



# Full wwPDB EM Validation Report ⓘ

Mar 4, 2025 – 04:24 PM JST

PDB ID : 5XF8  
EMDB ID : EMD-6671  
Title : Cryo-EM structure of the Cdt1-MCM2-7 complex in AMPPNP state  
Authors : Zhai, Y.; Cheng, E.; Wu, H.; Li, N.; Yung, P.Y.; Gao, N.; Tye, B.K.  
Deposited on : 2017-04-09  
Resolution : 7.10 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.2

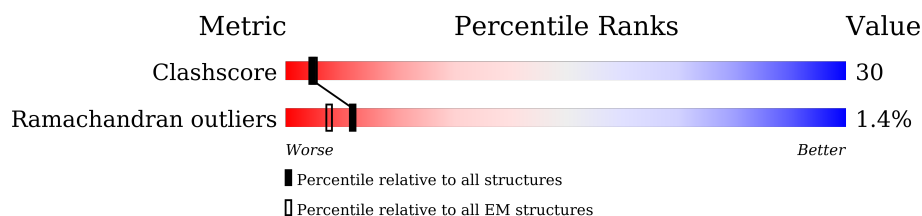
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


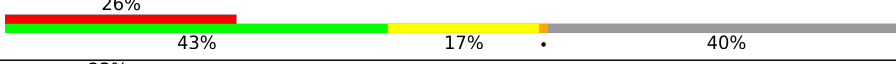
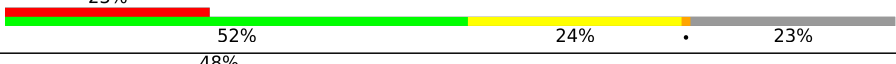

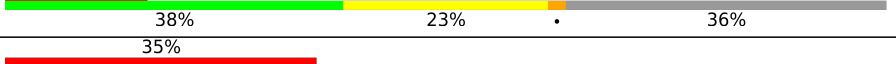
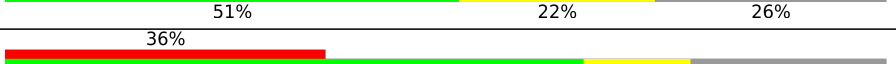
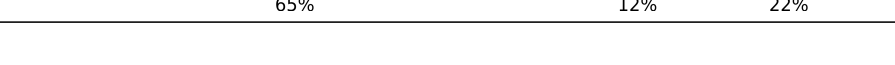
The reported resolution of this entry is 7.10 Å.

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	210492	15764
Ramachandran outliers	207382	16835

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  $\geq 3$ , 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	2	868	 19% 47% 20% . 32%
2	3	997	 26% 43% 17% . 40%
3	4	933	 23% 52% 24% . 23%
4	5	775	 48% 62% 19% 18%
5	6	1017	 16% 38% 23% . 36%
6	7	845	 35% 51% 22% 26%
7	C	604	 36% 65% 12% 22%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 21215 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2	591	Total	C	N	O	0	0
			2924	1742	591	591		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	601	Total	C	N	O	0	0
			2974	1772	601	601		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-25	MET	-	initiating methionine	UNP P24279
3	-24	ASP	-	expression tag	UNP P24279
3	-23	TYR	-	expression tag	UNP P24279
3	-22	LYS	-	expression tag	UNP P24279
3	-21	ASP	-	expression tag	UNP P24279
3	-20	HIS	-	expression tag	UNP P24279
3	-19	ASP	-	expression tag	UNP P24279
3	-18	GLY	-	expression tag	UNP P24279
3	-17	ASP	-	expression tag	UNP P24279
3	-16	TYR	-	expression tag	UNP P24279
3	-15	LYS	-	expression tag	UNP P24279
3	-14	ASP	-	expression tag	UNP P24279
3	-13	HIS	-	expression tag	UNP P24279
3	-12	ASP	-	expression tag	UNP P24279
3	-11	ILE	-	expression tag	UNP P24279
3	-10	ASP	-	expression tag	UNP P24279
3	-9	TYR	-	expression tag	UNP P24279
3	-8	LYS	-	expression tag	UNP P24279
3	-7	ASP	-	expression tag	UNP P24279
3	-6	ASP	-	expression tag	UNP P24279
3	-5	ASP	-	expression tag	UNP P24279

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Chain	Residue	Modelled	Actual	Comment	Reference
3	-4	ASP	-	expression tag	UNP P24279
3	-3	LYS	-	expression tag	UNP P24279
3	-2	GLY	-	expression tag	UNP P24279
3	-1	GLY	-	expression tag	UNP P24279
3	0	ARG	-	expression tag	UNP P24279

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	4	716	Total	C	N	O	0	0
			3551	2119	716	716		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	5	632	Total	C	N	O	0	0
			3130	1866	632	632		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	6	652	Total	C	N	O	0	0
			3230	1926	652	652		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	7	622	Total	C	N	O	0	0
			3076	1832	622	622		

- Molecule 7 is a protein called Cell division cycle protein CDT1.

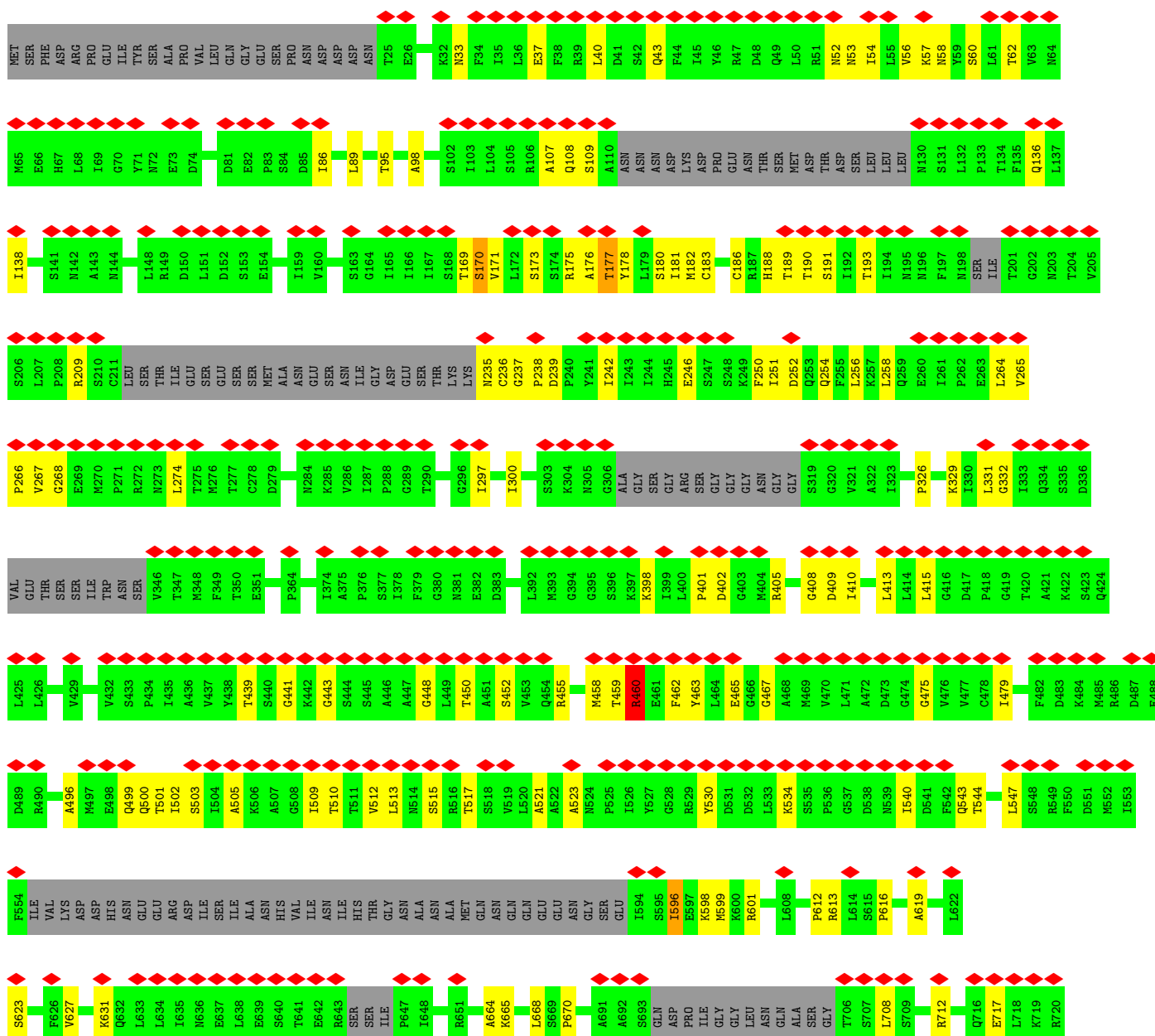
Mol	Chain	Residues	Atoms				AltConf	Trace
7	C	469	Total	C	N	O	0	0
			2330	1392	469	469		



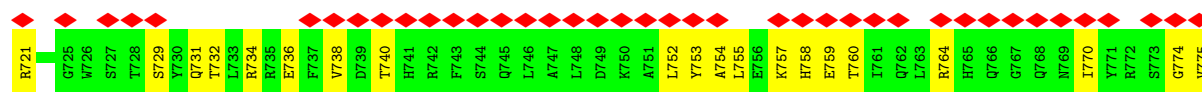




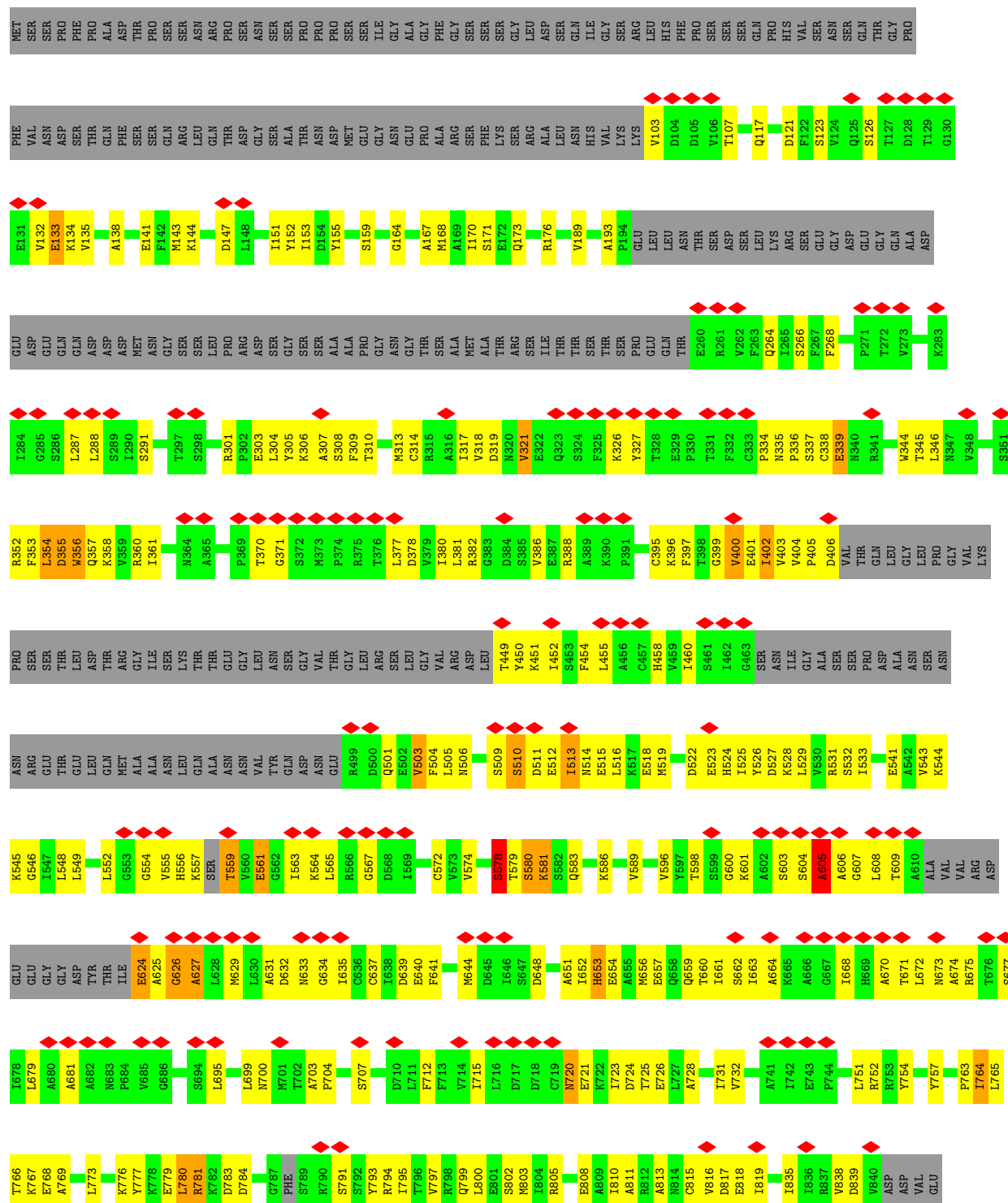
- Molecule 4: Minichromosome maintenance protein 5

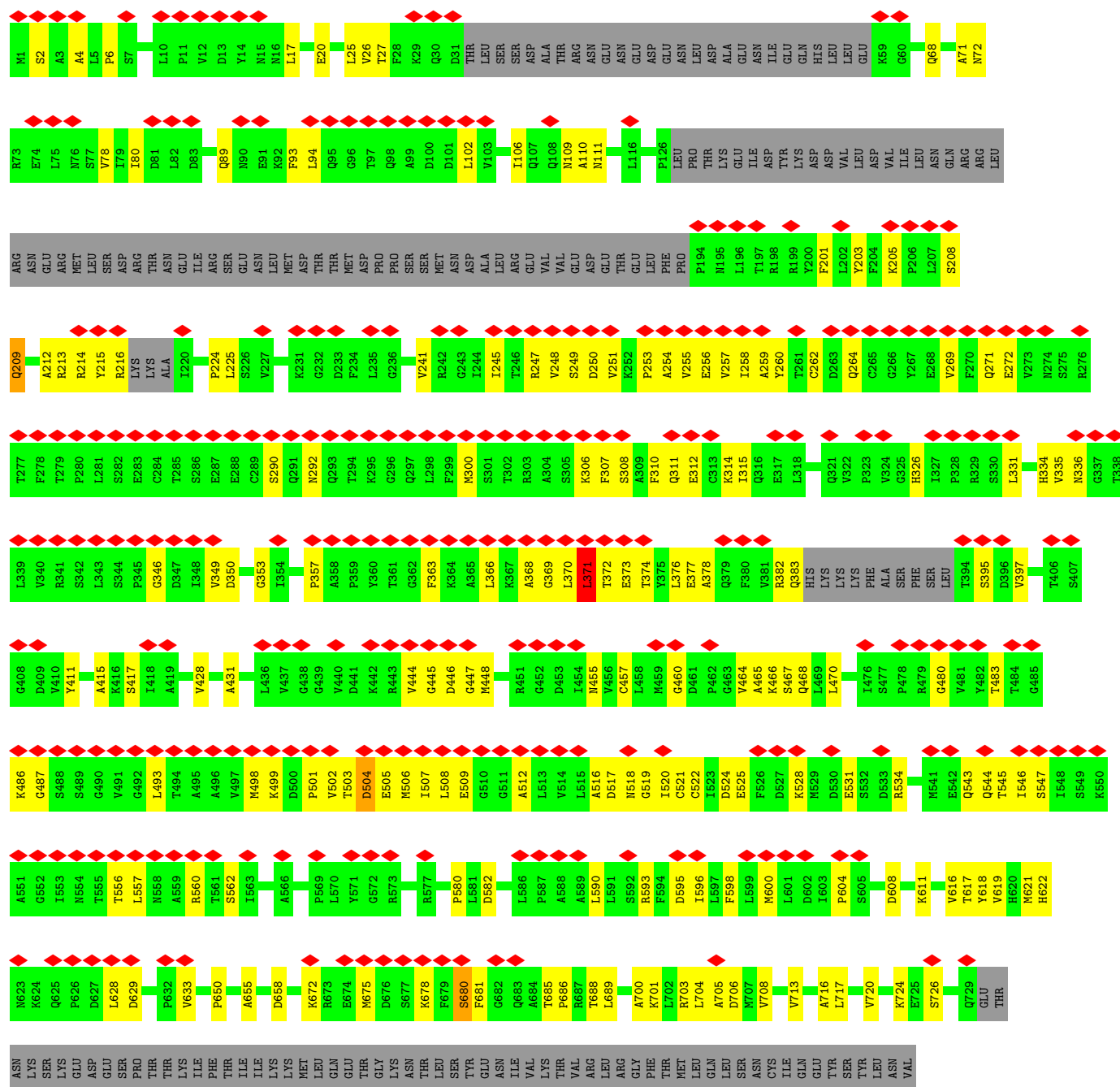




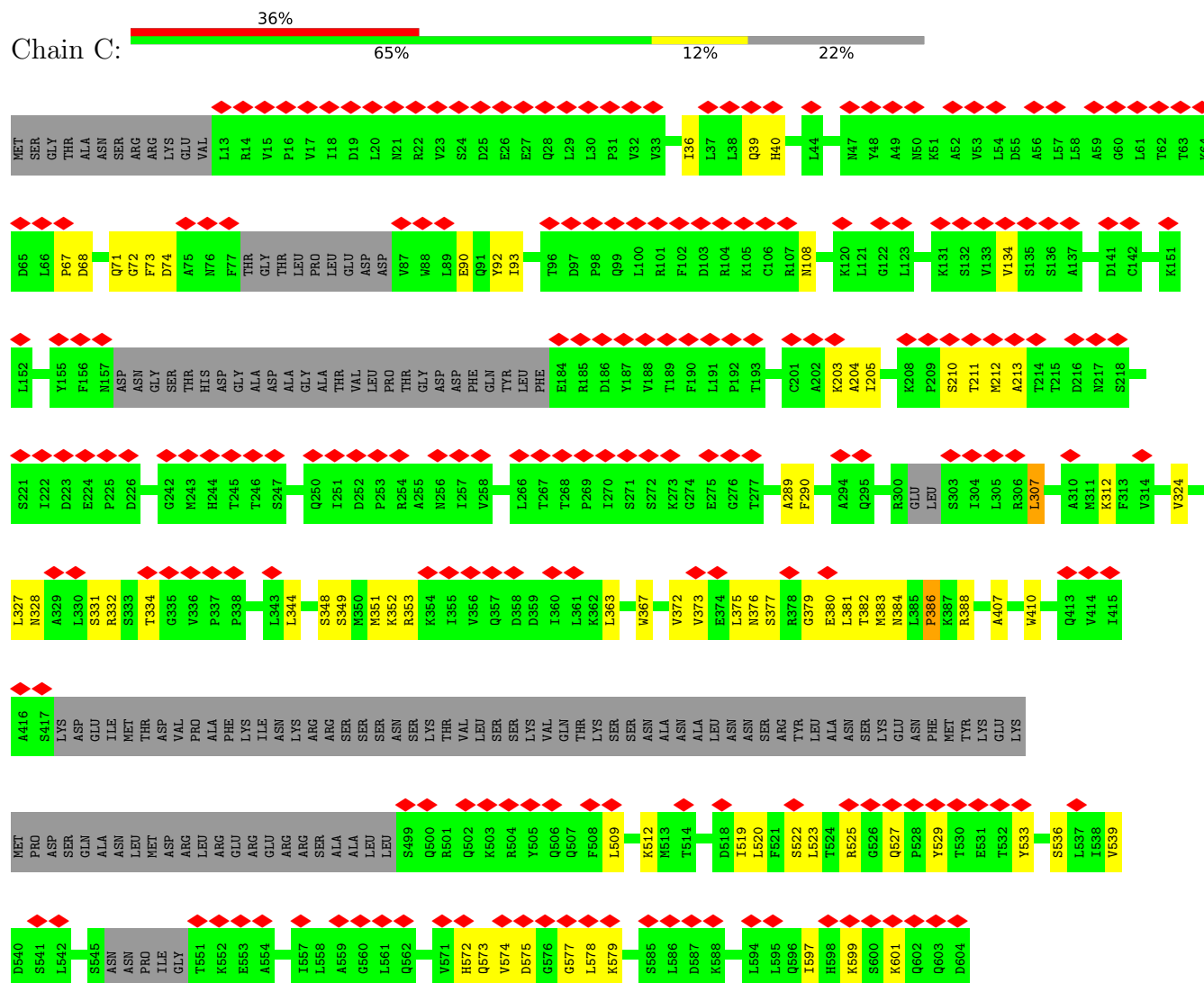


• Molecule 5: DNA replication licensing factor MCM6





## Chain C:



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	22.0	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	0.068	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0253	Depositor
Map size ( $\text{\AA}$ )	264.0, 264.0, 264.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.32, 1.32, 1.32	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	2	0.52	0/2920	0.69	3/4063 (0.1%)
2	3	0.45	0/2968	0.62	0/4127
3	4	0.51	0/3546	0.69	4/4939 (0.1%)
4	5	0.39	0/3121	0.56	0/4337
5	6	0.54	0/3221	0.77	5/4477 (0.1%)
6	7	0.46	0/3071	0.64	0/4271
7	C	0.38	0/2324	0.60	0/3235
All	All	0.47	0/21171	0.66	12/29449 (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
1	2	0	6
2	3	0	5
3	4	0	6
4	5	0	2
5	6	0	19
6	7	0	6
7	C	0	4
All	All	0	48

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	6	626	GLY	N-CA-C	-6.63	96.52	113.10
5	6	561	GLU	N-CA-C	-6.51	93.41	111.00
1	2	334	LEU	N-CA-C	-6.49	93.48	111.00
1	2	570	GLY	N-CA-C	6.27	128.77	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	920	GLY	C-N-CA	-5.95	106.81	121.70
5	6	767	LYS	N-CA-C	5.84	126.78	111.00
5	6	624	GLU	C-N-CA	-5.57	107.78	121.70
5	6	720	ASN	N-CA-C	-5.53	96.06	111.00
1	2	366	ASN	C-N-CA	5.29	134.93	121.70
3	4	919	LEU	N-CA-C	5.22	125.10	111.00
3	4	376	CYS	C-N-CA	5.21	134.73	121.70
3	4	376	CYS	CA-C-N	5.18	128.60	117.20

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	218	TYR	Peptide
1	2	298	SER	Peptide
1	2	367	CYS	Peptide
1	2	434	TYR	Peptide
1	2	588	GLU	Peptide
1	2	803	PHE	Peptide
2	3	172	THR	Peptide
2	3	237	GLU	Peptide
2	3	300	SER	Peptide
2	3	428	LEU	Peptide
2	3	498	ALA	Peptide
3	4	179	ILE	Peptide
3	4	373	ARG	Peptide
3	4	393	ASP	Peptide
3	4	408	ASP	Peptide
3	4	714	GLU	Peptide
3	4	927	VAL	Peptide
4	5	170	SER	Peptide
4	5	460	ARG	Mainchain
5	6	133	GLU	Peptide
5	6	321	VAL	Peptide
5	6	339	GLU	Peptide
5	6	354	LEU	Peptide
5	6	355	ASP	Peptide
5	6	356	TRP	Peptide
5	6	400	VAL	Peptide
5	6	402	ILE	Peptide
5	6	559	THR	Peptide
5	6	561	GLU	Peptide

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Mol	Chain	Res	Type	Group
5	6	578	SER	Peptide
5	6	581	LYS	Peptide
5	6	605	ALA	Peptide
5	6	627	ALA	Peptide
5	6	662	SER	Peptide
5	6	700	ASN	Peptide
5	6	764	ILE	Peptide
5	6	780	LEU	Peptide
5	6	972	ASP	Peptide
6	7	209	GLN	Peptide
6	7	371	LEU	Peptide
6	7	504	ASP	Peptide
6	7	678	LYS	Peptide
6	7	680	SER	Peptide
6	7	94	LEU	Peptide
7	C	307	LEU	Peptide
7	C	334	THR	Peptide
7	C	386	PRO	Peptide
7	C	599	LYS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2924	0	1308	146	0
2	3	2974	0	1349	134	0
3	4	3551	0	1537	162	0
4	5	3130	0	1369	97	0
5	6	3230	0	1449	202	0
6	7	3076	0	1381	157	0
7	C	2330	0	1004	47	0
All	All	21215	0	9397	908	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 30.

All (908) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:386:GLN:N	1:2:410:LEU:O	1.57	1.36
1:2:224:ARG:CB	7:C:212:MET:HA	1.55	1.34
3:4:856:VAL:HA	3:4:860:LYS:CB	1.73	1.19
5:6:625:ALA:HB3	5:6:629:MET:H	1.04	1.13
2:3:190:SER:HA	2:3:456:ARG:HA	1.34	1.09
1:2:386:GLN:O	1:2:410:LEU:N	1.86	1.08
5:6:512:GLU:O	5:6:515:GLU:N	1.86	1.08
1:2:224:ARG:CB	7:C:212:MET:CA	2.33	1.07
3:4:855:SER:HA	3:4:860:LYS:CB	1.81	1.06
5:6:608:LEU:HA	5:6:625:ALA:HA	1.37	1.05
6:7:250:ASP:N	6:7:505:GLU:O	1.89	1.04
2:3:197:ILE:O	2:3:198:ARG:O	1.75	1.02
6:7:249:SER:HA	6:7:507:ILE:HA	1.38	1.01
3:4:854:LYS:O	3:4:857:ILE:N	1.98	0.96
3:4:655:SER:HA	3:4:664:THR:HA	1.47	0.95
3:4:352:CYS:N	3:4:373:ARG:O	2.00	0.95
6:7:618:TYR:O	6:7:622:HIS:N	2.00	0.94
5:6:777:TYR:O	5:6:781:ARG:CB	2.17	0.93
3:4:856:VAL:CA	3:4:860:LYS:CB	2.46	0.92
1:2:355:SER:O	1:2:434:TYR:N	2.02	0.92
1:2:630:SER:HA	1:2:639:THR:HA	1.51	0.92
1:2:223:GLY:O	7:C:211:THR:O	1.88	0.90
5:6:405:PRO:HA	5:6:450:TYR:HA	1.51	0.89
2:3:434:GLY:N	2:3:473:ASP:O	2.05	0.89
1:2:526:ASN:HA	1:2:532:SER:HA	1.55	0.89
1:2:242:LEU:O	1:2:296:ARG:N	2.06	0.88
5:6:625:ALA:HB3	5:6:629:MET:N	1.87	0.88
6:7:254:ALA:N	6:7:308:SER:O	2.05	0.88
2:3:188:LYS:HA	2:3:458:GLU:HA	1.55	0.88
7:C:573:GLN:HA	7:C:578:LEU:HA	1.56	0.88
3:4:855:SER:CA	3:4:860:LYS:CB	2.46	0.87
1:2:341:CYS:HA	1:2:373:PHE:HA	1.55	0.87
3:4:550:LYS:O	3:4:557:ARG:N	2.07	0.87
5:6:525:ILE:O	5:6:529:LEU:N	2.07	0.87
6:7:334:HIS:HA	6:7:503:THR:N	1.89	0.87
5:6:159:SER:HA	5:6:167:ALA:HB2	1.57	0.86
5:6:503:VAL:O	5:6:506:ASN:N	2.09	0.85
1:2:425:GLU:O	1:2:457:LYS:N	2.09	0.85
5:6:404:VAL:O	5:6:451:LYS:N	2.10	0.85
3:4:441:SER:HA	3:4:459:THR:HA	1.58	0.84
3:4:733:PRO:CB	6:7:445:GLY:H	1.91	0.84
5:6:527:ASP:O	5:6:531:ARG:N	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:543:GLN:O	6:7:545:THR:N	2.11	0.83
1:2:386:GLN:C	1:2:410:LEU:H	1.80	0.83
3:4:378:GLU:O	3:4:380:ASN:N	2.11	0.83
1:2:560:ALA:HB3	1:2:563:ALA:HB2	1.60	0.82
2:3:504:THR:HA	6:7:326:HIS:HA	1.60	0.82
2:3:452:THR:HA	6:7:368:ALA:H	1.45	0.82
1:2:327:ARG:C	1:2:590:THR:HA	1.99	0.82
3:4:855:SER:H	3:4:859:ARG:CB	1.93	0.82
5:6:143:MET:O	5:6:147:ASP:N	2.11	0.82
2:3:449:ASP:HA	2:3:455:ARG:HA	1.62	0.81
3:4:608:ASP:N	3:4:613:GLN:O	2.12	0.81
5:6:151:ILE:N	5:6:264:GLN:O	2.13	0.81
5:6:578:SER:HA	5:6:581:LYS:N	1.96	0.81
6:7:80:ILE:N	6:7:203:TYR:O	2.13	0.81
1:2:548:ALA:O	1:2:551:GLN:N	2.14	0.81
2:3:190:SER:CA	2:3:456:ARG:HA	2.09	0.81
3:4:607:ARG:HA	3:4:614:LEU:HA	1.61	0.81
4:5:734:ARG:O	4:5:738:VAL:CB	2.29	0.81
5:6:578:SER:HA	5:6:581:LYS:H	1.45	0.81
3:4:343:LYS:O	3:4:360:ILE:N	2.12	0.80
5:6:779:GLU:O	5:6:783:ASP:CB	2.29	0.80
5:6:303:GLU:O	5:6:353:PHE:HA	1.80	0.80
5:6:794:ARG:H	5:6:795:ILE:HA	1.46	0.80
5:6:797:VAL:O	5:6:800:LEU:N	2.13	0.80
5:6:506:ASN:O	5:6:510:SER:N	2.12	0.80
5:6:314:CYS:N	5:6:336:PRO:O	2.14	0.80
5:6:123:SER:N	5:6:134:LYS:O	2.14	0.80
1:2:326:ARG:HA	1:2:591:LEU:C	2.01	0.80
5:6:608:LEU:CA	5:6:625:ALA:HA	2.11	0.80
5:6:288:LEU:O	5:6:399:GLY:N	2.15	0.79
5:6:596:VAL:O	5:6:637:CYS:N	2.14	0.79
3:4:485:LEU:N	7:C:575:ASP:O	2.15	0.79
5:6:720:ASN:O	5:6:724:ASP:N	2.15	0.79
5:6:406:ASP:N	5:6:449:THR:O	2.13	0.79
1:2:540:LEU:N	1:2:679:ILE:O	2.14	0.79
5:6:403:VAL:HA	5:6:452:ILE:HA	1.64	0.78
2:3:734:ARG:O	2:3:738:LEU:N	2.13	0.78
1:2:328:THR:CB	1:2:387:ARG:CB	2.61	0.78
2:3:537:ASP:O	2:3:540:LEU:N	2.16	0.77
4:5:171:VAL:N	4:5:254:GLN:O	2.16	0.77
3:4:399:LEU:O	3:4:415:ILE:N	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:255:VAL:HA	6:7:307:PHE:HA	1.66	0.77
2:3:30:GLU:O	2:3:34:THR:N	2.12	0.77
6:7:247:ARG:H	6:7:509:GLU:HA	1.49	0.77
3:4:856:VAL:C	3:4:860:LYS:CB	2.54	0.76
2:3:186:VAL:O	2:3:289:GLY:N	2.16	0.76
2:3:442:LEU:H	2:3:460:GLY:HA3	1.50	0.76
2:3:254:GLN:HA	2:3:454:GLU:CB	2.15	0.76
1:2:334:LEU:O	1:2:381:VAL:CB	2.33	0.76
6:7:225:LEU:H	6:7:241:VAL:HA	1.51	0.76
7:C:372:VAL:O	7:C:384:ASN:N	2.16	0.76
5:6:635:ILE:HA	5:6:677:SER:O	1.86	0.76
6:7:350:ASP:N	6:7:382:ARG:O	2.16	0.76
5:6:661:ILE:N	5:6:672:LEU:O	2.19	0.75
6:7:249:SER:HA	6:7:507:ILE:CA	2.15	0.75
1:2:497:ILE:O	1:2:500:SER:N	2.19	0.75
1:2:328:THR:N	1:2:387:ARG:O	2.16	0.75
3:4:605:ILE:HA	3:4:616:LEU:HA	1.68	0.75
6:7:311:GLN:HA	6:7:504:ASP:O	1.86	0.75
2:3:188:LYS:O	2:3:457:LEU:N	2.19	0.75
2:3:295:VAL:O	2:3:324:ASN:N	2.20	0.75
5:6:516:LEU:O	5:6:519:MET:N	2.20	0.74
2:3:408:VAL:N	2:3:547:PHE:O	2.19	0.74
5:6:598:THR:N	5:6:637:CYS:O	2.16	0.74
2:3:446:VAL:N	2:3:456:ARG:O	2.20	0.74
5:6:303:GLU:H	5:6:354:LEU:H	1.32	0.74
5:6:572:CYS:O	5:6:712:PHE:HA	1.86	0.74
2:3:191:LEU:N	2:3:455:ARG:O	2.20	0.74
3:4:733:PRO:C	6:7:445:GLY:HA2	2.07	0.73
2:3:496:THR:HA	2:3:505:THR:HA	1.70	0.73
3:4:573:SER:O	3:4:576:GLN:N	2.21	0.73
1:2:327:ARG:H	1:2:591:LEU:N	1.86	0.73
1:2:547:THR:C	1:2:549:LYS:H	1.90	0.73
7:C:527:GLN:O	7:C:529:TYR:N	2.20	0.73
3:4:853:GLY:C	3:4:858:GLN:H	1.91	0.73
5:6:303:GLU:N	5:6:354:LEU:H	1.86	0.73
5:6:581:LYS:CB	5:6:583:GLN:H	2.02	0.73
4:5:496:ALA:O	4:5:500:GLN:N	2.22	0.73
4:5:530:TYR:O	4:5:534:LYS:N	2.16	0.73
2:3:452:THR:HA	6:7:368:ALA:N	2.04	0.72
3:4:654:ILE:O	3:4:665:LEU:N	2.22	0.72
5:6:633:ASN:N	5:6:675:ARG:O	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:648:ASP:O	5:6:651:ALA:N	2.22	0.72
6:7:334:HIS:N	6:7:376:LEU:O	2.21	0.72
3:4:248:LEU:O	3:4:251:TYR:N	2.23	0.72
1:2:623:ALA:O	1:2:627:GLN:N	2.17	0.72
6:7:80:ILE:O	6:7:205:LYS:N	2.22	0.72
1:2:315:SER:N	1:2:430:TYR:O	2.17	0.72
2:3:190:SER:HA	2:3:456:ARG:CA	2.16	0.72
1:2:337:VAL:N	1:2:351:PHE:O	2.22	0.72
1:2:525:LYS:N	1:2:532:SER:O	2.23	0.72
1:2:331:PHE:O	1:2:384:ASN:N	2.23	0.71
4:5:171:VAL:CB	4:5:460:ARG:O	2.37	0.71
7:C:351:MET:C	7:C:353:ARG:H	1.90	0.71
6:7:254:ALA:O	6:7:308:SER:N	2.23	0.71
5:6:117:GLN:O	5:6:121:ASP:N	2.23	0.71
2:3:194:PRO:HA	2:3:252:ASP:HA	1.72	0.71
3:4:831:SER:O	3:4:835:ASP:N	2.23	0.71
2:3:61:ASP:HA	6:7:212:ALA:C	2.11	0.71
1:2:386:GLN:O	1:2:409:ILE:HA	1.90	0.71
2:3:461:ALA:O	2:3:465:ALA:N	2.24	0.71
4:5:452:SER:O	4:5:465:GLU:N	2.23	0.70
4:5:503:SER:HA	4:5:512:VAL:HA	1.74	0.70
5:6:608:LEU:H	5:6:626:GLY:H	1.39	0.70
1:2:695:LEU:O	1:2:698:PHE:N	2.25	0.70
2:3:690:ASP:O	2:3:694:LYS:N	2.25	0.70
3:4:918:VAL:CB	3:4:926:SER:O	2.38	0.70
6:7:650:PRO:HA	6:7:706:ASP:HA	1.73	0.70
2:3:443:THR:HA	2:3:458:GLU:O	1.91	0.70
3:4:202:LYS:HA	3:4:224:LEU:HA	1.73	0.70
5:6:396:LYS:N	5:6:460:ILE:O	2.24	0.70
2:3:191:LEU:H	2:3:455:ARG:N	1.90	0.70
5:6:664:ALA:HA	5:6:668:ILE:O	1.92	0.69
4:5:182:MET:O	4:5:242:ILE:N	2.22	0.69
4:5:183:CYS:N	4:5:188:HIS:O	2.23	0.69
6:7:249:SER:N	6:7:312:GLU:O	2.24	0.69
6:7:499:LYS:HA	6:7:506:MET:H	1.57	0.69
3:4:345:ALA:O	3:4:357:ALA:HB1	1.92	0.69
3:4:399:LEU:N	3:4:415:ILE:O	2.14	0.69
5:6:607:GLY:CA	5:6:627:ALA:H	2.04	0.69
4:5:505:ALA:HA	4:5:510:THR:HA	1.74	0.69
3:4:188:GLN:O	3:4:190:CYS:N	2.23	0.69
1:2:629:ILE:O	1:2:640:LEU:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:328:THR:HA	1:2:589:TRP:C	2.13	0.68
4:5:729:SER:O	4:5:732:THR:N	2.24	0.68
6:7:334:HIS:HA	6:7:503:THR:H	1.59	0.68
3:4:377:ASN:CB	3:4:378:GLU:HA	2.24	0.68
4:5:173:SER:O	4:5:252:ASP:HA	1.94	0.68
4:5:300:ILE:HA	4:5:326:PRO:HA	1.73	0.68
6:7:25:LEU:O	6:7:27:THR:N	2.25	0.68
5:6:608:LEU:H	5:6:626:GLY:N	1.92	0.67
2:3:103:LEU:O	2:3:107:ASP:N	2.27	0.67
5:6:603:SER:H	5:6:604:SER:HA	1.59	0.67
5:6:634:GLY:O	5:6:677:SER:N	2.28	0.67
6:7:357:PRO:HA	6:7:374:THR:HA	1.75	0.67
5:6:720:ASN:O	5:6:723:ILE:N	2.28	0.67
1:2:386:GLN:CA	1:2:410:LEU:O	2.43	0.67
2:3:391:LYS:O	2:3:399:LEU:N	2.26	0.67
3:4:348:LYS:O	3:4:383:SER:N	2.28	0.67
3:4:601:LEU:HA	3:4:620:ALA:HB3	1.76	0.67
3:4:734:GLU:N	6:7:445:GLY:HA2	2.10	0.67
1:2:326:ARG:HA	1:2:591:LEU:O	1.94	0.67
5:6:153:ILE:N	5:6:266:SER:O	2.24	0.67
2:3:61:ASP:O	6:7:213:ARG:HA	1.93	0.67
2:3:211:TYR:N	6:7:6:PRO:O	2.28	0.67
3:4:604:TYR:N	3:4:617:GLU:O	2.25	0.66
1:2:776:PRO:HA	1:2:827:GLU:C	2.16	0.66
5:6:524:HIS:O	5:6:527:ASP:N	2.27	0.66
6:7:25:LEU:C	6:7:27:THR:H	1.96	0.66
5:6:335:ASN:H	5:6:339:GLU:HA	1.60	0.66
2:3:98:ILE:O	2:3:158:LYS:N	2.27	0.66
2:3:194:PRO:O	6:7:372:THR:N	2.28	0.66
6:7:260:TYR:O	6:7:269:VAL:N	2.28	0.65
6:7:350:ASP:O	6:7:382:ARG:N	2.26	0.65
6:7:617:THR:O	6:7:621:MET:CB	2.44	0.65
1:2:354:ASP:O	1:2:356:ASN:HA	1.97	0.65
5:6:660:THR:HA	5:6:673:ASN:HA	1.77	0.65
6:7:89:GLN:O	6:7:93:PHE:N	2.30	0.65
1:2:542:LEU:N	1:2:681:CYS:O	2.29	0.65
4:5:502:ILE:O	4:5:513:LEU:N	2.30	0.65
1:2:777:LYS:H	1:2:828:PHE:HA	1.60	0.65
3:4:456:LEU:HA	6:7:253:PRO:O	1.97	0.65
2:3:495:VAL:O	2:3:506:LEU:N	2.28	0.65
3:4:918:VAL:CB	3:4:925:ARG:O	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:335:ASN:N	5:6:339:GLU:HA	2.12	0.65
4:5:176:ALA:O	4:5:178:TYR:N	2.30	0.64
6:7:68:GLN:O	6:7:72:ASN:N	2.26	0.64
4:5:770:ILE:O	4:5:774:GLY:N	2.31	0.64
5:6:103:VAL:O	5:6:107:THR:N	2.23	0.64
6:7:446:ASP:N	6:7:447:GLY:HA2	2.10	0.64
1:2:631:ILE:N	1:2:638:THR:O	2.25	0.64
5:6:355:ASP:CB	5:6:382:ARG:HA	2.27	0.64
6:7:249:SER:CA	6:7:507:ILE:HA	2.24	0.64
5:6:326:LYS:H	5:6:327:TYR:HA	1.62	0.64
5:6:765:LEU:CB	5:6:819:ILE:H	2.11	0.64
1:2:327:ARG:O	1:2:591:LEU:N	2.25	0.64
2:3:203:ALA:O	2:3:207:GLY:N	2.31	0.64
6:7:499:LYS:HA	6:7:506:MET:N	2.13	0.63
2:3:449:ASP:CA	2:3:455:ARG:HA	2.27	0.63
3:4:761:ILE:O	3:4:816:VAL:HA	1.99	0.63
2:3:191:LEU:O	2:3:454:GLU:HA	1.98	0.63
2:3:257:THR:HA	2:3:275:ASP:HA	1.79	0.63
4:5:53:ASN:O	4:5:58:ASN:N	2.22	0.63
4:5:175:ARG:O	4:5:251:ILE:N	2.32	0.63
6:7:78:VAL:N	6:7:201:PHE:O	2.30	0.63
6:7:411:TYR:O	6:7:415:ALA:HB2	1.98	0.63
2:3:113:GLY:O	2:3:117:GLU:N	2.26	0.63
3:4:206:ARG:O	3:4:211:GLU:N	2.30	0.63
2:3:389:VAL:O	2:3:401:GLY:HA3	1.99	0.63
4:5:169:THR:O	4:5:463:TYR:HA	1.98	0.63
2:3:422:VAL:O	2:3:426:ALA:HB2	1.99	0.62
5:6:189:VAL:O	5:6:193:ALA:N	2.31	0.62
5:6:301:ARG:N	5:6:355:ASP:O	2.32	0.62
1:2:337:VAL:O	1:2:351:PHE:N	2.25	0.62
3:4:855:SER:HA	3:4:856:VAL:C	2.19	0.62
5:6:304:LEU:O	5:6:306:LYS:N	2.30	0.62
3:4:679:GLY:HA3	3:4:681:ARG:O	1.99	0.62
7:C:372:VAL:N	7:C:384:ASN:O	2.29	0.62
1:2:631:ILE:O	1:2:637:VAL:HA	1.99	0.62
2:3:453:GLY:N	6:7:366:LEU:O	2.32	0.62
1:2:332:PRO:O	1:2:383:ARG:HA	1.98	0.62
3:4:626:GLY:N	3:4:668:ARG:O	2.22	0.62
5:6:631:ALA:O	5:6:634:GLY:N	2.33	0.62
3:4:352:CYS:N	3:4:353:ASP:HA	2.15	0.62
5:6:307:ALA:O	5:6:319:ASP:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:663:ILE:N	5:6:670:ALA:O	2.33	0.62
6:7:457:CYS:N	6:7:596:ILE:O	2.22	0.62
3:4:408:ASP:C	3:4:410:GLN:H	2.03	0.61
3:4:605:ILE:H	3:4:617:GLU:H	1.47	0.61
5:6:155:TYR:N	5:6:268:PHE:O	2.24	0.61
6:7:312:GLU:HA	6:7:503:THR:CB	2.30	0.61
6:7:310:PHE:HA	6:7:336:ASN:HA	1.81	0.61
6:7:335:VAL:H	6:7:503:THR:CB	2.13	0.61
3:4:341:ASP:H	3:4:392:ALA:N	1.98	0.61
6:7:260:TYR:HA	6:7:300:MET:HA	1.82	0.61
1:2:568:GLY:HA2	1:2:607:ASP:O	2.01	0.61
2:3:61:ASP:C	6:7:213:ARG:HA	2.20	0.61
6:7:334:HIS:O	6:7:378:ALA:N	2.30	0.61
3:4:761:ILE:N	3:4:815:ASN:O	2.33	0.61
5:6:358:LYS:HA	5:6:380:ILE:HA	1.82	0.61
5:6:607:GLY:HA2	5:6:627:ALA:H	1.66	0.61
1:2:427:THR:O	1:2:454:ASN:N	2.34	0.61
3:4:245:ALA:HB3	3:4:306:TYR:O	2.01	0.61
3:4:442:ILE:N	3:4:458:LYS:O	2.24	0.61
3:4:648:VAL:O	3:4:652:GLN:N	2.29	0.61
3:4:917:ILE:C	3:4:927:VAL:HA	2.21	0.61
2:3:404:ASN:O	2:3:544:ASP:N	2.33	0.61
5:6:632:ASP:HA	5:6:675:ARG:O	2.00	0.61
1:2:660:THR:O	1:2:850:LYS:HA	2.01	0.60
3:4:917:ILE:O	3:4:927:VAL:HA	2.01	0.60
1:2:327:ARG:N	1:2:591:LEU:N	2.49	0.60
4:5:175:ARG:O	4:5:250:PHE:HA	2.00	0.60
1:2:244:VAL:O	1:2:298:SER:N	2.34	0.60
2:3:314:LEU:CB	4:5:459:THR:H	2.15	0.60
5:6:134:LYS:N	5:6:135:VAL:HA	2.15	0.60
5:6:704:PRO:O	5:6:707:SER:N	2.34	0.60
7:C:36:ILE:O	7:C:40:HIS:N	2.35	0.60
2:3:669:PRO:O	2:3:720:THR:HA	2.02	0.60
1:2:821:ALA:O	1:2:825:LEU:N	2.34	0.60
2:3:462:MET:O	2:3:466:ASP:N	2.34	0.60
1:2:576:LEU:HA	1:2:595:ALA:H	1.66	0.60
5:6:344:TRP:CB	5:6:345:THR:HA	2.31	0.60
5:6:509:SER:O	5:6:511:ASP:N	2.35	0.60
3:4:919:LEU:O	3:4:923:VAL:O	2.20	0.60
5:6:512:GLU:O	5:6:514:ASN:N	2.35	0.60
7:C:572:HIS:O	7:C:579:LYS:N	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:394:LYS:CB	3:4:420:TYR:HA	2.31	0.59
3:4:913:GLU:C	3:4:915:LYS:H	2.06	0.59
6:7:486:LYS:N	6:7:487:GLY:HA3	2.17	0.59
5:6:153:ILE:O	5:6:268:PHE:N	2.34	0.59
5:6:578:SER:HA	5:6:581:LYS:CA	2.31	0.59
6:7:372:THR:C	6:7:374:THR:H	2.06	0.59
4:5:182:MET:HA	4:5:189:THR:HA	1.84	0.59
5:6:663:ILE:O	5:6:670:ALA:N	2.26	0.59
1:2:631:ILE:O	1:2:638:THR:N	2.29	0.59
5:6:309:PHE:N	5:6:317:ILE:HA	2.18	0.59
6:7:465:ALA:O	6:7:468:GLN:N	2.34	0.59
3:4:188:GLN:C	3:4:190:CYS:H	2.05	0.59
2:3:408:VAL:O	2:3:549:VAL:N	2.29	0.59
2:3:500:ALA:H	2:3:501:GLY:HA3	1.67	0.59
3:4:241:LEU:O	3:4:303:VAL:HA	2.02	0.59
5:6:360:ARG:HA	5:6:378:ASP:HA	1.85	0.59
1:2:328:THR:HA	1:2:589:TRP:O	2.03	0.58
1:2:356:ASN:N	1:2:434:TYR:O	2.36	0.58
6:7:258:ILE:N	6:7:271:GLN:O	2.34	0.58
1:2:333:GLN:HA	1:2:383:ARG:HA	1.85	0.58
6:7:311:GLN:HA	6:7:504:ASP:C	2.24	0.58
1:2:428:GLY:HA2	1:2:453:ALA:HA	1.84	0.58
3:4:656:ILE:N	3:4:663:THR:O	2.37	0.58
1:2:547:THR:C	1:2:549:LYS:N	2.56	0.58
2:3:686:LEU:O	2:3:690:ASP:CB	2.52	0.58
5:6:598:THR:O	5:6:639:ASP:N	2.21	0.58
3:4:546:GLY:HA2	3:4:807:ALA:HB2	1.86	0.58
4:5:398:LYS:O	4:5:405:ARG:HA	2.03	0.58
3:4:534:GLU:O	3:4:537:LYS:N	2.37	0.58
5:6:557:LYS:HA	5:6:564:LYS:HA	1.85	0.58
7:C:289:ALA:HA	7:C:290:PHE:O	2.04	0.58
2:3:237:GLU:O	2:3:239:ASN:N	2.37	0.57
3:4:233:MET:O	3:4:237:GLY:N	2.32	0.57
3:4:891:ASN:O	3:4:894:SER:HA	2.03	0.57
3:4:911:GLN:HA	3:4:916:VAL:O	2.04	0.57
6:7:608:ASP:O	6:7:611:LYS:N	2.37	0.57
2:3:432:THR:O	2:3:473:ASP:N	2.33	0.57
5:6:549:LEU:O	5:6:552:LEU:N	2.37	0.57
5:6:659:GLN:O	5:6:674:ALA:N	2.36	0.57
5:6:780:LEU:O	5:6:784:ASP:N	2.28	0.57
6:7:257:VAL:HA	6:7:272:GLU:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:575:GLY:C	1:2:577:THR:H	2.07	0.57
1:2:575:GLY:O	1:2:577:THR:N	2.37	0.57
3:4:609:VAL:HA	3:4:612:LYS:HA	1.86	0.57
4:5:181:ILE:N	4:5:190:THR:O	2.28	0.57
6:7:685:THR:O	6:7:688:THR:N	2.37	0.57
5:6:501:GLN:O	5:6:504:PHE:N	2.36	0.57
7:C:68:ASP:O	7:C:71:GLN:N	2.35	0.57
3:4:917:ILE:H	3:4:927:VAL:CA	2.18	0.57
4:5:175:ARG:N	4:5:251:ILE:O	2.37	0.57
2:3:675:ALA:O	2:3:678:VAL:N	2.38	0.57
3:4:629:CYS:N	3:4:670:SER:O	2.36	0.57
6:7:395:SER:C	6:7:397:VAL:H	2.08	0.56
3:4:344:VAL:HA	3:4:359:GLU:HA	1.86	0.56
6:7:335:VAL:N	6:7:503:THR:CB	2.68	0.56
1:2:477:THR:O	1:2:481:GLU:N	2.28	0.56
5:6:543:VAL:O	5:6:546:GLY:N	2.38	0.56
6:7:521:CYS:N	6:7:562:SER:O	2.37	0.56
1:2:632:SER:HA	1:2:637:VAL:HA	1.87	0.56
4:5:475:GLY:O	4:5:517:THR:HA	2.06	0.56
5:6:291:SER:HA	5:6:396:LYS:HA	1.87	0.56
5:6:554:GLY:O	5:6:567:GLY:HA2	2.05	0.56
6:7:310:PHE:O	6:7:504:ASP:O	2.23	0.56
6:7:498:MET:C	6:7:507:ILE:H	2.09	0.56
7:C:349:SER:O	7:C:352:LYS:N	2.39	0.56
3:4:567:CYS:O	3:4:708:VAL:N	2.37	0.56
5:6:607:GLY:CA	5:6:627:ALA:N	2.69	0.56
5:6:811:ALA:O	5:6:815:CYS:N	2.38	0.56
6:7:247:ARG:O	6:7:508:LEU:N	2.38	0.56
1:2:290:HIS:O	1:2:292:GLU:N	2.39	0.56
3:4:440:ARG:O	3:4:460:TYR:N	2.39	0.56
4:5:500:GLN:O	4:5:515:SER:N	2.33	0.56
1:2:332:PRO:C	1:2:383:ARG:HA	2.27	0.55
1:2:395:GLY:HA2	1:2:561:HIS:O	2.06	0.55
3:4:855:SER:HA	3:4:857:ILE:N	2.21	0.55
3:4:602:THR:N	3:4:619:GLY:HA3	2.22	0.55
5:6:135:VAL:O	5:6:138:ALA:N	2.39	0.55
5:6:754:TYR:O	5:6:757:TYR:N	2.40	0.55
7:C:522:SER:HA	7:C:525:ARG:CB	2.37	0.55
4:5:455:ARG:HA	4:5:462:PHE:HA	1.88	0.55
3:4:601:LEU:O	3:4:621:LEU:N	2.33	0.55
4:5:613:ARG:N	4:5:670:PRO:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:351:MET:C	7:C:353:ARG:N	2.59	0.55
2:3:202:TYR:N	2:3:242:THR:O	2.26	0.55
6:7:467:SER:O	6:7:470:LEU:N	2.39	0.55
5:6:763:PRO:HA	5:6:817:ASP:C	2.27	0.55
6:7:247:ARG:N	6:7:509:GLU:HA	2.18	0.55
1:2:702:SER:O	1:2:705:ARG:N	2.39	0.55
5:6:310:THR:C	5:6:345:THR:H	2.09	0.55
6:7:209:GLN:H	6:7:212:ALA:CB	2.20	0.55
6:7:262:CYS:C	6:7:264:GLN:H	2.11	0.55
5:6:126:SER:O	5:6:132:VAL:HA	2.07	0.55
5:6:525:ILE:HA	5:6:528:LYS:H	1.71	0.55
1:2:566:ALA:N	1:2:605:LEU:O	2.26	0.54
5:6:580:SER:O	5:6:581:LYS:C	2.45	0.54
3:4:540:ILE:O	3:4:543:GLN:N	2.40	0.54
4:5:266:PRO:C	4:5:268:GLY:H	2.10	0.54
5:6:404:VAL:N	5:6:451:LYS:O	2.37	0.54
6:7:686:PRO:O	6:7:689:LEU:N	2.41	0.54
2:3:441:GLY:HA2	2:3:461:ALA:N	2.22	0.54
3:4:677:PRO:O	3:4:680:SER:HA	2.07	0.54
5:6:303:GLU:H	5:6:354:LEU:N	2.03	0.54
3:4:594:LYS:C	3:4:596:SER:H	2.09	0.54
5:6:695:LEU:O	5:6:699:LEU:N	2.34	0.54
2:3:297:VAL:O	2:3:321:ILE:HA	2.06	0.54
3:4:334:ARG:O	3:4:398:LYS:N	2.38	0.54
5:6:794:ARG:N	5:6:795:ILE:HA	2.14	0.54
1:2:279:THR:O	1:2:283:TYR:N	2.29	0.54
3:4:832:ALA:O	3:4:836:TYR:N	2.41	0.54
6:7:460:GLY:HA3	6:7:600:MET:O	2.07	0.54
1:2:556:VAL:O	1:2:559:THR:N	2.41	0.54
3:4:517:ASP:O	3:4:520:SER:N	2.41	0.54
4:5:52:ASN:O	4:5:56:VAL:N	2.30	0.54
5:6:164:GLY:O	5:6:168:MET:N	2.30	0.54
3:4:341:ASP:H	3:4:392:ALA:H	1.55	0.54
5:6:661:ILE:O	5:6:672:LEU:N	2.38	0.54
2:3:432:THR:N	2:3:471:CYS:O	2.32	0.54
3:4:688:VAL:O	3:4:691:ASN:N	2.40	0.54
3:4:795:THR:O	3:4:798:LEU:N	2.41	0.54
4:5:544:THR:O	4:5:547:LEU:N	2.41	0.54
6:7:25:LEU:C	6:7:27:THR:N	2.61	0.54
6:7:619:VAL:HA	6:7:622:HIS:O	2.08	0.54
2:3:95:ARG:HA	2:3:154:LYS:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:308:SER:HA	5:6:318:VAL:O	2.08	0.54
2:3:437:SER:CB	2:3:438:SER:HA	2.38	0.53
4:5:441:GLY:HA3	4:5:443:GLY:N	2.23	0.53
5:6:607:GLY:HA2	5:6:627:ALA:N	2.23	0.53
1:2:386:GLN:O	1:2:409:ILE:CA	2.55	0.53
2:3:188:LYS:CA	2:3:458:GLU:HA	2.34	0.53
4:5:729:SER:O	4:5:731:GLN:N	2.40	0.53
5:6:586:LYS:O	5:6:589:VAL:N	2.40	0.53
6:7:68:GLN:HA	6:7:71:ALA:HB3	1.89	0.53
1:2:258:LEU:O	1:2:261:ALA:N	2.41	0.53
3:4:434:GLU:N	3:4:467:LYS:O	2.30	0.53
4:5:60:SER:HA	4:5:136:GLN:O	2.08	0.53
6:7:444:VAL:N	6:7:448:MET:O	2.42	0.53
1:2:777:LYS:O	1:2:828:PHE:HA	2.08	0.53
1:2:860:SER:O	1:2:864:TYR:N	2.42	0.53
5:6:559:THR:N	5:6:565:LEU:H	2.07	0.53
5:6:791:SER:HA	5:6:839:ASP:HA	1.88	0.53
1:2:333:GLN:HA	1:2:383:ARG:CB	2.38	0.53
2:3:377:ILE:O	2:3:380:ALA:HB3	2.08	0.53
3:4:833:ILE:C	3:4:836:TYR:H	2.12	0.53
4:5:33:ASN:O	4:5:37:GLU:N	2.40	0.53
4:5:170:SER:H	4:5:256:LEU:HA	1.73	0.53
5:6:777:TYR:O	5:6:780:LEU:N	2.36	0.53
2:3:452:THR:CA	6:7:368:ALA:H	2.18	0.53
3:4:915:LYS:HA	3:4:931:ASN:O	2.08	0.53
5:6:291:SER:HA	5:6:395:CYS:O	2.09	0.53
5:6:518:GLU:O	5:6:522:ASP:N	2.38	0.53
5:6:725:THR:O	5:6:728:ALA:HB3	2.08	0.53
2:3:183:GLU:HA	2:3:293:ASN:HA	1.90	0.53
4:5:627:VAL:O	4:5:631:LYS:CB	2.56	0.53
5:6:334:PRO:O	5:6:339:GLU:HA	2.08	0.53
1:2:699:VAL:O	1:2:702:SER:N	2.42	0.53
7:C:373:VAL:HA	7:C:383:MET:HA	1.91	0.53
3:4:397:ILE:O	3:4:416:SER:HA	2.09	0.53
1:2:244:VAL:H	1:2:297:ILE:C	2.12	0.52
2:3:270:LEU:HA	4:5:510:THR:H	1.75	0.52
5:6:151:ILE:O	5:6:266:SER:N	2.42	0.52
1:2:224:ARG:CB	7:C:212:MET:N	2.72	0.52
3:4:854:LYS:N	3:4:857:ILE:CB	2.72	0.52
3:4:917:ILE:H	3:4:927:VAL:HA	1.72	0.52
2:3:245:TYR:C	2:3:247:TYR:H	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:208:SER:O	6:7:212:ALA:HB2	2.10	0.52
3:4:608:ASP:C	3:4:610:ASP:H	2.12	0.52
6:7:457:CYS:O	6:7:598:PHE:N	2.36	0.52
7:C:344:LEU:O	7:C:348:SER:CB	2.57	0.52
4:5:598:LYS:O	4:5:601:ARG:N	2.43	0.52
6:7:353:GLY:HA3	6:7:377:GLU:O	2.08	0.52
5:6:751:LEU:O	5:6:754:TYR:N	2.43	0.52
5:6:764:ILE:CB	5:6:765:LEU:HA	2.40	0.52
6:7:245:ILE:O	6:7:346:GLY:N	2.42	0.52
1:2:600:ASP:C	1:2:602:GLY:H	2.13	0.52
2:3:392:ASN:HA	2:3:398:HIS:HA	1.91	0.52
3:4:563:ASN:O	3:4:703:ASP:N	2.43	0.52
6:7:700:ALA:HB1	6:7:705:ALA:CB	2.40	0.52
3:4:721:ALA:O	3:4:725:THR:CB	2.58	0.52
5:6:525:ILE:O	5:6:528:LYS:N	2.43	0.52
5:6:773:LEU:O	5:6:776:LYS:N	2.42	0.52
5:6:816:VAL:N	5:6:817:ASP:HA	2.24	0.52
1:2:347:ILE:C	1:2:349:GLY:H	2.12	0.52
1:2:663:LEU:O	1:2:667:VAL:N	2.42	0.52
2:3:197:ILE:N	2:3:249:THR:O	2.42	0.52
3:4:588:GLY:HA2	3:4:628:VAL:O	2.10	0.52
3:4:917:ILE:H	3:4:927:VAL:CB	2.23	0.52
4:5:458:MET:C	4:5:460:ARG:H	2.14	0.52
4:5:717:GLU:O	4:5:721:ARG:CB	2.58	0.52
4:5:753:TYR:O	4:5:757:LYS:CB	2.58	0.52
5:6:661:ILE:H	5:6:672:LEU:C	2.13	0.52
6:7:628:LEU:N	6:7:629:ASP:HA	2.24	0.52
1:2:327:ARG:HA	1:2:388:VAL:HA	1.92	0.51
2:3:723:LYS:O	2:3:726:ALA:HB3	2.10	0.51
4:5:596:ILE:HA	4:5:599:MET:CB	2.41	0.51
1:2:674:LEU:O	1:2:677:PHE:N	2.43	0.51
1:2:321:THR:HA	1:2:425:GLU:HA	1.91	0.51
6:7:512:ALA:O	6:7:516:ALA:N	2.33	0.51
7:C:327:LEU:O	7:C:331:SER:CB	2.58	0.51
2:3:197:ILE:O	2:3:249:THR:O	2.29	0.51
2:3:411:PRO:C	2:3:413:THR:H	2.14	0.51
6:7:713:VAL:O	6:7:716:ALA:N	2.43	0.51
1:2:433:ASN:HA	1:2:434:TYR:CB	2.40	0.51
5:6:361:ILE:N	5:6:377:LEU:O	2.42	0.51
3:4:657:ALA:HA	3:4:662:ILE:HA	1.92	0.51
1:2:327:ARG:O	1:2:590:THR:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:599:ALA:O	1:2:602:GLY:N	2.44	0.51
2:3:195:LYS:HA	6:7:371:LEU:C	2.31	0.51
3:4:188:GLN:C	3:4:190:CYS:N	2.64	0.51
5:6:523:GLU:O	5:6:525:ILE:N	2.37	0.51
5:6:608:LEU:N	5:6:625:ALA:HA	2.25	0.51
6:7:314:LYS:HA	6:7:331:LEU:O	2.11	0.51
2:3:197:ILE:CA	2:3:249:THR:O	2.59	0.51
3:4:608:ASP:O	3:4:610:ASP:N	2.43	0.51
6:7:214:ARG:N	6:7:215:TYR:HA	2.25	0.51
7:C:519:ILE:O	7:C:523:LEU:CB	2.58	0.51
3:4:566:LEU:HA	3:4:706:TYR:O	2.10	0.51
4:5:757:LYS:C	4:5:759:GLU:H	2.14	0.51
5:6:721:GLU:O	5:6:725:THR:CB	2.59	0.51
1:2:629:ILE:O	1:2:639:THR:HA	2.10	0.51
2:3:270:LEU:CB	4:5:509:ILE:HA	2.41	0.51
3:4:393:ASP:O	3:4:394:LYS:C	2.50	0.51
6:7:357:PRO:HA	6:7:374:THR:CA	2.40	0.51
6:7:417:SER:CB	6:7:633:VAL:H	2.24	0.51
3:4:378:GLU:C	3:4:380:ASN:N	2.64	0.50
5:6:541:GLU:O	5:6:544:LYS:N	2.44	0.50
6:7:483:THR:N	6:7:522:CYS:O	2.41	0.50
2:3:346:ASP:O	2:3:349:ASN:N	2.44	0.50
5:6:641:PHE:O	5:6:644:MET:CB	2.59	0.50
3:4:888:LYS:O	3:4:892:GLU:CB	2.59	0.50
3:4:592:SER:HA	3:4:632:ASP:CB	2.41	0.50
4:5:54:ILE:O	4:5:57:LYS:N	2.39	0.50
4:5:664:ALA:O	4:5:668:LEU:N	2.45	0.50
5:6:661:ILE:O	5:6:671:THR:HA	2.12	0.50
5:6:600:GLY:H	5:6:639:ASP:CB	2.24	0.50
1:2:663:LEU:O	1:2:666:ASN:N	2.44	0.50
5:6:141:GLU:O	5:6:144:LYS:N	2.45	0.50
4:5:180:SER:HA	4:5:191:SER:HA	1.92	0.50
5:6:334:PRO:C	5:6:339:GLU:HA	2.32	0.49
5:6:397:PHE:HA	5:6:458:HIS:O	2.12	0.49
5:6:835:ILE:O	5:6:838:VAL:N	2.45	0.49
3:4:331:LEU:HA	3:4:431:ASP:O	2.12	0.49
6:7:256:GLU:N	6:7:306:LYS:O	2.31	0.49
6:7:446:ASP:N	6:7:447:GLY:CA	2.75	0.49
1:2:388:VAL:N	1:2:408:VAL:O	2.39	0.49
6:7:590:LEU:O	6:7:593:ARG:N	2.45	0.49
3:4:727:LEU:HA	3:4:728:TYR:C	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:289:ILE:C	1:2:291:SER:H	2.16	0.49
2:3:173:ALA:HB1	4:5:250:PHE:O	2.12	0.49
3:4:571:SER:C	3:4:573:SER:H	2.16	0.49
5:6:523:GLU:C	5:6:525:ILE:H	2.15	0.49
5:6:401:GLU:O	5:6:454:PHE:HA	2.13	0.49
6:7:253:PRO:HA	6:7:308:SER:O	2.13	0.49
4:5:612:PRO:HA	4:5:670:PRO:HA	1.94	0.49
5:6:309:PHE:HA	5:6:345:THR:O	2.13	0.49
5:6:793:TYR:HA	5:6:794:ARG:HA	1.60	0.49
2:3:406:LEU:O	2:3:547:PHE:N	2.44	0.49
2:3:414:ALA:O	2:3:417:GLN:N	2.46	0.48
1:2:481:GLU:O	1:2:484:PHE:N	2.45	0.48
2:3:190:SER:N	2:3:456:ARG:HA	2.28	0.48
6:7:480:GLY:HA2	6:7:520:ILE:O	2.13	0.48
1:2:357:GLU:N	1:2:435:ASP:CB	2.77	0.48
4:5:169:THR:O	4:5:462:PHE:O	2.31	0.48
4:5:186:CYS:C	4:5:188:HIS:H	2.16	0.48
5:6:529:LEU:O	5:6:532:SER:N	2.45	0.48
1:2:510:ASP:O	1:2:513:THR:N	2.46	0.48
3:4:202:LYS:CA	3:4:224:LEU:HA	2.40	0.48
4:5:107:ALA:O	4:5:109:SER:HA	2.13	0.48
6:7:546:ILE:O	6:7:557:LEU:N	2.47	0.48
7:C:324:VAL:O	7:C:327:LEU:N	2.47	0.48
1:2:242:LEU:O	1:2:295:VAL:HA	2.13	0.48
2:3:191:LEU:H	2:3:455:ARG:C	2.17	0.48
2:3:193:ARG:O	2:3:253:HIS:N	2.45	0.48
2:3:449:ASP:HA	2:3:455:ARG:CA	2.41	0.48
3:4:249:LEU:HA	3:4:250:ALA:HA	1.50	0.48
3:4:341:ASP:N	3:4:392:ALA:O	2.46	0.48
3:4:850:VAL:O	3:4:853:GLY:N	2.47	0.48
4:5:177:THR:O	4:5:193:THR:HA	2.14	0.48
5:6:574:VAL:O	5:6:715:ILE:N	2.46	0.48
1:2:547:THR:O	1:2:549:LYS:N	2.47	0.48
1:2:630:SER:HA	1:2:639:THR:CA	2.35	0.48
1:2:826:SER:C	1:2:828:PHE:H	2.17	0.48
3:4:645:LEU:O	3:4:648:VAL:N	2.47	0.48
4:5:450:THR:C	4:5:467:GLY:HA3	2.34	0.48
4:5:736:GLU:O	4:5:740:THR:N	2.44	0.48
5:6:288:LEU:N	5:6:399:GLY:HA3	2.29	0.48
4:5:729:SER:H	4:5:775:VAL:C	2.17	0.48
5:6:721:GLU:HA	5:6:724:ASP:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:650:PRO:CA	6:7:706:ASP:HA	2.43	0.48
7:C:73:PHE:HA	7:C:92:TYR:HA	1.95	0.48
7:C:376:ASN:N	7:C:380:GLU:O	2.31	0.48
5:6:554:GLY:HA2	5:6:808:GLU:CB	2.43	0.47
7:C:203:LYS:O	7:C:205:ILE:N	2.46	0.47
1:2:333:GLN:HA	1:2:383:ARG:CA	2.44	0.47
4:5:297:ILE:N	4:5:329:LYS:O	2.33	0.47
7:C:328:ASN:HA	7:C:332:ARG:CB	2.44	0.47
4:5:441:GLY:HA3	4:5:443:GLY:H	1.78	0.47
5:6:802:SER:O	5:6:805:ARG:N	2.47	0.47
6:7:17:LEU:O	6:7:20:GLU:N	2.47	0.47
6:7:290:SER:C	6:7:292:ASN:H	2.18	0.47
5:6:661:ILE:C	5:6:672:LEU:H	2.17	0.47
6:7:580:PRO:C	6:7:582:ASP:H	2.18	0.47
2:3:294:VAL:HA	2:3:326:VAL:HA	1.96	0.47
3:4:651:GLN:C	3:4:653:THR:H	2.18	0.47
3:4:719:GLU:O	3:4:722:LYS:N	2.45	0.47
5:6:357:GLN:O	5:6:381:LEU:N	2.42	0.47
5:6:768:GLU:HA	5:6:769:ALA:HA	1.49	0.47
1:2:540:LEU:O	1:2:681:CYS:N	2.36	0.47
2:3:447:THR:HA	2:3:448:THR:HA	1.45	0.47
5:6:799:GLN:O	5:6:802:SER:N	2.47	0.47
6:7:249:SER:CB	6:7:505:GLU:C	2.83	0.47
6:7:493:LEU:HA	6:7:512:ALA:HB3	1.96	0.47
7:C:533:TYR:O	7:C:536:SER:N	2.48	0.47
1:2:219:THR:CB	1:2:225:SER:HA	2.44	0.47
3:4:705:VAL:O	3:4:832:ALA:HB2	2.15	0.47
5:6:601:LYS:CB	5:6:640:GLU:O	2.63	0.47
5:6:606:ALA:O	5:6:609:THR:N	2.47	0.47
5:6:661:ILE:H	5:6:672:LEU:N	2.12	0.47
6:7:250:ASP:CA	6:7:505:GLU:O	2.61	0.47
1:2:343:LYS:CB	1:2:371:GLY:HA3	2.45	0.47
1:2:528:ASN:HA	1:2:529:GLY:HA2	1.50	0.47
2:3:201:HIS:O	2:3:209:PHE:HA	2.15	0.47
3:4:913:GLU:C	3:4:915:LYS:N	2.65	0.47
4:5:540:ILE:O	4:5:543:GLN:N	2.47	0.47
6:7:102:LEU:O	6:7:106:ILE:N	2.37	0.47
6:7:680:SER:CB	6:7:681:PHE:HA	2.45	0.47
2:3:435:ARG:HA	2:3:436:GLY:HA3	1.62	0.47
5:6:399:GLY:O	5:6:400:VAL:C	2.53	0.47
5:6:913:MET:O	5:6:916:MET:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:334:HIS:HA	6:7:503:THR:CA	2.43	0.47
6:7:446:ASP:H	6:7:447:GLY:HA2	1.78	0.47
2:3:443:THR:C	2:3:445:ALA:H	2.18	0.47
2:3:462:MET:HA	2:3:465:ALA:HB3	1.97	0.47
1:2:386:GLN:CB	1:2:410:LEU:O	2.56	0.46
2:3:270:LEU:CB	4:5:510:THR:H	2.27	0.46
4:5:459:THR:C	4:5:460:ARG:O	2.54	0.46
7:C:407:ALA:O	7:C:410:TRP:N	2.47	0.46
2:3:500:ALA:N	2:3:501:GLY:HA3	2.29	0.46
3:4:603:ALA:H	3:4:619:GLY:H	1.63	0.46
4:5:408:GLY:HA2	4:5:409:ASP:HA	1.59	0.46
5:6:652:ILE:O	5:6:656:MET:N	2.31	0.46
2:3:187:THR:CB	2:3:459:ALA:H	2.29	0.46
2:3:188:LYS:O	2:3:457:LEU:C	2.54	0.46
4:5:448:GLY:O	4:5:467:GLY:HA2	2.15	0.46
6:7:78:VAL:O	6:7:203:TYR:N	2.32	0.46
6:7:717:LEU:O	6:7:720:VAL:N	2.49	0.46
1:2:600:ASP:CB	1:2:642:ALA:HA	2.46	0.46
1:2:630:SER:HA	1:2:638:THR:O	2.15	0.46
2:3:18:ASP:O	2:3:21:PHE:N	2.49	0.46
7:C:307:LEU:CB	7:C:312:LYS:H	2.28	0.46
7:C:375:LEU:HA	7:C:381:LEU:HA	1.97	0.46
1:2:245:ASN:HA	1:2:298:SER:CB	2.46	0.46
1:2:385:TYR:CB	1:2:410:LEU:O	2.63	0.46
2:3:195:LYS:O	2:3:251:ILE:O	2.33	0.46
3:4:485:LEU:HA	7:C:575:ASP:CB	2.46	0.46
5:6:370:THR:HA	5:6:371:GLY:HA2	1.63	0.46
3:4:342:MET:HA	3:4:390:SER:O	2.16	0.46
4:5:54:ILE:C	4:5:57:LYS:H	2.17	0.46
1:2:333:GLN:O	1:2:334:LEU:CB	2.63	0.46
4:5:264:LEU:HA	4:5:265:VAL:HA	1.56	0.46
6:7:501:PRO:O	6:7:503:THR:N	2.49	0.46
6:7:547:SER:HA	6:7:556:THR:HA	1.96	0.46
1:2:652:PRO:O	1:2:653:ASN:C	2.54	0.46
4:5:502:ILE:N	4:5:513:LEU:O	2.41	0.46
5:6:326:LYS:N	5:6:327:TYR:HA	2.30	0.46
6:7:312:GLU:CB	6:7:504:ASP:HA	2.45	0.46
1:2:242:LEU:N	1:2:294:HIS:O	2.42	0.46
2:3:449:ASP:HA	2:3:454:GLU:C	2.36	0.46
5:6:310:THR:N	5:6:317:ILE:H	2.12	0.46
6:7:349:VAL:HA	6:7:383:GLN:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:322:GLY:O	1:2:423:GLU:HA	2.15	0.45
2:3:562:SER:CB	4:5:623:SER:HA	2.45	0.45
3:4:242:ASN:O	3:4:305:PRO:HA	2.16	0.45
3:4:577:ILE:O	3:4:580:TYR:N	2.49	0.45
6:7:247:ARG:H	6:7:509:GLU:CA	2.23	0.45
6:7:251:VAL:HA	6:7:310:PHE:O	2.16	0.45
1:2:224:ARG:O	1:2:226:VAL:N	2.50	0.45
4:5:209:ARG:HA	4:5:239:ASP:CB	2.45	0.45
5:6:608:LEU:H	5:6:625:ALA:HA	1.81	0.45
1:2:327:ARG:H	1:2:591:LEU:H	1.64	0.45
2:3:666:ARG:HA	2:3:667:VAL:HA	1.72	0.45
6:7:106:ILE:O	6:7:110:ALA:HB2	2.17	0.45
1:2:327:ARG:C	1:2:591:LEU:H	2.16	0.45
1:2:776:PRO:HA	1:2:827:GLU:CA	2.46	0.45
2:3:418:LEU:O	2:3:421:PHE:N	2.49	0.45
3:4:854:LYS:H	3:4:857:ILE:CB	2.30	0.45
4:5:108:GLN:HA	4:5:109:SER:HA	1.69	0.45
3:4:245:ALA:HA	3:4:246:ARG:HA	1.52	0.45
4:5:616:PRO:O	4:5:619:ALA:HB3	2.16	0.45
5:6:601:LYS:CB	5:6:644:MET:N	2.79	0.45
1:2:268:LEU:O	1:2:271:PHE:N	2.50	0.45
1:2:329:GLY:N	1:2:589:TRP:O	2.50	0.45
1:2:359:ILE:HA	1:2:360:ARG:HA	1.60	0.45
3:4:339:ILE:O	3:4:392:ALA:O	2.35	0.45
3:4:854:LYS:C	3:4:857:ILE:H	2.08	0.45
4:5:53:ASN:O	4:5:57:LYS:N	2.49	0.45
5:6:308:SER:C	5:6:317:ILE:HA	2.37	0.45
5:6:654:GLU:O	5:6:657:GLU:N	2.45	0.45
5:6:659:GLN:CB	5:6:674:ALA:HB3	2.46	0.45
6:7:224:PRO:HA	6:7:241:VAL:HA	1.98	0.45
4:5:439:THR:O	4:5:479:ILE:HA	2.17	0.45
5:6:356:TRP:HA	5:6:381:LEU:O	2.16	0.45
5:6:559:THR:N	5:6:563:ILE:O	2.50	0.45
2:3:429:ALA:HB3	2:3:469:VAL:O	2.17	0.45
4:5:258:LEU:N	4:5:274:LEU:O	2.49	0.45
1:2:280:GLU:HA	1:2:283:TYR:O	2.17	0.45
3:4:502:THR:O	3:4:505:ASP:N	2.50	0.45
4:5:266:PRO:O	4:5:268:GLY:N	2.39	0.45
5:6:405:PRO:CA	5:6:450:TYR:HA	2.36	0.45
2:3:449:ASP:HA	2:3:454:GLU:O	2.17	0.44
4:5:413:LEU:HA	4:5:521:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:723:ILE:O	5:6:726:GLU:N	2.50	0.44
6:7:315:ILE:O	6:7:331:LEU:N	2.49	0.44
6:7:517:ASP:C	6:7:519:GLY:H	2.20	0.44
1:2:224:ARG:CB	7:C:211:THR:O	2.65	0.44
1:2:224:ARG:O	1:2:225:SER:C	2.54	0.44
1:2:318:VAL:N	1:2:428:GLY:O	2.26	0.44
2:3:301:LEU:O	2:3:318:LYS:O	2.35	0.44
5:6:545:LYS:O	5:6:548:LEU:N	2.51	0.44
5:6:605:ALA:C	5:6:607:GLY:N	2.70	0.44
6:7:311:GLN:O	6:7:503:THR:CB	2.65	0.44
2:3:406:LEU:N	2:3:545:LEU:O	2.50	0.44
2:3:690:ASP:O	2:3:693:LYS:N	2.51	0.44
3:4:822:VAL:O	3:4:825:ALA:HB3	2.18	0.44
6:7:310:PHE:C	6:7:504:ASP:O	2.55	0.44
6:7:369:GLY:HA2	6:7:370:LEU:HA	1.56	0.44
6:7:428:VAL:O	6:7:431:ALA:HB3	2.17	0.44
5:6:310:THR:O	5:6:345:THR:N	2.46	0.44
6:7:655:ALA:O	6:7:658:ASP:N	2.50	0.44
2:3:684:THR:O	2:3:688:ASN:CB	2.66	0.44
3:4:800:SER:O	3:4:801:MET:C	2.55	0.44
4:5:95:THR:HA	4:5:98:ALA:HB3	2.00	0.44
6:7:334:HIS:HA	6:7:503:THR:CB	2.48	0.44
7:C:373:VAL:HA	7:C:382:THR:O	2.18	0.44
5:6:305:TYR:CB	5:6:352:ARG:CB	2.96	0.44
5:6:313:MET:HA	5:6:314:CYS:HA	1.49	0.44
3:4:733:PRO:CB	6:7:445:GLY:N	2.71	0.44
6:7:209:GLN:H	6:7:212:ALA:H	1.65	0.44
7:C:72:GLY:N	7:C:93:ILE:O	2.50	0.44
5:6:624:GLU:O	5:6:626:GLY:N	2.51	0.44
6:7:251:VAL:HA	6:7:504:ASP:O	2.18	0.44
2:3:530:HIS:C	2:3:532:ASN:H	2.20	0.44
7:C:574:VAL:N	7:C:577:GLY:O	2.25	0.44
3:4:760:PRO:HA	3:4:815:ASN:HA	2.00	0.43
6:7:109:ASN:C	6:7:111:ASN:H	2.21	0.43
6:7:250:ASP:N	6:7:506:MET:O	2.51	0.43
1:2:629:ILE:N	1:2:640:LEU:O	2.39	0.43
3:4:910:LEU:O	3:4:915:LYS:N	2.51	0.43
5:6:287:LEU:HA	5:6:400:VAL:H	1.83	0.43
5:6:304:LEU:C	5:6:306:LYS:N	2.72	0.43
6:7:531:GLU:O	6:7:534:ARG:N	2.52	0.43
3:4:685:ASN:C	3:4:686:LEU:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:133:GLU:CB	5:6:134:LYS:HA	2.47	0.43
5:6:641:PHE:N	5:6:681:ALA:O	2.45	0.43
7:C:377:SER:C	7:C:379:GLY:H	2.21	0.43
2:3:412:SER:C	2:3:414:ALA:H	2.22	0.43
3:4:804:LEU:O	3:4:807:ALA:N	2.51	0.43
1:2:331:PHE:O	1:2:384:ASN:CA	2.59	0.43
2:3:29:GLN:N	2:3:31:PHE:O	2.52	0.43
2:3:404:ASN:HA	2:3:512:VAL:O	2.19	0.43
3:4:336:THR:N	3:4:396:VAL:O	2.46	0.43
5:6:505:LEU:O	5:6:509:SER:N	2.33	0.43
5:6:524:HIS:O	5:6:526:TYR:N	2.52	0.43
1:2:524:PRO:CB	1:2:525:LYS:HA	2.48	0.43
1:2:600:ASP:HA	1:2:643:ARG:H	1.83	0.43
3:4:501:ILE:O	3:4:502:THR:C	2.54	0.43
4:5:331:LEU:HA	4:5:332:GLY:HA2	1.63	0.43
5:6:802:SER:O	5:6:803:MET:C	2.56	0.43
2:3:223:THR:H	4:5:246:GLU:HA	1.82	0.43
5:6:123:SER:CB	5:6:135:VAL:H	2.32	0.43
6:7:724:LYS:C	6:7:726:SER:H	2.22	0.43
7:C:39:GLN:O	7:C:213:ALA:HB2	2.18	0.43
2:3:236:THR:HA	2:3:237:GLU:C	2.39	0.43
2:3:711:ALA:O	2:3:714:LYS:N	2.52	0.43
3:4:593:GLY:C	3:4:595:GLY:H	2.22	0.43
3:4:833:ILE:O	3:4:836:TYR:N	2.49	0.43
5:6:764:ILE:C	5:6:818:GLU:HA	2.39	0.43
6:7:2:SER:C	6:7:4:ALA:H	2.22	0.43
3:4:408:ASP:C	3:4:410:GLN:N	2.68	0.43
3:4:738:GLN:HA	3:4:739:ASP:HA	1.70	0.43
4:5:235:ASN:HA	4:5:236:CYS:HA	1.87	0.43
4:5:499:GLN:C	4:5:501:THR:H	2.22	0.43
5:6:653:HIS:O	5:6:657:GLU:N	2.51	0.43
6:7:395:SER:O	6:7:397:VAL:N	2.50	0.43
6:7:616:VAL:O	6:7:619:VAL:O	2.37	0.43
5:6:309:PHE:CA	5:6:317:ILE:HA	2.48	0.43
6:7:262:CYS:O	6:7:264:GLN:N	2.50	0.43
6:7:672:LYS:O	6:7:675:MET:N	2.48	0.43
6:7:701:LYS:C	6:7:704:LEU:H	2.22	0.43
7:C:386:PRO:O	7:C:388:ARG:N	2.51	0.43
1:2:244:VAL:H	1:2:297:ILE:CA	2.32	0.42
1:2:826:SER:O	1:2:828:PHE:N	2.51	0.42
2:3:198:ARG:HA	2:3:212:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:375:ASP:HA	3:4:377:ASN:O	2.19	0.42
5:6:510:SER:HA	5:6:513:ILE:CB	2.48	0.42
1:2:564:VAL:O	1:2:605:LEU:N	2.37	0.42
2:3:270:LEU:CA	4:5:510:THR:H	2.32	0.42
5:6:152:TYR:HA	5:6:266:SER:O	2.19	0.42
5:6:288:LEU:H	5:6:399:GLY:HA3	1.84	0.42
6:7:334:HIS:CB	6:7:377:GLU:HA	2.50	0.42
7:C:74:ASP:O	7:C:90:GLU:HA	2.18	0.42
2:3:536:PRO:HA	2:3:537:ASP:HA	1.55	0.42
2:3:669:PRO:HA	2:3:719:LYS:C	2.39	0.42
4:5:401:PRO:HA	4:5:402:ASP:C	2.38	0.42
5:6:810:ILE:O	5:6:813:ALA:HB3	2.19	0.42
1:2:220:ASP:O	1:2:223:GLY:O	2.38	0.42
1:2:221:GLU:CB	7:C:210:SER:CB	2.97	0.42
2:3:38:TYR:O	2:3:41:SER:N	2.52	0.42
3:4:329:LYS:HA	3:4:433:ILE:O	2.19	0.42
3:4:880:SER:CB	3:4:926:SER:H	2.32	0.42
3:4:917:ILE:O	3:4:926:SER:O	2.38	0.42
3:4:917:ILE:CB	3:4:928:ARG:H	2.32	0.42
5:6:559:THR:N	5:6:564:LYS:HA	2.35	0.42
4:5:752:LEU:O	4:5:755:LEU:N	2.51	0.42
3:4:598:ALA:HB2	3:4:640:SER:O	2.19	0.42
4:5:708:LEU:O	4:5:712:ARG:CB	2.66	0.42
5:6:336:PRO:C	5:6:338:CYS:H	2.21	0.42
1:2:497:ILE:C	1:2:500:SER:H	2.21	0.42
3:4:408:ASP:CB	3:4:409:GLY:HA2	2.50	0.42
3:4:594:LYS:C	3:4:596:SER:N	2.73	0.42
5:6:600:GLY:HA2	5:6:640:GLU:CB	2.50	0.42
6:7:395:SER:C	6:7:397:VAL:N	2.73	0.42
1:2:254:ALA:O	1:2:257:ALA:N	2.53	0.42
3:4:339:ILE:O	3:4:393:ASP:HA	2.19	0.42
4:5:760:THR:O	4:5:764:ARG:N	2.43	0.42
5:6:399:GLY:O	5:6:455:LEU:O	2.38	0.42
6:7:357:PRO:CA	6:7:374:THR:HA	2.44	0.42
6:7:703:ARG:C	6:7:705:ALA:H	2.23	0.42
1:2:425:GLU:O	1:2:456:ILE:HA	2.20	0.42
2:3:534:ALA:HA	4:5:758:HIS:O	2.20	0.42
3:4:377:ASN:CB	3:4:378:GLU:CA	2.96	0.42
4:5:62:THR:HA	4:5:138:ILE:O	2.19	0.42
5:6:603:SER:N	5:6:604:SER:HA	2.23	0.42
6:7:455:ASN:O	6:7:595:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:465:ALA:O	6:7:466:LYS:C	2.58	0.42
7:C:536:SER:O	7:C:539:VAL:N	2.53	0.42
1:2:370:LYS:C	1:2:372:PRO:N	2.74	0.42
2:3:314:LEU:C	4:5:459:THR:HA	2.40	0.42
3:4:256:ASP:O	3:4:259:HIS:N	2.53	0.42
5:6:386:VAL:C	5:6:388:ARG:H	2.22	0.42
5:6:797:VAL:C	5:6:799:GLN:N	2.73	0.42
6:7:525:GLU:O	6:7:528:LYS:N	2.41	0.42
1:2:505:ILE:C	1:2:507:GLY:H	2.23	0.41
1:2:552:ILE:O	1:2:555:TYR:N	2.53	0.41
2:3:100:LEU:H	2:3:159:GLY:H	1.67	0.41
2:3:191:LEU:N	2:3:455:ARG:C	2.73	0.41
2:3:201:HIS:HA	2:3:243:THR:HA	2.02	0.41
6:7:259:ALA:HA	6:7:269:VAL:O	2.20	0.41
1:2:332:PRO:O	1:2:382:TYR:O	2.38	0.41
5:6:309:PHE:CB	5:6:346:LEU:HA	2.50	0.41
5:6:337:SER:C	5:6:339:GLU:H	2.24	0.41
1:2:317:LEU:HA	1:2:429:ILE:HA	2.02	0.41
1:2:324:VAL:CB	1:2:420:PRO:HA	2.50	0.41
2:3:234:GLU:HA	2:3:240:LYS:HA	2.01	0.41
3:4:484:GLU:O	3:4:487:GLN:N	2.52	0.41
1:2:244:VAL:O	1:2:297:ILE:C	2.58	0.41
3:4:447:ASN:C	3:4:449:ARG:H	2.23	0.41
3:4:855:SER:CA	3:4:857:ILE:N	2.83	0.41
6:7:247:ARG:O	6:7:508:LEU:O	2.38	0.41
6:7:483:THR:O	6:7:524:ASP:N	2.53	0.41
7:C:203:LYS:C	7:C:205:ILE:H	2.24	0.41
2:3:338:ALA:HB3	2:3:339:ARG:C	2.41	0.41
6:7:499:LYS:CA	6:7:506:MET:H	2.31	0.41
1:2:207:ILE:O	1:2:208:ALA:C	2.59	0.41
2:3:323:GLY:HA3	2:3:324:ASN:HA	1.55	0.41
2:3:688:ASN:HA	6:7:604:PRO:CB	2.50	0.41
3:4:713:ASP:O	3:4:716:ASN:N	2.54	0.41
4:5:40:LEU:O	4:5:43:GLN:N	2.54	0.41
4:5:665:LYS:C	4:5:668:LEU:H	2.23	0.41
7:C:348:SER:O	7:C:352:LYS:N	2.54	0.41
1:2:290:HIS:C	1:2:292:GLU:H	2.23	0.41
3:4:445:ARG:HA	3:4:453:LEU:HA	2.03	0.41
4:5:86:ILE:O	4:5:89:LEU:N	2.52	0.41
6:7:518:ASN:H	6:7:560:ARG:C	2.24	0.41
7:C:597:ILE:O	7:C:601:LYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:787:SER:O	1:2:790:TYR:N	2.53	0.41
2:3:411:PRO:C	2:3:413:THR:N	2.73	0.41
4:5:754:ALA:O	4:5:758:HIS:N	2.51	0.41
5:6:301:ARG:N	5:6:356:TRP:O	2.45	0.41
5:6:543:VAL:O	5:6:544:LYS:C	2.58	0.41
7:C:509:LEU:O	7:C:512:LYS:N	2.54	0.41
1:2:500:SER:HA	1:2:757:PRO:CB	2.50	0.41
1:2:802:SER:HA	1:2:803:PHE:HA	1.80	0.41
2:3:448:THR:CB	6:7:363:PHE:H	2.33	0.41
3:4:608:ASP:C	3:4:610:ASP:N	2.74	0.41
3:4:729:LEU:HA	3:4:730:GLU:HA	1.68	0.41
4:5:415:LEU:HA	4:5:523:ALA:O	2.20	0.41
5:6:637:CYS:HA	5:6:679:LEU:O	2.20	0.41
5:6:751:LEU:O	5:6:752:ARG:C	2.58	0.41
5:6:763:PRO:HA	5:6:817:ASP:CB	2.51	0.41
5:6:766:THR:C	5:6:768:GLU:O	2.59	0.41
6:7:212:ALA:O	6:7:216:ARG:N	2.46	0.41
1:2:425:GLU:N	1:2:457:LYS:O	2.38	0.41
2:3:449:ASP:CB	6:7:366:LEU:CB	2.99	0.41
3:4:771:VAL:O	3:4:772:ARG:C	2.59	0.41
5:6:173:GLN:O	5:6:176:ARG:N	2.54	0.41
6:7:208:SER:CB	6:7:209:GLN:HA	2.51	0.41
3:4:335:SER:HA	3:4:396:VAL:O	2.22	0.40
3:4:766:ALA:O	3:4:767:LYS:C	2.59	0.40
3:4:811:MET:C	3:4:813:LEU:H	2.24	0.40
4:5:237:GLY:HA2	4:5:238:PRO:O	2.21	0.40
6:7:249:SER:CA	6:7:507:ILE:CA	2.92	0.40
2:3:474:GLU:O	2:3:477:LYS:N	2.54	0.40
2:3:735:PHE:HA	2:3:738:LEU:O	2.21	0.40
3:4:621:LEU:O	3:4:624:SER:N	2.54	0.40
5:6:170:ILE:O	5:6:171:SER:C	2.58	0.40
5:6:731:ILE:O	5:6:732:VAL:C	2.58	0.40
1:2:602:GLY:O	1:2:644:CYS:HA	2.22	0.40
2:3:235:ASP:N	2:3:239:ASN:O	2.54	0.40
2:3:539:LEU:O	2:3:542:ARG:N	2.53	0.40
5:6:512:GLU:O	5:6:513:ILE:C	2.60	0.40
7:C:520:LEU:O	7:C:523:LEU:N	2.55	0.40
2:3:96:ILE:O	2:3:155:LEU:HA	2.22	0.40
3:4:910:LEU:O	3:4:916:VAL:N	2.55	0.40
4:5:415:LEU:CB	4:5:523:ALA:HB3	2.50	0.40
5:6:512:GLU:C	5:6:514:ASN:N	2.73	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:533:ILE:O	2:3:534:ALA:HB3	2.21	0.40
3:4:292:ASP:N	3:4:293:LEU:HA	2.35	0.40
3:4:488:ASN:C	3:4:490:VAL:H	2.23	0.40
3:4:778:ARG:HA	3:4:793:ALA:HB3	2.02	0.40
7:C:363:LEU:O	7:C:367:TRP:N	2.51	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	2	583/868 (67%)	503 (86%)	69 (12%)	11 (2%)	6	32
2	3	589/997 (59%)	516 (88%)	65 (11%)	8 (1%)	9	41
3	4	706/933 (76%)	603 (85%)	95 (14%)	8 (1%)	12	47
4	5	614/775 (79%)	564 (92%)	45 (7%)	5 (1%)	16	55
5	6	634/1017 (62%)	539 (85%)	80 (13%)	15 (2%)	5	27
6	7	612/845 (72%)	542 (89%)	62 (10%)	8 (1%)	10	43
7	C	457/604 (76%)	407 (89%)	46 (10%)	4 (1%)	14	52
All	All	4195/6039 (70%)	3674 (88%)	462 (11%)	59 (1%)	12	41

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	305	SER
1	2	334	LEU
2	3	198	ARG
3	4	179	ILE
3	4	490	VAL
3	4	609	VAL

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Mol	Chain	Res	Type
4	5	267	VAL
4	5	596	ILE
5	6	510	SER
5	6	513	ILE
5	6	578	SER
5	6	605	ALA
6	7	26	VAL
6	7	464	VAL
6	7	544	GLN
1	2	297	ILE
1	2	533	ILE
1	2	548	ALA
2	3	389	VAL
3	4	419	VAL
3	4	857	ILE
4	5	177	THR
5	6	321	VAL
5	6	402	ILE
5	6	580	SER
6	7	502	VAL
1	2	585	ILE
2	3	230	ILE
4	5	410	ILE
5	6	555	VAL
5	6	579	THR
5	6	703	ALA
6	7	373	GLU
4	5	460	ARG
5	6	781	ARG
6	7	371	LEU
7	C	134	VAL
7	C	204	ALA
1	2	256	LEU
1	2	550	SER
2	3	158	LYS
2	3	440	VAL
3	4	773	ALA
5	6	556	HIS
5	6	653	HIS
1	2	265	GLU
1	2	291	SER
7	C	67	PRO

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Mol	Chain	Res	Type
7	C	108	ASN
3	4	463	VAL
5	6	533	ILE
6	7	248	VAL
1	2	840	VAL
3	4	526	ILE
2	3	326	VAL
2	3	20	VAL
2	3	533	ILE
5	6	503	VAL
6	7	708	VAL

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

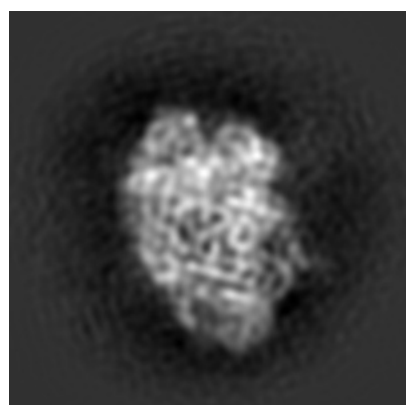
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6671. These allow visual inspection of the internal detail of the map and identification of artifacts.

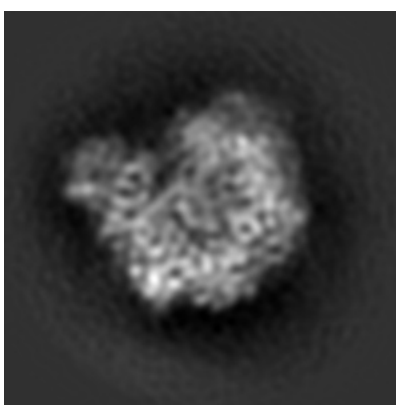
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

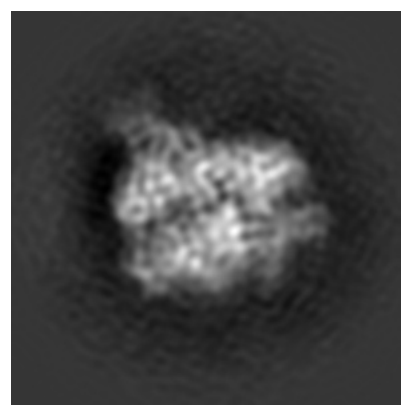
#### 6.1.1 Primary map



X



Y

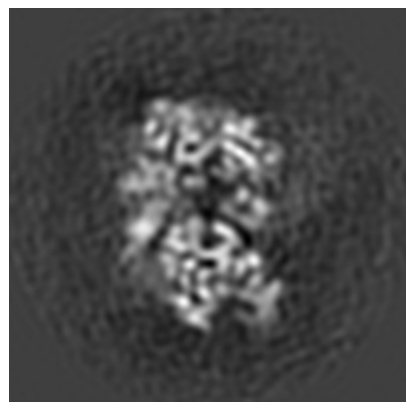


Z

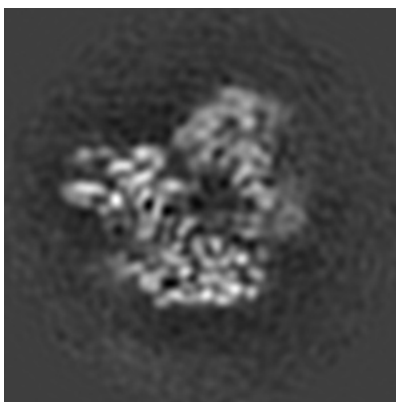
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

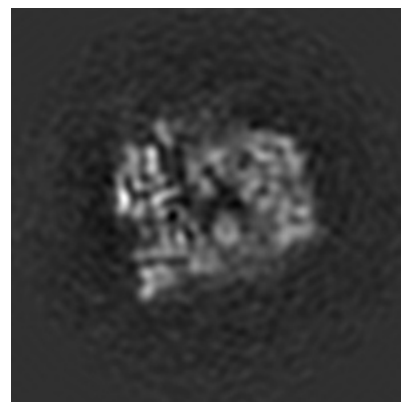
#### 6.2.1 Primary map



X Index: 100



Y Index: 100

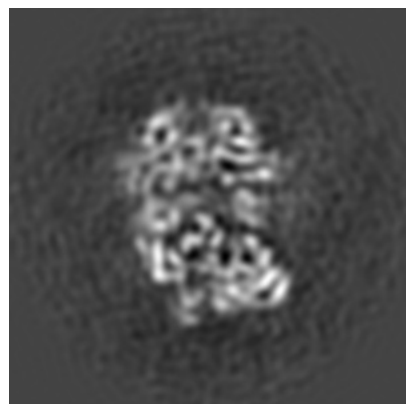


Z Index: 100

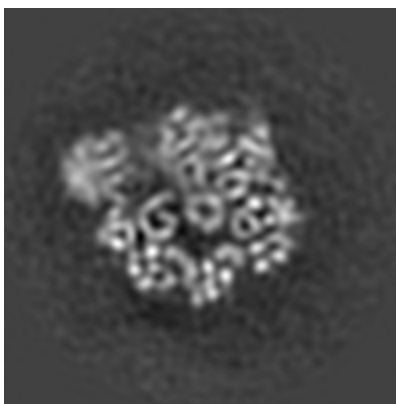
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

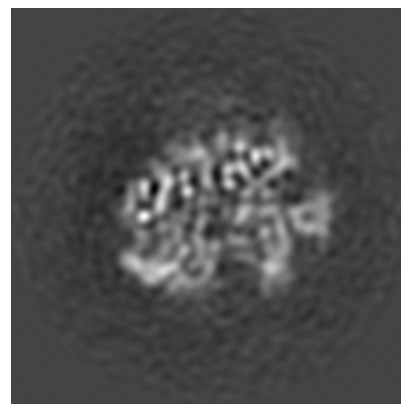
### 6.3.1 Primary map



X Index: 93



Y Index: 118

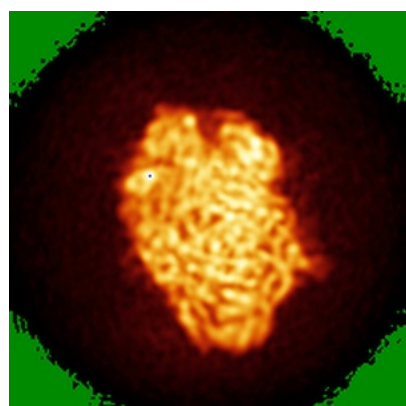


Z Index: 118

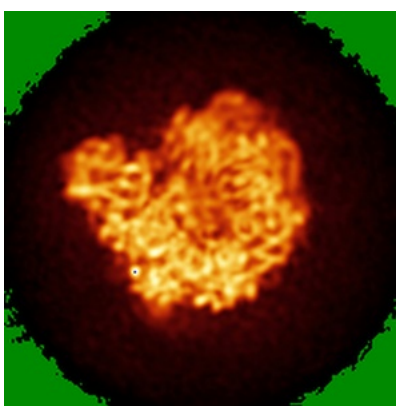
The images above show the largest variance slices of the map in three orthogonal directions.

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

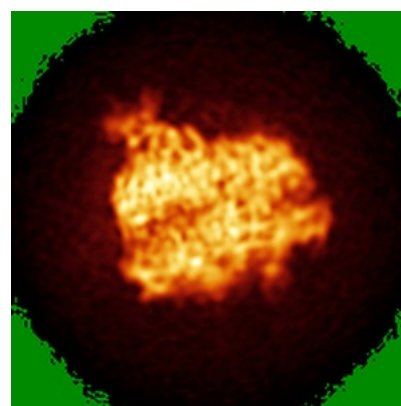
### 6.4.1 Primary map



X



Y

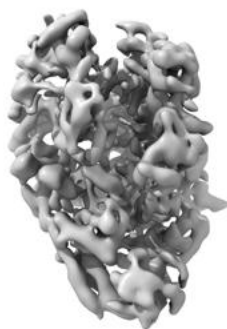


Z

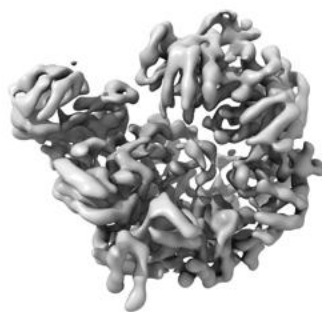
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

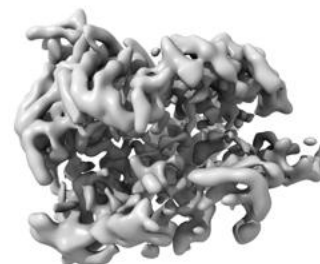
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0253. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

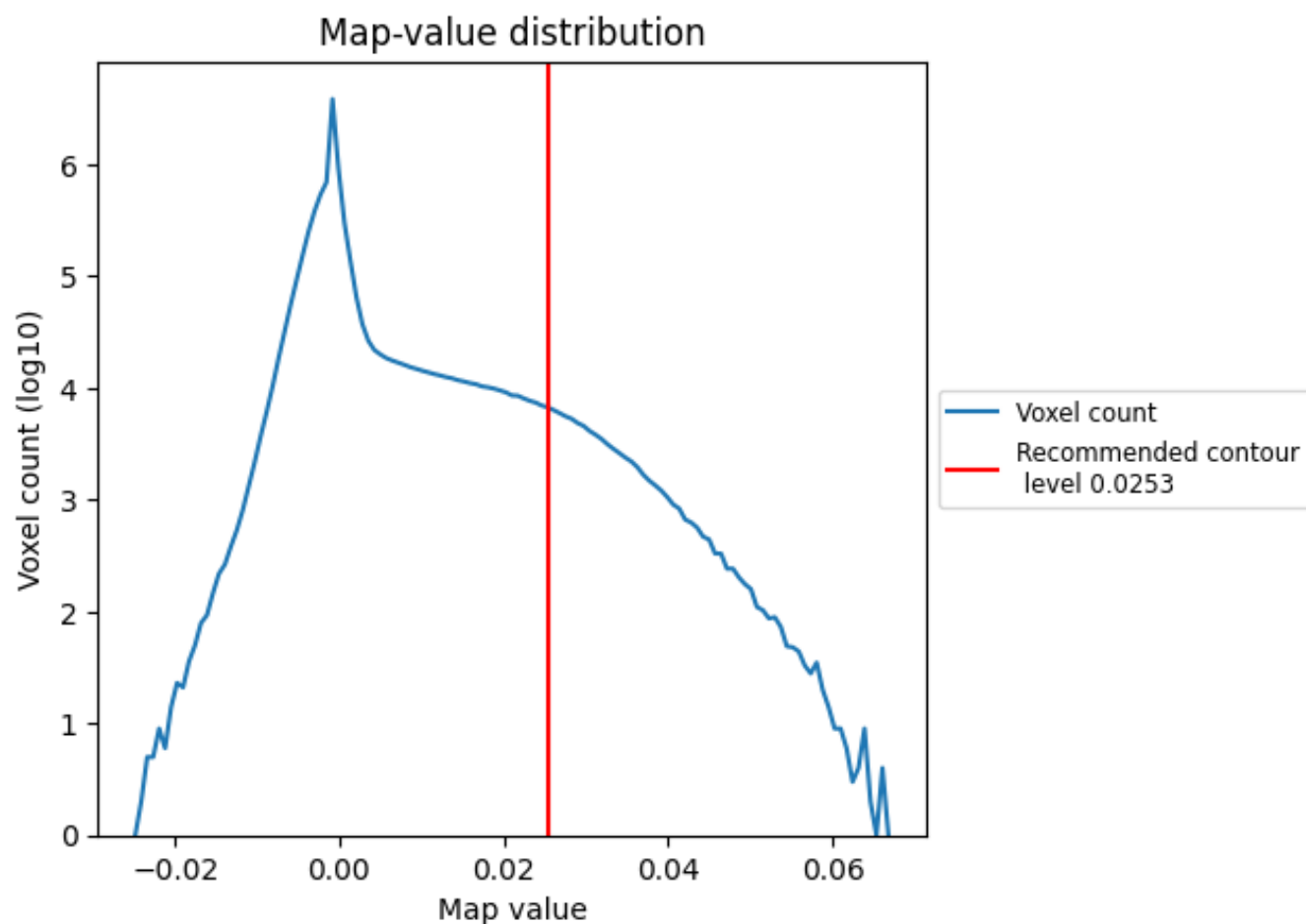
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

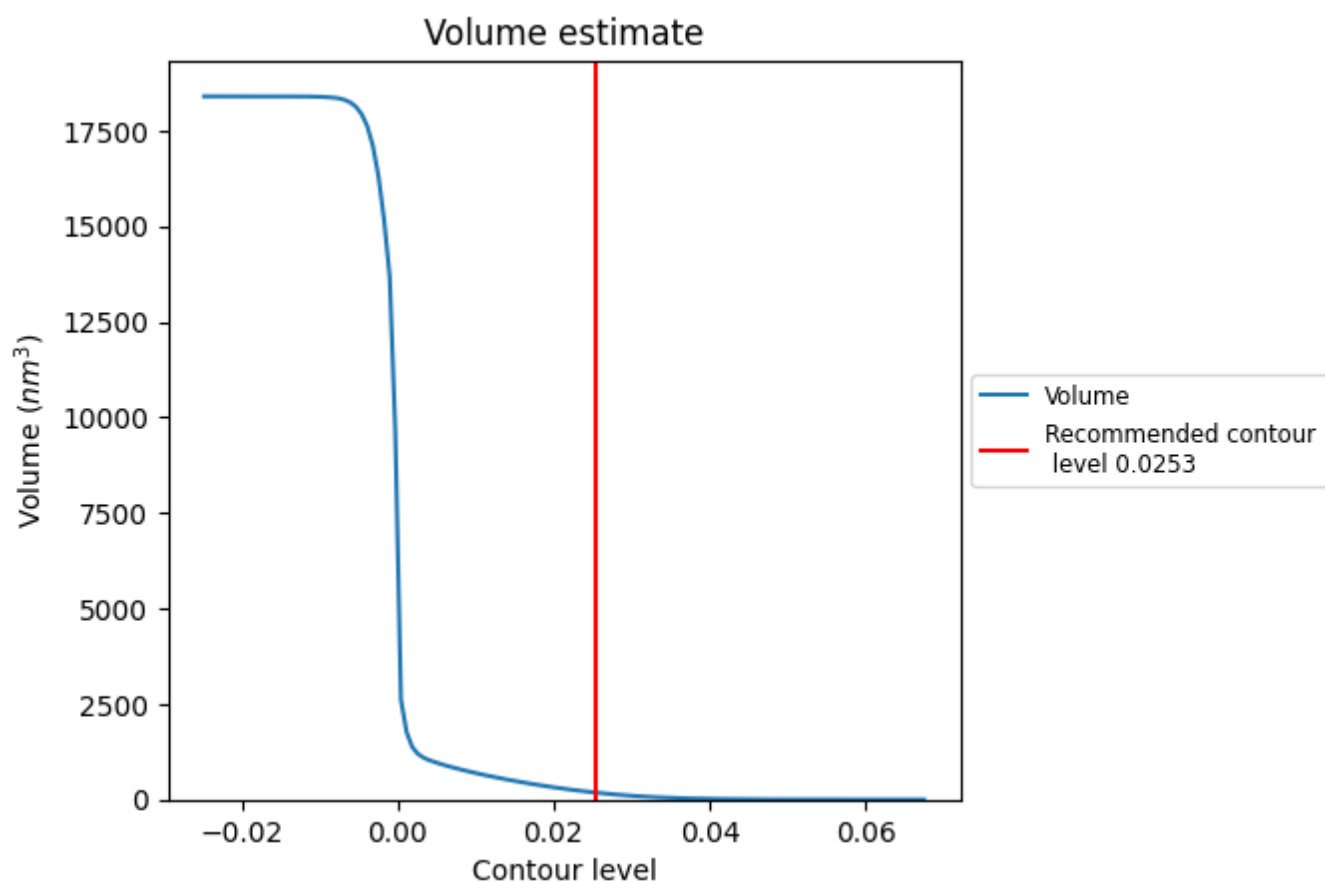
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

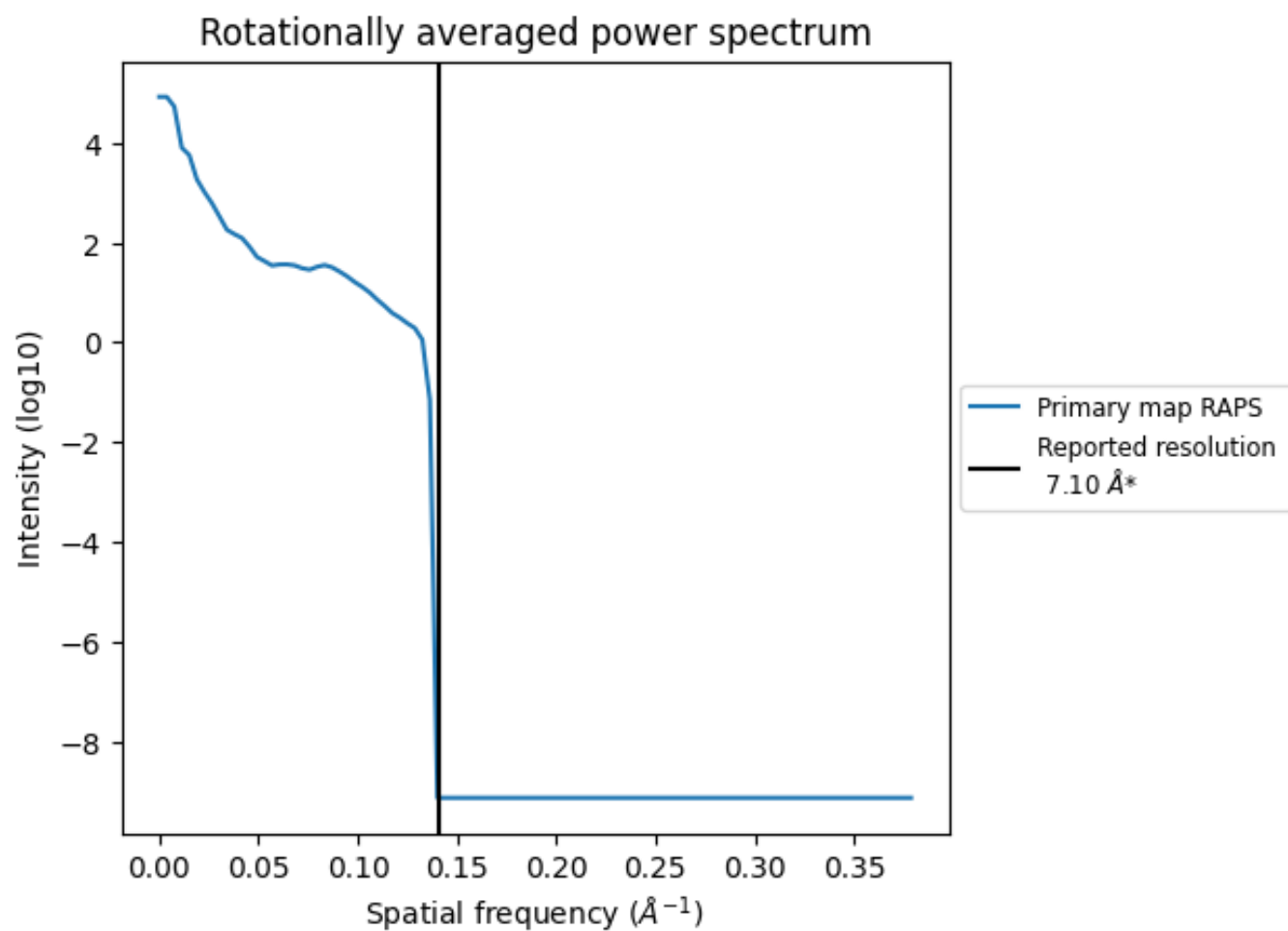
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 185 nm<sup>3</sup>; this corresponds to an approximate mass of 167 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.141 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

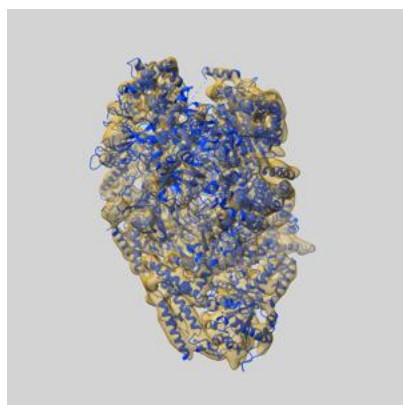
This section was not generated. No FSC curve or half-maps provided.



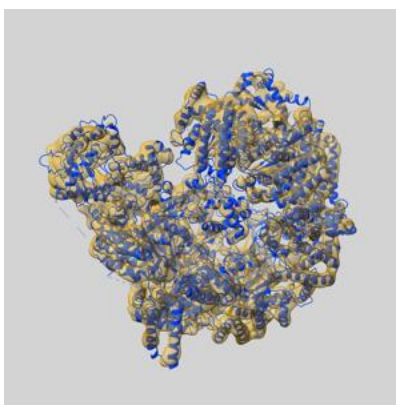
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6671 and PDB model 5XF8. Per-residue inclusion information can be found in section [3](#) on page [5](#).

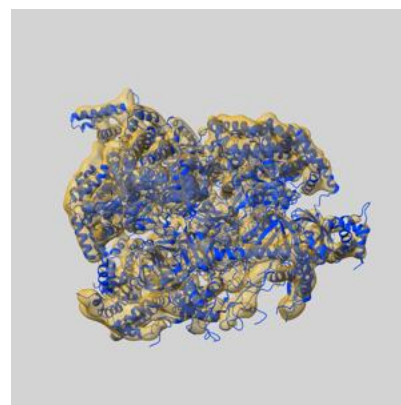
### 9.1 Map-model overlay [i](#)



X



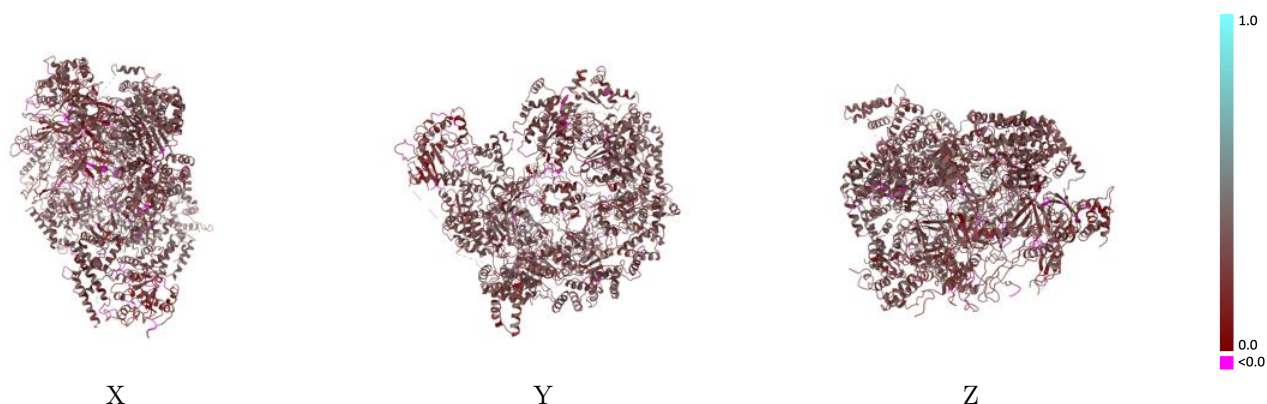
Y



Z

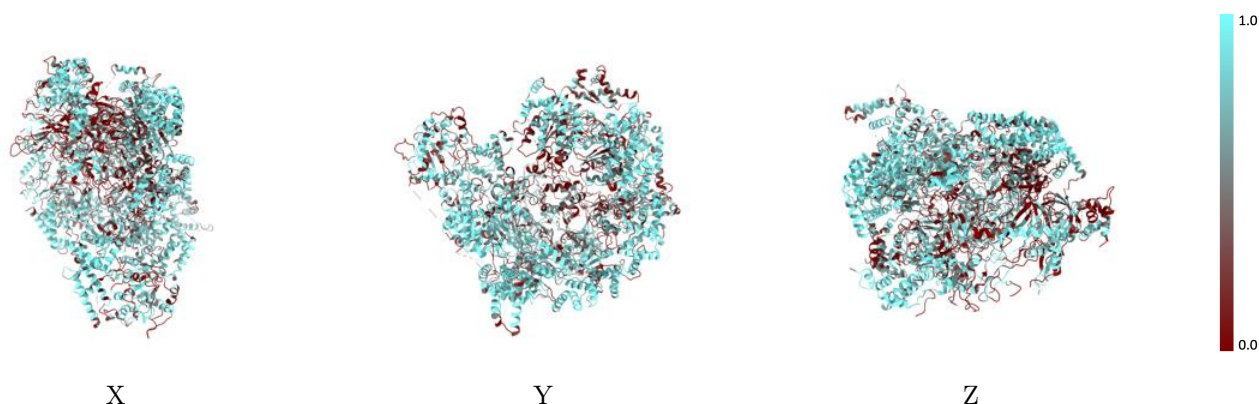
The images above show the 3D surface view of the map at the recommended contour level 0.0253 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



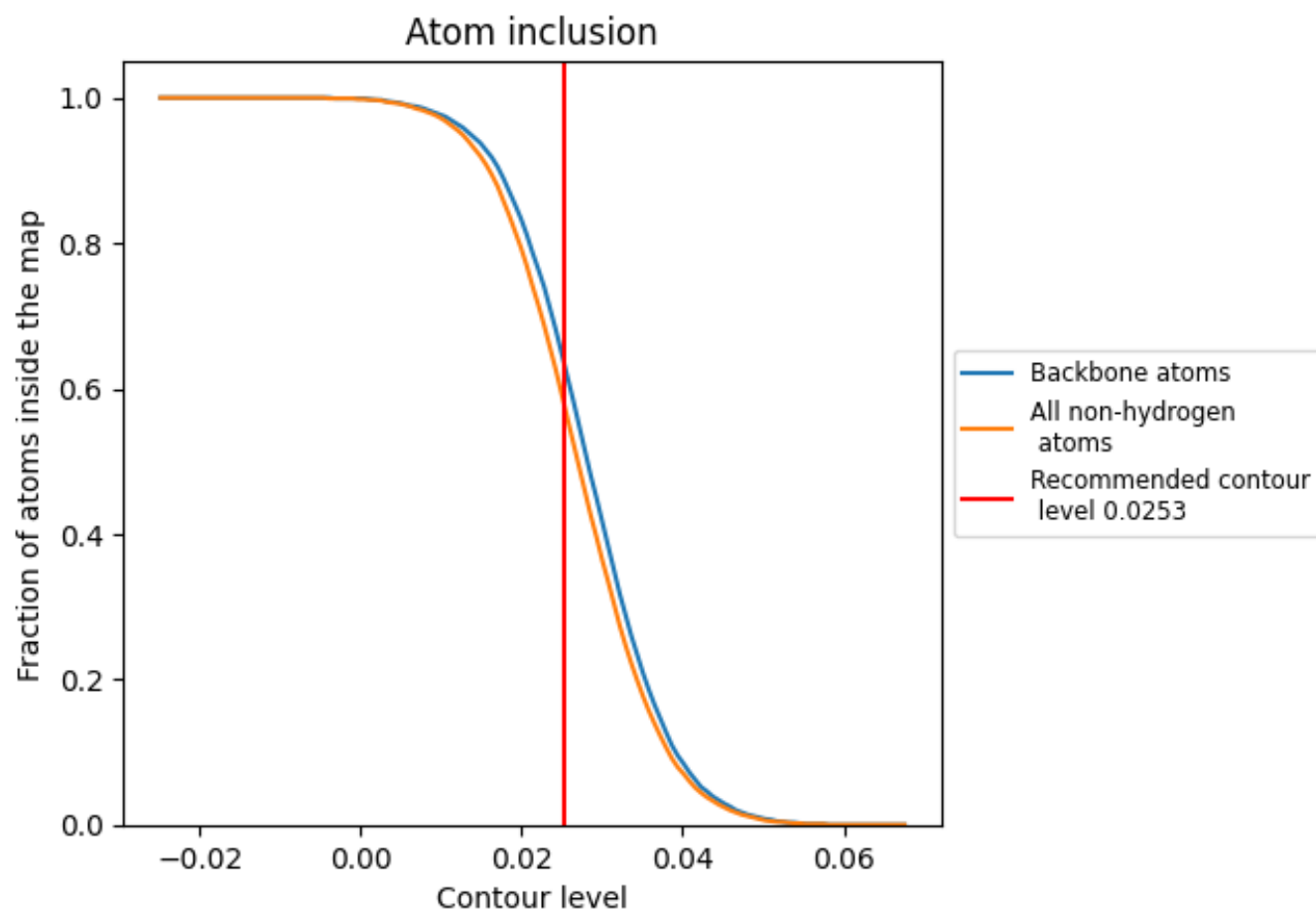
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0253).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 58% 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 (0.0253) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5770	<div></div> 0.2570
2	<div></div> 0.6710	<div></div> 0.2760
3	<div></div> 0.5460	<div></div> 0.2630
4	<div></div> 0.6590	<div></div> 0.2670
5	<div></div> 0.4120	<div></div> 0.2320
6	<div></div> 0.7080	<div></div> 0.2840
7	<div></div> 0.4990	<div></div> 0.2580
C	<div></div> 0.5150	<div></div> 0.2100

1.0

0.0

<0.0