	0.88
7:G:151:ILE:HG21	7:G:297:ILE:HG12	1.55	0.88
1:B:2748:GLU:HB3	1:B:2752:HIS:CD2	2.07	0.87
6:F:213:LYS:HE3	6:F:213:LYS:C	1.99	0.87
6:F:428:LEU:HB3	6:F:437:PHE:HE2	1.37	0.87
1:B:2821:ILE:CB	1:B:2849:TYR:CE2	2.57	0.87
1:B:3474:PHE:CZ	1:B:3526:VAL:HG22	2.09	0.87
5:A:511:ASP:O	5:A:515:GLU:N	2.07	0.87
6:F:87:GLN:HG3	6:F:132:MET:HE2	1.55	0.87
1:B:3354:ILE:HA	1:B:3371:ILE:H	1.39	0.87
1:B:3219:TYR:H	1:B:3220:PRO:HD3	1.38	0.87
1:B:3418:ARG:O	1:B:3422:LEU:CD2	2.23	0.87
1:B:3106:TRP:CZ2	1:B:3668:ARG:CB	2.58	0.86
1:B:3388:TYR:CB	1:B:3404:ALA:HB1	2.04	0.86
1:B:3418:ARG:CB	1:B:3418:ARG:HH11	1.88	0.86
1:B:3551:GLN:O	1:B:3554:SER:N	2.08	0.86
6:F:428:LEU:HB3	6:F:437:PHE:CE2	2.09	0.86
1:B:3474:PHE:HE2	1:B:3526:VAL:CG2	1.52	0.86
5:A:2567:VAL:C	5:A:2569:LYS:H	1.84	0.86
7:G:16:MET:N	7:G:16:MET:SD	2.49	0.86
5:A:1506:LEU:C	5:A:1508:GLU:H	1.84	0.86
5:A:1650:PHE:O	5:A:1652:ILE:N	2.09	0.86
1:B:3055:LYS:CB	1:B:3059:GLN:HG3	2.06	0.86
1:B:3652:LEU:O	1:B:3652:LEU:HD22	1.76	0.85
1:B:3169:PHE:CE1	1:B:3451:LEU:HD21	2.09	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:138:ALA:HA	7:G:152:VAL:HG11	1.56	0.85
1:B:3526:VAL:O	1:B:3530:HIS:N	2.08	0.85
1:B:2633:TRP:CB	5:A:2624:LYS:C	2.50	0.85
1:B:3424:ARG:CD	1:B:3445:LEU:CB	2.53	0.85
6:F:62:ILE:O	6:F:71:LEU:CD2	2.24	0.85
1:B:2651:ASN:O	1:B:2653:LYS:N	2.09	0.85
6:F:45:GLY:HA3	6:F:56:ILE:HG22	1.56	0.85
5:A:1993:PRO:O	5:A:1998:ASN:N	2.10	0.85
7:G:16:MET:CE	7:G:16:MET:H	1.88	0.85
7:G:138:ALA:HB3	7:G:165:ILE:HD11	1.58	0.84
1:B:2821:ILE:HA	1:B:2849:TYR:OH	1.76	0.84
1:B:3731:ARG:HD2	2:C:694:TRP:CD1	2.12	0.84
1:B:3068:LEU:CB	1:B:3078:ALA:CB	2.55	0.84
1:B:3427:ASN:N	1:B:3443:PHE:CZ	2.45	0.84
5:A:430:THR:O	5:A:431:VAL:C	2.21	0.84
6:F:91:GLN:OE1	6:F:132:MET:SD	2.34	0.84
1:B:3576:LYS:H	1:B:3576:LYS:HD3	1.43	0.84
1:B:3618:GLU:O	1:B:3620:VAL:O	1.96	0.84
6:F:72:LYS:HB3	6:F:72:LYS:HZ3	1.43	0.84
3:D:155:UNK:O	3:D:159:UNK:N	2.09	0.84
5:A:302:THR:O	5:A:304:PHE:N	2.10	0.84
1:B:3481:ASP:CB	1:B:3482:PRO:CD	2.55	0.84
1:B:3568:THR:CG2	1:B:3569:PRO:HD3	2.07	0.83
5:A:1859:LEU:O	5:A:1862:PHE:N	2.11	0.83
1:B:3418:ARG:HH11	1:B:3418:ARG:HB2	1.43	0.83
1:B:3062:PHE:CZ	1:B:3657:ASN:C	2.57	0.83
1:B:3168:HIS:O	1:B:3172:ARG:HB3	1.78	0.83
6:F:87:GLN:C	6:F:132:MET:CE	2.51	0.83
1:B:3168:HIS:HA	1:B:3171:LEU:HD22	1.61	0.83
1:B:3411:ARG:HD2	1:B:3587:LEU:CB	2.08	0.83
6:F:91:GLN:HB2	6:F:132:MET:SD	2.19	0.83
1:B:3106:TRP:CB	1:B:3665:LEU:HD13	2.07	0.83
1:B:3731:ARG:HD2	2:C:694:TRP:HE1	1.05	0.83
5:A:1097:ASP:O	5:A:1100:MET:N	2.10	0.83
5:A:996:GLY:O	5:A:998:GLN:N	2.12	0.82
2:C:722:GLN:O	2:C:726:GLU:CB	2.27	0.82
6:F:87:GLN:CG	6:F:132:MET:CE	2.54	0.82
7:G:140:LEU:CD1	7:G:343:GLY:N	2.42	0.82
1:B:2744:ASP:O	1:B:2747:THR:HG23	1.78	0.82
5:A:1006:SER:CB	5:A:1009:SER:CB	2.58	0.82
5:A:1097:ASP:O	5:A:1098:ASP:C	2.21	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:442:THR:HG21	6:F:448:ARG:CG	2.10	0.81
1:B:3404:ALA:N	1:B:3457:ILE:HG22	1.94	0.81
5:A:239:LYS:C	5:A:241:LEU:N	2.35	0.81
1:B:3173:THR:CB	1:B:3451:LEU:HA	2.10	0.81
1:B:3667:ILE:HD11	1:B:3692:VAL:CB	2.08	0.81
5:A:1629:GLN:O	5:A:1630:ARG:O	1.97	0.81
7:G:140:LEU:HD12	7:G:343:GLY:N	1.94	0.81
1:B:3171:LEU:O	1:B:3174:THR:OG1	1.97	0.81
5:A:976:ALA:O	5:A:977:ILE:CB	2.28	0.81
7:G:242:LEU:HD12	7:G:246:GLN:HB2	1.60	0.81
5:A:736:PHE:N	5:A:1543:LEU:C	2.38	0.81
1:B:3489:MET:HE2	1:B:3511:VAL:CG2	2.09	0.80
1:B:3719:PHE:CA	1:B:3722:ASP:OD2	2.25	0.80
5:A:1361:LEU:O	5:A:1363:LEU:N	2.14	0.80
7:G:14:SER:HA	7:G:71:ILE:HB	1.62	0.80
7:G:18:LYS:HG2	7:G:30:VAL:HG13	1.63	0.80
1:B:3106:TRP:CE3	1:B:3665:LEU:HD12	2.17	0.80
1:B:3253:LEU:HD12	1:B:3318:ARG:HG3	1.64	0.80
5:A:976:ALA:HA	5:A:992:SER:CB	2.12	0.80
1:B:3466:THR:HG22	1:B:3573:HIS:HB2	1.63	0.80
1:B:3493:LEU:O	1:B:3510:LYS:NZ	2.14	0.80
5:A:1300:ASN:C	5:A:1302:LYS:H	1.89	0.80
7:G:298:VAL:HG22	7:G:330:ILE:HB	1.63	0.80
1:B:3169:PHE:HE1	1:B:3451:LEU:CD2	1.95	0.80
1:B:3656:ASP:O	1:B:3658:GLU:N	2.14	0.79
1:B:3423:TYR:CB	1:B:3558:MET:HE1	2.11	0.79
1:B:3060:TRP:CE3	1:B:3064:ASN:ND2	2.49	0.79
1:B:3486:GLN:NE2	1:B:3486:GLN:O	2.16	0.79
5:A:1200:LEU:O	5:A:1203:ASP:CB	2.31	0.79
7:G:178:ILE:HD11	7:G:277:THR:HG21	1.65	0.79
1:B:3705:GLN:CB	1:B:3709:LEU:CB	2.61	0.78
1:B:3100:LEU:CD1	1:B:3101:LEU:N	2.44	0.78
5:A:217:SER:O	5:A:220:SER:N	2.14	0.78
5:A:1590:SER:O	5:A:1591:PRO:CB	2.31	0.78
1:B:3116:MET:O	1:B:3118:THR:N	2.16	0.78
1:B:3247:ARG:HG2	1:B:3248:LEU:H	1.49	0.78
1:B:3555:PHE:O	1:B:3559:SER:N	2.13	0.78
5:A:1650:PHE:O	5:A:1653:SER:N	2.17	0.78
7:G:286:ASP:CB	7:G:288:ASP:OD1	2.31	0.78
1:B:3068:LEU:CD2	1:B:3081:ALA:CB	2.53	0.78
1:B:3731:ARG:CZ	2:C:694:TRP:CD1	2.63	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:890:TYR:O	5:A:893:LEU:N	2.16	0.78
5:A:1091:SER:C	5:A:1099:ALA:HB2	2.08	0.78
6:F:72:LYS:HB3	6:F:72:LYS:NZ	1.99	0.78
1:B:2853:LEU:O	1:B:2856:THR:OG1	2.02	0.78
5:A:1650:PHE:O	5:A:1651:TYR:C	2.26	0.78
1:B:3102:CYS:SG	1:B:3134:ILE:CB	2.72	0.77
8:E:390:ALA:O	8:E:394:TYR:N	2.16	0.77
1:B:2944:ALA:HA	1:B:2970:ILE:HD12	1.66	0.77
1:B:3068:LEU:HB3	1:B:3078:ALA:HA	1.66	0.77
5:A:1091:SER:CB	5:A:1099:ALA:HB1	2.15	0.77
1:B:3461:SER:CB	1:B:3464:PHE:CZ	2.67	0.77
7:G:140:LEU:HD12	7:G:343:GLY:H	1.49	0.77
3:D:140:UNK:O	6:F:178:LYS:NZ	2.15	0.77
5:A:2567:VAL:O	5:A:2569:LYS:N	2.18	0.77
1:B:3719:PHE:HA	1:B:3722:ASP:CG	2.09	0.77
6:F:71:LEU:HD12	6:F:229:LEU:HD22	1.66	0.77
1:B:2655:ILE:HG22	1:B:2656:GLU:N	1.97	0.77
1:B:3656:ASP:C	1:B:3658:GLU:H	1.92	0.77
1:B:2818:ASP:O	1:B:2821:ILE:CB	2.33	0.77
1:B:3496:ALA:CB	2:C:684:TYR:CE1	2.65	0.77
5:A:1032:SER:O	5:A:1033:ALA:CB	2.33	0.77
1:B:2967:LEU:HD12	1:B:2967:LEU:O	1.84	0.77
1:B:3047:VAL:O	1:B:3050:ASP:O	2.03	0.77
2:C:805:GLN:O	2:C:809:ALA:N	2.12	0.77
1:B:3106:TRP:CH2	1:B:3668:ARG:HG3	2.00	0.76
5:A:1090:THR:C	5:A:1092:ILE:H	1.92	0.76
5:A:1091:SER:HA	5:A:1099:ALA:CB	2.14	0.76
5:A:328:LEU:O	5:A:332:LEU:CB	2.33	0.76
5:A:410:GLU:C	5:A:412:GLU:H	1.94	0.76
1:B:3618:GLU:C	1:B:3620:VAL:N	2.44	0.76
5:A:1372:GLU:O	5:A:1373:GLU:C	2.29	0.76
6:F:213:LYS:HB3	6:F:214:PRO:HD3	1.67	0.76
6:F:66:ARG:HB3	6:F:66:ARG:HH11	1.47	0.76
1:B:3618:GLU:O	1:B:3620:VAL:C	2.28	0.76
7:G:108:ALA:HB1	7:G:109:PRO:CD	2.15	0.76
5:A:1296:LEU:HA	5:A:1356:ALA:HB2	1.68	0.76
1:B:3219:TYR:N	1:B:3220:PRO:CD	2.49	0.75
5:A:1605:ASN:O	5:A:1608:THR:N	2.19	0.75
3:D:439:UNK:O	3:D:443:UNK:N	2.19	0.75
5:A:976:ALA:CA	5:A:992:SER:CB	2.65	0.75
7:G:9:VAL:O	7:G:340:TRP:NE1	2.17	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:19:ALA:HB3	7:G:29:ALA:HB3	1.67	0.75
7:G:150:GLY:O	7:G:293:LEU:CD2	2.33	0.75
6:F:87:GLN:HG3	6:F:132:MET:CE	2.16	0.75
6:F:444:HIS:O	6:F:445:THR:C	2.29	0.75
7:G:102:PRO:HB3	7:G:131:ALA:HB3	1.68	0.75
7:G:237:GLU:HG2	7:G:251:GLY:HA2	1.68	0.75
6:F:213:LYS:HE3	6:F:213:LYS:CA	2.16	0.75
7:G:163:VAL:HG23	7:G:175:ILE:CG2	2.16	0.75
7:G:220:ALA:HB1	7:G:226:GLU:HG3	1.69	0.75
5:A:1093:LYS:C	5:A:1095:LEU:H	1.92	0.75
1:B:3457:ILE:HD12	1:B:3457:ILE:O	1.86	0.75
1:B:3247:ARG:HG3	1:B:3247:ARG:NH2	1.99	0.75
1:B:3435:GLU:OE1	1:B:3435:GLU:N	2.20	0.75
1:B:3100:LEU:HD13	1:B:3101:LEU:CA	2.16	0.75
1:B:3625:THR:N	1:B:3626:PRO:HD3	2.02	0.75
3:D:55:UNK:O	3:D:59:UNK:N	2.20	0.75
5:A:1255:ALA:O	5:A:1258:ASP:N	2.19	0.75
6:F:211:GLN:OE1	6:F:217:ILE:CD1	2.34	0.75
2:C:717:ALA:O	2:C:718:HIS:CB	2.35	0.74
5:A:900:THR:CB	5:A:948:ILE:CD1	2.64	0.74
1:B:2777:GLU:O	1:B:2781:LYS:N	2.16	0.74
1:B:3099:GLU:HB2	1:B:3425:LEU:CD1	2.08	0.74
5:A:1605:ASN:O	5:A:1606:PRO:C	2.27	0.74
1:B:3474:PHE:CD2	1:B:3526:VAL:CG2	2.58	0.74
1:B:2941:HIS:H	1:B:2941:HIS:CD2	2.04	0.74
1:B:3169:PHE:HE1	1:B:3451:LEU:CG	2.00	0.74
5:A:410:GLU:C	5:A:412:GLU:N	2.45	0.74
1:B:3404:ALA:H	1:B:3457:ILE:CG2	1.98	0.74
1:B:3740:PHE:CA	1:B:3742:PRO:HD3	2.17	0.74
1:B:3097:ILE:HD13	1:B:3097:ILE:N	2.03	0.74
3:D:419:UNK:CB	6:F:439:ILE:HD12	2.17	0.74
5:A:1068:ASN:O	5:A:1070:ARG:N	2.21	0.74
5:A:1859:LEU:O	5:A:1860:PHE:C	2.29	0.74
1:B:3171:LEU:HD23	1:B:3172:ARG:H	0.92	0.74
1:B:3427:ASN:ND2	1:B:3428:LYS:N	2.36	0.74
1:B:3494:ASN:HA	1:B:3497:HIS:HB3	1.70	0.74
1:B:3062:PHE:HZ	1:B:3658:GLU:N	1.85	0.74
1:B:3244:ASP:CA	1:B:3247:ARG:HD2	2.15	0.73
1:B:3659:LEU:O	1:B:3662:TYR:CB	2.36	0.73
2:C:721:GLN:O	2:C:724:LEU:CA	2.36	0.73
1:B:2638:ASN:C	1:B:2642:SER:HB3	2.13	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3057:TRP:O	1:B:3061:GLY:N	2.17	0.73
5:A:2005:SER:O	5:A:2009:HIS:N	2.18	0.73
1:B:3462:VAL:O	1:B:3464:PHE:CD2	2.41	0.73
7:G:163:VAL:CG2	7:G:175:ILE:HD13	1.76	0.73
7:G:185:LEU:O	7:G:189:LEU:N	2.17	0.73
1:B:3492:LYS:HE3	1:B:3492:LYS:CA	2.18	0.73
2:C:722:GLN:C	2:C:724:LEU:N	2.38	0.73
6:F:129:LEU:HD22	6:F:129:LEU:N	2.03	0.73
5:A:516:GLU:O	5:A:519:ARG:N	2.20	0.73
5:A:578:ASP:O	5:A:582:ASP:N	2.21	0.73
6:F:455:GLY:HA2	6:F:458:ILE:HD12	1.69	0.73
7:G:164:PRO:HG2	7:G:174:ALA:HB3	1.71	0.73
5:A:976:ALA:C	5:A:992:SER:CB	2.62	0.73
7:G:138:ALA:HB1	7:G:165:ILE:CD1	2.18	0.73
7:G:287:VAL:HG12	7:G:290:ARG:NH1	2.04	0.73
1:B:3741:MET:N	1:B:3742:PRO:HD2	2.03	0.73
7:G:236:ILE:O	7:G:254:ARG:NH1	2.21	0.73
1:B:2882:GLN:HA	1:B:2885:ARG:HG3	1.70	0.72
1:B:3625:THR:H	1:B:3626:PRO:HD3	1.52	0.72
1:B:3649:SER:HB2	1:B:3705:GLN:HA	1.70	0.72
5:A:239:LYS:O	5:A:242:THR:N	2.22	0.72
5:A:516:GLU:O	5:A:517:PHE:C	2.30	0.72
1:B:3055:LYS:C	1:B:3059:GLN:HB2	2.13	0.72
5:A:1069:LYS:CB	5:A:1072:TYR:CB	2.68	0.72
6:F:129:LEU:H	6:F:129:LEU:CD2	2.01	0.72
6:F:210:LYS:HB2	6:F:219:LYS:HA	1.72	0.72
6:F:415:SER:HA	6:F:420:LEU:HD23	1.71	0.72
5:A:972:LEU:O	5:A:973:ASP:O	2.07	0.72
1:B:3062:PHE:HZ	1:B:3658:GLU:CA	2.03	0.72
2:C:713:LYS:O	2:C:714:GLY:C	2.32	0.72
5:A:856:GLU:O	5:A:860:GLU:N	2.21	0.72
6:F:442:THR:OG1	6:F:443:GLY:N	2.06	0.72
4:H:57:ASN:O	4:H:61:ASN:N	2.16	0.72
6:F:8:VAL:HG22	8:E:368:TRP:HB3	1.70	0.72
5:A:1292:ILE:C	5:A:1294:CYS:N	2.36	0.71
1:B:3105:LEU:C	1:B:3105:LEU:HD12	2.15	0.71
1:B:3247:ARG:NH1	1:B:3407:TYR:CB	2.53	0.71
1:B:3388:TYR:HA	1:B:3405:VAL:CB	2.20	0.71
1:B:3424:ARG:HH12	1:B:3447:ILE:CA	1.96	0.71
6:F:92:TRP:O	6:F:96:ASN:ND2	2.23	0.71
1:B:3667:ILE:HD13	1:B:3692:VAL:C	2.14	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3105:LEU:HD12	1:B:3105:LEU:O	1.91	0.71
1:B:3444:ASN:O	1:B:3446:PRO:HD3	1.91	0.71
3:D:426:UNK:O	3:D:430:UNK:N	2.22	0.71
3:D:440:UNK:O	3:D:444:UNK:N	2.23	0.71
5:A:897:GLY:O	5:A:901:LEU:N	2.18	0.71
1:B:3509:LEU:HD11	2:C:687:ASN:HD22	1.54	0.71
3:D:150:UNK:O	3:D:153:UNK:N	2.23	0.71
1:B:2899:ASN:OD1	1:B:2899:ASN:N	2.17	0.71
1:B:3169:PHE:CZ	1:B:3451:LEU:HD21	2.25	0.71
1:B:3424:ARG:HD3	1:B:3445:LEU:CB	2.21	0.71
5:A:1032:SER:O	5:A:1033:ALA:HB3	1.89	0.71
1:B:3167:LEU:HD12	1:B:3167:LEU:O	1.90	0.71
3:D:151:UNK:O	3:D:155:UNK:N	2.24	0.71
1:B:2944:ALA:HA	1:B:2970:ILE:CD1	2.21	0.71
1:B:3644:ASN:CA	1:B:3647:THR:OG1	2.39	0.71
1:B:3106:TRP:CZ2	1:B:3668:ARG:HB2	2.24	0.71
5:A:1093:LYS:C	5:A:1095:LEU:N	2.48	0.71
7:G:16:MET:H	7:G:16:MET:HE3	1.54	0.70
1:B:3375:LEU:CB	1:B:3376:PRO:CD	2.68	0.70
5:A:583:ALA:O	5:A:587:TYR:N	2.23	0.70
6:F:212:ARG:O	6:F:275:ASN:ND2	2.20	0.70
1:B:3169:PHE:HE1	1:B:3451:LEU:HG	1.56	0.70
1:B:3171:LEU:C	1:B:3174:THR:HG1	1.98	0.70
1:B:3427:ASN:N	1:B:3443:PHE:CE1	2.58	0.70
1:B:3719:PHE:C	1:B:3722:ASP:HB2	2.15	0.70
6:F:442:THR:HG22	6:F:448:ARG:HE	1.49	0.70
7:G:151:ILE:CG2	7:G:297:ILE:HA	2.21	0.70
1:B:3086:LEU:N	1:B:3104:ILE:HD13	2.07	0.70
1:B:3418:ARG:O	1:B:3422:LEU:HD21	1.90	0.70
5:A:814:THR:O	5:A:818:SER:N	2.18	0.70
5:A:2415:ARG:O	5:A:2419:PRO:N	2.24	0.70
1:B:3101:LEU:HD13	1:B:3101:LEU:C	2.15	0.70
5:A:1090:THR:O	5:A:1092:ILE:N	2.25	0.70
5:A:1605:ASN:O	5:A:1607:VAL:N	2.24	0.70
5:A:2243:ILE:CB	5:A:2253:VAL:CA	2.69	0.70
7:G:132:PHE:N	7:G:357:ILE:O	2.25	0.70
5:A:2389:SER:O	5:A:2392:LYS:N	2.25	0.70
6:F:204:ILE:HB	6:F:274:TRP:CE3	2.26	0.70
1:B:3168:HIS:O	1:B:3172:ARG:N	2.25	0.70
2:C:754:ARG:O	2:C:758:ALA:N	2.24	0.70
1:B:3646:PHE:O	1:B:3649:SER:OG	2.08	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3667:ILE:HD13	1:B:3692:VAL:CA	2.21	0.70
3:D:172:UNK:N	8:E:357:THR:OG1	2.25	0.69
7:G:124:PHE:CZ	7:G:132:PHE:HB3	2.27	0.69
1:B:3101:LEU:O	1:B:3101:LEU:HD22	1.92	0.69
1:B:3391:LEU:H	1:B:3402:SER:CB	2.03	0.69
5:A:424:ASP:C	5:A:426:SER:N	2.50	0.69
5:A:1964:ASP:O	5:A:1968:ASN:N	2.21	0.69
1:B:3247:ARG:HG2	1:B:3248:LEU:N	2.05	0.69
1:B:3094:ASN:CB	1:B:3097:ILE:HG12	2.22	0.69
1:B:3253:LEU:CD1	1:B:3318:ARG:HG3	2.22	0.69
2:C:699:ARG:N	2:C:699:ARG:HD2	2.04	0.69
7:G:163:VAL:HG22	7:G:175:ILE:HG12	0.99	0.69
7:G:9:VAL:HG21	7:G:344:SER:HA	1.75	0.69
1:B:3173:THR:O	1:B:3452:SER:HB2	1.93	0.69
1:B:2914:ASN:OD1	1:B:2915:ALA:N	2.25	0.69
1:B:3100:LEU:HD13	1:B:3100:LEU:C	2.17	0.69
1:B:3737:ASP:OD2	1:B:3739:ASN:ND2	2.26	0.69
5:A:900:THR:CB	5:A:948:ILE:HD13	2.23	0.69
5:A:2181:MET:O	5:A:2185:PRO:N	2.26	0.69
6:F:428:LEU:CB	6:F:437:PHE:HE2	2.05	0.69
1:B:3422:LEU:H	1:B:3422:LEU:CD2	2.06	0.69
1:B:2962:VAL:HA	1:B:2965:SER:HB3	1.74	0.69
1:B:2967:LEU:HD12	1:B:2967:LEU:C	2.17	0.69
7:G:297:ILE:HB	7:G:329:ILE:HG13	1.76	0.68
1:B:2670:GLN:N	1:B:2837:PRO:CG	2.56	0.68
7:G:212:ILE:HG23	7:G:216:LEU:HD12	1.74	0.68
1:B:2817:CYS:CB	1:B:2852:PHE:HZ	2.07	0.68
1:B:3068:LEU:HD23	1:B:3081:ALA:HB1	1.71	0.68
1:B:3652:LEU:HD22	1:B:3652:LEU:C	2.17	0.68
5:A:1152:ALA:C	5:A:1154:SER:H	1.97	0.68
1:B:3670:GLU:O	1:B:3673:SER:OG	2.12	0.68
4:H:12:GLN:O	4:H:16:THR:N	2.27	0.68
5:A:369:TYR:O	5:A:373:GLU:N	2.26	0.68
6:F:1:MET:H	7:G:371:HIS:CG	2.12	0.68
1:B:3100:LEU:C	1:B:3100:LEU:HD22	2.17	0.68
7:G:121:GLN:O	7:G:362:TYR:OH	2.12	0.68
1:B:3568:THR:CB	1:B:3569:PRO:HD2	2.07	0.68
1:B:3644:ASN:O	1:B:3647:THR:OG1	2.09	0.68
6:F:91:GLN:CB	6:F:132:MET:HE1	2.20	0.68
1:B:3229:LEU:C	1:B:3229:LEU:HD12	2.18	0.68
1:B:3625:THR:N	1:B:3626:PRO:CD	2.56	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:444:HIS:C	6:F:446:ILE:N	2.52	0.68
6:F:266:ALA:C	6:F:282:ASN:HD21	2.01	0.68
1:B:3432:LYS:HB2	1:B:3432:LYS:HZ2	1.59	0.67
1:B:3514:PHE:O	1:B:3518:GLN:N	2.22	0.67
5:A:967:THR:O	5:A:968:GLU:O	2.11	0.67
7:G:151:ILE:CG2	7:G:297:ILE:HG12	2.24	0.67
1:B:3468:HIS:HB2	1:B:3570:HIS:HA	1.77	0.67
4:H:261:ARG:O	4:H:265:PHE:N	2.28	0.67
5:A:2243:ILE:CB	5:A:2253:VAL:HA	2.24	0.67
1:B:2651:ASN:O	1:B:2652:THR:C	2.37	0.67
7:G:24:ASP:HB2	7:G:340:TRP:HH2	1.60	0.67
7:G:299:MET:HE3	7:G:304:THR:HG22	1.76	0.67
8:E:382:ALA:O	8:E:385:THR:OG1	2.11	0.67
1:B:3703:VAL:C	1:B:3704:ALA:O	2.36	0.67
5:A:1249:GLN:O	5:A:1251:GLU:N	2.24	0.67
1:B:3481:ASP:CB	1:B:3482:PRO:HD2	2.24	0.67
1:B:3493:LEU:HD13	1:B:3493:LEU:C	2.19	0.67
1:B:3649:SER:CB	1:B:3704:ALA:O	2.43	0.67
5:A:430:THR:C	5:A:432:GLN:N	2.53	0.67
5:A:2243:ILE:CB	5:A:2252:SER:CB	2.72	0.67
2:C:684:TYR:HA	2:C:687:ASN:HB3	1.76	0.67
1:B:2670:GLN:HA	1:B:2837:PRO:HG3	1.72	0.67
1:B:3407:TYR:N	1:B:3408:PRO:HD2	2.04	0.67
6:F:11:GLY:N	6:F:461:SER:O	2.26	0.67
6:F:233:ALA:O	6:F:237:GLY:N	2.27	0.67
7:G:137:GLN:OE1	7:G:137:GLN:N	2.27	0.67
5:A:137:LEU:O	5:A:138:ASP:C	2.37	0.67
5:A:1069:LYS:O	5:A:1070:ARG:C	2.37	0.67
5:A:1345:LEU:HA	5:A:1349:MET:CB	2.25	0.67
7:G:347:ALA:O	7:G:353:GLN:NE2	2.27	0.67
7:G:163:VAL:HG21	7:G:175:ILE:HD11	1.58	0.67
1:B:3448:ALA:HA	1:B:3458:MET:HA	1.77	0.67
5:A:217:SER:O	5:A:218:MET:C	2.38	0.67
5:A:424:ASP:C	5:A:426:SER:H	2.03	0.67
1:B:3060:TRP:CZ3	1:B:3064:ASN:ND2	2.62	0.66
1:B:3169:PHE:CE1	1:B:3451:LEU:CD2	2.73	0.66
5:A:486:MET:O	5:A:490:GLY:N	2.28	0.66
5:A:1036:PRO:C	5:A:1038:ASN:H	2.02	0.66
7:G:312:ARG:NE	7:G:316:GLU:OE2	2.18	0.66
3:D:156:UNK:O	3:D:160:UNK:N	2.28	0.66
5:A:1090:THR:C	5:A:1092:ILE:N	2.53	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:242:LEU:N	7:G:246:GLN:O	2.26	0.66
1:B:3019:LYS:CG	1:B:3020:ALA:N	2.58	0.66
1:B:3116:MET:O	1:B:3117:LEU:C	2.38	0.66
1:B:3461:SER:CB	1:B:3464:PHE:HZ	2.06	0.66
7:G:275:ASP:OD1	7:G:276:GLN:N	2.24	0.66
1:B:2633:TRP:CB	5:A:2624:LYS:CA	2.73	0.66
4:H:113:LEU:O	4:H:117:LYS:N	2.24	0.66
5:A:353:HIS:O	5:A:357:THR:N	2.25	0.66
5:A:1859:LEU:C	5:A:1861:ARG:N	2.53	0.66
6:F:47:TYR:O	6:F:53:ASN:OD1	2.13	0.66
6:F:174:MET:HA	6:F:489[B]:ARG:HB3	1.78	0.66
7:G:239:SER:HA	7:G:249:THR:HA	1.78	0.66
1:B:3644:ASN:C	1:B:3647:THR:HG1	2.02	0.66
5:A:588:ARG:O	5:A:592:SER:N	2.17	0.66
1:B:2885:ARG:HD3	1:B:2885:ARG:C	2.20	0.66
1:B:3060:TRP:O	1:B:3063:PHE:N	2.28	0.66
1:B:3527:LEU:O	1:B:3531:PHE:N	2.25	0.66
7:G:99:GLU:HA	7:G:129:VAL:HA	1.78	0.66
1:B:3062:PHE:CZ	1:B:3657:ASN:O	2.49	0.66
1:B:3253:LEU:HD11	1:B:3318:ARG:HB2	1.78	0.66
2:C:695:GLN:O	2:C:699:ARG:HD3	1.96	0.65
3:D:64:UNK:O	6:F:434:SER:OG	2.06	0.65
3:D:396:UNK:HA	6:F:436:LYS:HE3	1.78	0.65
6:F:72:LYS:HD2	6:F:73:PRO:HD2	1.77	0.65
1:B:3086:LEU:N	1:B:3104:ILE:CD1	2.58	0.65
1:B:3423:TYR:CB	1:B:3558:MET:CE	2.74	0.65
5:A:1296:LEU:HA	5:A:1356:ALA:CB	2.26	0.65
6:F:169:PRO:HB2	6:F:176:LEU:HB2	1.79	0.65
7:G:163:VAL:HG23	7:G:175:ILE:HG23	1.78	0.65
1:B:3494:ASN:HD22	1:B:3497:HIS:HB3	1.61	0.65
5:A:1646:ASN:O	5:A:1649:ASP:N	2.30	0.65
5:A:1763:LYS:O	5:A:1767:PHE:N	2.30	0.65
1:B:3101:LEU:HD13	1:B:3101:LEU:O	1.96	0.65
5:A:1036:PRO:O	5:A:1038:ASN:N	2.29	0.65
5:A:2567:VAL:C	5:A:2569:LYS:N	2.52	0.65
1:B:3437:ARG:O	1:B:3440:SER:N	2.28	0.65
5:A:1201:CYS:HA	5:A:1209:LYS:HA	1.79	0.65
5:A:1452:SER:O	5:A:1456:ILE:N	2.30	0.65
8:E:366:ALA:C	8:E:368:TRP:H	2.05	0.65
1:B:2748:GLU:HB3	1:B:2752:HIS:HD2	1.59	0.65
1:B:3241:THR:O	1:B:3242:ASP:CB	2.43	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3541:PHE:O	1:B:3544:PHE:N	2.25	0.65
4:H:115:ASP:O	4:H:119:ASP:N	2.24	0.65
4:H:183:LYS:O	4:H:187:LEU:N	2.27	0.65
1:B:2998:GLU:O	1:B:3001:THR:N	2.30	0.64
1:B:2635:GLN:N	1:B:2635:GLN:OE1	2.28	0.64
5:A:2389:SER:O	5:A:2390:LEU:C	2.39	0.64
6:F:191:ASN:HA	6:F:194:ILE:HD12	1.79	0.64
6:F:254:THR:O	6:F:258:THR:N	2.29	0.64
1:B:2821:ILE:CB	1:B:2849:TYR:HE2	2.06	0.64
1:B:3509:LEU:HA	1:B:3512:GLU:HB3	1.79	0.64
1:B:3253:LEU:HD21	1:B:3314:LEU:CA	2.27	0.64
1:B:3062:PHE:CZ	1:B:3658:GLU:CA	2.80	0.64
7:G:138:ALA:CB	7:G:165:ILE:CD1	2.69	0.64
1:B:3489:MET:CE	1:B:3511:VAL:HG23	2.16	0.64
5:A:1247:ASP:O	5:A:1248:THR:CB	2.44	0.64
1:B:3159:ILE:O	1:B:3163:TYR:N	2.31	0.64
5:A:2243:ILE:CB	5:A:2252:SER:O	2.46	0.64
7:G:16:MET:HE1	7:G:157:ASP:CB	2.28	0.64
1:B:3427:ASN:HD22	1:B:3428:LYS:N	1.94	0.64
1:B:2691:GLY:O	1:B:2695:GLU:N	2.31	0.64
1:B:3509:LEU:O	1:B:3513:ILE:N	2.27	0.64
5:A:217:SER:O	5:A:219:PHE:N	2.30	0.64
5:A:389:PRO:O	5:A:392:TYR:N	2.30	0.64
5:A:483:ASP:O	5:A:487:LYS:N	2.30	0.64
5:A:1646:ASN:O	5:A:1647:PHE:C	2.39	0.64
1:B:2670:GLN:C	1:B:2837:PRO:HG3	2.23	0.63
4:H:189:ARG:O	4:H:193:LEU:N	2.20	0.63
5:A:122:LEU:CB	5:A:219:PHE:CB	2.75	0.63
5:A:579:PRO:O	5:A:583:ALA:N	2.31	0.63
7:G:138:ALA:HA	7:G:152:VAL:CG1	2.28	0.63
1:B:3474:PHE:HE2	1:B:3526:VAL:HG21	0.93	0.63
5:A:976:ALA:O	5:A:992:SER:CB	2.46	0.63
5:A:1091:SER:O	5:A:1099:ALA:HB2	1.98	0.63
1:B:2651:ASN:O	1:B:2654:ILE:N	2.31	0.63
1:B:3646:PHE:CB	1:B:3720:ILE:HD11	2.28	0.63
5:A:1117:THR:O	5:A:1121:ASN:N	2.29	0.63
3:D:278:UNK:O	3:D:282:UNK:N	2.31	0.63
6:F:16:ALA:HB2	6:F:107:PRO:HG2	1.80	0.63
6:F:71:LEU:CD1	6:F:229:LEU:HD22	2.29	0.63
5:A:686:LEU:O	5:A:690:PHE:N	2.20	0.63
6:F:107:PRO:HB2	6:F:469:TRP:CZ3	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1580:LEU:O	5:A:1583:LYS:CB	2.47	0.63
6:F:213:LYS:HE3	6:F:213:LYS:HA	1.80	0.63
1:B:2779:SER:O	1:B:2783:VAL:N	2.27	0.63
5:A:1372:GLU:C	5:A:1374:LEU:N	2.57	0.63
1:B:3040:ASN:OD1	1:B:3060:TRP:CZ2	2.52	0.62
1:B:3462:VAL:O	1:B:3464:PHE:N	2.32	0.62
1:B:3740:PHE:HB3	1:B:3742:PRO:HD3	1.80	0.62
3:D:277:UNK:O	3:D:281:UNK:N	2.31	0.62
2:C:673:SER:O	2:C:675:HIS:N	2.32	0.62
4:H:24:GLU:O	4:H:28:ASN:N	2.27	0.62
7:G:73:HIS:HA	7:G:159:VAL:HG13	1.82	0.62
1:B:3644:ASN:C	1:B:3647:THR:OG1	2.42	0.62
1:B:3244:ASP:O	1:B:3247:ARG:CG	2.45	0.62
1:B:3474:PHE:CG	1:B:3526:VAL:CG1	2.75	0.62
7:G:163:VAL:HG23	7:G:175:ILE:CB	2.28	0.62
7:G:273:GLY:O	7:G:277:THR:N	2.28	0.62
5:A:487:LYS:O	5:A:491:ARG:N	2.17	0.62
6:F:413:GLY:HA3	6:F:449:GLN:HE21	1.64	0.62
1:B:2912:ILE:HD13	1:B:2912:ILE:N	2.14	0.62
1:B:3404:ALA:C	1:B:3457:ILE:HG22	2.24	0.62
1:B:3492:LYS:N	1:B:3492:LYS:HD2	2.14	0.62
5:A:2256:GLY:O	5:A:2260:ALA:N	2.28	0.62
6:F:112:GLU:OE1	6:F:116:ASN:ND2	2.24	0.62
6:F:301:PRO:HG2	6:F:304:TRP:HB2	1.81	0.62
1:B:3055:LYS:CB	1:B:3059:GLN:CG	2.78	0.62
1:B:3404:ALA:O	1:B:3457:ILE:CG2	2.48	0.62
4:H:51:GLN:O	4:H:54:LEU:N	2.32	0.62
4:H:191:THR:O	4:H:195:LYS:N	2.33	0.62
5:A:2369:VAL:O	5:A:2370:LYS:C	2.42	0.62
1:B:2822:GLN:O	1:B:2824:SER:N	2.32	0.62
1:B:3054:ALA:O	1:B:3055:LYS:C	2.43	0.62
5:A:1097:ASP:C	5:A:1099:ALA:N	2.58	0.62
3:D:161:UNK:O	3:D:166:UNK:N	2.33	0.61
5:A:346:GLU:O	5:A:350:ALA:N	2.25	0.61
1:B:2943:ILE:C	1:B:2970:ILE:HD11	2.25	0.61
5:A:897:GLY:HA2	5:A:948:ILE:HD11	1.81	0.61
7:G:131:ALA:HA	7:G:358:SER:HA	1.82	0.61
3:D:74:UNK:O	3:D:75:UNK:CB	2.48	0.61
6:F:32:GLY:HA2	8:E:373:PHE:HZ	1.65	0.61
8:E:360:ASN:O	8:E:364:GLU:HG3	1.99	0.61
1:B:3418:ARG:O	1:B:3422:LEU:HD22	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3422:LEU:HD22	1:B:3422:LEU:N	2.09	0.61
2:C:739:SER:HA	3:D:328:UNK:O	2.01	0.61
1:B:3068:LEU:HD22	1:B:3081:ALA:HB3	1.79	0.61
1:B:3492:LYS:HA	1:B:3492:LYS:CE	2.28	0.61
2:C:721:GLN:O	2:C:724:LEU:N	2.32	0.61
3:D:168:UNK:O	3:D:171:UNK:N	2.34	0.61
4:H:119:ASP:O	4:H:122:LYS:N	2.30	0.61
6:F:80:VAL:HB	6:F:83:TRP:CZ2	2.36	0.61
7:G:150:GLY:HA3	7:G:296:ASN:HB2	1.81	0.61
1:B:3055:LYS:O	1:B:3056:ALA:C	2.43	0.61
1:B:3418:ARG:HH11	1:B:3418:ARG:CG	2.14	0.61
2:C:715:PRO:O	2:C:716:ARG:C	2.43	0.61
6:F:153:PRO:HB3	8:E:363:LEU:HD13	1.82	0.61
1:B:2651:ASN:ND2	1:B:2651:ASN:H	1.98	0.61
4:H:25:LEU:O	4:H:29:GLY:N	2.27	0.61
6:F:71:LEU:HD11	6:F:229:LEU:CD1	2.25	0.61
7:G:139:VAL:N	7:G:165:ILE:HD13	2.16	0.61
1:B:3062:PHE:HZ	1:B:3657:ASN:O	1.83	0.61
1:B:3062:PHE:CZ	1:B:3658:GLU:N	2.69	0.61
1:B:3354:ILE:CB	1:B:3355:PRO:CD	2.79	0.61
1:B:3427:ASN:HA	1:B:3443:PHE:HZ	1.58	0.61
4:H:231:SER:O	4:H:235:LEU:N	2.33	0.61
7:G:19:ALA:N	7:G:29:ALA:O	2.34	0.61
7:G:149:THR:HG23	7:G:166:TYR:HA	1.83	0.61
6:F:8:VAL:HG21	8:E:368:TRP:O	2.01	0.61
6:F:272:SER:OG	6:F:276:GLU:N	2.33	0.61
6:F:446:ILE:H	6:F:446:ILE:HD12	1.64	0.61
1:B:3101:LEU:HD22	1:B:3104:ILE:HB	1.81	0.60
1:B:3106:TRP:CZ2	1:B:3668:ARG:HB3	2.32	0.60
7:G:9:VAL:N	7:G:20:GLY:O	2.25	0.60
1:B:2895:VAL:O	1:B:2895:VAL:HG12	2.02	0.60
1:B:3556:VAL:O	1:B:3559:SER:OG	2.11	0.60
7:G:7:ALA:O	7:G:22:ALA:N	2.33	0.60
7:G:107:GLU:HB2	7:G:111:ASN:HD22	1.65	0.60
1:B:2636:SER:HA	1:B:2639:ILE:HG13	1.83	0.60
5:A:1152:ALA:C	5:A:1154:SER:N	2.57	0.60
1:B:3394:ARG:HA	1:B:3398:GLY:HA2	1.83	0.60
1:B:3437:ARG:C	1:B:3440:SER:H	2.09	0.60
1:B:3019:LYS:HG3	1:B:3020:ALA:N	2.17	0.60
1:B:3139:GLN:CB	1:B:3418:ARG:CZ	2.76	0.60
5:A:1036:PRO:C	5:A:1038:ASN:N	2.59	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1938:ALA:O	5:A:1942:VAL:N	2.31	0.60
6:F:308:ASN:OD1	6:F:309:SER:N	2.34	0.60
7:G:151:ILE:HG23	7:G:151:ILE:O	2.00	0.60
5:A:976:ALA:O	5:A:992:SER:CA	2.50	0.60
1:B:3068:LEU:HD12	1:B:3069:SER:N	2.17	0.60
5:A:424:ASP:O	5:A:425:GLU:C	2.45	0.60
5:A:634:PHE:O	5:A:638:PHE:N	2.33	0.60
5:A:872:LEU:O	5:A:876:LEU:N	2.28	0.60
1:B:3071:GLU:O	1:B:3072:PRO:O	2.19	0.60
2:C:739:SER:CB	3:D:328:UNK:O	2.49	0.60
7:G:147:ARG:NE	7:G:296:ASN:OD1	2.34	0.60
1:B:3169:PHE:CE1	1:B:3451:LEU:CG	2.85	0.60
1:B:3577:THR:O	5:A:965:ASP:N	2.35	0.60
5:A:878:PHE:O	5:A:881:LYS:N	2.34	0.60
5:A:995:PRO:CB	5:A:2558:ARG:CB	2.80	0.60
7:G:150:GLY:O	7:G:293:LEU:HD23	2.02	0.60
1:B:2638:ASN:O	1:B:2642:SER:CA	2.49	0.60
1:B:2690:ILE:CB	1:B:3715:VAL:CB	2.80	0.60
5:A:1103:LEU:C	5:A:1105:ASN:H	2.09	0.59
1:B:3441:ILE:O	1:B:3441:ILE:HG22	2.01	0.59
5:A:682:LEU:O	5:A:686:LEU:N	2.25	0.59
8:E:370:GLN:O	8:E:374:LYS:N	2.25	0.59
1:B:2822:GLN:O	1:B:2823:LEU:C	2.44	0.59
6:F:66:ARG:HB3	6:F:66:ARG:CZ	2.32	0.59
7:G:34:ILE:HD12	7:G:55:GLY:O	2.02	0.59
1:B:3169:PHE:CE1	1:B:3451:LEU:HG	2.37	0.59
1:B:3544:PHE:HE1	1:B:3579:GLY:HA2	1.67	0.59
5:A:1372:GLU:O	5:A:1374:LEU:C	2.44	0.59
6:F:87:GLN:HA	6:F:132:MET:HE3	1.83	0.59
6:F:171:VAL:O	6:F:174:MET:N	2.26	0.59
1:B:2970:ILE:O	1:B:2970:ILE:HG22	2.00	0.59
5:A:976:ALA:O	5:A:992:SER:HA	2.02	0.59
7:G:353:GLN:HA	7:G:356:TRP:CD1	2.38	0.59
1:B:2643:ILE:O	1:B:2643:ILE:HG23	2.00	0.59
5:A:914:ASP:O	5:A:917:ILE:N	2.35	0.59
6:F:99:TYR:OH	7:G:177:ARG:NH1	2.36	0.59
1:B:2835:TYR:O	1:B:2839:HIS:N	2.35	0.59
1:B:3085:TYR:CB	1:B:3104:ILE:CD1	2.81	0.59
5:A:430:THR:O	5:A:433:ILE:N	2.35	0.59
6:F:442:THR:HG21	6:F:448:ARG:CD	2.33	0.59
7:G:192:ILE:HD12	7:G:253:GLU:HG2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3366:VAL:HG13	1:B:3366:VAL:O	2.02	0.59
5:A:982:ILE:CB	5:A:2481:ASN:CA	2.80	0.59
5:A:1091:SER:O	5:A:1099:ALA:CB	2.51	0.59
6:F:171:VAL:HG11	6:F:400:LEU:HD13	1.84	0.59
1:B:3664:ALA:O	1:B:3667:ILE:HG13	2.03	0.58
7:G:287:VAL:HG23	7:G:287:VAL:O	2.02	0.58
5:A:894:VAL:O	5:A:897:GLY:N	2.33	0.58
1:B:3462:VAL:C	1:B:3464:PHE:H	2.10	0.58
5:A:474:ARG:O	5:A:478:LEU:N	2.35	0.58
5:A:594:LEU:O	5:A:597:ILE:N	2.36	0.58
5:A:1107:LEU:O	5:A:1111:CYS:N	2.36	0.58
5:A:1157:ILE:C	5:A:1159:GLU:H	2.06	0.58
6:F:211:GLN:HB2	6:F:217:ILE:HD12	1.84	0.58
7:G:172:PRO:HA	7:G:175:ILE:HD12	1.85	0.58
1:B:3097:ILE:O	1:B:3097:ILE:HG22	2.02	0.58
6:F:213:LYS:HA	6:F:213:LYS:CE	2.33	0.58
6:F:230:TYR:O	6:F:234:ASN:ND2	2.36	0.58
7:G:5:VAL:HB	7:G:101:HIS:CE1	2.37	0.58
7:G:159:VAL:HB	7:G:179:ASP:HA	1.83	0.58
1:B:3547:GLN:O	1:B:3551:GLN:N	2.31	0.58
7:G:357:ILE:HA	7:G:361:GLU:OE1	2.04	0.58
1:B:2817:CYS:CB	1:B:2852:PHE:CE2	2.86	0.58
1:B:2851:GLU:HA	1:B:2854:GLU:HB2	1.85	0.58
1:B:3106:TRP:HZ3	1:B:3668:ARG:CD	1.91	0.58
1:B:3483:ASP:N	1:B:3483:ASP:OD1	2.34	0.58
5:A:927:ALA:O	5:A:930:ASN:OD1	2.21	0.58
6:F:91:GLN:H	6:F:132:MET:HE1	1.69	0.58
7:G:144:SER:OG	7:G:338:SER:HB3	2.04	0.58
1:B:3171:LEU:O	1:B:3172:ARG:C	2.47	0.58
1:B:3354:ILE:CB	1:B:3369:ILE:O	2.51	0.58
4:H:109:ASP:O	4:H:113:LEU:N	2.22	0.58
5:A:341:SER:O	5:A:345:LYS:N	2.33	0.58
6:F:116:ASN:OD1	6:F:117:SER:N	2.37	0.58
1:B:3464:PHE:HA	1:B:3576:LYS:HZ1	1.69	0.58
6:F:94:LEU:O	6:F:100:LEU:N	2.35	0.58
1:B:2844:HIS:HA	1:B:2847:GLN:HB3	1.86	0.58
1:B:3421:GLN:OE1	1:B:3421:GLN:N	2.37	0.58
3:D:286:UNK:O	3:D:290:UNK:N	2.37	0.58
5:A:2601:ASN:O	5:A:2604:ASN:N	2.37	0.58
7:G:335:ARG:HA	7:G:338:SER:OG	2.04	0.58
7:G:139:VAL:HG13	7:G:165:ILE:CG2	2.29	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:58:SER:HB2	6:F:92:TRP:HH2	1.69	0.57
7:G:79:TRP:HZ2	7:G:115:ASN:OD1	1.85	0.57
6:F:444:HIS:O	6:F:446:ILE:CA	2.52	0.57
6:F:483:LEU:HG	6:F:487:ARG:HH12	1.70	0.57
1:B:3168:HIS:O	1:B:3172:ARG:CB	2.49	0.57
1:B:3515:ASN:ND2	1:B:3733:LEU:HD22	2.20	0.57
5:A:1373:GLU:O	5:A:1377:LEU:N	2.34	0.57
6:F:70:GLU:HG2	6:F:70:GLU:O	2.04	0.57
6:F:261:GLU:O	6:F:265:THR:HB	2.05	0.57
1:B:3229:LEU:HD12	1:B:3229:LEU:O	2.02	0.57
1:B:3450:PRO:C	1:B:3451:LEU:HD13	2.27	0.57
5:A:982:ILE:CB	5:A:2480:PHE:C	2.78	0.57
5:A:1581:GLU:O	5:A:1585:ARG:CA	2.52	0.57
6:F:210:LYS:HB3	6:F:217:ILE:HG22	1.85	0.57
1:B:2941:HIS:CD2	1:B:2941:HIS:N	2.73	0.57
3:D:172:UNK:O	3:D:176:UNK:N	2.38	0.57
5:A:2179:TRP:O	5:A:2183:ASN:N	2.28	0.57
5:A:2410:THR:O	5:A:2414:VAL:N	2.35	0.57
2:C:689:GLU:C	2:C:691:ARG:H	2.12	0.57
1:B:3740:PHE:HB2	1:B:3742:PRO:HD3	1.85	0.57
3:D:185:UNK:O	6:F:9:TYR:N	2.38	0.57
6:F:25:THR:HG22	6:F:41:PRO:HA	1.87	0.57
6:F:83:TRP:HB3	6:F:127:VAL:HG21	1.87	0.57
7:G:137:GLN:HG3	7:G:339:VAL:HG11	1.87	0.57
7:G:279:TYR:CZ	7:G:283:MET:HG3	2.40	0.57
7:G:349:LEU:HB2	7:G:352:PHE:HB3	1.86	0.57
1:B:2637:ILE:HG13	1:B:2665:LEU:HD12	1.86	0.57
7:G:250:ILE:HG22	7:G:254:ARG:HG3	1.87	0.57
1:B:3576:LYS:H	1:B:3576:LYS:CD	2.13	0.57
1:B:2822:GLN:C	1:B:2824:SER:N	2.61	0.56
1:B:3503:ALA:HB1	1:B:3506:MET:HB2	1.87	0.56
5:A:516:GLU:C	5:A:518:MET:N	2.62	0.56
6:F:10:GLY:HA2	6:F:463:GLY:H	1.69	0.56
6:F:148:PHE:HD2	6:F:459:LEU:HD11	1.70	0.56
7:G:34:ILE:HG12	7:G:69:TYR:CE1	2.39	0.56
7:G:238:LYS:O	7:G:250:ILE:N	2.38	0.56
6:F:87:GLN:CA	6:F:132:MET:CE	2.82	0.56
1:B:3555:PHE:HB2	1:B:3558:MET:HB3	1.87	0.56
5:A:1295:GLU:O	5:A:1356:ALA:HB1	2.04	0.56
1:B:2964:ILE:HD13	1:B:2964:ILE:N	2.19	0.56
1:B:3171:LEU:CG	1:B:3172:ARG:N	2.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:120:ASN:HA	6:F:123:LYS:HB3	1.88	0.56
7:G:8:LEU:HD12	7:G:103:VAL:HG22	1.87	0.56
6:F:170:ILE:HD13	6:F:175:THR:HA	1.87	0.56
1:B:2847:GLN:HA	1:B:2847:GLN:OE1	2.04	0.56
5:A:389:PRO:O	5:A:390:LEU:C	2.48	0.56
6:F:462:LEU:HD21	8:E:369:MET:HB2	1.88	0.56
7:G:36:GLY:HA3	7:G:67:LEU:HD23	1.88	0.56
1:B:2998:GLU:O	1:B:2999:LEU:C	2.48	0.56
1:B:3068:LEU:HB3	1:B:3078:ALA:CA	2.36	0.56
3:D:79:UNK:O	3:D:80:UNK:C	2.50	0.56
5:A:1157:ILE:C	5:A:1159:GLU:N	2.60	0.56
5:A:2524:LYS:O	5:A:2528:ALA:N	2.38	0.56
7:G:287:VAL:HG12	7:G:290:ARG:CZ	2.35	0.56
1:B:2651:ASN:H	1:B:2651:ASN:HD22	1.54	0.56
1:B:3085:TYR:CA	1:B:3104:ILE:HD11	2.35	0.56
1:B:3568:THR:CG2	1:B:3569:PRO:CD	2.75	0.56
1:B:2991:CYS:CB	1:B:2999:LEU:CB	2.83	0.56
1:B:3089:ALA:HB1	1:B:3100:LEU:HD11	1.88	0.56
7:G:37:ARG:C	7:G:65:LEU:HB3	2.31	0.56
7:G:300:SER:N	7:G:304:THR:HG21	2.20	0.56
1:B:2849:TYR:HA	1:B:2852:PHE:HB3	1.87	0.56
1:B:2898:TRP:C	1:B:2898:TRP:HE3	2.13	0.56
1:B:3068:LEU:CB	1:B:3078:ALA:HB2	2.33	0.56
1:B:3106:TRP:CZ3	1:B:3668:ARG:NH2	2.74	0.56
1:B:3354:ILE:HA	1:B:3371:ILE:N	2.15	0.56
1:B:3432:LYS:HB2	1:B:3432:LYS:NZ	2.21	0.56
1:B:3517:ILE:O	1:B:3521:PHE:N	2.36	0.56
5:A:972:LEU:O	5:A:973:ASP:C	2.47	0.56
6:F:213:LYS:HE3	6:F:213:LYS:O	2.05	0.56
1:B:3366:VAL:O	1:B:3367:HIS:O	2.24	0.55
1:B:3551:GLN:CD	1:B:3580:ASN:HA	2.31	0.55
1:B:3573:HIS:HB3	1:B:3582:PHE:HB3	1.87	0.55
6:F:44:TYR:HB3	6:F:74:ILE:HD11	1.88	0.55
7:G:58:ALA:HB1	7:G:67:LEU:HD22	1.87	0.55
1:B:3085:TYR:CB	1:B:3104:ILE:HD11	2.36	0.55
1:B:3015:GLY:HA2	1:B:3019:LYS:HB3	1.88	0.55
6:F:245:THR:OG1	6:F:246:LEU:HD12	2.05	0.55
7:G:187:ASP:O	7:G:191:LYS:HG3	2.07	0.55
2:C:797:ALA:O	2:C:801:LEU:N	2.39	0.55
5:A:1249:GLN:C	5:A:1251:GLU:H	2.14	0.55
6:F:266:ALA:O	6:F:282:ASN:ND2	2.34	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:6:ALA:O	7:G:101:HIS:ND1	2.34	0.55
5:A:137:LEU:C	5:A:139:SER:N	2.63	0.55
5:A:591:MET:O	5:A:595:LYS:N	2.23	0.55
7:G:27:PRO:HB3	7:G:340:TRP:CE2	2.42	0.55
7:G:283:MET:HE1	7:G:290:ARG:HD3	1.87	0.55
5:A:1372:GLU:O	5:A:1374:LEU:CA	2.54	0.55
6:F:48:THR:C	6:F:50:ASP:H	2.14	0.55
6:F:308:ASN:HA	6:F:382:LEU:H	1.71	0.55
7:G:16:MET:O	7:G:18:LYS:HG3	2.06	0.55
1:B:2651:ASN:C	1:B:2653:LYS:N	2.64	0.55
7:G:150:GLY:O	7:G:293:LEU:HD22	2.07	0.55
1:B:3085:TYR:O	1:B:3104:ILE:HD11	2.06	0.55
5:A:681:GLU:O	5:A:685:TYR:N	2.26	0.55
5:A:1044:LYS:C	5:A:1046:ALA:N	2.62	0.55
7:G:332:PRO:HD2	7:G:335:ARG:HB3	1.88	0.55
1:B:3023:PHE:HB3	1:B:3046:ALA:HB1	1.89	0.55
1:B:3375:LEU:CB	1:B:3376:PRO:HD2	2.37	0.55
5:A:2564:PHE:CB	5:A:2607:LEU:O	2.55	0.55
1:B:2797:PHE:HA	1:B:2852:PHE:HE1	1.71	0.54
1:B:3217:THR:HA	1:B:3220:PRO:HG3	1.89	0.54
1:B:3717:THR:O	1:B:3720:ILE:HB	2.06	0.54
5:A:1038:ASN:O	5:A:1039:TYR:C	2.50	0.54
7:G:138:ALA:C	7:G:165:ILE:CD1	2.80	0.54
7:G:286:ASP:HB2	7:G:288:ASP:OD2	2.08	0.54
7:G:108:ALA:HB1	7:G:109:PRO:HD2	1.89	0.54
7:G:330:ILE:HG22	7:G:332:PRO:HD3	1.89	0.54
1:B:3062:PHE:CZ	1:B:3658:GLU:CB	2.91	0.54
1:B:3474:PHE:CD1	1:B:3474:PHE:C	2.85	0.54
5:A:2260:ALA:O	5:A:2261:TRP:C	2.50	0.54
7:G:10:ILE:HA	7:G:19:ALA:HA	1.88	0.54
7:G:54:VAL:HB	7:G:88:HIS:CG	2.42	0.54
7:G:84:LYS:HA	7:G:87:HIS:HB3	1.90	0.54
1:B:2634:TYR:CD1	1:B:2634:TYR:N	2.75	0.54
1:B:3462:VAL:C	1:B:3464:PHE:N	2.65	0.54
1:B:3731:ARG:CD	2:C:694:TRP:CD1	2.88	0.54
6:F:458:ILE:HG12	8:E:373:PHE:HD2	1.72	0.54
1:B:3055:LYS:O	1:B:3059:GLN:HB2	2.06	0.54
1:B:3479:GLY:O	1:B:3480:PHE:O	2.26	0.54
1:B:3712:THR:CB	1:B:3713:PRO:HD2	2.37	0.54
6:F:20:ASP:OD2	6:F:452:SER:OG	2.18	0.54
7:G:107:GLU:HB3	7:G:134:VAL:HG11	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3570:HIS:C	1:B:3570:HIS:CD2	2.85	0.54
1:B:3586:MET:N	1:B:3586:MET:SD	2.81	0.54
5:A:580:ILE:HA	5:A:583:ALA:CB	2.38	0.54
5:A:873:ALA:O	5:A:877:PRO:N	2.41	0.54
5:A:1090:THR:O	5:A:1093:LYS:N	2.39	0.54
5:A:2225:ILE:HA	5:A:2229:GLU:CB	2.38	0.54
6:F:0:PRO:HB3	7:G:371:HIS:HB3	1.90	0.54
5:A:1652:ILE:C	5:A:1654:ASN:H	2.15	0.54
6:F:428:LEU:CB	6:F:437:PHE:CE2	2.85	0.54
8:E:365:GLU:O	8:E:368:TRP:HB2	2.08	0.54
1:B:2635:GLN:NE2	1:B:3539:GLU:CB	2.70	0.54
3:D:168:UNK:O	3:D:170:UNK:N	2.41	0.54
6:F:438:ARG:HG2	6:F:440:LEU:HD22	1.90	0.54
1:B:2635:GLN:HE21	1:B:3539:GLU:CB	2.20	0.54
1:B:3100:LEU:HD22	1:B:3100:LEU:O	2.06	0.54
1:B:3247:ARG:HH12	1:B:3407:TYR:CB	2.21	0.54
6:F:35:PHE:CD1	6:F:36:PRO:HD2	2.43	0.54
1:B:3044:ALA:HB2	1:B:3060:TRP:CH2	2.43	0.53
1:B:3071:GLU:O	1:B:3072:PRO:C	2.48	0.53
2:C:697:PHE:CD1	2:C:697:PHE:C	2.85	0.53
3:D:424:UNK:O	3:D:428:UNK:N	2.42	0.53
6:F:66:ARG:HG3	6:F:69:TYR:CG	2.43	0.53
7:G:349:LEU:HD13	8:E:394:TYR:CD2	2.44	0.53
5:A:601:LEU:O	5:A:604:PHE:N	2.41	0.53
7:G:91:TYR:HA	7:G:95:ARG:HA	1.90	0.53
1:B:3062:PHE:CE2	1:B:3658:GLU:CB	2.91	0.53
1:B:3246:PHE:CD1	1:B:3246:PHE:C	2.85	0.53
3:D:65:UNK:O	3:D:66:UNK:O	2.27	0.53
6:F:302:ALA:HA	6:F:306:ARG:HH21	1.73	0.53
6:F:447:GLU:HG2	6:F:450:TYR:OH	2.08	0.53
3:D:285:UNK:O	3:D:289:UNK:N	2.42	0.53
1:B:2961:ASP:O	1:B:2963:CYS:N	2.41	0.53
7:G:83:GLU:O	7:G:87:HIS:N	2.38	0.53
1:B:3568:THR:HG21	1:B:3739:ASN:HB3	1.91	0.53
2:C:694:TRP:HA	2:C:697:PHE:HD2	1.74	0.53
3:D:171:UNK:O	3:D:175:UNK:N	2.42	0.53
6:F:465:PHE:CE1	6:F:468:LEU:HD22	2.43	0.53
6:F:466:HIS:HA	6:F:469:TRP:CD1	2.44	0.53
7:G:371:HIS:O	8:E:380:LYS:NZ	2.33	0.53
1:B:3099:GLU:O	1:B:3099:GLU:HG2	2.08	0.53
1:B:3493:LEU:HD13	1:B:3497:HIS:HB2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:677:THR:O	2:C:678:HIS:O	2.26	0.53
5:A:1045:THR:CB	5:A:2511:VAL:CB	2.87	0.53
5:A:2036:LEU:O	5:A:2039:GLU:N	2.42	0.53
6:F:84:ASP:O	6:F:87:GLN:HB3	2.08	0.53
6:F:211:GLN:HB2	6:F:217:ILE:HB	1.90	0.53
1:B:3020:ALA:HB1	1:B:3050:ASP:CB	2.39	0.53
1:B:3354:ILE:CB	1:B:3355:PRO:HD2	2.38	0.53
1:B:3649:SER:HB2	1:B:3704:ALA:C	2.33	0.53
3:D:170:UNK:O	3:D:174:UNK:N	2.42	0.53
5:A:1652:ILE:O	5:A:1654:ASN:N	2.41	0.53
5:A:410:GLU:O	5:A:412:GLU:N	2.42	0.53
1:B:2791:ARG:O	1:B:2792:GLN:C	2.51	0.53
3:D:180:UNK:C	3:D:182:UNK:H	2.21	0.53
6:F:151:GLY:H	8:E:370:GLN:HE22	1.57	0.53
1:B:3107:LEU:HD12	1:B:3110:ILE:HD12	1.90	0.52
1:B:3389:ARG:O	1:B:3404:ALA:HA	2.10	0.52
5:A:1012:HIS:C	5:A:1014:ARG:H	2.15	0.52
1:B:3505:ASP:HA	1:B:3508:ILE:HB	1.91	0.52
6:F:249:ILE:HD12	6:F:420:LEU:HB2	1.91	0.52
1:B:3489:MET:CE	1:B:3511:VAL:CG2	2.83	0.52
1:B:3517:ILE:O	1:B:3520:MET:N	2.43	0.52
6:F:190:ILE:O	6:F:194:ILE:HG13	2.09	0.52
7:G:80:ASP:O	7:G:83:GLU:HB3	2.08	0.52
1:B:3246:PHE:HE2	1:B:3322:GLU:HA	1.75	0.52
1:B:2941:HIS:C	1:B:2943:ILE:H	2.18	0.52
1:B:2944:ALA:N	1:B:2970:ILE:CD1	2.73	0.52
1:B:3541:PHE:HE2	1:B:3545:ARG:NE	2.07	0.52
1:B:3656:ASP:C	1:B:3658:GLU:N	2.59	0.52
6:F:8:VAL:CG2	8:E:368:TRP:HB3	2.38	0.52
7:G:33:SER:O	7:G:33:SER:OG	2.18	0.52
1:B:3085:TYR:O	1:B:3104:ILE:CD1	2.56	0.52
1:B:3436:THR:O	1:B:3440:SER:N	2.43	0.52
6:F:19:ILE:HG22	6:F:21:PRO:HD3	1.91	0.52
6:F:80:VAL:HB	6:F:83:TRP:CH2	2.43	0.52
1:B:2898:TRP:C	1:B:2898:TRP:CE3	2.88	0.52
1:B:3576:LYS:CD	1:B:3576:LYS:N	2.73	0.52
6:F:119:GLU:O	6:F:123:LYS:N	2.24	0.52
2:C:692:THR:N	2:C:693:PRO:CD	2.73	0.52
5:A:430:THR:O	5:A:432:GLN:CA	2.56	0.52
5:A:787:HIS:O	5:A:791:LEU:N	2.28	0.52
6:F:62:ILE:HG12	6:F:71:LEU:HD23	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:86:TRP:NE1	7:G:105:LEU:HD21	2.24	0.52
1:B:3160:ALA:HA	1:B:3167:LEU:CD2	2.39	0.52
1:B:3387:SER:O	1:B:3388:TYR:O	2.27	0.52
1:B:3553:SER:O	1:B:3556:VAL:HG22	2.10	0.52
6:F:114:VAL:HG11	6:F:180:THR:HG21	1.92	0.52
6:F:442:THR:HG21	6:F:448:ARG:HG2	1.91	0.52
6:F:447:GLU:HG2	6:F:450:TYR:CZ	2.45	0.52
7:G:255:PHE:C	7:G:258:PRO:HD2	2.35	0.52
1:B:3432:LYS:NZ	1:B:3432:LYS:CB	2.73	0.52
1:B:3721:LEU:HA	1:B:3724:ILE:HD12	1.91	0.52
2:C:722:GLN:O	2:C:724:LEU:N	2.42	0.52
6:F:151:GLY:H	8:E:370:GLN:NE2	2.07	0.52
6:F:272:SER:HG	6:F:274:TRP:CD1	2.26	0.52
7:G:169:PHE:CE1	8:E:381:VAL:HG22	2.45	0.52
1:B:3246:PHE:CE2	1:B:3322:GLU:HA	2.45	0.51
1:B:3706:LEU:CB	1:B:3720:ILE:HG13	2.40	0.51
5:A:1027:LEU:O	5:A:1030:LYS:N	2.37	0.51
6:F:291:GLU:HG3	6:F:296:LYS:H	1.75	0.51
7:G:208:ILE:HD12	7:G:208:ILE:H	1.75	0.51
3:D:438:UNK:O	6:F:266:ALA:N	2.42	0.51
5:A:1201:CYS:C	5:A:1203:ASP:H	2.18	0.51
5:A:1581:GLU:C	5:A:1583:LYS:H	2.17	0.51
1:B:2659:GLU:HG2	1:B:2681:ARG:CB	2.36	0.51
1:B:3020:ALA:CB	1:B:3050:ASP:CB	2.89	0.51
1:B:3418:ARG:CG	1:B:3418:ARG:NH1	2.73	0.51
1:B:3492:LYS:N	1:B:3492:LYS:CD	2.73	0.51
1:B:3492:LYS:HD2	1:B:3492:LYS:H	1.75	0.51
6:F:20:ASP:OD2	6:F:453:TRP:N	2.43	0.51
6:F:151:GLY:O	8:E:367:LYS:HE2	2.11	0.51
1:B:3366:VAL:O	1:B:3367:HIS:C	2.51	0.51
1:B:3551:GLN:O	1:B:3553:SER:N	2.43	0.51
2:C:739:SER:CA	3:D:328:UNK:O	2.58	0.51
3:D:414:UNK:C	3:D:416:UNK:H	2.22	0.51
5:A:958:GLN:O	5:A:960:LEU:N	2.43	0.51
5:A:348:LEU:O	5:A:352:ARG:N	2.36	0.51
7:G:286:ASP:HB2	7:G:288:ASP:CG	2.35	0.51
5:A:2012:ASN:O	5:A:2016:PHE:N	2.43	0.51
6:F:48:THR:O	6:F:50:ASP:N	2.44	0.51
1:B:3171:LEU:O	1:B:3174:THR:CB	2.59	0.51
1:B:3464:PHE:HA	1:B:3576:LYS:NZ	2.26	0.51
1:B:3666:PHE:HA	1:B:3669:ASP:OD2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1103:LEU:O	5:A:1105:ASN:N	2.40	0.51
7:G:9:VAL:HG13	7:G:104:LEU:HD23	1.93	0.51
1:B:3097:ILE:N	1:B:3097:ILE:CD1	2.73	0.51
1:B:3555:PHE:CD1	1:B:3581:VAL:HG11	2.45	0.51
5:A:957:ARG:O	5:A:959:PHE:N	2.44	0.51
5:A:2541:PHE:O	5:A:2544:SER:N	2.44	0.51
6:F:241:GLU:HA	6:F:244:GLU:HG3	1.92	0.51
7:G:190:MET:HE1	7:G:206:ARG:NH2	2.26	0.51
1:B:3444:ASN:ND2	1:B:3580:ASN:HD22	2.08	0.51
1:B:3461:SER:CB	1:B:3464:PHE:CE2	2.94	0.51
5:A:978:ALA:O	5:A:990:PRO:HA	2.11	0.51
5:A:1867:LEU:O	5:A:1871:PHE:N	2.41	0.51
1:B:3242:ASP:O	1:B:3245:LEU:N	2.44	0.51
1:B:3504:PRO:O	1:B:3507:THR:OG1	2.24	0.51
1:B:3576:LYS:HD3	1:B:3576:LYS:N	2.20	0.51
6:F:24:TYR:CD2	6:F:25:THR:HG23	2.46	0.50
5:A:1589:ASP:O	5:A:1590:SER:C	2.54	0.50
7:G:109:PRO:HD2	7:G:161:HIS:CD2	2.46	0.50
7:G:132:PHE:CG	7:G:133:TYR:N	2.78	0.50
7:G:313:MET:O	7:G:317:ILE:HG12	2.11	0.50
1:B:3085:TYR:C	1:B:3104:ILE:HD13	2.24	0.50
1:B:3247:ARG:CG	1:B:3248:LEU:N	2.74	0.50
1:B:3474:PHE:CD2	1:B:3526:VAL:CB	2.94	0.50
5:A:328:LEU:O	5:A:332:LEU:N	2.39	0.50
1:B:2639:ILE:O	1:B:2643:ILE:N	2.43	0.50
1:B:3242:ASP:O	1:B:3243:GLU:C	2.52	0.50
5:A:871:VAL:O	5:A:874:PRO:N	2.45	0.50
6:F:27:ASN:ND2	6:F:450:TYR:HA	2.26	0.50
7:G:78:ASN:ND2	7:G:81:ASP:OD2	2.44	0.50
7:G:109:PRO:HG2	7:G:161:HIS:CD2	2.46	0.50
1:B:2633:TRP:CB	5:A:2625:TYR:N	2.75	0.50
5:A:425:GLU:O	5:A:426:SER:CB	2.60	0.50
6:F:187:GLY:O	6:F:243:LYS:NZ	2.44	0.50
7:G:99:GLU:C	7:G:130:PRO:HD3	2.37	0.50
5:A:511:ASP:O	5:A:515:GLU:CA	2.60	0.50
5:A:1441:LEU:O	5:A:1445:PHE:CB	2.59	0.50
7:G:355:MET:HA	7:G:373:LYS:HZ1	1.77	0.50
1:B:2888:LEU:HA	5:A:953:GLY:HA2	1.94	0.50
1:B:3060:TRP:O	1:B:3061:GLY:C	2.53	0.50
1:B:3668:ARG:HG2	1:B:3672:ILE:HG23	1.93	0.50
5:A:967:THR:O	5:A:968:GLU:C	2.55	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:982:ILE:CB	5:A:2481:ASN:N	2.75	0.50
7:G:208:ILE:HG12	7:G:243:PRO:HG3	1.92	0.50
1:B:3068:LEU:HB2	1:B:3078:ALA:HB2	1.83	0.50
1:B:3106:TRP:HE3	1:B:3665:LEU:HD12	1.73	0.50
1:B:3574:VAL:HA	1:B:3580:ASN:O	2.12	0.50
1:B:3618:GLU:O	1:B:3620:VAL:CA	2.60	0.50
2:C:695:GLN:O	2:C:699:ARG:HG2	2.11	0.50
3:D:11:UNK:O	3:D:13:UNK:N	2.44	0.50
5:A:2381:ALA:O	5:A:2384:ILE:CB	2.60	0.50
1:B:3096:LYS:C	1:B:3097:ILE:HD13	2.35	0.49
1:B:3171:LEU:O	1:B:3174:THR:CA	2.60	0.49
1:B:3699:ILE:O	1:B:3700:ILE:C	2.55	0.49
5:A:1207:TYR:O	5:A:1208:ASN:C	2.55	0.49
7:G:345:ILE:O	7:G:349:LEU:HG	2.12	0.49
1:B:3467:LEU:CD1	1:B:3467:LEU:C	2.86	0.49
5:A:580:ILE:C	5:A:583:ALA:H	2.19	0.49
5:A:1650:PHE:C	5:A:1652:ILE:N	2.70	0.49
7:G:139:VAL:N	7:G:165:ILE:CD1	2.75	0.49
7:G:155:SER:HA	7:G:160:THR:HG23	1.93	0.49
1:B:2737:ALA:CB	1:B:2746:LEU:HD11	2.42	0.49
1:B:2885:ARG:C	1:B:2885:ARG:CD	2.85	0.49
1:B:2912:ILE:N	1:B:2912:ILE:CD1	2.74	0.49
5:A:239:LYS:O	5:A:240:GLN:C	2.47	0.49
6:F:128:LEU:HD13	6:F:134:PHE:CE2	2.48	0.49
6:F:182:ARG:N	6:F:388:LEU:HD11	2.26	0.49
7:G:275:ASP:OD2	7:G:316:GLU:HB3	2.12	0.49
7:G:360:GLN:O	7:G:364:GLU:N	2.45	0.49
2:C:690:ARG:HH12	2:C:763:ALA:HB1	1.78	0.49
4:H:185:LEU:O	4:H:189:ARG:N	2.32	0.49
7:G:125:GLU:HG3	7:G:362:TYR:OH	2.13	0.49
1:B:2874:ALA:C	1:B:2876:GLU:H	2.18	0.49
1:B:3015:GLY:C	1:B:3019:LYS:HB3	2.38	0.49
1:B:3040:ASN:OD1	1:B:3060:TRP:HZ2	1.93	0.49
1:B:3424:ARG:NH2	1:B:3424:ARG:HG2	2.27	0.49
6:F:148:PHE:CD2	6:F:459:LEU:HD11	2.47	0.49
7:G:10:ILE:HG12	7:G:19:ALA:HB1	1.94	0.49
7:G:312:ARG:O	7:G:316:GLU:HG2	2.12	0.49
1:B:2944:ALA:CA	1:B:2970:ILE:CD1	2.88	0.49
5:A:736:PHE:N	5:A:1543:LEU:O	2.46	0.49
6:F:58:SER:HB2	6:F:92:TRP:CH2	2.47	0.49
7:G:138:ALA:HB1	7:G:163:VAL:HG12	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:286:ASP:HB2	7:G:288:ASP:OD1	2.11	0.49
1:B:3393:ILE:CB	1:B:3400:VAL:HA	2.43	0.49
1:B:3407:TYR:N	1:B:3408:PRO:HD3	2.20	0.49
1:B:3617:ASN:O	1:B:3618:GLU:C	2.55	0.49
3:D:3:UNK:O	3:D:7:UNK:N	2.45	0.49
5:A:302:THR:C	5:A:304:PHE:N	2.71	0.49
5:A:1012:HIS:C	5:A:1014:ARG:N	2.67	0.49
5:A:1745:LEU:O	5:A:1749:ASP:N	2.32	0.49
6:F:72:LYS:CD	6:F:73:PRO:HD2	2.41	0.49
6:F:122:LYS:HG2	6:F:484:LEU:HD11	1.94	0.49
1:B:2670:GLN:O	1:B:2837:PRO:HB3	2.11	0.49
1:B:3583:THR:O	1:B:3586:MET:HE1	2.12	0.49
5:A:741:LEU:O	5:A:744:LEU:N	2.46	0.49
6:F:10:GLY:C	6:F:12:ASP:H	2.19	0.49
1:B:2844:HIS:C	1:B:2846:PHE:N	2.70	0.49
1:B:3474:PHE:CE2	1:B:3526:VAL:CB	2.88	0.49
4:H:183:LYS:O	4:H:184:LEU:C	2.56	0.49
6:F:118:THR:HA	6:F:121:ARG:HD2	1.95	0.49
6:F:132:MET:HB2	6:F:134:PHE:CZ	2.47	0.49
6:F:193:LEU:HD21	6:F:299:ASP:HB3	1.95	0.49
6:F:475:TYR:C	6:F:475:TYR:CD1	2.85	0.49
5:A:806:LEU:O	5:A:809:PHE:N	2.46	0.49
5:A:2169:TYR:O	5:A:2173:LYS:N	2.46	0.49
5:A:2539:SER:O	5:A:2543:ASP:N	2.30	0.49
6:F:87:GLN:CA	6:F:132:MET:HE3	2.42	0.49
6:F:205:PRO:HG3	6:F:230:TYR:CD1	2.48	0.49
7:G:349:LEU:HD13	8:E:394:TYR:CE2	2.48	0.49
1:B:3086:LEU:HA	1:B:3104:ILE:HD12	1.94	0.48
5:A:1605:ASN:C	5:A:1607:VAL:N	2.71	0.48
6:F:70:GLU:HB2	6:F:226:ASP:OD2	2.11	0.48
6:F:466:HIS:HA	6:F:469:TRP:HD1	1.76	0.48
7:G:139:VAL:CA	7:G:165:ILE:HD13	2.43	0.48
1:B:3697:ASP:O	1:B:3701:ARG:HG3	2.13	0.48
3:D:215:UNK:O	3:D:216:UNK:CB	2.59	0.48
1:B:3068:LEU:HD12	1:B:3068:LEU:C	2.39	0.48
1:B:3143:SER:OG	1:B:3204:PRO:CB	2.61	0.48
2:C:763:ALA:O	2:C:767:CYS:N	2.42	0.48
6:F:297:GLU:O	6:F:300:ILE:N	2.44	0.48
1:B:3040:ASN:O	1:B:3060:TRP:HZ2	1.95	0.48
1:B:3098:ARG:O	1:B:3134:ILE:CB	2.61	0.48
1:B:3360:LEU:CB	1:B:3424:ARG:HH22	2.18	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3372:ALA:HB3	1:B:3395:GLY:HA2	1.95	0.48
5:A:1653:SER:O	5:A:1654:ASN:C	2.56	0.48
1:B:3503:ALA:O	1:B:3506:MET:HB3	2.13	0.48
1:B:3556:VAL:C	1:B:3559:SER:HG	2.14	0.48
1:B:3674:TRP:CZ3	1:B:3678:LEU:HB2	2.48	0.48
6:F:145:CYS:O	6:F:455:GLY:HA3	2.14	0.48
1:B:3068:LEU:CB	1:B:3078:ALA:HA	2.40	0.48
5:A:1962:THR:O	5:A:1966:TRP:N	2.31	0.48
7:G:124:PHE:HB2	7:G:362:TYR:CD2	2.48	0.48
7:G:336:LYS:HG2	7:G:337:TYR:CE1	2.48	0.48
1:B:3468:HIS:ND1	1:B:3569:PRO:HB2	2.28	0.48
7:G:16:MET:N	7:G:16:MET:HE3	2.26	0.48
7:G:101:HIS:O	7:G:103:VAL:HG23	2.13	0.48
7:G:310:ALA:O	7:G:313:MET:HB2	2.14	0.48
1:B:3236:ARG:NE	1:B:3338:CYS:CB	2.76	0.48
1:B:3646:PHE:CB	1:B:3720:ILE:CD1	2.92	0.48
5:A:1044:LYS:C	5:A:1046:ALA:H	2.22	0.48
5:A:1255:ALA:O	5:A:1256:ILE:C	2.56	0.48
7:G:312:ARG:O	7:G:316:GLU:N	2.28	0.48
8:E:357:THR:N	8:E:361:ILE:HD12	2.29	0.48
1:B:2874:ALA:C	1:B:2876:GLU:N	2.71	0.48
1:B:3062:PHE:HZ	1:B:3658:GLU:HA	1.77	0.48
1:B:3650:ARG:O	1:B:3654:GLU:N	2.45	0.48
6:F:92:TRP:CD1	6:F:96:ASN:HD21	2.31	0.48
7:G:190:MET:SD	7:G:203:THR:HG22	2.53	0.48
1:B:2663:LEU:HD13	1:B:2663:LEU:HA	1.72	0.48
1:B:3509:LEU:HD12	1:B:3510:LYS:N	2.28	0.48
3:D:2:UNK:CB	3:D:16:UNK:HA	2.44	0.48
3:D:162:UNK:O	3:D:165:UNK:N	2.47	0.48
5:A:1859:LEU:C	5:A:1861:ARG:H	2.20	0.48
6:F:118:THR:O	6:F:121:ARG:HB2	2.13	0.48
1:B:3493:LEU:C	1:B:3493:LEU:CD1	2.86	0.47
2:C:679:ARG:C	2:C:681:THR:H	2.22	0.47
5:A:2257:VAL:O	5:A:2261:TRP:N	2.41	0.47
6:F:48:THR:C	6:F:50:ASP:N	2.71	0.47
6:F:87:GLN:C	6:F:132:MET:HE2	2.38	0.47
6:F:190:ILE:HD11	6:F:292:LEU:HD11	1.96	0.47
6:F:412:GLY:O	6:F:415:SER:OG	2.28	0.47
6:F:444:HIS:O	6:F:447:GLU:N	2.47	0.47
6:F:447:GLU:HA	6:F:450:TYR:CE1	2.49	0.47
1:B:2748:GLU:HB3	1:B:2752:HIS:NE2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1560:HIS:CB	5:A:1598:ARG:CB	2.92	0.47
5:A:1646:ASN:O	5:A:1648:TYR:N	2.47	0.47
7:G:261:LEU:HB3	7:G:274:ILE:HD13	1.96	0.47
3:D:168:UNK:O	3:D:169:UNK:C	2.62	0.47
5:A:834:ILE:O	5:A:838:LEU:N	2.27	0.47
6:F:213:LYS:CB	6:F:214:PRO:HD3	2.35	0.47
6:F:241:GLU:O	6:F:244:GLU:HB2	2.14	0.47
6:F:244:GLU:HB3	7:G:287:VAL:CG1	2.44	0.47
1:B:3449:ILE:HG22	1:B:3451:LEU:HD11	1.97	0.47
2:C:695:GLN:O	2:C:699:ARG:CD	2.61	0.47
2:C:702:GLN:OE1	2:C:702:GLN:HA	2.14	0.47
5:A:982:ILE:CB	5:A:2481:ASN:HA	2.42	0.47
6:F:36:PRO:HB3	6:F:453:TRP:CE2	2.48	0.47
6:F:174:MET:HA	6:F:489[A]:ARG:HB3	1.95	0.47
6:F:432:LEU:HD21	6:F:435:LEU:HD22	1.96	0.47
7:G:72:GLU:HB2	7:G:77:THR:HG21	1.97	0.47
7:G:124:PHE:HB2	7:G:362:TYR:CE2	2.49	0.47
1:B:3427:ASN:CA	1:B:3443:PHE:HZ	2.17	0.47
1:B:3427:ASN:HD22	1:B:3428:LYS:H	1.61	0.47
6:F:107:PRO:HB2	6:F:469:TRP:CH2	2.49	0.47
1:B:3491:ASP:HB3	1:B:3492:LYS:NZ	2.30	0.47
1:B:3545:ARG:NH1	1:B:3633:GLY:HA2	2.29	0.47
5:A:1091:SER:HA	5:A:1099:ALA:CA	2.44	0.47
5:A:1417:LYS:HA	5:A:1420:ALA:HB3	1.97	0.47
5:A:1581:GLU:O	5:A:1585:ARG:CB	2.63	0.47
7:G:82:MET:HE3	7:G:86:TRP:NE1	2.29	0.47
7:G:351:THR:O	7:G:354:GLN:HG2	2.15	0.47
8:E:392:LYS:O	8:E:396:THR:HG23	2.15	0.47
1:B:2637:ILE:HA	1:B:2640:LEU:HB3	1.95	0.47
1:B:2839:HIS:O	1:B:2843:LEU:HG	2.15	0.47
1:B:3168:HIS:ND1	1:B:3168:HIS:C	2.73	0.47
1:B:3296:PHE:CD1	1:B:3296:PHE:C	2.92	0.47
1:B:3481:ASP:CB	1:B:3482:PRO:HD3	2.42	0.47
1:B:3658:GLU:O	1:B:3662:TYR:N	2.38	0.47
1:B:3699:ILE:O	1:B:3702:LYS:N	2.48	0.47
1:B:3721:LEU:HG	1:B:3724:ILE:HD12	1.96	0.47
5:A:461:LYS:O	5:A:465:MET:N	2.32	0.47
5:A:1086:VAL:O	5:A:1090:THR:N	2.38	0.47
5:A:2352:ILE:O	5:A:2356:SER:N	2.46	0.47
6:F:442:THR:HG21	6:F:448:ARG:HG3	1.92	0.47
7:G:9:VAL:O	7:G:20:GLY:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3065:ASP:O	1:B:3068:LEU:HG	2.14	0.47
1:B:3391:LEU:C	1:B:3402:SER:CB	2.87	0.47
1:B:3493:LEU:O	1:B:3493:LEU:HD13	2.14	0.47
3:D:4:UNK:O	3:D:8:UNK:N	2.47	0.47
4:H:86:ASN:O	4:H:89:PRO:N	2.47	0.47
1:B:2635:GLN:N	1:B:2635:GLN:CD	2.72	0.47
1:B:2969:ARG:O	1:B:2969:ARG:HD3	2.15	0.47
1:B:3100:LEU:HD13	1:B:3101:LEU:HA	1.97	0.47
1:B:3731:ARG:HB3	2:C:694:TRP:HE1	1.80	0.47
3:D:420:UNK:C	3:D:422:UNK:N	2.77	0.47
7:G:180:LEU:HD23	7:G:184:ASP:OD2	2.14	0.47
7:G:359:LYS:O	7:G:362:TYR:HB3	2.15	0.47
1:B:3163:TYR:CB	1:B:3167:LEU:HB3	2.45	0.47
5:A:31:LEU:O	5:A:35:MET:N	2.48	0.47
5:A:330:ILE:O	5:A:334:GLN:CB	2.63	0.47
5:A:566:TYR:C	5:A:568:PRO:N	2.73	0.47
8:E:391:ILE:CA	8:E:394:TYR:HB2	2.32	0.47
1:B:2837:PRO:O	1:B:2840:LYS:N	2.47	0.46
1:B:3649:SER:HB2	1:B:3705:GLN:CA	2.42	0.46
1:B:3668:ARG:NE	1:B:3672:ILE:HD13	2.15	0.46
5:A:1043:LEU:O	5:A:1046:ALA:N	2.46	0.46
6:F:264:SER:O	6:F:265:THR:OG1	2.30	0.46
7:G:82:MET:HG3	7:G:86:TRP:CZ2	2.50	0.46
1:B:3244:ASP:O	1:B:3247:ARG:CD	2.63	0.46
1:B:3740:PHE:CB	1:B:3742:PRO:CD	2.84	0.46
3:D:61:UNK:C	3:D:63:UNK:N	2.78	0.46
5:A:1036:PRO:O	5:A:1039:TYR:N	2.33	0.46
5:A:1345:LEU:CA	5:A:1349:MET:CB	2.92	0.46
5:A:2092:LEU:O	5:A:2095:ALA:HB3	2.14	0.46
6:F:61:SER:OG	7:G:270:GLU:O	2.25	0.46
1:B:3496:ALA:CB	2:C:684:TYR:CD1	2.98	0.46
1:B:3668:ARG:NE	1:B:3672:ILE:HG21	2.29	0.46
6:F:152:ARG:HD3	6:F:407:ASN:OD1	2.15	0.46
1:B:3229:LEU:C	1:B:3229:LEU:CD1	2.85	0.46
4:H:183:LYS:O	4:H:186:LYS:N	2.49	0.46
5:A:981:LYS:CB	5:A:988:ASP:HA	2.44	0.46
5:A:1673:PHE:O	5:A:1674:ASN:C	2.58	0.46
6:F:302:ALA:C	6:F:304:TRP:H	2.22	0.46
1:B:3427:ASN:N	1:B:3443:PHE:HZ	2.09	0.46
5:A:1003:ILE:CB	5:A:1017:ALA:HB2	2.45	0.46
5:A:1948:VAL:O	5:A:1952:VAL:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:72:LYS:NZ	6:F:72:LYS:CB	2.73	0.46
6:F:110:LEU:HD23	6:F:111:THR:N	2.31	0.46
6:F:285:ARG:HA	6:F:288:PHE:CE2	2.50	0.46
7:G:14:SER:HB2	7:G:157:ASP:CB	2.45	0.46
8:E:361:ILE:HA	8:E:364:GLU:CD	2.41	0.46
1:B:2690:ILE:C	1:B:3715:VAL:CB	2.89	0.46
1:B:3107:LEU:HD12	1:B:3110:ILE:CD1	2.45	0.46
3:D:139:UNK:O	6:F:178:LYS:HE3	2.16	0.46
5:A:635:LYS:O	5:A:636:ASP:C	2.58	0.46
5:A:1102:LEU:O	5:A:1106:LEU:N	2.38	0.46
6:F:241:GLU:HG3	6:F:244:GLU:OE1	2.15	0.46
7:G:101:HIS:O	7:G:130:PRO:HD2	2.15	0.46
8:E:358:HIS:CG	8:E:359:GLN:H	2.34	0.46
3:D:102:UNK:C	3:D:233:UNK:HA	2.45	0.46
5:A:1222:ASN:O	5:A:1223:VAL:C	2.58	0.46
5:A:2036:LEU:O	5:A:2037:TYR:C	2.59	0.46
6:F:47:TYR:CD1	6:F:50:ASP:OD2	2.68	0.46
6:F:95:GLN:O	6:F:99:TYR:HA	2.16	0.46
7:G:277:THR:HA	7:G:280:ASN:HD22	1.81	0.46
7:G:286:ASP:O	7:G:290:ARG:NE	2.49	0.46
1:B:2737:ALA:HB3	1:B:2746:LEU:HD11	1.98	0.46
1:B:3082:ILE:CB	1:B:3108:ILE:HD11	2.46	0.46
1:B:3316:TYR:CD1	1:B:3316:TYR:C	2.90	0.46
5:A:1868:SER:O	5:A:1872:ILE:N	2.48	0.46
6:F:43:VAL:HG22	6:F:73:PRO:HA	1.97	0.46
5:A:914:ASP:O	5:A:916:ILE:N	2.47	0.46
6:F:390:TYR:HD1	6:F:432:LEU:HD12	1.80	0.46
6:F:444:HIS:CE1	8:E:377:HIS:HE1	2.34	0.46
1:B:3505:ASP:HA	1:B:3508:ILE:HD12	1.97	0.46
2:C:721:GLN:C	2:C:724:LEU:CB	2.77	0.46
5:A:709:VAL:O	5:A:713:MET:N	2.49	0.46
5:A:1041:GLU:HA	5:A:2514:VAL:CB	2.46	0.46
7:G:33:SER:CB	7:G:71:ILE:HG13	2.46	0.46
7:G:162:VAL:HG11	7:G:278:THR:HA	1.98	0.46
8:E:378:LYS:O	8:E:382:ALA:N	2.42	0.46
1:B:2639:ILE:HA	1:B:2642:SER:HB3	1.98	0.45
1:B:3404:ALA:CA	1:B:3457:ILE:HG22	2.46	0.45
1:B:3555:PHE:CE1	1:B:3581:VAL:HG11	2.51	0.45
2:C:699:ARG:N	2:C:699:ARG:CD	2.73	0.45
5:A:1300:ASN:C	5:A:1302:LYS:N	2.56	0.45
5:A:2334:SER:O	5:A:2338:LEU:N	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:140:LEU:HD11	7:G:343:GLY:CA	2.45	0.45
7:G:180:LEU:HD21	7:G:269:LEU:HD21	1.97	0.45
7:G:227:MET:HE1	7:G:252:ASN:ND2	2.31	0.45
1:B:2957:HIS:HA	1:B:3434:VAL:CB	2.46	0.45
1:B:3068:LEU:CB	1:B:3078:ALA:CA	2.94	0.45
1:B:3496:ALA:HB3	1:B:3510:LYS:HZ2	1.81	0.45
5:A:1044:LYS:O	5:A:1045:THR:C	2.58	0.45
7:G:108:ALA:HB1	7:G:109:PRO:HD3	1.96	0.45
7:G:309:ILE:O	7:G:313:MET:HG2	2.16	0.45
1:B:2675:PHE:O	1:B:2675:PHE:CG	2.69	0.45
1:B:2941:HIS:C	1:B:2943:ILE:N	2.74	0.45
1:B:3427:ASN:ND2	1:B:3427:ASN:C	2.73	0.45
6:F:443:GLY:O	6:F:444:HIS:HD2	1.99	0.45
7:G:273:GLY:N	7:G:276:GLN:HB3	2.31	0.45
1:B:3038:GLU:N	1:B:3038:GLU:CD	2.73	0.45
5:A:996:GLY:C	5:A:998:GLN:N	2.73	0.45
6:F:122:LYS:HA	6:F:125:LEU:HD12	1.98	0.45
7:G:360:GLN:O	7:G:364:GLU:HG3	2.17	0.45
5:A:1091:SER:CA	5:A:1099:ALA:CA	2.90	0.45
6:F:156:LEU:HD12	6:F:168:SER:O	2.17	0.45
7:G:24:ASP:HB2	7:G:340:TRP:CH2	2.46	0.45
1:B:3731:ARG:CB	2:C:694:TRP:HE1	2.29	0.45
1:B:3220:PRO:C	1:B:3222:LEU:H	2.24	0.45
1:B:3236:ARG:HA	1:B:3236:ARG:HD2	1.48	0.45
1:B:3296:PHE:CD1	1:B:3296:PHE:O	2.70	0.45
1:B:3435:GLU:N	1:B:3435:GLU:CD	2.73	0.45
1:B:3437:ARG:O	1:B:3439:ARG:N	2.50	0.45
1:B:3555:PHE:CZ	1:B:3583:THR:HG21	2.52	0.45
3:D:310:UNK:O	3:D:313:UNK:N	2.49	0.45
6:F:272:SER:HB3	6:F:278:ILE:HG12	1.99	0.45
6:F:291:GLU:OE2	6:F:296:LYS:HB2	2.17	0.45
1:B:3486:GLN:NE2	1:B:3486:GLN:C	2.73	0.45
6:F:216:PHE:CE2	6:F:218:LYS:HG3	2.52	0.45
7:G:124:PHE:HD1	7:G:359:LYS:HG2	1.82	0.45
7:G:143:TYR:CG	8:E:391:ILE:HG21	2.51	0.45
1:B:3099:GLU:CD	1:B:3099:GLU:C	2.85	0.45
1:B:3424:ARG:HH21	1:B:3424:ARG:CG	2.30	0.45
1:B:3474:PHE:CE2	1:B:3526:VAL:CG1	2.92	0.45
2:C:704:ASN:CB	2:C:711:ASP:HA	2.46	0.45
3:D:420:UNK:O	3:D:422:UNK:N	2.50	0.45
5:A:1103:LEU:C	5:A:1105:ASN:N	2.74	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1581:GLU:C	5:A:1583:LYS:N	2.74	0.45
5:A:1673:PHE:O	5:A:1676:MET:N	2.50	0.45
6:F:175:THR:N	6:F:489[B]:ARG:HG2	2.31	0.45
6:F:406:HIS:CD2	6:F:406:HIS:O	2.70	0.45
7:G:138:ALA:CA	7:G:152:VAL:HG11	2.40	0.45
7:G:148:THR:HB	8:E:388:ALA:HB1	1.99	0.45
7:G:346:LEU:HG	7:G:352:PHE:CE2	2.52	0.45
8:E:366:ALA:C	8:E:368:TRP:N	2.70	0.45
2:C:689:GLU:C	2:C:691:ARG:N	2.75	0.45
5:A:592:SER:O	5:A:596:THR:N	2.38	0.45
7:G:216:LEU:HD22	7:G:238:LYS:HD2	1.99	0.45
7:G:271:SER:OG	7:G:272:ALA:N	2.50	0.45
1:B:2821:ILE:HA	1:B:2849:TYR:CZ	2.52	0.44
1:B:3159:ILE:O	1:B:3163:TYR:CB	2.65	0.44
1:B:3358:TYR:CG	1:B:3358:TYR:O	2.70	0.44
4:H:60:THR:C	4:H:63:ARG:H	2.24	0.44
1:B:3100:LEU:HD13	1:B:3101:LEU:H	1.67	0.44
1:B:3316:TYR:CD1	1:B:3316:TYR:O	2.70	0.44
1:B:3592:PRO:CB	1:B:3671:ILE:HB	2.47	0.44
1:B:3649:SER:CB	1:B:3705:GLN:CA	2.82	0.44
3:D:38:UNK:O	3:D:39:UNK:C	2.65	0.44
3:D:373:UNK:H	8:E:379:TYR:HE1	1.57	0.44
6:F:204:ILE:HD12	6:F:274:TRP:CD2	2.52	0.44
6:F:253:LYS:HB3	6:F:256:GLU:HG2	1.98	0.44
7:G:73:HIS:ND1	7:G:73:HIS:N	2.64	0.44
7:G:81:ASP:O	7:G:84:LYS:N	2.51	0.44
1:B:2898:TRP:CE3	1:B:2898:TRP:O	2.70	0.44
1:B:3467:LEU:C	1:B:3467:LEU:HD12	2.43	0.44
1:B:3653:ILE:O	1:B:3654:GLU:C	2.59	0.44
3:D:384:UNK:O	3:D:386:UNK:N	2.50	0.44
5:A:119:MET:O	5:A:123:THR:N	2.46	0.44
6:F:127:VAL:HG12	6:F:128:LEU:HD23	1.99	0.44
1:B:3366:VAL:C	1:B:3367:HIS:O	2.61	0.44
1:B:3504:PRO:O	1:B:3508:ILE:HG13	2.18	0.44
1:B:2651:ASN:HD22	1:B:2651:ASN:N	2.13	0.44
1:B:3100:LEU:CD1	1:B:3100:LEU:C	2.86	0.44
1:B:3220:PRO:C	1:B:3222:LEU:N	2.75	0.44
1:B:3424:ARG:HH11	1:B:3447:ILE:HA	1.65	0.44
1:B:3439:ARG:HG3	1:B:3441:ILE:HG12	2.00	0.44
1:B:3570:HIS:O	1:B:3570:HIS:CG	2.70	0.44
5:A:2549:PHE:HZ	5:A:2556:ILE:HA	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:258:THR:HA	6:F:261:GLU:HG2	1.99	0.44
7:G:187:ASP:OD1	7:G:206:ARG:NH1	2.51	0.44
7:G:210:ARG:O	7:G:213:LYS:HB3	2.17	0.44
1:B:3106:TRP:CB	1:B:3665:LEU:CD1	2.81	0.44
1:B:3172:ARG:NH2	1:B:3173:THR:HA	2.32	0.44
5:A:1207:TYR:O	5:A:1210:ARG:N	2.51	0.44
6:F:57:PHE:CE1	6:F:89:GLN:HB2	2.53	0.44
6:F:400:LEU:O	6:F:404:LEU:HG	2.18	0.44
7:G:117:GLU:HG2	7:G:367:PRO:O	2.17	0.44
7:G:230:ALA:CB	7:G:252:ASN:HB3	2.47	0.44
1:B:3563:MET:C	1:B:3565:ASN:H	2.24	0.44
2:C:688:ILE:HA	2:C:691:ARG:HE	1.82	0.44
6:F:18:VAL:O	6:F:28:ILE:HG23	2.18	0.44
7:G:24:ASP:HB3	7:G:26:ALA:H	1.83	0.44
1:B:2675:PHE:O	1:B:2675:PHE:CD1	2.71	0.44
1:B:2843:LEU:O	1:B:2846:PHE:N	2.39	0.44
2:C:732:GLN:O	2:C:734:GLN:N	2.50	0.44
5:A:890:TYR:C	5:A:892:ASP:N	2.75	0.44
1:B:3247:ARG:HH11	1:B:3407:TYR:CB	2.29	0.44
1:B:3358:TYR:O	1:B:3358:TYR:CD2	2.71	0.44
2:C:691:ARG:HG3	2:C:692:THR:N	2.33	0.44
6:F:186:ALA:O	6:F:189:PHE:N	2.49	0.44
6:F:484:LEU:HA	6:F:487:ARG:HH11	1.82	0.44
7:G:35:VAL:N	7:G:68:ARG:O	2.43	0.44
8:E:364:GLU:O	8:E:368:TRP:HD1	2.01	0.44
1:B:3015:GLY:CA	1:B:3019:LYS:HB3	2.48	0.43
1:B:3116:MET:C	1:B:3118:THR:N	2.72	0.43
1:B:3570:HIS:CD2	1:B:3570:HIS:O	2.70	0.43
5:A:1038:ASN:O	5:A:1041:GLU:N	2.52	0.43
6:F:267:LYS:HA	6:F:282:ASN:HD21	1.83	0.43
8:E:375:GLU:O	8:E:378:LYS:N	2.51	0.43
1:B:3516:SER:O	1:B:3519:THR:OG1	2.37	0.43
4:H:193:LEU:O	4:H:196:LEU:N	2.46	0.43
5:A:2243:ILE:CB	5:A:2252:SER:CA	2.94	0.43
5:A:2389:SER:O	5:A:2391:SER:N	2.50	0.43
6:F:390:TYR:CD1	6:F:432:LEU:HD12	2.53	0.43
7:G:257:ALA:HB3	7:G:258:PRO:HD3	2.00	0.43
1:B:3552:TYR:CD1	1:B:3552:TYR:O	2.70	0.43
2:C:712:LEU:O	2:C:716:ARG:CB	2.66	0.43
5:A:838:LEU:O	5:A:842:LEU:N	2.49	0.43
5:A:1249:GLN:C	5:A:1251:GLU:N	2.74	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:253:GLU:HG2	7:G:256:ARG:HD3	2.00	0.43
7:G:326:LYS:HE3	7:G:328:LYS:HD2	2.01	0.43
1:B:3070:GLU:OE1	1:B:3070:GLU:HA	2.18	0.43
2:C:670:GLU:O	2:C:674:ALA:N	2.37	0.43
3:D:150:UNK:O	3:D:152:UNK:N	2.51	0.43
6:F:177:SER:HA	6:F:180:THR:HG23	2.00	0.43
6:F:244:GLU:HB3	7:G:287:VAL:HG11	1.99	0.43
7:G:18:LYS:HE3	7:G:337:TYR:CD1	2.53	0.43
7:G:140:LEU:CD1	7:G:343:GLY:CA	2.96	0.43
1:B:3085:TYR:CB	1:B:3104:ILE:HD13	2.48	0.43
1:B:3253:LEU:CD1	1:B:3318:ARG:HB2	2.45	0.43
1:B:3411:ARG:O	1:B:3415:ARG:CB	2.66	0.43
1:B:3546:LYS:NZ	1:B:3550:SER:HB2	2.34	0.43
2:C:649:ILE:O	2:C:652:SER:N	2.51	0.43
3:D:79:UNK:C	3:D:80:UNK:O	2.59	0.43
5:A:1044:LYS:O	5:A:1046:ALA:N	2.52	0.43
7:G:137:GLN:HG3	7:G:339:VAL:CG1	2.48	0.43
7:G:223:PHE:HD1	7:G:259:GLU:HG3	1.84	0.43
3:D:11:UNK:C	3:D:13:UNK:N	2.82	0.43
5:A:2526:HIS:O	5:A:2530:MET:N	2.51	0.43
6:F:180:THR:O	6:F:181:ARG:NH1	2.42	0.43
7:G:227:MET:HE1	7:G:252:ASN:HD22	1.83	0.43
7:G:275:ASP:CG	7:G:276:GLN:N	2.76	0.43
8:E:377:HIS:O	8:E:381:VAL:HG23	2.19	0.43
1:B:2898:TRP:CZ3	1:B:2902:VAL:HG21	2.53	0.43
1:B:3108:ILE:HD12	1:B:3108:ILE:HA	1.74	0.43
1:B:3443:PHE:CD1	1:B:3443:PHE:N	2.73	0.43
1:B:3585:GLU:C	1:B:3586:MET:SD	3.01	0.43
1:B:3733:LEU:HD21	1:B:3742:PRO:HG2	2.00	0.43
6:F:94:LEU:O	6:F:99:TYR:N	2.52	0.43
7:G:253:GLU:HA	7:G:256:ARG:HB2	2.00	0.43
1:B:3488:PHE:CE1	1:B:3492:LYS:HG2	2.54	0.43
6:F:413:GLY:HA3	6:F:449:GLN:NE2	2.33	0.43
7:G:107:GLU:HB2	7:G:111:ASN:ND2	2.32	0.43
1:B:2819:GLU:C	1:B:2821:ILE:N	2.75	0.43
1:B:3019:LYS:O	1:B:3020:ALA:C	2.61	0.43
1:B:3171:LEU:C	1:B:3174:THR:OG1	2.56	0.43
1:B:3668:ARG:O	1:B:3671:ILE:HG13	2.18	0.43
5:A:871:VAL:C	5:A:873:ALA:N	2.76	0.43
5:A:1988:PHE:O	5:A:1991:SER:N	2.42	0.43
5:A:2168:LEU:O	5:A:2172:PHE:N	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:128:LEU:HD13	6:F:134:PHE:CD2	2.53	0.43
6:F:416:SER:HA	6:F:448:ARG:NH1	2.34	0.43
6:F:462:LEU:HD23	6:F:462:LEU:HA	1.84	0.43
1:B:2898:TRP:HE3	1:B:2898:TRP:O	2.00	0.43
1:B:2947:ILE:CB	1:B:2970:ILE:HD12	2.49	0.43
1:B:3394:ARG:CA	1:B:3398:GLY:HA2	2.49	0.43
1:B:3551:GLN:C	1:B:3553:SER:N	2.77	0.43
5:A:1417:LYS:O	5:A:1421:ILE:N	2.51	0.43
5:A:1506:LEU:C	5:A:1508:GLU:N	2.51	0.43
5:A:1986:TYR:HA	5:A:1989:LEU:CB	2.49	0.43
6:F:440:LEU:HD13	6:F:440:LEU:HA	1.75	0.43
7:G:116:ARG:HG2	7:G:370:VAL:HG21	2.01	0.43
7:G:203:THR:C	7:G:205:GLU:H	2.27	0.43
1:B:3062:PHE:CZ	1:B:3658:GLU:HA	2.50	0.42
5:A:21:LEU:O	5:A:25:TYR:N	2.44	0.42
5:A:2556:ILE:C	5:A:2558:ARG:H	2.27	0.42
6:F:40:LEU:HB3	6:F:89:GLN:HE21	1.84	0.42
6:F:116:ASN:OD1	6:F:120:ASN:HB2	2.19	0.42
7:G:103:VAL:O	7:G:132:PHE:HD1	2.02	0.42
7:G:151:ILE:CG2	7:G:297:ILE:CG1	2.95	0.42
6:F:10:GLY:HA2	6:F:463:GLY:N	2.34	0.42
6:F:272:SER:HB3	6:F:278:ILE:CG1	2.49	0.42
1:B:2966:GLN:OE1	1:B:2966:GLN:HA	2.19	0.42
1:B:3493:LEU:CD1	1:B:3497:HIS:HB2	2.49	0.42
7:G:70:PRO:HG2	7:G:85:ILE:HD11	2.01	0.42
1:B:2844:HIS:HA	1:B:2847:GLN:CB	2.47	0.42
1:B:3378:VAL:O	1:B:3379:ASP:C	2.62	0.42
1:B:3667:ILE:HG21	1:B:3696:VAL:CB	2.49	0.42
6:F:56:ILE:HD12	6:F:56:ILE:HA	1.68	0.42
7:G:105:LEU:HD13	7:G:132:PHE:CE1	2.54	0.42
7:G:255:PHE:O	7:G:259:GLU:HG2	2.19	0.42
1:B:2648:SER:O	1:B:2649:ILE:CB	2.68	0.42
1:B:3244:ASP:C	1:B:3247:ARG:CD	2.92	0.42
5:A:369:TYR:O	5:A:372:ASP:N	2.52	0.42
5:A:1581:GLU:O	5:A:1585:ARG:N	2.53	0.42
6:F:2:SER:HB2	7:G:371:HIS:O	2.19	0.42
6:F:151:GLY:H	8:E:370:GLN:CD	2.27	0.42
6:F:238:PHE:HZ	6:F:278:ILE:HG21	1.85	0.42
7:G:102:PRO:HA	7:G:131:ALA:O	2.20	0.42
1:B:2761:GLU:O	1:B:2765:ARG:N	2.52	0.42
1:B:3071:GLU:C	1:B:3072:PRO:O	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3163:TYR:CB	1:B:3167:LEU:CB	2.98	0.42
1:B:3247:ARG:O	1:B:3251:VAL:HG23	2.18	0.42
1:B:3418:ARG:HA	1:B:3418:ARG:HD3	1.26	0.42
1:B:3462:VAL:O	1:B:3464:PHE:CG	2.72	0.42
2:C:691:ARG:O	2:C:695:GLN:HG3	2.20	0.42
4:H:223:ASP:O	4:H:227:GLU:N	2.44	0.42
1:B:2885:ARG:HD3	1:B:2886:ASP:N	2.34	0.42
1:B:3236:ARG:C	1:B:3238:LYS:H	2.28	0.42
1:B:3512:GLU:O	1:B:3515:ASN:HB3	2.19	0.42
1:B:3724:ILE:O	1:B:3727:ALA:N	2.50	0.42
2:C:649:ILE:O	2:C:653:GLU:N	2.49	0.42
3:D:424:UNK:O	3:D:425:UNK:C	2.67	0.42
5:A:1345:LEU:O	5:A:1349:MET:CB	2.67	0.42
6:F:175:THR:O	6:F:489[B]:ARG:NH2	2.48	0.42
6:F:243:LYS:HG2	6:F:247:CYS:SG	2.59	0.42
6:F:287:GLY:HA2	6:F:290:GLU:HB3	2.01	0.42
6:F:437:PHE:N	6:F:437:PHE:CD1	2.86	0.42
7:G:109:PRO:C	7:G:111:ASN:N	2.77	0.42
7:G:230:ALA:HB2	7:G:252:ASN:HB3	2.02	0.42
4:H:186:LYS:O	4:H:190:ASP:N	2.51	0.42
6:F:62:ILE:HG12	6:F:71:LEU:CD2	2.49	0.42
6:F:484:LEU:O	6:F:487:ARG:HG2	2.19	0.42
7:G:355:MET:HA	7:G:373:LYS:NZ	2.34	0.42
1:B:3360:LEU:CB	1:B:3424:ARG:HG2	2.50	0.42
1:B:3451:LEU:CD1	1:B:3451:LEU:N	2.73	0.42
5:A:217:SER:C	5:A:219:PHE:N	2.77	0.42
5:A:1296:LEU:O	5:A:1352:GLY:C	2.63	0.42
5:A:2236:ILE:O	5:A:2237:GLN:C	2.63	0.42
6:F:19:ILE:HA	6:F:28:ILE:HG12	2.02	0.42
6:F:213:LYS:CA	6:F:213:LYS:CE	2.86	0.42
6:F:272:SER:HG	6:F:274:TRP:CG	2.37	0.42
1:B:3106:TRP:CH2	1:B:3668:ARG:CZ	3.00	0.42
1:B:3492:LYS:O	1:B:3510:LYS:HE2	2.20	0.42
3:D:396:UNK:CA	6:F:436:LYS:HE3	2.48	0.42
5:A:2180:ILE:O	5:A:2184:LEU:N	2.52	0.42
6:F:30:TYR:HB2	7:G:113:LYS:HE3	2.02	0.42
7:G:133:TYR:CZ	7:G:374:CYS:HA	2.54	0.42
1:B:2778:GLN:O	1:B:2782:SER:N	2.30	0.41
1:B:3720:ILE:O	1:B:3723:CYS:N	2.52	0.41
5:A:982:ILE:CB	5:A:2481:ASN:C	2.93	0.41
6:F:164:THR:HG22	6:F:184:PHE:CD1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:406:HIS:O	6:F:406:HIS:CG	2.70	0.41
7:G:109:PRO:CD	7:G:161:HIS:CD2	3.03	0.41
7:G:163:VAL:HA	7:G:164:PRO:HD3	1.65	0.41
1:B:3354:ILE:CA	1:B:3371:ILE:H	2.22	0.41
1:B:3540:ASP:HA	1:B:3543:LEU:HD13	2.02	0.41
5:A:434:MET:O	5:A:435:SER:C	2.62	0.41
5:A:2606:LEU:C	5:A:2608:ASP:N	2.78	0.41
6:F:151:GLY:N	8:E:370:GLN:OE1	2.53	0.41
6:F:213:LYS:CG	6:F:214:PRO:HD3	2.50	0.41
7:G:149:THR:HG21	7:G:292:GLU:OE1	2.19	0.41
7:G:151:ILE:HD12	7:G:152:VAL:N	2.36	0.41
7:G:180:LEU:HD21	7:G:269:LEU:HD11	2.01	0.41
1:B:2826:ILE:C	1:B:2826:ILE:HD13	2.44	0.41
1:B:3437:ARG:C	1:B:3439:ARG:N	2.78	0.41
2:C:694:TRP:HA	2:C:697:PHE:CD2	2.53	0.41
5:A:580:ILE:HA	5:A:583:ALA:HB3	2.01	0.41
6:F:122:LYS:HA	6:F:125:LEU:CD1	2.50	0.41
1:B:2844:HIS:C	1:B:2846:PHE:H	2.27	0.41
1:B:3068:LEU:HB3	1:B:3078:ALA:CB	2.44	0.41
4:H:59:LEU:O	4:H:63:ARG:N	2.54	0.41
6:F:110:LEU:HD13	6:F:124:SER:HB3	2.01	0.41
7:G:190:MET:SD	7:G:206:ARG:NE	2.93	0.41
1:B:2663:LEU:HD21	1:B:2678:LEU:CB	2.50	0.41
1:B:3553:SER:O	1:B:3555:PHE:N	2.54	0.41
6:F:6:LEU:HA	6:F:6:LEU:HD23	1.84	0.41
6:F:71:LEU:CD1	6:F:229:LEU:HA	2.50	0.41
6:F:213:LYS:HG3	6:F:214:PRO:HD3	2.02	0.41
6:F:434:SER:O	6:F:435:LEU:HD12	2.20	0.41
6:F:487:ARG:HA	6:F:487:ARG:NE	2.36	0.41
1:B:2634:TYR:H	1:B:2634:TYR:HD1	1.66	0.41
1:B:3418:ARG:HB2	1:B:3418:ARG:NH1	2.24	0.41
1:B:3663:LEU:O	1:B:3667:ILE:HG23	2.20	0.41
2:C:701:VAL:HG13	2:C:711:ASP:CB	2.51	0.41
2:C:724:LEU:C	2:C:726:GLU:N	2.77	0.41
7:G:8:LEU:HD13	7:G:10:ILE:HD11	2.03	0.41
7:G:18:LYS:HA	7:G:30:VAL:HA	2.02	0.41
7:G:351:THR:HG22	7:G:354:GLN:NE2	2.36	0.41
8:E:390:ALA:HB1	8:E:394:TYR:CE2	2.55	0.41
1:B:3249:ILE:O	1:B:3253:LEU:HG	2.21	0.41
1:B:3492:LYS:O	1:B:3510:LYS:CE	2.68	0.41
5:A:1286:GLU:O	5:A:1290:THR:N	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:105:GLY:O	6:F:106:ILE:HD13	2.21	0.41
7:G:18:LYS:HB3	7:G:30:VAL:HG22	2.02	0.41
1:B:2654:ILE:HD12	1:B:2654:ILE:HA	1.81	0.41
1:B:2783:VAL:C	1:B:2785:ASP:H	2.28	0.41
5:A:244:THR:C	5:A:245:SER:O	2.59	0.41
6:F:304:TRP:O	6:F:306:ARG:HG3	2.21	0.41
7:G:163:VAL:HG22	7:G:175:ILE:HG13	1.67	0.41
1:B:3068:LEU:HD22	1:B:3078:ALA:O	2.20	0.41
1:B:3464:PHE:CD2	1:B:3575:ASP:CB	3.04	0.41
1:B:3666:PHE:O	1:B:3669:ASP:N	2.54	0.41
3:D:442:UNK:O	3:D:443:UNK:C	2.69	0.41
5:A:137:LEU:O	5:A:140:PHE:N	2.51	0.41
5:A:1262:LYS:O	5:A:1265:ILE:N	2.54	0.41
5:A:2259:LEU:O	5:A:2260:ALA:C	2.64	0.41
6:F:70:GLU:HB2	6:F:226:ASP:CG	2.46	0.41
6:F:397:ASP:O	6:F:401:ARG:HG3	2.21	0.41
7:G:124:PHE:CD1	7:G:359:LYS:HG2	2.56	0.41
7:G:149:THR:HG22	7:G:150:GLY:N	2.36	0.41
8:E:361:ILE:HA	8:E:364:GLU:OE1	2.21	0.41
8:E:384:CYS:O	8:E:387:MET:HB2	2.20	0.41
1:B:2849:TYR:HA	1:B:2852:PHE:CB	2.50	0.41
1:B:3078:ALA:O	1:B:3081:ALA:HB3	2.21	0.41
1:B:3360:LEU:CB	1:B:3424:ARG:CG	2.99	0.41
1:B:3404:ALA:C	1:B:3457:ILE:CG2	2.91	0.41
3:D:418:UNK:C	3:D:420:UNK:N	2.83	0.41
7:G:9:VAL:HG12	7:G:340:TRP:CD1	2.55	0.41
1:B:3236:ARG:CD	1:B:3338:CYS:CB	2.95	0.40
1:B:3741:MET:N	1:B:3742:PRO:HD3	2.00	0.40
5:A:2345:ASP:C	5:A:2347:ASN:N	2.79	0.40
6:F:425:MET:HE3	6:F:429:ASN:OD1	2.20	0.40
5:A:890:TYR:O	5:A:892:ASP:N	2.54	0.40
5:A:1027:LEU:C	5:A:1029:THR:N	2.77	0.40
6:F:23:SER:HB3	6:F:163:ASP:H	1.85	0.40
6:F:94:LEU:HA	6:F:98:LEU:HB2	2.02	0.40
6:F:444:HIS:C	6:F:446:ILE:H	2.22	0.40
6:F:463:GLY:O	6:F:466:HIS:HD2	2.04	0.40
7:G:27:PRO:HA	7:G:340:TRP:CZ2	2.56	0.40
1:B:3136:PHE:O	1:B:3141:LEU:N	2.54	0.40
1:B:3733:LEU:O	1:B:3733:LEU:HD23	2.21	0.40
5:A:811:LEU:C	5:A:813:ARG:H	2.28	0.40
5:A:1295:GLU:O	5:A:1356:ALA:CB	2.68	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3253:LEU:HD21	1:B:3314:LEU:C	2.46	0.40
1:B:3354:ILE:C	1:B:3356:GLY:N	2.78	0.40
1:B:3437:ARG:O	1:B:3438:ARG:C	2.64	0.40
5:A:1456:ILE:O	5:A:1457:ASN:C	2.64	0.40
5:A:2517:LEU:O	5:A:2519:LEU:N	2.54	0.40
7:G:282:ILE:HG22	7:G:283:MET:HE2	2.04	0.40
7:G:310:ALA:O	7:G:314:GLN:N	2.36	0.40
1:B:3071:GLU:O	1:B:3071:GLU:HG2	2.21	0.40
1:B:3544:PHE:CE1	1:B:3579:GLY:HA2	2.52	0.40
1:B:3661:THR:HA	1:B:3664:ALA:HB2	2.04	0.40
1:B:3668:ARG:O	1:B:3671:ILE:N	2.52	0.40
1:B:3719:PHE:HA	1:B:3722:ASP:CB	2.49	0.40
4:H:183:LYS:O	4:H:185:LEU:N	2.54	0.40
5:A:1652:ILE:C	5:A:1654:ASN:N	2.79	0.40
6:F:297:GLU:C	6:F:299:ASP:N	2.78	0.40
7:G:103:VAL:O	7:G:356:TRP:HZ3	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	935/1115 (84%)	658 (70%)	205 (22%)	72 (8%)	1	10
2	C	136/336 (40%)	99 (73%)	24 (18%)	13 (10%)	0	7
4	H	136/279 (49%)	120 (88%)	14 (10%)	2 (2%)	8	38
5	A	1857/2627 (71%)	1494 (80%)	251 (14%)	112 (6%)	1	13
6	F	417/490 (85%)	350 (84%)	62 (15%)	5 (1%)	10	43
7	G	345/375 (92%)	311 (90%)	32 (9%)	2 (1%)	21	59
8	E	39/41 (95%)	29 (74%)	10 (26%)	0	100	100
All	All	3865/5263 (73%)	3061 (79%)	598 (16%)	206 (5%)	2	15

All (206) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2649	ILE
1	B	2652	THR
1	B	2787	PRO
1	B	2788	THR
1	B	3056	ALA
1	B	3117	LEU
1	B	3164	PRO
1	B	3223	ALA
1	B	3242	ASP
1	B	3293	ARG
1	B	3367	HIS
1	B	3401	HIS
1	B	3407	TYR
1	B	3453	PRO
1	B	3463	SER
1	B	3480	PHE
1	B	3481	ASP
1	B	3552	TYR
1	B	3592	PRO
1	B	3598	PRO
1	B	3657	ASN
1	B	3704	ALA
1	B	3742	PRO
2	C	674	ALA
2	C	678	HIS
2	C	714	GLY
2	C	715	PRO
2	C	716	ARG
2	C	739	SER
2	C	740	PRO
5	A	138	ASP
5	A	218	MET
5	A	231	MET
5	A	240	GLN
5	A	245	SER
5	A	303	SER
5	A	411	ILE
5	A	425	GLU
5	A	431	VAL
5	A	517	PHE
5	A	567	ALA
5	A	777	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	866	PRO
5	A	924	VAL
5	A	958	GLN
5	A	962	PRO
5	A	963	PRO
5	A	968	GLU
5	A	970	THR
5	A	973	ASP
5	A	977	ILE
5	A	994	THR
5	A	997	ILE
5	A	1035	PHE
5	A	1069	LYS
5	A	1094	GLU
5	A	1098	ASP
5	A	1153	LEU
5	A	1158	PRO
5	A	1223	VAL
5	A	1250	SER
5	A	1293	VAL
5	A	1301	PRO
5	A	1346	PRO
5	A	1362	SER
5	A	1364	PRO
5	A	1373	GLU
5	A	1507	LEU
5	A	1591	PRO
5	A	1605	ASN
5	A	1630	ARG
5	A	1651	TYR
5	A	1860	PHE
5	A	2369	VAL
5	A	2419	PRO
5	A	2497	PRO
5	A	2506	GLU
5	A	2568	TYR
5	A	2572	PRO
6	F	49	ALA
6	F	213	LYS
6	F	445	THR
7	G	16	MET
1	B	2997	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3368	PHE
1	B	3388	TYR
1	B	3394	ARG
1	B	3403	PHE
1	B	3455	VAL
1	B	3568	THR
1	B	3595	ARG
5	A	572	LEU
5	A	959	PHE
5	A	976	ALA
5	A	980	PHE
5	A	1011	ILE
5	A	1033	ALA
5	A	1037	THR
5	A	1091	SER
5	A	1295	GLU
5	A	1653	SER
5	A	2384	ILE
5	A	2401	LEU
5	A	2491	ILE
1	B	2823	LEU
1	B	3115	GLY
1	B	3149	ALA
1	B	3150	ASN
1	B	3366	VAL
1	B	3482	PRO
1	B	3590	ARG
1	B	3599	LEU
1	B	3619	PRO
1	B	3707	GLY
1	B	3709	LEU
1	B	3717	THR
1	B	3737	ASP
1	B	3743	TRP
2	C	680	LEU
2	C	718	HIS
2	C	719	SER
4	H	131	MET
5	A	389	PRO
5	A	426	SER
5	A	889	GLN
5	A	967	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	995	PRO
5	A	1070	ARG
5	A	1104	ASN
5	A	1204	GLU
5	A	1225	SER
5	A	1229	PHE
5	A	1302	LYS
5	A	1335	SER
5	A	1606	PRO
5	A	1615	MET
5	A	1895	LYS
5	A	2226	ILE
5	A	2518	GLU
6	F	405	ALA
1	B	2647	THR
1	B	2958	ASN
1	B	2962	VAL
1	B	3291	TYR
1	B	3356	GLY
1	B	3409	ALA
1	B	3410	VAL
1	B	3462	VAL
1	B	3706	LEU
1	B	3741	MET
2	C	679	ARG
2	C	690	ARG
4	H	129	ILE
5	A	833	PRO
5	A	978	ALA
5	A	983	ASN
5	A	986	PRO
5	A	1006	SER
5	A	1095	LEU
5	A	1105	ASN
5	A	1207	TYR
5	A	1898	ASP
5	A	2612	LYS
6	F	70	GLU
1	B	2671	GLU
1	B	2942	GLU
1	B	2961	ASP
1	B	3054	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3165	GLN
1	B	3219	TYR
1	B	3618	GLU
5	A	637	LEU
5	A	1067	VAL
5	A	1203	ASP
5	A	1321	PRO
5	A	1650	PHE
5	A	1894	ILE
5	A	2390	LEU
5	A	2557	HIS
5	A	2570	SER
1	B	2789	PRO
1	B	3344	PHE
1	B	3602	ASN
1	B	3625	THR
1	B	3627	ASN
2	C	675	HIS
5	A	246	LEU
5	A	314	ALA
5	A	890	TYR
5	A	991	LEU
5	A	1051	LYS
5	A	1583	LYS
5	A	1596	LEU
5	A	1647	PHE
5	A	1897	GLU
1	B	2902	VAL
1	B	3400	VAL
5	A	776	PHE
5	A	993	VAL
5	A	1036	PRO
1	B	3393	ILE
1	B	3612	PRO
1	B	3381	VAL
5	A	1256	ILE
7	G	287	VAL
5	A	982	ILE

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	B	300/1012 (30%)	201 (67%)	99 (33%)	0	2
2	C	26/309 (8%)	12 (46%)	14 (54%)	0	0
5	A	7/2438 (0%)	5 (71%)	2 (29%)	0	3
6	F	372/435 (86%)	355 (95%)	17 (5%)	24	46
7	G	297/320 (93%)	284 (96%)	13 (4%)	25	47
8	E	34/34 (100%)	33 (97%)	1 (3%)	37	58
All	All	1036/4548 (23%)	890 (86%)	146 (14%)	5	15

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2636	SER
1	B	2637	ILE
1	B	2639	ILE
1	B	2643	ILE
1	B	2651	ASN
1	B	2652	THR
1	B	2654	ILE
1	B	2655	ILE
1	B	2663	LEU
1	B	2665	LEU
1	B	2674	MET
1	B	2735	GLN
1	B	2826	ILE
1	B	2847	GLN
1	B	2854	GLU
1	B	2856	THR
1	B	2882	GLN
1	B	2885	ARG
1	B	2894	ASP
1	B	2896	ASN
1	B	2897	MET
1	B	2898	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2899	ASN
1	B	2900	ASP
1	B	2902	VAL
1	B	2906	GLN
1	B	2912	ILE
1	B	2941	HIS
1	B	2946	VAL
1	B	2952	HIS
1	B	2964	ILE
1	B	2965	SER
1	B	2966	GLN
1	B	2967	LEU
1	B	2970	ILE
1	B	2971	TYR
1	B	3007	SER
1	B	3019	LYS
1	B	3038	GLU
1	B	3041	GLN
1	B	3059	GLN
1	B	3066	ARG
1	B	3067	ARG
1	B	3069	SER
1	B	3095	SER
1	B	3097	ILE
1	B	3099	GLU
1	B	3100	LEU
1	B	3104	ILE
1	B	3105	LEU
1	B	3107	LEU
1	B	3108	ILE
1	B	3145	SER
1	B	3162	SER
1	B	3167	LEU
1	B	3168	HIS
1	B	3171	LEU
1	B	3172	ARG
1	B	3180	VAL
1	B	3219	TYR
1	B	3229	LEU
1	B	3236	ARG
1	B	3247	ARG
1	B	3317	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3318	ARG
1	B	3367	HIS
1	B	3411	ARG
1	B	3417	GLU
1	B	3418	ARG
1	B	3421	GLN
1	B	3422	LEU
1	B	3424	ARG
1	B	3427	ASN
1	B	3432	LYS
1	B	3435	GLU
1	B	3440	SER
1	B	3441	ILE
1	B	3443	PHE
1	B	3444	ASN
1	B	3449	ILE
1	B	3457	ILE
1	B	3462	VAL
1	B	3467	LEU
1	B	3468	HIS
1	B	3472	ASN
1	B	3484	ASP
1	B	3485	ILE
1	B	3486	GLN
1	B	3487	ASP
1	B	3489	MET
1	B	3492	LYS
1	B	3494	ASN
1	B	3499	ASP
1	B	3568	THR
1	B	3570	HIS
1	B	3571	LYS
1	B	3647	THR
1	B	3652	LEU
1	B	3714	THR
2	C	680	LEU
2	C	681	THR
2	C	684	TYR
2	C	685	LEU
2	C	687	ASN
2	C	688	ILE
2	C	689	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	695	GLN
2	C	696	CYS
2	C	697	PHE
2	C	699	ARG
2	C	701	VAL
2	C	702	GLN
2	C	703	LEU
5	A	948	ILE
5	A	1896	LEU
6	F	47	TYR
6	F	56	ILE
6	F	66	ARG
6	F	67	LYS
6	F	70	GLU
6	F	71	LEU
6	F	72	LYS
6	F	125	LEU
6	F	127	VAL
6	F	128	LEU
6	F	129	LEU
6	F	137	CYS
6	F	213	LYS
6	F	406	HIS
6	F	440	LEU
6	F	442	THR
6	F	472	LYS
7	G	16	MET
7	G	71	ILE
7	G	73	HIS
7	G	135	SER
7	G	136	ILE
7	G	137	GLN
7	G	139	VAL
7	G	151	ILE
7	G	152	VAL
7	G	153	LEU
7	G	159	VAL
7	G	163	VAL
7	G	288	ASP
8	E	394	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2735	GLN
1	B	2752	HIS
1	B	2941	HIS
1	B	3041	GLN
1	B	3059	GLN
1	B	3367	HIS
1	B	3427	ASN
1	B	3444	ASN
1	B	3486	GLN
1	B	3494	ASN
1	B	3570	HIS
1	B	3732	ASN
2	C	687	ASN
6	F	89	GLN
6	F	91	GLN
6	F	96	ASN
6	F	120	ASN
6	F	162	HIS
6	F	234	ASN
6	F	248	HIS
6	F	406	HIS
6	F	444	HIS
6	F	449	GLN
6	F	467	GLN
7	G	87	HIS
7	G	280	ASN
8	E	377	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

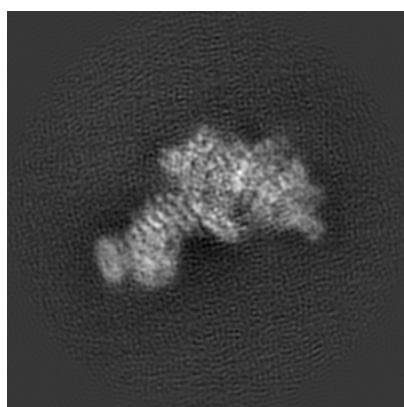
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6816. These allow visual inspection of the internal detail of the map and identification of artifacts.

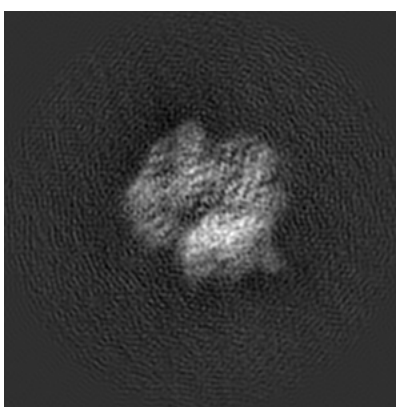
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

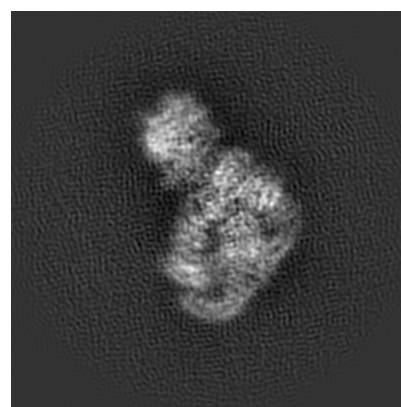
6.1.1 Primary map



X



Y

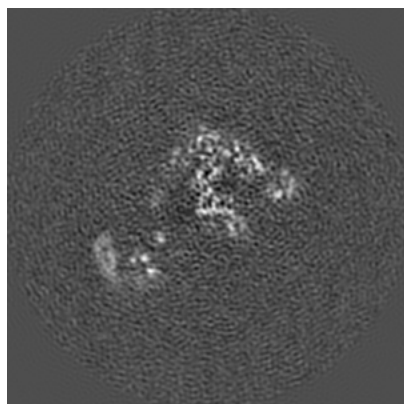


Z

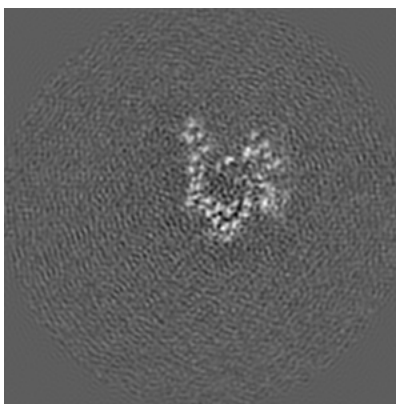
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

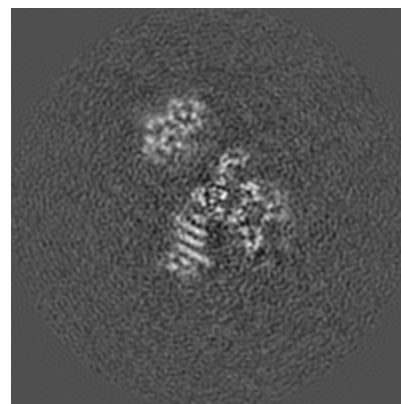
6.2.1 Primary map



X Index: 144



Y Index: 144

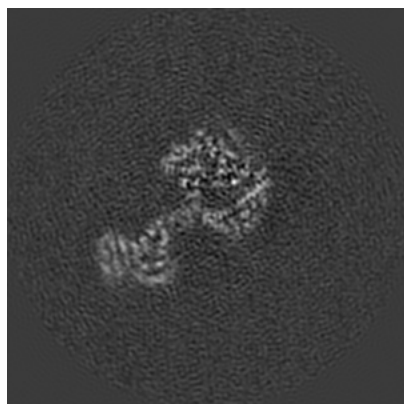


Z Index: 144

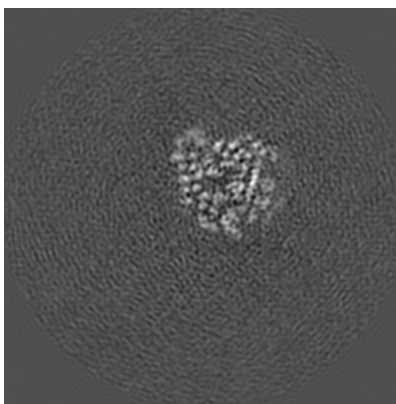
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

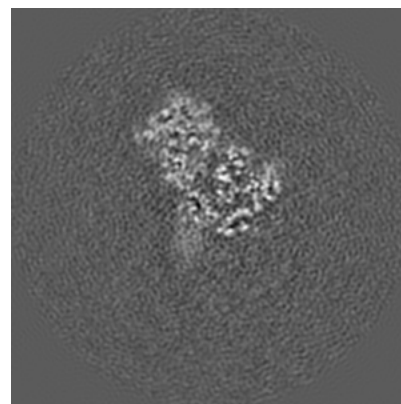
6.3.1 Primary map



X Index: 158



Y Index: 153

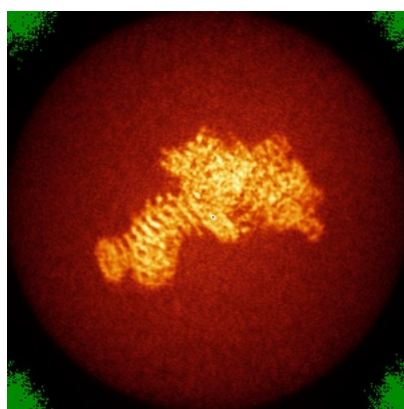


Z Index: 160

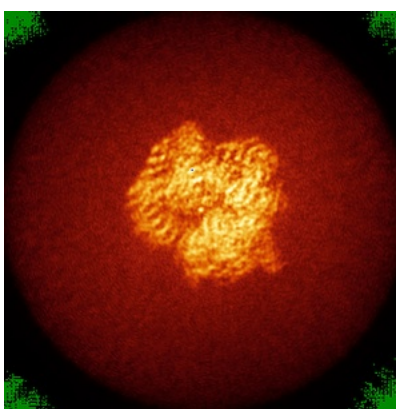
The images above show the largest variance slices of the map in three orthogonal directions.

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

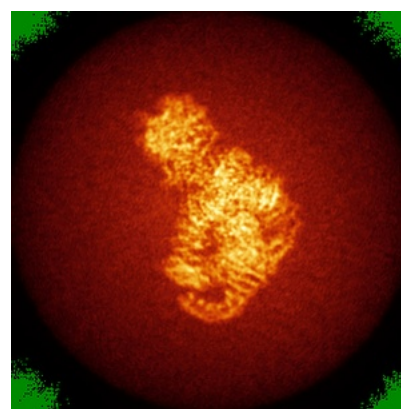
6.4.1 Primary map



X



Y

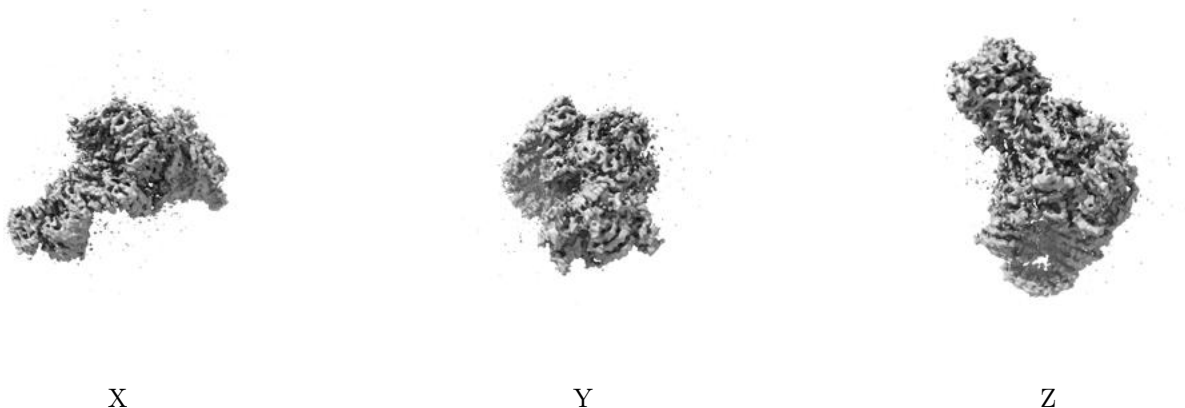


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0225. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

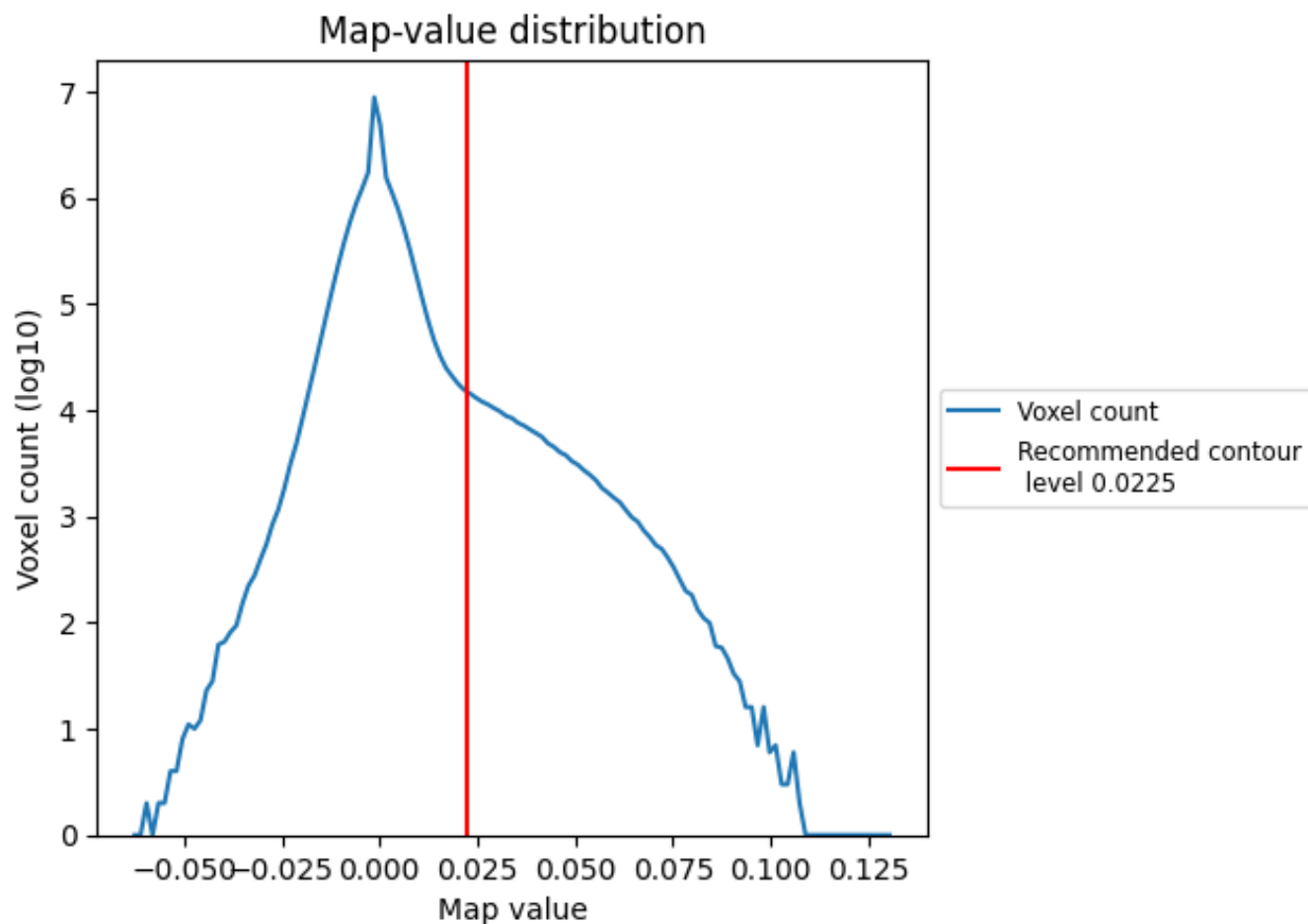
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

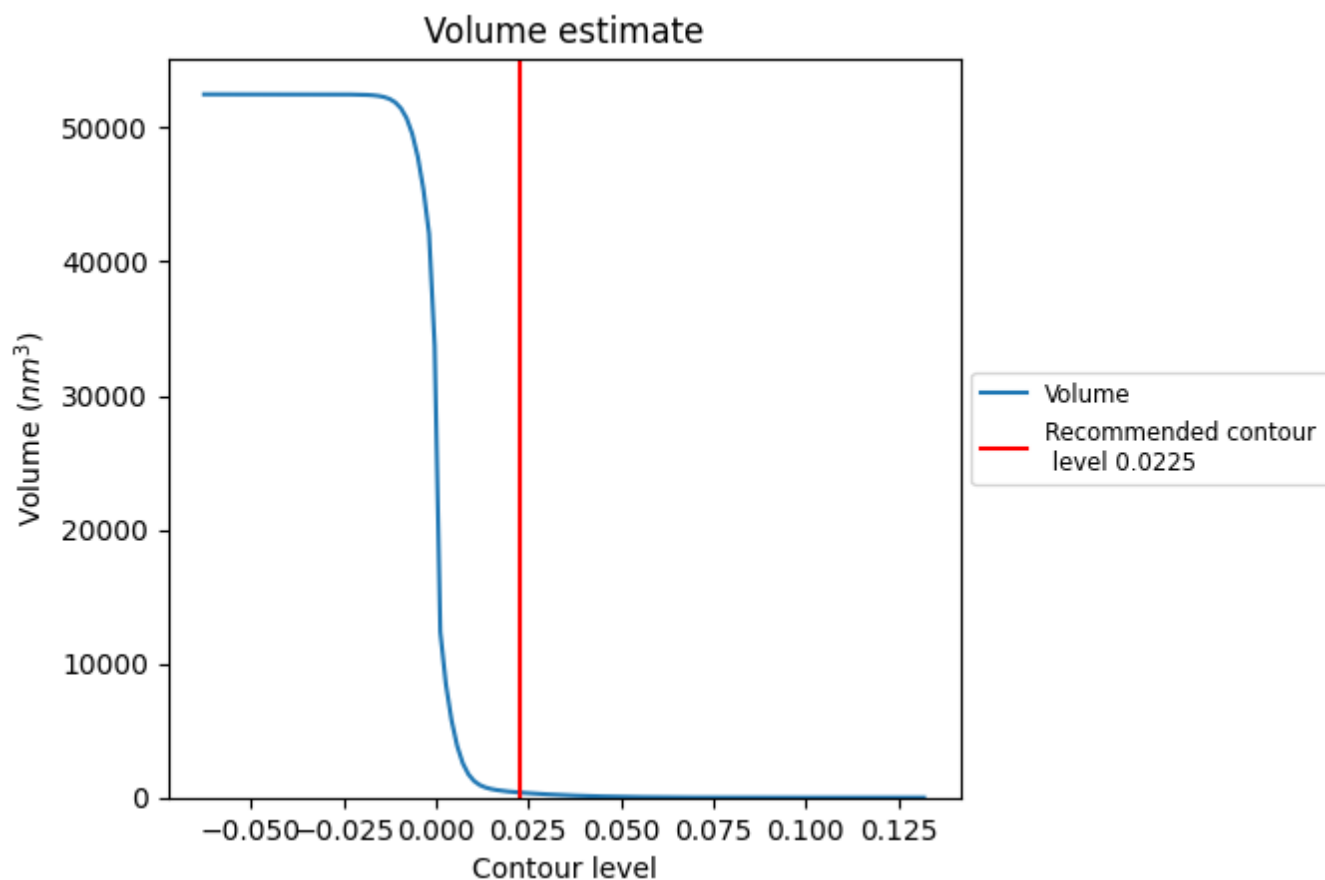
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

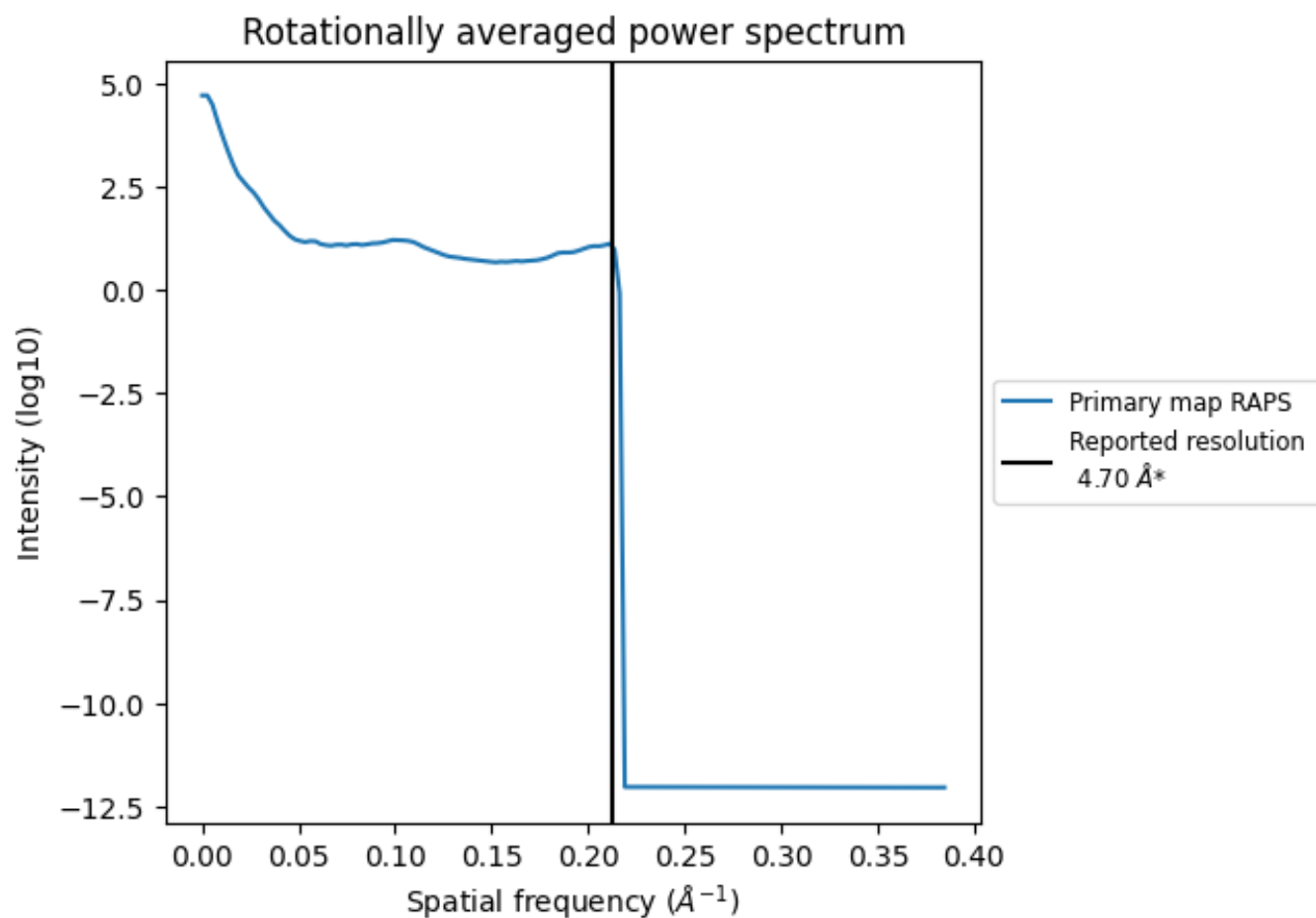
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm³; this corresponds to an approximate mass of 341 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 0.213 Å⁻¹

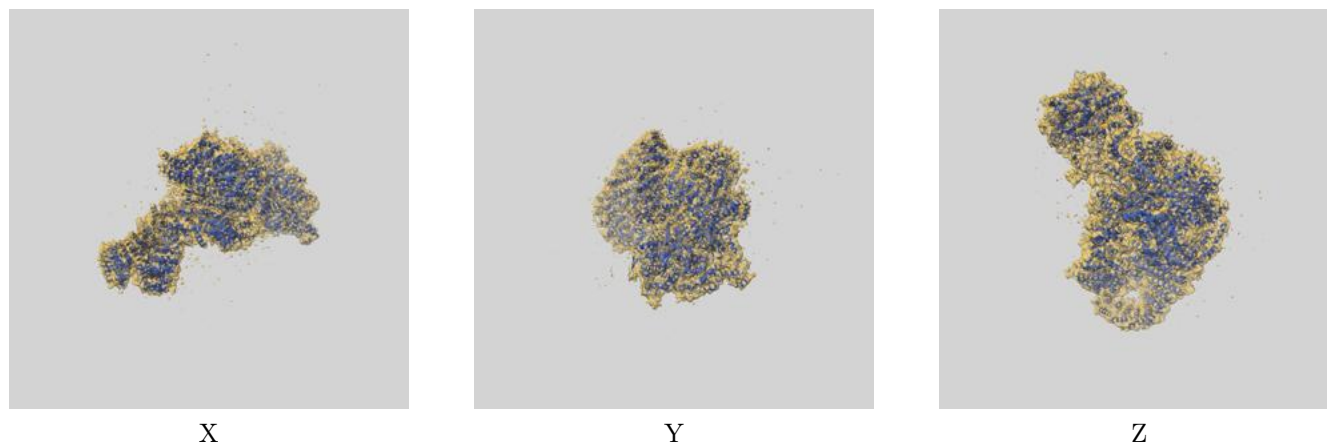
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

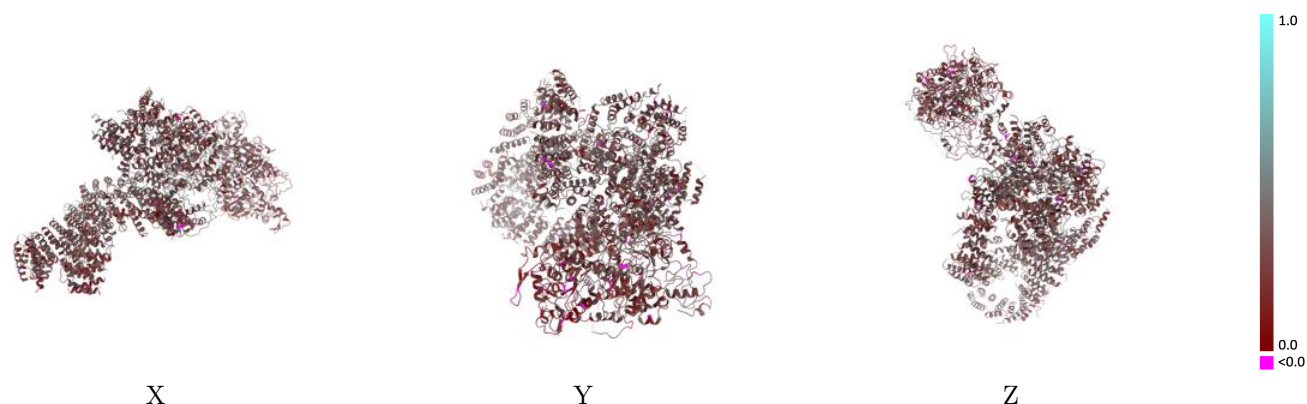
This section contains information regarding the fit between EMDB map EMD-6816 and PDB model 5Y81. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



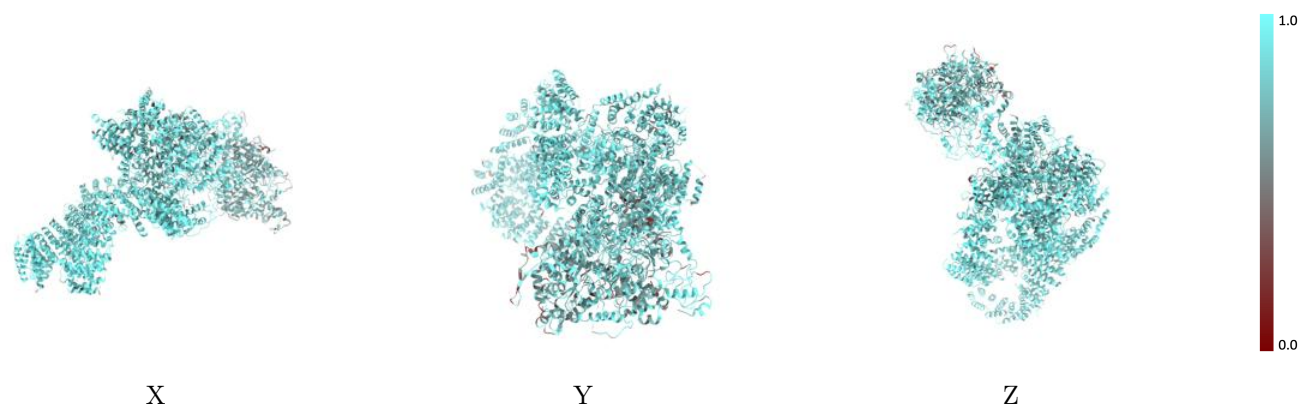
The images above show the 3D surface view of the map at the recommended contour level 0.0225 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



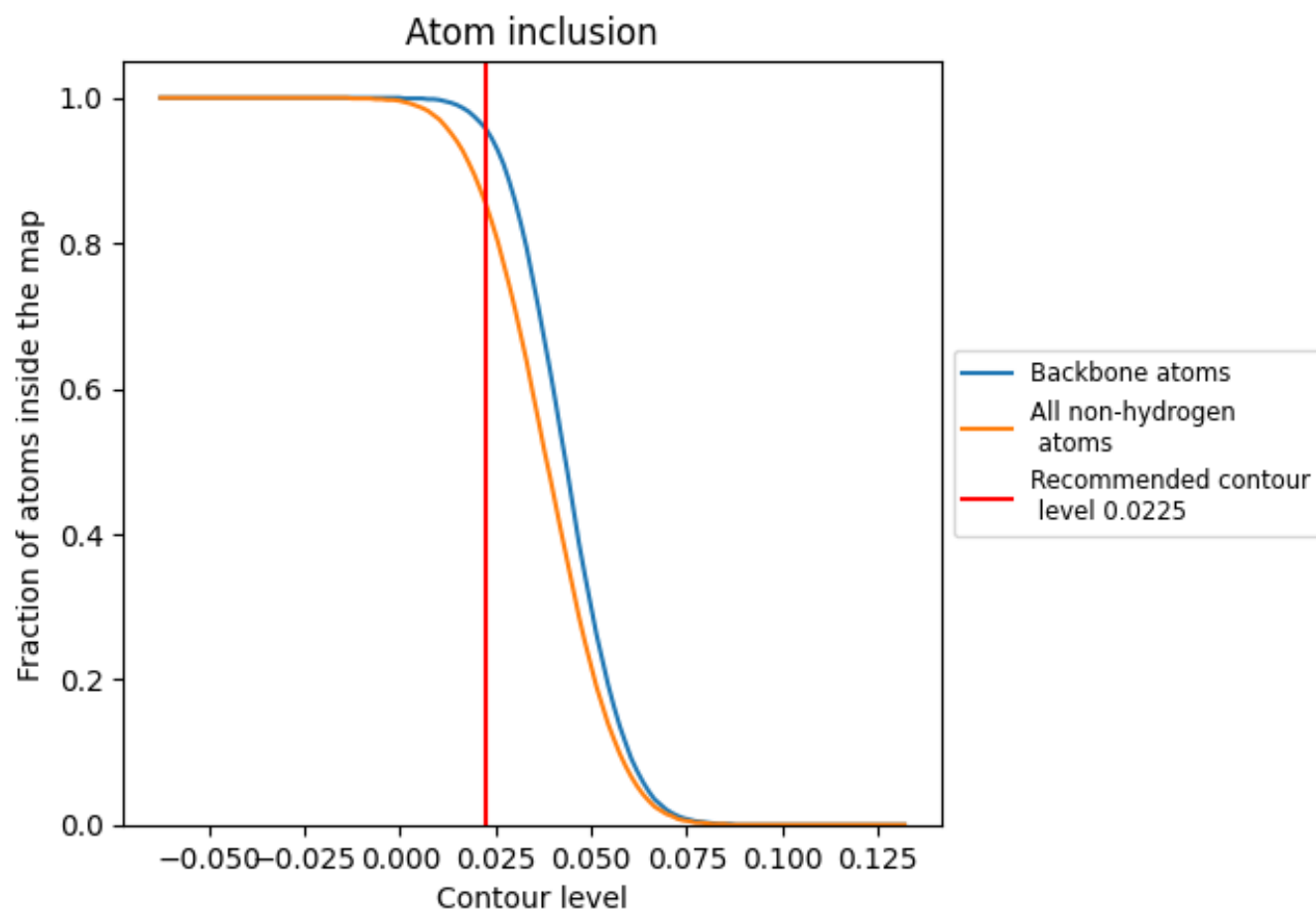
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0225).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 85% 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 (0.0225) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8530	0.3080
A	0.9250	0.3230
B	0.8590	0.3370
C	0.8950	0.3300
D	0.8830	0.3430
E	0.7090	0.2490
F	0.7100	0.2630
G	0.7180	0.2240
H	0.9020	0.3050

1.0

0.0

<0.0