



Full wwPDB EM Validation Report ⓘ

Jan 20, 2022 – 12:36 pm GMT

PDB ID : 7QE7
EMDB ID : EMD-13931
Title : High-resolution structure of the Anaphase-promoting complex/cyclosome (APC/C) bound to co-activator Cdh1
Authors : Hoefler, A.; Yu, J.; Chang, L.; Zhang, Z.; Yang, J.; Boland, A.; Barford, D.
Deposited on : 2021-12-01
Resolution : 2.90 Å (reported)
Based on initial model : 4UI9

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

EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.24

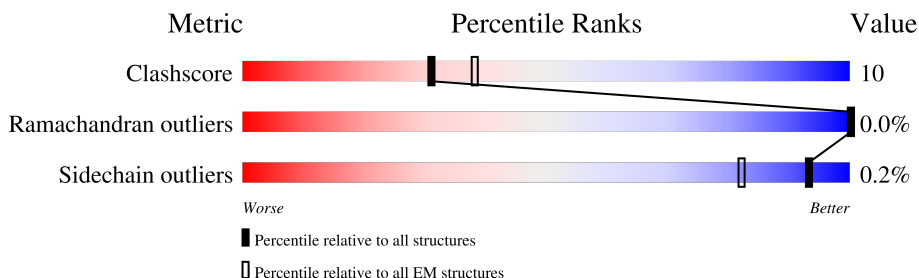
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.







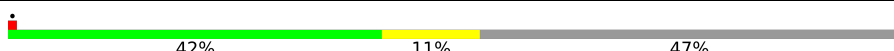
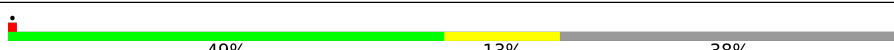
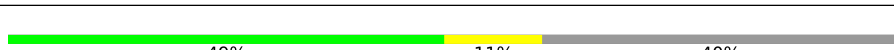
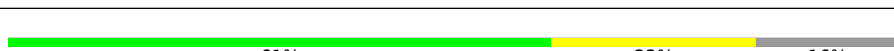


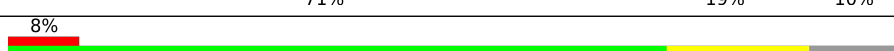

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	L	185	
2	D	121	
3	A	1944	
4	N	822	
5	I	814	
6	O	755	
7	S	447	
8	K	620	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	Q	620	
9	G	85	
9	W	85	
10	M	74	
11	H	110	
12	J	824	
12	P	824	
13	Y	599	
13	Z	599	
14	U	597	
14	V	597	
15	R	496	
16	C	84	

2 Entry composition i

There are 17 unique types of molecules in this entry. The entry contains 71432 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 Anaphase-promoting complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	183	1479	926	268	278	7	0	0

- Molecule 2 is a protein called Anaphase-promoting complex subunit 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	56	470	299	81	89	1	1	0

- Molecule 3 is a protein called Anaphase-promoting complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	1648	12968	8284	2191	2407	86	0	0

- Molecule 4 is a protein called Anaphase-promoting complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	682	5505	3484	973	1021	27	0	0

- Molecule 5 is a protein called Anaphase-promoting complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	742	5925	3793	989	1109	34	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	809	GLU	-	expression tag	UNP Q9UJX5
I	810	ASN	-	expression tag	UNP Q9UJX5
I	811	LEU	-	expression tag	UNP Q9UJX5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	812	TYR	-	expression tag	UNP Q9UJX5
I	813	PHE	-	expression tag	UNP Q9UJX5
I	814	GLN	-	expression tag	UNP Q9UJX5

- Molecule 6 is a protein called Anaphase-promoting complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	O	707	5593	3567	972	1024	30	0	0

- Molecule 7 is a protein called F-box only protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	S	100	784	483	148	144	9	0	0

- Molecule 8 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	K	531	4323	2775	726	794	28	0	0
8	Q	506	4103	2630	694	754	25	1	0

- Molecule 9 is a protein called Anaphase-promoting complex subunit CDC26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	G	27	233	146	43	43	1	0	0
9	W	26	225	142	42	40	1	0	0

- Molecule 10 is a protein called Anaphase-promoting complex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	68	553	342	91	118	2	0	0

- Molecule 11 is a protein called Anaphase-promoting complex subunit 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	58	Total	C	N	O	S	0	0
			475	304	79	90	2		

- Molecule 12 is a protein called Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	510	Total	C	N	O	S	1	0
			4097	2632	691	748	26		
12	P	496	Total	C	N	O	S	0	0
			3994	2569	671	728	26		

- Molecule 13 is a protein called Anaphase-promoting complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	502	Total	C	N	O	S	0	0
			3922	2480	682	731	29		
13	Z	488	Total	C	N	O	S	1	0
			3830	2426	664	714	26		

- Molecule 14 is a protein called Cell division cycle protein 23 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	540	Total	C	N	O	S	0	0
			4442	2859	747	810	26		
14	V	534	Total	C	N	O	S	1	0
			4380	2817	732	805	26		

- Molecule 15 is a protein called Fizzy-related protein homolog.

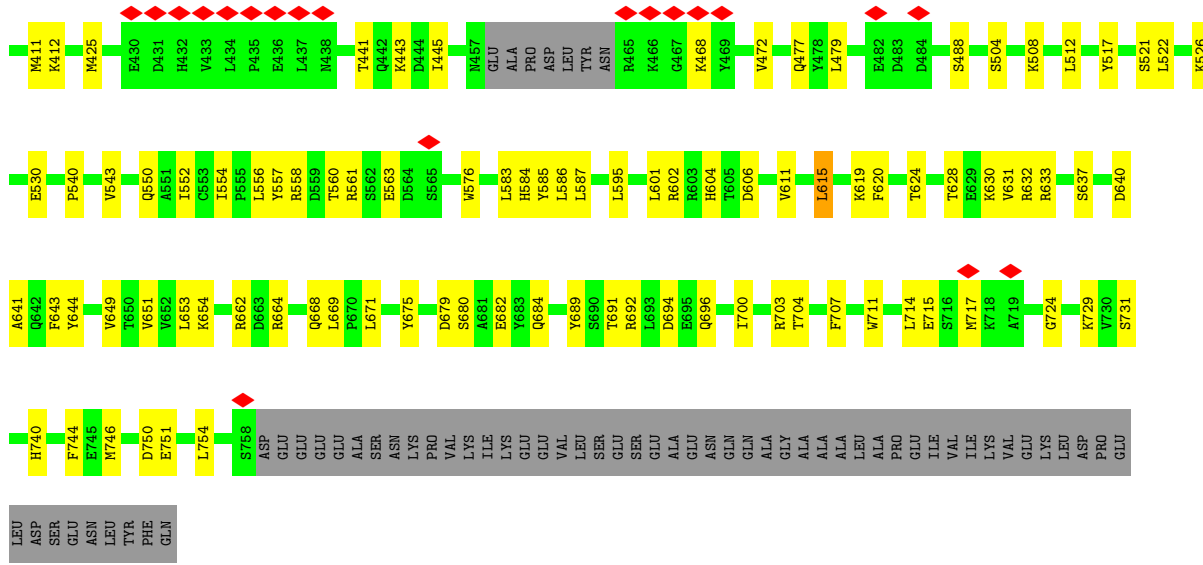
Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	440	Total	C	N	O	S	0	0
			3445	2161	627	646	11		

- Molecule 16 is a protein called Anaphase-promoting complex subunit 11.

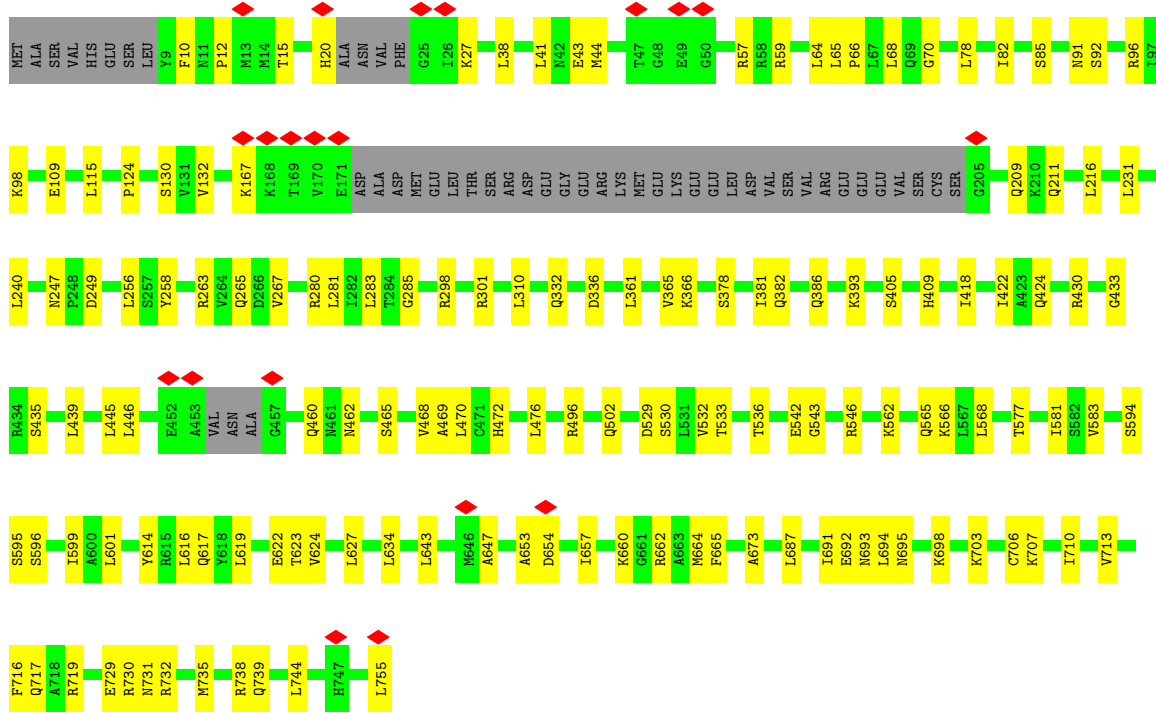
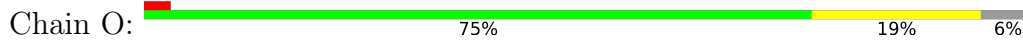
Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	84	Total	C	N	O	S	0	0
			680	431	123	110	16		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

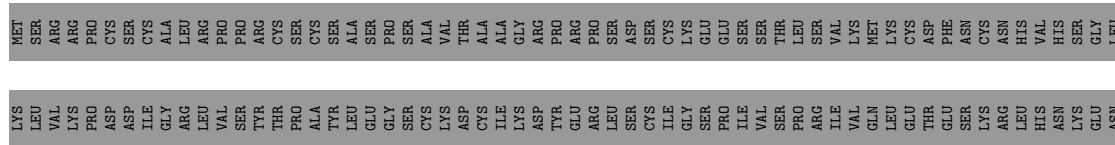
Mol	Chain	Residues	Atoms		AltConf
17	N	1	Total 1	Zn 1	0
17	S	2	Total 2	Zn 2	0
17	C	3	Total 3	Zn 3	0

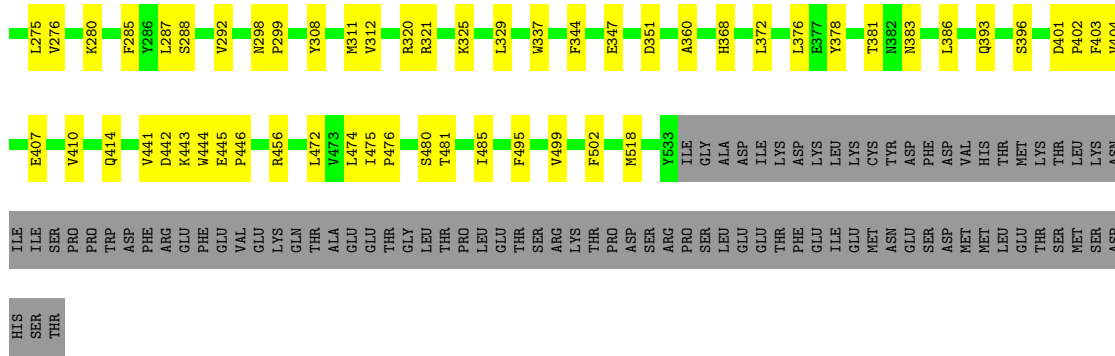


• Molecule 6: Anaphase-promoting complex subunit 5

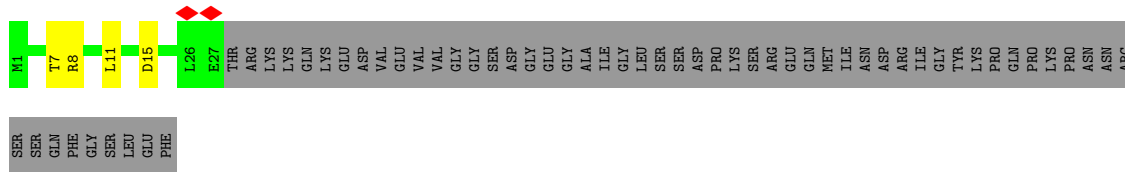


• Molecule 7: F-box only protein 5

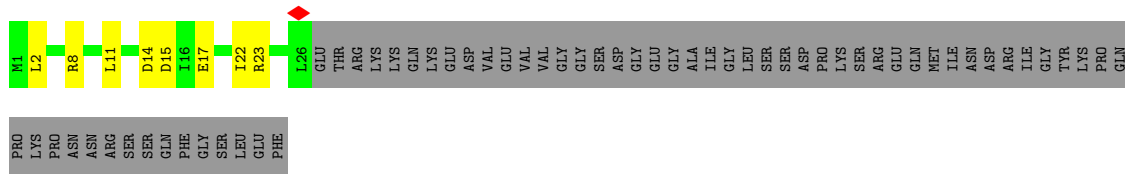




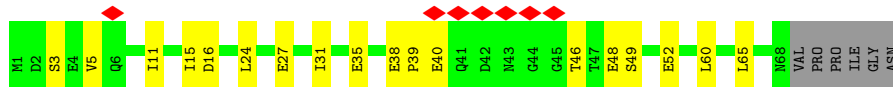
● Molecule 9: Anaphase-promoting complex subunit CDC26



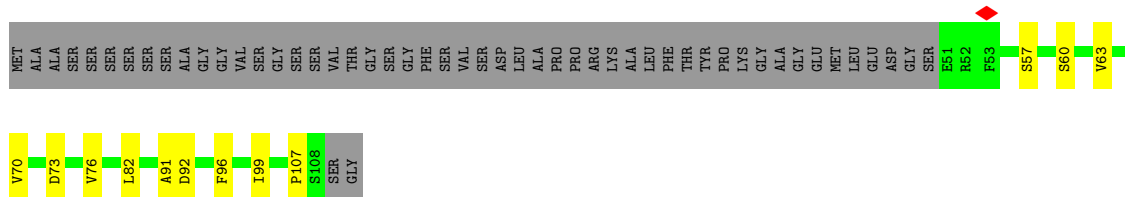
● Molecule 9: Anaphase-promoting complex subunit CDC26



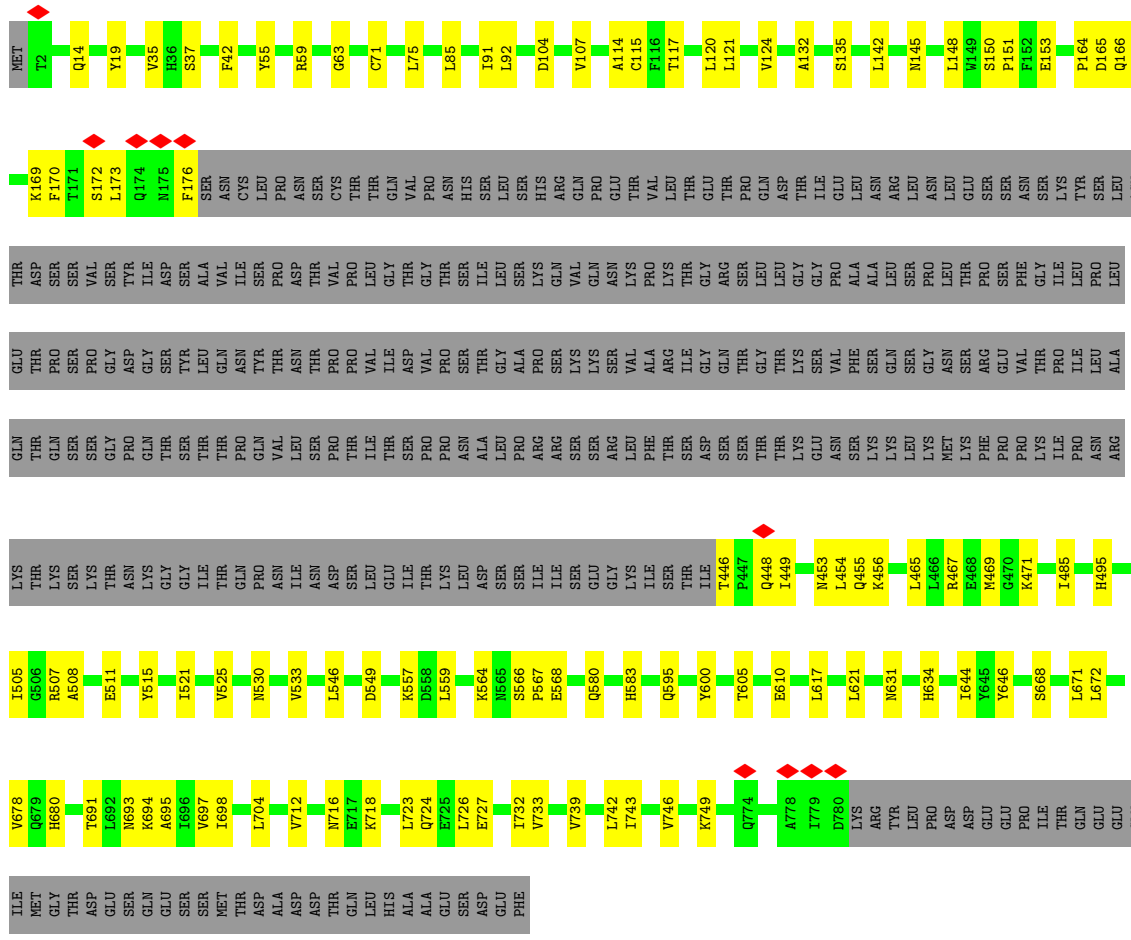
● Molecule 10: Anaphase-promoting complex subunit 13



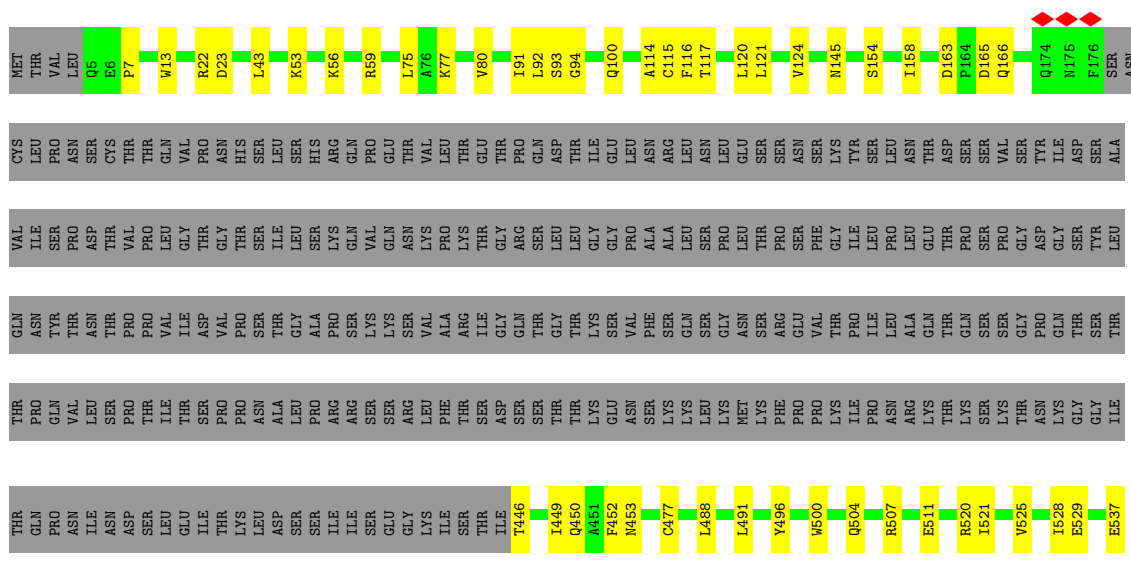
● Molecule 11: Anaphase-promoting complex subunit 16

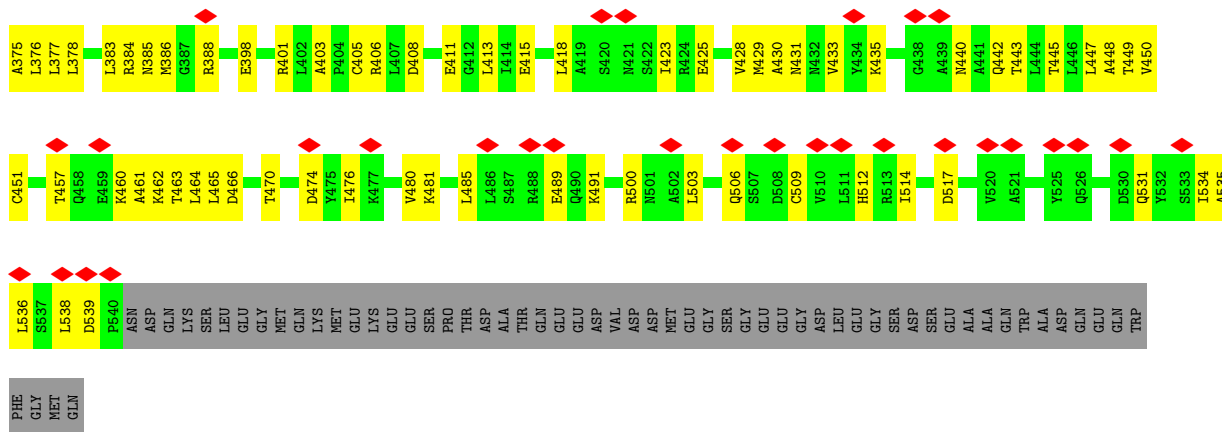


● Molecule 12: Cell division cycle protein 27 homolog

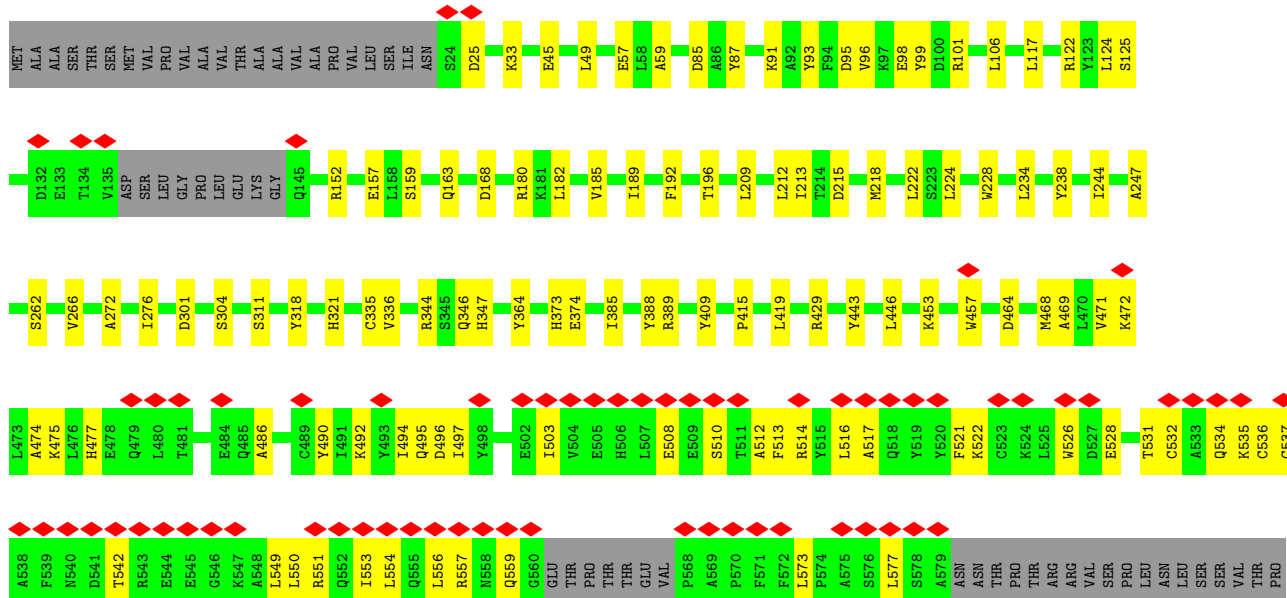


• Molecule 12: Cell division cycle protein 27 homolog

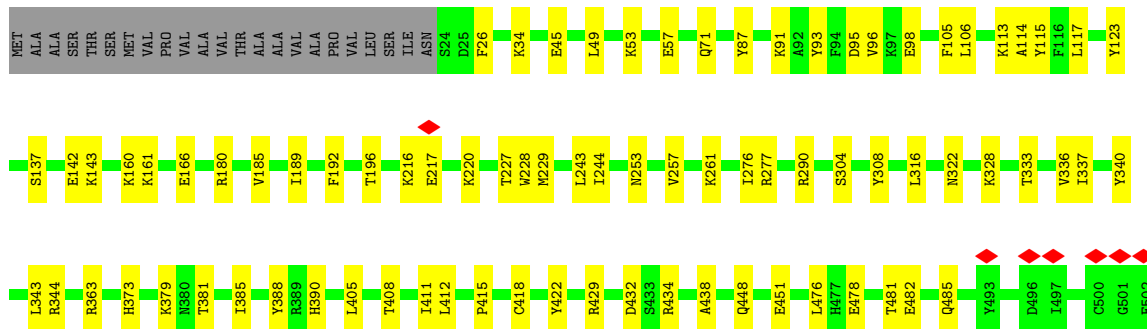


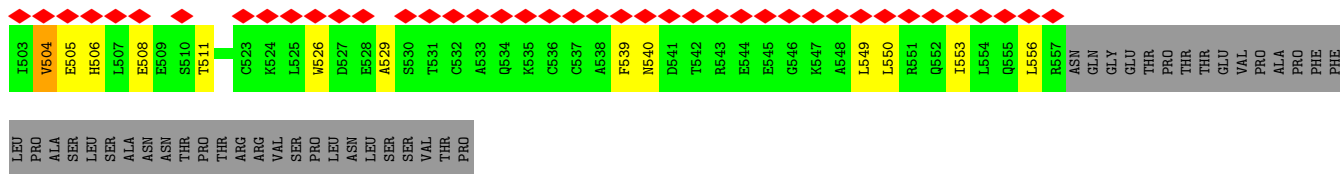


• Molecule 14: Cell division cycle protein 23 homolog

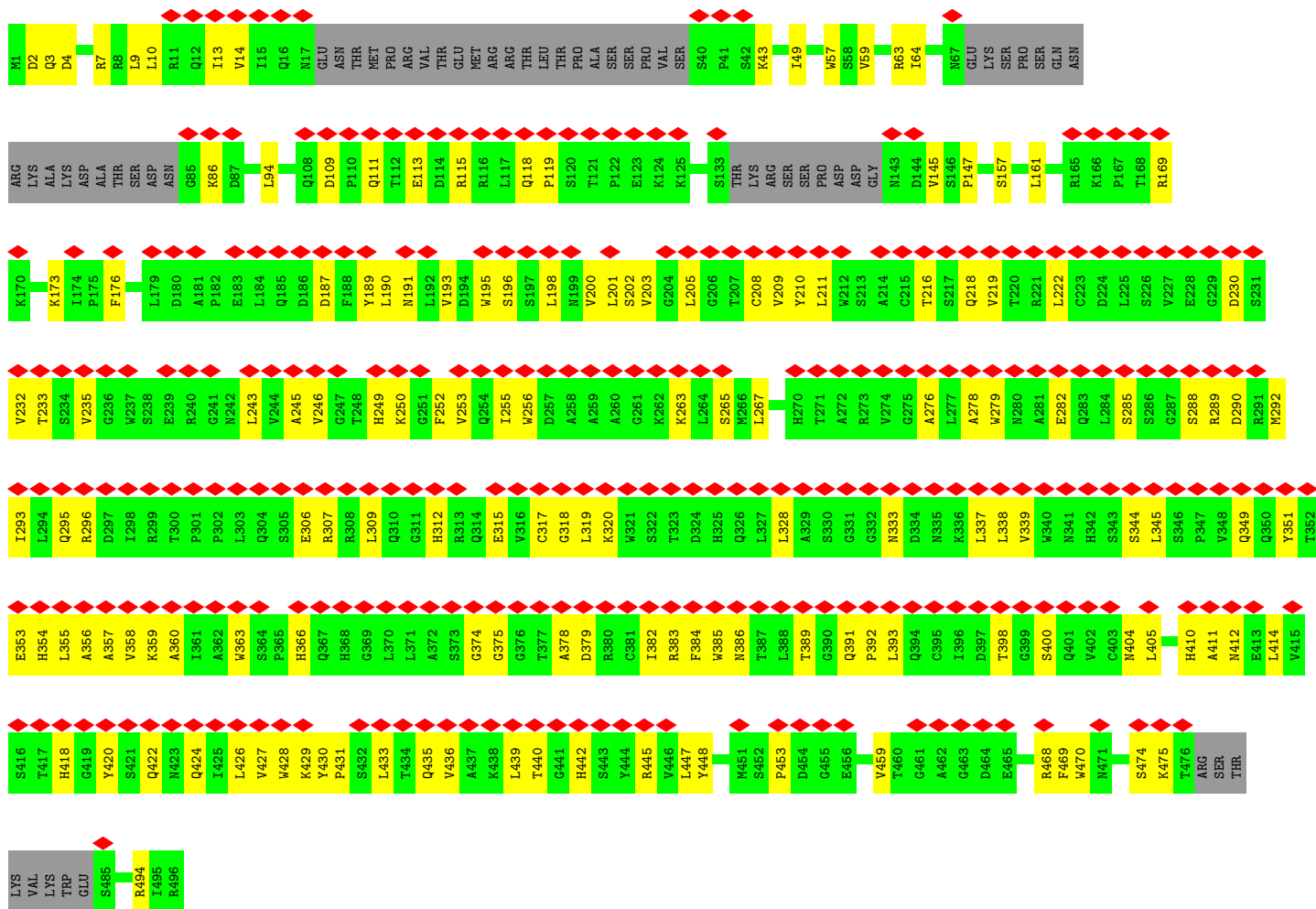


• Molecule 14: Cell division cycle protein 23 homolog

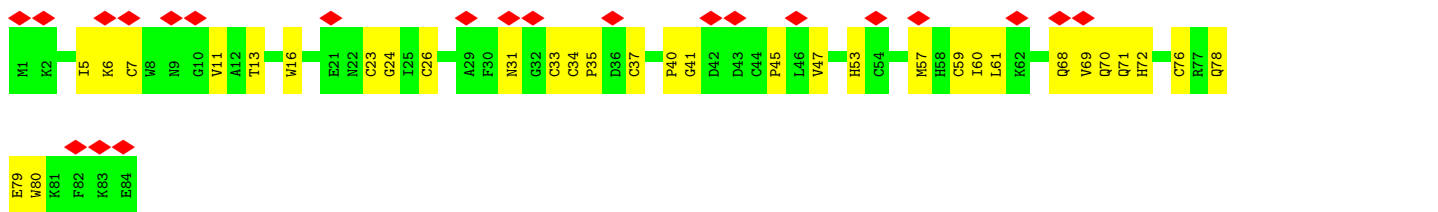




• Molecule 15: Fizzy-related protein homolog



• Molecule 16: Anaphase-promoting complex subunit 11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	364331	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.000	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

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	L	0.30	0/1514	0.47	0/2051
2	D	0.29	0/485	0.45	0/662
3	A	0.32	0/13269	0.45	0/18041
4	N	0.28	0/5618	0.46	0/7605
5	I	0.29	0/6050	0.45	0/8188
6	O	0.32	0/5697	0.43	0/7694
7	S	0.37	0/794	0.56	0/1055
8	K	0.33	0/4431	0.41	0/5998
8	Q	0.33	0/4205	0.42	0/5691
9	G	0.26	0/234	0.38	0/310
9	W	0.27	0/226	0.41	0/299
10	M	0.30	0/563	0.45	0/765
11	H	0.29	0/484	0.39	0/651
12	J	0.32	0/4196	0.42	0/5672
12	P	0.33	0/4090	0.41	0/5527
13	Y	0.26	0/3982	0.44	0/5380
13	Z	0.26	0/3893	0.49	0/5262
14	U	0.32	0/4544	0.43	0/6133
14	V	0.36	0/4483	0.43	0/6056
15	R	0.27	0/3518	0.49	0/4769
16	C	0.24	0/703	0.44	0/951
All	All	0.31	0/72979	0.44	0/98760

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1479	0	1462	33	0
2	D	470	0	458	3	0
3	A	12968	0	12918	247	0
4	N	5505	0	5487	154	0
5	I	5925	0	5902	115	0
6	O	5593	0	5659	100	0
7	S	784	0	794	33	0
8	K	4323	0	4229	62	0
8	Q	4103	0	4026	71	0
9	G	233	0	246	5	0
9	W	225	0	242	10	0
10	M	553	0	516	15	0
11	H	475	0	469	12	0
12	J	4097	0	4058	71	0
12	P	3994	0	3955	68	0
13	Y	3922	0	3989	93	0
13	Z	3830	0	3909	133	0
14	U	4442	0	4409	83	0
14	V	4380	0	4326	69	0
15	R	3445	0	3411	117	0
16	C	680	0	640	25	0
17	C	3	0	0	0	0
17	N	1	0	0	0	0
17	S	2	0	0	0	0
All	All	71432	0	71105	1384	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 10.

All (1384) 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)
13:Z:451:CYS:HB2	13:Z:457:THR:HG21	1.24	1.11
4:N:666:ILE:HD11	4:N:685:VAL:HG11	1.53	0.87
15:R:195:TRP:HE1	15:R:453:PRO:HD3	1.40	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:267:LEU:HD21	13:Z:273:LEU:HD22	1.58	0.86
13:Z:451:CYS:HB2	13:Z:457:THR:CG2	2.06	0.86
13:Z:457:THR:HG22	13:Z:457:THR:O	1.81	0.81
15:R:255:ILE:HB	15:R:265:SER:HB3	1.60	0.81
16:C:47:VAL:HG13	16:C:57:MET:HG2	1.63	0.80
16:C:34:CYS:SG	16:C:37:CYS:HB2	2.22	0.79
12:P:80:VAL:HG11	12:P:120:LEU:HD11	1.65	0.78
16:C:76:CYS:SG	16:C:78:GLN:NE2	2.56	0.78
6:O:735:MET:SD	6:O:739:GLN:NE2	2.57	0.78
15:R:195:TRP:NE1	15:R:453:PRO:HD3	1.99	0.77
3:A:617:LEU:HD11	3:A:786:LEU:HD12	1.67	0.76
15:R:253:VAL:HB	15:R:267:LEU:O	1.85	0.75
3:A:1668:VAL:O	3:A:1675:GLU:HA	1.87	0.74
1:L:98:VAL:HB	1:L:134:THR:HG21	1.68	0.74
3:A:1096:PRO:O	6:O:332:GLN:NE2	2.21	0.73
1:L:74:VAL:HG21	1:L:137:ILE:HD11	1.70	0.73
4:N:689:VAL:HA	4:N:692:LEU:HD12	1.71	0.73
8:Q:445:GLU:HG3	8:Q:446:PRO:HD3	1.71	0.72
15:R:427:VAL:HG23	15:R:436:VAL:HB	1.71	0.72
8:Q:276:VAL:HA	8:Q:311:MET:HE1	1.72	0.72
3:A:183:THR:HG22	3:A:249:LEU:HD21	1.71	0.72
4:N:646:MET:HG3	4:N:657:VAL:HG23	1.70	0.72
4:N:701:GLN:NE2	4:N:702:GLN:OE1	2.23	0.72
4:N:612:PRO:HD3	4:N:665:VAL:HG13	1.72	0.71
12:J:726:LEU:HD21	12:J:742:LEU:HD23	1.72	0.71
14:V:504:VAL:HG23	14:V:505:GLU:H	1.55	0.71
1:L:141:VAL:HG11	1:L:151:THR:HG21	1.73	0.71
15:R:355:LEU:HB2	15:R:379:ASP:HA	1.73	0.70
4:N:594:VAL:HB	16:C:11:VAL:HG22	1.73	0.70
15:R:317:CYS:HB2	15:R:359:LYS:HE3	1.72	0.70
4:N:666:ILE:HD11	4:N:685:VAL:CG1	2.20	0.70
3:A:591:VAL:HG12	3:A:592:HIS:H	1.55	0.70
3:A:795:ARG:NH2	3:A:815:ARG:O	2.24	0.70
15:R:278:ALA:HB2	15:R:319:LEU:HB3	1.74	0.70
15:R:328:LEU:O	15:R:339:VAL:HA	1.92	0.70
8:Q:368:HIS:NE2	8:Q:401:ASP:OD2	2.25	0.69
13:Z:250:ASP:OD2	13:Z:253:ARG:NH1	2.25	0.69
13:Y:271:VAL:HG21	13:Y:301:ASP:HB2	1.73	0.69
14:V:217:GLU:HA	14:V:220:LYS:HG3	1.74	0.69
3:A:1267:ARG:NH1	3:A:1315:GLY:O	2.25	0.69
8:K:524:GLU:OE2	9:W:23:ARG:NH2	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:411:HIS:NE2	3:A:414:THR:OG1	2.24	0.69
3:A:1716:GLN:HE22	4:N:327:HIS:HB2	1.57	0.69
12:J:617:LEU:HD12	12:J:644:ILE:HG23	1.74	0.69
13:Y:62:THR:HG21	13:Z:270:ASN:HB2	1.74	0.69
7:S:417:LYS:HD3	7:S:417:LYS:O	1.93	0.68
6:O:43:GLU:OE2	6:O:96:ARG:NH2	2.26	0.68
13:Z:386:MET:SD	13:Z:388:ARG:NH2	2.66	0.68
3:A:766:LEU:HB3	3:A:790:LEU:HD21	1.75	0.68
3:A:1826:HIS:O	3:A:1830:LEU:HB3	1.94	0.68
12:J:530:ASN:OD1	12:P:59:ARG:NH1	2.27	0.68
8:K:400:GLU:HB2	8:K:431:LYS:HE3	1.75	0.68
3:A:594:ARG:HG2	3:A:608:THR:HG22	1.76	0.67
13:Z:406:ARG:HH21	13:Z:408:ASP:HB3	1.59	0.67
13:Y:164:SER:HA	13:Y:167:ARG:HD2	1.76	0.67
15:R:339:VAL:HB	15:R:349:GLN:HB2	1.76	0.67
15:R:169:ARG:HH12	15:R:474:SER:H	1.39	0.67
15:R:205:LEU:HD21	15:R:210:TYR:HD2	1.60	0.67
5:I:116:MET:HG2	5:I:210:LEU:HB3	1.77	0.67
4:N:189:ARG:HG3	4:N:196:ASP:HB2	1.76	0.67
6:O:240:LEU:HD21	6:O:256:LEU:HD23	1.77	0.67
5:I:211:SER:HB3	5:I:584:HIS:HE2	1.60	0.66
4:N:311:ARG:HB2	4:N:312:PRO:HD3	1.77	0.66
7:S:325:LEU:HD21	15:R:203:VAL:HG21	1.78	0.66
3:A:506:VAL:HG22	3:A:639:VAL:HG22	1.78	0.66
3:A:1721:GLN:HA	3:A:1724:ALA:HB2	1.78	0.66
12:P:94:GLY:HA3	12:P:100:GLN:HA	1.77	0.66
13:Z:261:LEU:HB2	13:Z:267:LEU:HD22	1.78	0.66
15:R:320:LYS:HE2	15:R:363:TRP:H	1.59	0.66
3:A:94:TYR:CE2	3:A:96:ALA:HB2	2.32	0.65
15:R:360:ALA:HB1	15:R:405:LEU:HD13	1.77	0.65
5:I:327:VAL:HG22	5:I:425:MET:HE3	1.77	0.65
13:Z:258:ILE:HD11	13:Z:277:LEU:HD13	1.79	0.65
4:N:162:PHE:O	4:N:255:ARG:NH2	2.29	0.65
6:O:249:ASP:OD1	6:O:280:ARG:NH2	2.29	0.65
13:Z:252:SER:HA	13:Z:255:ILE:HD12	1.77	0.65
3:A:1067:GLU:OE2	3:A:1124:ASN:ND2	2.28	0.65
12:J:166:GLN:O	12:J:169:LYS:NZ	2.25	0.65
12:J:533:VAL:HG23	12:J:559:LEU:HD22	1.78	0.65
3:A:775:LEU:HD11	3:A:844:ILE:HD13	1.80	0.64
13:Y:194:GLU:OE1	13:Y:197:ARG:NH2	2.30	0.64
14:U:464:ASP:OD2	14:U:468:MET:N	2.29	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:188:LEU:HD11	3:A:223:LEU:HD13	1.77	0.64
4:N:706:ARG:HB2	4:N:716:ILE:HD11	1.80	0.64
13:Y:192:TYR:HB3	13:Y:209:LEU:HD12	1.80	0.64
15:R:289:ARG:HG3	15:R:315:GLU:HB2	1.79	0.64
15:R:384:PHE:O	15:R:393:LEU:N	2.30	0.64
7:S:392:GLN:HG3	7:S:408:LYS:HE3	1.80	0.64
13:Z:210:LEU:HD11	13:Z:219:VAL:HG11	1.80	0.64
13:Y:373:VAL:HG11	13:Y:403:ALA:HB2	1.80	0.63
4:N:229:GLN:OE1	4:N:229:GLN:N	2.26	0.63
12:J:85:LEU:HB2	12:J:124:VAL:HG23	1.79	0.63
7:S:358:ARG:NH1	7:S:382:ASN:O	2.31	0.63
12:P:93:SER:HB2	12:P:121:LEU:HD21	1.80	0.63
3:A:1635:GLU:HB2	3:A:1669:LYS:HD2	1.80	0.63
10:M:60:LEU:HD11	12:J:549:ASP:HB3	1.79	0.63
12:P:730:LYS:HE3	12:P:740:TYR:HE1	1.63	0.63
14:U:554:LEU:HA	14:U:557:ARG:HG2	1.79	0.63
15:R:356:ALA:HB2	15:R:378:ALA:HB3	1.79	0.63
4:N:652:ASP:HB3	4:N:718:GLU:HB2	1.81	0.63
13:Z:460:LYS:HA	13:Z:463:THR:HG22	1.80	0.63
14:U:531:THR:O	14:U:535:LYS:HG2	1.98	0.63
3:A:137:LYS:HE2	3:A:273:ARG:HH11	1.63	0.63
12:P:163:ASP:HB3	12:P:166:GLN:HB2	1.80	0.63
3:A:271:LEU:HD11	3:A:407:LEU:HD23	1.81	0.62
3:A:1354:GLU:OE2	3:A:1359:ASN:ND2	2.31	0.62
4:N:227:ASP:OD1	4:N:227:ASP:N	2.27	0.62
13:Z:474:ASP:HB2	13:Z:506:GLN:HE22	1.63	0.62
14:V:333:THR:O	14:V:337:ILE:HG12	1.99	0.62
11:H:92:ASP:OD1	12:J:595:GLN:NE2	2.32	0.62
3:A:247:VAL:HG11	3:A:427:ALA:HB3	1.82	0.62
4:N:528:LEU:HD11	4:N:641:LEU:HD11	1.82	0.62
3:A:1726:ARG:NH2	3:A:1780:THR:OG1	2.24	0.62
8:K:171:THR:HB	8:K:209:LEU:HD21	1.82	0.62
14:V:550:LEU:HD23	14:V:553:ILE:HD12	1.80	0.62
5:I:714:LEU:HD13	5:I:717:MET:HE3	1.83	0.61
12:J:92:LEU:HD11	12:J:120:LEU:HD23	1.82	0.61
3:A:45:ALA:O	14:V:180:ARG:NH1	2.30	0.61
5:I:441:THR:HG22	5:I:443:LYS:H	1.65	0.61
3:A:720:GLU:O	3:A:725:ASN:ND2	2.33	0.61
1:L:163:GLU:CD	1:L:164:GLU:H	2.03	0.61
5:I:312:LYS:NZ	6:O:124:PRO:O	2.33	0.61
15:R:296:ARG:NH2	15:R:306:GLU:OE2	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:193:VAL:HG22	15:R:203:VAL:HG12	1.81	0.61
12:J:153:GLU:OE1	12:P:22:ARG:NH2	2.33	0.61
13:Z:309:ASP:HB2	13:Z:340:GLU:HG3	1.83	0.61
4:N:162:PHE:HE2	4:N:252:LEU:HD13	1.65	0.61
6:O:601:LEU:HD11	6:O:634:LEU:HD11	1.83	0.61
14:U:25:ASP:HB3	14:U:228:TRP:HB3	1.82	0.61
14:U:464:ASP:OD2	14:U:469:ALA:N	2.34	0.61
13:Z:308:MET:HA	13:Z:311:TYR:HB3	1.83	0.61
12:J:691:THR:HA	12:J:694:LYS:HE3	1.82	0.60
3:A:252:ASP:HB2	3:A:253:PRO:HD3	1.82	0.60
8:Q:194:CYS:SG	8:Q:195:ASN:N	2.74	0.60
4:N:609:LEU:HD12	4:N:639:HIS:HB2	1.83	0.60
5:I:107:GLU:OE1	5:I:197:ARG:NH2	2.33	0.60
6:O:542:GLU:OE1	6:O:546:ARG:NH1	2.33	0.60
5:I:269:LEU:HD22	5:I:526:LYS:HD3	1.83	0.60
13:Y:373:VAL:HA	13:Y:376:LEU:HD12	1.83	0.60
4:N:365:LEU:HD11	4:N:374:LEU:HD13	1.84	0.60
4:N:646:MET:HA	16:C:6:LYS:H	1.66	0.60
5:I:230:GLU:HB2	5:I:558:ARG:HG3	1.84	0.60
5:I:619:LYS:O	5:I:704:THR:HA	2.02	0.60
11:H:91:ALA:O	12:J:595:GLN:NE2	2.33	0.60
14:V:290:ARG:NH2	14:V:322:ASN:OD1	2.34	0.60
14:V:540:ASN:ND2	15:R:145:VAL:O	2.35	0.60
16:C:68:GLN:HG3	16:C:69:VAL:H	1.67	0.60
3:A:1827:GLN:NE2	4:N:143:GLY:O	2.35	0.60
13:Y:40:HIS:HE1	13:Z:200:PRO:HD2	1.67	0.60
5:I:272:MET:HG3	5:I:347:LEU:HD23	1.83	0.60
8:K:177:THR:HB	8:K:180:GLU:HG3	1.83	0.60
3:A:845:TYR:HB3	3:A:1812:TRP:CE2	2.37	0.59
8:Q:320:ARG:NH2	8:Q:347:GLU:OE1	2.35	0.59
13:Z:44:MET:HB3	13:Z:49:LEU:HD11	1.83	0.59
3:A:1925:VAL:HG21	4:N:70:VAL:HB	1.84	0.59
13:Z:227:ILE:HD11	13:Z:234:ASP:HA	1.82	0.59
5:I:682:GLU:OE2	5:I:703:ARG:NH1	2.34	0.59
13:Z:206:ILE:HG23	13:Z:219:VAL:HG21	1.84	0.59
3:A:880:TYR:HB2	3:A:930:LEU:HD22	1.85	0.59
6:O:729:GLU:HA	6:O:732:ARG:HG2	1.84	0.59
13:Y:268:ARG:O	13:Z:66:ASN:ND2	2.32	0.59
14:U:513:PHE:HB3	14:U:536:CYS:HB3	1.83	0.59
15:R:191:ASN:ND2	15:R:235:VAL:O	2.36	0.59
5:I:231:VAL:HG23	5:I:556:LEU:HB2	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:325:LYS:HE3	8:Q:329:LEU:HD11	1.84	0.59
3:A:1167:GLU:HG3	3:A:1168:LEU:HG	1.84	0.59
16:C:70:GLN:HB2	16:C:72:HIS:HD2	1.68	0.59
3:A:1797:ILE:HG21	3:A:1848:VAL:HG23	1.83	0.59
1:L:113:LEU:HB3	1:L:116:PRO:HG3	1.85	0.59
5:I:560:THR:HB	5:I:563:GLU:HB2	1.85	0.59
13:Z:159:LEU:HD22	13:Z:171:ILE:HG23	1.84	0.59
13:Y:143:ALA:O	13:Y:147:THR:HG23	2.03	0.58
14:U:517:ALA:HB1	14:U:549:LEU:HD13	1.86	0.58
14:U:521:PHE:HD2	14:U:522:LYS:HD2	1.66	0.58
13:Y:71:PHE:HB3	13:Y:75:GLN:HB2	1.85	0.58
5:I:117:GLU:OE1	5:I:172:ARG:NH2	2.36	0.58
8:Q:372:LEU:HD13	8:Q:404:VAL:HG12	1.85	0.58
13:Y:418:LEU:HD21	13:Y:450:VAL:HG23	1.85	0.58
3:A:1537:GLN:NE2	4:N:478:GLU:OE1	2.35	0.58
6:O:624:VAL:HG11	6:O:647:ALA:HB1	1.85	0.58
13:Y:42:ARG:HH2	13:Y:131:CYS:HB3	1.67	0.58
12:J:507:ARG:NH1	12:J:511:GLU:OE2	2.37	0.58
15:R:412:ASN:HD21	15:R:430:TYR:HD2	1.49	0.58
5:I:60:PRO:HB2	5:I:66:LYS:HG2	1.85	0.58
8:Q:445:GLU:HB3	8:Q:474:LEU:HD23	1.85	0.58
4:N:229:GLN:H	4:N:229:GLN:CD	2.05	0.58
4:N:395:ASP:HB3	7:S:444:LEU:HD21	1.86	0.58
5:I:557:TYR:OH	5:I:561:ARG:NH2	2.37	0.58
14:U:91:LYS:NZ	14:U:95:ASP:OD1	2.37	0.58
14:V:526:TRP:HA	14:V:529:ALA:HB3	1.86	0.58
3:A:1797:ILE:HD12	3:A:1851:THR:HG21	1.86	0.58
4:N:112:LEU:HD21	4:N:243:LEU:HB2	1.86	0.58
5:I:380:GLY:HA3	5:I:543:VAL:HG21	1.86	0.58
3:A:963:ARG:NH2	3:A:1782:GLU:O	2.37	0.57
6:O:430:ARG:HD3	6:O:472:HIS:CD2	2.39	0.57
14:V:244:ILE:HG21	14:V:276:ILE:HG13	1.86	0.57
15:R:422:GLN:HG3	15:R:424:GLN:HG2	1.86	0.57
3:A:1281:PRO:HB2	3:A:1349:SER:HB2	1.86	0.57
3:A:1306:CYS:HB2	3:A:1374:ILE:HG12	1.86	0.57
4:N:440:ALA:O	4:N:443:THR:OG1	2.23	0.57
4:N:513:ASP:OD2	7:S:380:ARG:NH2	2.27	0.57
10:M:27:GLU:OE1	14:V:344:ARG:NH1	2.38	0.57
10:M:46:THR:HG23	10:M:48:GLU:H	1.69	0.57
4:N:546:LYS:O	4:N:550:GLY:N	2.37	0.57
7:S:381:CYS:SG	7:S:401:CYS:HB3	2.44	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:35:GLU:HB3	8:Q:40:ILE:HD11	1.86	0.57
3:A:757:THR:HG22	3:A:830:PHE:HB3	1.86	0.57
12:P:93:SER:OG	12:P:94:GLY:N	2.37	0.57
15:R:442:HIS:CE1	15:R:468:ARG:HG3	2.39	0.57
1:L:164:GLU:CD	1:L:165:SER:H	2.07	0.57
5:I:187:LEU:HB2	5:I:196:ALA:HB3	1.87	0.57
8:K:453:HIS:HE1	9:W:11:LEU:HG	1.70	0.57
12:P:92:LEU:HD22	12:P:117:THR:OG1	2.05	0.57
3:A:249:LEU:HD13	3:A:256:VAL:HG22	1.87	0.57
5:I:325:LEU:HD21	5:I:330:LEU:HD13	1.87	0.57
13:Y:186:ARG:HE	13:Y:190:THR:HG23	1.69	0.57
13:Y:508:ASP:O	13:Y:512:HIS:ND1	2.35	0.57
4:N:51:LYS:HB3	4:N:54:GLU:HB2	1.87	0.57
5:I:9:PRO:HD3	5:I:754:LEU:HB3	1.86	0.57
14:V:411:ILE:HG12	15:R:57:TRP:HB3	1.87	0.57
5:I:7:CYS:SG	5:I:628:THR:OG1	2.62	0.57
13:Z:296:GLN:O	13:Z:299:MET:HG2	2.04	0.57
7:S:388:ASP:O	7:S:392:GLN:N	2.38	0.57
15:R:195:TRP:CE3	15:R:201:LEU:HB2	2.39	0.57
5:I:504:SER:O	5:I:508:LYS:NZ	2.37	0.56
14:V:478:GLU:O	14:V:481:THR:N	2.31	0.56
3:A:1766:GLU:OE1	3:A:1798:ARG:NH2	2.37	0.56
11:H:63:VAL:HG21	13:Y:364:LYS:HB2	1.86	0.56
4:N:234:ARG:HE	4:N:234:ARG:N	2.02	0.56
12:J:142:LEU:HG	12:J:151:PRO:HB2	1.87	0.56
15:R:200:VAL:HG11	15:R:211:LEU:HD13	1.86	0.56
3:A:1694:ASP:HB3	3:A:1696:VAL:HG23	1.85	0.56
13:Z:291:VAL:HG23	13:Z:311:TYR:HE1	1.69	0.56
3:A:705:ASP:OD1	6:O:738:ARG:NH1	2.39	0.56
4:N:666:ILE:CG1	4:N:685:VAL:HG21	2.36	0.56
9:W:14:ASP:O	9:W:17:GLU:HG2	2.06	0.56
13:Z:295:GLU:OE2	13:Z:298:GLN:NE2	2.39	0.56
3:A:98:ASN:HA	3:A:123:VAL:HG23	1.88	0.56
3:A:100:VAL:HG13	3:A:117:PHE:HB2	1.88	0.56
13:Z:246:VAL:HG22	13:Z:280:LEU:HD21	1.87	0.56
3:A:961:HIS:HB3	3:A:1836:ARG:HH11	1.71	0.56
4:N:577:GLU:OE1	4:N:581:ARG:NH1	2.39	0.56
8:K:35:GLU:HB3	8:K:40:ILE:HD11	1.87	0.56
12:J:165:ASP:OD1	12:J:471:LYS:NZ	2.32	0.56
6:O:59:ARG:NH2	6:O:85:SER:O	2.35	0.56
15:R:196:SER:HB2	15:R:200:VAL:H	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:502:ILE:HB	4:N:548:ARG:HH21	1.71	0.56
13:Y:246:VAL:HG13	13:Y:280:LEU:HD21	1.87	0.56
15:R:307:ARG:NH2	15:R:344:SER:O	2.39	0.56
3:A:637:MET:HA	3:A:667:MET:HE1	1.88	0.56
3:A:1918:PHE:HD2	3:A:1921:LEU:HD11	1.71	0.56
15:R:285:SER:OG	15:R:295:GLN:NE2	2.38	0.56
5:I:303:GLU:HB3	5:I:317:LEU:HD13	1.88	0.55
10:M:3:SER:OG	14:U:180:ARG:NH2	2.38	0.55
14:U:301:ASP:OD2	14:U:364:TYR:OH	2.24	0.55
13:Z:509:CYS:HA	13:Z:512:HIS:HB2	1.88	0.55
13:Z:457:THR:CG2	13:Z:457:THR:O	2.52	0.55
3:A:724:LEU:O	3:A:727:SER:OG	2.24	0.55
5:I:341:TYR:HB3	5:I:411:MET:HE2	1.88	0.55
3:A:1284:GLU:HG2	3:A:1285:MET:H	1.71	0.55
4:N:224:CYS:SG	4:N:226:SER:HB2	2.46	0.55
12:P:477:CYS:O	12:P:633:ARG:NH2	2.40	0.55
13:Y:160:ASP:HA	13:Y:167:ARG:NH2	2.21	0.55
13:Z:220:ALA:O	13:Z:224:MET:HG2	2.06	0.55
4:N:517:ASN:ND2	7:S:409:CYS:HB3	2.22	0.55
8:Q:376:LEU:HD21	8:Q:407:GLU:HG3	1.89	0.55
14:U:550:LEU:O	14:U:553:ILE:HG22	2.07	0.55
3:A:1086:MET:HG2	3:A:1610:TYR:CZ	2.42	0.55
3:A:1437:ASN:HB2	3:A:1457:LEU:HD23	1.88	0.55
13:Y:37:VAL:HG12	13:Z:233:LEU:HD11	1.87	0.55
13:Z:201:LEU:HD21	13:Z:233:LEU:HD13	1.89	0.55
15:R:276:ALA:HB3	15:R:319:LEU:HD23	1.88	0.55
6:O:66:PRO:O	6:O:70:GLY:N	2.37	0.55
8:Q:60:LEU:HD22	8:Q:72:CYS:HB3	1.88	0.55
4:N:682:SER:O	4:N:686:LYS:N	2.39	0.55
5:I:75:PRO:HG2	5:I:117:GLU:HB2	1.88	0.55
5:I:408:ASP:OD2	5:I:412:LYS:NZ	2.40	0.55
5:I:477:GLN:NE2	5:I:488:SER:OG	2.39	0.55
5:I:717:MET:HG2	5:I:740:HIS:CE1	2.42	0.55
14:U:453:LYS:HZ3	14:U:457:TRP:HE1	1.54	0.55
14:V:508:GLU:HA	14:V:511:THR:HG22	1.89	0.55
15:R:94:LEU:HD11	15:R:161:LEU:HD21	1.87	0.55
4:N:289:PHE:O	4:N:293:ILE:HG12	2.07	0.55
12:J:724:GLN:O	12:J:724:GLN:NE2	2.39	0.55
14:U:304:SER:HB3	14:U:336:VAL:HG22	1.88	0.55
14:U:106:LEU:HD11	14:U:117:LEU:HD23	1.88	0.54
14:V:316:LEU:HD23	14:V:343:LEU:HD12	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:360:ALA:HA	15:R:404:ASN:HA	1.89	0.54
1:L:115:GLU:H	1:L:145:HIS:CE1	2.26	0.54
4:N:169:PHE:HA	4:N:172:MET:HG2	1.90	0.54
13:Y:532:TYR:HB3	13:Y:549:MET:HG2	1.89	0.54
13:Z:373:VAL:O	13:Z:377:LEU:HD12	2.08	0.54
3:A:205:GLU:HG2	15:R:13:ILE:HG21	1.90	0.54
3:A:501:THR:HG23	3:A:504:VAL:HB	1.89	0.54
6:O:568:LEU:HB2	6:O:583:VAL:HG11	1.88	0.54
8:K:225:ASP:HA	8:K:228:GLN:HE22	1.73	0.54
14:V:381:THR:HG21	14:V:412:LEU:HD21	1.90	0.54
7:S:362:PHE:CD2	16:C:35:PRO:HG3	2.43	0.54
12:J:583:HIS:ND1	12:J:610:GLU:OE2	2.28	0.54
13:Y:346:GLY:HA3	13:Y:378:LEU:HD21	1.90	0.54
14:V:540:ASN:HB2	15:R:147:PRO:HG3	1.89	0.54
13:Z:408:ASP:O	13:Z:411:GLU:HG3	2.07	0.54
6:O:562:LYS:O	6:O:566:LYS:HG3	2.08	0.54
8:K:174:HIS:CE1	8:K:211:LYS:HD2	2.42	0.54
14:U:222:LEU:HD23	14:U:224:LEU:HD21	1.88	0.54
14:U:385:ILE:O	14:U:389:ARG:HG2	2.07	0.54
3:A:1430:VAL:O	3:A:1435:ARG:NH2	2.41	0.54
12:P:115:CYS:SG	12:P:145:ASN:HB2	2.48	0.54
13:Z:339:ALA:O	13:Z:343:VAL:HG23	2.08	0.54
13:Z:440:ASN:HB3	13:Z:443:THR:HG23	1.89	0.54
15:R:232:VAL:HG13	15:R:246:VAL:HG13	1.90	0.54
1:L:46:ARG:NH1	1:L:156:ILE:O	2.41	0.54
6:O:439:LEU:HG	6:O:476:LEU:HD13	1.89	0.54
14:V:385:ILE:HG23	14:V:405:LEU:HD11	1.90	0.54
13:Z:376:LEU:HD21	13:Z:398:GLU:HB3	1.90	0.54
3:A:443:CYS:HB3	3:A:452:LEU:HD11	1.90	0.54
4:N:574:ILE:HA	4:N:577:GLU:HG3	1.90	0.54
13:Z:38:ILE:HA	13:Z:41:VAL:HG12	1.90	0.54
13:Z:373:VAL:HG21	13:Z:403:ALA:HB2	1.90	0.54
13:Z:413:LEU:HD23	13:Z:429:MET:HE2	1.90	0.54
6:O:281:LEU:HD21	6:O:283:LEU:HD13	1.89	0.54
13:Y:87:LEU:HD13	13:Y:95:ASN:HB3	1.90	0.54
14:U:45:GLU:O	14:U:87:TYR:OH	2.26	0.54
14:V:137:SER:O	14:V:143:LYS:NZ	2.41	0.54
5:I:284:ASP:OD1	5:I:472:VAL:HG12	2.08	0.53
6:O:460:GLN:OE1	6:O:496:ARG:NH2	2.40	0.53
12:J:631:ASN:HB3	12:J:634:HIS:HB2	1.89	0.53
12:P:724:GLN:O	12:P:728:GLU:HG3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:45:GLU:O	14:V:91:LYS:HE3	2.08	0.53
3:A:23:PHE:HB2	3:A:111:LEU:HD21	1.90	0.53
3:A:1328:TYR:HA	3:A:1358:ILE:HG21	1.90	0.53
5:I:370:ALA:HB2	5:I:381:LEU:HG	1.90	0.53
12:J:732:ILE:HG22	12:J:733:VAL:HG13	1.90	0.53
8:Q:146:ARG:O	8:Q:150:THR:HG23	2.09	0.53
14:V:106:LEU:HD11	14:V:117:LEU:HD23	1.90	0.53
15:R:201:LEU:O	15:R:211:LEU:HA	2.08	0.53
15:R:337:LEU:HB2	15:R:351:TYR:HB2	1.88	0.53
15:R:391:GLN:OE1	15:R:392:PRO:HD2	2.07	0.53
8:K:157:LEU:HD12	8:K:170:LEU:HD12	1.91	0.53
10:M:11:ILE:O	10:M:15:ILE:HG12	2.08	0.53
14:U:95:ASP:HB3	14:V:49:LEU:HD22	1.90	0.53
14:U:215:ASP:N	14:U:215:ASP:OD1	2.41	0.53
15:R:386:ASN:ND2	15:R:393:LEU:HB2	2.24	0.53
16:C:53:HIS:HE1	16:C:76:CYS:SG	2.32	0.53
3:A:838:THR:HG22	3:A:840:GLU:H	1.72	0.53
4:N:439:VAL:HG13	4:N:519:TYR:HD1	1.73	0.53
6:O:581:ILE:HD12	6:O:616:LEU:HD12	1.90	0.53
8:K:8:LYS:HG2	8:K:12:GLN:HE21	1.73	0.53
13:Z:143:ALA:O	13:Z:147:THR:HG23	2.07	0.53
13:Z:238:VAL:HG11	13:Z:261:LEU:HD21	1.90	0.53
13:Z:259:CYS:HA	13:Z:262:GLU:OE1	2.08	0.53
3:A:12:ILE:O	3:A:510:PHE:N	2.39	0.53
4:N:186:GLN:HG3	4:N:223:GLY:H	1.72	0.53
5:I:13:VAL:HG22	5:I:744:PHE:CE1	2.43	0.53
12:J:453:ASN:OD1	12:J:454:LEU:N	2.41	0.53
12:J:723:LEU:HG	12:J:746:VAL:HG11	1.91	0.53
13:Z:224:MET:HA	13:Z:227:ILE:HG22	1.91	0.53
3:A:710:LEU:O	3:A:713:SER:OG	2.26	0.53
5:I:185:ILE:HG12	5:I:201:ILE:HG13	1.90	0.53
3:A:1247:HIS:NE2	3:A:1290:ASP:O	2.40	0.53
6:O:301:ARG:NH1	6:O:336:ASP:OD2	2.31	0.53
4:N:53:GLU:HA	4:N:56:ARG:HB2	1.89	0.53
12:J:114:ALA:HA	12:J:117:THR:HG22	1.90	0.53
1:L:50:LEU:O	1:L:154:ARG:NH1	2.40	0.53
5:I:288:THR:HA	5:I:291:VAL:HG12	1.91	0.53
6:O:462:ASN:OD1	6:O:496:ARG:NE	2.38	0.53
8:K:193:LEU:HD23	8:K:197:GLU:HG2	1.91	0.53
9:G:8:ARG:HH21	8:Q:480:SER:HB2	1.74	0.53
10:M:39:PRO:O	10:M:40:GLU:HB3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:381:ILE:HG21	6:O:405:SER:HB3	1.91	0.52
6:O:468:VAL:O	6:O:472:HIS:ND1	2.42	0.52
6:O:695:ASN:OD1	6:O:717:GLN:NE2	2.42	0.52
8:Q:476:PRO:HG2	14:U:182:LEU:HD22	1.91	0.52
14:U:556:LEU:HD23	14:U:559:GLN:NE2	2.24	0.52
13:Z:239:TRP:HZ3	13:Z:273:LEU:HD11	1.73	0.52
4:N:224:CYS:HB3	4:N:233:CYS:SG	2.48	0.52
4:N:540:ARG:NH1	4:N:541:ASN:HB3	2.23	0.52
6:O:15:THR:HB	6:O:20:HIS:NE2	2.24	0.52
8:K:190:LEU:HD22	8:K:201:LEU:HD23	1.91	0.52
3:A:1828:GLU:O	3:A:1832:ASN:ND2	2.43	0.52
4:N:182:ARG:HB3	4:N:223:GLY:HA2	1.92	0.52
5:I:668:GLN:NE2	5:I:746:MET:SD	2.82	0.52
13:Y:59:LEU:O	13:Y:62:THR:HG22	2.10	0.52
13:Y:165:ARG:O	13:Y:165:ARG:NH1	2.37	0.52
13:Y:475:TYR:CE2	13:Y:477:LYS:HB2	2.43	0.52
15:R:169:ARG:HH12	15:R:474:SER:N	2.06	0.52
12:J:549:ASP:OD1	12:J:580:GLN:NE2	2.39	0.52
13:Y:377:LEU:HD21	13:Y:409:CYS:SG	2.50	0.52
6:O:378:SER:O	6:O:382:GLN:HG2	2.10	0.52
12:J:455:GLN:HE21	12:P:7:PRO:HB3	1.73	0.52
13:Z:50:HIS:O	13:Z:86:SER:OG	2.27	0.52
1:L:77:LEU:HD11	1:L:139:ILE:HD11	1.91	0.52
6:O:386:GLN:HB2	6:O:424:GLN:HE21	1.74	0.52
14:U:531:THR:O	14:U:534:GLN:HG3	2.09	0.52
13:Z:267:LEU:O	13:Z:267:LEU:HD23	2.10	0.52
1:L:90:THR:HG21	1:L:116:PRO:HD2	1.91	0.52
3:A:94:TYR:O	3:A:100:VAL:HA	2.10	0.52
3:A:1016:MET:HG2	3:A:1088:THR:HG21	1.92	0.52
3:A:1815:LYS:O	3:A:1819:GLU:HG2	2.10	0.52
4:N:699:TRP:CE3	4:N:702:GLN:HG3	2.45	0.52
8:Q:251:TYR:HA	8:Q:254:THR:HG22	1.92	0.52
1:L:22:VAL:HB	1:L:159:TYR:HB3	1.92	0.52
3:A:27:HIS:HB3	3:A:101:ILE:HD13	1.92	0.52
3:A:931:VAL:HA	3:A:934:MET:HG2	1.92	0.52
13:Y:431:ASN:O	13:Y:435:LYS:HG2	2.09	0.52
14:U:494:ILE:O	14:U:497:ILE:HG22	2.10	0.52
1:L:174:THR:HG22	12:P:737:SER:H	1.74	0.52
6:O:209:GLN:OE1	6:O:247:ASN:ND2	2.43	0.52
8:Q:495:PHE:O	8:Q:499:VAL:HG23	2.10	0.52
13:Y:499:LEU:O	13:Y:503:LEU:HG	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:23:PHE:CE2	3:A:113:VAL:HG23	2.45	0.52
8:K:231:LEU:HA	8:K:234:VAL:HG22	1.92	0.52
12:J:14:GLN:HE21	12:P:116:PHE:HE2	1.58	0.52
3:A:94:TYR:HE2	3:A:96:ALA:HB2	1.74	0.51
3:A:1573:SER:HB2	3:A:1656:LEU:HD22	1.92	0.51
12:J:172:SER:OG	12:J:173:LEU:N	2.41	0.51
12:P:449:ILE:HA	12:P:452:PHE:HB3	1.92	0.51
5:I:368:GLY:HA3	6:O:653:ALA:HB2	1.91	0.51
10:M:16:ASP:OD1	10:M:16:ASP:N	2.43	0.51
14:U:33:LYS:NZ	14:U:59:ALA:O	2.42	0.51
15:R:256:TRP:CE2	15:R:263:LYS:HB2	2.45	0.51
3:A:133:ILE:HG12	3:A:146:GLU:HA	1.92	0.51
3:A:234:SER:OG	3:A:235:ARG:N	2.44	0.51
4:N:386:LEU:HD22	4:N:399:LEU:HD22	1.93	0.51
6:O:698:LYS:HB2	6:O:713:VAL:HG11	1.91	0.51
12:P:507:ARG:O	12:P:511:GLU:HG2	2.11	0.51
13:Y:242:ALA:O	13:Y:246:VAL:HG23	2.09	0.51
13:Z:476:ILE:HD12	13:Z:476:ILE:H	1.75	0.51
15:R:315:GLU:HB3	15:R:333:ASN:OD1	2.10	0.51
3:A:77:ARG:NH2	3:A:91:GLU:OE1	2.32	0.51
3:A:489:LEU:HD11	3:A:509:VAL:HG21	1.92	0.51
6:O:231:LEU:O	6:O:263:ARG:NH2	2.32	0.51
8:K:391:PHE:CG	8:K:408:VAL:HG12	2.45	0.51
13:Z:531:GLN:HA	13:Z:534:ILE:HG22	1.92	0.51
3:A:455:VAL:HB	3:A:471:VAL:HG12	1.92	0.51
3:A:1617:ARG:HA	3:A:1691:LEU:HD13	1.93	0.51
3:A:1918:PHE:CD2	3:A:1921:LEU:HD11	2.44	0.51
5:I:576:TRP:CG	5:I:643:PHE:HD2	2.29	0.51
15:R:360:ALA:HB3	15:R:374:GLY:O	2.11	0.51
3:A:11:MET:SD	3:A:510:PHE:HB2	2.51	0.51
3:A:665:MET:HE1	3:A:792:GLN:HG2	1.92	0.51
4:N:130:GLU:HG3	4:N:150:ARG:HH22	1.76	0.51
4:N:576:GLU:HA	4:N:579:GLU:HG3	1.92	0.51
6:O:446:LEU:HD21	6:O:470:LEU:HG	1.92	0.51
7:S:323:THR:HB	7:S:324:PRO:HD2	1.92	0.51
9:G:11:LEU:HD21	8:Q:456:ARG:HH12	1.74	0.51
14:U:301:ASP:OD1	14:U:301:ASP:N	2.40	0.51
14:U:347:HIS:ND1	14:U:374:GLU:OE1	2.39	0.51
1:L:87:GLU:HG2	1:L:88:SER:N	2.26	0.51
1:L:91:PRO:HB2	1:L:94:ILE:HD11	1.93	0.51
3:A:1915:LEU:HB3	4:N:67:LEU:HD11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:613:GLU:OE1	4:N:616:ARG:NE	2.30	0.51
6:O:386:GLN:HB2	6:O:424:GLN:NE2	2.25	0.51
6:O:542:GLU:O	6:O:546:ARG:HG2	2.11	0.51
6:O:581:ILE:HB	6:O:619:LEU:HD13	1.92	0.51
12:J:605:THR:OG1	12:J:634:HIS:NE2	2.35	0.51
8:K:386:LEU:HD11	14:V:550:LEU:HB3	1.93	0.51
14:U:472:LYS:HA	14:U:475:LYS:HB2	1.93	0.51
4:N:681:LEU:O	4:N:685:VAL:N	2.33	0.51
5:I:640:ASP:OD1	5:I:641:ALA:N	2.44	0.51
8:K:342:HIS:HD2	9:W:2:LEU:HD23	1.75	0.51
13:Z:457:THR:HG23	13:Z:460:LYS:HE3	1.92	0.51
4:N:545:LEU:O	4:N:549:PHE:HB2	2.11	0.51
4:N:586:GLN:HG2	4:N:587:PRO:HD2	1.93	0.51
4:N:650:LEU:HD11	4:N:717:GLU:HA	1.92	0.51
13:Y:62:THR:HA	13:Y:65:ASN:ND2	2.26	0.51
14:U:535:LYS:HE2	14:U:577:LEU:HD22	1.91	0.51
13:Z:323:ASP:OD1	13:Z:324:VAL:N	2.44	0.51
13:Z:442:GLN:HA	13:Z:445:THR:HG22	1.93	0.51
15:R:279:TRP:HE3	15:R:282:GLU:HA	1.76	0.51
13:Y:322:GLU:HA	13:Y:325:GLU:HG2	1.93	0.50
13:Y:384:ARG:NH1	13:Y:385:ASN:OD1	2.44	0.50
15:R:202:SER:HB2	15:R:222:LEU:HD11	1.92	0.50
3:A:1889:LEU:HD13	3:A:1894:VAL:HB	1.93	0.50
15:R:173:LYS:NZ	15:R:440:THR:H	2.09	0.50
3:A:496:ASN:HB2	3:A:508:LYS:HE3	1.93	0.50
5:I:188:TYR:HA	5:I:194:LYS:HA	1.94	0.50
5:I:266:ASN:ND2	5:I:530:GLU:OE2	2.42	0.50
6:O:70:GLY:O	6:O:211:GLN:NE2	2.44	0.50
15:R:358:VAL:HA	15:R:375:GLY:HA2	1.93	0.50
3:A:1058:SER:OG	3:A:1059:ASP:N	2.43	0.50
3:A:1059:ASP:CG	7:S:399:GLU:HB3	2.31	0.50
3:A:1230:ILE:HA	3:A:1236:LEU:HD21	1.93	0.50
8:Q:410:VAL:O	8:Q:414:GLN:HG2	2.11	0.50
13:Y:267:LEU:HD23	13:Y:267:LEU:H	1.77	0.50
3:A:88:ASP:OD1	3:A:594:ARG:NH2	2.44	0.50
7:S:410:LEU:N	7:S:410:LEU:HD12	2.26	0.50
12:J:621:LEU:HG	12:J:644:ILE:HG21	1.93	0.50
4:N:685:VAL:HG12	4:N:685:VAL:O	2.12	0.50
5:I:308:LEU:HD21	5:I:445:ILE:HG23	1.92	0.50
12:J:723:LEU:O	12:J:727:GLU:HG2	2.11	0.50
8:Q:325:LYS:O	8:Q:329:LEU:HD12	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:312:GLY:O	13:Z:315:LEU:HB2	2.11	0.50
15:R:366:HIS:NE2	15:R:411:ALA:O	2.45	0.50
8:K:250:CYS:SG	8:K:274:THR:HG21	2.51	0.50
13:Z:227:ILE:HA	13:Z:230:VAL:HG22	1.93	0.50
13:Z:536:LEU:HA	13:Z:539:ASP:HB2	1.93	0.50
3:A:729:CYS:HB2	6:O:673:ALA:HA	1.94	0.50
6:O:465:SER:HA	6:O:468:VAL:HG22	1.94	0.50
13:Y:226:VAL:HA	13:Y:229:THR:HG22	1.93	0.50
13:Y:411:GLU:HG3	13:Y:446:LEU:HD22	1.93	0.50
15:R:354:HIS:CD2	15:R:383:ARG:HD2	2.47	0.50
2:D:21:ASP:OD2	5:I:443:LYS:NZ	2.44	0.50
3:A:641:TRP:HA	3:A:644:VAL:HG12	1.93	0.50
14:V:227:THR:HG22	14:V:229:MET:H	1.77	0.50
15:R:426:LEU:HD22	15:R:435:GLN:HG2	1.94	0.50
2:D:54:ILE:O	14:U:409:TYR:OH	2.20	0.49
3:A:210:MET:HE2	3:A:223:LEU:HD22	1.93	0.49
4:N:574:ILE:O	4:N:577:GLU:HG3	2.12	0.49
5:I:552:ILE:HG23	5:I:554:ILE:HG23	1.93	0.49
8:K:513:THR:HA	8:K:516:VAL:HG12	1.94	0.49
12:J:173:LEU:HD23	12:J:176:PHE:H	1.77	0.49
14:U:213:ILE:HG23	14:U:218:MET:HB2	1.94	0.49
14:U:453:LYS:NZ	14:U:457:TRP:HE1	2.09	0.49
16:C:71:GLN:NE2	16:C:80:TRP:HB3	2.27	0.49
4:N:63:ARG:HH21	4:N:140:LEU:HA	1.77	0.49
5:I:671:LEU:HB2	5:I:675:TYR:HD2	1.77	0.49
8:K:261:ASP:OD2	8:Q:55:ARG:NH2	2.44	0.49
8:Q:441:VAL:HG23	8:Q:444:TRP:HB2	1.94	0.49
13:Z:264:LYS:HZ3	13:Z:266:LEU:HD12	1.77	0.49
5:I:643:PHE:CD1	5:I:649:VAL:HB	2.46	0.49
13:Y:40:HIS:NE2	13:Z:201:LEU:HB2	2.27	0.49
14:U:415:PRO:HB2	14:U:446:LEU:HD13	1.93	0.49
15:R:209:VAL:HG23	15:R:222:LEU:HB2	1.94	0.49
15:R:309:LEU:HD13	15:R:345:LEU:HG	1.94	0.49
15:R:439:LEU:HD23	15:R:470:TRP:CE3	2.47	0.49
3:A:1794:ASP:O	3:A:1797:ILE:HG12	2.11	0.49
4:N:224:CYS:SG	4:N:231:CYS:HA	2.52	0.49
13:Z:68:PRO:O	13:Z:69:GLU:HB3	2.13	0.49
15:R:173:LYS:HZ3	15:R:440:THR:H	1.60	0.49
3:A:767:HIS:O	3:A:770:TYR:HB3	2.12	0.49
4:N:442:LEU:HB3	4:N:456:LEU:HD22	1.95	0.49
13:Y:206:ILE:HG23	13:Y:219:VAL:HG11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:471:VAL:HG11	14:U:508:GLU:OE1	2.12	0.49
13:Z:384:ARG:NH2	13:Z:385:ASN:OD1	2.44	0.49
15:R:173:LYS:HZ1	15:R:440:THR:HG22	1.77	0.49
3:A:47:GLU:OE2	14:V:123:TYR:OH	2.23	0.49
3:A:966:PRO:HG3	3:A:980:ARG:HH12	1.77	0.49
3:A:1910:SER:N	3:A:1913:GLU:OE2	2.43	0.49
8:K:171:THR:HG22	8:K:176:LEU:HD12	1.93	0.49
8:K:342:HIS:O	8:K:346:VAL:HG23	2.12	0.49
14:U:185:VAL:HG13	14:U:212:LEU:HD22	1.95	0.49
15:R:250:LYS:HE2	15:R:252:PHE:HE2	1.78	0.49
4:N:83:LEU:HB3	4:N:160:VAL:HG11	1.93	0.49
5:I:585:TYR:HE1	5:I:602:ARG:HE	1.59	0.49
7:S:325:LEU:HD12	15:R:219:VAL:HG13	1.95	0.49
8:Q:321:ARG:NH1	15:R:113:GLU:OE2	2.45	0.49
13:Y:91:LYS:O	13:Z:338:HIS:NE2	2.45	0.49
13:Y:429:MET:HA	13:Y:432:ASN:ND2	2.28	0.49
14:U:192:PHE:O	14:U:196:THR:HG23	2.13	0.49
14:U:532:CYS:HA	14:U:535:LYS:CG	2.43	0.49
3:A:885:GLU:O	3:A:888:VAL:HG22	2.12	0.49
3:A:1376:LEU:HG	3:A:1377:LYS:HG3	1.93	0.49
4:N:51:LYS:HG3	4:N:53:GLU:H	1.78	0.49
12:J:566:SER:OG	12:J:568:GLU:OE1	2.30	0.49
13:Z:292:LEU:O	13:Z:296:GLN:HG2	2.13	0.49
13:Z:342:TRP:HE3	13:Z:361:LEU:HG	1.78	0.49
3:A:1421:PRO:HG3	3:A:1476:PHE:CZ	2.48	0.49
3:A:1860:LEU:HD11	3:A:1888:PHE:HE2	1.77	0.49
6:O:694:LEU:HD11	6:O:716:PHE:HD2	1.77	0.49
3:A:137:LYS:HG3	3:A:273:ARG:NH1	2.28	0.49
3:A:633:ILE:HG23	3:A:754:LEU:HD11	1.94	0.49
3:A:824:ASP:O	3:A:828:THR:OG1	2.23	0.49
5:I:74:ARG:O	5:I:77:GLY:N	2.37	0.49
8:K:342:HIS:NE2	9:W:2:LEU:O	2.32	0.49
12:J:693:ASN:O	12:J:697:VAL:HG13	2.13	0.49
13:Y:238:VAL:HA	13:Y:241:LYS:HG2	1.93	0.49
13:Y:458:GLN:HE21	13:Y:485:LEU:HD11	1.77	0.49
14:V:87:TYR:CZ	14:V:113:LYS:HD3	2.48	0.49
13:Z:509:CYS:SG	13:Z:538:LEU:HD22	2.53	0.49
15:R:288:SER:OG	15:R:289:ARG:N	2.46	0.49
16:C:72:HIS:HA	16:C:79:GLU:HA	1.95	0.49
1:L:178:PHE:CE2	12:P:736:GLU:HG2	2.48	0.48
3:A:720:GLU:OE2	6:O:719:ARG:NH1	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1196:TYR:O	3:A:1199:LYS:HG2	2.13	0.48
3:A:1776:TYR:CZ	3:A:1780:THR:HG21	2.47	0.48
14:V:379:LYS:HD2	15:R:64:ILE:HB	1.95	0.48
15:R:414:LEU:HB3	15:R:428:TRP:HB2	1.94	0.48
4:N:230:GLN:HE21	4:N:230:GLN:HA	1.78	0.48
5:I:202:ALA:O	5:I:221:THR:OG1	2.30	0.48
8:K:423:LYS:NZ	8:K:427:ASP:OD2	2.44	0.48
8:Q:93:LEU:HD22	8:Q:132:ILE:HG23	1.94	0.48
13:Y:229:THR:HG23	13:Y:230:VAL:HG23	1.94	0.48
14:U:344:ARG:NH1	14:U:346:GLN:OE1	2.38	0.48
14:V:429:ARG:HB3	14:V:432:ASP:HB2	1.93	0.48
15:R:400:SER:CB	15:R:422:GLN:HB2	2.44	0.48
5:I:671:LEU:HB2	5:I:675:TYR:CD2	2.48	0.48
12:P:528:ILE:HG22	12:P:529:GLU:HG3	1.96	0.48
14:V:93:TYR:HE2	14:V:105:PHE:HE2	1.61	0.48
13:Z:343:VAL:HG22	13:Z:375:ALA:HB2	1.95	0.48
13:Z:535:ALA:O	13:Z:539:ASP:N	2.46	0.48
3:A:791:VAL:HG21	3:A:814:VAL:HG22	1.94	0.48
3:A:1895:PRO:HG3	3:A:1921:LEU:HD13	1.94	0.48
8:Q:337:TRP:HB3	8:Q:360:ALA:HB2	1.95	0.48
8:Q:442:ASP:N	8:Q:442:ASP:OD1	2.46	0.48
13:Z:192:TYR:HB3	13:Z:209:LEU:CD1	2.43	0.48
12:P:75:LEU:HG	12:P:91:ILE:HD13	1.95	0.48
13:Z:264:LYS:NZ	13:Z:266:LEU:HB2	2.27	0.48
4:N:358:ILE:HG21	4:N:409:VAL:HG13	1.96	0.48
5:I:73:TRP:CZ3	5:I:95:VAL:HG11	2.48	0.48
13:Y:455:PRO:HA	13:Y:458:GLN:HB2	1.95	0.48
14:U:534:GLN:HA	14:U:537:CYS:SG	2.53	0.48
14:V:482:GLU:HB2	14:V:485:GLN:OE1	2.14	0.48
13:Z:457:THR:CG2	13:Z:460:LYS:HE3	2.44	0.48
3:A:745:GLN:HG2	3:A:746:ASN:H	1.79	0.48
5:I:679:ASP:O	5:I:682:GLU:HG2	2.14	0.48
14:U:96:VAL:HG21	14:V:53:LYS:HD3	1.94	0.48
13:Z:398:GLU:OE2	13:Z:401:ARG:NH2	2.22	0.48
3:A:1909:THR:N	3:A:1913:GLU:OE2	2.41	0.48
5:I:604:HIS:HB2	5:I:611:VAL:HG13	1.96	0.48
6:O:78:LEU:O	6:O:82:ILE:HG12	2.13	0.48
8:K:251:TYR:HA	8:K:254:THR:HG22	1.96	0.48
12:J:19:TYR:HB2	12:P:77:LYS:HE2	1.95	0.48
14:V:506:HIS:HD1	14:V:539:PHE:HE1	1.62	0.48
15:R:405:LEU:HD23	15:R:414:LEU:HD11	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:573:ASN:HA	4:N:576:GLU:OE1	2.12	0.48
8:K:86:HIS:HB3	8:K:139:ILE:HG23	1.96	0.48
13:Z:93:TYR:CZ	13:Z:148:MET:HG2	2.48	0.48
3:A:1360:VAL:HG13	3:A:1364:CYS:HB2	1.94	0.48
13:Z:476:ILE:O	13:Z:480:VAL:HG13	2.14	0.48
15:R:2:ASP:OD1	15:R:3:GLN:N	2.47	0.48
3:A:1463:TYR:HE1	3:A:1511:ASN:HB3	1.79	0.47
3:A:1596:SER:O	3:A:1597:THR:OG1	2.28	0.47
3:A:1653:ALA:O	3:A:1655:THR:N	2.46	0.47
11:H:70:VAL:HG22	13:Y:357:ARG:HD3	1.95	0.47
13:Z:230:VAL:HG21	13:Z:233:LEU:HD12	1.97	0.47
13:Z:500[B]:ARG:HA	13:Z:503:LEU:HB2	1.96	0.47
3:A:42:LEU:HD22	14:V:363:ARG:HG2	1.96	0.47
3:A:925:SER:OG	3:A:926:LEU:N	2.46	0.47
13:Y:429:MET:HA	13:Y:432:ASN:HD21	1.78	0.47
13:Z:359:LEU:HD11	13:Z:383:LEU:HD22	1.95	0.47
15:R:418:HIS:NE2	15:R:426:LEU:HD12	2.29	0.47
3:A:1284:GLU:HG2	3:A:1285:MET:N	2.29	0.47
3:A:1284:GLU:HB2	3:A:1350:TYR:CD2	2.49	0.47
4:N:666:ILE:HA	4:N:669:TYR:HB2	1.96	0.47
12:J:465:LEU:HD11	12:J:495:HIS:CG	2.49	0.47
12:P:730:LYS:HE3	12:P:740:TYR:CE1	2.47	0.47
8:Q:378:TYR:HA	8:Q:381:THR:HG22	1.96	0.47
13:Z:318:GLU:OE2	13:Z:320:ARG:HG2	2.14	0.47
13:Z:500[A]:ARG:HA	13:Z:503:LEU:HB2	1.96	0.47
15:R:187:ASP:HB3	15:R:190:LEU:HG	1.97	0.47
15:R:386:ASN:HB2	15:R:389:THR:OG1	2.14	0.47
4:N:273:MET:HA	4:N:289:PHE:CZ	2.49	0.47
7:S:405:TYR:HA	7:S:411:CYS:O	2.15	0.47
13:Y:170:LYS:HE3	13:Z:48:GLY:HA3	1.95	0.47
3:A:1186:THR:HG23	3:A:1215:ALA:HB1	1.95	0.47
4:N:341:ILE:HG12	4:N:374:LEU:HD12	1.96	0.47
4:N:696:MET:HG2	4:N:713:PHE:CD2	2.49	0.47
5:I:360:LEU:HD11	5:I:390:ILE:HG23	1.96	0.47
8:K:500:ASP:O	8:K:504:THR:HG23	2.14	0.47
12:P:691:THR:HA	12:P:694:LYS:HE3	1.97	0.47
13:Y:414:ILE:HD12	13:Y:446:LEU:HD21	1.97	0.47
13:Z:466:ASP:O	13:Z:470:THR:HG23	2.14	0.47
1:L:24:GLU:OE2	1:L:46:ARG:NH2	2.39	0.47
3:A:1409:LEU:HA	3:A:1471:SER:OG	2.15	0.47
3:A:1680:LEU:HD21	3:A:1687:LEU:HD23	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1729:GLU:O	3:A:1733:PHE:N	2.47	0.47
5:I:349:ILE:HG12	5:I:404:LEU:HD11	1.96	0.47
6:O:530:SER:O	6:O:533:THR:HG22	2.14	0.47
8:Q:167:PHE:HE2	8:Q:208:LYS:HB2	1.79	0.47
8:Q:185:LEU:HA	8:Q:188:LEU:HD13	1.96	0.47
8:Q:476:PRO:HD3	14:U:152:ARG:HD3	1.97	0.47
13:Y:38:ILE:HG13	13:Y:75:GLN:HB3	1.96	0.47
13:Z:138:VAL:O	13:Z:142:MET:HG3	2.14	0.47
13:Z:233:LEU:HB3	13:Z:236:LEU:HD23	1.96	0.47
4:N:646:MET:HB3	16:C:5:ILE:HG23	1.97	0.47
4:N:666:ILE:HG13	4:N:685:VAL:HG21	1.96	0.47
5:I:285:SER:O	5:I:288:THR:HG22	2.15	0.47
6:O:619:LEU:O	6:O:623:THR:HG22	2.14	0.47
8:K:284:LEU:HD21	8:K:307:CYS:SG	2.54	0.47
8:K:472:LEU:HG	8:K:481:THR:HG21	1.96	0.47
12:J:115:CYS:SG	12:J:145:ASN:HB2	2.54	0.47
13:Y:153:LYS:O	13:Y:156:ILE:HG12	2.15	0.47
13:Y:259:CYS:O	13:Y:263:LYS:HG2	2.15	0.47
14:V:216:LYS:HD3	14:V:243:LEU:HD21	1.97	0.47
15:R:94:LEU:HD22	15:R:157:SER:OG	2.14	0.47
15:R:205:LEU:HD21	15:R:210:TYR:CD2	2.45	0.47
5:I:47:HIS:CE1	5:I:54:ARG:HB2	2.49	0.47
8:K:190:LEU:HA	8:K:193:LEU:HD13	1.97	0.47
10:M:35:GLU:O	10:M:49:SER:OG	2.31	0.47
11:H:99:ILE:HG12	12:P:591:GLN:HG2	1.97	0.47
14:V:304:SER:HB3	14:V:336:VAL:HG22	1.96	0.47
14:V:328:LYS:HA	14:V:333:THR:HG21	1.97	0.47
13:Z:461:ALA:O	13:Z:465:LEU:HG	2.15	0.47
15:R:243:LEU:HD23	15:R:255:ILE:HG21	1.97	0.47
1:L:53:TYR:HB3	1:L:154:ARG:HG2	1.95	0.47
3:A:23:PHE:HE2	3:A:113:VAL:HG23	1.80	0.47
3:A:248:PHE:HB2	3:A:430:VAL:HB	1.97	0.47
3:A:796:ASP:C	3:A:798:LYS:H	2.17	0.47
3:A:1236:LEU:HD22	15:R:161:LEU:HD11	1.97	0.47
8:K:306:GLY:HA3	8:K:323:LEU:HG	1.96	0.47
8:Q:254:THR:OG1	8:Q:267:CYS:SG	2.73	0.47
13:Y:83:HIS:HD2	13:Y:99:LYS:HG2	1.79	0.47
14:U:168:ASP:OD1	14:U:168:ASP:N	2.47	0.47
13:Z:457:THR:HG23	13:Z:460:LYS:HB3	1.96	0.47
16:C:16:TRP:HD1	16:C:31:ASN:HA	1.80	0.47
1:L:103:HIS:ND1	3:A:1594:ALA:HB2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:137:LYS:HE3	3:A:406:GLU:HB3	1.96	0.47
3:A:1089:LEU:HB3	3:A:1568:GLY:HA2	1.97	0.47
3:A:1119:ASP:OD1	3:A:1120:LEU:N	2.48	0.47
4:N:408:ARG:HD3	4:N:499:SER:HB2	1.97	0.47
4:N:541:ASN:OD1	4:N:542:VAL:N	2.48	0.47
5:I:307:LEU:HD13	5:I:313:ALA:HB2	1.97	0.47
13:Y:227:ILE:HD11	13:Y:236:LEU:HD23	1.96	0.47
13:Z:514:ILE:HA	13:Z:517:ASP:HB2	1.96	0.47
6:O:665:PHE:CD2	6:O:755:LEU:HD11	2.50	0.46
8:Q:393:GLN:O	8:Q:396:SER:OG	2.25	0.46
14:U:93:TYR:OH	14:V:57:GLU:OE2	2.23	0.46
14:V:96:VAL:HG23	14:V:98:GLU:HG3	1.96	0.46
3:A:1892:HIS:HB3	3:A:1927:ALA:HB2	1.97	0.46
4:N:401:ILE:HG23	4:N:501:ILE:HD12	1.97	0.46
5:I:601:LEU:HB2	5:I:615:LEU:HD12	1.98	0.46
12:P:753:THR:HA	12:P:756:ALA:HB3	1.97	0.46
8:Q:6:LEU:O	8:Q:10:VAL:HG13	2.15	0.46
14:U:528:GLU:HG3	14:U:573:LEU:HD21	1.96	0.46
3:A:1335:ARG:NE	11:H:107:PRO:HD3	2.29	0.46
3:A:1717:SER:OG	3:A:1718:LEU:N	2.47	0.46
8:K:496:GLU:OE2	12:P:660:LYS:NZ	2.46	0.46
12:P:543:LEU:HB2	12:P:552:LEU:HD13	1.98	0.46
4:N:657:VAL:HB	4:N:659:VAL:HG13	1.97	0.46
4:N:663:GLN:HB2	4:N:699:TRP:NE1	2.30	0.46
7:S:387:TYR:HE1	7:S:407:THR:HB	1.80	0.46
8:K:10:VAL:HG21	8:K:26:ALA:HB2	1.96	0.46
10:M:24:LEU:HD21	14:V:337:ILE:HG23	1.97	0.46
12:J:170:PHE:HB3	12:J:456:LYS:HG3	1.98	0.46
12:J:521:ILE:O	12:J:525:VAL:HG23	2.15	0.46
8:Q:188:LEU:HB3	8:Q:190:LEU:HD13	1.97	0.46
13:Z:271:VAL:HG11	13:Z:301:ASP:HB2	1.96	0.46
15:R:312:HIS:CE1	15:R:338:LEU:HD12	2.50	0.46
15:R:337:LEU:HD21	15:R:354:HIS:CD2	2.49	0.46
5:I:219:VAL:HG13	5:I:234:PHE:HB2	1.97	0.46
9:G:11:LEU:HD21	8:Q:456:ARG:NH1	2.31	0.46
12:J:694:LYS:O	12:J:698:ILE:HG23	2.16	0.46
13:Y:85:ASP:OD1	13:Y:86:SER:N	2.49	0.46
14:U:99:TYR:HB2	14:U:125:SER:HB3	1.97	0.46
14:V:549:LEU:O	14:V:553:ILE:HG13	2.16	0.46
13:Z:314:LEU:O	13:Z:317:ARG:HB3	2.15	0.46
4:N:523:LEU:HD21	4:N:561:LEU:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:651:VAL:HG21	5:I:669:LEU:HD23	1.97	0.46
5:I:692:ARG:HH11	5:I:694:ASP:HB3	1.79	0.46
10:M:38:GLU:HG3	10:M:39:PRO:O	2.15	0.46
8:Q:481:THR:O	8:Q:485:ILE:HG13	2.16	0.46
13:Y:342:TRP:HB2	13:Y:365:ALA:HB2	1.96	0.46
14:U:512:ALA:O	14:U:516:LEU:HG	2.15	0.46
5:I:356:SER:HB2	5:I:397:ILE:HG12	1.98	0.46
6:O:577:THR:HG21	6:O:614:TYR:CD2	2.51	0.46
6:O:664:MET:SD	6:O:693:ASN:ND2	2.87	0.46
8:K:171:THR:O	8:K:171:THR:OG1	2.30	0.46
13:Y:140:TYR:HD2	13:Y:171:ILE:HG22	1.81	0.46
14:U:373:HIS:ND1	14:U:388:TYR:OH	2.43	0.46
14:V:26:PHE:CE1	14:V:228:TRP:HB2	2.51	0.46
3:A:594:ARG:CG	3:A:608:THR:HG22	2.44	0.46
3:A:1719:LEU:HB3	3:A:1723:VAL:HG13	1.98	0.46
4:N:441:GLY:HA3	4:N:452:LEU:HD23	1.96	0.46
5:I:381:LEU:HD12	5:I:381:LEU:HA	1.70	0.46
5:I:556:LEU:HD11	5:I:586:LEU:HD21	1.97	0.46
5:I:750:ASP:OD1	5:I:751:GLU:N	2.44	0.46
6:O:258:TYR:HE1	6:O:310:LEU:HD13	1.80	0.46
8:Q:210:LYS:HB3	8:Q:210:LYS:HE2	1.70	0.46
13:Y:40:HIS:CE1	13:Z:201:LEU:H	2.33	0.46
14:U:98:GLU:OE1	14:U:101:ARG:NH2	2.49	0.46
14:U:528:GLU:OE1	14:U:528:GLU:N	2.49	0.46
16:C:68:GLN:HG3	16:C:69:VAL:N	2.30	0.46
3:A:796:ASP:O	3:A:798:LYS:N	2.49	0.46
3:A:1100:LEU:HD22	3:A:1147:ILE:HD11	1.98	0.46
3:A:1439:ILE:O	3:A:1443:GLU:HG3	2.15	0.46
3:A:1735:PRO:HB2	3:A:1756:LYS:HG3	1.97	0.46
4:N:439:VAL:HG11	4:N:519:TYR:HA	1.98	0.46
5:I:221:THR:O	5:I:231:VAL:HA	2.16	0.46
5:I:624:THR:O	5:I:711:TRP:NE1	2.27	0.46
7:S:406:CYS:SG	7:S:408:LYS:HB2	2.56	0.46
12:J:165:ASP:HA	12:J:467:ARG:HD3	1.98	0.46
12:J:564:LYS:HB3	12:J:564:LYS:HE2	1.66	0.46
8:Q:472:LEU:O	8:Q:476:PRO:HA	2.15	0.46
14:U:510:SER:O	14:U:542:THR:HG21	2.15	0.46
14:V:277:ARG:HH12	14:V:434:ARG:HH12	1.64	0.46
15:R:295:GLN:HB3	15:R:307:ARG:HB3	1.98	0.46
15:R:447:LEU:HD23	15:R:447:LEU:H	1.81	0.46
6:O:435:SER:H	6:O:654:ASP:HB3	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:445:LEU:HD23	6:O:469:ALA:HB2	1.98	0.46
7:S:359:HIS:NE2	16:C:59:CYS:HA	2.31	0.46
13:Y:168:THR:O	13:Y:171:ILE:HG12	2.16	0.46
3:A:1054:TYR:HB2	3:A:1057:LEU:HB2	1.98	0.45
3:A:1652:MET:HG2	8:K:556:LYS:HA	1.98	0.45
5:I:620:PHE:HD2	5:I:707:PHE:HE2	1.63	0.45
8:K:194:CYS:SG	8:K:195:ASN:N	2.89	0.45
12:P:726:LEU:HD21	12:P:742:LEU:HB3	1.98	0.45
13:Y:391:GLU:HA	13:Y:394:ILE:HG12	1.97	0.45
14:U:57:GLU:OE2	14:V:93:TYR:OH	2.24	0.45
13:Z:461:ALA:O	13:Z:464:LEU:HD23	2.16	0.45
1:L:87:GLU:HG2	1:L:88:SER:H	1.82	0.45
3:A:1915:LEU:HD21	3:A:1925:VAL:HG13	1.98	0.45
7:S:392:GLN:HG3	7:S:408:LYS:HG2	1.98	0.45
3:A:72:GLU:HG3	3:A:94:TYR:CE1	2.50	0.45
3:A:1084:ARG:NH2	3:A:1139:ASN:OD1	2.49	0.45
4:N:252:LEU:O	4:N:256:VAL:HG12	2.15	0.45
6:O:91:ASN:OD1	6:O:92:SER:N	2.49	0.45
6:O:657:ILE:HG21	6:O:703:LYS:HB2	1.97	0.45
6:O:706:CYS:O	6:O:710:ILE:HG13	2.16	0.45
8:K:525:MET:HE1	9:W:23:ARG:HG3	1.98	0.45
12:J:446:THR:HB	12:J:449:ILE:HG12	1.98	0.45
14:U:551:ARG:O	14:U:554:LEU:HG	2.17	0.45
15:R:216:THR:HG23	15:R:218:GLN:H	1.80	0.45
4:N:290:HIS:CE1	8:K:566:ARG:HD3	2.51	0.45
5:I:554:ILE:HG21	5:I:689:TYR:HB3	1.99	0.45
6:O:10:PHE:O	6:O:249:ASP:HB2	2.17	0.45
13:Y:146:TYR:HB3	13:Y:151:GLN:O	2.16	0.45
15:R:196:SER:HB3	15:R:198:LEU:H	1.82	0.45
4:N:170:GLN:O	4:N:173:ILE:HG22	2.16	0.45
4:N:293:ILE:HD12	4:N:328:VAL:HG12	1.98	0.45
5:I:393:VAL:O	5:I:397:ILE:HG13	2.16	0.45
10:M:65:LEU:HD11	12:J:557:LYS:HG3	1.98	0.45
12:J:145:ASN:HB3	12:J:148:LEU:HG	1.99	0.45
3:A:716:HIS:HA	3:A:719:VAL:HG12	1.99	0.45
3:A:1141:VAL:HG11	3:A:1608:HIS:CG	2.52	0.45
3:A:1621:PRO:HA	3:A:1697:LEU:O	2.17	0.45
4:N:387:LEU:HD11	4:N:424:ILE:HG12	1.97	0.45
5:I:649:VAL:HG13	5:I:669:LEU:HG	1.97	0.45
8:K:523:ILE:HG21	12:P:653:LEU:HG	1.99	0.45
14:V:192:PHE:O	14:V:196:THR:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:175:LEU:HG	13:Z:179:TYR:CE2	2.52	0.45
13:Z:300:LEU:H	13:Z:300:LEU:HD23	1.80	0.45
3:A:465:GLN:HE21	3:A:467:ILE:HD11	1.82	0.45
4:N:317:ALA:O	4:N:320:THR:HG22	2.17	0.45
5:I:198:VAL:HG11	5:I:236:LEU:HD13	1.98	0.45
5:I:296:THR:HG22	5:I:298:THR:H	1.81	0.45
5:I:628:THR:HG22	5:I:630:LYS:HB3	1.98	0.45
11:H:57:SER:OG	13:Z:361:LEU:HD11	2.16	0.45
8:Q:245:CYS:SG	8:Q:443:LYS:HD2	2.57	0.45
15:R:353:GLU:HB2	15:R:385:TRP:HH2	1.82	0.45
12:J:446:THR:HG22	12:J:448:GLN:H	1.82	0.45
12:J:515:TYR:HB2	12:J:546:LEU:HD21	1.99	0.45
12:J:726:LEU:HD13	12:J:743:ILE:HG12	1.97	0.45
14:U:495:GLN:NE2	14:U:496:ASP:OD1	2.49	0.45
13:Z:466:ASP:N	13:Z:466:ASP:OD1	2.46	0.45
4:N:378:LEU:HD22	4:N:420:ALA:HB1	1.98	0.45
4:N:699:TRP:HE3	4:N:702:GLN:HG3	1.82	0.45
7:S:370:LYS:O	7:S:373:GLU:HB2	2.17	0.45
7:S:441:LYS:O	7:S:445:ARG:HG3	2.16	0.45
12:J:164:PRO:O	12:J:467:ARG:HG3	2.17	0.45
13:Y:321:LEU:O	13:Y:324:VAL:HG22	2.16	0.45
13:Z:200:PRO:HB2	13:Z:201:LEU:HD12	1.99	0.45
16:C:45:PRO:HG2	16:C:57:MET:SD	2.56	0.45
3:A:253:PRO:HB2	3:A:255:ILE:HG23	1.99	0.45
3:A:452:LEU:HD23	3:A:474:ILE:HD11	1.99	0.45
3:A:963:ARG:HG3	3:A:980:ARG:HG2	1.98	0.45
3:A:1845:LEU:HA	3:A:1848:VAL:HG12	1.99	0.45
3:A:1932:ALA:N	3:A:1933:PRO:HD2	2.32	0.45
4:N:708:GLU:O	4:N:708:GLU:HG2	2.17	0.45
8:K:167:PHE:HE2	8:K:208:LYS:HD3	1.81	0.45
8:Q:125:GLN:O	8:Q:128:ILE:HG22	2.16	0.45
8:Q:285:PHE:HB2	8:Q:308:TYR:CE1	2.52	0.45
14:U:159:SER:O	14:U:163:GLN:HG2	2.16	0.45
14:U:318:TYR:HA	14:U:321:HIS:CD2	2.52	0.45
14:V:373:HIS:ND1	14:V:388:TYR:OH	2.49	0.45
13:Z:108:LYS:HB2	13:Z:108:LYS:HE3	1.73	0.45
16:C:33:CYS:SG	16:C:40:PRO:HD3	2.57	0.45
4:N:434:THR:O	4:N:438:ILE:HG13	2.17	0.44
5:I:58:PHE:HE1	5:I:64:THR:HG21	1.82	0.44
8:K:168:ASP:O	8:K:172:SER:HB3	2.17	0.44
8:K:445:GLU:OE2	9:W:8:ARG:NH1	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:82:LEU:HB3	12:P:577:PHE:CE2	2.53	0.44
12:J:121:LEU:HA	12:J:124:VAL:HG12	1.98	0.44
12:P:717:GLU:HA	12:P:719:TYR:CE1	2.52	0.44
15:R:118:GLN:HB3	15:R:119:PRO:HD3	1.99	0.44
1:L:175:THR:HG21	12:P:733:VAL:HG11	1.98	0.44
3:A:772:GLU:HG3	3:A:867:CYS:HA	1.97	0.44
3:A:942:ARG:HG2	6:O:565:GLN:HG2	2.00	0.44
4:N:351:PHE:O	4:N:354:SER:N	2.50	0.44
4:N:611:VAL:HG12	4:N:665:VAL:HG21	1.99	0.44
5:I:347:LEU:HD12	5:I:351:HIS:CD2	2.53	0.44
5:I:691:THR:HG23	5:I:696:GLN:NE2	2.32	0.44
6:O:109:GLU:HB3	14:U:344:ARG:CZ	2.48	0.44
6:O:109:GLU:HB3	14:U:344:ARG:NH2	2.32	0.44
10:M:49:SER:HB2	10:M:52:GLU:HG2	1.99	0.44
12:P:114:ALA:HA	12:P:117:THR:HG22	1.98	0.44
12:P:752:GLN:N	12:P:752:GLN:OE1	2.50	0.44
13:Z:224:MET:O	13:Z:228:GLN:HG2	2.17	0.44
13:Z:291:VAL:HG23	13:Z:311:TYR:CE1	2.52	0.44
13:Z:418:LEU:HA	13:Z:423:ILE:HG22	1.97	0.44
15:R:429:LYS:O	15:R:433:LEU:N	2.50	0.44
3:A:845:TYR:HB3	3:A:1812:TRP:NE1	2.32	0.44
4:N:335:ILE:HG13	4:N:336:TYR:N	2.31	0.44
5:I:587:LEU:HD21	5:I:643:PHE:CE1	2.52	0.44
12:P:154:SER:O	12:P:158:ILE:HG13	2.18	0.44
13:Z:474:ASP:HB2	13:Z:506:GLN:NE2	2.31	0.44
3:A:1100:LEU:HD21	3:A:1143:ALA:O	2.17	0.44
3:A:1917:LYS:O	3:A:1920:GLN:NE2	2.45	0.44
4:N:108:LEU:HB2	4:N:176:LEU:HD11	1.99	0.44
4:N:381:ALA:HA	4:N:384:THR:HG22	1.99	0.44
5:I:236:LEU:HD23	5:I:550:GLN:HA	1.99	0.44
5:I:512:LEU:HD13	6:O:439:LEU:HD11	1.99	0.44
12:P:500:TRP:O	12:P:504:GLN:HG2	2.18	0.44
12:P:521:ILE:O	12:P:525:VAL:HG23	2.18	0.44
12:P:605:THR:HG1	12:P:634:HIS:CD2	2.34	0.44
12:P:747:TYR:CE2	12:P:755:LEU:HB3	2.53	0.44
13:Y:100:TYR:CD1	13:Y:138:VAL:HG13	2.51	0.44
14:V:185:VAL:O	14:V:189:ILE:HG13	2.17	0.44
13:Z:283:ARG:NH1	13:Z:405:CYS:O	2.50	0.44
16:C:23:CYS:SG	16:C:24:GLY:N	2.90	0.44
3:A:1053:GLN:NE2	3:A:1059:ASP:OD1	2.50	0.44
3:A:1378:THR:HG23	3:A:1380:ASN:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1470:LEU:HA	3:A:1522:SER:OG	2.17	0.44
4:N:90:GLU:OE2	4:N:121:ARG:NH1	2.50	0.44
4:N:696:MET:HG2	4:N:713:PHE:CE2	2.53	0.44
5:I:288:THR:HG21	5:I:468:LYS:HD2	2.00	0.44
5:I:521:SER:OG	5:I:522:LEU:N	2.51	0.44
6:O:366:LYS:HA	6:O:366:LYS:HD3	1.75	0.44
7:S:374:SER:HB3	7:S:387:TYR:HD2	1.82	0.44
9:G:7:THR:HG23	8:Q:410:VAL:HG21	1.99	0.44
10:M:5:VAL:HG22	14:U:124:LEU:HD22	1.99	0.44
13:Y:396:PHE:O	13:Y:400:ILE:HG12	2.18	0.44
14:U:311:SER:O	14:U:311:SER:OG	2.36	0.44
3:A:86:ASP:N	3:A:86:ASP:OD1	2.42	0.44
3:A:707:TRP:CD2	6:O:730:ARG:HD3	2.53	0.44
3:A:959:ILE:HG23	3:A:978:ILE:HA	2.00	0.44
4:N:364:CYS:O	4:N:368:THR:HG22	2.18	0.44
6:O:27:LYS:HB3	6:O:209:GLN:HG3	1.99	0.44
12:J:694:LYS:HA	12:J:697:VAL:HG22	1.99	0.44
8:Q:36:GLU:HB2	8:Q:39:ASP:OD2	2.17	0.44
13:Y:550:GLN:HA	13:Y:553:GLU:HG3	1.99	0.44
13:Z:363:ALA:O	13:Z:366:ILE:HG22	2.18	0.44
2:D:50:ASN:OD1	2:D:51:LEU:N	2.50	0.44
3:A:74:TRP:HZ2	3:A:604:MET:CE	2.30	0.44
3:A:796:ASP:C	3:A:798:LYS:N	2.71	0.44
3:A:843:SER:HB3	3:A:846:GLN:HB3	1.99	0.44
3:A:942:ARG:HD3	3:A:942:ARG:HA	1.83	0.44
3:A:943:ASP:O	3:A:946:THR:OG1	2.32	0.44
3:A:1812:TRP:CE3	3:A:1890:VAL:HG13	2.53	0.44
9:G:15:ASP:OD2	8:Q:456:ARG:NH2	2.50	0.44
12:P:646:TYR:CD1	12:P:678:VAL:HG12	2.53	0.44
13:Z:299:MET:HG3	13:Z:300:LEU:N	2.33	0.44
15:R:190:LEU:HD13	15:R:233:THR:HA	1.98	0.44
3:A:1432:GLN:NE2	3:A:1436:GLU:OE2	2.34	0.44
3:A:1726:ARG:NH2	3:A:1781:GLN:HG3	2.33	0.44
5:I:306:HIS:CG	6:O:57:ARG:HH21	2.36	0.44
5:I:583:LEU:HD11	5:I:611:VAL:HG21	1.99	0.44
5:I:662:ARG:HB3	5:I:715:GLU:HG3	2.00	0.44
6:O:10:PHE:HD1	14:V:390:HIS:CD2	2.35	0.44
7:S:396:CYS:O	7:S:402:GLY:HA2	2.18	0.44
7:S:437:THR:O	7:S:441:LYS:HG2	2.17	0.44
12:J:465:LEU:O	12:J:469:MET:HG3	2.16	0.44
12:J:704:LEU:HD22	15:R:494:ARG:HG3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:93:TYR:HE2	14:V:105:PHE:CE2	2.35	0.44
13:Z:425:GLU:HA	13:Z:428:VAL:HG12	2.00	0.44
1:L:178:PHE:HE1	12:P:703:PRO:HB2	1.83	0.44
4:N:186:GLN:CG	4:N:223:GLY:H	2.31	0.44
4:N:234:ARG:NE	4:N:234:ARG:CA	2.81	0.44
4:N:581:ARG:HB3	4:N:585:GLU:HG2	2.00	0.44
4:N:687:MET:HB3	4:N:692:LEU:HG	1.99	0.44
6:O:65:LEU:HB3	6:O:66:PRO:HD3	2.00	0.44
6:O:361:LEU:O	6:O:365:VAL:HG23	2.18	0.44
7:S:396:CYS:HB3	7:S:403:PHE:H	1.83	0.44
8:K:40:ILE:HD13	8:K:63:ARG:HD3	1.99	0.44
13:Y:74:PRO:HB3	13:Y:132:LEU:HD11	1.99	0.44
13:Y:97:VAL:HG21	13:Y:146:TYR:CE1	2.53	0.44
14:V:161:LYS:HE3	14:V:166:GLU:HG3	2.00	0.44
13:Z:61:LEU:O	13:Z:65:ASN:ND2	2.36	0.44
4:N:119:GLU:HA	4:N:250:LEU:HD21	2.00	0.43
4:N:177:TYR:HE2	4:N:303:VAL:HG21	1.82	0.43
12:J:485:ILE:HD11	12:J:508:ALA:HB3	2.00	0.43
8:Q:60:LEU:HD23	8:Q:65:LEU:HD23	2.00	0.43
8:Q:231:LEU:HG	8:Q:257:VAL:HG13	1.98	0.43
14:U:238:TYR:HB3	14:U:247:ALA:HB2	1.99	0.43
13:Z:430:ALA:HA	13:Z:433:VAL:HG12	2.00	0.43
15:R:195:TRP:CZ3	15:R:201:LEU:HB2	2.53	0.43
3:A:257:MET:HE1	3:A:444:PHE:HB3	2.00	0.43
4:N:174:GLN:HE22	4:N:263:THR:HG22	1.83	0.43
4:N:574:ILE:HG21	4:N:622:TYR:HE1	1.84	0.43
5:I:595:LEU:HD13	5:I:637:SER:HB3	2.00	0.43
12:J:485:ILE:HD12	12:J:505:ILE:HG23	2.00	0.43
12:P:672:LEU:HB3	12:P:695:ALA:HB2	1.99	0.43
13:Z:233:LEU:O	13:Z:236:LEU:HG	2.18	0.43
3:A:1060:HIS:O	3:A:1064:GLU:HG2	2.18	0.43
4:N:199:LEU:HD23	4:N:295:ARG:HE	1.84	0.43
4:N:405:LYS:HG2	4:N:408:ARG:HH21	1.83	0.43
5:I:526:LYS:HB3	5:I:526:LYS:HE3	1.83	0.43
6:O:529:ASP:O	6:O:532:VAL:HG12	2.18	0.43
7:S:406:CYS:O	7:S:408:LYS:N	2.51	0.43
12:J:92:LEU:HD22	12:J:117:THR:OG1	2.17	0.43
12:P:449:ILE:HG22	12:P:453:ASN:OD1	2.18	0.43
13:Y:62:THR:HA	13:Y:65:ASN:HD21	1.83	0.43
13:Z:342:TRP:HB2	13:Z:365:ALA:HB2	2.00	0.43
15:R:404:ASN:ND2	15:R:447:LEU:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:420:TYR:CE1	15:R:445:ARG:HD3	2.53	0.43
1:L:90:THR:HB	1:L:145:HIS:HD2	1.83	0.43
3:A:422:GLU:HG2	3:A:449:GLN:HG2	2.01	0.43
3:A:465:GLN:OE1	3:A:465:GLN:N	2.49	0.43
3:A:731:SER:O	6:O:719:ARG:NH2	2.52	0.43
4:N:224:CYS:HB2	4:N:232:TRP:CD1	2.53	0.43
4:N:391:VAL:O	4:N:431:ARG:NH2	2.51	0.43
4:N:433:ASP:O	4:N:437:GLN:HG2	2.18	0.43
5:I:310:TRP:HZ2	6:O:44:MET:HE2	1.84	0.43
6:O:12:PRO:HG3	6:O:247:ASN:HA	2.00	0.43
6:O:596:SER:O	6:O:599:ILE:HG12	2.18	0.43
8:K:226:GLY:HA2	8:Q:34:ARG:HH12	1.83	0.43
12:P:496:TYR:CZ	13:Z:105:GLN:HG3	2.54	0.43
8:Q:208:LYS:HE3	8:Q:208:LYS:HB3	1.88	0.43
13:Z:289:ASN:HA	13:Z:292:LEU:HG	2.00	0.43
15:R:357:ALA:HB1	15:R:359:LYS:NZ	2.34	0.43
3:A:137:LYS:NZ	3:A:273:ARG:HB3	2.34	0.43
3:A:1872:LEU:HD11	3:A:1931:LEU:HD13	2.00	0.43
5:I:557:TYR:HA	5:I:694:ASP:HB2	1.99	0.43
5:I:632:ARG:HH12	5:I:711:TRP:HH2	1.67	0.43
7:S:398:ARG:HB3	7:S:401:CYS:O	2.19	0.43
8:K:491:LEU:HD22	9:W:22:ILE:HD12	2.00	0.43
11:H:96:PHE:HB3	12:P:595:GLN:HB3	2.01	0.43
12:J:35:VAL:HG23	12:J:37:SER:H	1.82	0.43
8:Q:351:ASP:OD2	15:R:393:LEU:HD13	2.18	0.43
14:U:234:LEU:HD23	14:U:234:LEU:HA	1.88	0.43
14:U:550:LEU:HA	14:U:553:ILE:HG22	2.00	0.43
14:V:308:TYR:CD2	14:V:343:LEU:HG	2.53	0.43
15:R:293:ILE:HB	15:R:309:LEU:HB2	1.99	0.43
15:R:430:TYR:CG	15:R:431:PRO:HA	2.54	0.43
1:L:175:THR:HG22	12:P:736:GLU:OE1	2.18	0.43
3:A:464:THR:OG1	3:A:465:GLN:OE1	2.34	0.43
3:A:1843:GLU:HA	3:A:1846:PRO:HG2	2.00	0.43
4:N:691:LEU:HD12	4:N:694:ARG:HB2	2.00	0.43
8:K:487:TYR:OH	9:W:15:ASP:O	2.25	0.43
12:P:742:LEU:HD23	12:P:742:LEU:HA	1.83	0.43
8:Q:218:THR:HG21	8:Q:241:HIS:CD2	2.54	0.43
8:Q:402:PRO:HB2	8:Q:444:TRP:CZ2	2.54	0.43
14:V:253:ASN:O	14:V:257:VAL:HG23	2.19	0.43
15:R:109:ASP:O	15:R:111:GLN:N	2.52	0.43
15:R:318:GLY:O	15:R:319:LEU:HD22	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:214:LEU:HD11	3:A:407:LEU:HD13	2.00	0.43
3:A:1860:LEU:HD11	3:A:1888:PHE:CE2	2.52	0.43
8:K:28:LYS:HA	8:K:28:LYS:HD3	1.81	0.43
8:K:157:LEU:HD11	8:K:167:PHE:HA	2.00	0.43
13:Y:146:TYR:HE2	13:Y:158:ILE:HG13	1.83	0.43
14:U:49:LEU:HD22	14:V:95:ASP:HB3	2.01	0.43
13:Z:321:LEU:HA	13:Z:324:VAL:HG12	2.00	0.43
3:A:1441:LEU:HD12	3:A:1454:LEU:HD21	2.00	0.43
4:N:543:GLU:HA	4:N:546:LYS:HD3	2.00	0.43
5:I:628:THR:HG22	5:I:630:LYS:H	1.84	0.43
6:O:265:GLN:HE21	6:O:502:GLN:HB2	1.82	0.43
12:J:672:LEU:HB3	12:J:695:ALA:HB2	2.01	0.43
12:P:446:THR:O	12:P:450:GLN:HB2	2.18	0.43
8:Q:6:LEU:HD23	8:Q:6:LEU:HA	1.89	0.43
13:Y:40:HIS:CE1	13:Z:200:PRO:HD2	2.51	0.43
13:Y:147:THR:HG22	13:Y:178:LEU:HD21	2.01	0.43
13:Y:246:VAL:HG22	13:Y:280:LEU:HD11	2.00	0.43
13:Y:330:ARG:O	13:Y:334:ILE:HG23	2.18	0.43
13:Z:237:SER:O	13:Z:241:LYS:HG2	2.18	0.43
1:L:178:PHE:CE1	12:P:703:PRO:HB2	2.54	0.43
3:A:477:LYS:N	3:A:491:LEU:O	2.47	0.43
3:A:1656:LEU:O	8:K:553:LYS:HE2	2.19	0.43
3:A:1821:PHE:HZ	3:A:1839:PHE:HD2	1.67	0.43
5:I:540:PRO:HA	5:I:543:VAL:HG22	2.01	0.43
6:O:38:LEU:HB3	6:O:115:LEU:HD11	2.00	0.43
8:Q:88:GLN:O	8:Q:92:VAL:HG23	2.19	0.43
8:Q:445:GLU:HG2	8:Q:475:ILE:HD12	2.01	0.43
14:U:262:SER:O	14:U:266:VAL:HG23	2.19	0.43
14:U:494:ILE:HD11	14:U:512:ALA:HB1	2.00	0.43
14:U:526:TRP:HA	14:U:553:ILE:HD11	2.00	0.43
3:A:1543:HIS:HD2	3:A:1544:MET:SD	2.42	0.43
4:N:51:LYS:HB3	4:N:54:GLU:CB	2.49	0.43
5:I:155:ILE:O	5:I:161:SER:OG	2.23	0.43
5:I:309:LEU:O	6:O:130:SER:HB3	2.19	0.43
6:O:378:SER:HB3	6:O:409:HIS:NE2	2.34	0.43
12:J:42:PHE:HB2	12:J:71:CYS:SG	2.59	0.43
12:J:104:ASP:HA	12:J:107:VAL:HG12	2.01	0.43
12:P:165:ASP:N	12:P:165:ASP:OD1	2.45	0.43
8:Q:502:PHE:CE2	8:Q:518:MET:HG3	2.54	0.43
14:U:85:ASP:OD1	14:U:85:ASP:N	2.52	0.43
14:U:318:TYR:HA	14:U:321:HIS:NE2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:504:VAL:HG23	14:V:505:GLU:N	2.30	0.43
13:Z:60:LEU:HD12	13:Z:71:PHE:CZ	2.54	0.43
3:A:1489:HIS:O	3:A:1493:LYS:HG2	2.19	0.42
4:N:321:LEU:HD12	4:N:324:TRP:HE3	1.84	0.42
4:N:690:ALA:O	4:N:694:ARG:HG2	2.19	0.42
4:N:693:ARG:HD2	4:N:693:ARG:HA	1.75	0.42
4:N:694:ARG:O	4:N:698:VAL:HG23	2.19	0.42
5:I:48:ARG:HG3	5:I:55:VAL:CG2	2.48	0.42
5:I:615:LEU:HD21	5:I:700:ILE:HD12	2.00	0.42
6:O:216:LEU:HD22	6:O:256:LEU:HD22	2.01	0.42
7:S:410:LEU:N	7:S:410:LEU:CD1	2.82	0.42
8:K:55:ARG:HD2	8:Q:263:PHE:O	2.18	0.42
12:P:738:LEU:HA	12:P:738:LEU:HD23	1.80	0.42
14:U:474:ALA:HA	14:U:477:HIS:ND1	2.33	0.42
14:V:106:LEU:HD22	14:V:114:ALA:HB1	2.01	0.42
3:A:15:ARG:HB2	3:A:608:THR:OG1	2.19	0.42
3:A:40:ARG:HB3	14:V:142:GLU:HG3	2.01	0.42
4:N:144:THR:HG21	4:N:152:GLU:OE1	2.19	0.42
4:N:416:ILE:O	4:N:420:ALA:CB	2.67	0.42
12:J:63:GLY:O	13:Y:296:GLN:HG3	2.19	0.42
12:J:680:HIS:ND1	12:J:712:VAL:HG23	2.34	0.42
14:V:115:TYR:OH	14:V:161:LYS:HD3	2.18	0.42
14:V:160:LYS:HE3	14:V:160:LYS:HB2	1.72	0.42
13:Z:168:THR:O	13:Z:172:ASN:ND2	2.52	0.42
15:R:59:VAL:O	15:R:63:ARG:HG2	2.19	0.42
15:R:290:ASP:O	15:R:292:MET:HG2	2.19	0.42
3:A:862:TYR:CZ	3:A:864:PRO:HA	2.54	0.42
3:A:1533:LEU:HD11	4:N:482:PRO:HD3	2.01	0.42
3:A:1575:SER:HG	3:A:1580:SER:HG	1.61	0.42
3:A:1793:MET:HG2	3:A:1814:ILE:HG12	2.02	0.42
4:N:234:ARG:N	4:N:234:ARG:NE	2.67	0.42
5:I:90:ILE:HD11	5:I:110:VAL:HG21	2.00	0.42
5:I:631:VAL:HG21	5:I:633:ARG:HE	1.84	0.42
6:O:285:GLY:HA3	6:O:298:ARG:NE	2.34	0.42
7:S:399:GLU:HA	7:S:399:GLU:OE1	2.20	0.42
7:S:406:CYS:C	7:S:408:LYS:N	2.71	0.42
8:K:405:MET:HA	8:K:408:VAL:HG22	1.99	0.42
13:Y:551:LYS:HE3	13:Y:551:LYS:HB2	1.83	0.42
13:Z:186:ARG:O	13:Z:190:THR:HG23	2.19	0.42
13:Z:431:ASN:O	13:Z:435:LYS:HG2	2.19	0.42
15:R:43:LYS:HD3	15:R:43:LYS:HA	1.90	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:R:245:ALA:HB2	15:R:279:TRP:HZ2	1.84	0.42
15:R:429:LYS:HG2	15:R:436:VAL:HG22	2.01	0.42
3:A:224:VAL:HG12	3:A:238:TYR:HD1	1.84	0.42
3:A:1323:GLU:HG3	8:K:513:THR:HG23	2.00	0.42
3:A:1825:SER:OG	3:A:1829:ARG:NH1	2.52	0.42
8:K:134:LEU:HD22	8:K:163:CYS:SG	2.60	0.42
10:M:11:ILE:HD13	10:M:11:ILE:HA	1.94	0.42
10:M:31:ILE:HD13	10:M:31:ILE:HA	1.88	0.42
13:Y:547:GLU:O	13:Y:550:GLN:HG3	2.20	0.42
14:U:492:LYS:O	14:U:495:GLN:HG3	2.19	0.42
14:U:551:ARG:NH2	14:U:554:LEU:HD21	2.34	0.42
15:R:4:ASP:OD1	15:R:7:ARG:NH1	2.52	0.42
15:R:193:VAL:HB	15:R:448:TYR:HB3	2.00	0.42
15:R:430:TYR:CD1	15:R:431:PRO:HA	2.54	0.42
16:C:60:ILE:HG13	16:C:61:LEU:N	2.34	0.42
3:A:777:THR:HB	6:O:594:SER:O	2.20	0.42
4:N:186:GLN:CD	4:N:222:ALA:HB3	2.39	0.42
4:N:483:ASP:OD2	4:N:497:ARG:NH2	2.46	0.42
4:N:660:THR:HG22	4:N:663:GLN:OE1	2.20	0.42
6:O:687:LEU:O	6:O:691:ILE:HG13	2.19	0.42
8:Q:176:LEU:O	8:Q:210:LYS:NZ	2.51	0.42
14:U:486:ALA:O	14:U:490:TYR:HB2	2.19	0.42
13:Z:462:LYS:HE2	13:Z:485:LEU:HD21	2.01	0.42
1:L:79:ILE:HG22	1:L:156:ILE:HG12	2.01	0.42
3:A:1033:ARG:O	3:A:1037:VAL:HG23	2.19	0.42
4:N:633:ARG:NH2	16:C:41:GLY:HA2	2.34	0.42
5:I:7:CYS:HG	5:I:628:THR:HG1	1.56	0.42
6:O:532:VAL:HG23	6:O:546:ARG:HB2	2.01	0.42
6:O:622:GLU:OE2	6:O:662:ARG:NH2	2.52	0.42
8:K:342:HIS:ND1	8:K:357:TYR:OH	2.40	0.42
12:P:53:LYS:HB3	12:P:56:LYS:HG3	2.01	0.42
8:Q:320:ARG:HD3	8:Q:344:PHE:CZ	2.54	0.42
14:U:514:ARG:NE	14:U:542:THR:HG22	2.34	0.42
15:R:410:HIS:CD2	15:R:475:LYS:HA	2.55	0.42
1:L:32:SER:HB2	1:L:65:ASN:HD22	1.85	0.42
3:A:497:LEU:HD11	3:A:597:LEU:HD21	2.02	0.42
3:A:1313:LEU:HB3	3:A:1316:MET:HE3	2.01	0.42
4:N:573:ASN:HA	4:N:576:GLU:CD	2.39	0.42
6:O:433:GLY:HA3	6:O:617:GLN:HB3	2.01	0.42
13:Y:430:ALA:O	13:Y:433:VAL:HG12	2.20	0.42
14:V:385:ILE:HG13	14:V:408:THR:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:49:LEU:HD13	13:Z:52:ASN:HB2	2.02	0.42
3:A:709:TYR:HE2	6:O:738:ARG:HA	1.83	0.42
3:A:811:PRO:HD2	3:A:1806:SER:O	2.19	0.42
3:A:1434:ILE:O	3:A:1438:SER:OG	2.27	0.42
3:A:1621:PRO:HG3	3:A:1653:ALA:CB	2.50	0.42
5:I:64:THR:O	5:I:84:LEU:HD13	2.20	0.42
5:I:230:GLU:HA	5:I:558:ARG:HA	2.00	0.42
6:O:622:GLU:CD	6:O:662:ARG:HH22	2.23	0.42
12:P:520:ARG:NH1	13:Z:154:ASP:OD1	2.51	0.42
8:Q:7:ARG:O	8:Q:10:VAL:HG22	2.19	0.42
8:Q:403:PHE:O	8:Q:407:GLU:HG2	2.19	0.42
14:U:419:LEU:HD21	14:U:443:TYR:CE1	2.54	0.42
13:Z:449:THR:HG23	13:Z:481:LYS:NZ	2.35	0.42
3:A:115:LYS:HD3	6:O:267:VAL:HG21	2.01	0.42
3:A:224:VAL:HG12	3:A:238:TYR:CD1	2.53	0.42
3:A:1153:ILE:O	3:A:1187:LYS:HD2	2.20	0.42
3:A:1409:LEU:HD22	3:A:1470:LEU:HD23	2.02	0.42
4:N:616:ARG:O	4:N:620:GLU:HG2	2.20	0.42
5:I:654:LYS:HA	5:I:664:ARG:HG2	2.02	0.42
5:I:680:SER:O	5:I:684:GLN:NE2	2.53	0.42
8:K:514:PHE:CE2	9:W:11:LEU:HD13	2.54	0.42
11:H:73:ASP:HA	11:H:76:VAL:HG12	2.02	0.42
12:P:727:GLU:HA	12:P:730:LYS:HB2	2.00	0.42
8:Q:288:SER:O	8:Q:292:VAL:HG22	2.19	0.42
8:Q:308:TYR:O	8:Q:312:VAL:HG13	2.20	0.42
13:Z:364:LYS:HA	13:Z:364:LYS:HD2	1.90	0.42
3:A:178:ALA:HB2	3:A:192:SER:HB3	2.01	0.42
3:A:435:ASP:OD1	3:A:436:LEU:N	2.53	0.42
4:N:56:ARG:NH1	4:N:140:LEU:HD21	2.35	0.42
4:N:512:LYS:HE3	4:N:549:PHE:CD1	2.55	0.42
4:N:644:VAL:HG21	4:N:661:PRO:HA	2.01	0.42
5:I:344:ILE:HD13	5:I:479:LEU:HD11	2.00	0.42
12:J:739:VAL:O	12:J:743:ILE:HG13	2.19	0.42
12:P:23:ASP:OD1	12:P:23:ASP:N	2.46	0.42
12:P:488:LEU:HA	12:P:491:LEU:HD13	2.01	0.42
8:Q:275:LEU:HD22	8:Q:280:LYS:HB2	2.02	0.42
13:Y:78:GLN:HA	13:Y:81:VAL:HG22	2.02	0.42
13:Y:309:ASP:OD1	13:Y:309:ASP:N	2.52	0.42
13:Z:135:GLU:O	13:Z:139:LYS:HG2	2.20	0.42
15:R:113:GLU:HG2	15:R:115:ARG:H	1.85	0.42
15:R:201:LEU:HD13	15:R:469:PHE:CZ	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:181:TRP:HB2	3:A:249:LEU:HD23	2.00	0.41
3:A:497:LEU:HB3	3:A:509:VAL:HB	2.01	0.41
3:A:1667:LYS:HZ3	3:A:1677:LEU:HD13	1.85	0.41
3:A:1797:ILE:O	3:A:1801:GLY:N	2.48	0.41
6:O:98:LYS:HB3	6:O:98:LYS:HE2	1.86	0.41
8:K:372:LEU:HD22	8:K:404:VAL:HG22	2.01	0.41
12:P:689:LEU:HD23	12:P:689:LEU:HA	1.86	0.41
12:P:736:GLU:OE2	12:P:738:LEU:N	2.48	0.41
14:U:122:ARG:NH1	14:U:157:GLU:OE1	2.41	0.41
14:U:535:LYS:CE	14:U:577:LEU:HD22	2.50	0.41
15:R:176:PHE:CE2	15:R:469:PHE:HB3	2.55	0.41
15:R:353:GLU:OE1	15:R:353:GLU:N	2.53	0.41
15:R:382:ILE:HD11	15:R:398:THR:HG22	2.02	0.41
3:A:436:LEU:HD23	3:A:638:LEU:HD13	2.02	0.41
4:N:400:TYR:O	4:N:404:ILE:HG13	2.20	0.41
4:N:682:SER:HB2	4:N:692:LEU:HD11	2.02	0.41
6:O:64:LEU:O	6:O:68:LEU:HG	2.20	0.41
6:O:249:ASP:HA	6:O:280:ARG:HH22	1.85	0.41
7:S:364:GLU:HA	7:S:367:LYS:HG2	2.01	0.41
8:K:88:GLN:O	8:K:92:VAL:HG23	2.20	0.41
8:Q:175:MET:HB2	8:Q:175:MET:HE3	1.94	0.41
8:Q:474:LEU:HD12	8:Q:474:LEU:HA	1.86	0.41
13:Y:59:LEU:HD21	13:Z:239:TRP:CH2	2.55	0.41
15:R:9:LEU:HD23	15:R:9:LEU:HA	1.89	0.41
1:L:76:THR:HG22	1:L:159:TYR:HB2	2.02	0.41
3:A:1636:VAL:CG1	3:A:1663:LEU:HD11	2.50	0.41
4:N:640:THR:O	4:N:661:PRO:HD2	2.20	0.41
5:I:265:ILE:HD13	5:I:265:ILE:HA	1.85	0.41
6:O:536:THR:HB	6:O:543:GLY:HA3	2.02	0.41
8:Q:264:HIS:HB3	8:Q:267:CYS:HB3	2.02	0.41
14:U:335:CYS:SG	14:U:364:TYR:HE2	2.43	0.41
14:V:388:TYR:HB2	14:V:405:LEU:HD13	2.03	0.41
16:C:16:TRP:CD1	16:C:31:ASN:HA	2.55	0.41
3:A:628:ILE:HD12	3:A:628:ILE:HA	1.93	0.41
4:N:108:LEU:HD13	4:N:176:LEU:HD12	2.02	0.41
4:N:598:SER:HB3	16:C:13:THR:HB	2.01	0.41
6:O:594:SER:O	6:O:594:SER:OG	2.33	0.41
7:S:403:PHE:CE2	7:S:405:TYR:HB3	2.55	0.41
8:K:74:TYR:HB2	8:K:132:ILE:HD11	2.02	0.41
12:J:75:LEU:HG	12:J:91:ILE:HD13	2.03	0.41
14:V:34:LYS:HB3	14:V:71:GLN:HE21	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:V:340:TYR:CZ	14:V:344:ARG:HD2	2.56	0.41
13:Z:448:ALA:HA	13:Z:451:CYS:SG	2.61	0.41
15:R:189:TYR:HB3	15:R:317:CYS:SG	2.60	0.41
3:A:17:LEU:HD21	3:A:511:ILE:HG22	2.01	0.41
3:A:248:PHE:HB3	3:A:257:MET:HB3	2.03	0.41
3:A:1043:SER:O	3:A:1043:SER:OG	2.37	0.41
5:I:731:SER:HB3	5:I:746:MET:CE	2.50	0.41
6:O:660:LYS:HE3	6:O:660:LYS:HB2	1.88	0.41
7:S:359:HIS:HE2	16:C:59:CYS:HA	1.86	0.41
12:P:537:GLU:HG3	12:P:538:ILE:H	1.86	0.41
13:Y:447:LEU:O	13:Y:450:VAL:HG12	2.19	0.41
14:V:415:PRO:HA	14:V:418:CYS:SG	2.60	0.41
13:Z:309:ASP:HB2	13:Z:340:GLU:CG	2.50	0.41
13:Z:489:GLU:HG3	13:Z:491:LYS:HG2	2.03	0.41
15:R:10:LEU:O	15:R:14:VAL:HG23	2.20	0.41
15:R:201:LEU:HD11	15:R:459:VAL:HG21	2.03	0.41
15:R:289:ARG:HA	15:R:315:GLU:HG3	2.03	0.41
1:L:167:ILE:HG23	1:L:170:PHE:H	1.85	0.41
3:A:1199:LYS:HE2	3:A:1201:HIS:HB2	2.02	0.41
3:A:1847:VAL:HA	3:A:1850:CYS:SG	2.61	0.41
5:I:724:GLY:HA2	5:I:731:SER:HA	2.03	0.41
8:K:209:LEU:HD23	8:K:209:LEU:HA	1.79	0.41
12:J:567:PRO:HB2	12:J:600:TYR:CD2	2.56	0.41
12:P:53:LYS:HG3	12:P:56:LYS:HE2	2.01	0.41
13:Y:159:LEU:HB3	13:Y:175:LEU:HG	2.02	0.41
13:Y:191:SER:O	13:Y:194:GLU:HB3	2.19	0.41
14:V:261:LYS:HE3	14:V:261:LYS:HB2	1.80	0.41
3:A:1208:LEU:HD23	3:A:1208:LEU:HA	1.86	0.41
3:A:1216:LYS:HA	3:A:1216:LYS:HD3	1.80	0.41
4:N:607:GLU:H	4:N:607:GLU:HG2	1.58	0.41
5:I:620:PHE:CE1	5:I:653:LEU:HD21	2.56	0.41
5:I:644:TYR:OH	5:I:729:LYS:HA	2.20	0.41
6:O:418:ILE:O	6:O:422:ILE:HG13	2.21	0.41
6:O:430:ARG:HD3	6:O:472:HIS:HD2	1.83	0.41
8:K:258:MET:HG3	8:K:271:HIS:CD2	2.55	0.41
12:J:132:ALA:O	12:J:135:SER:OG	2.33	0.41
12:J:150:SER:H	12:P:23:ASP:HB3	1.86	0.41
12:J:668:SER:OG	12:J:671:LEU:HB2	2.20	0.41
13:Y:94:ARG:HA	13:Y:97:VAL:HG12	2.03	0.41
14:U:517:ALA:HA	14:U:532:CYS:SG	2.61	0.41
14:V:526:TRP:HE1	14:V:556:LEU:HD23	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:304:LEU:O	13:Z:305:ILE:HD13	2.21	0.41
15:R:203:VAL:O	15:R:209:VAL:HA	2.20	0.41
3:A:704:ASP:OD1	6:O:731:ASN:ND2	2.47	0.41
4:N:53:GLU:OE1	4:N:53:GLU:N	2.54	0.41
4:N:340:ARG:HB2	4:N:361:LEU:HD13	2.03	0.41
4:N:556:PHE:HA	4:N:559:VAL:HG12	2.01	0.41
4:N:571:ASN:HD22	4:N:574:ILE:HD12	1.85	0.41
4:N:650:LEU:HD21	4:N:716:ILE:O	2.21	0.41
5:I:653:LEU:HD23	5:I:653:LEU:HA	1.78	0.41
13:Y:185:GLU:O	13:Y:189:VAL:HG23	2.20	0.41
15:R:205:LEU:HG	15:R:208:CYS:HB2	2.03	0.41
3:A:93:LEU:HD21	3:A:151:ILE:HD11	2.02	0.41
3:A:93:LEU:HD12	3:A:102:TRP:HA	2.03	0.41
3:A:489:LEU:HG	3:A:497:LEU:HD22	2.03	0.41
3:A:780:GLY:HA3	6:O:595:SER:HB3	2.03	0.41
3:A:1014:ASP:OD1	3:A:1014:ASP:N	2.54	0.41
3:A:1155:SER:HB2	3:A:1187:LYS:O	2.21	0.41
3:A:1871:TYR:CE1	3:A:1889:LEU:HD11	2.56	0.41
4:N:28:SER:O	4:N:32:VAL:HG12	2.20	0.41
4:N:404:ILE:HA	4:N:417:LEU:HD13	2.03	0.41
5:I:214:LEU:HD12	5:I:245:LEU:HD12	2.02	0.41
12:J:55:TYR:O	12:J:59:ARG:HG3	2.20	0.41
12:P:662:LEU:HD13	12:P:675:ILE:HD12	2.02	0.41
8:Q:61:ARG:HD2	8:Q:66:ASP:CG	2.41	0.41
8:Q:298:ASN:OD1	8:Q:299:PRO:HD2	2.21	0.41
13:Y:277:LEU:HD12	13:Y:277:LEU:HA	1.92	0.41
13:Y:402:LEU:HD23	13:Y:402:LEU:HA	1.97	0.41
14:V:142:GLU:OE2	14:V:390:HIS:HE1	2.03	0.41
14:V:448:GLN:HB3	14:V:451:GLU:OE1	2.21	0.41
13:Z:49:LEU:O	13:Z:49:LEU:HD12	2.20	0.41
13:Z:384:ARG:HD2	13:Z:415:GLU:OE1	2.21	0.41
13:Z:449:THR:HA	13:Z:481:LYS:NZ	2.36	0.41
15:R:230:ASP:OD1	15:R:249:HIS:HB3	2.21	0.41
3:A:628:ILE:HD11	3:A:836:PHE:CZ	2.55	0.41
3:A:827:GLN:HB3	3:A:830:PHE:CD2	2.56	0.41
3:A:1307:LEU:HD12	3:A:1307:LEU:HA	1.91	0.41
3:A:1719:LEU:HD11	4:N:304:PHE:CZ	2.56	0.41
5:I:399:LYS:NZ	5:I:517:TYR:O	2.43	0.41
6:O:41:LEU:HD13	6:O:132:VAL:HG13	2.01	0.41
6:O:643:LEU:O	6:O:647:ALA:HB3	2.21	0.41
12:J:749:LYS:HD3	12:J:749:LYS:HA	1.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:25:TRP:O	8:Q:29:VAL:HG23	2.21	0.41
13:Y:244:ALA:O	13:Y:248:THR:HG23	2.21	0.41
13:Y:507:SER:OG	13:Y:538:LEU:HD11	2.21	0.41
14:U:503:ILE:HG13	14:U:503:ILE:O	2.21	0.41
3:A:953:LEU:HD21	3:A:1821:PHE:CE2	2.56	0.40
3:A:1090:PHE:HE1	3:A:1182:ASN:OD1	2.04	0.40
4:N:186:GLN:OE1	4:N:189:ARG:NH2	2.54	0.40
4:N:269:THR:HB	4:N:331:PHE:HE2	1.86	0.40
8:K:94:ASP:OD1	8:K:95:MET:N	2.53	0.40
12:J:14:GLN:NE2	12:P:116:PHE:HE2	2.19	0.40
12:P:13:TRP:NE1	12:P:43:LEU:HD21	2.36	0.40
12:P:668:SER:HB3	12:P:671:LEU:HB2	2.04	0.40
8:Q:134:LEU:HG	8:Q:138:LYS:HE3	2.02	0.40
8:Q:383:ASN:ND2	8:Q:386:LEU:HD12	2.36	0.40
14:V:505:GLU:HG3	14:V:508:GLU:OE2	2.21	0.40
13:Z:192:TYR:HB3	13:Z:209:LEU:HD12	2.02	0.40
16:C:23:CYS:HB3	16:C:26:CYS:SG	2.60	0.40
3:A:435:ASP:OD1	3:A:501:THR:OG1	2.33	0.40
3:A:1619:LEU:HD21	3:A:1697:LEU:HD22	2.02	0.40
4:N:172:MET:HG3	4:N:173:ILE:N	2.37	0.40
4:N:592:TYR:HE2	16:C:7:CYS:HB3	1.87	0.40
5:I:174:ASN:OD1	5:I:190:TYR:HA	2.22	0.40
5:I:374:GLN:HE21	6:O:692:GLU:HB3	1.86	0.40
5:I:604:HIS:CD2	5:I:606:ASP:H	2.40	0.40
8:K:270:VAL:O	8:K:274:THR:HG23	2.21	0.40
11:H:82:LEU:HB3	12:P:577:PHE:HE2	1.86	0.40
13:Y:77:TYR:O	13:Y:81:VAL:HG13	2.21	0.40
13:Y:152:ASP:O	13:Y:156:ILE:HG23	2.21	0.40
13:Y:160:ASP:HA	13:Y:167:ARG:HH21	1.85	0.40
14:U:244:ILE:HG21	14:U:276:ILE:HB	2.03	0.40
14:V:434:ARG:HH21	15:R:49:ILE:HD12	1.85	0.40
14:V:476:LEU:HD23	14:V:476:LEU:HA	1.81	0.40
3:A:462:ASP:OD2	3:A:464:THR:OG1	2.39	0.40
3:A:1163:PRO:HB2	3:A:1168:LEU:HB2	2.03	0.40
3:A:1794:ASP:OD1	3:A:1798:ARG:HD2	2.21	0.40
3:A:1931:LEU:HD23	3:A:1931:LEU:HA	1.88	0.40
4:N:575:ARG:HD2	4:N:592:TYR:CE1	2.55	0.40
6:O:627:LEU:HD23	6:O:627:LEU:HA	1.94	0.40
6:O:707:LYS:HB3	6:O:744:LEU:HD11	2.04	0.40
8:Q:271:HIS:HD2	8:Q:287:LEU:HD22	1.87	0.40
13:Y:393:ILE:O	13:Y:397:ARG:HG3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:244:ILE:HG23	14:U:272:ALA:HB1	2.02	0.40
15:R:386:ASN:HD21	15:R:393:LEU:HB2	1.84	0.40
1:L:54:TRP:O	1:L:152:HIS:HA	2.21	0.40
4:N:334:ARG:HG3	4:N:335:ILE:H	1.87	0.40
4:N:627:GLU:HG2	4:N:633:ARG:O	2.21	0.40
8:K:551:THR:OG1	8:K:553:LYS:HG3	2.22	0.40
12:P:120:LEU:O	12:P:124:VAL:HG23	2.22	0.40
13:Y:76:LYS:HE2	13:Y:76:LYS:HB3	1.91	0.40
13:Y:466:ASP:OD1	13:Y:467:LYS:N	2.54	0.40
14:U:189:ILE:HG23	14:U:209:LEU:HD11	2.04	0.40
14:V:422:TYR:CZ	14:V:438:ALA:HB1	2.56	0.40
13:Z:100:TYR:HB3	13:Z:142:MET:SD	2.61	0.40
13:Z:347:CYS:SG	13:Z:378:LEU:HD12	2.62	0.40
13:Z:447:LEU:HA	13:Z:450:VAL:HG12	2.03	0.40
1:L:43:ASP:O	1:L:47:ASP:N	2.54	0.40
1:L:82:ASP:HA	1:L:117:SER:HA	2.04	0.40
1:L:101:ASN:ND2	3:A:1402:GLU:OE2	2.52	0.40
3:A:956:ARG:HD2	3:A:1786:MET:SD	2.62	0.40
4:N:31:LEU:HD13	4:N:132:LEU:HD11	2.02	0.40
4:N:566:ASP:OD1	4:N:569:ARG:NH2	2.47	0.40
6:O:393:LYS:HE2	6:O:393:LYS:HB3	1.89	0.40
11:H:60:SER:HA	11:H:63:VAL:HG12	2.04	0.40
12:J:646:TYR:CD1	12:J:678:VAL:HG12	2.57	0.40
12:J:716:ASN:HB3	12:J:718:LYS:NZ	2.36	0.40
12:P:644:ILE:O	12:P:648:GLN:HG3	2.21	0.40
14:U:429:ARG:HD3	14:U:429:ARG:HA	1.87	0.40
13:Z:72:SER:H	13:Z:75:GLN:HE21	1.69	0.40
13:Z:512:HIS:O	13:Z:531:GLN:HB3	2.21	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	L	181/185 (98%)	171 (94%)	10 (6%)	0	100	100
2	D	55/121 (46%)	51 (93%)	4 (7%)	0	100	100
3	A	1628/1944 (84%)	1537 (94%)	90 (6%)	1 (0%)	51	82
4	N	674/822 (82%)	640 (95%)	34 (5%)	0	100	100
5	I	736/814 (90%)	696 (95%)	40 (5%)	0	100	100
6	O	699/755 (93%)	683 (98%)	16 (2%)	0	100	100
7	S	94/447 (21%)	82 (87%)	12 (13%)	0	100	100
8	K	525/620 (85%)	507 (97%)	18 (3%)	0	100	100
8	Q	503/620 (81%)	494 (98%)	9 (2%)	0	100	100
9	G	25/85 (29%)	25 (100%)	0	0	100	100
9	W	24/85 (28%)	24 (100%)	0	0	100	100
10	M	66/74 (89%)	62 (94%)	4 (6%)	0	100	100
11	H	56/110 (51%)	55 (98%)	1 (2%)	0	100	100
12	J	507/824 (62%)	490 (97%)	17 (3%)	0	100	100
12	P	492/824 (60%)	483 (98%)	9 (2%)	0	100	100
13	Y	498/599 (83%)	487 (98%)	11 (2%)	0	100	100
13	Z	485/599 (81%)	470 (97%)	15 (3%)	0	100	100
14	U	534/597 (89%)	510 (96%)	24 (4%)	0	100	100
14	V	533/597 (89%)	519 (97%)	13 (2%)	1 (0%)	47	78
15	R	430/496 (87%)	401 (93%)	29 (7%)	0	100	100
16	C	82/84 (98%)	74 (90%)	8 (10%)	0	100	100
All	All	8827/11302 (78%)	8461 (96%)	364 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	797	LEU
14	V	504	VAL

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	168/170 (99%)	168 (100%)	0	100	100
2	D	54/115 (47%)	54 (100%)	0	100	100
3	A	1450/1720 (84%)	1450 (100%)	0	100	100
4	N	600/724 (83%)	594 (99%)	6 (1%)	76	92
5	I	663/736 (90%)	661 (100%)	2 (0%)	92	98
6	O	604/650 (93%)	603 (100%)	1 (0%)	93	98
7	S	88/403 (22%)	85 (97%)	3 (3%)	37	71
8	K	463/548 (84%)	463 (100%)	0	100	100
8	Q	437/548 (80%)	437 (100%)	0	100	100
9	G	26/77 (34%)	26 (100%)	0	100	100
9	W	25/77 (32%)	25 (100%)	0	100	100
10	M	61/67 (91%)	61 (100%)	0	100	100
11	H	52/89 (58%)	52 (100%)	0	100	100
12	J	439/727 (60%)	439 (100%)	0	100	100
12	P	429/727 (59%)	429 (100%)	0	100	100
13	Y	425/513 (83%)	423 (100%)	2 (0%)	88	96
13	Z	417/513 (81%)	416 (100%)	1 (0%)	93	98
14	U	471/520 (91%)	471 (100%)	0	100	100
14	V	463/520 (89%)	463 (100%)	0	100	100
15	R	378/431 (88%)	377 (100%)	1 (0%)	92	98
16	C	75/75 (100%)	75 (100%)	0	100	100
All	All	7788/9950 (78%)	7772 (100%)	16 (0%)	93	98

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	N	221	CYS
4	N	227	ASP
4	N	230	GLN
4	N	540	ARG
4	N	580	LYS
4	N	687	MET
5	I	332	LYS
5	I	615	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	O	167	LYS
7	S	401	CYS
7	S	403	PHE
7	S	414	HIS
13	Y	88	PHE
13	Y	108	LYS
13	Z	264	LYS
15	R	86	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	146	GLN
4	N	230	GLN
4	N	245	GLN
4	N	329	GLN
4	N	517	ASN
4	N	571	ASN
4	N	701	GLN
4	N	702	GLN
5	I	292	GLN
5	I	604	HIS
5	I	613	ASN
5	I	668	GLN
5	I	720	GLN
6	O	693	ASN
7	S	414	HIS
8	K	12	GLN
8	K	125	GLN
12	J	98	ASN
12	J	455	GLN
8	Q	88	GLN
13	Y	50	HIS
13	Y	83	HIS
13	Y	95	ASN
13	Y	421	ASN
13	Y	458	GLN
13	Y	541	ASN
14	U	236	HIS
14	U	555	GLN
14	U	559	GLN
14	V	71	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	V	242	GLN
14	V	447	ASN
15	R	295	GLN
15	R	310	GLN
15	R	435	GLN
16	C	71	GLN
16	C	72	HIS
16	C	78	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

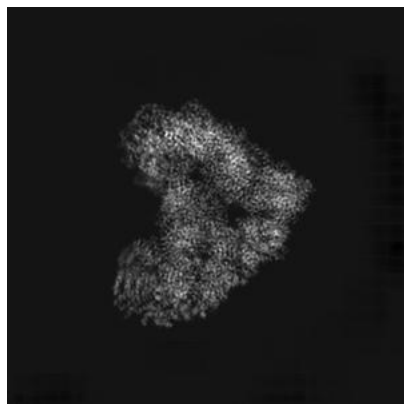
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13931. These allow visual inspection of the internal detail of the map and identification of artifacts.

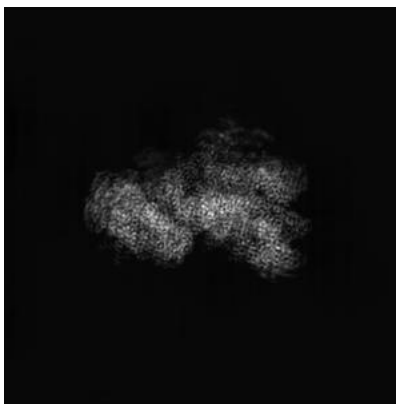
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

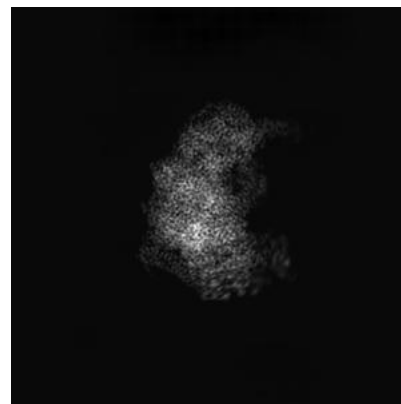
6.1.1 Primary map



X

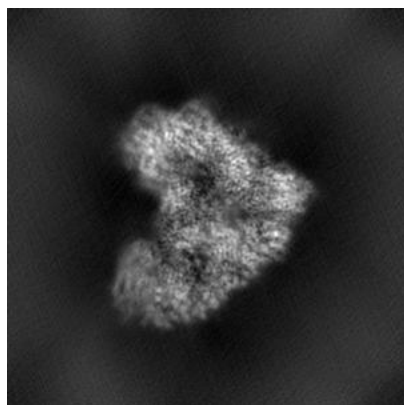


Y

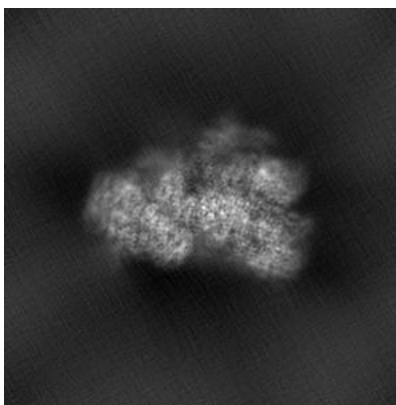


Z

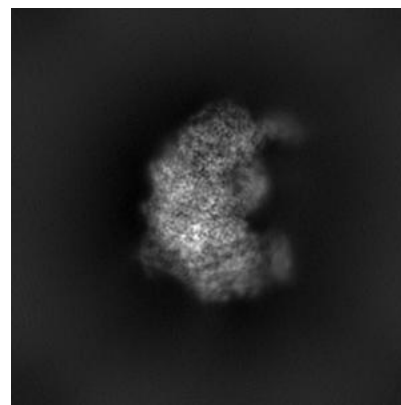
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180

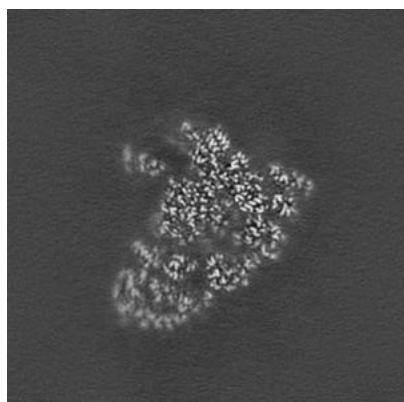


Y Index: 180

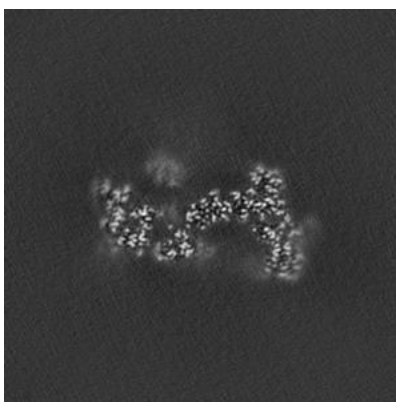


Z Index: 180

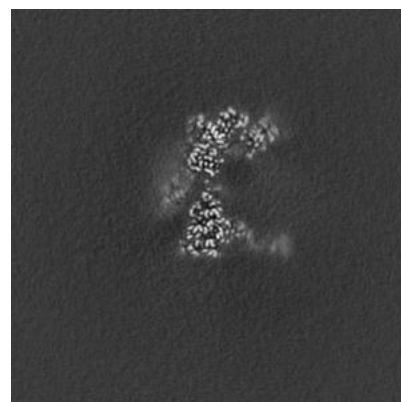
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

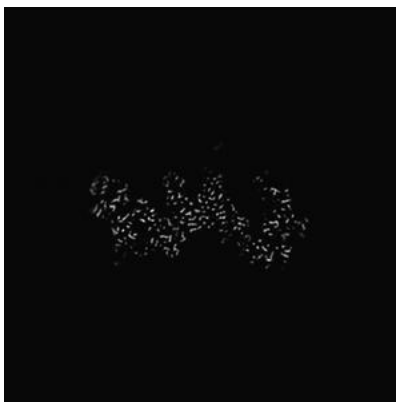
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 175

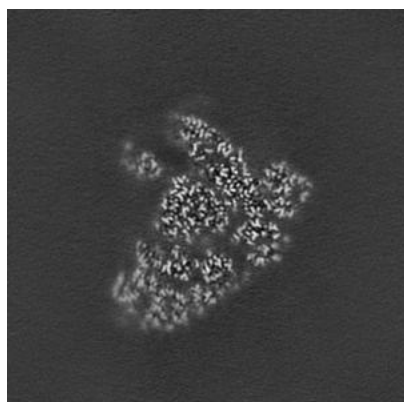


Y Index: 160

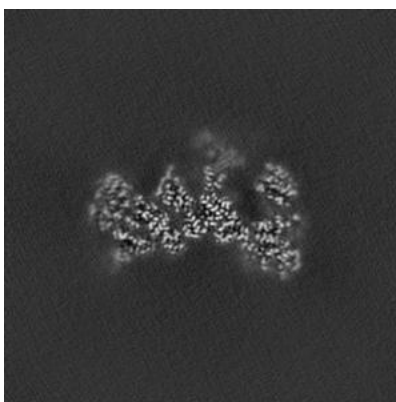


Z Index: 233

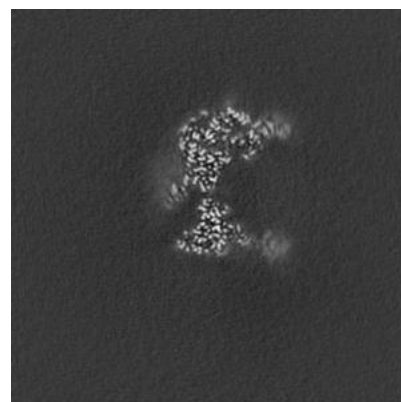
6.3.2 Raw map



X Index: 175



Y Index: 154



Z Index: 188

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

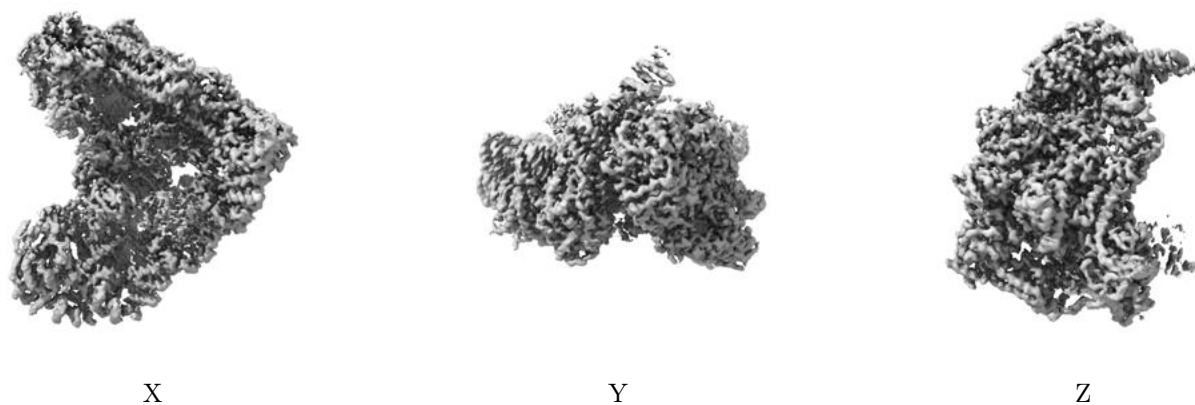
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

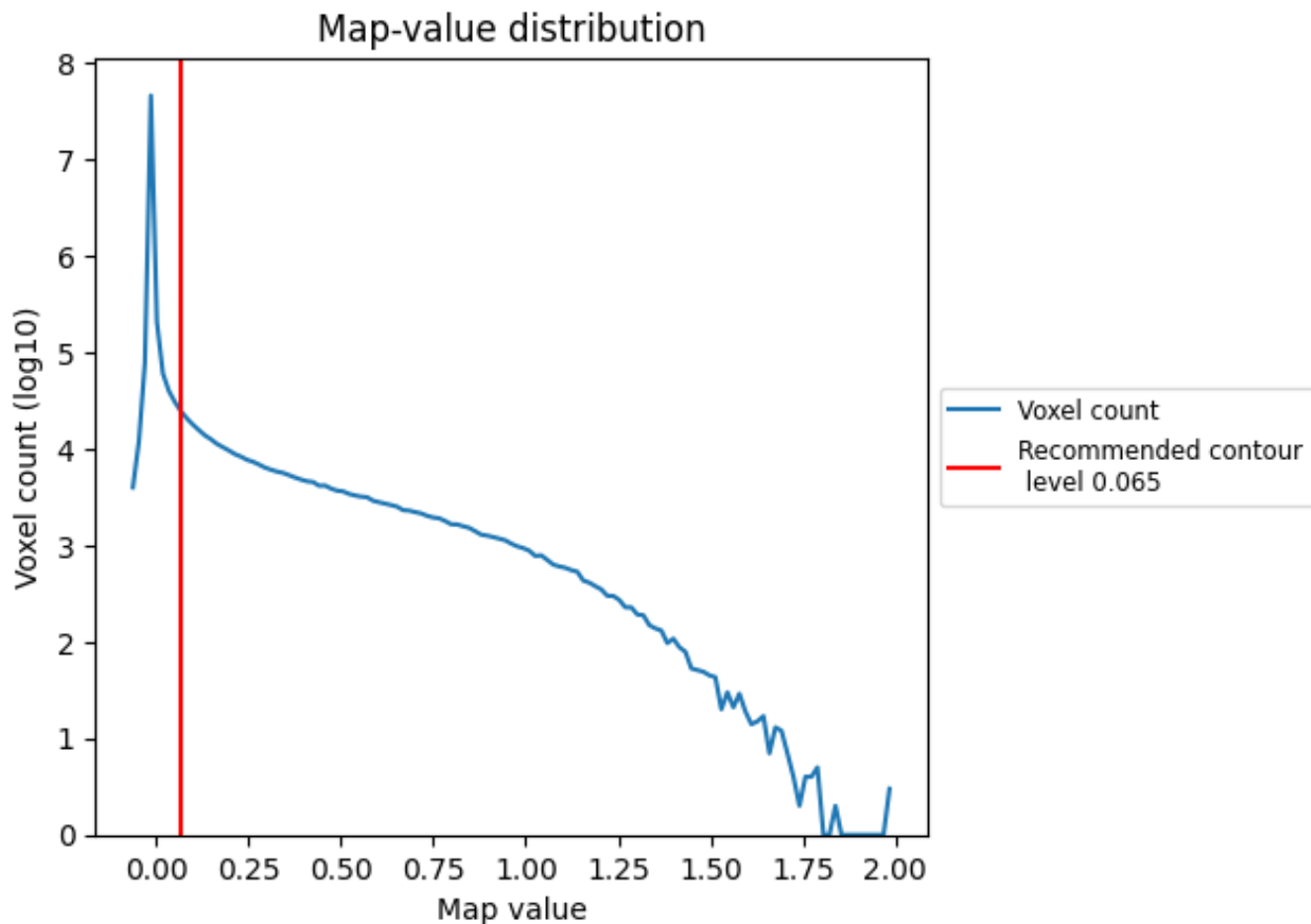
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

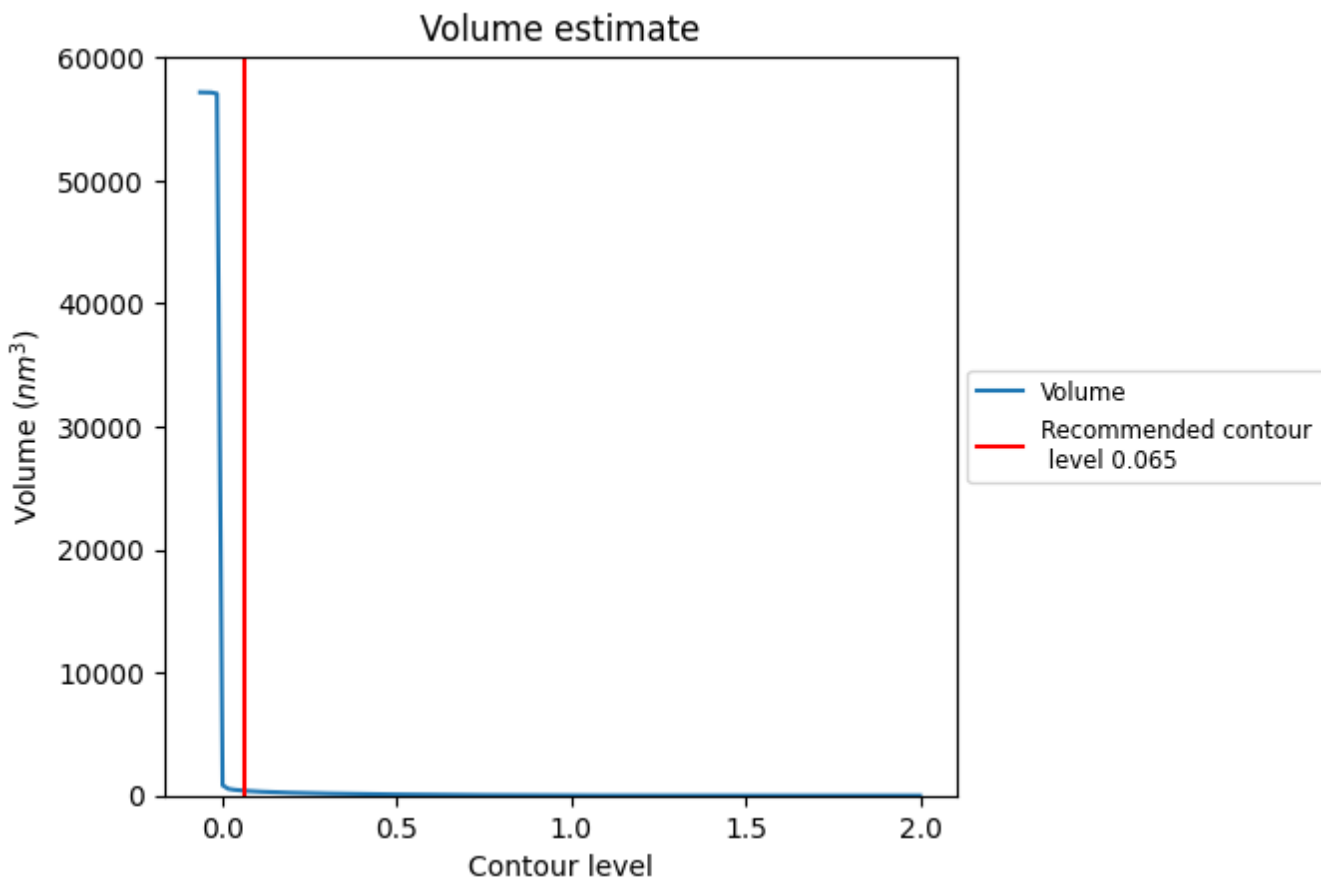
This section contains the results of statistical analysis of the map.

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.

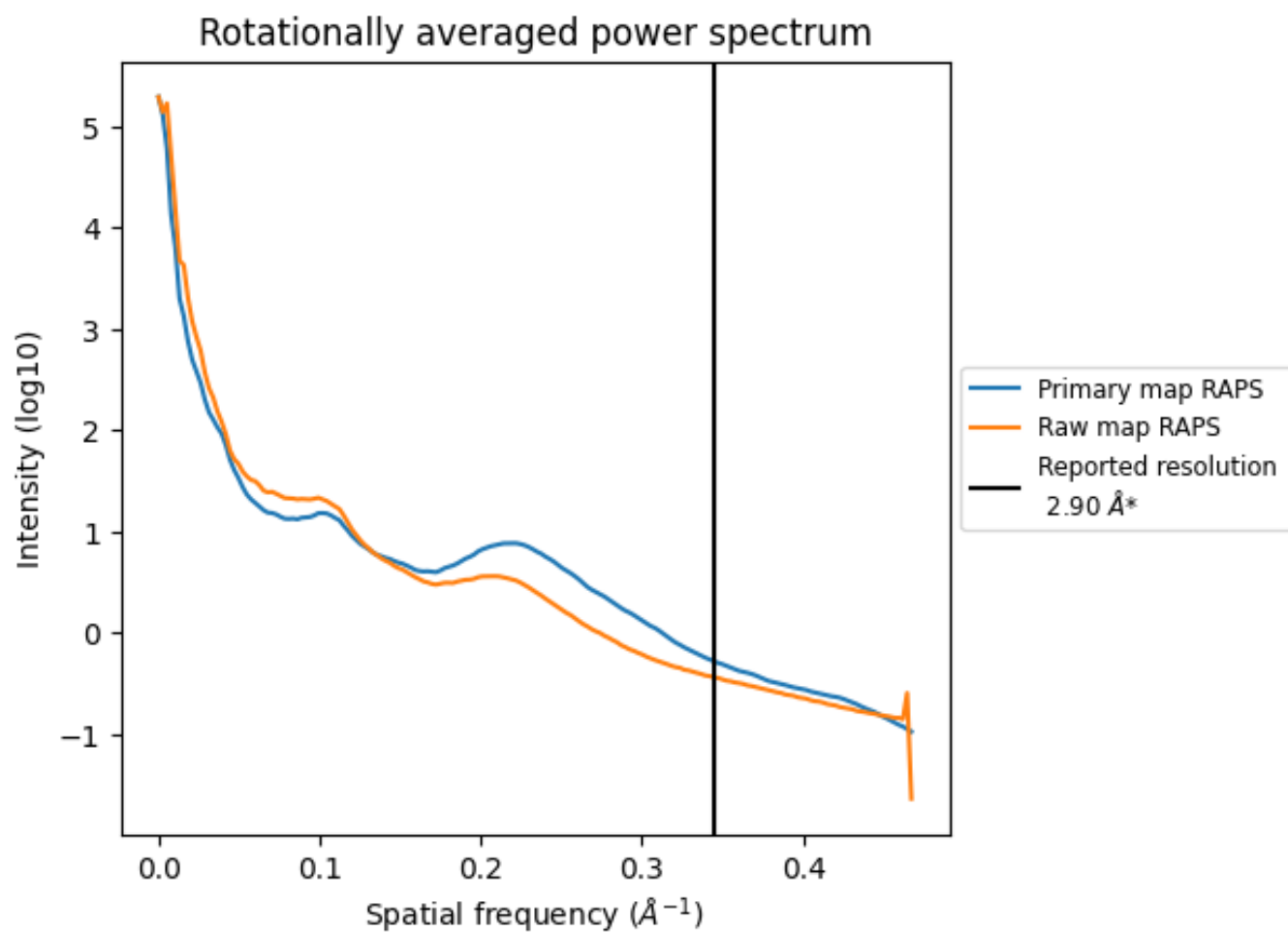
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 392 nm³; this corresponds to an approximate mass of 354 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 [i](#)

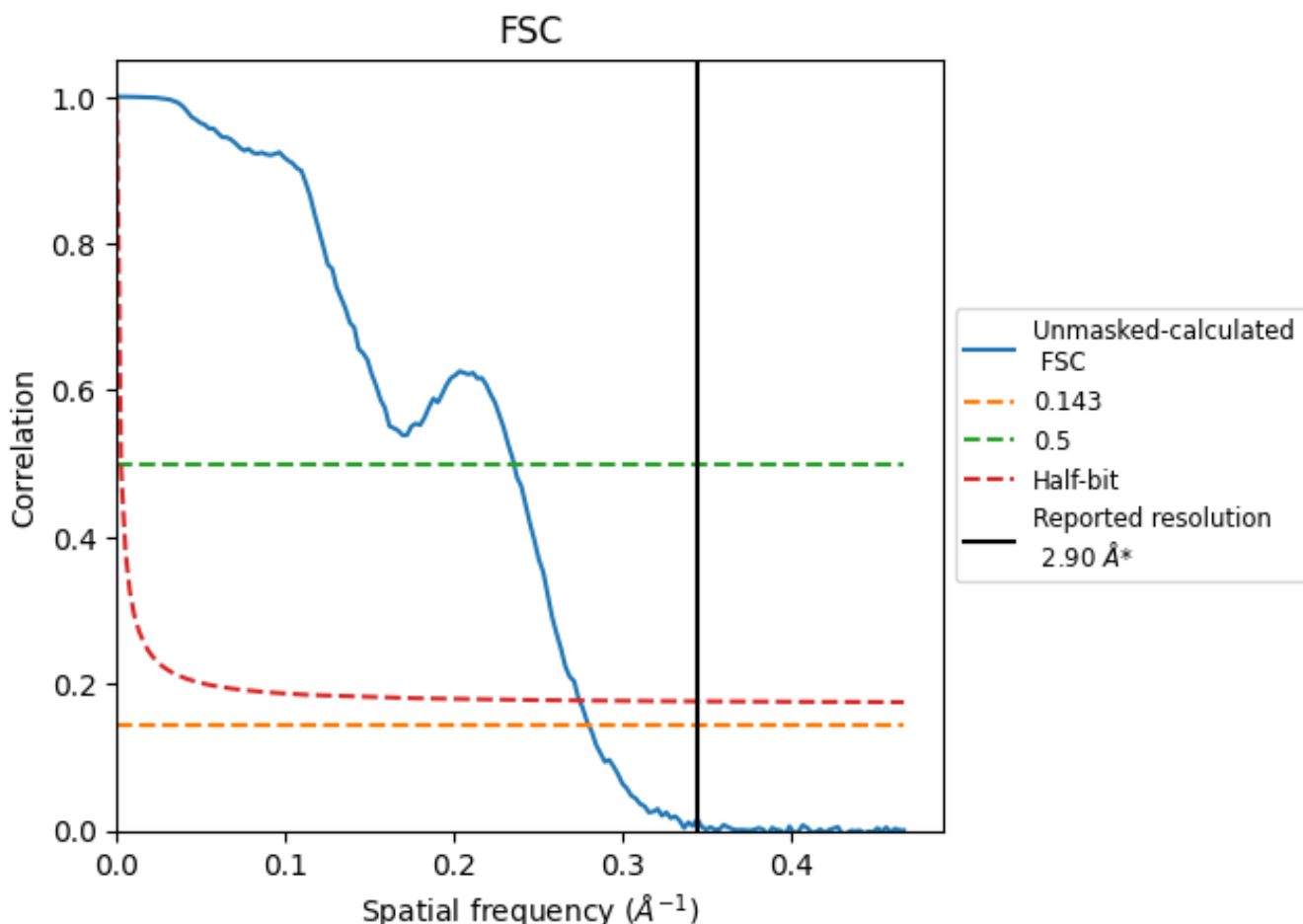


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

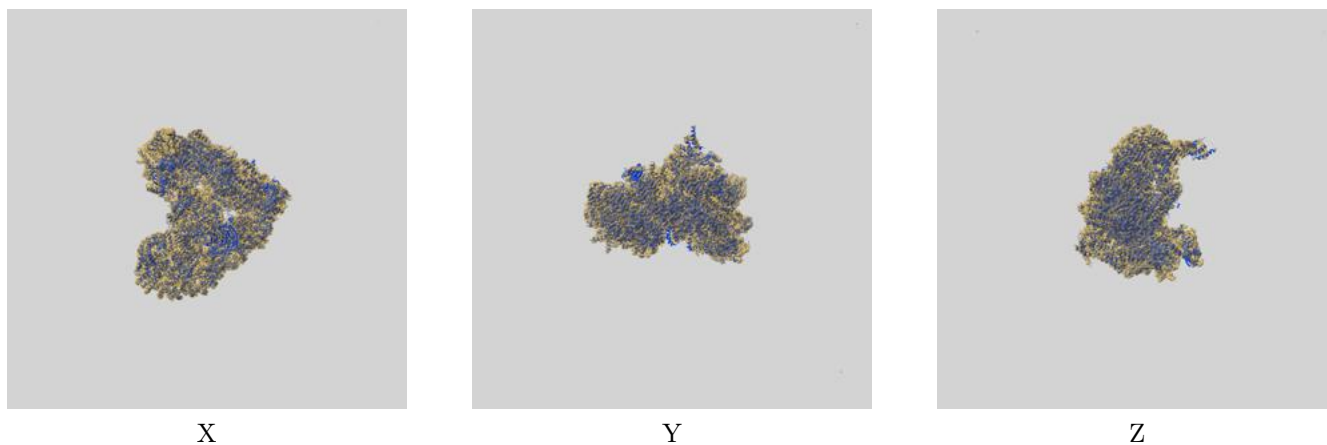
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.57	4.24	3.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.57 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

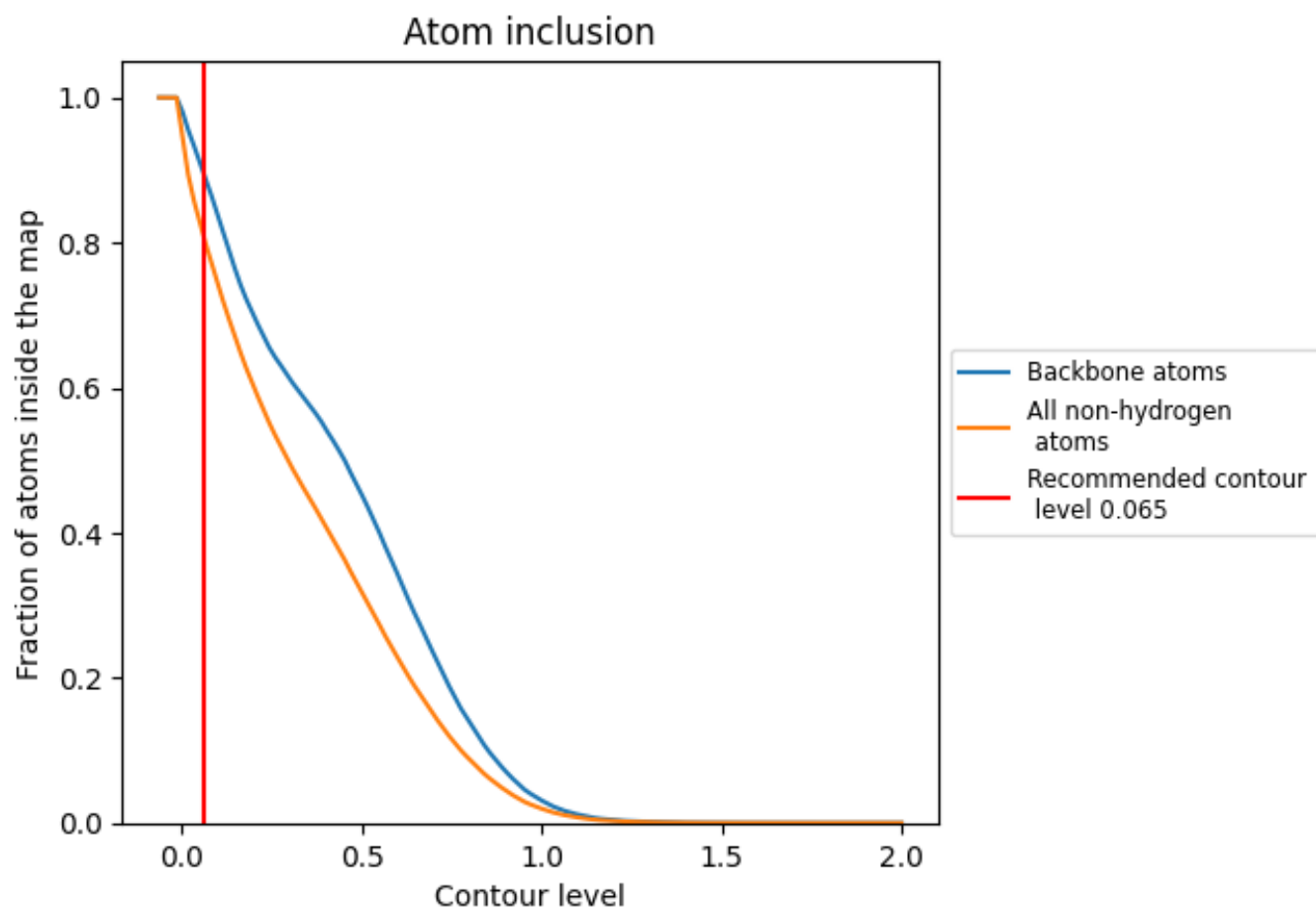
This section contains information regarding the fit between EMDB map EMD-13931 and PDB model 7QE7. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.065 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 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.