



Full wwPDB EM Validation Report ⓘ

Feb 27, 2025 – 06:30 pm GMT

PDB ID : 9GJW
EMDB ID : EMD-51407
Title : OCCM maturation intermediate stalled with an Arginine Finger mutation in Mcm2
Authors : Butryn, A.; Costa, A.
Deposited on : 2024-08-22
Resolution : 3.30 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.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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

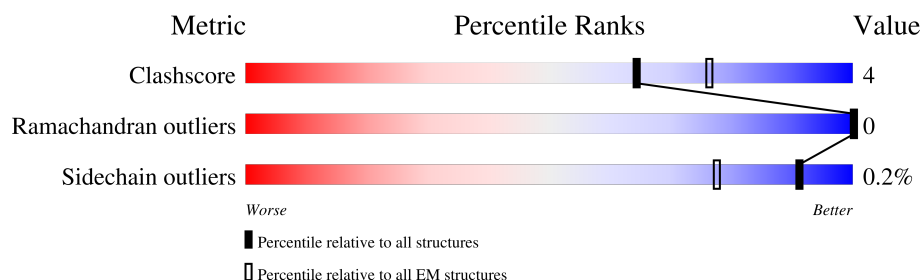
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.





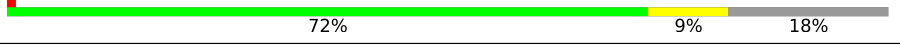

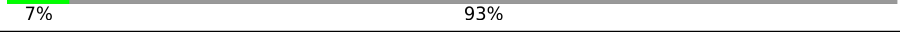
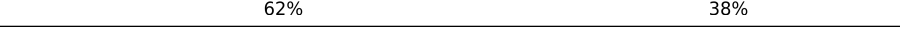
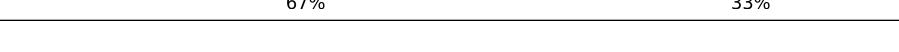
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	868	
2	3	1006	
3	4	933	
4	5	775	
5	6	1017	
6	7	845	
7	8	604	
8	A	949	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	B	620	
10	C	616	
11	D	529	
12	E	479	
13	F	435	
14	X	42	
14	Y	42	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 52380 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	590	Total	C	N	O	S	0	0
			4681	2940	842	884	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	676	ALA	ARG	engineered mutation	UNP P29469

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	573	Total	C	N	O	S	0	0
			4489	2839	794	844	12		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-34	MET	-	initiating methionine	UNP P24279
3	-33	LYS	-	expression tag	UNP P24279
3	-32	ARG	-	expression tag	UNP P24279
3	-31	ARG	-	expression tag	UNP P24279
3	-30	TRP	-	expression tag	UNP P24279
3	-29	LYS	-	expression tag	UNP P24279
3	-28	LYS	-	expression tag	UNP P24279
3	-27	ASN	-	expression tag	UNP P24279
3	-26	PHE	-	expression tag	UNP P24279
3	-25	ILE	-	expression tag	UNP P24279
3	-24	ALA	-	expression tag	UNP P24279
3	-23	VAL	-	expression tag	UNP P24279
3	-22	SER	-	expression tag	UNP P24279
3	-21	ALA	-	expression tag	UNP P24279
3	-20	ALA	-	expression tag	UNP P24279
3	-19	ASN	-	expression tag	UNP P24279

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
3	-18	ARG	-	expression tag	UNP P24279
3	-17	PHE	-	expression tag	UNP P24279
3	-16	LYS	-	expression tag	UNP P24279
3	-15	LYS	-	expression tag	UNP P24279
3	-14	ILE	-	expression tag	UNP P24279
3	-13	SER	-	expression tag	UNP P24279
3	-12	SER	-	expression tag	UNP P24279
3	-11	SER	-	expression tag	UNP P24279
3	-10	GLY	-	expression tag	UNP P24279
3	-9	ALA	-	expression tag	UNP P24279
3	-8	LEU	-	expression tag	UNP P24279
3	-7	GLU	-	expression tag	UNP P24279
3	-6	ASN	-	expression tag	UNP P24279
3	-5	LEU	-	expression tag	UNP P24279
3	-4	TYR	-	expression tag	UNP P24279
3	-3	PHE	-	expression tag	UNP P24279
3	-2	GLN	-	expression tag	UNP P24279
3	-1	GLY	-	expression tag	UNP P24279
3	0	GLU	-	expression tag	UNP P24279

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	658	Total	C	N	O	S	0	0
			5225	3275	901	1018	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	566	Total	C	N	O	S	0	0
			4460	2813	768	856	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	679	Total	C	N	O	S	0	0
			5420	3436	938	1017	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	651	Total	C	N	O	S	0	0
			5128	3239	883	975	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	505	Total	C	N	O	S	0	0
			4047	2583	688	757	19		

- Molecule 8 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	416	Total	C	N	O	S	0	0
			3318	2116	566	618	18		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP P54784
A	-33	LYS	-	expression tag	UNP P54784
A	-32	ARG	-	expression tag	UNP P54784
A	-31	ARG	-	expression tag	UNP P54784
A	-30	TRP	-	expression tag	UNP P54784
A	-29	LYS	-	expression tag	UNP P54784
A	-28	LYS	-	expression tag	UNP P54784
A	-27	ASN	-	expression tag	UNP P54784
A	-26	PHE	-	expression tag	UNP P54784
A	-25	ILE	-	expression tag	UNP P54784
A	-24	ALA	-	expression tag	UNP P54784
A	-23	VAL	-	expression tag	UNP P54784
A	-22	SER	-	expression tag	UNP P54784
A	-21	ALA	-	expression tag	UNP P54784
A	-20	ALA	-	expression tag	UNP P54784
A	-19	ASN	-	expression tag	UNP P54784
A	-18	ARG	-	expression tag	UNP P54784
A	-17	PHE	-	expression tag	UNP P54784
A	-16	LYS	-	expression tag	UNP P54784
A	-15	LYS	-	expression tag	UNP P54784
A	-14	ILE	-	expression tag	UNP P54784
A	-13	SER	-	expression tag	UNP P54784
A	-12	SER	-	expression tag	UNP P54784
A	-11	SER	-	expression tag	UNP P54784
A	-10	GLY	-	expression tag	UNP P54784

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	expression tag	UNP P54784
A	-8	LEU	-	expression tag	UNP P54784
A	-7	GLU	-	expression tag	UNP P54784
A	-6	ASN	-	expression tag	UNP P54784
A	-5	LEU	-	expression tag	UNP P54784
A	-4	TYR	-	expression tag	UNP P54784
A	-3	PHE	-	expression tag	UNP P54784
A	-2	GLN	-	expression tag	UNP P54784
A	-1	GLY	-	expression tag	UNP P54784
A	0	GLU	-	expression tag	UNP P54784

- Molecule 9 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	221	Total	C	N	O	S	0	0
			1840	1201	298	331	10		

- Molecule 10 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	552	Total	C	N	O	S	0	0
			4581	2964	754	847	16		

- Molecule 11 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	433	Total	C	N	O	S	0	0
			3533	2268	599	653	13		

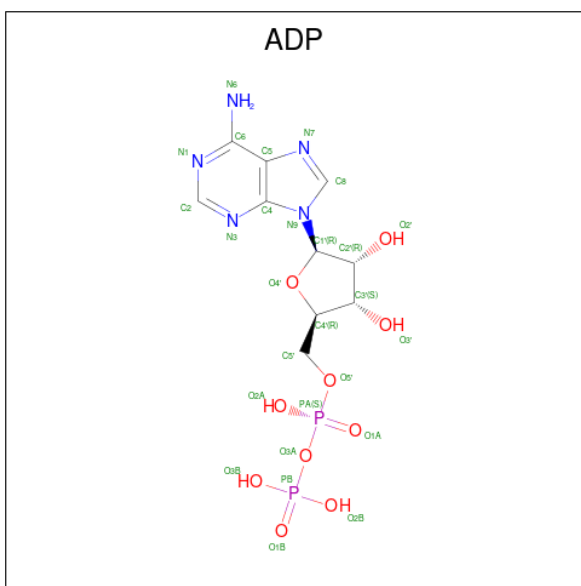
- Molecule 12 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	416	Total	C	N	O	S	0	0
			3410	2226	538	632	14		

- Molecule 13 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	31	Total	C	N	O	S	0	0
			267	172	45	49	1		

- Molecule 15 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).

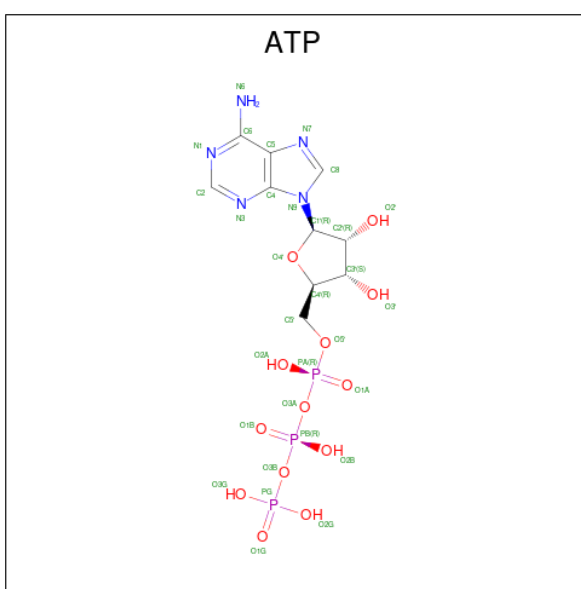


Mol	Chain	Residues	Atoms					AltConf
15	2	1	Total 27	C 10	N 5	O 10	P 2	0
15	3	1	Total 27	C 10	N 5	O 10	P 2	0
15	4	1	Total 27	C 10	N 5	O 10	P 2	0
15	5	1	Total 27	C 10	N 5	O 10	P 2	0
15	6	1	Total 27	C 10	N 5	O 10	P 2	0
15	7	1	Total 27	C 10	N 5	O 10	P 2	0

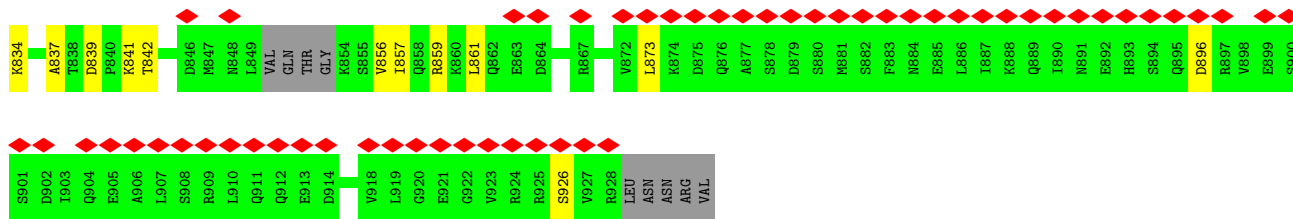
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	4	1	Total	Zn	0
			1	1	
16	5	1	Total	Zn	0
			1	1	
16	6	1	Total	Zn	0
			1	1	
16	7	1	Total	Zn	0
			1	1	

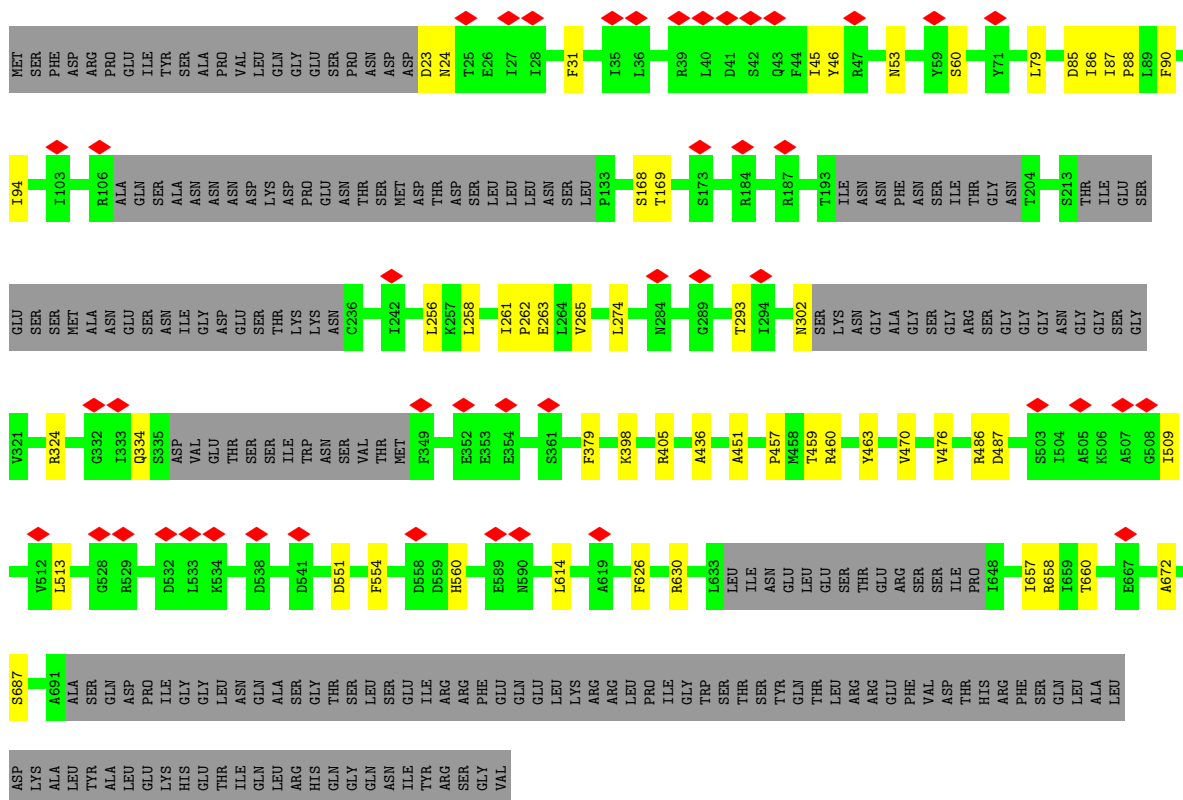
- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



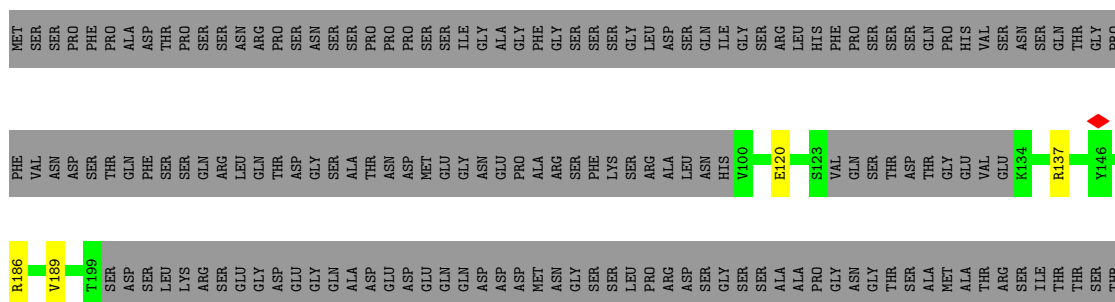
Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
17	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
17	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

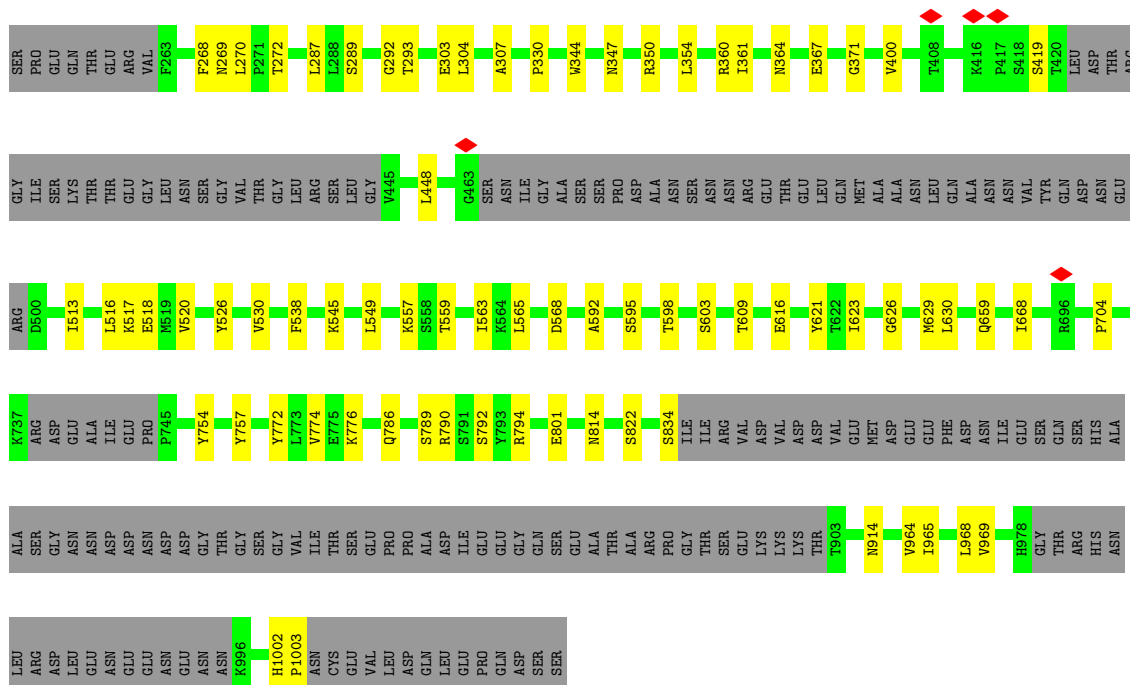


- Molecule 4: Minichromosome maintenance protein 5

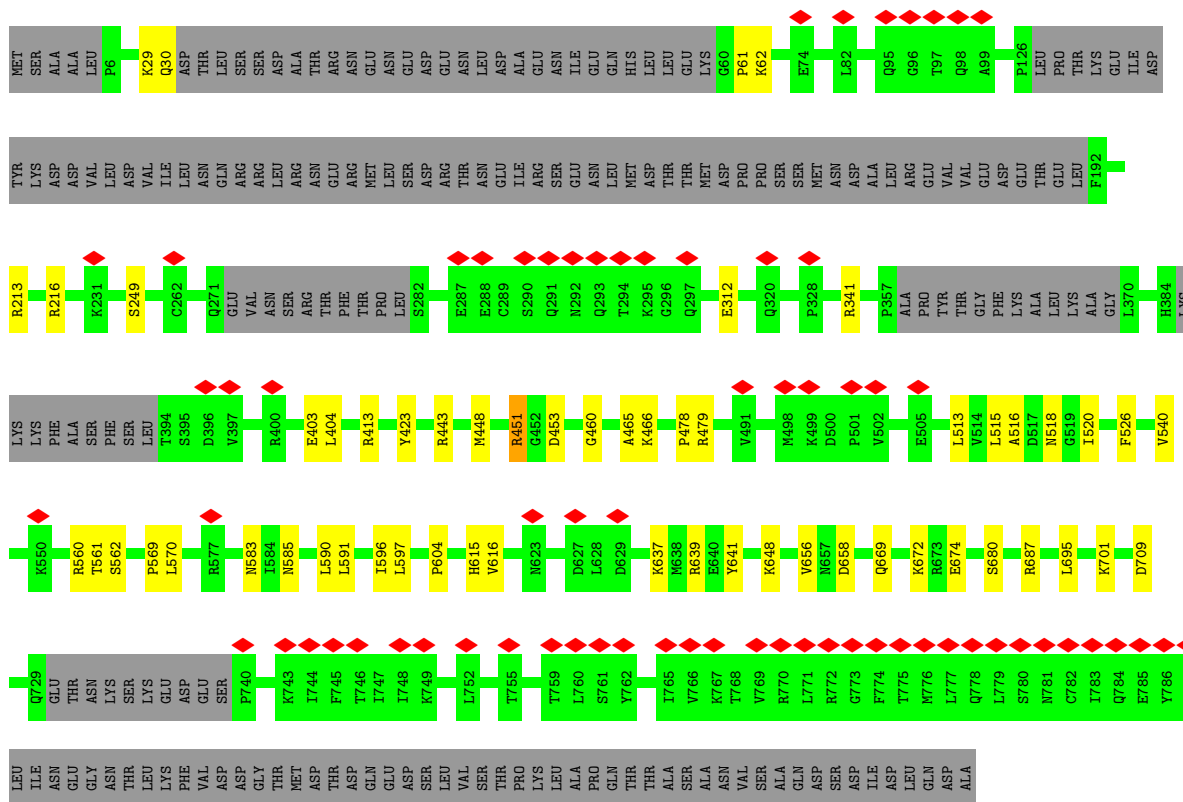


- Molecule 5: DNA replication licensing factor MCM6






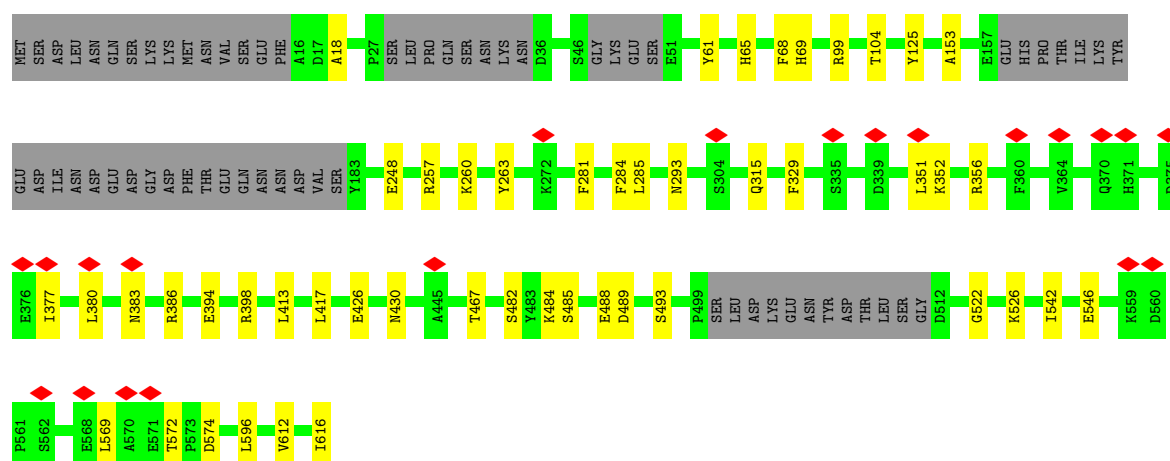
- Molecule 6: DNA replication licensing factor MCM7



- Molecule 7: Cell division cycle protein CDT1

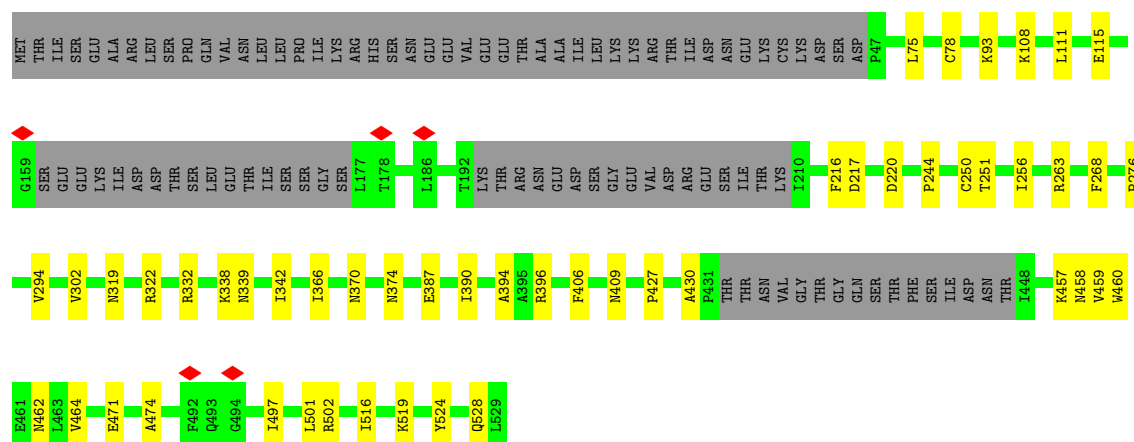


Chain C: 




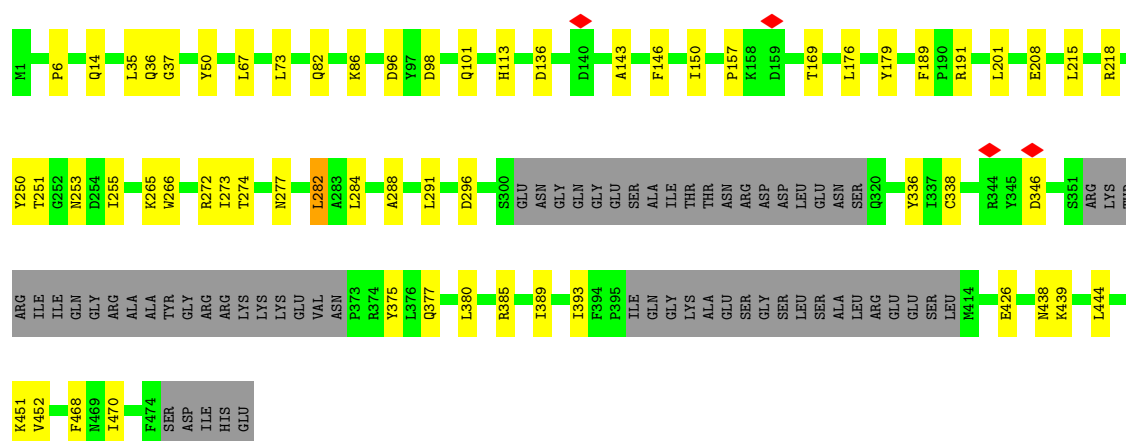
• Molecule 11: Origin recognition complex subunit 4

Chain D: 

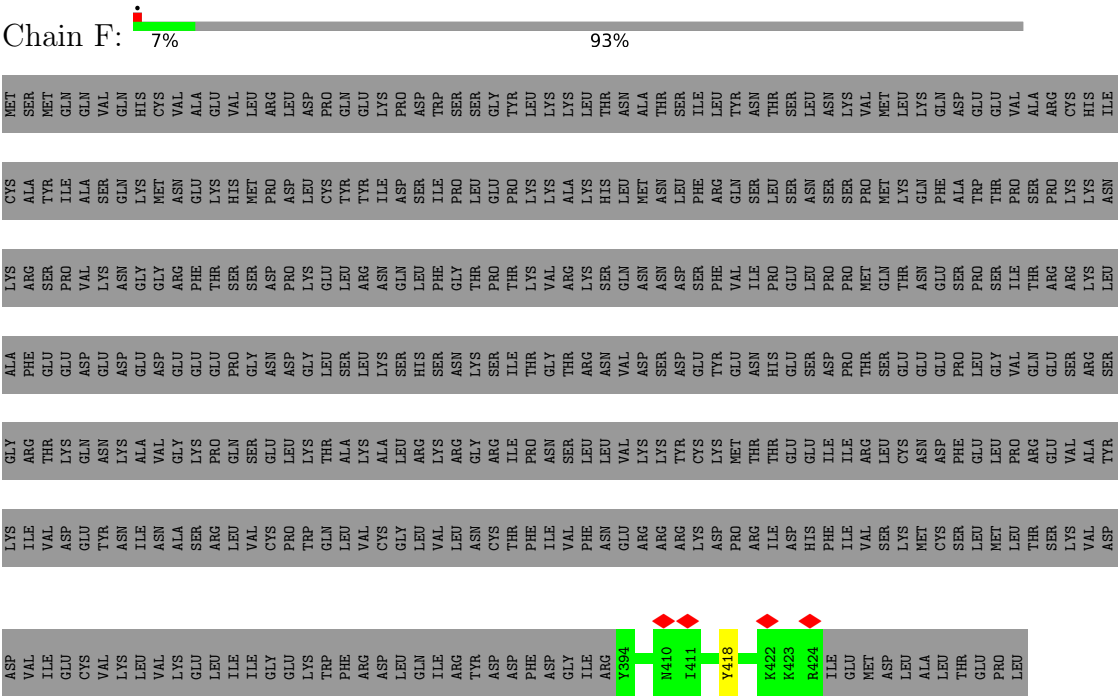


• Molecule 12: Origin recognition complex subunit 5

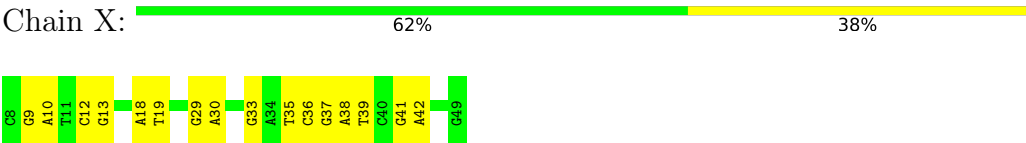
Chain E: 



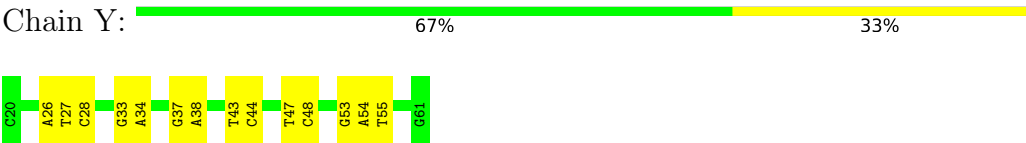
● Molecule 13: Origin recognition complex subunit 6



● Molecule 14: DNA (42-MER)



● Molecule 14: DNA (42-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	178450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.34	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.811	Depositor
Minimum map value	-0.309	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	418.0, 418.0, 418.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/4758	0.50	0/6427
2	3	0.24	0/4565	0.49	0/6191
3	4	0.24	0/5289	0.48	0/7132
4	5	0.24	0/4521	0.48	0/6103
5	6	0.24	0/5509	0.48	0/7425
6	7	0.24	0/5204	0.47	0/7026
7	8	0.24	0/4123	0.47	0/5588
8	A	0.24	0/3366	0.45	0/4530
9	B	0.25	0/1887	0.45	0/2549
10	C	0.24	0/4679	0.44	0/6313
11	D	0.24	0/3597	0.45	0/4862
12	E	0.25	0/3492	0.43	0/4747
13	F	0.24	0/271	0.47	0/364
14	X	0.51	0/965	0.93	0/1487
14	Y	0.50	0/965	0.93	0/1487
All	All	0.25	0/53191	0.50	0/72231

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	4681	0	4741	43	0
2	3	4489	0	4560	32	0
3	4	5225	0	5296	51	0
4	5	4460	0	4549	34	0
5	6	5420	0	5468	50	0
6	7	5128	0	5209	37	0
7	8	4047	0	4117	39	0
8	A	3318	0	3410	27	0
9	B	1840	0	1810	17	0
10	C	4581	0	4555	31	0
11	D	3533	0	3597	37	0
12	E	3410	0	3421	41	0
13	F	267	0	271	2	0
14	X	861	0	473	9	0
14	Y	861	0	473	12	0
15	2	27	0	12	2	0
15	3	27	0	12	2	0
15	4	27	0	12	2	0
15	5	27	0	12	1	0
15	6	27	0	12	1	0
15	7	27	0	12	6	0
16	4	1	0	0	0	0
16	5	1	0	0	0	0
16	6	1	0	0	0	0
16	7	1	0	0	0	0
17	A	31	0	12	0	0
17	D	31	0	12	1	0
17	E	31	0	12	0	0
All	All	52380	0	52058	410	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 4.

All (410) 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)
1:2:530:LYS:HD2	1:2:531:HIS:H	1.39	0.86
3:4:402:THR:HG1	3:4:413:HIS:N	1.73	0.86
3:4:527:ALA:HB3	3:4:537:LYS:HE3	1.60	0.83
10:C:257:ARG:NH2	11:D:458:ASN:OD1	2.16	0.78
4:5:457:PRO:O	4:5:460:ARG:NH1	2.19	0.76
3:4:859:ARG:NH1	8:A:908:ASP:O	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:601:LEU:HB2	3:4:621:LEU:HD23	1.73	0.71
6:7:596:ILE:HD11	6:7:695:LEU:HD11	1.73	0.71
5:6:592:ALA:HB3	5:6:595:SER:HB2	1.74	0.70
12:E:274:THR:H	12:E:277:ASN:HB2	1.58	0.68
11:D:462:ASN:ND2	12:E:251:THR:O	2.27	0.68
3:4:526:ILE:HD11	3:4:541:LEU:HD13	1.76	0.67
1:2:387:ARG:NH1	1:2:407:GLU:OE1	2.28	0.67
10:C:248:GLU:O	11:D:457:LYS:NZ	2.28	0.67
1:2:247:ARG:O	1:2:247:ARG:NH1	2.26	0.67
2:3:352:LYS:O	2:3:356:LYS:NZ	2.27	0.66
7:8:387:LYS:HG3	7:8:395:THR:HG21	1.76	0.66
3:4:317:LEU:O	6:7:341:ARG:NH2	2.29	0.66
1:2:247:ARG:HE	7:8:320:VAL:HA	1.62	0.65
6:7:513:LEU:HD13	6:7:540:VAL:HG21	1.77	0.64
9:B:316:PHE:CD2	9:B:480:ILE:HG13	2.33	0.64
1:2:242:LEU:HD12	1:2:295:VAL:HG22	1.80	0.63
10:C:99:ARG:NH1	12:E:208:GLU:OE2	2.29	0.63
1:2:631:ILE:HD11	1:2:633:LYS:HD3	1.80	0.62
3:4:856:VAL:HA	3:4:859:ARG:HD2	1.81	0.62
5:6:794:ARG:NH1	5:6:834:SER:OG	2.33	0.62
6:7:479:ARG:NH2	6:7:515:LEU:O	2.32	0.62
1:2:551:GLN:HG3	15:2:901:ADP:H3'	1.83	0.61
6:7:466:LYS:NZ	15:7:902:ADP:O2B	2.33	0.61
8:A:837:GLY:HA2	8:A:842:VAL:HG11	1.82	0.61
14:Y:26:DA:H2'	14:Y:27:DT:H71	1.82	0.61
12:E:272:ARG:O	12:E:277:ASN:ND2	2.34	0.60
6:7:29:LYS:HA	6:7:61:PRO:HA	1.84	0.60
9:B:467:ASN:ND2	12:E:426:GLU:OE2	2.33	0.60
4:5:87:ILE:HG22	4:5:88:PRO:HD3	1.82	0.60
11:D:338:LYS:NZ	17:D:601:ATP:O2'	2.32	0.60
1:2:188:ASN:HD22	7:8:393:THR:HG22	1.66	0.60
1:2:656:ARG:NH1	5:6:792:SER:O	2.35	0.60
1:2:530:LYS:HD2	1:2:531:HIS:N	2.15	0.60
3:4:758:ILE:HG21	3:4:810:LYS:HA	1.82	0.60
3:4:873:LEU:HD21	3:4:926:SER:HA	1.83	0.60
12:E:82:GLN:NE2	12:E:96:ASP:OD1	2.35	0.60
1:2:183:LEU:HD23	1:2:186:LEU:HD12	1.84	0.60
2:3:372:TYR:O	15:3:1001:ADP:N6	2.34	0.59
5:6:621:TYR:HB2	5:6:668:ILE:HD11	1.84	0.59
2:3:195:LYS:N	2:3:251:ILE:O	2.30	0.58
10:C:484:LYS:NZ	10:C:616:ILE:O	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:188:ASN:HD21	7:8:392:THR:HA	1.66	0.58
3:4:896:ASP:O	8:A:840:LYS:NZ	2.36	0.58
9:B:306:PHE:O	9:B:309:THR:OG1	2.20	0.58
12:E:288:ALA:HB1	12:E:291:LEU:HD12	1.86	0.58
5:6:347:ASN:OD1	5:6:350:ARG:N	2.35	0.58
11:D:75:LEU:HD23	11:D:276:PRO:HG2	1.86	0.58
3:4:304:ARG:NH2	3:4:422:GLU:OE2	2.32	0.57
3:4:402:THR:OG1	3:4:413:HIS:N	2.36	0.57
4:5:53:ASN:ND2	4:5:60:SER:O	2.38	0.57
1:2:333:GLN:OE1	1:2:383:ARG:NH1	2.38	0.57
9:B:468:MET:SD	9:B:472:ASN:ND2	2.78	0.57
6:7:403:GLU:OE1	6:7:637:LYS:NZ	2.37	0.56
5:6:786:GLN:OE1	5:6:789:SER:OG	2.23	0.56
3:4:714:GLU:OE2	6:7:669:GLN:NE2	2.37	0.56
5:6:568:ASP:OD2	5:6:659:GLN:NE2	2.32	0.56
8:A:842:VAL:HA	8:A:845:ILE:HG22	1.87	0.56
8:A:553:VAL:HB	8:A:558:LYS:HE3	1.88	0.56
6:7:443:ARG:NH1	6:7:448:MET:O	2.39	0.56
11:D:108:LYS:NZ	11:D:251:THR:O	2.38	0.56
12:E:346:ASP:OD2	12:E:385:ARG:NE	2.34	0.55
8:A:600:ASN:OD1	8:A:601:THR:N	2.39	0.55
3:4:280:MET:HG3	3:4:296:ILE:HG21	1.89	0.55
6:7:249:SER:HB3	6:7:312:GLU:H	1.72	0.54
2:3:167:SER:H	2:3:170:THR:HG1	1.55	0.54
10:C:482:SER:HB3	10:C:485:SER:HB2	1.89	0.54
6:7:451:ARG:NH2	6:7:453:ASP:O	2.39	0.54
2:3:190:SER:O	2:3:254:GLN:NE2	2.39	0.54
1:2:601:LYS:N	1:2:643:ARG:O	2.40	0.54
8:A:797:LEU:O	11:D:332:ARG:NH2	2.41	0.53
14:Y:37:DG:H2"	14:Y:38:DA:C8	2.44	0.53
4:5:459:THR:HG1	4:5:463:TYR:HH	1.53	0.53
2:3:480:ASP:OD1	2:3:483:ARG:NH2	2.30	0.53
5:6:914:ASN:ND2	11:D:427:PRO:O	2.41	0.53
3:4:282:SER:O	3:4:287:ASN:ND2	2.34	0.53
7:8:61:LEU:HA	7:8:65:ASP:HB2	1.89	0.53
4:5:79:LEU:HD11	4:5:87:ILE:HD12	1.91	0.53
5:6:623:ILE:HG23	5:6:668:ILE:HG21	1.90	0.52
8:A:810:ASN:ND2	8:A:828:GLU:OE2	2.37	0.52
1:2:447:PHE:HE1	5:6:304:LEU:HB2	1.74	0.52
1:2:778:LEU:HD23	1:2:829:VAL:HG21	1.90	0.52
2:3:495:VAL:HG23	2:3:508:ALA:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:505:TYR:OH	7:8:553:GLU:OE2	2.26	0.52
11:D:409:ASN:HB3	12:E:375:TYR:HD1	1.74	0.52
1:2:255:ILE:HG23	7:8:393:THR:HB	1.92	0.52
1:2:696:ALA:HB3	5:6:774:VAL:HG23	1.92	0.52
3:4:437:GLY:HA2	3:4:464:VAL:HG23	1.91	0.52
7:8:61:LEU:O	7:8:154:ARG:NH2	2.43	0.52
11:D:458:ASN:ND2	12:E:250:TYR:OH	2.43	0.52
1:2:506:TYR:HB2	1:2:698:PHE:CD2	2.44	0.51
2:3:150:ARG:NH1	2:3:247:TYR:O	2.40	0.51
10:C:352:LYS:O	10:C:356:ARG:HG3	2.10	0.51
3:4:285:VAL:O	3:4:288:ASN:ND2	2.44	0.51
3:4:834:LYS:HG2	3:4:837:ALA:HB3	1.92	0.51
11:D:338:LYS:O	11:D:342:ILE:HG13	2.11	0.51
12:E:282:LEU:H	12:E:282:LEU:HD12	1.73	0.51
12:E:67:LEU:HD13	12:E:73:LEU:HA	1.93	0.51
14:X:41:DG:H2"	14:X:42:DA:C8	2.45	0.51
12:E:6:PRO:HG3	12:E:50:TYR:HA	1.92	0.51
12:E:218:ARG:NH2	12:E:273:ILE:O	2.35	0.51
4:5:614:LEU:HA	4:5:672:ALA:HB3	1.93	0.51
5:6:303:GLU:N	5:6:354:LEU:O	2.33	0.51
1:2:774:ILE:HG22	1:2:776:PRO:HD3	1.92	0.51
1:2:655:GLY:HA3	5:6:704:PRO:HD3	1.93	0.50
5:6:304:LEU:HD11	5:6:307:ALA:HB2	1.92	0.50
5:6:557:LYS:HB2	5:6:565:LEU:HD12	1.93	0.50
11:D:497:ILE:HD11	11:D:502:ARG:HA	1.93	0.50
4:5:258:LEU:O	4:5:274:LEU:N	2.44	0.50
9:B:471:GLN:HG3	10:C:315:GLN:HG2	1.94	0.50
1:2:576:LEU:HD13	1:2:620:ILE:HD11	1.93	0.50
8:A:708:LYS:NZ	11:D:268:PHE:O	2.42	0.50
12:E:201:LEU:HD21	12:E:255:ILE:HG23	1.93	0.50
5:6:598:THR:OG1	5:6:603:SER:OG	2.21	0.50
8:A:865:SER:HB2	8:A:868:PHE:HB3	1.94	0.50
12:E:215:LEU:HD11	12:E:266:TRP:CZ2	2.47	0.50
14:X:38:DA:H2'	14:X:39:DT:H71	1.94	0.50
3:4:760:PRO:HB2	3:4:817:VAL:HG23	1.94	0.50
7:8:36:ILE:O	7:8:40:HIS:N	2.44	0.50
12:E:468:PHE:HD2	12:E:470:ILE:HG23	1.76	0.50
3:4:602:THR:HG23	3:4:654:ILE:HG21	1.94	0.49
7:8:81:LEU:HD12	7:8:82:PRO:HD2	1.93	0.49
9:B:323:ARG:HH11	9:B:488:VAL:HG21	1.75	0.49
2:3:700:ARG:NH2	15:7:902:ADP:O1B	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:1002:HIS:ND1	5:6:1003:PRO:HD2	2.27	0.49
8:A:822:LEU:HD22	8:A:866:TRP:HZ2	1.77	0.49
14:Y:27:DT:H2"	14:Y:28:DC:C6	2.47	0.49
3:4:664:THR:HG23	5:6:371:GLY:HA2	1.94	0.49
6:7:791:VAL:O	8:A:694:ARG:NH1	2.46	0.49
6:7:30:GLN:HA	6:7:62:LYS:HB2	1.93	0.49
7:8:568:ASP:HB3	7:8:584:ASN:H	1.76	0.49
14:X:18:DA:C8	14:X:19:DT:H72	2.48	0.49
1:2:247:ARG:HH12	1:2:251:GLU:N	2.10	0.49
8:A:839:ASN:HB2	8:A:842:VAL:HG23	1.92	0.49
3:4:754:ALA:HA	3:4:758:ILE:HD13	1.94	0.49
7:8:507:GLN:HA	7:8:510:ALA:HB3	1.95	0.49
14:Y:53:DG:H2"	14:Y:54:DA:C8	2.47	0.49
1:2:556:VAL:HG11	1:2:647:ILE:HD12	1.95	0.49
3:4:243:LEU:HD23	3:4:305:PRO:HB3	1.94	0.49
3:4:857:ILE:O	3:4:861:LEU:HG	2.13	0.49
15:4:1102:ADP:O1B	6:7:687:ARG:NH1	2.46	0.49
7:8:337:PRO:HB3	7:8:384:ASN:HB2	1.94	0.49
1:2:530:LYS:CD	1:2:531:HIS:H	2.17	0.49
3:4:805:ALA:HB1	3:4:817:VAL:HG11	1.94	0.49
8:A:847:LYS:HG3	8:A:853:GLY:HA2	1.94	0.48
9:B:272:GLU:O	9:B:276:LEU:HG	2.12	0.48
11:D:374:ASN:ND2	12:E:36:GLN:OE1	2.41	0.48
8:A:558:LYS:NZ	8:A:590:ASN:O	2.46	0.48
12:E:146:PHE:O	12:E:150:ILE:HG13	2.14	0.48
12:E:98:ASP:HB3	12:E:101:GLN:HG2	1.95	0.48
3:4:515:ARG:NE	3:4:517:ASP:OD1	2.40	0.48
9:B:371:ASN:HD21	9:B:373:ARG:HB2	1.77	0.48
11:D:294:VAL:HB	11:D:302:VAL:HG13	1.93	0.48
11:D:396:ARG:NH2	11:D:528:GLN:O	2.46	0.48
2:3:387:GLY:O	2:3:714:LYS:NZ	2.46	0.48
10:C:356:ARG:HA	13:F:418:TYR:CE2	2.49	0.48
3:4:374:ILE:O	3:4:377:ASN:ND2	2.46	0.48
8:A:569:ASP:OD2	11:D:263:ARG:NH2	2.39	0.48
1:2:613:ASN:ND2	1:2:616:ASP:OD2	2.47	0.48
2:3:307:ASN:ND2	2:3:308:GLN:OE1	2.34	0.48
4:5:551:ASP:OD2	4:5:658:ARG:NH1	2.44	0.48
6:7:423:TYR:HB2	6:7:615:HIS:CG	2.49	0.48
11:D:519:LYS:HG2	11:D:524:TYR:CZ	2.49	0.48
1:2:188:ASN:ND2	7:8:393:THR:H	2.11	0.48
6:7:213:ARG:HG3	6:7:216:ARG:HH21	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:X:35:DT:H2"	14:X:36:DC:C5	2.49	0.48
2:3:271:PRO:HG3	4:5:509:ILE:HG21	1.94	0.48
3:4:714:GLU:HA	3:4:717:ASP:HB2	1.95	0.47
2:3:291:ARG:HB3	2:3:329:LEU:HD12	1.97	0.47
6:7:656:VAL:HG11	6:7:709:ASP:HA	1.97	0.47
12:E:338:CYS:SG	12:E:389:ILE:HD12	2.54	0.47
7:8:570:SER:H	7:8:581:TYR:HB3	1.79	0.47
5:6:518:GLU:OE2	7:8:504:ARG:NH1	2.45	0.47
4:5:31:PHE:HE2	4:5:94:ILE:HB	1.78	0.47
6:7:591:LEU:HD22	6:7:597:LEU:HD11	1.96	0.47
2:3:412:SER:HA	15:3:1001:ADP:H5'1	1.96	0.47
3:4:712:VAL:HG11	6:7:672:LYS:HD3	1.97	0.47
10:C:293:ASN:HB2	10:C:467:THR:HG22	1.97	0.47
1:2:188:ASN:HD22	7:8:393:THR:H	1.62	0.47
2:3:672:THR:HG22	2:3:674:GLU:H	1.79	0.47
12:E:143:ALA:O	12:E:179:TYR:OH	2.32	0.47
7:8:539:VAL:HG11	7:8:551:THR:HA	1.97	0.46
12:E:380:LEU:HD23	12:E:451:LYS:HB3	1.96	0.46
2:3:533:ILE:HG22	2:3:535:LEU:HG	1.96	0.46
7:8:73:PHE:CD1	7:8:81:LEU:HB2	2.50	0.46
10:C:104:THR:HB	10:C:263:TYR:HA	1.98	0.46
1:2:522:GLY:O	1:2:822:LYS:NZ	2.43	0.46
7:8:587:ASP:OD2	7:8:590:ARG:HD3	2.14	0.46
8:A:774:HIS:CE1	8:A:775:ILE:HG22	2.50	0.46
4:5:554:PHE:CZ	4:5:687:SER:HB2	2.50	0.46
3:4:194:PHE:CZ	3:4:257:LEU:HD21	2.51	0.46
6:7:569:PRO:HB3	6:7:583:ASN:HB3	1.97	0.46
6:7:465:ALA:HA	15:7:902:ADP:H5'1	1.96	0.46
9:B:305:TRP:O	9:B:309:THR:HG23	2.15	0.46
3:4:696:PRO:N	3:4:697:PRO:HD2	2.31	0.46
6:7:466:LYS:HZ3	15:7:902:ADP:PB	2.38	0.46
12:E:338:CYS:O	12:E:385:ARG:NH1	2.49	0.46
2:3:194:PRO:HA	2:3:252:ASP:HA	1.98	0.46
7:8:202:ALA:HB2	7:8:229:LEU:HB2	1.97	0.46
10:C:351:LEU:HD13	10:C:386:ARG:NE	2.30	0.46
4:5:486:ARG:HD3	4:5:487:ASP:N	2.31	0.45
5:6:287:LEU:HA	5:6:400:VAL:HG12	1.98	0.45
3:4:725:THR:HA	3:4:728:TYR:CE2	2.52	0.45
5:6:292:GLY:HA3	5:6:361:ILE:HD12	1.98	0.45
7:8:485:ASP:OD1	7:8:488:ARG:NH2	2.49	0.45
11:D:339:ASN:HA	11:D:342:ILE:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:356:LYS:HD3	2:3:356:LYS:N	2.31	0.45
4:5:168:SER:OG	4:5:463:TYR:HB3	2.16	0.45
1:2:447:PHE:CE1	5:6:304:LEU:HB2	2.51	0.45
15:2:901:ADP:O2'	5:6:801:GLU:OE2	2.25	0.45
3:4:203:TYR:HB3	3:4:221:ASP:HA	1.98	0.45
5:6:563:ILE:HD13	5:6:563:ILE:HA	1.81	0.45
8:A:606:GLU:OE2	8:A:621:ARG:NH2	2.34	0.45
14:Y:33:DG:H2''	14:Y:34:DA:C8	2.52	0.45
3:4:251:TYR:CE2	3:4:253:GLN:HB2	2.52	0.45
10:C:522:GLY:O	10:C:526:LYS:HG3	2.16	0.45
12:E:136:ASP:OD1	12:E:136:ASP:N	2.50	0.45
2:3:462:MET:HE3	2:3:489:VAL:HG21	1.99	0.45
3:4:616:LEU:HD12	3:4:618:SER:H	1.82	0.45
5:6:772:TYR:CZ	5:6:776:LYS:HE2	2.51	0.45
3:4:365:ILE:HB	5:6:419:SER:HA	1.98	0.45
8:A:836:ASN:O	8:A:842:VAL:HG21	2.17	0.45
14:Y:54:DA:H2'	14:Y:55:DT:H71	1.98	0.45
3:4:570:PRO:HA	3:4:574:LYS:HZ1	1.82	0.45
3:4:841:LYS:HG3	3:4:842:THR:HG23	1.99	0.45
5:6:965:ILE:O	5:6:969:VAL:HG23	2.16	0.45
12:E:438:ASN:OD1	12:E:439:LYS:NZ	2.41	0.45
6:7:570:LEU:HD13	6:7:585:ASN:HB2	1.98	0.44
2:3:25:VAL:HG13	2:3:128:ALA:HB2	1.99	0.44
3:4:238:THR:HG22	3:4:240:ASN:H	1.82	0.44
4:5:87:ILE:HA	4:5:90:PHE:HD2	1.83	0.44
4:5:261:ILE:HG22	4:5:263:GLU:H	1.81	0.44
1:2:260:LEU:HA	1:2:267:MET:HG3	1.99	0.44
2:3:687:ARG:HH21	6:7:604:PRO:HG3	1.82	0.44
3:4:839:ASP:OD1	3:4:842:THR:N	2.49	0.44
6:7:460:GLY:O	6:7:569:PRO:HD3	2.18	0.44
6:7:520:ILE:HG12	6:7:562:SER:HB2	1.99	0.44
7:8:23:VAL:HG13	7:8:28:GLN:HB3	1.99	0.44
10:C:383:ASN:OD1	10:C:386:ARG:NE	2.50	0.44
12:E:113:HIS:CE1	12:E:157:PRO:HG3	2.52	0.44
11:D:220:ASP:OD1	11:D:220:ASP:N	2.50	0.44
3:4:610:ASP:OD1	3:4:611:THR:N	2.51	0.44
4:5:379:PHE:H	15:5:901:ADP:HN62	1.64	0.44
8:A:568:LEU:HD22	8:A:597:ALA:HB1	1.99	0.44
12:E:336:TYR:HA	12:E:452:VAL:HG21	1.99	0.44
14:X:12:DC:H2''	14:X:13:DG:C8	2.52	0.44
2:3:314:LEU:HD13	4:5:460:ARG:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:716:ARG:NH2	2:3:722:ASN:OD1	2.51	0.44
1:2:286:TYR:CE1	1:2:293:ILE:HD11	2.52	0.44
3:4:331:LEU:N	3:4:400:GLN:O	2.49	0.44
4:5:470:VAL:HG13	4:5:513:LEU:HD21	1.98	0.44
6:7:674:GLU:HB3	6:7:680:SER:HB2	1.99	0.44
7:8:524:THR:HB	7:8:583:TRP:CZ2	2.53	0.44
10:C:542:ILE:O	10:C:546:GLU:HG2	2.17	0.44
2:3:141:HIS:CG	2:3:144:ALA:HB3	2.52	0.44
9:B:242:THR:HG23	9:B:244:GLU:H	1.83	0.44
11:D:78:CYS:SG	11:D:276:PRO:HD3	2.57	0.44
5:6:526:TYR:O	5:6:530:VAL:HG23	2.17	0.44
3:4:441:SER:HG	3:4:457:TYR:N	2.16	0.43
4:5:86:ILE:HG22	4:5:90:PHE:CE2	2.53	0.43
5:6:304:LEU:HD21	5:6:307:ALA:HB2	1.99	0.43
11:D:217:ASP:HA	11:D:250:CYS:HB2	2.00	0.43
2:3:154:LYS:HE2	2:3:154:LYS:HA	1.99	0.43
4:5:302:ASN:OD1	4:5:324:ARG:NH1	2.51	0.43
2:3:177:ASN:N	2:3:298:PHE:O	2.49	0.43
6:7:404:LEU:HD23	6:7:641:TYR:CD2	2.54	0.43
2:3:552:ASP:OD2	2:3:557:ARG:NH1	2.40	0.43
3:4:276:ILE:O	3:4:280:MET:HG2	2.17	0.43
4:5:23:ASP:OD1	4:5:24:ASN:N	2.51	0.43
4:5:85:ASP:C	4:5:88:PRO:HD2	2.39	0.43
12:E:191:ARG:NH2	12:E:253:ASN:OD1	2.40	0.43
7:8:506:GLN:O	7:8:510:ALA:N	2.47	0.43
11:D:394:ALA:HB1	11:D:406:PHE:CE2	2.54	0.43
2:3:138:ASP:OD1	2:3:138:ASP:N	2.51	0.43
7:8:206:ARG:HH21	7:8:220:VAL:N	2.17	0.43
10:C:68:PHE:CZ	10:C:284:PHE:HD1	2.37	0.43
4:5:436:ALA:HA	4:5:476:VAL:O	2.18	0.43
5:6:268:PHE:CG	5:6:269:ASN:N	2.86	0.43
10:C:125:TYR:OH	10:C:153:ALA:O	2.33	0.43
10:C:426:GLU:O	10:C:430:ASN:ND2	2.47	0.43
11:D:471:GLU:HB3	11:D:474:ALA:HB2	2.01	0.43
5:6:330:PRO:HD2	5:6:344:TRP:CD1	2.54	0.43
5:6:516:LEU:HD21	5:6:757:TYR:CG	2.54	0.43
7:8:95:ASP:OD1	7:8:96:THR:N	2.52	0.43
9:B:323:ARG:NH2	10:C:18:ALA:HB2	2.33	0.43
11:D:216:PHE:O	11:D:250:CYS:N	2.52	0.43
4:5:262:PRO:HA	4:5:265:VAL:HG23	2.01	0.42
5:6:272:THR:HB	7:8:519:ILE:HG23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:423:TYR:HB3	15:7:902:ADP:HN62	1.84	0.42
7:8:322:GLU:OE2	7:8:371:TYR:OH	2.33	0.42
10:C:484:LYS:NZ	10:C:488:GLU:OE2	2.50	0.42
12:E:468:PHE:CD2	12:E:470:ILE:HG23	2.54	0.42
7:8:392:THR:HG22	7:8:395:THR:H	1.84	0.42
8:A:849:LEU:O	8:A:864:ILE:HG12	2.19	0.42
11:D:387:GLU:CG	11:D:459:VAL:HG13	2.50	0.42
14:Y:43:DT:H2"	14:Y:44:DC:C5	2.55	0.42
1:2:262:LYS:HE3	7:8:330:LEU:HB3	2.02	0.42
2:3:301:LEU:HB2	2:3:318:LYS:HB2	2.02	0.42
3:4:350:ASN:OD1	3:4:351:VAL:HG13	2.19	0.42
5:6:270:LEU:HD12	5:6:289:SER:HB2	2.01	0.42
5:6:364:ASN:ND2	5:6:367:GLU:OE2	2.52	0.42
5:6:822:SER:HA	11:D:430:ALA:HB2	2.00	0.42
8:A:647:PHE:CD1	8:A:679:LYS:HE3	2.54	0.42
10:C:489:ASP:O	10:C:493:SER:N	2.47	0.42
11:D:319:ASN:OD1	11:D:322:ARG:NH2	2.40	0.42
1:2:424:VAL:HG21	1:2:456:ILE:HD11	2.01	0.42
3:4:722:LYS:NZ	6:7:658:ASP:OD1	2.42	0.42
6:7:518:ASN:N	6:7:560:ARG:O	2.52	0.42
8:A:898:VAL:HG12	8:A:902:LYS:HE3	2.00	0.42
10:C:61:TYR:HB2	10:C:329:PHE:CG	2.55	0.42
10:C:394:GLU:OE1	10:C:398:ARG:NE	2.52	0.42
14:Y:47:DT:H2"	14:Y:48:DC:C5	2.55	0.42
11:D:501:LEU:HD13	12:E:377:GLN:HA	2.01	0.42
1:2:798:ILE:HB	4:5:560:HIS:CE1	2.55	0.42
12:E:86:LYS:NZ	12:E:96:ASP:OD1	2.50	0.42
10:C:413:LEU:HD23	10:C:417:LEU:HD12	2.02	0.42
1:2:688:ASP:OD2	5:6:790:ARG:NH1	2.41	0.42
3:4:240:ASN:CG	3:4:304:ARG:HH22	2.23	0.42
4:5:79:LEU:HD13	4:5:90:PHE:HE2	1.84	0.42
4:5:451:ALA:HB2	4:5:513:LEU:HD13	2.02	0.42
5:6:513:ILE:O	5:6:517:LYS:N	2.41	0.42
5:6:609:THR:O	5:6:629:MET:HG3	2.20	0.42
6:7:648:LYS:HB2	6:7:701:LYS:HG3	2.02	0.42
9:B:321:SER:HB2	9:B:486:SER:HA	2.01	0.42
11:D:390:ILE:HD12	11:D:459:VAL:HG11	2.02	0.42
4:5:459:THR:OG1	4:5:463:TYR:OH	2.25	0.42
6:7:478:PRO:HB3	6:7:639:ARG:NH1	2.35	0.42
7:8:48:TYR:CE2	7:8:50:ASN:HB2	2.54	0.42
9:B:433:ARG:HG2	12:E:444:LEU:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:37:GLY:HA3	12:E:189:PHE:HB2	2.02	0.42
1:2:617:ARG:HG2	1:2:673:ILE:HD13	2.01	0.41
4:5:293:THR:N	4:5:334:GLN:O	2.44	0.41
4:5:398:LYS:HE2	4:5:398:LYS:HB2	1.94	0.41
11:D:366:ILE:O	11:D:370:ASN:ND2	2.51	0.41
3:4:769:GLU:HG3	3:4:819:LEU:HD13	2.01	0.41
4:5:45:ILE:HG13	4:5:46:TYR:N	2.35	0.41
4:5:626:PHE:CE2	4:5:630:ARG:HD2	2.55	0.41
6:7:526:PHE:CE1	6:7:590:LEU:HD21	2.55	0.41
11:D:460:TRP:O	11:D:464:VAL:HG23	2.20	0.41
2:3:551:ASP:OD1	2:3:551:ASP:N	2.49	0.41
9:B:326:LEU:HD11	9:B:455:SER:HB3	2.03	0.41
9:B:479:ASP:C	9:B:480:ILE:HD13	2.40	0.41
10:C:65:HIS:CE1	10:C:69:HIS:CD2	3.08	0.41
10:C:572:THR:HG22	10:C:574:ASP:H	1.86	0.41
1:2:274:VAL:HA	1:2:277:GLU:HG2	2.01	0.41
1:2:701:ASP:HA	1:2:704:VAL:HG12	2.01	0.41
5:6:772:TYR:OH	5:6:776:LYS:HE2	2.21	0.41
10:C:596:LEU:HD23	10:C:612:VAL:HG11	2.02	0.41
14:Y:33:DG:H2"	14:Y:34:DA:N7	2.35	0.41
7:8:361:LEU:HB3	7:8:428:PHE:H	1.85	0.41
7:8:534:LEU:O	7:8:538:ILE:HG12	2.21	0.41
12:E:35:LEU:O	12:E:169:THR:HA	2.21	0.41
4:5:169:THR:HG22	4:5:256:LEU:HD23	2.03	0.41
5:6:520:VAL:HG22	5:6:754:TYR:CE1	2.55	0.41
9:B:276:LEU:HD12	10:C:569:LEU:HD22	2.03	0.41
12:E:389:ILE:O	12:E:393:ILE:HG12	2.21	0.41
1:2:333:GLN:N	1:2:383:ARG:O	2.52	0.41
5:6:120:GLU:OE1	5:6:137:ARG:NH2	2.50	0.41
7:8:372:VAL:O	7:8:383:MET:HA	2.20	0.41
12:E:273:ILE:HG12	12:E:284:LEU:HD21	2.02	0.41
14:X:9:DG:H2"	14:X:10:DA:C8	2.56	0.41
5:6:293:THR:HG21	5:6:630:LEU:HD22	2.03	0.41
8:A:829:ILE:O	8:A:833:ILE:HG12	2.21	0.41
8:A:861:LEU:HD21	11:D:516:ILE:HD11	2.02	0.41
11:D:93:LYS:HG3	11:D:244:PRO:HG2	2.03	0.41
11:D:111:LEU:O	11:D:115:GLU:HG2	2.19	0.41
4:5:657:ILE:O	4:5:660:THR:OG1	2.26	0.41
6:7:616:VAL:HG22	15:7:902:ADP:C2	2.55	0.41
7:8:514:THR:HA	7:8:517:PHE:CE2	2.56	0.41
7:8:524:THR:HB	7:8:583:TRP:HZ2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:791:ILE:O	8:A:795:THR:HG23	2.21	0.41
8:A:822:LEU:HD21	8:A:892:VAL:HG21	2.03	0.41
10:C:356:ARG:HA	13:F:418:TYR:CZ	2.56	0.41
14:X:33:DG:C2	14:Y:37:DG:C2	3.09	0.41
3:4:601:LEU:HA	3:4:620:ALA:HB3	2.03	0.41
5:6:626:GLY:O	5:6:630:LEU:HG	2.21	0.41
5:6:964:VAL:O	5:6:968:LEU:HG	2.20	0.41
9:B:294:PHE:O	9:B:298:LYS:HG3	2.21	0.41
11:D:256:ILE:H	11:D:256:ILE:HG13	1.63	0.41
14:X:29:DG:H2''	14:X:30:DA:H8	1.86	0.41
3:4:530:ILE:HA	15:4:1102:ADP:C2	2.56	0.40
5:6:186:ARG:HA	5:6:189:VAL:HG22	2.03	0.40
5:6:545:LYS:O	5:6:549:LEU:HG	2.20	0.40
6:7:674:GLU:CB	6:7:680:SER:HB2	2.51	0.40
12:E:14:GLN:HG2	12:E:189:PHE:CE1	2.57	0.40
5:6:360:ARG:NH2	5:6:616:GLU:OE1	2.53	0.40
5:6:559:THR:HB	5:6:563:ILE:HB	2.03	0.40
6:7:516:ALA:O	6:7:561:THR:HG22	2.22	0.40
10:C:281:PHE:O	10:C:285:LEU:HG	2.21	0.40
3:4:312:LYS:HE2	3:4:317:LEU:HA	2.03	0.40
12:E:265:LYS:NZ	12:E:296:ASP:OD2	2.50	0.40
1:2:508:HIS:HB3	1:2:511:ILE:HD12	2.04	0.40
2:3:167:SER:N	2:3:170:THR:OG1	2.43	0.40
7:8:479:SER:OG	7:8:482:ASN:HB2	2.21	0.40
10:C:260:LYS:HE2	12:E:296:ASP:O	2.21	0.40
10:C:377:ILE:O	10:C:380:LEU:HG	2.21	0.40
14:X:37:DG:C2	14:Y:33:DG:C2	3.09	0.40
14:Y:53:DG:H2''	14:Y:54:DA:H8	1.85	0.40
1:2:227:TYR:CD1	1:2:230:ARG:HD2	2.57	0.40
1:2:604:CYS:O	1:2:646:ILE:HA	2.22	0.40
2:3:442:LEU:HD12	2:3:482:ASP:HB3	2.03	0.40
5:6:538:PHE:HB3	15:6:1101:ADP:HN62	1.87	0.40
7:8:73:PHE:CZ	7:8:77:PHE:HA	2.56	0.40
11:D:519:LYS:HG2	11:D:524:TYR:CE2	2.56	0.40
12:E:36:GLN:HG3	12:E:176:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	582/868 (67%)	569 (98%)	13 (2%)	0	100	100
2	3	559/1006 (56%)	546 (98%)	13 (2%)	0	100	100
3	4	642/933 (69%)	622 (97%)	20 (3%)	0	100	100
4	5	552/775 (71%)	545 (99%)	7 (1%)	0	100	100
5	6	663/1017 (65%)	652 (98%)	11 (2%)	0	100	100
6	7	637/845 (75%)	624 (98%)	13 (2%)	0	100	100
7	8	497/604 (82%)	489 (98%)	8 (2%)	0	100	100
8	A	408/949 (43%)	408 (100%)	0	0	100	100
9	B	213/620 (34%)	207 (97%)	6 (3%)	0	100	100
10	C	542/616 (88%)	527 (97%)	15 (3%)	0	100	100
11	D	425/529 (80%)	421 (99%)	4 (1%)	0	100	100
12	E	408/479 (85%)	398 (98%)	10 (2%)	0	100	100
13	F	29/435 (7%)	29 (100%)	0	0	100	100
All	All	6157/9676 (64%)	6037 (98%)	120 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	516/769 (67%)	513 (99%)	3 (1%)	84	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3	498/864 (58%)	498 (100%)	0	100	100
3	4	597/848 (70%)	596 (100%)	1 (0%)	92	95
4	5	507/688 (74%)	506 (100%)	1 (0%)	92	95
5	6	597/886 (67%)	595 (100%)	2 (0%)	91	94
6	7	577/753 (77%)	575 (100%)	2 (0%)	91	94
7	8	459/545 (84%)	459 (100%)	0	100	100
8	A	367/842 (44%)	367 (100%)	0	100	100
9	B	208/573 (36%)	208 (100%)	0	100	100
10	C	515/576 (89%)	515 (100%)	0	100	100
11	D	399/488 (82%)	399 (100%)	0	100	100
12	E	388/440 (88%)	387 (100%)	1 (0%)	91	94
13	F	30/406 (7%)	30 (100%)	0	100	100
All	All	5658/8678 (65%)	5648 (100%)	10 (0%)	91	95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	183	LEU
1	2	777	LYS
1	2	784	ASP
3	4	386	HIS
4	5	405	ARG
5	6	448	LEU
5	6	814	ASN
6	7	413	ARG
6	7	451	ARG
12	E	282	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	188	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	ADP	3	1001	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
15	ADP	7	902	-	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
15	ADP	5	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.51	4 (13%)
17	ATP	D	601	-	26,33,33	0.60	0	31,52,52	0.81	1 (3%)
17	ATP	A	1001	-	26,33,33	0.59	0	31,52,52	0.82	2 (6%)
15	ADP	6	1101	-	24,29,29	0.95	1 (4%)	29,45,45	1.52	4 (13%)
15	ADP	2	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.51	4 (13%)
15	ADP	4	1102	-	24,29,29	0.96	1 (4%)	29,45,45	1.39	4 (13%)
17	ATP	E	501	-	26,33,33	0.59	0	31,52,52	0.81	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ADP	3	1001	-	-	2/12/32/32	0/3/3/3
15	ADP	7	902	-	-	4/12/32/32	0/3/3/3
15	ADP	5	901	-	-	4/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ATP	D	601	-	-	4/18/38/38	0/3/3/3
17	ATP	A	1001	-	-	4/18/38/38	0/3/3/3
15	ADP	6	1101	-	-	4/12/32/32	0/3/3/3
15	ADP	2	901	-	-	2/12/32/32	0/3/3/3
15	ADP	4	1102	-	-	4/12/32/32	0/3/3/3
17	ATP	E	501	-	-	2/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	5	901	ADP	C5-C4	2.55	1.47	1.40
15	7	902	ADP	C5-C4	2.52	1.47	1.40
15	4	1102	ADP	C5-C4	2.50	1.47	1.40
15	3	1001	ADP	C5-C4	2.49	1.47	1.40
15	6	1101	ADP	C5-C4	2.46	1.47	1.40
15	2	901	ADP	C5-C4	2.45	1.47	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	2	901	ADP	PA-O3A-PB	-3.96	119.24	132.83
15	5	901	ADP	PA-O3A-PB	-3.87	119.56	132.83
15	6	1101	ADP	PA-O3A-PB	-3.72	120.05	132.83
15	6	1101	ADP	C3'-C2'-C1'	3.67	106.51	100.98
15	7	902	ADP	C3'-C2'-C1'	3.55	106.32	100.98
15	5	901	ADP	C3'-C2'-C1'	3.49	106.23	100.98
15	2	901	ADP	C3'-C2'-C1'	3.44	106.16	100.98
15	4	1102	ADP	C3'-C2'-C1'	3.42	106.12	100.98
15	3	1001	ADP	C3'-C2'-C1'	3.31	105.95	100.98
15	3	1001	ADP	PA-O3A-PB	-3.27	121.60	132.83
15	3	1001	ADP	N3-C2-N1	-3.22	123.65	128.68
15	5	901	ADP	N3-C2-N1	-3.17	123.73	128.68
15	6	1101	ADP	N3-C2-N1	-3.11	123.82	128.68
15	7	902	ADP	N3-C2-N1	-3.09	123.85	128.68
15	4	1102	ADP	N3-C2-N1	-3.07	123.88	128.68
15	2	901	ADP	N3-C2-N1	-2.93	124.10	128.68
15	7	902	ADP	PA-O3A-PB	-2.84	123.08	132.83
15	4	1102	ADP	PA-O3A-PB	-2.72	123.50	132.83
15	2	901	ADP	C4-C5-N7	-2.64	106.65	109.40
15	5	901	ADP	C4-C5-N7	-2.60	106.69	109.40
15	3	1001	ADP	C4-C5-N7	-2.60	106.69	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	6	1101	ADP	C4-C5-N7	-2.52	106.78	109.40
15	7	902	ADP	C4-C5-N7	-2.50	106.80	109.40
15	4	1102	ADP	C4-C5-N7	-2.49	106.81	109.40
17	D	601	ATP	C5-C6-N6	2.29	123.84	120.35
17	E	501	ATP	C5-C6-N6	2.29	123.83	120.35
17	A	1001	ATP	C5-C6-N6	2.25	123.78	120.35
17	A	1001	ATP	PB-O3B-PG	2.07	139.94	132.83

There are no chirality outliers.

All (30) torsion outliers are listed below:

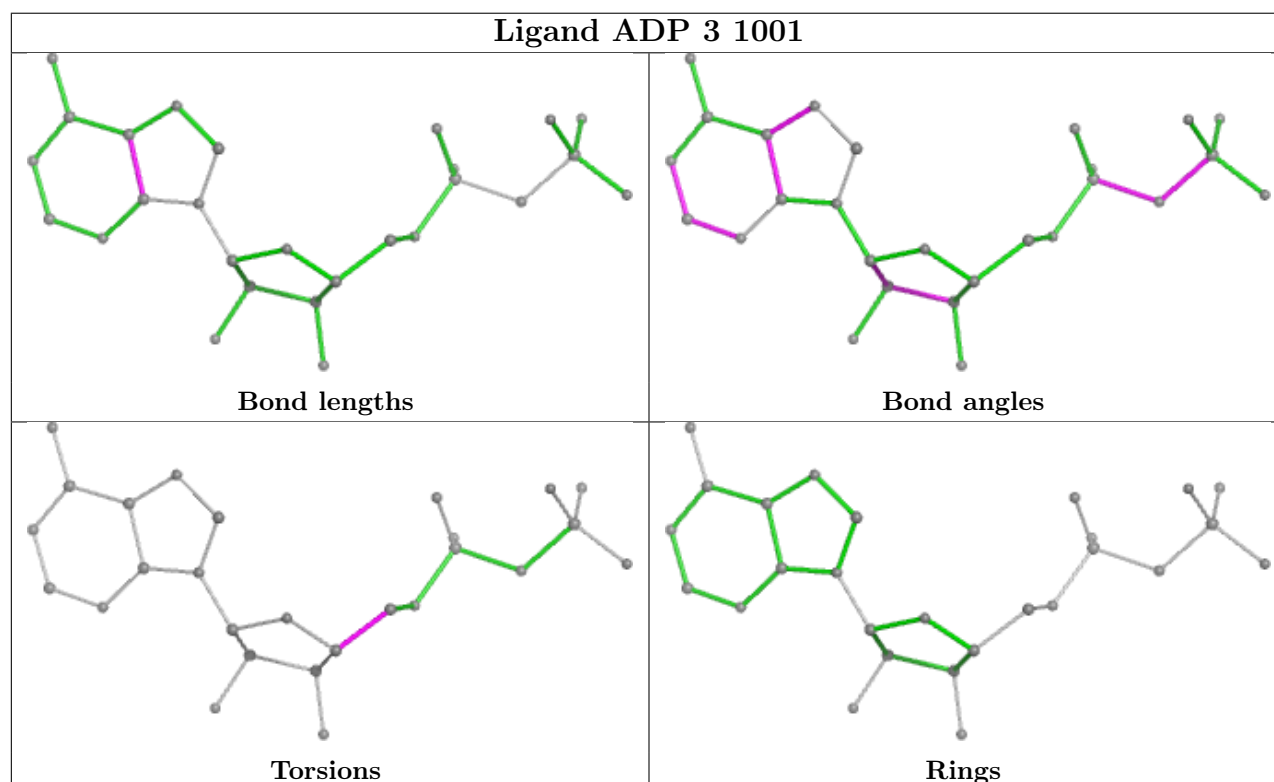
Mol	Chain	Res	Type	Atoms
15	3	1001	ADP	O4'-C4'-C5'-O5'
15	4	1102	ADP	C5'-O5'-PA-O2A
15	5	901	ADP	C5'-O5'-PA-O1A
15	5	901	ADP	C5'-O5'-PA-O2A
15	6	1101	ADP	C5'-O5'-PA-O2A
15	6	1101	ADP	C5'-O5'-PA-O3A
15	7	902	ADP	O4'-C4'-C5'-O5'
17	A	1001	ATP	PB-O3B-PG-O2G
17	D	601	ATP	C5'-O5'-PA-O1A
15	3	1001	ADP	C3'-C4'-C5'-O5'
15	7	902	ADP	C3'-C4'-C5'-O5'
17	A	1001	ATP	PB-O3B-PG-O1G
15	4	1102	ADP	O4'-C4'-C5'-O5'
15	6	1101	ADP	O4'-C4'-C5'-O5'
15	4	1102	ADP	C5'-O5'-PA-O3A
15	5	901	ADP	C5'-O5'-PA-O3A
15	7	902	ADP	PB-O3A-PA-O2A
17	D	601	ATP	C4'-C5'-O5'-PA
17	D	601	ATP	C5'-O5'-PA-O2A
15	5	901	ADP	O4'-C4'-C5'-O5'
17	E	501	ATP	C4'-C5'-O5'-PA
17	A	1001	ATP	PB-O3A-PA-O1A
15	2	901	ADP	C3'-C4'-C5'-O5'
15	6	1101	ADP	C3'-C4'-C5'-O5'
15	2	901	ADP	PA-O3A-PB-O3B
17	D	601	ATP	C5'-O5'-PA-O3A
15	7	902	ADP	PB-O3A-PA-O1A
17	A	1001	ATP	PB-O3A-PA-O2A
15	4	1102	ADP	C5'-O5'-PA-O1A
17	E	501	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

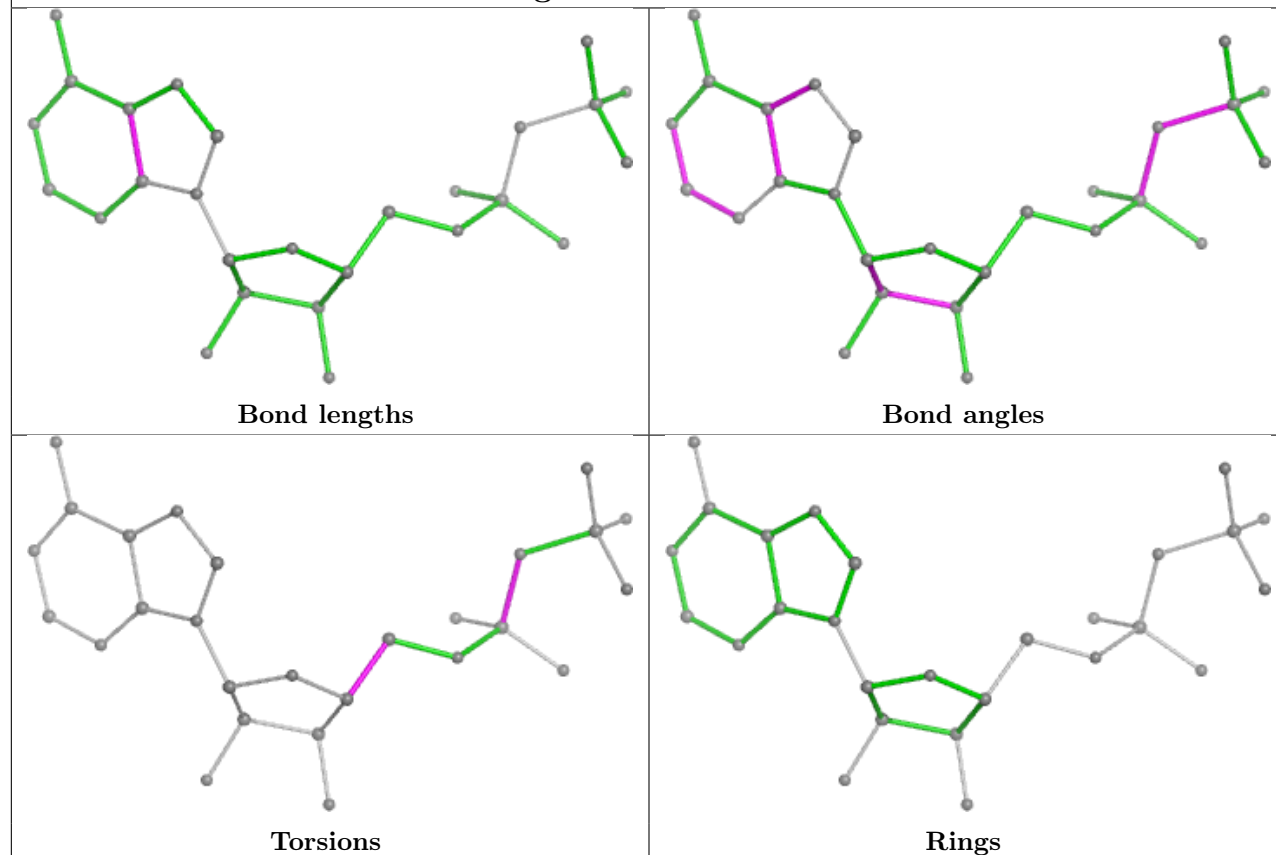
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	1001	ADP	2	0
15	7	902	ADP	6	0
15	5	901	ADP	1	0
17	D	601	ATP	1	0
15	6	1101	ADP	1	0
15	2	901	ADP	2	0
15	4	1102	ADP	2	0

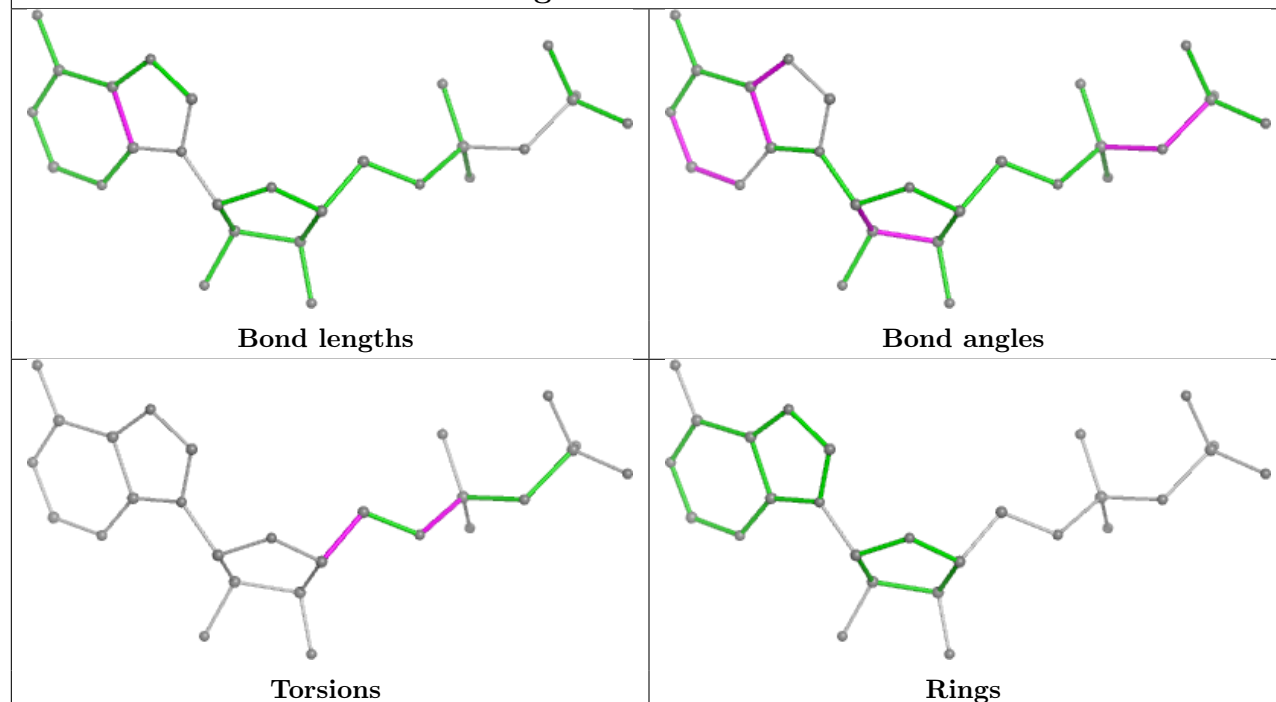
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

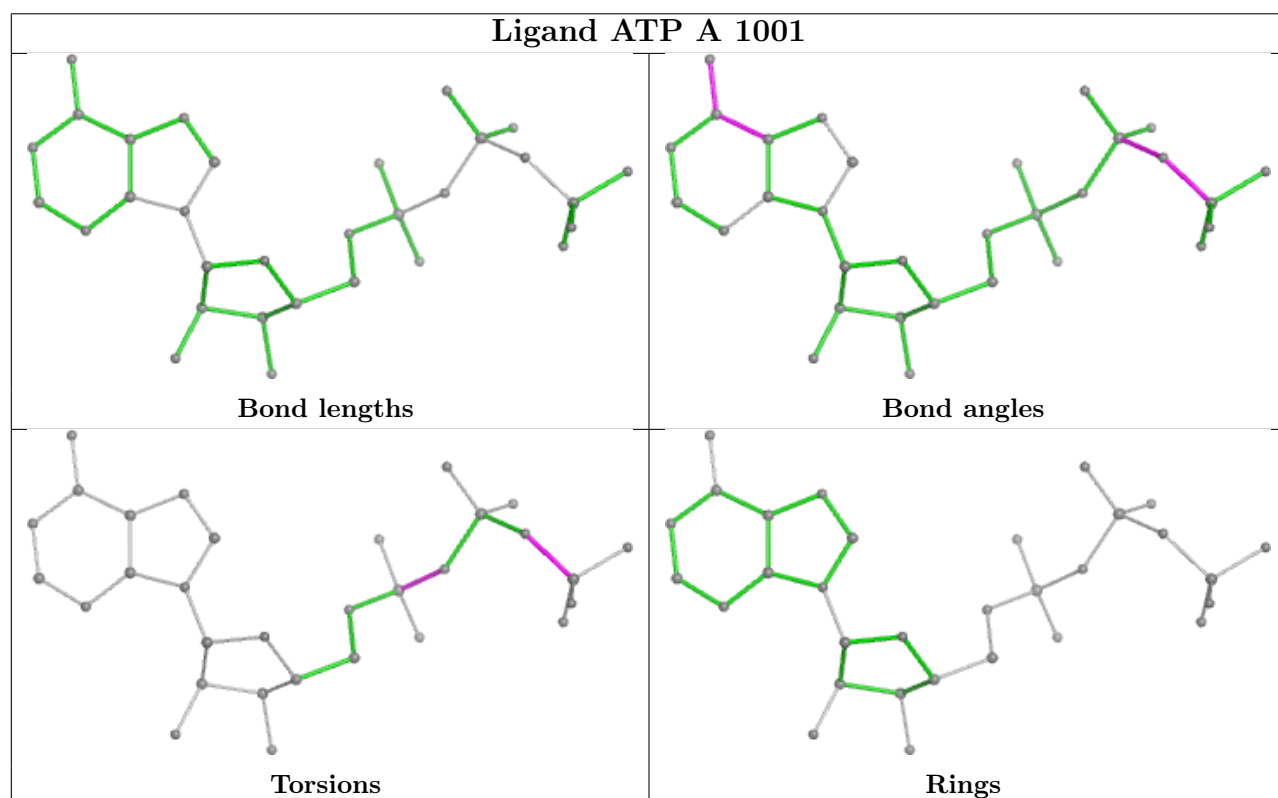
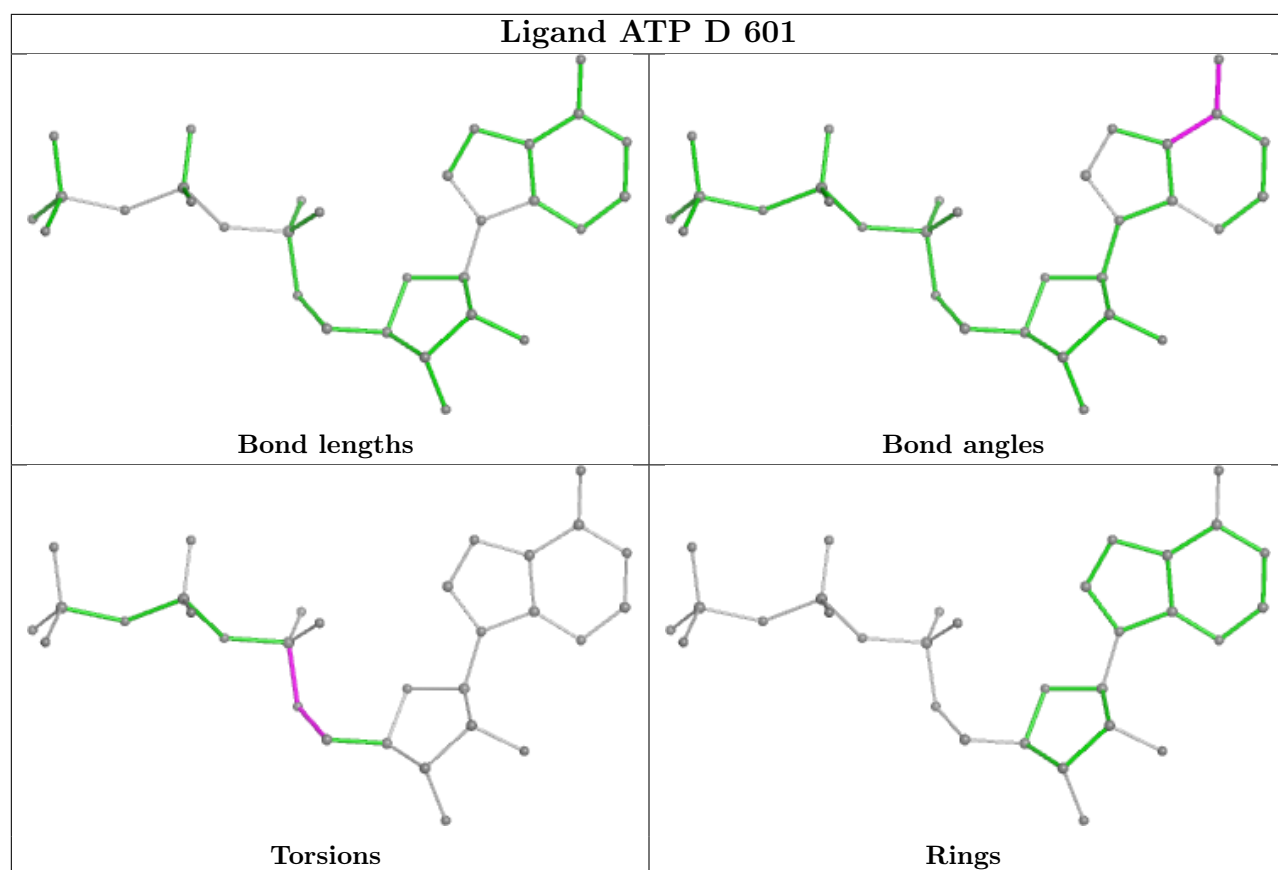


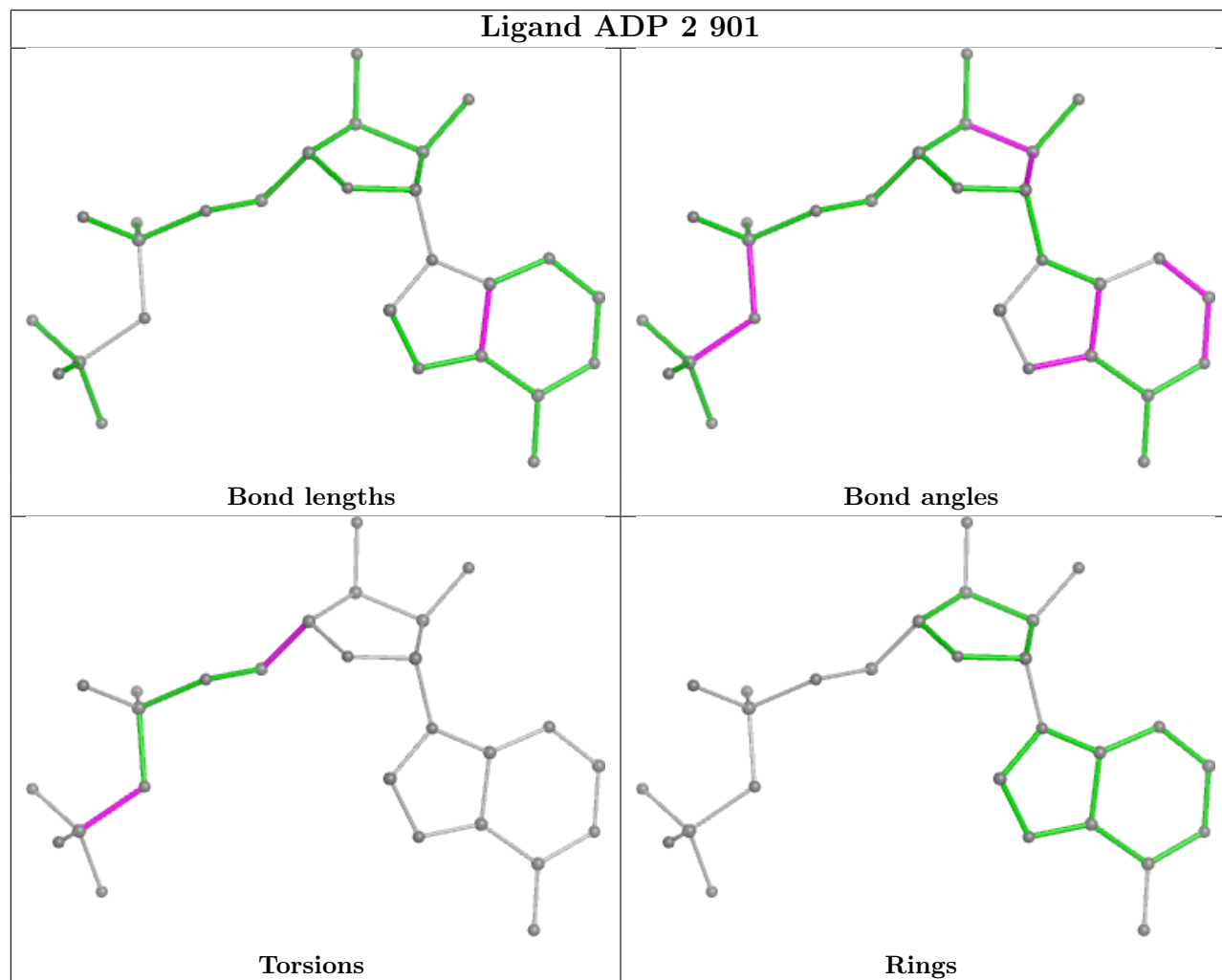
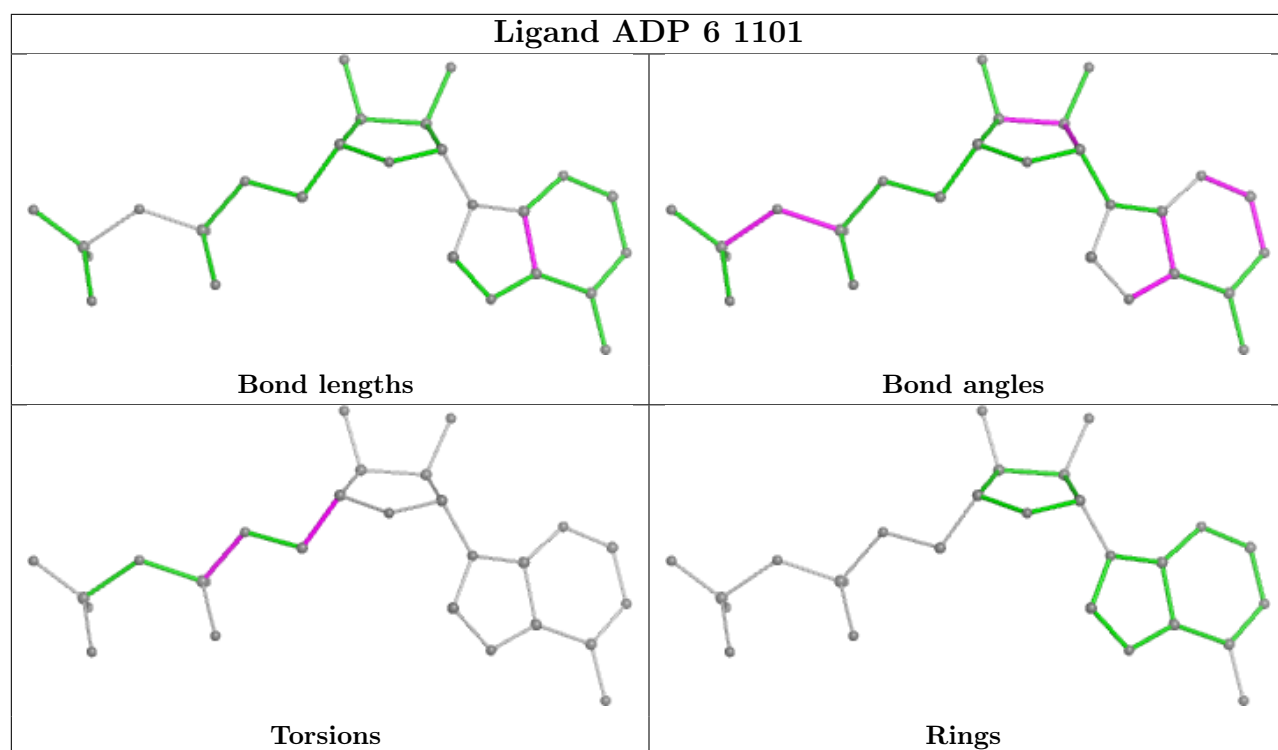
Ligand ADP 7 902

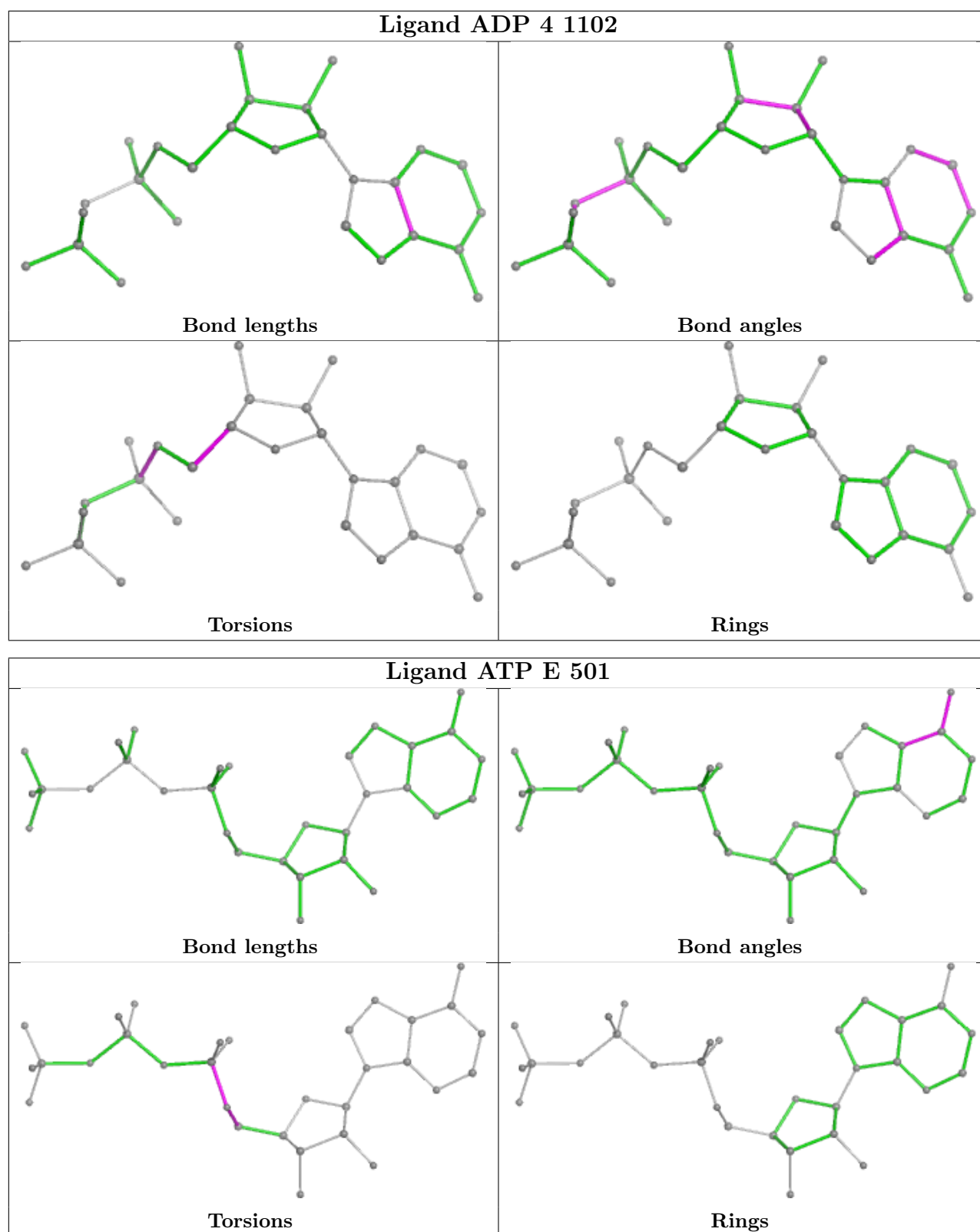


Ligand ADP 5 901









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

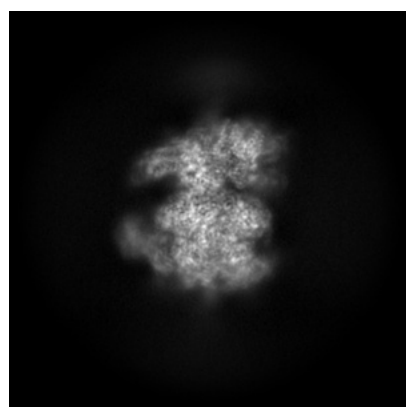
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51407. These allow visual inspection of the internal detail of the map and identification of artifacts.

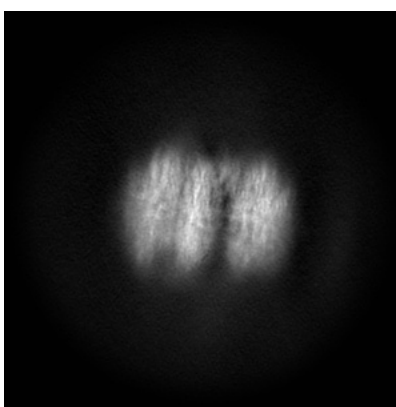
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

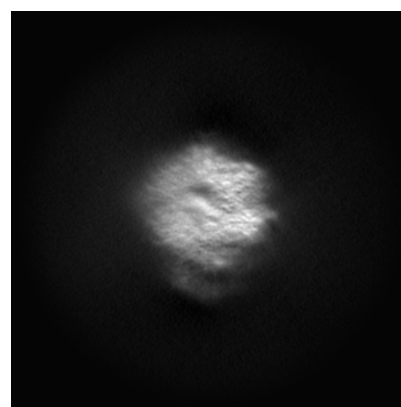
6.1.1 Primary map



X



Y

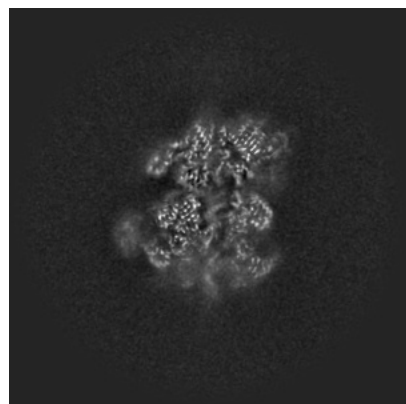


Z

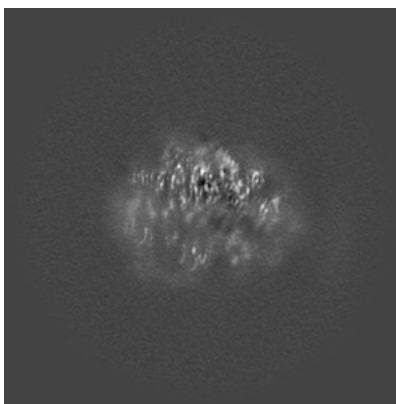
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

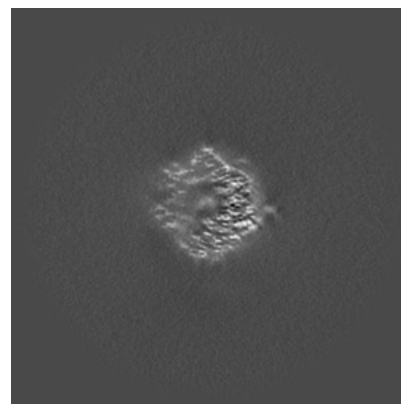
6.2.1 Primary map



X Index: 220



Y Index: 220

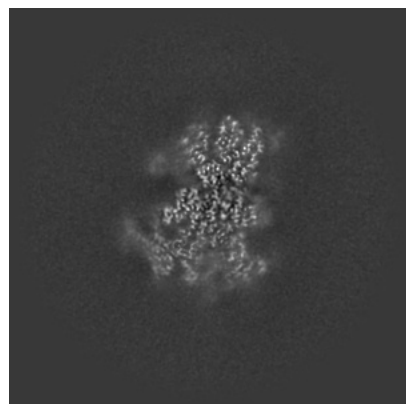


Z Index: 220

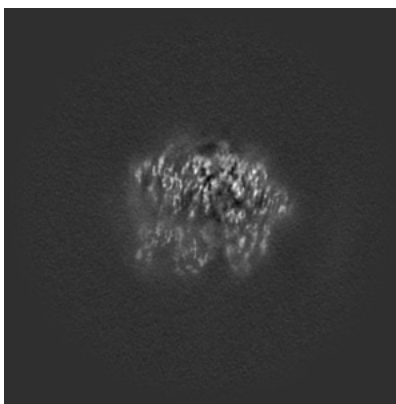
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

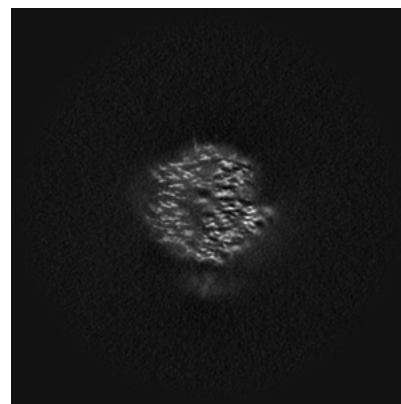
6.3.1 Primary map



X Index: 235



Y Index: 209

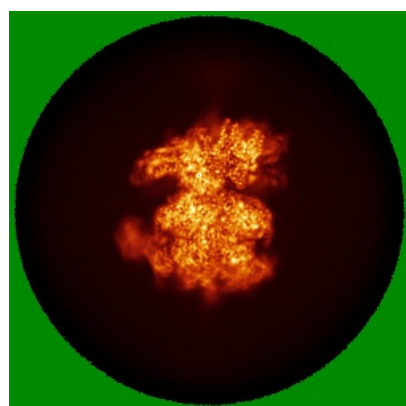


Z Index: 210

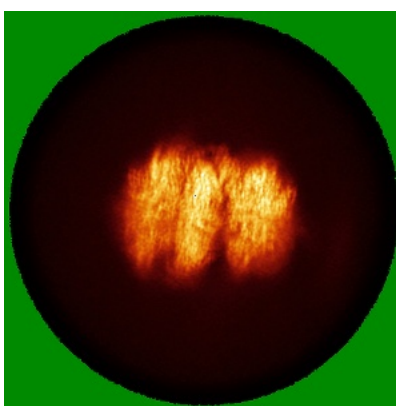
The images above show the largest variance slices of the map in three orthogonal directions.

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

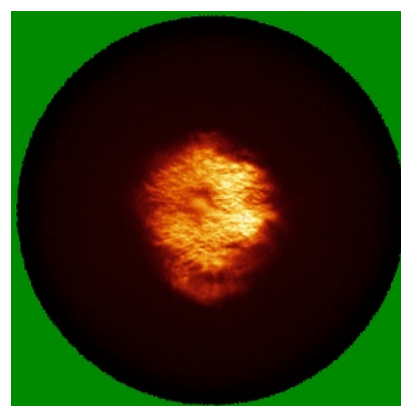
6.4.1 Primary map



X



Y

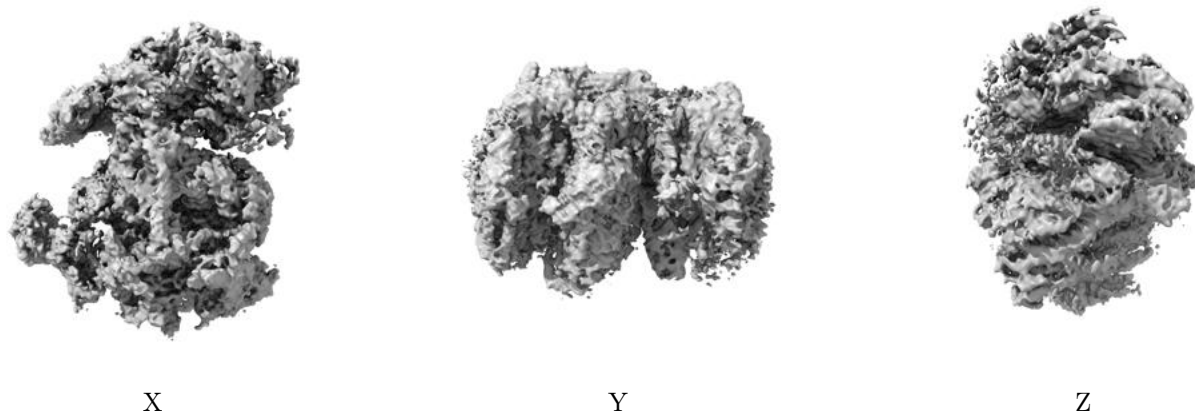


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

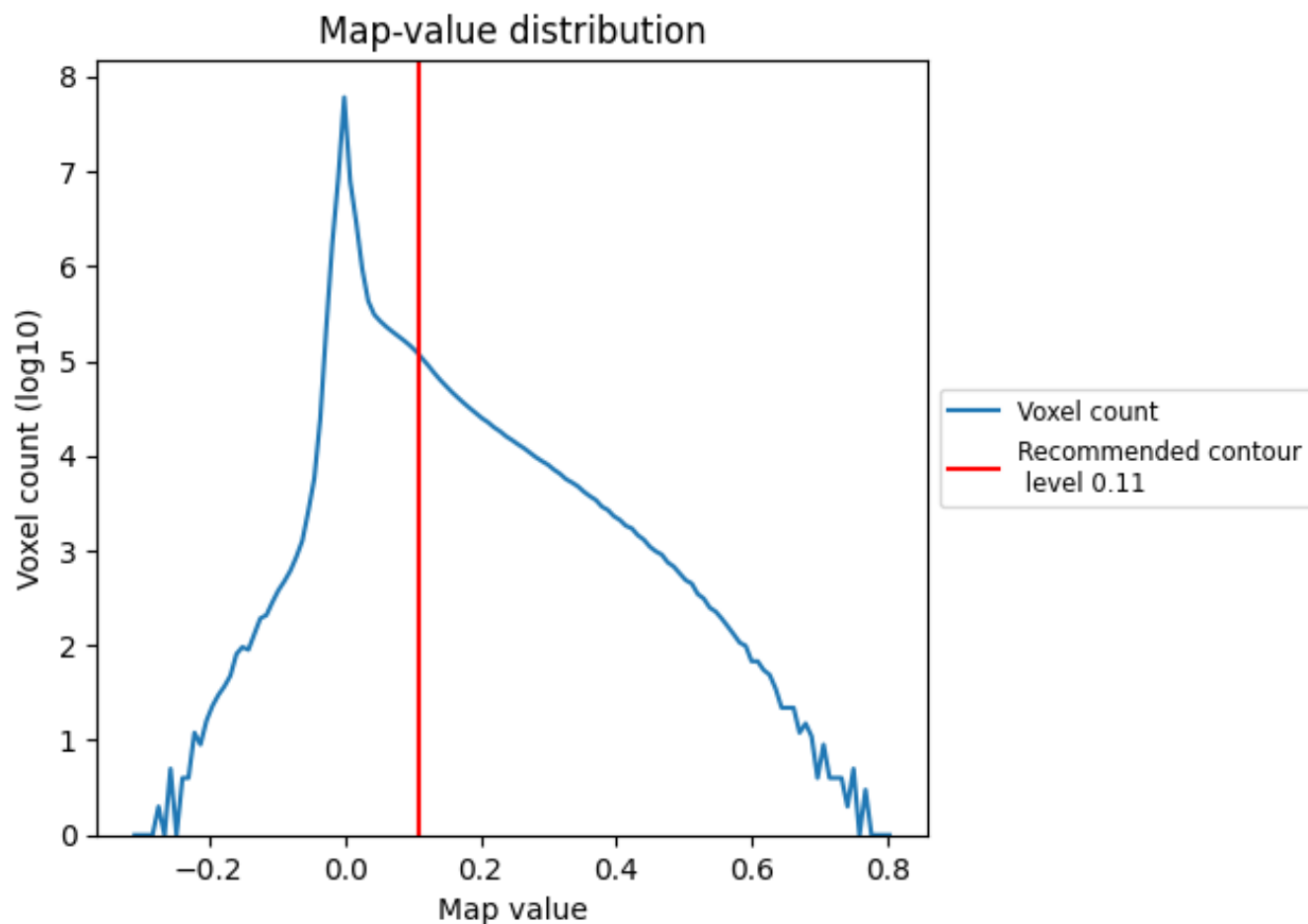
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

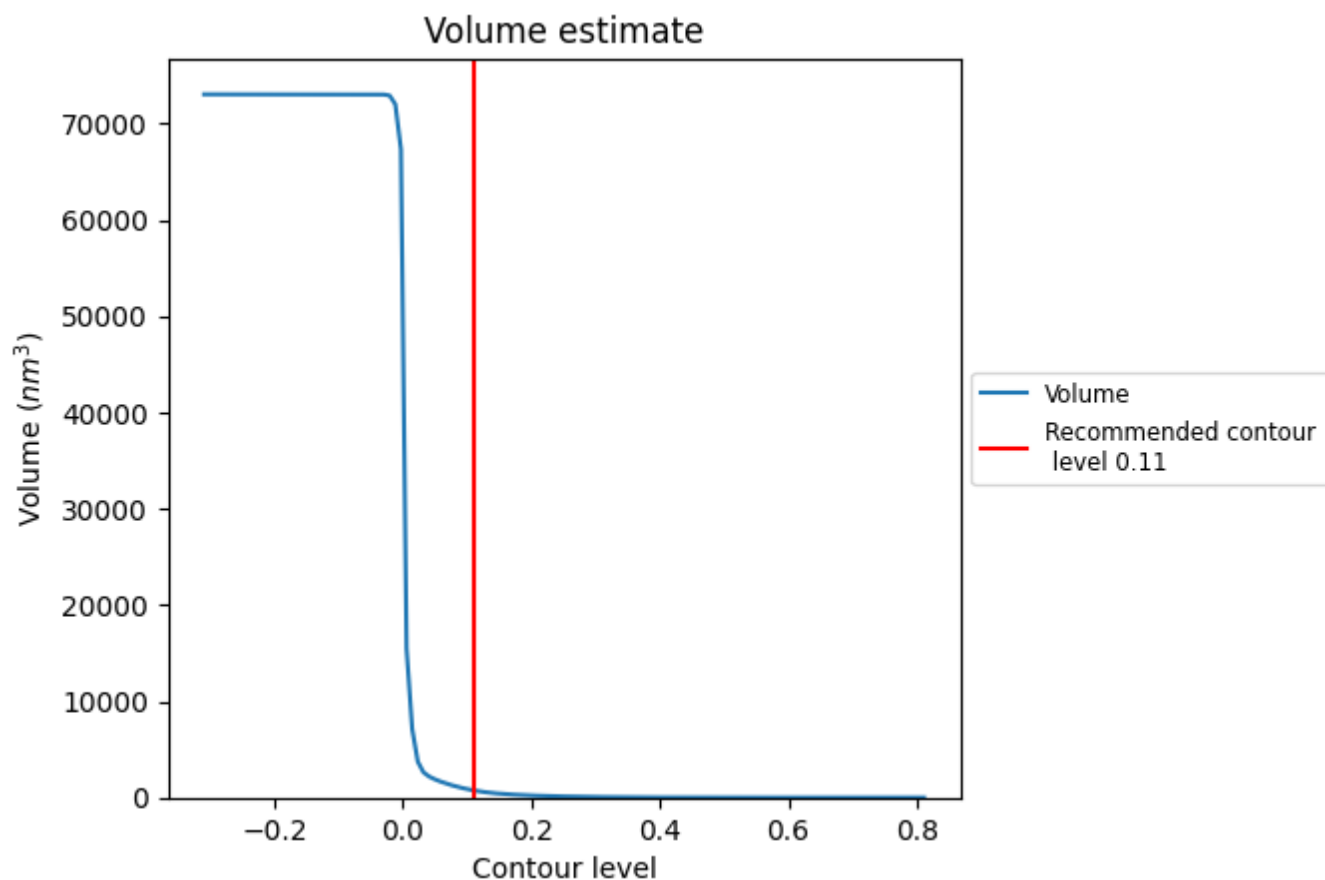
This section contains the results of statistical analysis of the map.

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.

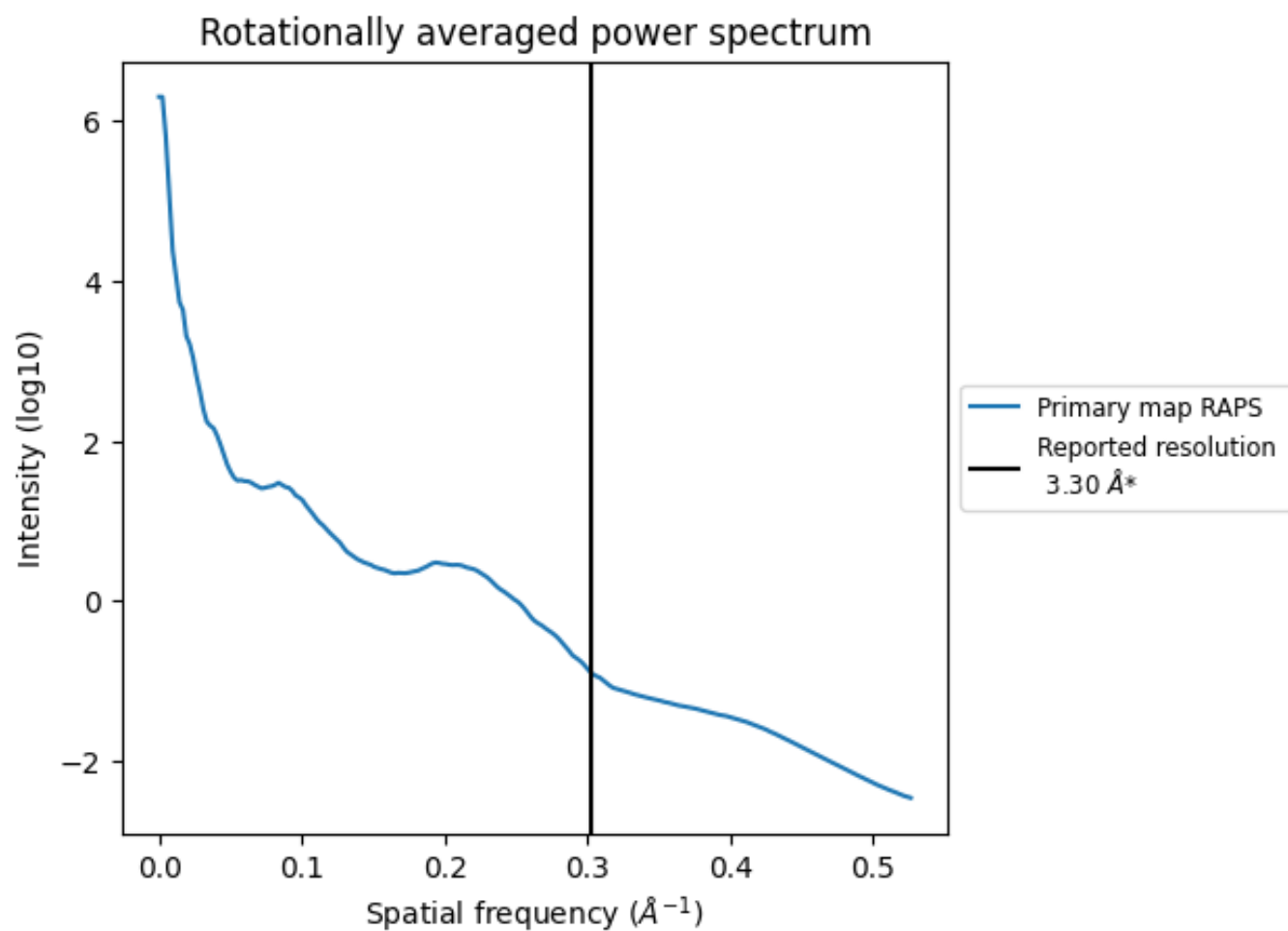
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 747 nm^3 ; this corresponds to an approximate mass of 675 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 0.303 Å⁻¹

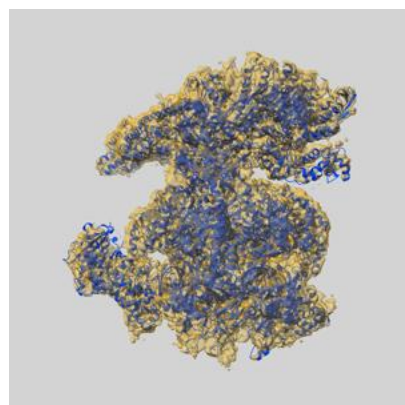
8 Fourier-Shell correlation

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

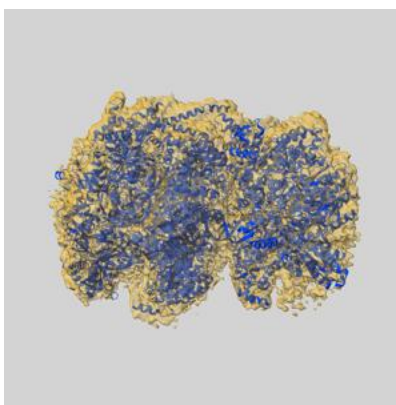
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51407 and PDB model 9GJW. Per-residue inclusion information can be found in section [3](#) on page [10](#).

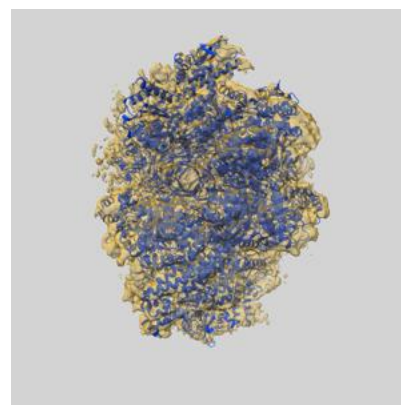
9.1 Map-model overlay [i](#)



X



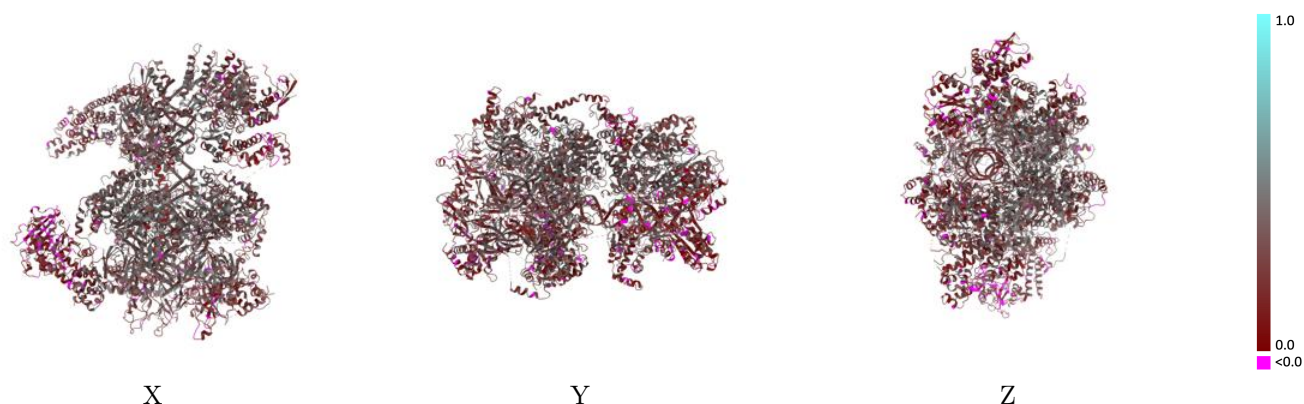
Y



Z

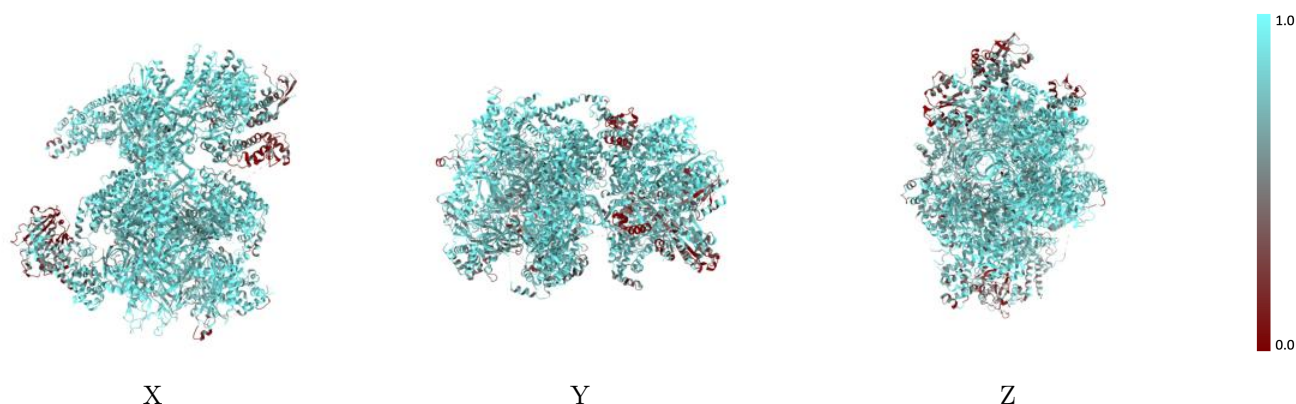
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



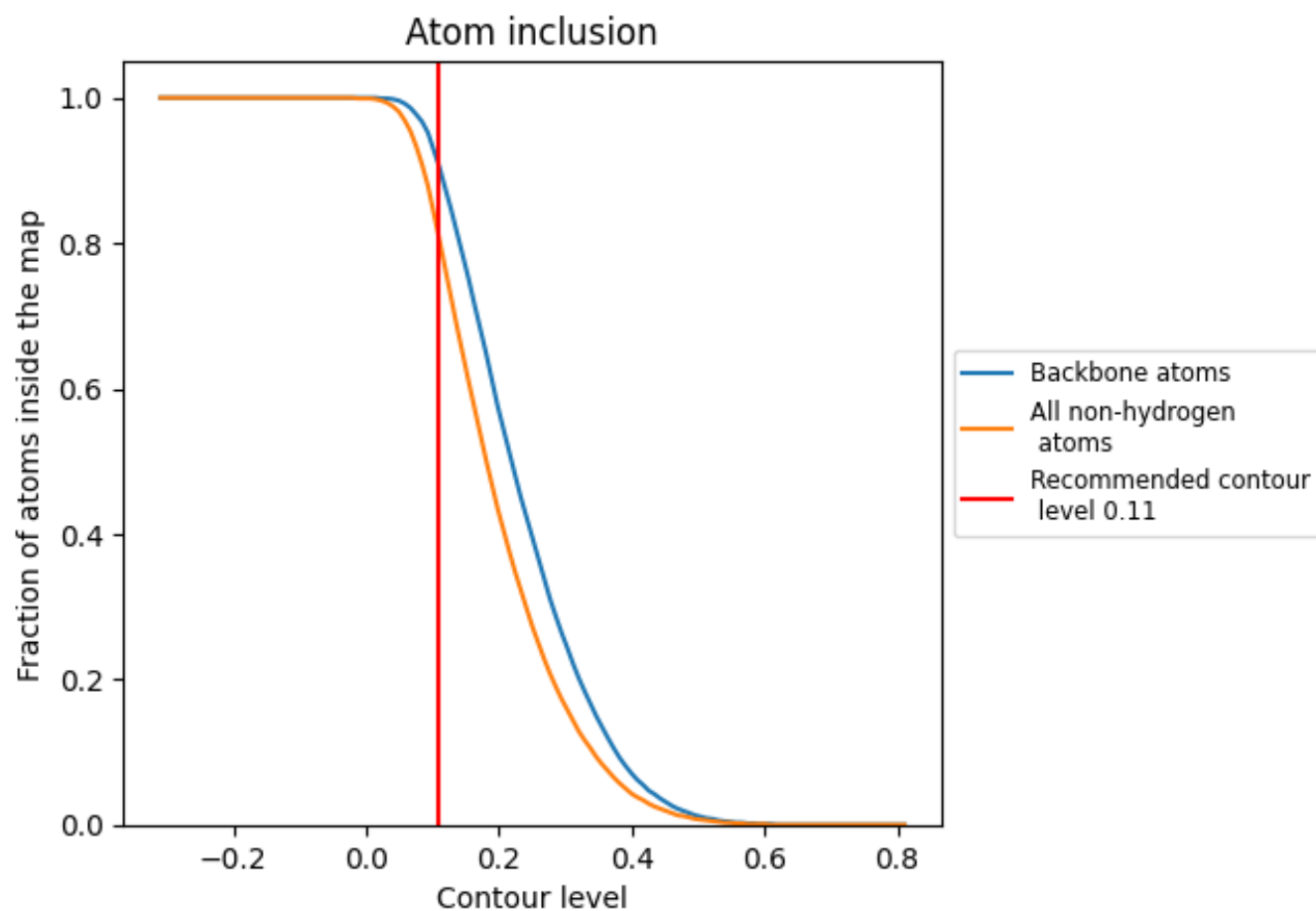
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 81% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.2960
2	 0.8640	 0.3340
3	 0.7940	 0.2840
4	 0.8060	 0.3230
5	 0.7860	 0.2510
6	 0.9010	 0.3700
7	 0.7840	 0.2790
8	 0.5730	 0.1720
A	 0.6130	 0.2240
B	 0.8310	 0.2910
C	 0.8410	 0.2800
D	 0.9060	 0.3450
E	 0.9110	 0.3790
F	 0.7460	 0.2720
X	 0.9410	 0.2740
Y	 0.9160	 0.2820

