Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 12:17 pm GMT

PDB ID	:	6Q6H
EMDB ID	:	EMD-4466
Title	:	Cryo-EM structure of the APC/C-Cdc20-Cdk2-cyclinA2-Cks2 complex, the D2 box class
Authors	:	Zhang, S.; Barford, D.
Deposited on	:	2018-12-11
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

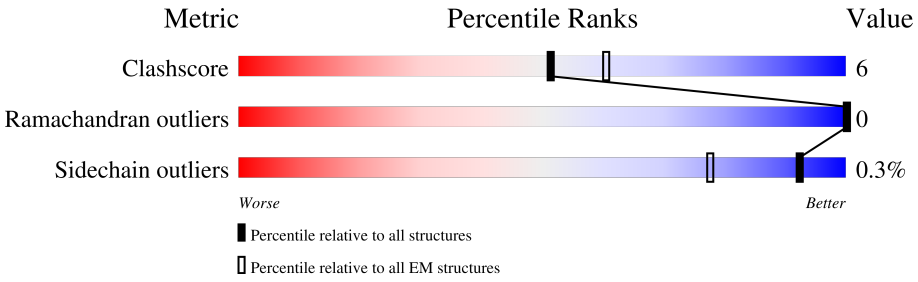
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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.



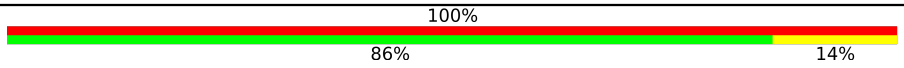
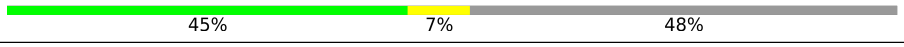
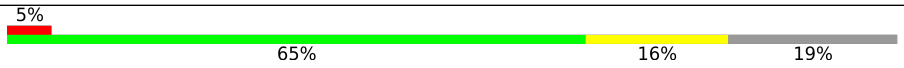
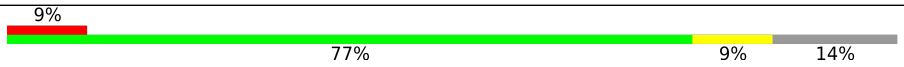
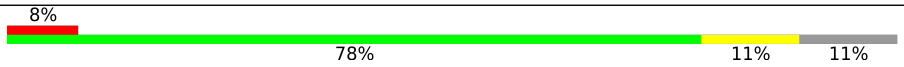
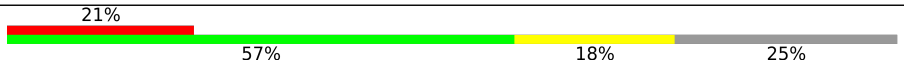
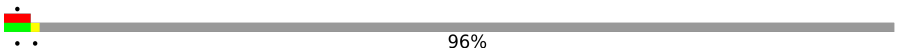
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	76% 21%
2	D	121	40% 6% 54%
3	A	1855	68% 16% 16%
4	N	822	35% 64% 16% 21%
5	I	808	9% 75% 15% 10%
6	O	755	5% 81% 12% 7%
7	K	620	73% 11% 16%
7	Q	620	72% 9% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	C	84	
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	499	
16	S	394	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 67944 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	179	1446	906	263	270	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 Apc1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	1551	12131	7785	2041	2222	83	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	653	5238	3337	932	944	25	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	729	5752	3685	956	1077	34	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	O	703	5532	3529	963	1011	29	0	0

- Molecule 7 is a protein called Cell division cycle protein 16 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	518	Total	C	N	O	S	0	0
			4187	2694	704	764	25		
7	Q	504	Total	C	N	O	S	0	0
			4055	2606	684	741	24		

- Molecule 8 is a protein called Anaphase-promoting complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	84	Total	C	N	O	S	0	0
			657	418	120	103	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	27	Total	C	N	O	S	0	0
			226	142	42	41	1		
9	W	26	Total	C	N	O	S	0	0
			225	142	42	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	61	Total	C	N	O	S	0	0
			499	314	81	102	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	57	Total	C	N	O	S	0	0
			459	296	75	86	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	496	Total	C	N	O	S	0	0
			3964	2547	668	723	26		
12	P	484	Total	C	N	O	S	0	0
			3883	2497	653	707	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	499	Total	C	N	O	S	1	0
			3911	2474	682	728	27		
13	Z	486	Total	C	N	O	S	1	0
			3807	2413	664	705	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	515	Total	C	N	O	S	0	0
			4160	2678	700	758	24		
14	V	530	Total	C	N	O	S	0	0
			4311	2778	720	789	24		

- Molecule 15 is a protein called Cell division cycle protein 20 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	375	Total	C	N	O	S	2	0
			2897	1818	529	538	12		

- Molecule 16 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	S	17	Total	C	N	O	0	0
			134	83	22	29		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	?	-	ASN	deletion	UNP P20248
S	?	-	PRO	deletion	UNP P20248
S	?	-	GLU	deletion	UNP P20248
S	?	-	LYS	deletion	UNP P20248
S	?	-	ALA	deletion	UNP P20248
S	?	-	ALA	deletion	UNP P20248
S	?	-	PRO	deletion	UNP P20248
S	?	-	VAL	deletion	UNP P20248
S	?	-	GLN	deletion	UNP P20248
S	?	-	GLN	deletion	UNP P20248
S	?	-	PRO	deletion	UNP P20248
S	?	-	ARG	deletion	UNP P20248
S	?	-	THR	deletion	UNP P20248
S	?	-	ARG	deletion	UNP P20248
S	?	-	ALA	deletion	UNP P20248

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
S	?	-	ALA	deletion	UNP P20248
S	?	-	LEU	deletion	UNP P20248
S	?	-	ALA	deletion	UNP P20248
S	?	-	VAL	deletion	UNP P20248
S	?	-	LEU	deletion	UNP P20248
S	?	-	LYS	deletion	UNP P20248
S	?	-	SER	deletion	UNP P20248
S	?	-	GLY	deletion	UNP P20248
S	?	-	ASN	deletion	UNP P20248
S	?	-	PRO	deletion	UNP P20248
S	?	-	ARG	deletion	UNP P20248
S	?	-	GLY	deletion	UNP P20248
S	?	-	LEU	deletion	UNP P20248
S	?	-	ALA	deletion	UNP P20248
S	?	-	GLN	deletion	UNP P20248
S	?	-	GLN	deletion	UNP P20248
S	?	-	GLN	deletion	UNP P20248
S	?	-	ARG	deletion	UNP P20248
S	?	-	PRO	deletion	UNP P20248
S	?	-	LYS	deletion	UNP P20248
S	?	-	THR	deletion	UNP P20248
S	?	-	ARG	deletion	UNP P20248
S	?	-	ARG	deletion	UNP P20248

3 Residue-property plots (i)

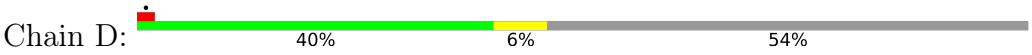
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

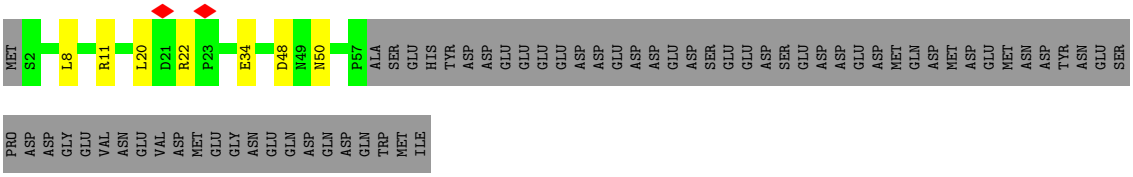
• Molecule 1: Anaphase-promoting complex subunit 10

Chain L:

• Molecule 2: Anaphase-promoting complex subunit 15

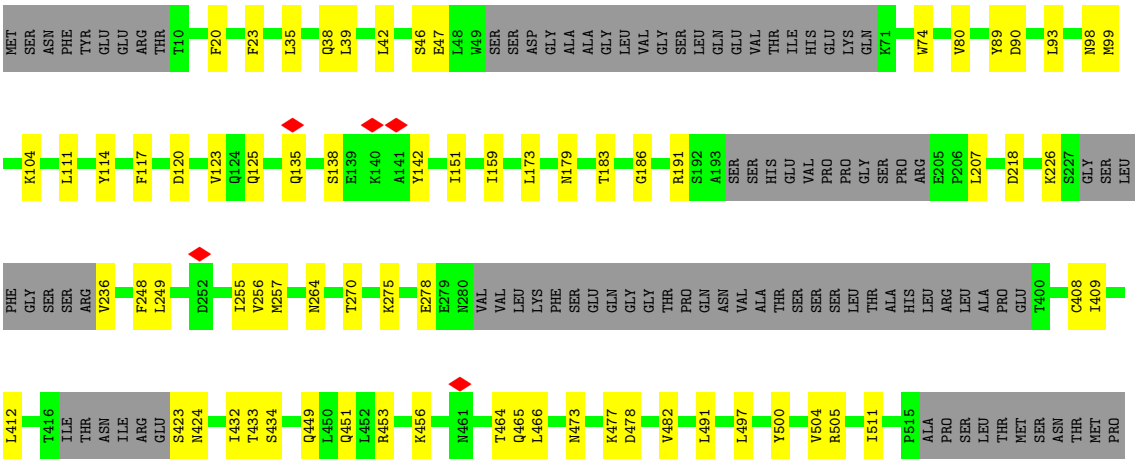
Chain D:

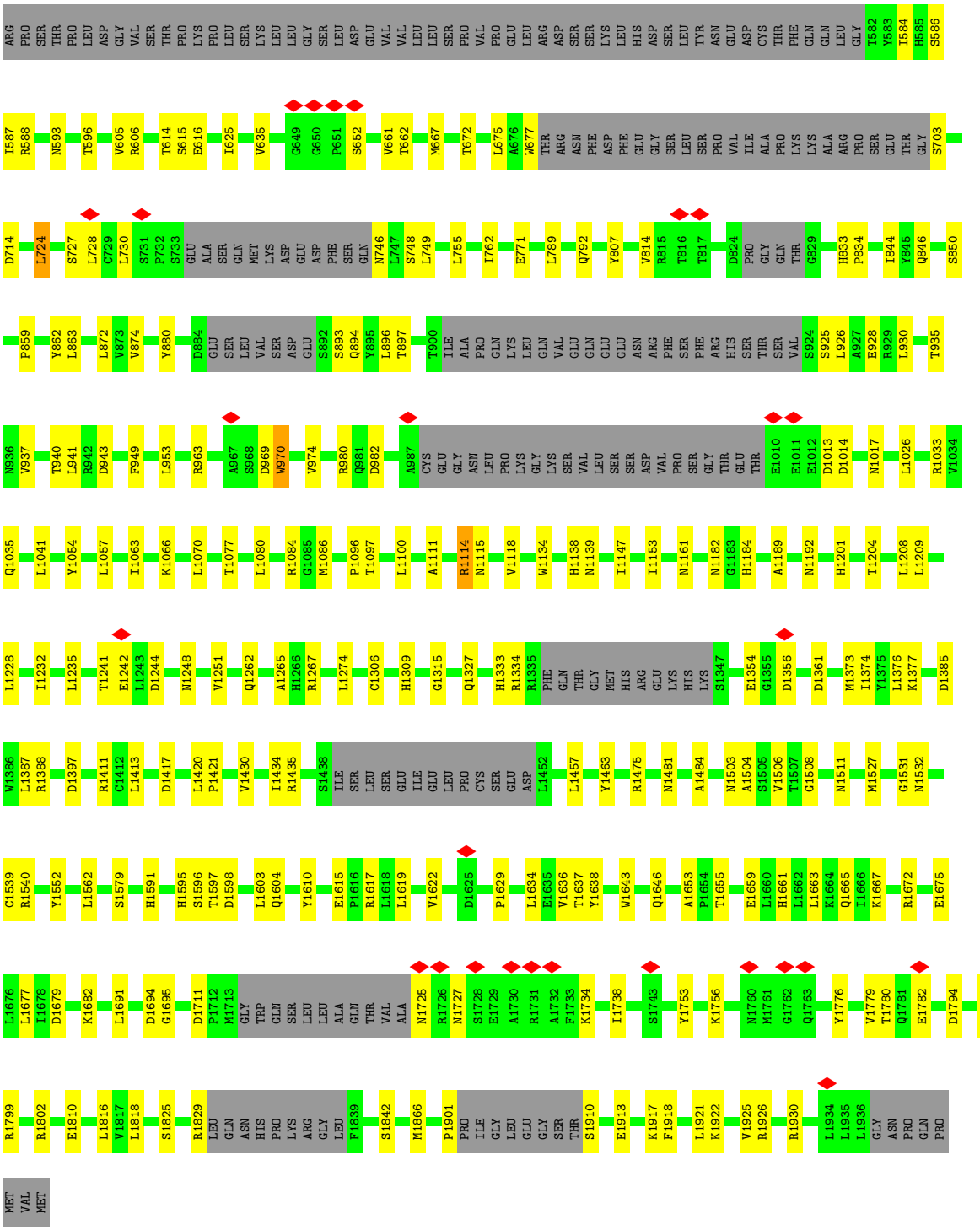




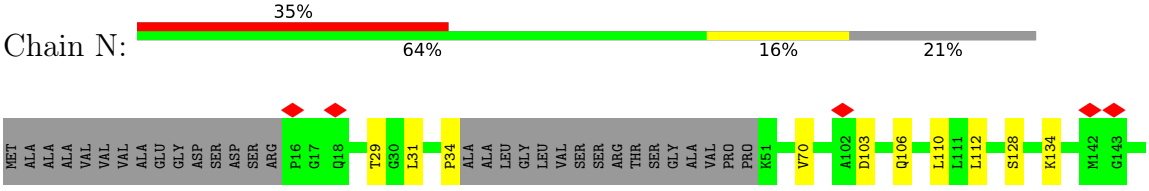
• Molecule 3: Apc1

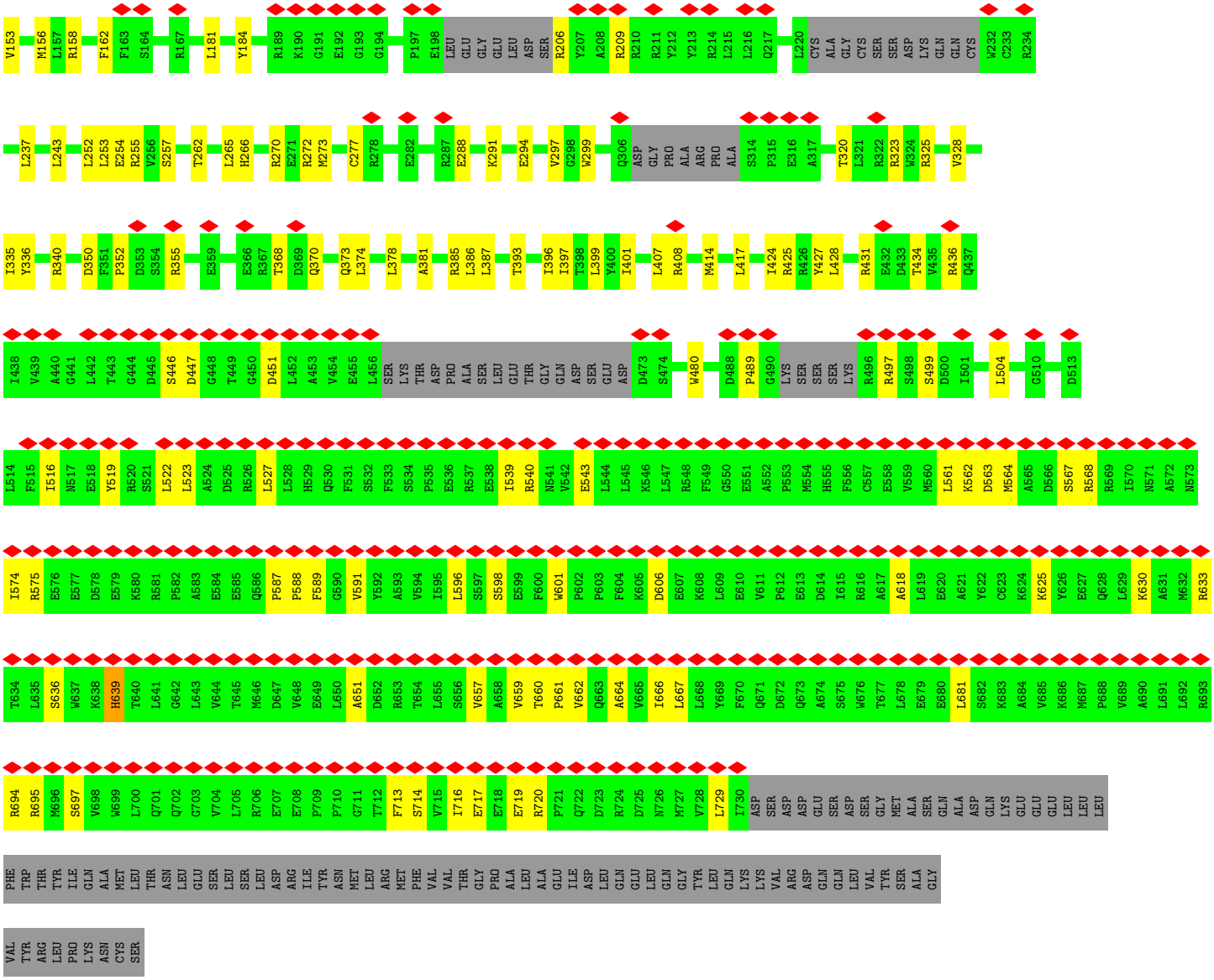
Chain A:





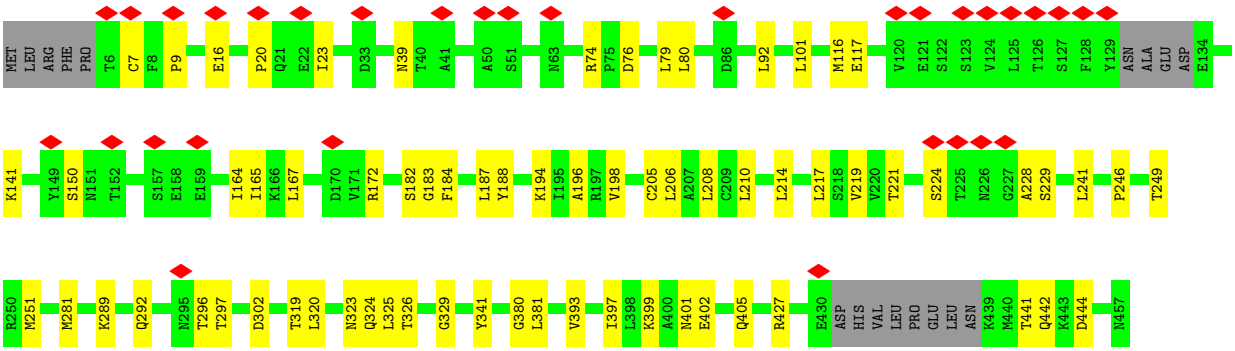
• Molecule 4: Anaphase-promoting complex subunit 2

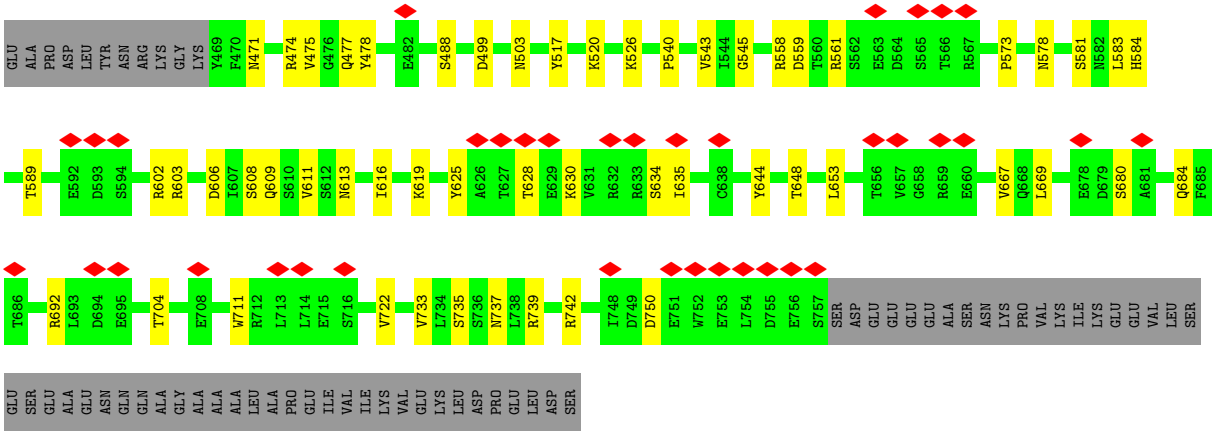




• Molecule 5: Anaphase-promoting complex subunit 4

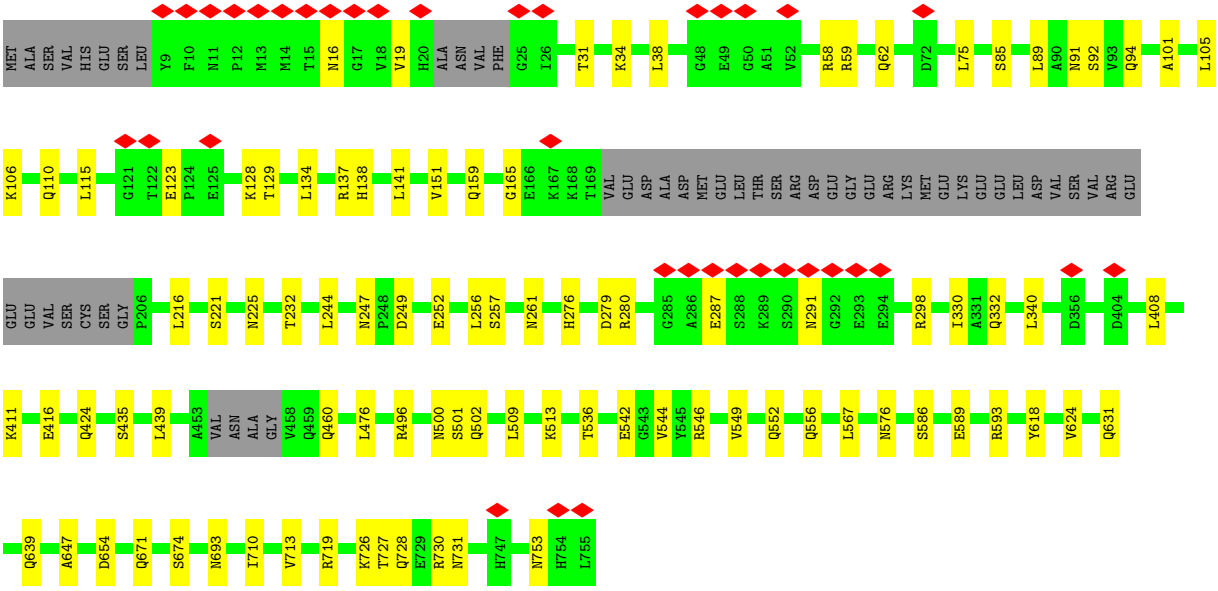
Chain I:





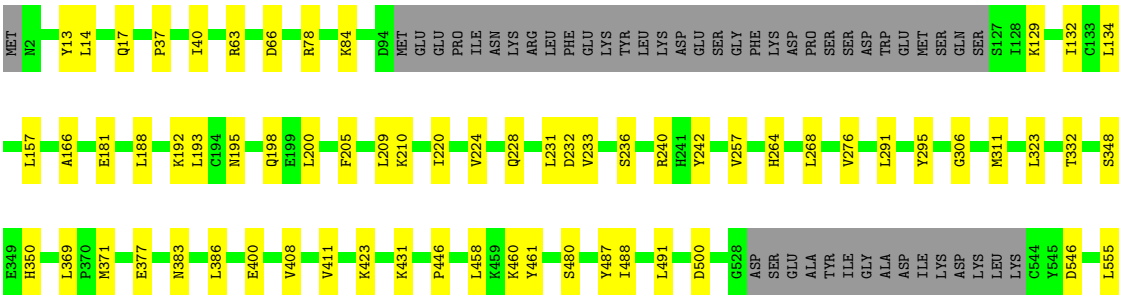
• Molecule 6: Anaphase-promoting complex subunit 5

Chain O:



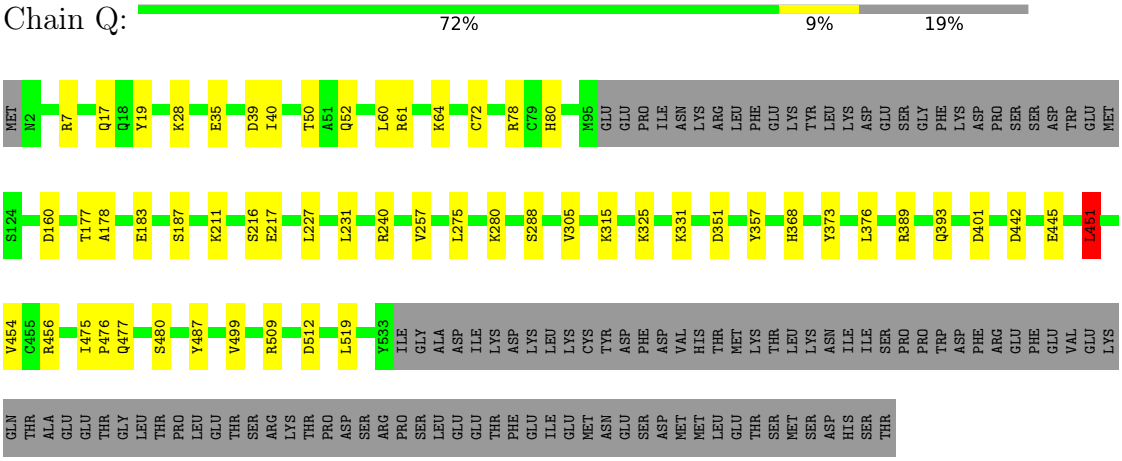
• Molecule 7: Cell division cycle protein 16 homolog

Chain K:



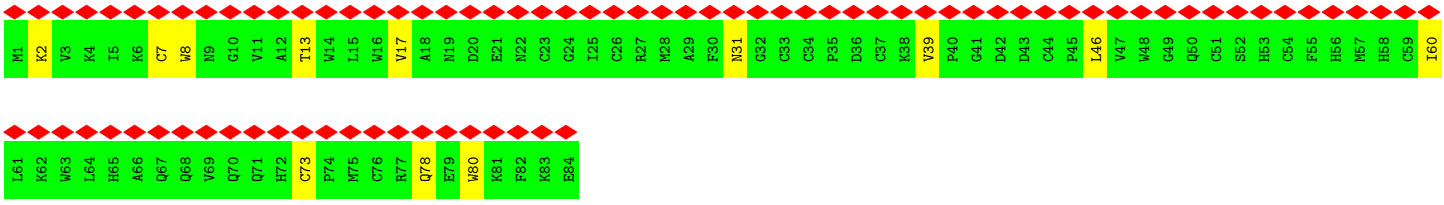
• Molecule 7: Cell division cycle protein 16 homolog

Chain Q:



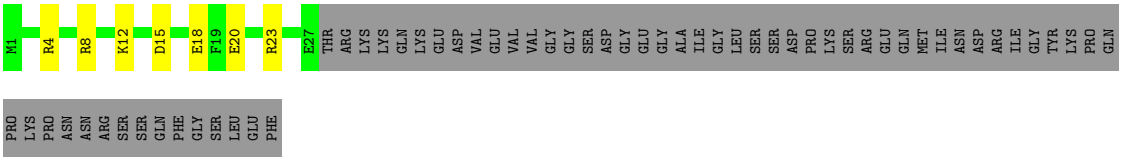
• Molecule 8: Anaphase-promoting complex subunit 11

Chain C:



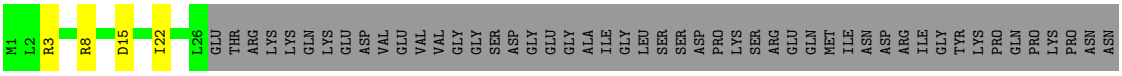
• Molecule 9: Anaphase-promoting complex subunit CDC26

Chain G:



• Molecule 9: Anaphase-promoting complex subunit CDC26

Chain W:

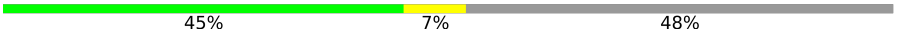


• Molecule 10: Anaphase-promoting complex subunit 13

Chain M:

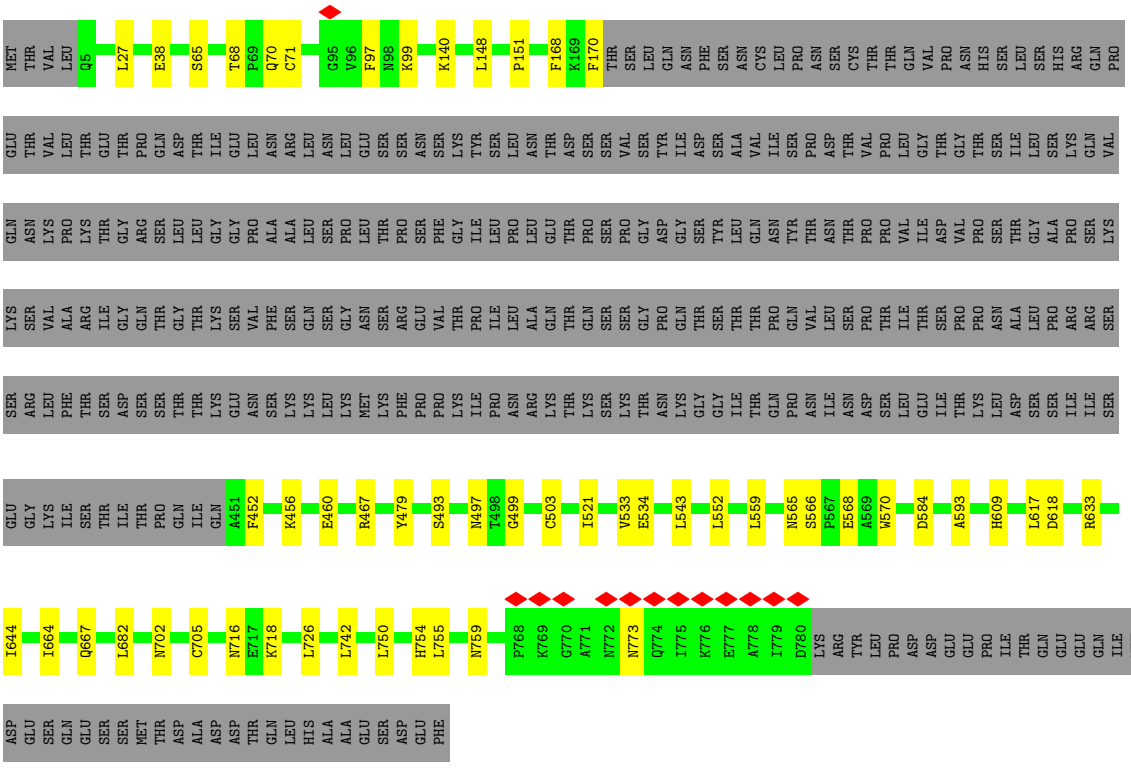
• Molecule 11: Anaphase-promoting complex subunit 16

Chain H:



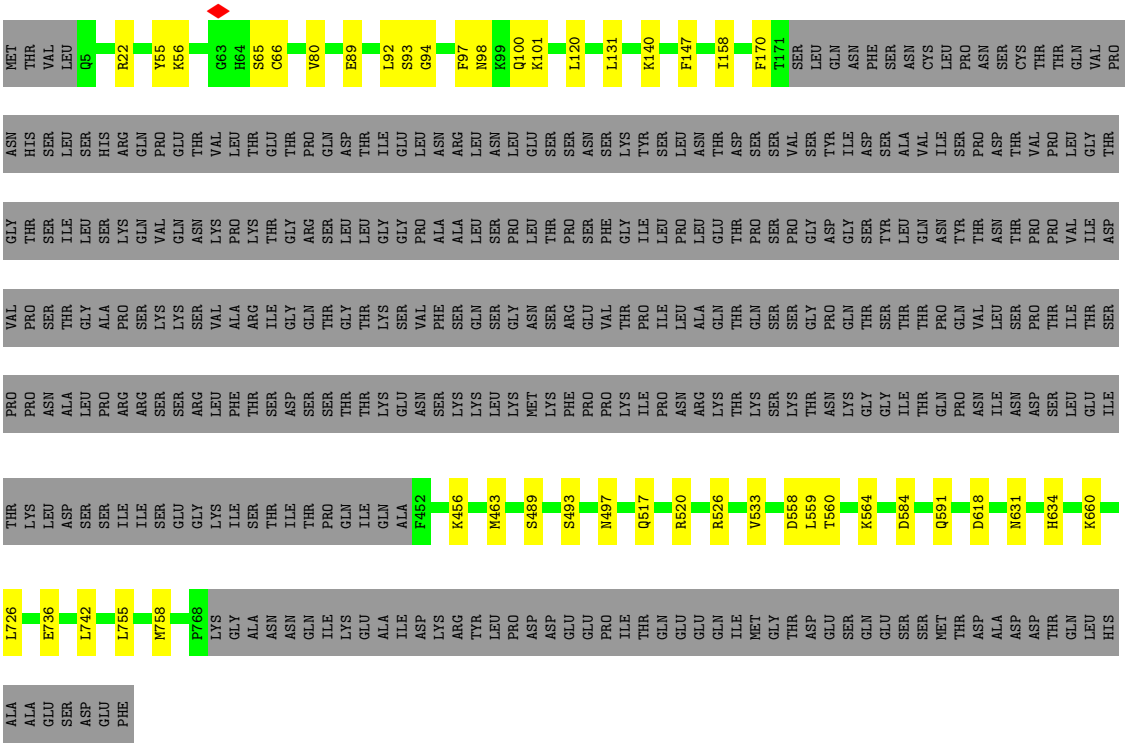
• Molecule 12: Cell division cycle protein 27 homolog

Chain J:



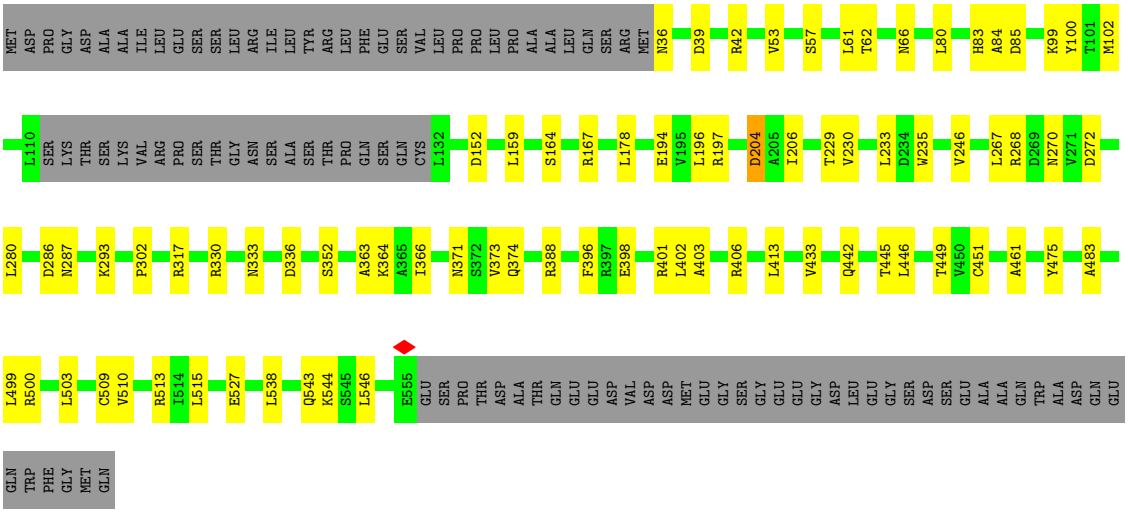
• Molecule 12: Cell division cycle protein 27 homolog

Chain P:



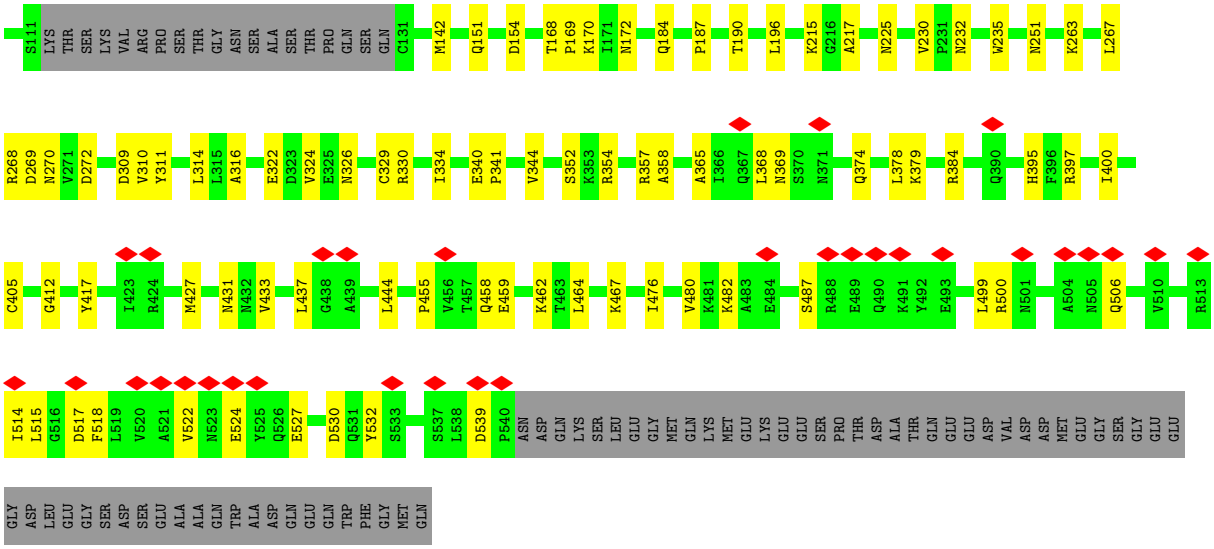
• Molecule 13: Anaphase-promoting complex subunit 7

Chain Y:



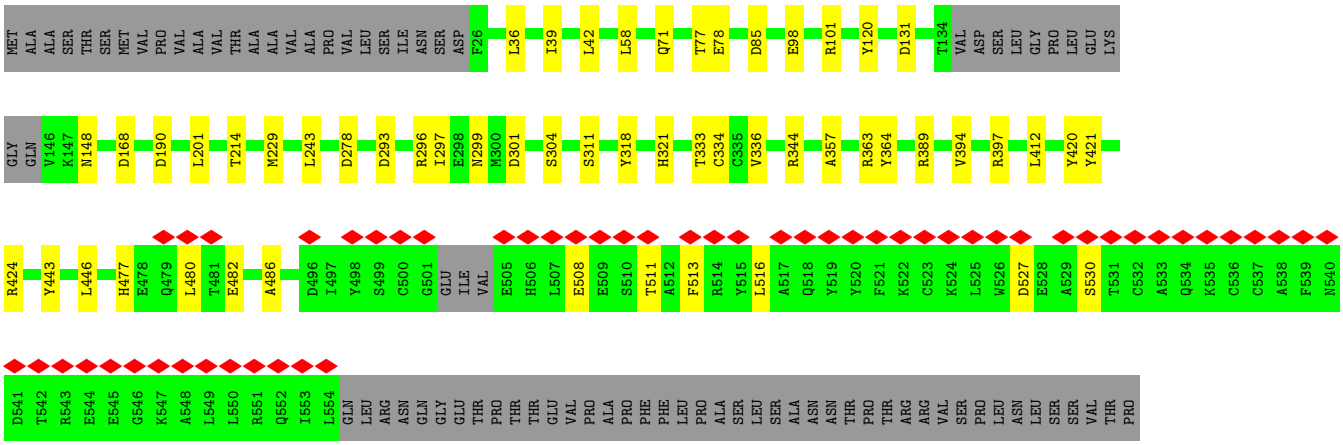
• Molecule 13: Anaphase-promoting complex subunit 7

Chain Z:



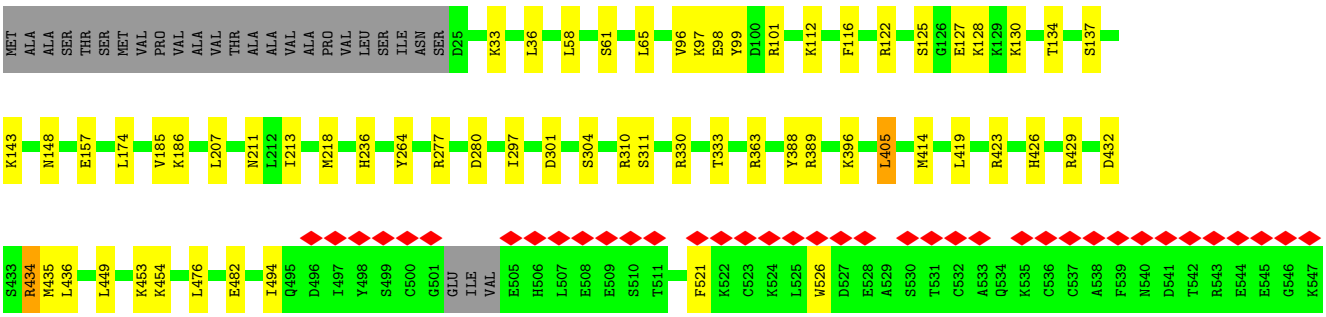
• Molecule 14: Cell division cycle protein 23 homolog

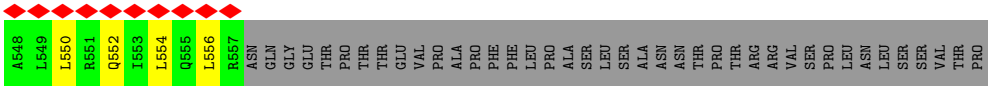
Chain U:



• Molecule 14: Cell division cycle protein 23 homolog

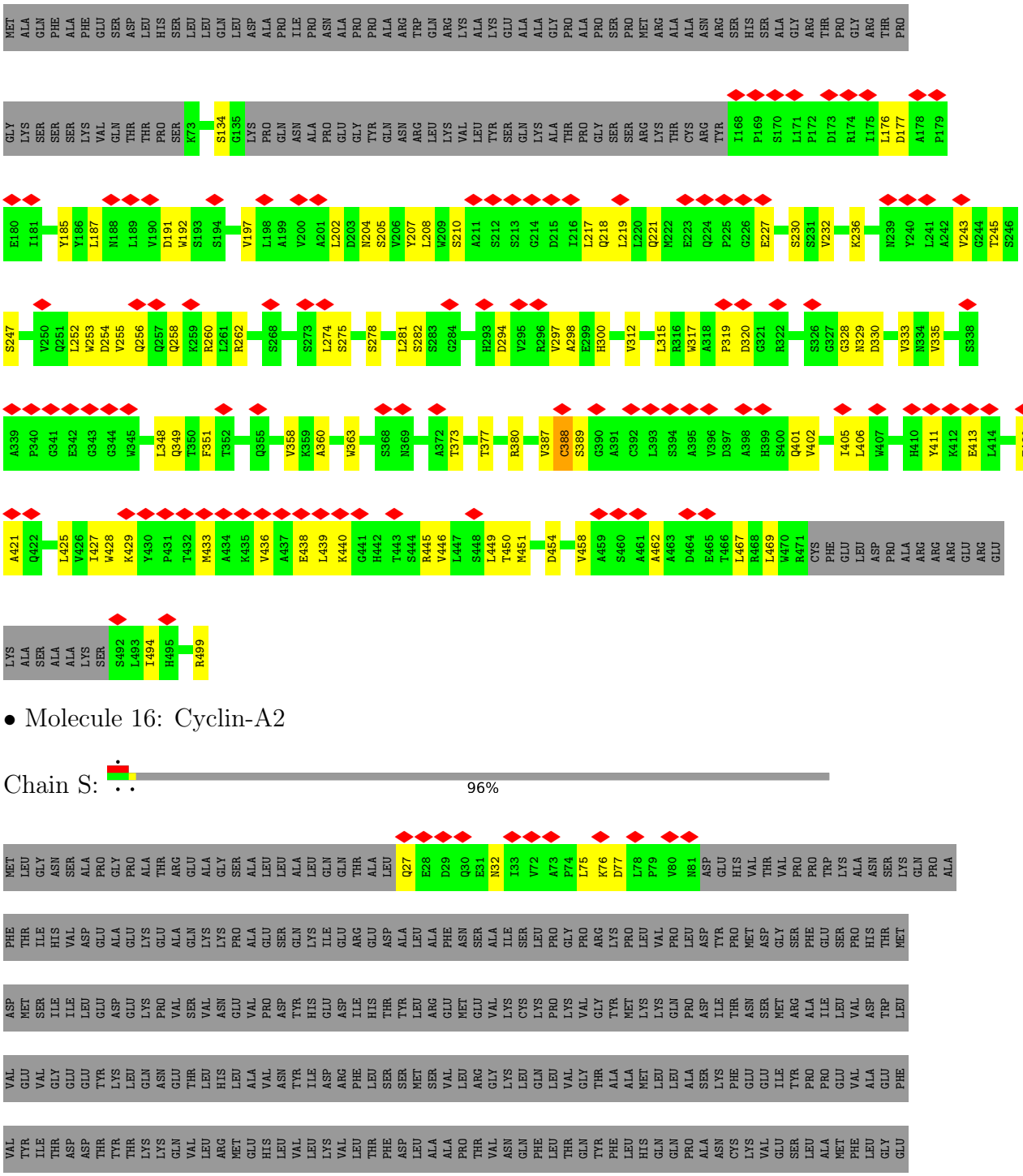
Chain V:





• Molecule 15: Cell division cycle protein 20 homolog

Chain R:



• Molecule 16: Cyclin-A2

Chain S:


LEU SER LEU ILE ASP ALA ASP PRO TYR LEU LYS TYR LEU PRO SER VAL ILE ALA GLY ALA ALA PHE HIS LEU ALA LEU TYR THR VAL THR GLY GLN SER TRP PRO GLU SER LEU ILE ARG LYS THR GLY TYR THR LEU GLU SER LEU LYS PRO CYS LEU MET ASP LEU HIS GLN THR TYR


LEU LYS ALA PRO GLN HIS ALA GLN GLN SER ILE ARG GLU LYS TYR LYS ASN SER LYS TYR HIS GLY VAL SER LEU LEU ASN PRO PRO GLU THR LEU ASN LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	117044	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 ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.016	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	418.80002, 418.80002, 418.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	L	0.38	0/1480	0.53	0/2005
2	D	0.33	0/485	0.51	0/662
3	A	0.38	1/12411 (0.0%)	0.56	6/16877 (0.0%)
4	N	0.29	0/5343	0.56	1/7236 (0.0%)
5	I	0.32	0/5871	0.52	1/7954 (0.0%)
6	O	0.36	0/5634	0.50	0/7612
7	K	0.38	0/4291	0.50	0/5812
7	Q	0.42	0/4154	0.52	2/5627 (0.0%)
8	C	0.28	0/680	0.56	1/921 (0.1%)
9	G	0.35	0/227	0.46	0/302
9	W	0.33	0/226	0.51	0/299
10	M	0.37	0/508	0.52	0/689
11	H	0.39	0/468	0.48	0/631
12	J	0.42	0/4058	0.47	0/5485
12	P	0.44	0/3975	0.47	0/5371
13	Y	0.34	0/3974	0.53	4/5369 (0.1%)
13	Z	0.33	0/3870	0.52	1/5233 (0.0%)
14	U	0.38	0/4255	0.48	1/5753 (0.0%)
14	V	0.41	0/4409	0.49	1/5958 (0.0%)
15	R	0.30	0/2969	0.56	1/4038 (0.0%)
16	S	0.29	0/134	0.58	0/181
All	All	0.37	1/69422 (0.0%)	0.52	19/94015 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	2
4	N	0	1
6	O	0	1
15	R	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
16	S	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1591	HIS	C-N	-5.06	1.22	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Q	442	ASP	CB-CG-OD1	10.05	127.35	118.30
3	A	120	ASP	CB-CG-OD1	8.10	125.59	118.30
3	A	728	LEU	CA-CB-CG	7.81	133.26	115.30
13	Z	334	ILE	CG1-CB-CG2	-7.05	95.89	111.40
3	A	1694	ASP	CB-CG-OD1	7.03	124.63	118.30
5	I	325	LEU	CA-CB-CG	6.94	131.27	115.30
3	A	1356	ASP	CB-CG-OD1	6.74	124.36	118.30
13	Y	204	ASP	CB-CG-OD2	6.70	124.33	118.30
7	Q	451	LEU	CA-CB-CG	6.70	130.71	115.30
3	A	724	LEU	CA-CB-CG	6.65	130.59	115.30
3	A	1596	SER	C-N-CA	5.95	136.58	121.70
13	Y	233	LEU	CA-CB-CG	5.87	128.80	115.30
14	U	243	LEU	CA-CB-CG	5.72	128.46	115.30
4	N	522	LEU	CA-CB-CG	5.69	128.38	115.30
14	V	405	LEU	CB-CG-CD2	-5.58	101.52	111.00
13	Y	336	ASP	CB-CG-OD1	5.51	123.26	118.30
13	Y	267	LEU	CA-CB-CG	5.27	127.42	115.30
15	R	252	LEU	CA-CB-CG	5.24	127.35	115.30
8	C	60	ILE	CG1-CB-CG2	-5.02	100.35	111.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	969	ASP	Peptide
3	A	970	TRP	Peptide
4	N	630	LYS	Peptide
6	O	123	GLU	Peptide
15	R	202	LEU	Peptide
16	S	76	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1446	0	1423	23	0
2	D	470	0	458	6	0
3	A	12131	0	12059	178	0
4	N	5238	0	5220	77	0
5	I	5752	0	5680	77	0
6	O	5532	0	5570	61	0
7	K	4187	0	4099	45	0
7	Q	4055	0	3959	40	0
8	C	657	0	611	7	0
9	G	226	0	233	6	0
9	W	225	0	242	6	0
10	M	499	0	469	4	0
11	H	459	0	449	7	0
12	J	3964	0	3903	37	0
12	P	3883	0	3836	29	0
13	Y	3911	0	3986	49	0
13	Z	3807	0	3885	65	0
14	U	4160	0	4038	34	0
14	V	4311	0	4237	43	0
15	R	2897	0	2789	60	0
16	S	134	0	129	4	0
All	All	67944	0	67275	777	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 6.

All (777) 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)
7:K:205:PHE:O	7:K:209:LEU:HB2	1.85	0.77
4:N:273:MET:O	4:N:277:CYS:HB2	1.88	0.71
13:Y:66:ASN:HD21	13:Z:269:ASP:H	1.38	0.71
3:A:1638:TYR:O	3:A:1646:GLN:HA	1.93	0.69
15:R:208:LEU:HB3	15:R:217:LEU:HB2	1.75	0.67
12:P:80:VAL:HG11	12:P:120:LEU:HD11	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:103:ASP:HB3	4:N:106:GLN:HB2	1.77	0.65
5:I:625:TYR:HB2	5:I:628:THR:HG22	1.79	0.65
5:I:644:TYR:HB3	5:I:648:THR:HG23	1.78	0.65
13:Y:53:VAL:O	13:Y:57:SER:HB3	1.97	0.65
4:N:633:ARG:HD3	8:C:17:VAL:HG22	1.78	0.64
15:R:245:THR:HG23	15:R:247:SER:H	1.62	0.64
3:A:862:TYR:HB2	3:A:896:LEU:HD22	1.78	0.64
3:A:1097:THR:HG23	6:O:340:LEU:HB3	1.80	0.64
1:L:24:GLU:HG3	1:L:26:GLY:H	1.63	0.64
5:I:380:GLY:HA3	5:I:543:VAL:HG11	1.79	0.64
6:O:542:GLU:OE2	6:O:546:ARG:NH1	2.31	0.63
15:R:176:LEU:HB2	15:R:467:LEU:HB2	1.80	0.63
3:A:1376:LEU:HD23	3:A:1377:LYS:HG3	1.79	0.63
4:N:523:LEU:O	4:N:527:LEU:HB2	1.99	0.62
4:N:262:THR:O	4:N:266:HIS:ND1	2.33	0.62
6:O:593:ARG:HG2	6:O:753:ASN:HB3	1.82	0.61
15:R:333:VAL:HB	15:R:351:PHE:HB2	1.80	0.61
12:J:456:LYS:O	12:J:460:GLU:HB2	2.00	0.61
12:J:702:ASN:ND2	12:J:705:CYS:SG	2.72	0.61
5:I:187:LEU:HB2	5:I:196:ALA:HB3	1.82	0.60
3:A:482:VAL:HG13	3:A:593:ASN:HA	1.84	0.60
6:O:110:GLN:HA	14:U:344:ARG:HH21	1.67	0.60
7:K:78:ARG:NH2	7:Q:17:GLN:O	2.31	0.60
3:A:1096:PRO:O	6:O:332:GLN:NE2	2.35	0.60
5:I:16:GLU:HG3	5:I:742:ARG:HG3	1.84	0.59
3:A:859:PRO:HB2	3:A:897:THR:HG23	1.84	0.59
13:Y:513:ARG:HD2	13:Y:544:LYS:HB2	1.84	0.59
14:U:296:ARG:HH22	14:U:299:ASN:HD22	1.51	0.59
3:A:1100:LEU:H	3:A:1161:ASN:HD21	1.49	0.59
5:I:214:LEU:HD23	5:I:241:LEU:HB3	1.84	0.59
3:A:42:LEU:HD22	14:V:363:ARG:HG2	1.84	0.58
1:L:79:ILE:HG13	1:L:156:ILE:HG12	1.84	0.58
14:V:127:GLU:OE1	14:V:148:ASN:ND2	2.36	0.58
13:Z:499:LEU:HD11	13:Z:514:ILE:HG13	1.85	0.58
15:R:425:LEU:HB2	15:R:439:LEU:HB2	1.85	0.58
1:L:66:ILE:HB	1:L:137:ILE:HG23	1.86	0.58
5:I:606:ASP:HB3	5:I:609:GLN:HB2	1.86	0.58
13:Z:54:ARG:NH2	13:Z:92:GLU:OE2	2.37	0.58
14:U:98:GLU:OE2	14:U:101:ARG:NH1	2.36	0.58
3:A:1527:MET:SD	3:A:1532:ASN:ND2	2.77	0.58
3:A:449:GLN:HG3	3:A:453:ARG:HH12	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:420:TYR:OH	14:U:424:ARG:NH1	2.37	0.57
15:R:177:ASP:H	16:S:75:LEU:HA	1.69	0.57
12:J:584:ASP:N	12:J:584:ASP:OD1	2.37	0.57
13:Y:302:PRO:O	13:Y:330:ARG:NH1	2.37	0.57
13:Z:476:ILE:HG12	13:Z:506:GLN:HE21	1.68	0.57
13:Y:194:GLU:OE1	13:Y:197:ARG:NH2	2.37	0.57
4:N:153:VAL:HA	4:N:156:MET:HG2	1.86	0.57
5:I:648:THR:HA	5:I:669:LEU:O	2.05	0.57
5:I:722:VAL:HG12	5:I:733:VAL:HG22	1.85	0.57
7:K:242:TYR:O	9:W:3:ARG:NH2	2.38	0.57
15:R:255:VAL:O	15:R:258:GLN:NE2	2.38	0.57
3:A:90:ASP:OD1	3:A:90:ASP:N	2.37	0.57
7:K:17:GLN:OE1	7:Q:78:ARG:NH1	2.38	0.57
12:P:89:GLU:HA	12:P:92:LEU:HD12	1.86	0.57
3:A:1799:ARG:NH1	3:A:1810:GLU:OE2	2.38	0.57
6:O:408:LEU:HA	6:O:411:LYS:HB3	1.87	0.57
3:A:1111:ALA:O	3:A:1115:ASN:HA	2.04	0.57
3:A:1727:ASN:ND2	3:A:1842:SER:O	2.37	0.57
12:J:754:HIS:HD2	7:Q:389:ARG:HE	1.53	0.57
3:A:1244:ASP:OD2	3:A:1244:ASP:N	2.38	0.57
6:O:552:GLN:HE22	6:O:589:GLU:HG3	1.69	0.57
7:K:458:LEU:HD23	7:K:460:LYS:HE2	1.86	0.56
12:P:533:VAL:HG23	12:P:559:LEU:HD22	1.86	0.56
13:Y:196:LEU:HD11	13:Y:206:ILE:HG12	1.87	0.56
1:L:73:THR:OG1	1:L:133:ARG:NH1	2.38	0.56
15:R:312:VAL:HA	15:R:328:GLY:HA2	1.87	0.56
3:A:249:LEU:HD13	3:A:256:VAL:HG22	1.87	0.56
3:A:1926:ARG:O	3:A:1930:ARG:NH1	2.38	0.56
7:K:480:SER:HB2	9:W:8:ARG:HH21	1.70	0.56
13:Z:459:GLU:HA	13:Z:462:LYS:HD3	1.88	0.56
3:A:1417:ASP:O	3:A:1643:TRP:NE1	2.38	0.56
12:J:170:PHE:HB3	12:J:456:LYS:HE3	1.86	0.56
1:L:39:GLY:O	1:L:44:GLN:NE2	2.39	0.56
13:Z:433:VAL:O	13:Z:437:LEU:HB2	2.06	0.56
1:L:57:ASP:OD1	1:L:57:ASP:N	2.38	0.56
4:N:660:THR:HG23	4:N:729:LEU:HD11	1.88	0.56
6:O:257:SER:O	6:O:261:ASN:ND2	2.39	0.56
15:R:360:ALA:HB1	15:R:405:ILE:HG13	1.87	0.56
3:A:1825:SER:HB2	3:A:1829:ARG:HH12	1.70	0.56
3:A:1084:ARG:NH2	3:A:1139:ASN:OD1	2.39	0.55
7:K:210:LYS:HB2	7:K:240:ARG:HH21	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:517:ASP:OD2	13:Z:532:TYR:OH	2.24	0.55
6:O:58:ARG:O	6:O:62:GLN:NE2	2.40	0.55
11:H:63:VAL:HG21	13:Y:364:LYS:HB2	1.87	0.55
12:P:618:ASP:OD1	12:P:618:ASP:N	2.38	0.55
1:L:86:ASP:O	1:L:90:THR:OG1	2.24	0.55
15:R:262:ARG:NH2	15:R:298:ALA:O	2.40	0.55
3:A:1306:CYS:HB2	3:A:1374:ILE:HG12	1.88	0.55
13:Y:500[B]:ARG:NH2	13:Y:527:GLU:OE1	2.38	0.55
15:R:197:VAL:HA	15:R:210:SER:HA	1.89	0.55
13:Z:270:ASN:ND2	13:Z:272:ASP:OD1	2.39	0.55
4:N:386:LEU:HD13	4:N:399:LEU:HD23	1.89	0.55
6:O:59:ARG:NH1	6:O:85:SER:O	2.40	0.55
7:Q:477:GLN:OE1	14:U:148:ASN:ND2	2.40	0.55
13:Y:84:ALA:HB2	13:Y:99:LYS:HB2	1.89	0.55
5:I:79:LEU:HD11	5:I:167:LEU:HD13	1.88	0.55
9:G:18:GLU:OE1	7:Q:456:ARG:NH1	2.40	0.55
13:Y:503:LEU:HD12	13:Y:515:LEU:HD13	1.88	0.55
4:N:162:PHE:O	4:N:255:ARG:NH2	2.40	0.54
11:H:57:SER:OG	13:Z:357:ARG:NH2	2.39	0.54
13:Y:398:GLU:OE2	13:Y:401:ARG:NH2	2.40	0.54
3:A:771:GLU:HG3	3:A:844:ILE:HG22	1.89	0.54
5:I:680:SER:O	5:I:684:GLN:NE2	2.40	0.54
10:M:5:VAL:O	10:M:7:ARG:NH1	2.40	0.54
14:U:190:ASP:OD1	14:U:190:ASP:N	2.36	0.54
15:R:406:LEU:HD21	15:R:451[B]:MET:HB2	1.89	0.54
3:A:714:ASP:N	3:A:714:ASP:OD1	2.39	0.54
3:A:748:SER:OG	3:A:749:LEU:N	2.40	0.54
3:A:1262:GLN:NE2	3:A:1579:SER:OG	2.40	0.54
3:A:1063:ILE:HA	3:A:1066:LYS:HE2	1.90	0.54
5:I:441:THR:HG23	5:I:444:ASP:H	1.71	0.54
7:Q:509:ARG:NH1	7:Q:512:ASP:OD2	2.40	0.54
5:I:101:LEU:HD11	5:I:164:ILE:HD12	1.90	0.54
5:I:281:MET:SD	5:I:281:MET:N	2.76	0.54
4:N:387:LEU:HD21	4:N:424:ILE:HD13	1.90	0.54
14:U:301:ASP:OD1	14:U:301:ASP:N	2.41	0.54
14:V:449:LEU:HD22	14:V:476:LEU:HD11	1.89	0.54
6:O:624:VAL:HG11	6:O:647:ALA:HB3	1.88	0.54
6:O:101:ALA:O	6:O:159:GLN:NE2	2.40	0.54
13:Y:246:VAL:HG13	13:Y:280:LEU:HD21	1.89	0.54
11:H:99:ILE:HG12	12:P:591:GLN:HG2	1.91	0.53
12:J:452:PHE:O	12:J:456:LYS:HB2	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:493:SER:O	12:J:497:ASN:ND2	2.41	0.53
13:Y:229:THR:HG23	13:Y:230:VAL:HG23	1.90	0.53
3:A:38:GLN:HE21	14:V:396:LYS:HG2	1.73	0.53
5:I:251:MET:HE3	5:I:381:LEU:HB2	1.90	0.53
6:O:38:LEU:HD22	6:O:115:LEU:HD21	1.91	0.53
14:V:137:SER:O	14:V:143:LYS:NZ	2.41	0.53
3:A:807:TYR:HA	3:A:814:VAL:HG21	1.90	0.53
12:P:170:PHE:HB2	12:P:463:MET:HG3	1.89	0.53
3:A:880:TYR:HB2	3:A:930:LEU:HD22	1.91	0.53
3:A:980:ARG:NH2	3:A:1675:GLU:O	2.41	0.53
12:P:94:GLY:H	12:P:101:LYS:HE3	1.73	0.53
6:O:128:LYS:O	6:O:137:ARG:NH1	2.40	0.53
3:A:408:CYS:SG	3:A:409:ILE:N	2.82	0.53
5:I:477:GLN:NE2	5:I:488:SER:O	2.41	0.53
12:J:27:LEU:HD11	12:P:147:PHE:HB3	1.90	0.53
12:P:560:THR:O	12:P:564:LYS:NZ	2.42	0.53
15:R:274:LEU:HD23	15:R:281:LEU:HD11	1.91	0.53
3:A:125:GLN:NE2	3:A:179:ASN:OD1	2.42	0.53
3:A:1866:MET:SD	3:A:1866:MET:N	2.76	0.53
15:R:377:THR:O	15:R:380:ARG:NH1	2.37	0.53
2:D:11:ARG:NH1	6:O:416:GLU:OE2	2.42	0.53
5:I:401:ASN:OD1	5:I:405:GLN:NE2	2.41	0.53
6:O:221:SER:O	6:O:225:ASN:ND2	2.37	0.53
14:V:236:HIS:HD1	14:V:264:TYR:HH	1.57	0.53
14:V:97:LYS:O	14:V:128:LYS:NZ	2.43	0.52
14:V:213:ILE:HG23	14:V:218:MET:HB3	1.91	0.52
3:A:677:TRP:HH2	3:A:792:GLN:HE21	1.58	0.52
15:R:187:LEU:HD22	15:R:230:SER:HB2	1.91	0.52
15:R:207:TYR:HA	15:R:218:GLN:HA	1.90	0.52
14:U:334:CYS:HB2	14:U:357:ALA:HB2	1.92	0.52
14:U:477:HIS:HB2	14:U:486:ALA:HB2	1.91	0.52
1:L:6:LYS:NZ	1:L:7:THR:O	2.42	0.52
3:A:925:SER:OG	3:A:926:LEU:N	2.42	0.52
7:K:200:LEU:HD13	7:K:224:VAL:HG11	1.91	0.52
15:R:428:TRP:HB3	15:R:433:MET:HA	1.90	0.52
3:A:1725:ASN:ND2	4:N:254:GLU:O	2.42	0.52
6:O:247:ASN:OD1	6:O:247:ASN:N	2.43	0.52
12:J:755:LEU:O	12:J:759:ASN:ND2	2.38	0.52
7:K:487:TYR:OH	9:W:15:ASP:O	2.23	0.52
2:D:8:LEU:HD11	6:O:424:GLN:HE22	1.75	0.52
12:J:38:GLU:HB2	13:Y:268:ARG:HH12	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:500[B]:ARG:HG3	13:Y:515:LEU:HD11	1.91	0.52
3:A:661:VAL:HG12	3:A:789:LEU:HD12	1.92	0.51
3:A:662:THR:HG22	3:A:672:THR:HG21	1.91	0.51
3:A:1637:THR:HG1	3:A:1665:GLN:H	1.58	0.51
5:I:74:ARG:HH11	5:I:79:LEU:HD13	1.75	0.51
5:I:474:ARG:NH1	5:I:488:SER:OG	2.44	0.51
5:I:634:SER:OG	5:I:635:ILE:N	2.44	0.51
13:Y:85:ASP:OD1	13:Y:100:TYR:OH	2.25	0.51
13:Z:215:LYS:HE2	13:Z:217:ALA:HB3	1.92	0.51
3:A:615:SER:OG	3:A:616:GLU:N	2.43	0.51
4:N:540:ARG:HA	4:N:543:GLU:HG2	1.91	0.51
12:J:479:TYR:O	12:J:667:GLN:NE2	2.43	0.51
14:V:36:LEU:HD21	14:V:58:LEU:HB3	1.91	0.51
13:Z:358:ALA:HB1	13:Z:378:LEU:HD11	1.92	0.51
5:I:540:PRO:HA	5:I:543:VAL:HG12	1.91	0.51
6:O:249:ASP:OD2	6:O:280:ARG:NH2	2.43	0.51
7:Q:351:ASP:OD1	7:Q:351:ASP:N	2.39	0.51
13:Z:397:ARG:NH2	13:Z:417:TYR:OH	2.44	0.51
3:A:1615:GLU:OE2	3:A:1617:ARG:NE	2.43	0.51
5:I:116:MET:HG2	5:I:210:LEU:HB3	1.92	0.51
5:I:229:SER:O	5:I:558:ARG:HA	2.09	0.51
4:N:575:ARG:HH21	4:N:591:VAL:HG13	1.75	0.51
10:M:7:ARG:HH21	14:U:131:ASP:HB2	1.76	0.51
15:R:445:ARG:NH1	16:S:32:ASN:OD1	2.44	0.51
3:A:1539:CYS:HB3	3:A:1562:LEU:HD12	1.93	0.51
3:A:1679:ASP:OD2	3:A:1682:LYS:NZ	2.43	0.51
4:N:265:LEU:HD21	4:N:328:VAL:HG23	1.93	0.51
14:V:122:ARG:NH1	14:V:157:GLU:OE1	2.40	0.51
3:A:159:ILE:HD11	3:A:173:LEU:HD21	1.93	0.51
3:A:412:LEU:HD21	3:A:466:LEU:HB2	1.93	0.51
3:A:1667:LYS:HD3	3:A:1677:LEU:HD12	1.92	0.51
3:A:1753:TYR:O	6:O:631:GLN:NE2	2.44	0.51
13:Z:487:SER:HB3	13:Z:518:PHE:HE1	1.76	0.51
3:A:183:THR:HG22	3:A:249:LEU:HD21	1.93	0.51
5:I:184:PHE:HA	5:I:198:VAL:O	2.11	0.51
5:I:205:CYS:HA	5:I:221:THR:HA	1.92	0.51
13:Z:184:GLN:HB3	13:Z:187:PRO:HD2	1.93	0.51
12:J:148:LEU:HD23	12:J:151:PRO:HG2	1.93	0.51
14:U:214:THR:HA	14:U:397:ARG:HE	1.75	0.51
13:Z:329:CYS:SG	13:Z:330:ARG:N	2.84	0.51
13:Z:427:MET:O	13:Z:431:ASN:ND2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1138:HIS:HE1	3:A:1604:GLN:HE21	1.58	0.50
3:A:1361:ASP:N	3:A:1361:ASP:OD1	2.44	0.50
3:A:1756:LYS:O	6:O:639:GLN:NE2	2.44	0.50
5:I:198:VAL:HG22	5:I:545:GLY:HA2	1.93	0.50
7:K:555:LEU:HA	7:K:558:ILE:HD12	1.93	0.50
12:P:489:SER:O	13:Z:105:GLN:NE2	2.44	0.50
13:Z:169:PRO:HA	13:Z:172:ASN:HD22	1.76	0.50
2:D:34:GLU:HG2	6:O:141:LEU:HD13	1.93	0.50
3:A:1267:ARG:NH2	7:K:348:SER:OG	2.44	0.50
7:Q:451:LEU:HA	7:Q:454:VAL:HG22	1.92	0.50
16:S:77:ASP:OD2	16:S:77:ASP:N	2.42	0.50
12:J:609:HIS:NE2	15:R:499:ARG:OXT	2.42	0.50
7:K:350:HIS:ND1	7:K:377:GLU:OE1	2.42	0.50
7:K:400:GLU:HB2	7:K:431:LYS:HE2	1.94	0.50
14:U:85:ASP:N	14:U:85:ASP:OD1	2.44	0.50
3:A:23:PHE:HB2	3:A:111:LEU:HD22	1.92	0.50
5:I:499:ASP:O	5:I:503:ASN:ND2	2.44	0.50
7:K:220:ILE:HD13	7:K:228:GLN:HB3	1.93	0.50
14:U:508:GLU:OE2	14:U:511:THR:OG1	2.28	0.50
7:K:369:LEU:HD21	9:W:3:ARG:HG2	1.94	0.50
13:Z:272:ASP:OD1	13:Z:272:ASP:N	2.39	0.50
4:N:451:ASP:OD2	4:N:451:ASP:N	2.45	0.50
6:O:91:ASN:HA	6:O:94:GLN:HB3	1.93	0.50
13:Z:354:ARG:HH11	13:Z:357:ARG:HG2	1.76	0.50
3:A:703:SER:HB2	6:O:731:ASN:HB3	1.93	0.50
13:Z:168:THR:HG22	13:Z:170:LYS:H	1.77	0.50
1:L:61:PRO:HB3	1:L:142:LEU:HD23	1.93	0.49
15:R:204:ASN:ND2	15:R:227:GLU:O	2.45	0.49
15:R:335:VAL:O	15:R:348:LEU:N	2.43	0.49
3:A:1033:ARG:NH1	3:A:1531:GLY:O	2.45	0.49
3:A:1327:GLN:NE2	3:A:1333:HIS:O	2.45	0.49
4:N:336:TYR:OH	4:N:340:ARG:NH2	2.46	0.49
12:P:493:SER:O	12:P:497:ASN:ND2	2.45	0.49
13:Y:152:ASP:HB3	13:Y:178:LEU:HD22	1.93	0.49
3:A:1463:TYR:HE1	3:A:1511:ASN:HB3	1.77	0.49
7:K:37:PRO:HA	7:K:40:ILE:HD12	1.95	0.49
3:A:614:THR:O	6:O:556:GLN:NE2	2.45	0.49
3:A:1248:ASN:HA	3:A:1251:VAL:HG12	1.95	0.49
15:R:388[A]:CYS:O	15:R:389:SER:N	2.44	0.49
6:O:513:LYS:HE2	6:O:542:GLU:HG2	1.94	0.49
3:A:80:VAL:O	3:A:89:TYR:OH	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1070:LEU:HD22	3:A:1118:VAL:HG23	1.93	0.49
12:P:520:ARG:NH2	13:Z:154:ASP:OD1	2.46	0.49
12:P:584:ASP:OD1	12:P:584:ASP:N	2.46	0.49
3:A:1552:TYR:OH	3:A:1604:GLN:NE2	2.45	0.49
3:A:1918:PHE:HA	3:A:1921:LEU:HB2	1.94	0.49
4:N:563:ASP:O	4:N:567:SER:N	2.42	0.49
7:K:232:ASP:OD1	7:K:264:HIS:NE2	2.41	0.49
7:K:446:PRO:HB3	9:W:8:ARG:HB2	1.93	0.49
7:K:500:ASP:OD1	12:P:660:LYS:NZ	2.45	0.49
3:A:451:GLN:NE2	3:A:473:ASN:OD1	2.45	0.49
6:O:75:LEU:HB3	6:O:165:GLY:HA3	1.95	0.49
12:J:534:GLU:OE2	12:P:22:ARG:NH2	2.45	0.49
13:Y:499:LEU:HB3	13:Y:515:LEU:HD12	1.95	0.49
15:R:451[B]:MET:HG3	15:R:458:VAL:HG12	1.94	0.49
4:N:381:ALA:O	4:N:385:ARG:HB2	2.12	0.49
5:I:289:LYS:HA	5:I:292:GLN:HE21	1.78	0.49
12:P:65:SER:OG	12:P:66:CYS:N	2.45	0.49
14:U:304:SER:HB3	14:U:336:VAL:HG22	1.95	0.49
14:V:311:SER:HB2	15:R:134:SER:HB2	1.95	0.49
13:Z:455:PRO:HA	13:Z:458:GLN:HB2	1.94	0.49
7:Q:480:SER:HB3	7:Q:509:ARG:HH22	1.78	0.48
3:A:1041:LEU:HA	3:A:1080:LEU:HD22	1.94	0.48
13:Z:94:ARG:HH12	13:Z:151:GLN:HE22	1.61	0.48
15:R:262:ARG:NH1	15:R:297:VAL:O	2.46	0.48
15:R:360:ALA:O	15:R:373:THR:HA	2.13	0.48
1:L:79:ILE:HG22	1:L:120:ILE:HB	1.94	0.48
3:A:1672:ARG:NH1	3:A:1711:ASP:O	2.39	0.48
7:K:276:VAL:HG23	7:K:311:MET:HB2	1.95	0.48
12:J:726:LEU:HD21	12:J:742:LEU:HD23	1.95	0.48
14:U:278:ASP:N	14:U:278:ASP:OD1	2.46	0.48
3:A:218:ASP:OD2	14:V:454:LYS:NZ	2.45	0.48
4:N:516:ILE:HD12	4:N:519:TYR:HB3	1.95	0.48
7:K:129:LYS:HA	7:K:132:ILE:HD12	1.95	0.48
12:J:97:PHE:CG	13:Y:286:ASP:HB3	2.49	0.48
5:I:559:ASP:OD1	5:I:559:ASP:N	2.46	0.48
13:Y:270:ASN:HD21	13:Y:272:ASP:HB3	1.77	0.48
13:Z:232:ASN:O	13:Z:235:TRP:NE1	2.46	0.48
3:A:74:TRP:O	3:A:588:ARG:NH2	2.44	0.48
3:A:183:THR:HG1	3:A:186:GLY:H	1.61	0.48
4:N:431:ARG:HB2	4:N:434:THR:HB	1.95	0.48
7:K:195:ASN:HA	7:K:198:GLN:HB2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:80:LEU:HD21	13:Y:102:MET:HB2	1.95	0.48
4:N:272:ARG:NH2	4:N:288:GLU:OE2	2.46	0.48
4:N:407:LEU:HB2	4:N:417:LEU:HB3	1.96	0.48
4:N:651:ALA:HA	4:N:717:GLU:HG2	1.96	0.48
14:U:293:ASP:OD2	14:V:101:ARG:NH1	2.46	0.48
3:A:497:LEU:HD12	3:A:511:ILE:HD11	1.94	0.48
13:Y:39:ASP:OD1	13:Y:42:ARG:NH2	2.46	0.48
15:R:262:ARG:NH1	15:R:294:ASP:O	2.47	0.48
15:R:333:VAL:HG22	15:R:358:VAL:HG21	1.96	0.48
3:A:1738:ILE:HD11	3:A:1779:VAL:HG11	1.95	0.48
5:I:117:GLU:OE2	5:I:172:ARG:NH2	2.45	0.48
5:I:326:THR:OG1	5:I:329:GLY:N	2.42	0.48
5:I:399:LYS:NZ	5:I:517:TYR:O	2.38	0.48
4:N:414:MET:HE2	4:N:497:ARG:HB3	1.96	0.47
6:O:276:HIS:CG	14:V:389:ARG:HH21	2.32	0.47
12:J:168:PHE:O	12:J:467:ARG:NH2	2.44	0.47
12:P:517:GLN:OE1	12:P:520:ARG:NH1	2.47	0.47
5:I:188:TYR:HA	5:I:194:LYS:HA	1.95	0.47
13:Y:374:GLN:OE1	13:Y:406:ARG:NH2	2.46	0.47
5:I:182:SER:OG	5:I:183:GLY:N	2.46	0.47
14:V:550:LEU:O	14:V:554:LEU:HB2	2.14	0.47
12:J:65:SER:OG	12:J:65:SER:O	2.32	0.47
12:P:755:LEU:HA	12:P:758:MET:HG2	1.97	0.47
7:Q:183:GLU:O	7:Q:187:SER:HB3	2.14	0.47
13:Y:445:THR:O	13:Y:449:THR:OG1	2.28	0.47
3:A:970:TRP:CD1	3:A:974:VAL:HG11	2.50	0.47
3:A:1925:VAL:HG21	4:N:70:VAL:HB	1.97	0.47
6:O:134:LEU:O	6:O:138:HIS:ND1	2.43	0.47
6:O:216:LEU:HD22	6:O:256:LEU:HG	1.95	0.47
14:U:36:LEU:HD21	14:U:58:LEU:HB3	1.95	0.47
14:V:58:LEU:O	14:V:61:SER:OG	2.31	0.47
15:R:236:LYS:NZ	15:R:278:SER:O	2.39	0.47
15:R:406:LEU:HD21	15:R:451[A]:MET:HB2	1.94	0.47
1:L:75:LYS:HD2	1:L:161:PRO:HG3	1.96	0.47
4:N:294:GLU:HA	4:N:297:VAL:HG12	1.96	0.47
4:N:719:GLU:O	4:N:720:ARG:NE	2.46	0.47
6:O:576:ASN:N	6:O:576:ASN:OD1	2.45	0.47
7:K:461:TYR:HD1	7:K:488:ILE:HG23	1.78	0.47
13:Y:287:ASN:OD1	13:Y:317:ARG:NH1	2.47	0.47
15:R:438:GLU:OE2	15:R:440:LYS:NZ	2.45	0.47
3:A:1014:ASP:N	3:A:1014:ASP:OD1	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:76:ASP:OD1	5:I:76:ASP:N	2.41	0.47
5:I:583:LEU:HD12	5:I:602:ARG:HB2	1.96	0.47
6:O:89:LEU:HA	6:O:92:SER:HB3	1.97	0.47
6:O:726:LYS:HB3	6:O:728:GLN:HE22	1.79	0.47
7:K:546:ASP:N	7:K:546:ASP:OD1	2.47	0.47
9:G:20:GLU:HA	9:G:23:ARG:HD3	1.97	0.47
14:U:301:ASP:OD2	14:U:364:TYR:OH	2.31	0.47
14:V:277:ARG:HH22	14:V:434:ARG:HH22	1.63	0.47
3:A:846:GLN:OE1	3:A:850:SER:OG	2.32	0.47
12:J:68:THR:OG1	12:J:71:CYS:SG	2.72	0.47
15:R:282:SER:HG	15:R:317:TRP:HE1	1.59	0.47
3:A:1503:ASN:O	3:A:1506:VAL:HB	2.15	0.47
4:N:427:TYR:OH	4:N:431:ARG:NH2	2.48	0.47
4:N:681:LEU:HD22	4:N:713:PHE:HZ	1.80	0.47
11:H:73:ASP:HA	11:H:76:VAL:HG12	1.95	0.47
4:N:29:THR:HG22	4:N:34:PRO:HB3	1.97	0.47
8:C:73:CYS:HB3	8:C:78:GLN:H	1.79	0.47
15:R:425:LEU:HD11	15:R:449:LEU:HD11	1.96	0.47
1:L:71:LYS:HA	1:L:134:THR:O	2.16	0.46
3:A:255:ILE:HD11	3:A:432:ILE:HD11	1.96	0.46
3:A:1267:ARG:NH1	3:A:1315:GLY:O	2.48	0.46
7:K:66:ASP:OD1	7:K:66:ASP:N	2.48	0.46
12:J:533:VAL:HG23	12:J:559:LEU:HD22	1.97	0.46
3:A:596:THR:HA	3:A:605:VAL:O	2.14	0.46
15:R:192:TRP:HB2	15:R:450:THR:HB	1.97	0.46
15:R:219:LEU:HD11	15:R:255:VAL:HG12	1.97	0.46
15:R:454:ASP:OD1	15:R:454:ASP:N	2.47	0.46
5:I:625:TYR:OH	5:I:711:TRP:O	2.30	0.46
7:K:332:THR:O	7:K:332:THR:OG1	2.34	0.46
7:K:408:VAL:HA	7:K:411:VAL:HG12	1.97	0.46
5:I:210:LEU:HD13	5:I:217:LEU:HB2	1.97	0.46
7:Q:368:HIS:NE2	7:Q:401:ASP:OD2	2.48	0.46
15:R:411:TYR:O	15:R:429:LYS:NZ	2.39	0.46
3:A:652:SER:O	3:A:652:SER:OG	2.34	0.46
3:A:1147:ILE:O	3:A:1182:ASN:ND2	2.44	0.46
4:N:370:GLN:NE2	4:N:373:GLN:OE1	2.42	0.46
4:N:574:ILE:HG21	4:N:625:LYS:HZ3	1.80	0.46
7:K:134:LEU:HD13	7:K:166:ALA:HB2	1.98	0.46
7:Q:288:SER:HB2	7:Q:305:VAL:HG22	1.97	0.46
13:Z:379:LYS:HG2	13:Z:395:HIS:CD2	2.51	0.46
3:A:248:PHE:HB3	3:A:257:MET:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1617:ARG:HA	3:A:1691:LEU:HD13	1.97	0.46
12:P:55:TYR:OH	12:P:56:LYS:NZ	2.49	0.46
13:Y:159:LEU:O	13:Y:167:ARG:NH2	2.49	0.46
14:V:526:TRP:HE1	14:V:552:GLN:HE22	1.64	0.46
13:Z:522:VAL:HG23	13:Z:524:GLU:HG2	1.97	0.46
5:I:561:ARG:NH1	5:I:589:THR:OG1	2.48	0.46
6:O:287:GLU:HB2	6:O:291:ASN:HD22	1.80	0.46
7:Q:216:SER:OG	7:Q:217:GLU:N	2.49	0.46
3:A:925:SER:HB3	3:A:928:GLU:HG3	1.98	0.46
4:N:206:ARG:O	4:N:209:ARG:NE	2.49	0.46
6:O:330:ILE:HD11	14:V:414:MET:HG2	1.97	0.46
13:Z:311:TYR:HA	13:Z:314:LEU:HD12	1.98	0.46
15:R:205:SER:HA	15:R:221:GLN:HA	1.98	0.46
3:A:1798:ARG:HB3	3:A:1802:ARG:HH12	1.81	0.46
6:O:105:LEU:HD11	6:O:151:VAL:HG12	1.97	0.46
11:H:100:GLU:HG3	11:H:105:PHE:HD2	1.81	0.46
12:J:499:GLY:O	12:J:503:CYS:HB2	2.16	0.46
15:R:427:ILE:HG23	15:R:436:VAL:HG23	1.98	0.46
1:L:67:GLN:HG2	1:L:136:MET:HG3	1.98	0.46
6:O:544:VAL:HG23	6:O:567:LEU:HD22	1.96	0.46
7:K:157:LEU:HG	7:K:188:LEU:HD22	1.98	0.46
7:Q:211:LYS:HG2	7:Q:240:ARG:HG2	1.97	0.46
14:U:39:ILE:HA	14:U:42:LEU:HB2	1.99	0.46
14:U:201:LEU:HA	14:U:229:MET:HG3	1.98	0.46
14:V:453:LYS:HG3	14:V:476:LEU:HD23	1.97	0.46
13:Z:187:PRO:HA	13:Z:190:THR:HG22	1.96	0.46
3:A:183:THR:OG1	3:A:186:GLY:N	2.47	0.45
3:A:504:VAL:HG11	3:A:635:VAL:HG11	1.98	0.45
5:I:150:SER:O	5:I:150:SER:OG	2.33	0.45
9:G:15:ASP:O	7:Q:487:TYR:OH	2.25	0.45
12:J:543:LEU:HB2	12:J:552:LEU:HD13	1.98	0.45
3:A:477:LYS:N	3:A:491:LEU:O	2.44	0.45
3:A:1659:GLU:OE1	3:A:1661:HIS:NE2	2.49	0.45
5:I:9:PRO:HG2	5:I:750:ASP:HB3	1.98	0.45
14:U:77:THR:OG1	14:U:78:GLU:N	2.49	0.45
13:Z:263:LYS:O	13:Z:268:ARG:NH2	2.44	0.45
12:P:97:PHE:O	12:P:98:ASN:ND2	2.49	0.45
13:Z:464:LEU:HD23	13:Z:467:LYS:HD3	1.98	0.45
3:A:1035:GLN:HE22	4:N:489:PRO:HB3	1.80	0.45
12:J:754:HIS:ND1	7:Q:393:GLN:OE1	2.50	0.45
7:Q:475:ILE:HA	7:Q:476:PRO:HD3	1.75	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:371:ASN:HA	13:Y:402:LEU:HD21	1.99	0.45
13:Y:396:PHE:HB3	13:Y:413:LEU:HB2	1.98	0.45
15:R:420:PHE:HA	15:R:421:ALA:HA	1.60	0.45
3:A:1387:LEU:HB3	3:A:1411:ARG:HB2	1.99	0.45
3:A:1816:LEU:HD23	3:A:1816:LEU:HA	1.86	0.45
6:O:435:SER:OG	6:O:618:TYR:OH	2.29	0.45
6:O:727:THR:HA	6:O:730:ARG:HB3	1.99	0.45
11:H:99:ILE:HD12	11:H:99:ILE:HA	1.86	0.45
12:P:131:LEU:HD11	12:P:158:ILE:HG12	1.97	0.45
13:Z:251:ASN:OD1	13:Z:251:ASN:N	2.50	0.45
3:A:874:VAL:HG21	3:A:896:LEU:HD21	1.97	0.45
5:I:141:LYS:HD2	5:I:141:LYS:HA	1.76	0.45
9:G:8:ARG:NH1	7:Q:445:GLU:OE1	2.46	0.45
13:Y:373:VAL:HG11	13:Y:403:ALA:HB2	1.99	0.45
13:Z:53:VAL:O	13:Z:57:SER:HB3	2.16	0.45
3:A:46:SER:OG	3:A:47:GLU:N	2.49	0.45
13:Y:53:VAL:O	13:Y:57:SER:CB	2.64	0.45
13:Y:164:SER:OG	13:Y:167:ARG:NH1	2.49	0.45
14:V:207:LEU:O	14:V:211:ASN:ND2	2.49	0.45
13:Z:100:TYR:HB3	13:Z:142:MET:HE2	1.99	0.45
3:A:1077:THR:HA	3:A:1080:LEU:HD12	1.99	0.45
4:N:408:ARG:NH2	4:N:499:SER:O	2.49	0.45
6:O:501:SER:OG	6:O:502:GLN:N	2.49	0.45
13:Z:310:VAL:HA	13:Z:374:GLN:HE22	1.81	0.45
3:A:191:ARG:HH12	3:A:207:LEU:HD22	1.82	0.45
3:A:1636:VAL:HB	3:A:1663:LEU:HD11	1.99	0.45
5:I:208:LEU:HD23	5:I:219:VAL:HG22	1.99	0.45
7:K:13:TYR:OH	7:Q:160:ASP:OD2	2.30	0.45
14:U:443:TYR:HA	14:U:446:LEU:HB2	1.99	0.45
13:Z:405:CYS:HA	13:Z:437:LEU:HD21	1.98	0.45
3:A:93:LEU:HD12	3:A:93:LEU:HA	1.82	0.45
5:I:578:ASN:ND2	5:I:581:SER:OG	2.49	0.45
7:K:233:VAL:O	7:K:236:SER:OG	2.28	0.45
1:L:71:LYS:N	3:A:1397:ASP:O	2.46	0.44
3:A:1691:LEU:HA	3:A:1695:GLY:HA2	1.99	0.44
4:N:446:SER:OG	4:N:447:ASP:N	2.50	0.44
5:I:206:LEU:HD23	5:I:573:PRO:HD2	1.99	0.44
5:I:427:ARG:NH1	6:O:129:THR:O	2.50	0.44
13:Z:196:LEU:HD12	13:Z:196:LEU:HA	1.85	0.44
3:A:104:LYS:HG3	3:A:114:TYR:HB2	1.99	0.44
3:A:724:LEU:O	3:A:727:SER:OG	2.36	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:270:ARG:HE	4:N:270:ARG:HB2	1.59	0.44
4:N:662:VAL:O	4:N:695:ARG:NH1	2.51	0.44
5:I:224:SER:HA	5:I:229:SER:HA	1.97	0.44
5:I:735:SER:OG	5:I:737:ASN:OD1	2.30	0.44
6:O:671:GLN:NE2	6:O:693:ASN:OD1	2.49	0.44
12:J:773:ASN:HD22	15:R:494:ILE:HG21	1.82	0.44
14:U:318:TYR:HA	14:U:321:HIS:CE1	2.52	0.44
13:Z:57:SER:OG	13:Z:83:HIS:ND1	2.50	0.44
15:R:185:TYR:OH	15:R:402:VAL:O	2.34	0.44
3:A:99:MET:HA	3:A:117:PHE:O	2.17	0.44
3:A:264:ASN:O	3:A:424:ASN:ND2	2.49	0.44
3:A:1901:PRO:HG2	3:A:1917:LYS:HD3	1.98	0.44
4:N:606:ASP:OD2	4:N:639:HIS:N	2.49	0.44
4:N:714:SER:HB2	4:N:716:ILE:HG23	1.98	0.44
7:K:371:MET:H	7:K:371:MET:HG2	1.66	0.44
14:U:527:ASP:O	14:U:530:SER:OG	2.34	0.44
14:V:280:ASP:OD1	14:V:310:ARG:NH2	2.44	0.44
13:Z:309:ASP:HB2	13:Z:340:GLU:HG3	1.99	0.44
13:Z:500[B]:ARG:HE	13:Z:515:LEU:HD21	1.83	0.44
3:A:1134:TRP:HD1	3:A:1597:THR:HA	1.82	0.44
3:A:1209:LEU:HD22	3:A:1228:LEU:HD23	1.99	0.44
3:A:1232:ILE:HD12	3:A:1235:LEU:HD12	1.99	0.44
3:A:1504:ALA:O	3:A:1508:GLY:N	2.49	0.44
4:N:368:THR:OG1	4:N:370:GLN:OE1	2.35	0.44
6:O:509:LEU:HG	6:O:513:LYS:HE3	1.99	0.44
7:Q:315:LYS:HD2	7:Q:315:LYS:HA	1.87	0.44
14:V:185:VAL:HG13	14:V:186:LYS:HD2	1.98	0.44
3:A:500:TYR:HE1	3:A:505:ARG:HG3	1.82	0.44
4:N:158:ARG:HB3	4:N:255:ARG:HE	1.82	0.44
14:V:419:LEU:O	14:V:423:ARG:HB2	2.18	0.44
3:A:433:THR:OG1	3:A:434:SER:N	2.49	0.44
3:A:1540:ARG:HD2	4:N:480:TRP:CD2	2.53	0.44
4:N:320:THR:HA	4:N:323:ARG:HG2	2.00	0.44
7:K:231:LEU:HD23	7:K:257:VAL:HG13	2.00	0.44
12:J:618:ASP:N	12:J:618:ASP:OD1	2.48	0.44
7:Q:61:ARG:HD3	7:Q:80:HIS:HE1	1.83	0.44
14:V:33:LYS:HD3	14:V:65:LEU:HG	1.99	0.44
13:Z:482:LYS:HD2	13:Z:482:LYS:HA	1.74	0.44
3:A:935:THR:HG21	3:A:974:VAL:HG23	1.99	0.44
3:A:1153:ILE:HD11	3:A:1184:HIS:HB3	1.98	0.44
9:G:4:ARG:NH2	7:Q:357:TYR:OH	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:543:GLN:HA	13:Y:546:LEU:HB2	1.99	0.44
15:R:413:GLU:HG3	15:R:429:LYS:HA	1.98	0.44
3:A:1251:VAL:HG13	3:A:1603:LEU:HD22	1.99	0.44
3:A:1265:ALA:HB2	3:A:1309:HIS:HD2	1.82	0.44
3:A:1385:ASP:OD1	3:A:1388:ARG:NH2	2.51	0.44
5:I:23:ILE:HA	5:I:39:ASN:HA	1.99	0.44
5:I:319:THR:HA	5:I:323:ASN:HD22	1.83	0.44
5:I:341:TYR:HE1	5:I:475:VAL:HG11	1.81	0.44
5:I:558:ARG:H	5:I:692:ARG:NH2	2.16	0.44
5:I:613:ASN:HB3	5:I:616:ILE:HD11	2.00	0.44
7:K:268:LEU:HD22	7:K:291:LEU:HD11	2.00	0.44
7:Q:231:LEU:HD23	7:Q:257:VAL:HG13	2.00	0.44
13:Y:204:ASP:H	13:Z:52:ASN:HD22	1.65	0.44
13:Y:442:GLN:HE21	13:Y:475:TYR:HE1	1.64	0.44
1:L:30:VAL:HG23	3:A:1354:GLU:HA	2.00	0.44
3:A:275:LYS:NZ	3:A:278:GLU:OE2	2.50	0.44
3:A:1086:MET:HG2	3:A:1610:TYR:CZ	2.53	0.44
4:N:664:ALA:HA	4:N:667:LEU:HB2	2.00	0.44
5:I:606:ASP:OD1	5:I:608:SER:OG	2.35	0.44
5:I:619:LYS:O	5:I:704:THR:HA	2.18	0.44
14:V:476:LEU:HD12	14:V:476:LEU:HA	1.87	0.44
15:R:253:TRP:HZ2	15:R:260:ARG:HH21	1.66	0.44
4:N:110:LEU:HD23	4:N:110:LEU:HA	1.91	0.43
4:N:564:MET:O	4:N:568:ARG:N	2.51	0.43
6:O:500:ASN:OD1	6:O:500:ASN:N	2.51	0.43
7:K:193:LEU:O	7:K:198:GLN:NE2	2.40	0.43
14:V:112:LYS:HA	14:V:112:LYS:HD3	1.83	0.43
14:V:116:PHE:HE1	14:V:174:LEU:HB2	1.83	0.43
14:V:236:HIS:ND1	14:V:264:TYR:OH	2.45	0.43
3:A:423:SER:OG	3:A:424:ASN:N	2.50	0.43
3:A:1910:SER:OG	3:A:1913:GLU:OE2	2.35	0.43
5:I:402:GLU:OE2	5:I:478:TYR:OH	2.32	0.43
5:I:526:LYS:HE3	5:I:526:LYS:HB3	1.84	0.43
7:K:306:GLY:HA3	7:K:323:LEU:HG	1.99	0.43
14:V:96:VAL:HG23	14:V:98:GLU:HG2	1.99	0.43
14:V:130:LYS:O	14:V:134:THR:OG1	2.31	0.43
3:A:730:LEU:HD22	6:O:719:ARG:HG2	1.99	0.43
4:N:393:THR:HA	4:N:396:ILE:HD12	2.00	0.43
12:J:754:HIS:CD2	7:Q:389:ARG:HE	2.33	0.43
14:U:168:ASP:OD1	14:U:168:ASP:N	2.51	0.43
13:Z:444:LEU:HD22	13:Z:464:LEU:HD22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:515:LEU:HD12	13:Z:518:PHE:HD2	1.83	0.43
3:A:982:ASP:N	3:A:982:ASP:OD1	2.51	0.43
4:N:587:PRO:HA	4:N:588:PRO:HD3	1.88	0.43
14:V:99:TYR:HB2	14:V:125:SER:HB3	2.01	0.43
14:V:388:TYR:HB2	14:V:405:LEU:HD13	2.00	0.43
13:Z:397:ARG:HA	13:Z:400:ILE:HG12	2.00	0.43
13:Z:527:GLU:HA	13:Z:530:ASP:HB3	2.01	0.43
15:R:275:SER:OG	15:R:315:LEU:O	2.36	0.43
3:A:270:THR:O	3:A:409:ILE:HA	2.18	0.43
3:A:667:MET:HB3	3:A:755:LEU:HD12	2.00	0.43
3:A:1054:TYR:HB2	3:A:1057:LEU:HB2	2.00	0.43
5:I:471:ASN:ND2	5:I:477:GLN:OE1	2.50	0.43
7:K:78:ARG:HH12	7:Q:17:GLN:HB2	1.82	0.43
13:Z:352:SER:O	13:Z:352:SER:OG	2.35	0.43
3:A:675:LEU:HD23	3:A:675:LEU:HA	1.92	0.43
4:N:206:ARG:HG2	4:N:209:ARG:HH21	1.83	0.43
4:N:666:ILE:HD11	4:N:695:ARG:HH22	1.83	0.43
12:P:631:ASN:HB3	12:P:634:HIS:HB2	2.00	0.43
7:Q:331:LYS:HA	7:Q:331:LYS:HD3	1.83	0.43
1:L:12:ASP:OD2	1:L:15:GLN:N	2.52	0.43
12:J:750:LEU:HD23	12:J:750:LEU:HA	1.88	0.43
12:P:140:LYS:HA	12:P:140:LYS:HD2	1.87	0.43
13:Y:235:TRP:NE1	13:Z:63:MET:SD	2.91	0.43
13:Y:333:ASN:O	13:Z:94:ARG:NE	2.52	0.43
15:R:254:ASP:OD1	15:R:256:GLN:NE2	2.52	0.43
3:A:1430:VAL:O	3:A:1435:ARG:NH2	2.52	0.43
12:P:726:LEU:HD21	12:P:742:LEU:HD23	2.01	0.43
13:Y:352:SER:O	13:Y:352:SER:OG	2.33	0.43
14:U:480:LEU:HG	14:U:482:GLU:H	1.84	0.43
13:Z:50:HIS:O	13:Z:86:SER:OG	2.27	0.43
3:A:1274:LEU:HD12	3:A:1274:LEU:HA	1.90	0.43
4:N:374:LEU:O	4:N:378:LEU:HB2	2.18	0.43
4:N:589:PHE:HZ	4:N:618:ALA:HB2	1.83	0.43
7:K:383:ASN:HB3	7:K:386:LEU:HB2	2.00	0.43
3:A:730:LEU:HD13	6:O:719:ARG:HD2	2.00	0.43
3:A:1595:HIS:CE1	3:A:1598:ASP:HB2	2.54	0.43
6:O:586:SER:HA	6:O:589:GLU:HG2	2.00	0.43
3:A:89:TYR:HB3	6:O:536:THR:HG23	2.01	0.42
3:A:746:ASN:OD1	3:A:746:ASN:N	2.52	0.42
4:N:350:ASP:N	4:N:350:ASP:OD1	2.52	0.42
4:N:352:PRO:HA	4:N:355:ARG:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:165:ILE:H	5:I:165:ILE:HG13	1.65	0.42
6:O:460:GLN:OE1	6:O:496:ARG:NH2	2.44	0.42
7:Q:509:ARG:HD2	7:Q:512:ASP:HB2	2.01	0.42
15:R:320:ASP:OD1	15:R:320:ASP:N	2.48	0.42
15:R:401:GLN:HE22	15:R:445:ARG:HD2	1.83	0.42
3:A:491:LEU:HD13	3:A:584:ILE:HD11	2.00	0.42
4:N:112:LEU:HD13	4:N:243:LEU:HD22	2.01	0.42
5:I:80:LEU:O	5:I:92:LEU:HA	2.18	0.42
7:K:423:LYS:HB3	7:K:423:LYS:HE3	1.85	0.42
3:A:456:LYS:HE2	3:A:456:LYS:HB3	1.90	0.42
5:I:320:LEU:HD12	5:I:324:GLN:HB3	2.02	0.42
14:U:513:PHE:HA	14:U:516:LEU:HB2	2.00	0.42
15:R:176:LEU:HD11	15:R:469:LEU:HB2	2.00	0.42
3:A:226:LYS:HB2	3:A:236:VAL:HG22	2.00	0.42
3:A:1241:THR:HG22	3:A:1242:GLU:H	1.85	0.42
12:J:682:LEU:HD23	12:J:682:LEU:HA	1.91	0.42
13:Y:61:LEU:HD23	13:Y:61:LEU:HA	1.91	0.42
14:U:389:ARG:NH1	14:U:421:TYR:OH	2.49	0.42
1:L:6:LYS:HA	1:L:114:VAL:HG13	2.00	0.42
1:L:129:LYS:HA	1:L:129:LYS:HD3	1.93	0.42
3:A:1413:LEU:HD23	3:A:1413:LEU:HA	1.88	0.42
4:N:253:LEU:O	4:N:257:SER:OG	2.29	0.42
10:M:34:ASN:HB3	10:M:51:LYS:HB2	2.00	0.42
7:Q:35:GLU:HB3	7:Q:40:ILE:HD11	2.00	0.42
7:Q:373:TYR:HD1	7:Q:376:LEU:HD12	1.84	0.42
13:Y:433:VAL:HG21	13:Y:446:LEU:HD23	2.00	0.42
13:Z:384:ARG:NH2	13:Z:412:GLY:O	2.52	0.42
3:A:1622:VAL:HA	3:A:1629:PRO:HA	2.02	0.42
4:N:694:ARG:O	4:N:697:SER:OG	2.37	0.42
12:P:526:ARG:NH2	12:P:558:ASP:OD1	2.46	0.42
13:Z:341:PRO:HA	13:Z:344:VAL:HG12	2.01	0.42
15:R:232:VAL:HG22	15:R:243:VAL:HG12	2.02	0.42
15:R:329:ASN:O	16:S:27:GLN:NE2	2.53	0.42
15:R:330:ASP:OD1	15:R:330:ASP:N	2.40	0.42
3:A:940:THR:OG1	3:A:941:LEU:N	2.52	0.42
4:N:31:LEU:HD22	4:N:128:SER:HB3	2.02	0.42
5:I:441:THR:OG1	5:I:442:GLN:N	2.53	0.42
5:I:628:THR:HG23	5:I:630:LYS:H	1.84	0.42
7:K:40:ILE:HG21	7:K:63:ARG:HD2	2.01	0.42
3:A:464:THR:OG1	3:A:465:GLN:OE1	2.38	0.42
4:N:325:ARG:HA	4:N:328:VAL:HG12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:653:LEU:HD12	5:I:667:VAL:HG21	2.02	0.42
12:J:570:TRP:HB2	12:J:593:ALA:HB2	2.02	0.42
7:Q:64:LYS:HE2	7:Q:64:LYS:HB3	1.83	0.42
15:R:335:VAL:HG12	15:R:348:LEU:HD12	2.01	0.42
1:L:78:CYS:SG	1:L:121:HIS:ND1	2.89	0.42
3:A:949:PHE:O	3:A:953:LEU:HB2	2.19	0.42
12:J:70:GLN:H	12:J:70:GLN:HG2	1.71	0.42
13:Z:267:LEU:HD23	13:Z:267:LEU:HA	1.90	0.42
15:R:294:ASP:HB2	15:R:300:HIS:HA	2.02	0.42
15:R:319:PRO:HD3	15:R:363:TRP:HB3	2.02	0.42
3:A:135:GLN:NE2	14:V:482:GLU:OE1	2.53	0.42
3:A:863:LEU:HD12	3:A:863:LEU:HA	1.85	0.42
4:N:633:ARG:HH21	8:C:46:LEU:HD11	1.85	0.42
5:I:246:PRO:HA	5:I:249:THR:HG22	2.02	0.42
5:I:517:TYR:HB3	5:I:520:LYS:HB2	2.01	0.42
6:O:31:THR:HG23	6:O:34:LYS:H	1.85	0.42
6:O:279:ASP:HB3	14:V:389:ARG:HG3	2.02	0.42
12:P:170:PHE:HD2	12:P:456:LYS:HD2	1.85	0.42
7:Q:28:LYS:HD3	7:Q:28:LYS:HA	1.80	0.42
4:N:252:LEU:HB2	4:N:255:ARG:HB3	2.01	0.41
10:M:2:ASP:O	14:U:120:TYR:OH	2.34	0.41
7:Q:499:VAL:HG23	7:Q:519:LEU:HD11	2.00	0.41
13:Z:444:LEU:HB3	13:Z:464:LEU:HB3	2.02	0.41
3:A:940:THR:HG23	3:A:943:ASP:H	1.85	0.41
5:I:188:TYR:CZ	5:I:194:LYS:HB2	2.55	0.41
6:O:291:ASN:HB3	6:O:298:ARG:HH22	1.85	0.41
14:V:426:HIS:HB2	14:V:435:MET:HB3	2.02	0.41
13:Z:480:VAL:HG13	13:Z:514:ILE:HD13	2.01	0.41
2:D:50:ASN:OD1	2:D:50:ASN:N	2.53	0.41
4:N:243:LEU:HD13	4:N:243:LEU:HA	1.85	0.41
4:N:639:HIS:CD2	4:N:661:PRO:HB2	2.56	0.41
7:K:14:LEU:HD23	7:K:14:LEU:HA	1.87	0.41
14:U:311:SER:O	14:U:311:SER:OG	2.33	0.41
14:V:301:ASP:O	14:V:304:SER:OG	2.38	0.41
14:V:552:GLN:HG2	14:V:556:LEU:HD12	2.03	0.41
13:Z:316:ALA:HB2	13:Z:324:VAL:HG21	2.02	0.41
15:R:191:ASP:OD1	15:R:191:ASP:N	2.53	0.41
3:A:138:SER:N	3:A:142:TYR:OH	2.45	0.41
3:A:478:ASP:OD2	3:A:587:ILE:N	2.49	0.41
4:N:425:ARG:HH22	4:N:504:LEU:HB3	1.85	0.41
4:N:428:LEU:HD23	4:N:428:LEU:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:657:VAL:HG22	4:N:659:VAL:HB	2.01	0.41
6:O:546:ARG:HA	6:O:549:VAL:HG12	2.02	0.41
12:J:617:LEU:HD23	12:J:644:ILE:HG23	2.02	0.41
3:A:35:LEU:HD23	3:A:35:LEU:HA	1.87	0.41
3:A:1667:LYS:HB3	3:A:1667:LYS:HE3	1.91	0.41
4:N:539:ILE:HD13	4:N:561:LEU:HD23	2.02	0.41
5:I:393:VAL:O	5:I:397:ILE:HG13	2.21	0.41
6:O:16:ASN:HB3	6:O:19:VAL:HG22	2.01	0.41
7:Q:227:LEU:HD23	7:Q:227:LEU:HA	1.93	0.41
13:Z:365:ALA:O	13:Z:369:ASN:N	2.45	0.41
3:A:1734:LYS:HA	3:A:1734:LYS:HD3	1.84	0.41
3:A:1922:LYS:HE2	3:A:1922:LYS:HB3	1.82	0.41
4:N:181:LEU:HD13	4:N:299:TRP:CD2	2.56	0.41
4:N:335:ILE:HD13	4:N:335:ILE:HG21	1.87	0.41
4:N:596:LEU:HD12	4:N:601:TRP:CD2	2.56	0.41
7:K:491:LEU:HD22	9:W:22:ILE:HD12	2.03	0.41
8:C:7:CYS:SG	8:C:8:TRP:N	2.94	0.41
12:J:716:ASN:HB3	12:J:718:LYS:HE3	2.01	0.41
13:Y:57:SER:HG	13:Y:83:HIS:HD1	1.68	0.41
14:U:71:GLN:H	14:U:71:GLN:HG2	1.71	0.41
14:U:297:ILE:HD11	14:U:333:THR:HB	2.02	0.41
1:L:22:VAL:HB	1:L:159:TYR:HB3	2.03	0.41
3:A:1481:ASN:HB3	3:A:1484:ALA:HB3	2.02	0.41
3:A:1794:ASP:N	3:A:1794:ASP:OD1	2.53	0.41
13:Z:539:ASP:OD1	13:Z:539:ASP:N	2.53	0.41
3:A:1013:ASP:OD1	3:A:1017:ASN:ND2	2.42	0.41
5:I:20:PRO:O	5:I:739:ARG:NH2	2.54	0.41
5:I:228:ALA:HA	5:I:559:ASP:O	2.21	0.41
7:Q:7:ARG:NH2	7:Q:39:ASP:OD2	2.44	0.41
13:Y:509:CYS:SG	13:Y:510:VAL:N	2.94	0.41
13:Z:322:GLU:O	13:Z:326:ASN:ND2	2.53	0.41
1:L:130:LYS:HD3	1:L:130:LYS:HA	1.75	0.41
3:A:39:LEU:HD13	6:O:244:LEU:HD13	2.02	0.41
3:A:833:HIS:HA	3:A:834:PRO:HD3	1.91	0.41
3:A:872:LEU:HD12	3:A:937:VAL:HG11	2.02	0.41
3:A:1026:LEU:HD11	3:A:1629:PRO:HB2	2.03	0.41
3:A:1201:HIS:ND1	3:A:1204:THR:OG1	2.45	0.41
3:A:1653:ALA:O	3:A:1655:THR:N	2.54	0.41
3:A:1776:TYR:CZ	3:A:1780:THR:HG21	2.56	0.41
5:I:584:HIS:O	5:I:602:ARG:HA	2.20	0.41
6:O:435:SER:H	6:O:654:ASP:HB3	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:73:CYS:HA	8:C:80:TRP:HE1	1.86	0.41
12:J:521:ILE:HD13	12:J:521:ILE:HA	1.94	0.41
12:P:93:SER:O	12:P:93:SER:OG	2.30	0.41
12:P:94:GLY:HA3	12:P:100:GLN:HA	2.03	0.41
7:Q:60:LEU:HD22	7:Q:72:CYS:HB3	2.03	0.41
7:Q:325:LYS:HD2	7:Q:325:LYS:HA	1.79	0.41
13:Y:36:ASN:HB3	13:Z:230:VAL:HG12	2.03	0.41
13:Y:270:ASN:HA	13:Z:62:THR:HG21	2.02	0.41
13:Y:293:LYS:HD3	13:Y:293:LYS:HA	1.87	0.41
13:Y:483:ALA:HB2	13:Y:499:LEU:HD11	2.03	0.41
14:V:58:LEU:HD23	14:V:58:LEU:HA	1.87	0.41
13:Z:85:ASP:OD1	13:Z:100:TYR:OH	2.28	0.41
13:Z:225:ASN:OD1	13:Z:225:ASN:N	2.54	0.41
15:R:236:LYS:HB2	15:R:236:LYS:HE2	1.76	0.41
3:A:586:SER:OG	3:A:587:ILE:N	2.53	0.41
3:A:1111:ALA:O	3:A:1115:ASN:CA	2.68	0.41
3:A:1189:ALA:HB3	3:A:1192:ASN:HD22	1.86	0.41
3:A:1818:LEU:HD23	3:A:1818:LEU:HA	1.90	0.41
5:I:319:THR:O	5:I:323:ASN:HB2	2.21	0.41
5:I:488:SER:O	5:I:488:SER:OG	2.39	0.41
12:J:140:LYS:HD2	12:J:140:LYS:HA	1.79	0.41
12:J:566:SER:OG	12:J:568:GLU:OE1	2.38	0.41
14:V:494:ILE:HD13	14:V:494:ILE:HA	1.95	0.41
15:R:275:SER:HB3	15:R:317:TRP:HD1	1.86	0.41
3:A:1208:LEU:HD23	3:A:1208:LEU:HA	1.90	0.40
3:A:1434:ILE:HG12	3:A:1457:LEU:HD22	2.03	0.40
12:J:633:ARG:HA	12:J:664:ILE:HD13	2.03	0.40
7:Q:177:THR:OG1	7:Q:178:ALA:N	2.54	0.40
14:V:429:ARG:HB3	14:V:432:ASP:HB2	2.03	0.40
15:R:446:VAL:HA	15:R:462:ALA:HA	2.03	0.40
1:L:96:VAL:HG13	1:L:137:ILE:HD11	2.03	0.40
2:D:48:ASP:OD1	2:D:48:ASP:N	2.54	0.40
3:A:893:SER:OG	3:A:894:GLN:N	2.54	0.40
3:A:963:ARG:NH2	3:A:1782:GLU:O	2.53	0.40
4:N:397:ILE:O	4:N:401:ILE:HG13	2.22	0.40
5:I:603:ARG:HA	5:I:611:VAL:HG11	2.03	0.40
6:O:674:SER:O	6:O:674:SER:OG	2.37	0.40
6:O:710:ILE:HA	6:O:713:VAL:HG12	2.02	0.40
7:K:295:TYR:HE1	7:Q:52:GLN:HG2	1.85	0.40
12:P:736:GLU:OE1	12:P:736:GLU:N	2.54	0.40
7:Q:19:TYR:HB3	7:Q:50:THR:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:53:TYR:HB3	1:L:154:ARG:HG2	2.03	0.40
3:A:625:ILE:HG12	3:A:762:ILE:HD12	2.04	0.40
3:A:1420:LEU:HA	3:A:1421:PRO:HD3	1.90	0.40
4:N:134:LYS:HE3	4:N:134:LYS:HB3	1.98	0.40
4:N:184:TYR:HD1	4:N:237:LEU:HD11	1.87	0.40
4:N:598:SER:H	8:C:31:ASN:HD21	1.69	0.40
4:N:636:SER:O	8:C:13:THR:N	2.52	0.40
14:U:363:ARG:HG2	14:U:394:VAL:HG13	2.02	0.40
2:D:20:LEU:HD13	6:O:252:GLU:HG2	2.03	0.40
3:A:20:PHE:HB2	3:A:606:ARG:HG2	2.03	0.40
3:A:1373:MET:HA	3:A:1376:LEU:HD12	2.04	0.40
5:I:7:CYS:HB2	5:I:628:THR:HA	2.04	0.40
5:I:296:THR:OG1	5:I:297:THR:N	2.54	0.40
5:I:302:ASP:HB2	6:O:58:ARG:HD2	2.03	0.40
9:G:12:LYS:NZ	9:G:15:ASP:OD1	2.39	0.40
11:H:95:ARG:HH12	12:J:565:ASN:HB3	1.86	0.40
13:Y:363:ALA:HA	13:Y:366:ILE:HG22	2.04	0.40
14:U:412:LEU:HD23	14:U:412:LEU:HA	1.92	0.40
14:V:330:ARG:HB2	14:V:333:THR:HG22	2.03	0.40
3:A:98:ASN:HA	3:A:123:VAL:HG23	2.03	0.40
3:A:1114:ARG:H	3:A:1114:ARG:HD3	1.85	0.40
3:A:1619:LEU:HD23	3:A:1634:LEU:HD21	2.03	0.40
4:N:436:ARG:H	4:N:436:ARG:HG3	1.65	0.40
6:O:439:LEU:HG	6:O:476:LEU:HD13	2.02	0.40
7:K:84:LYS:HA	7:K:84:LYS:HD3	1.92	0.40
7:K:181:GLU:HG2	7:K:209:LEU:HD11	2.02	0.40
7:Q:275:LEU:HD22	7:Q:280:LYS:HB2	2.04	0.40
13:Y:62:THR:HG21	13:Z:270:ASN:HA	2.03	0.40
13:Y:451:CYS:HB2	13:Y:461:ALA:HB2	2.02	0.40
13:Y:538:LEU:HD23	13:Y:538:LEU:HA	1.89	0.40
14:V:436:LEU:HD23	14:V:436:LEU:HA	1.96	0.40
13:Z:368:LEU:HD23	13:Z:368:LEU:HA	1.93	0.40
15:R:349:GLN:NE2	15:R:387:VAL:O	2.47	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	175/185 (95%)	163 (93%)	12 (7%)	0	100	100
2	D	55/121 (46%)	50 (91%)	5 (9%)	0	100	100
3	A	1515/1855 (82%)	1404 (93%)	111 (7%)	0	100	100
4	N	639/822 (78%)	607 (95%)	32 (5%)	0	100	100
5	I	721/808 (89%)	683 (95%)	38 (5%)	0	100	100
6	O	695/755 (92%)	674 (97%)	21 (3%)	0	100	100
7	K	512/620 (83%)	497 (97%)	15 (3%)	0	100	100
7	Q	500/620 (81%)	482 (96%)	18 (4%)	0	100	100
8	C	82/84 (98%)	74 (90%)	8 (10%)	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	57/74 (77%)	55 (96%)	2 (4%)	0	100	100
11	H	55/110 (50%)	55 (100%)	0	0	100	100
12	J	492/824 (60%)	476 (97%)	16 (3%)	0	100	100
12	P	480/824 (58%)	467 (97%)	13 (3%)	0	100	100
13	Y	496/599 (83%)	485 (98%)	11 (2%)	0	100	100
13	Z	483/599 (81%)	475 (98%)	8 (2%)	0	100	100
14	U	509/597 (85%)	488 (96%)	21 (4%)	0	100	100
14	V	526/597 (88%)	508 (97%)	18 (3%)	0	100	100
15	R	371/499 (74%)	348 (94%)	23 (6%)	0	100	100
16	S	13/394 (3%)	10 (77%)	3 (23%)	0	100	100
All	All	8425/11157 (76%)	8050 (96%)	375 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	163/170 (96%)	162 (99%)	1 (1%)	86 94
2	D	54/115 (47%)	52 (96%)	2 (4%)	34 68
3	A	1340/1639 (82%)	1336 (100%)	4 (0%)	92 96
4	N	560/724 (77%)	557 (100%)	3 (0%)	88 95
5	I	635/730 (87%)	635 (100%)	0	100 100
6	O	591/650 (91%)	589 (100%)	2 (0%)	92 96
7	K	445/548 (81%)	444 (100%)	1 (0%)	93 98
7	Q	426/548 (78%)	425 (100%)	1 (0%)	93 98
8	C	68/75 (91%)	66 (97%)	2 (3%)	42 74
9	G	24/77 (31%)	24 (100%)	0	100 100
9	W	25/77 (32%)	25 (100%)	0	100 100
10	M	54/67 (81%)	54 (100%)	0	100 100
11	H	49/89 (55%)	49 (100%)	0	100 100
12	J	420/727 (58%)	419 (100%)	1 (0%)	93 98
12	P	414/727 (57%)	414 (100%)	0	100 100
13	Y	424/513 (83%)	423 (100%)	1 (0%)	93 98
13	Z	412/513 (80%)	412 (100%)	0	100 100
14	U	423/520 (81%)	423 (100%)	0	100 100
14	V	448/520 (86%)	445 (99%)	3 (1%)	84 94
15	R	305/411 (74%)	303 (99%)	2 (1%)	84 94
16	S	16/348 (5%)	16 (100%)	0	100 100
All	All	7296/9788 (74%)	7273 (100%)	23 (0%)	92 96

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	25	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	22[A]	ARG
2	D	22[B]	ARG
3	A	151	ILE
3	A	1114	ARG
3	A	1334	ARG
3	A	1475	ARG
4	N	291	LYS
4	N	562	LYS
4	N	639	HIS
6	O	106	LYS
6	O	232	THR
7	K	192	LYS
8	C	2	LYS
8	C	39	VAL
12	J	99	LYS
7	Q	451	LEU
13	Y	388	ARG
14	V	297	ILE
14	V	434	ARG
14	V	521	PHE
15	R	388[A]	CYS
15	R	388[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	144	ASN
3	A	38	GLN
3	A	75	GLN
3	A	125	GLN
3	A	162	HIS
3	A	176	GLN
3	A	179	ASN
3	A	215	HIS
3	A	426	GLN
3	A	449	GLN
3	A	451	GLN
3	A	473	ASN
3	A	643	ASN
3	A	666	ASN
3	A	722	HIS
3	A	725	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	792	GLN
3	A	1138	HIS
3	A	1161	ASN
3	A	1170	ASN
3	A	1184	HIS
3	A	1192	ASN
3	A	1262	GLN
3	A	1309	HIS
3	A	1327	GLN
3	A	1543	HIS
3	A	1604	GLN
3	A	1813	GLN
4	N	186	GLN
4	N	235	GLN
4	N	248	HIS
4	N	541	ASN
5	I	292	GLN
5	I	323	ASN
5	I	405	GLN
5	I	503	ASN
5	I	506	HIS
5	I	577	ASN
5	I	578	ASN
5	I	684	GLN
6	O	91	ASN
6	O	150	GLN
6	O	291	ASN
6	O	424	GLN
6	O	440	GLN
6	O	449	ASN
6	O	512	GLN
6	O	552	GLN
6	O	671	GLN
6	O	693	ASN
6	O	722	HIS
6	O	731	ASN
7	K	174	HIS
7	K	271	HIS
7	K	318	HIS
7	K	352	GLN
7	K	382	ASN
7	K	557	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	C	31	ASN
12	J	486	ASN
12	J	497	ASN
12	J	583	HIS
12	J	674	HIS
12	J	702	ASN
12	J	773	ASN
12	P	98	ASN
12	P	680	HIS
12	P	702	ASN
12	P	759	ASN
7	Q	16	GLN
7	Q	58	HIS
7	Q	80	HIS
7	Q	316	ASN
7	Q	342	HIS
7	Q	503	HIS
13	Y	66	ASN
13	Y	270	ASN
13	Y	385	ASN
13	Y	431	ASN
13	Y	442	GLN
13	Y	506	GLN
14	U	299	ASN
14	U	321	HIS
14	V	104	HIS
14	V	202	HIS
14	V	287	ASN
14	V	305	ASN
14	V	346	GLN
14	V	347	HIS
14	V	373	HIS
14	V	477	HIS
14	V	488	GLN
13	Z	65	ASN
13	Z	67	ASN
13	Z	106	GLN
13	Z	151	GLN
13	Z	172	ASN
13	Z	326	ASN
13	Z	338	HIS
13	Z	431	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	Z	432	ASN
15	R	204	ASN
15	R	221	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
16	S	1
15	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	33:ILE	C	72:VAL	N	27.52
1	R	388[A]:CYS	C	389:SER	N	3.12

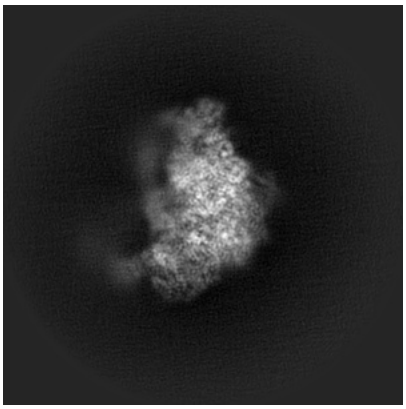
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4466. These allow visual inspection of the internal detail of the map and identification of artifacts.

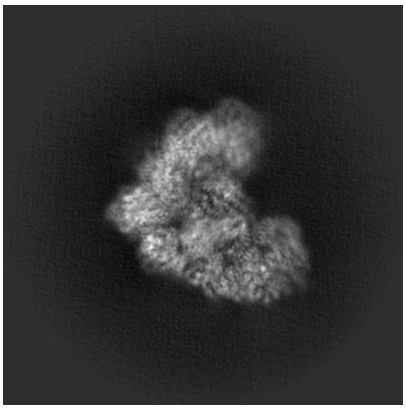
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

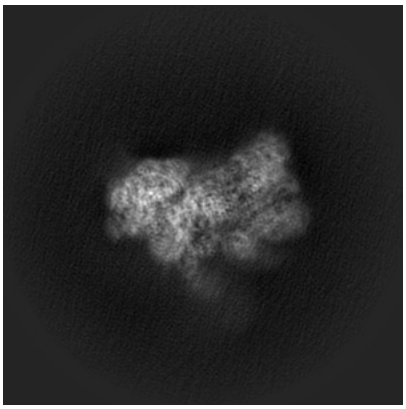
6.1.1 Primary map



X

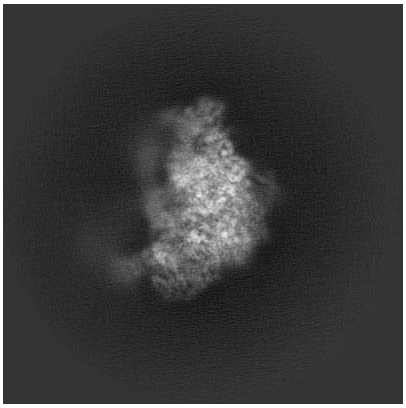


Y

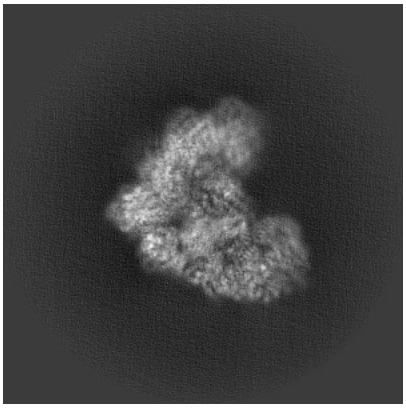


Z

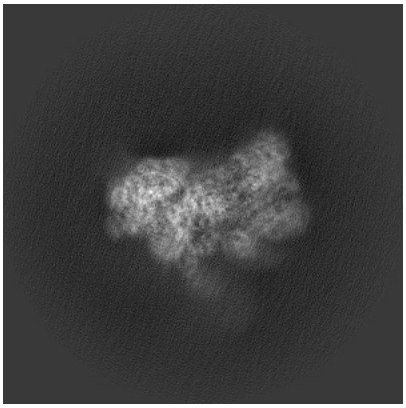
6.1.2 Raw map



X



Y

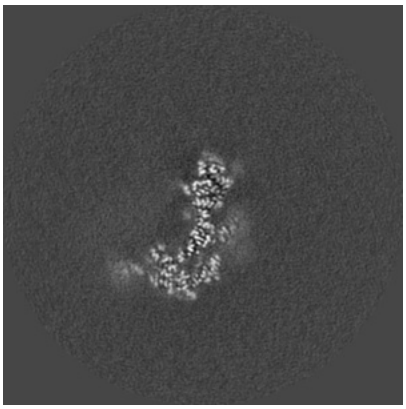


Z

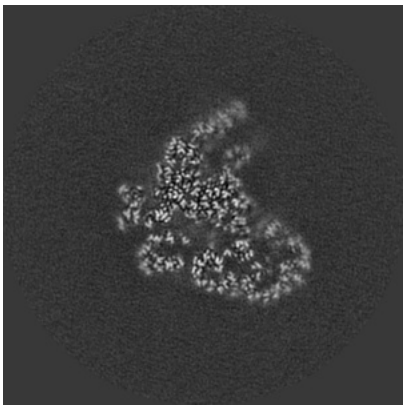
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

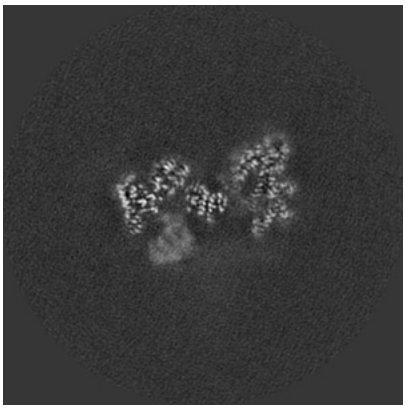
6.2.1 Primary map



X Index: 200

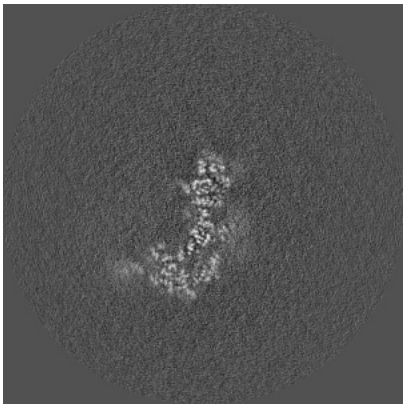


Y Index: 200

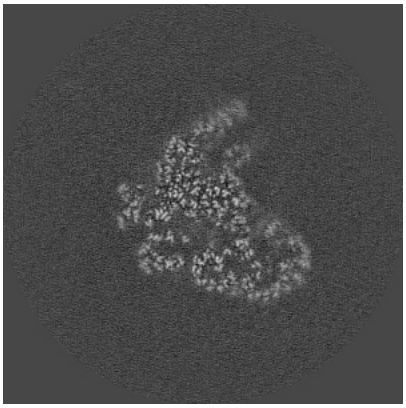


Z Index: 200

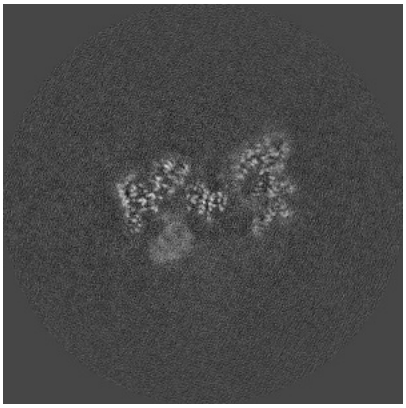
6.2.2 Raw map



X Index: 200



Y Index: 200

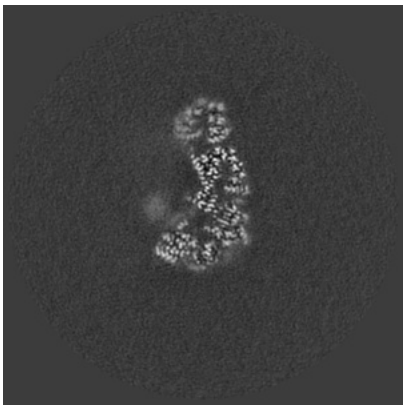


Z Index: 200

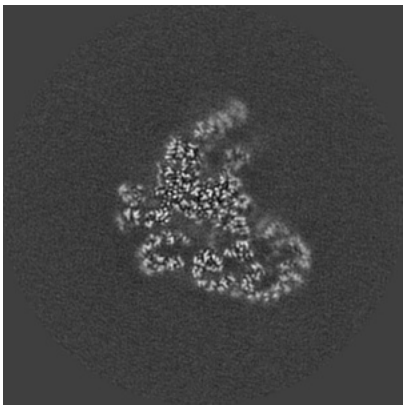
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

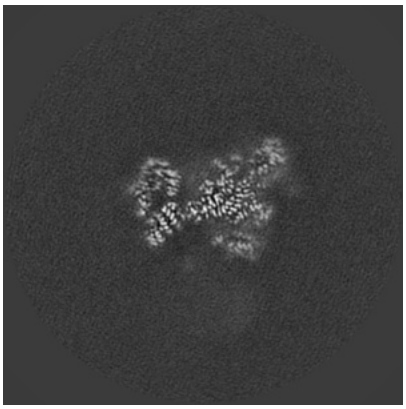
6.3.1 Primary map



X Index: 150

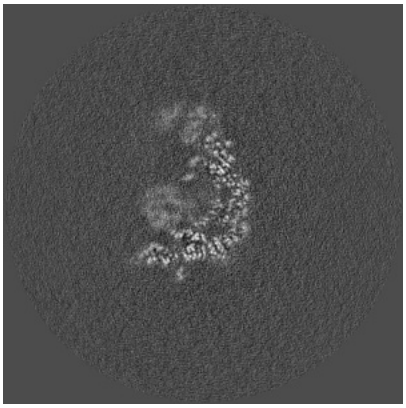


Y Index: 199

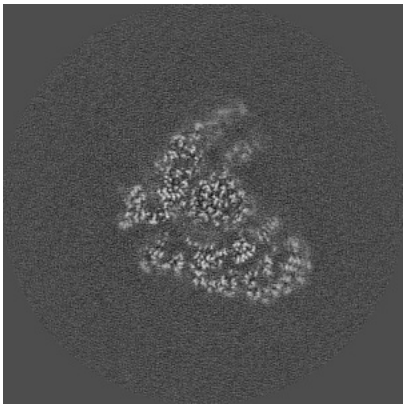


Z Index: 166

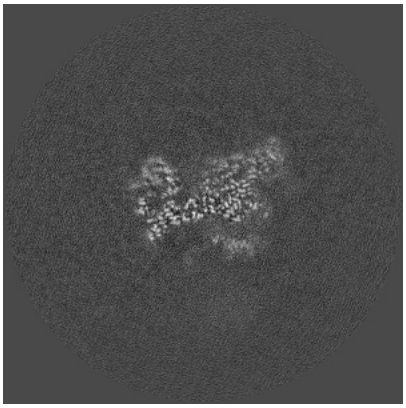
6.3.2 Raw map



X Index: 165



Y Index: 203

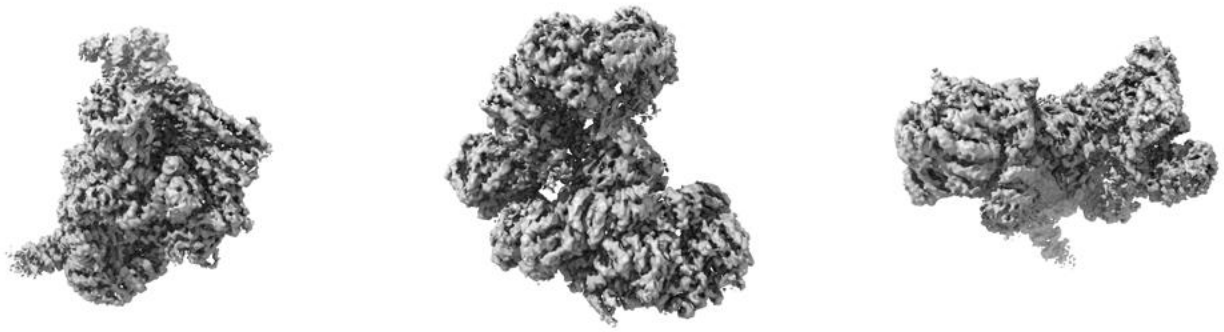


Z Index: 164

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



X Y Z

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

6.4.2 Raw map

X Y Z

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.

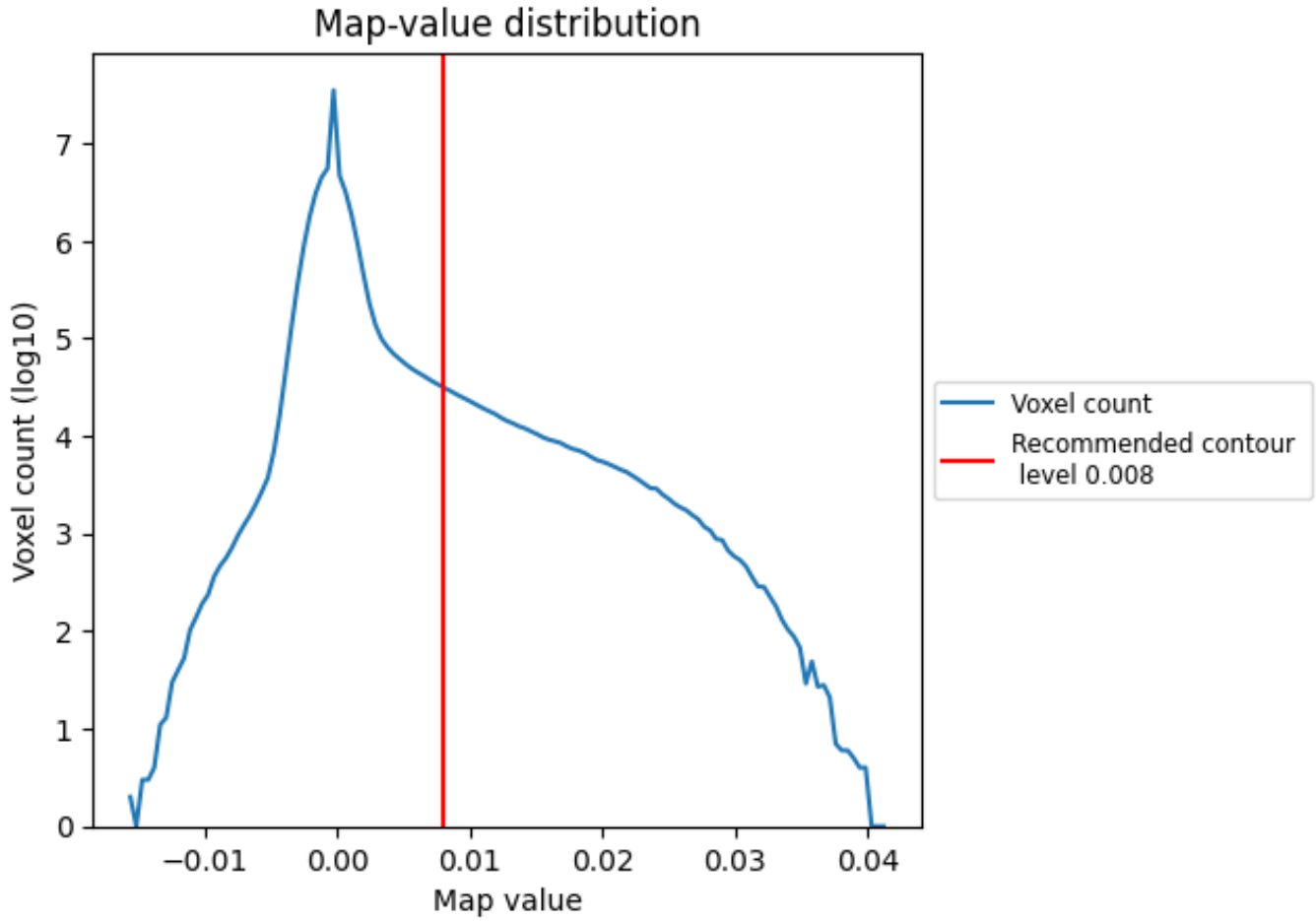
6.5 Mask visualisation (i)

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

7 Map analysis

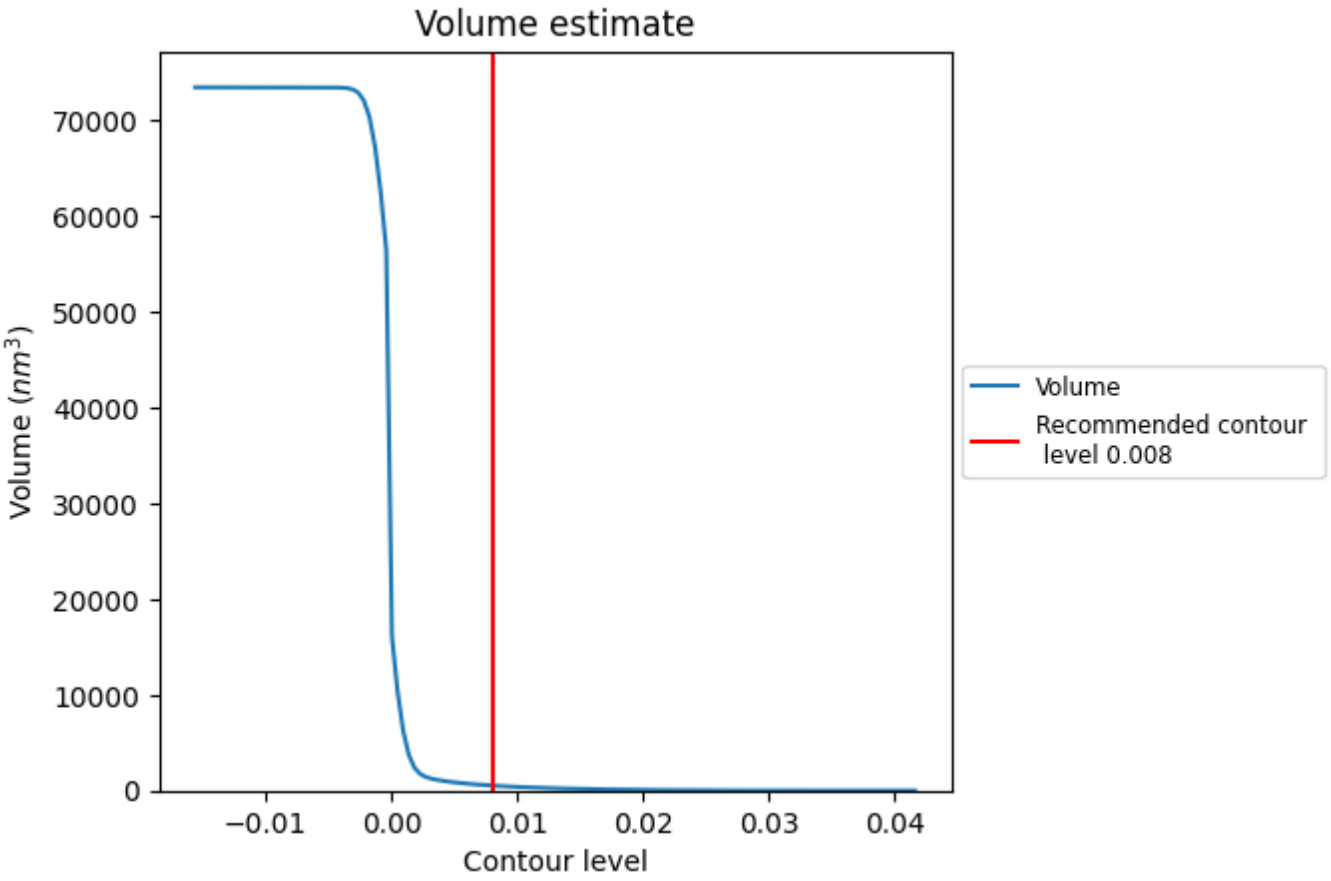
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

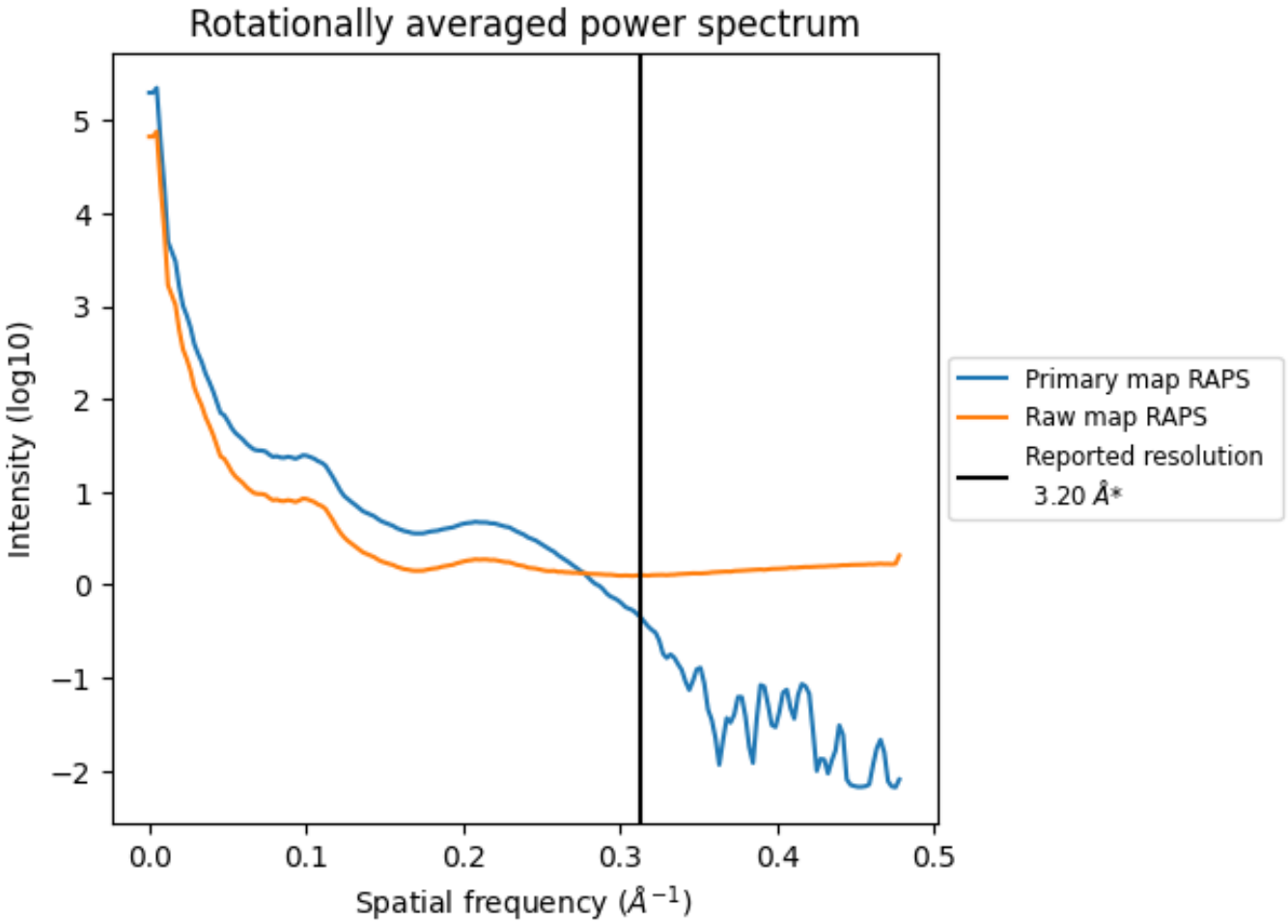
7.2 Volume estimate (i)



The volume at the recommended contour level is 522 nm^3; this corresponds to an approximate mass of 471 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)

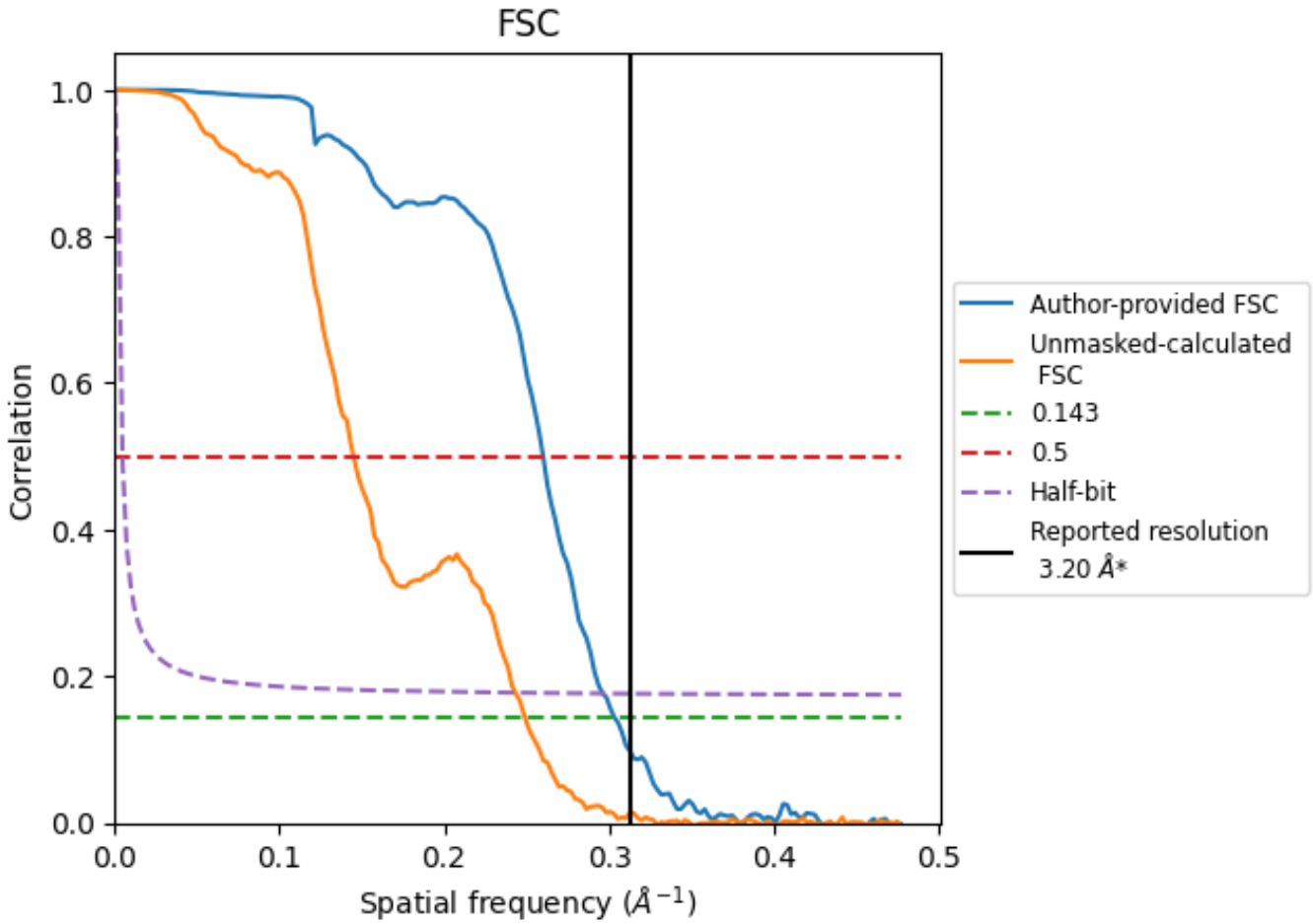


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

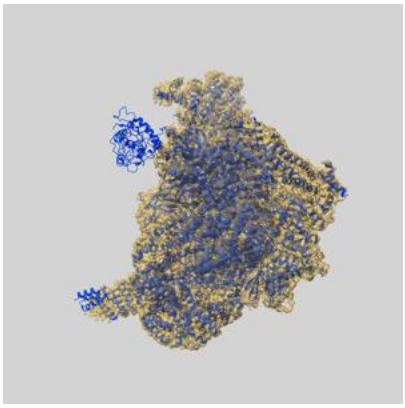
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.29	3.84	3.38
Unmasked-calculated*	4.01	6.90	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.2 by more than 10 %

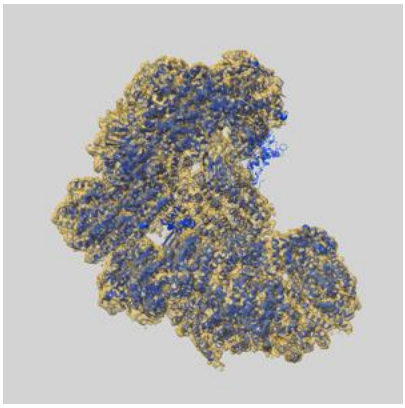
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4466 and PDB model 6Q6H. Per-residue inclusion information can be found in section 3 on page 8.

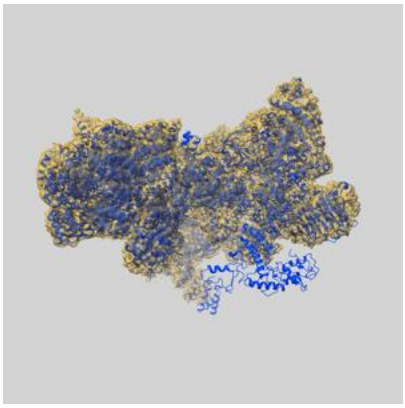
9.1 Map-model overlay



X



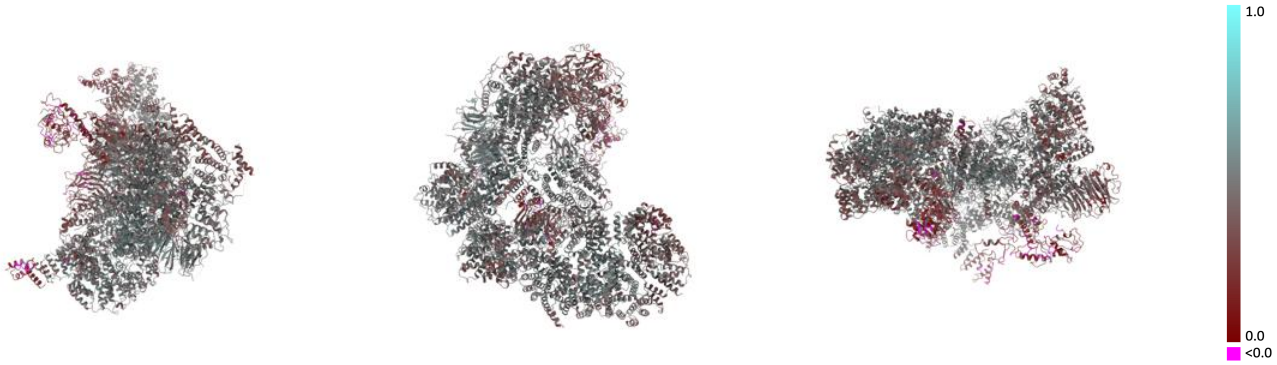
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

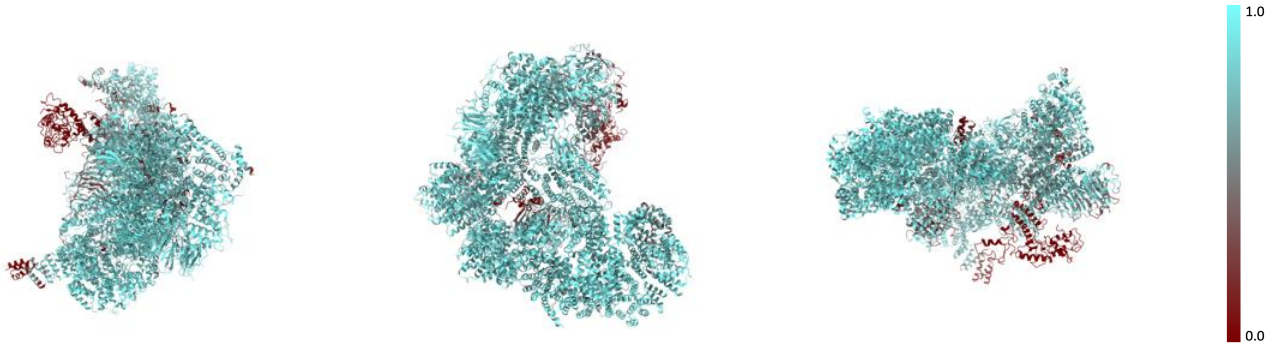
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

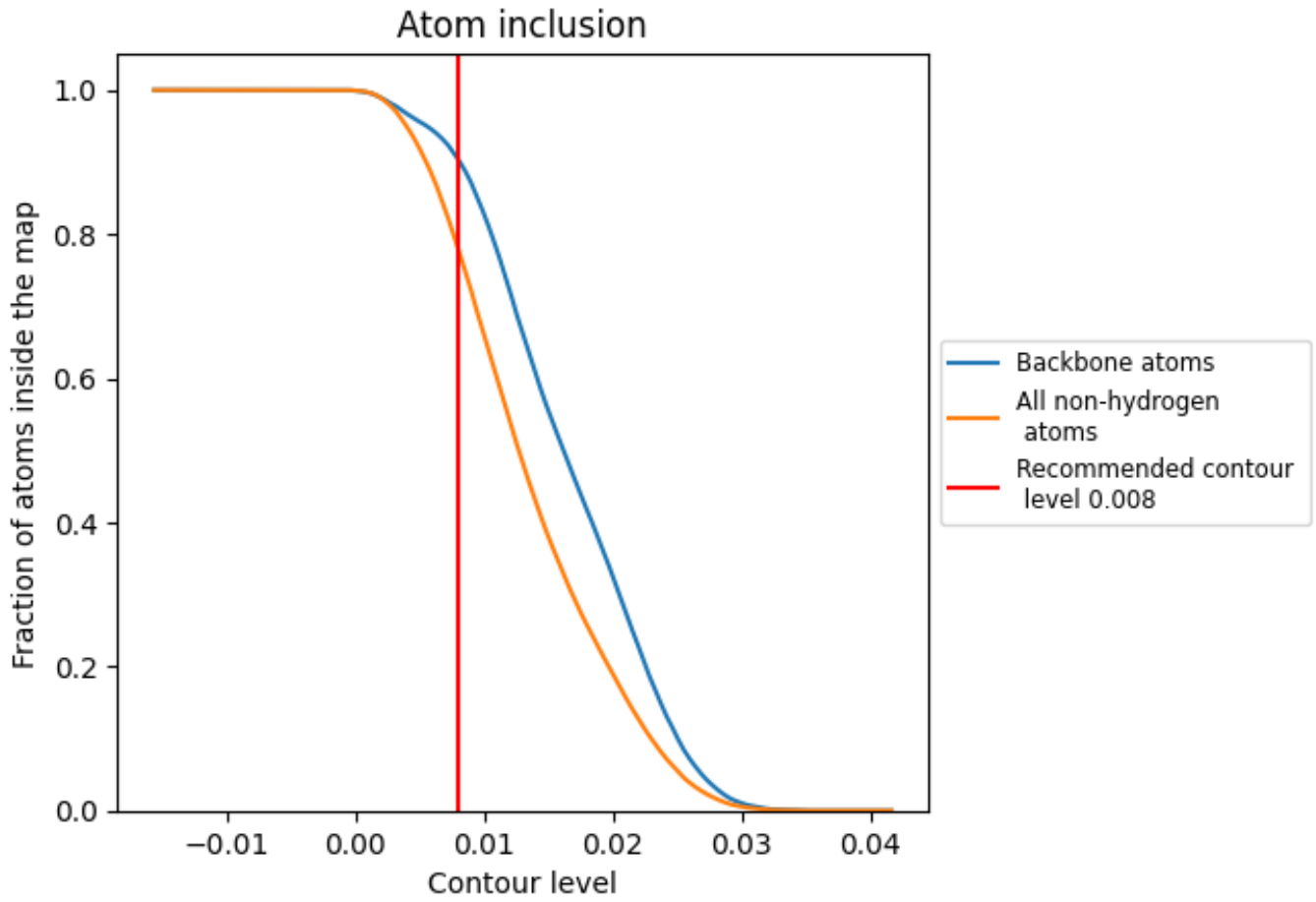
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7795	0.4340
A	0.8376	0.4710
C	0.0000	0.2030
D	0.7785	0.4920
G	0.8303	0.4860
H	0.8742	0.4810
I	0.7309	0.4020
J	0.8683	0.4890
K	0.8595	0.4600
L	0.8469	0.4490
M	0.7771	0.4970
N	0.4382	0.3090
O	0.8164	0.4750
P	0.8936	0.4950
Q	0.8908	0.4880
R	0.6171	0.2570
S	0.3284	0.2700
U	0.8000	0.4460
V	0.8030	0.4660
W	0.7880	0.4600
Y	0.8435	0.4350
Z	0.7827	0.3680