



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 09:53 PM UTC

PDB ID : 8W0G / pdb_00008w0g
EMDB ID : EMD-43709
Title : Cryo-EM structure of a human MCM2-7 dimer
Authors : Yang, R.; Hunker, O.; Bleichert, F.
Deposited on : 2024-02-13
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

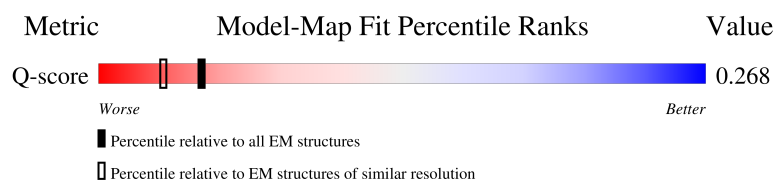
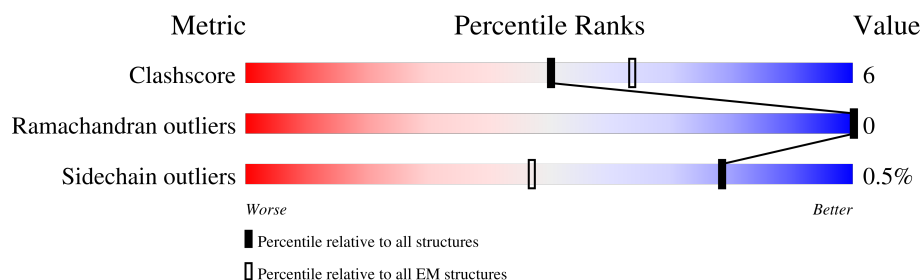
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



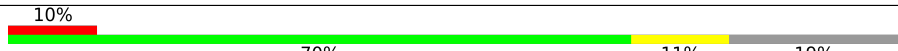
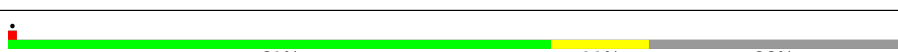
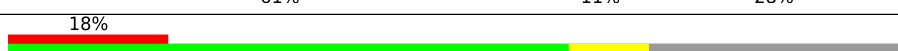
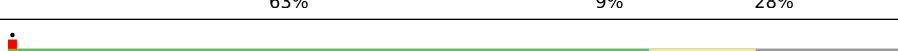
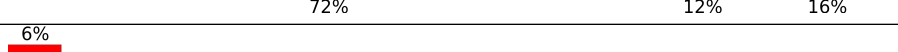
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	904	10% 54% 12% 34%
1	A	904	33% 56% 10% 34%
2	3	810	65% 9% 27%
2	B	810	66% 7% 27%

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Mol	Chain	Length	Quality of chain
3	4	866	
3	C	866	
4	5	734	
4	D	734	
5	6	821	
5	E	821	
6	7	719	
6	F	719	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	ATP	2	1002	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 114148 atoms, of which 57228 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	598	Total	C	H	N	O	S	0	0
			9472	2980	4740	844	879	29		
1	A	598	Total	C	H	N	O	S	0	0
			9472	2980	4740	844	879	29		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	3	594	Total	C	H	N	O	S	0	0
			9354	2916	4691	821	900	26		
2	B	594	Total	C	H	N	O	S	0	0
			9354	2916	4691	821	900	26		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-1	SER	-	expression tag	UNP P25205
3	0	ASN	-	expression tag	UNP P25205
3	1	ALA	-	expression tag	UNP P25205
B	-1	SER	-	expression tag	UNP P25205
B	0	ASN	-	expression tag	UNP P25205
B	1	ALA	-	expression tag	UNP P25205

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	4	580	Total	C	H	N	O	S	0	0
			9311	2928	4675	822	860	26		
3	C	580	Total	C	H	N	O	S	0	0
			9313	2928	4677	822	860	26		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	-2	SER	-	expression tag	UNP P33991
4	-1	ASN	-	expression tag	UNP P33991
4	0	ALA	-	expression tag	UNP P33991
4	650	MET	LEU	variant	UNP P33991
C	-2	SER	-	expression tag	UNP P33991
C	-1	ASN	-	expression tag	UNP P33991
C	0	ALA	-	expression tag	UNP P33991
C	650	MET	LEU	variant	UNP P33991

- Molecule 4 is a protein called DNA replication licensing factor MCM5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	5	597	Total	C	H	N	O	S	0	0
			9469	2953	4783	825	873	35		
4	D	597	Total	C	H	N	O	S	0	0
			9469	2953	4783	825	873	35		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	6	591	Total	C	H	N	O	S	0	0
			9496	2982	4759	836	893	26		
5	E	591	Total	C	H	N	O	S	0	0
			9497	2982	4760	836	893	26		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	7	607	Total	C	H	N	O	S	0	0
			9749	3044	4904	860	910	31		
6	F	607	Total	C	H	N	O	S	0	0
			9750	3044	4905	860	910	31		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	2	1	Total	Zn	0
			1	1	
7	4	1	Total	Zn	0
			1	1	
7	5	1	Total	Zn	0
			1	1	

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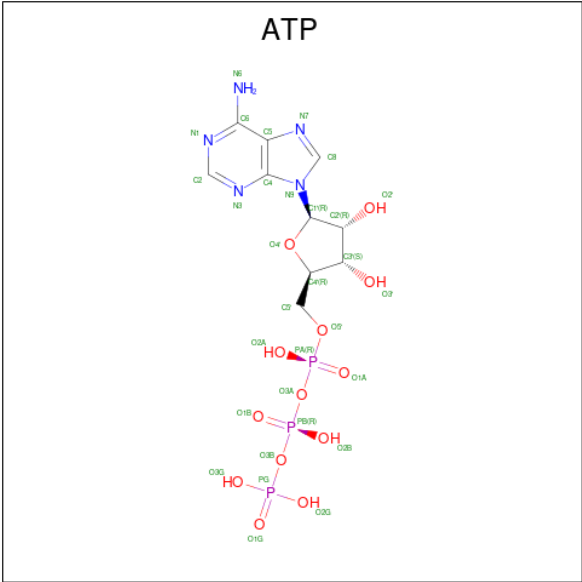
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Mol	Chain	Residues	Atoms		AltConf
7	6	1	Total 1	Zn 1	0
7	7	1	Total 1	Zn 1	0
7	A	1	Total 1	Zn 1	0
7	C	1	Total 1	Zn 1	0
7	D	1	Total 1	Zn 1	0
7	E	1	Total 1	Zn 1	0
7	F	1	Total 1	Zn 1	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

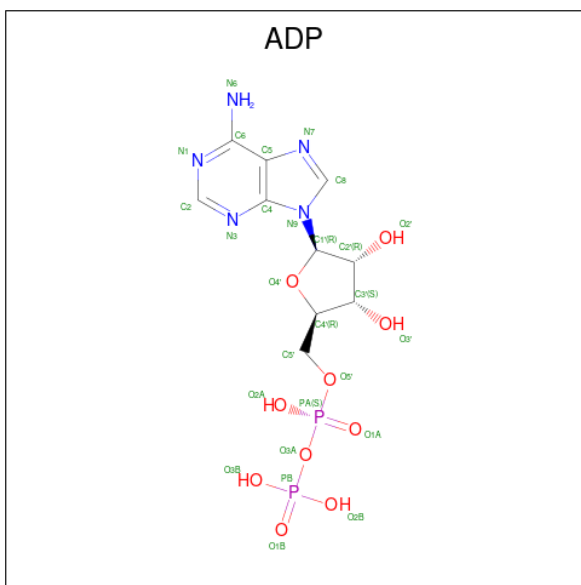
Mol	Chain	Residues	Atoms		AltConf
8	2	1	Total 1	Mg 1	0
8	3	1	Total 1	Mg 1	0
8	4	2	Total 2	Mg 2	0
8	7	1	Total 1	Mg 1	0
8	A	1	Total 1	Mg 1	0
8	B	1	Total 1	Mg 1	0
8	C	1	Total 1	Mg 1	0
8	E	1	Total 1	Mg 1	0
8	F	1	Total 1	Mg 1	0

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						AltConf
9	2	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
9	4	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
9	6	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
9	7	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
9	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
9	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
9	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
9	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms						AltConf
10	3	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
10	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

Chain A:



[illegible]

Chain B:

66% 7% 27%

Position 1: SER

Position 2: ASN

Position 3: ALA

Position 4: ALA

Position 5: GLY

Position 6: T4

Position 7: D25

Position 8: Q33

Position 9: H43

Position 10: V49

Position 11: F83

Position 12: S86

Position 13: Y95

Position 14: G101

Position 15: I130

Position 16: C148

Position 17: K152

Position 18: E156

Position 19: R157

Position 20: L162

Position 21: THR

Position 22: THR

Position 23: LEU

Position 24: VAL

Position 25: ALA

Position 26: PHE

Position 27: SER

Position 28: SER

Position 29: S172

Position 30: V173

Position 31: Y174

Position 32: T186

Position 33: E187

Position 34: D195

Position 35: H196

Position 36: D218

Position 37: G232

Position 38: C246

Position 39: LYS

Position 40: LYS

Position 41: GLY

Position 42: GLY

Position 43: T295

Position 44: K270

Position 45: D271

Position 46: A272

Position 47: Q273

Position 48: P274

Position 49: S275

Position 50: F276

Position 51: S277

Position 52: S292

Position 53: D480

Position 54: Y95

Position 55: T295

Position 56: L299

Position 57: L303

Position 58: T307

Position 59: R327

Position 60: S333

Position 61: H334

Position 62: T335

Position 63: R336

Position 64: G337

Position 65: D338

Position 66: S352

Position 67: T366

Position 68: G370

Position 69: R371

Position 70: G372

Position 71: S373

Position 72: S374

Position 73: G375

Position 74: L378

Position 75: D385

Position 76: Q386

Position 77: E387

Position 78: T388

Position 79: G389

Position 80: E390

Position 81: R391

Position 82: D409

Position 83: E410

Position 84: D412

Position 85: E427

Position 86: H439

Position 87: V448

Position 88: Y456

Position 89: G457

Position 90: R458

Position 91: M466

Position 92: C470

Position 93: R478

Position 94: F479

Position 95: L481

Position 96: L486

Position 97: Q513

Position 98: M518

Position 99: G521

Position 100: S522

Position 101: A523

Position 102: V524

Position 103: LYS

Position 104: VAL

Position 105: LEU

Position 106: LEU

Position 107: ALA

Position 108: THR

Position 109: ASP

Position 110: PRO

Position 111: ASP

Position 112: ASN

Position 113: PHE

Position 114: SER

Position 115: GLN

Position 116: GLN

Position 117: ASP

Position 118: ASP

Position 119: GLN

Position 120: GLN

Position 121: THR

Position 122: THR

Position 123: THR

Position 124: ILE

Position 125: TYR

Position 126: GLU

Position 127: LYS

Position 128: HIS

Position 129: ASP

Position 130: ASN

Position 131: LEU

Position 132: HIS

Position 133: GLY

Position 134: THR

Position 135: LYS

Position 136: LYS

Position 137: ARG

Position 138: LYS

Position 139: ALA

Position 140: ASP

Position 141: SER

Position 142: ALA

Position 143: SER

Position 144: GLN

Position 145: LEU

Position 146: LYS

Position 147: THR

Position 148: LYS

Position 149: MET

Position 150: GLN

Position 151: ASP

Position 152: ASN

Position 153: GLN

Position 154: VAL

Position 155: VAL

Position 156: MET

Position 157: VAL

Position 158: SER

Position 159: SER

Position 160: GLU

Position 161: GLY

Position 162: ARG

Position 163: THR

Position 164: GLU

Position 165: SER

Position 166: ILE

Position 167: ASN

Position 168: ARG

Position 169: ASP

Position 170: GLU

Position 171: ASP

Position 172: SER

Position 173: PHE

Position 174: SER

Position 175: VAL

Position 176: PRO

Position 177: VAL

Position 178: ILE

Position 179: GLN

Position 180: ALA

Position 181: ASP

Position 182: SER

Position 183: ALA

Position 184: SER

Position 185: GLN

Position 186: LEU

Position 187: LYS

Position 188: MET

Position 189: GLN

Position 190: ASP

Position 191: ASP

Position 192: ASN

Position 193: GLN

Position 194: VAL

Position 195: MET

Position 196: VAL

Position 197: SER

Position 198: SER

Position 199: GLU

Position 200: GLY

Position 201: THR

Position 202: LYS

Position 203: GLU

Position 204: LYS

Position 205: THR

Position 206: ASP

Position 207: THR

Position 208: ASP

Position 209: THR

Position 210: LYS

Position 211: ARG

Position 212: LYS

Position 213: THR

Position 214: THR

Position 215: THR

Position 216: THR

Position 217: THR

Position 218: THR

Position 219: THR

Position 220: THR

Position 221: THR

Position 222: THR

Position 223: THR

Position 224: THR

Position 225: THR

Position 226: THR

Position 227: THR

Position 228: THR

Position 229: THR

Position 230: THR

Position 231: THR

Position 232: THR

Position 233: THR

Position 234: THR

Position 235: THR

Position 236: THR

Position 237: THR

Position 238: THR

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Position 242: THR

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Position 244: THR

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Position 285: THR

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Position 287: THR

Position 288: THR

Position 289: THR

Position 290: THR

Position 291: THR

Position 292: THR

Position 293: THR

Position 294: THR

Position 295: THR

Position 296: THR

Position 297: THR

Position 298: THR

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Position 301: THR

Position 302: THR

Position 303: THR

Position 304: THR

Position 305: THR

Position 306: THR

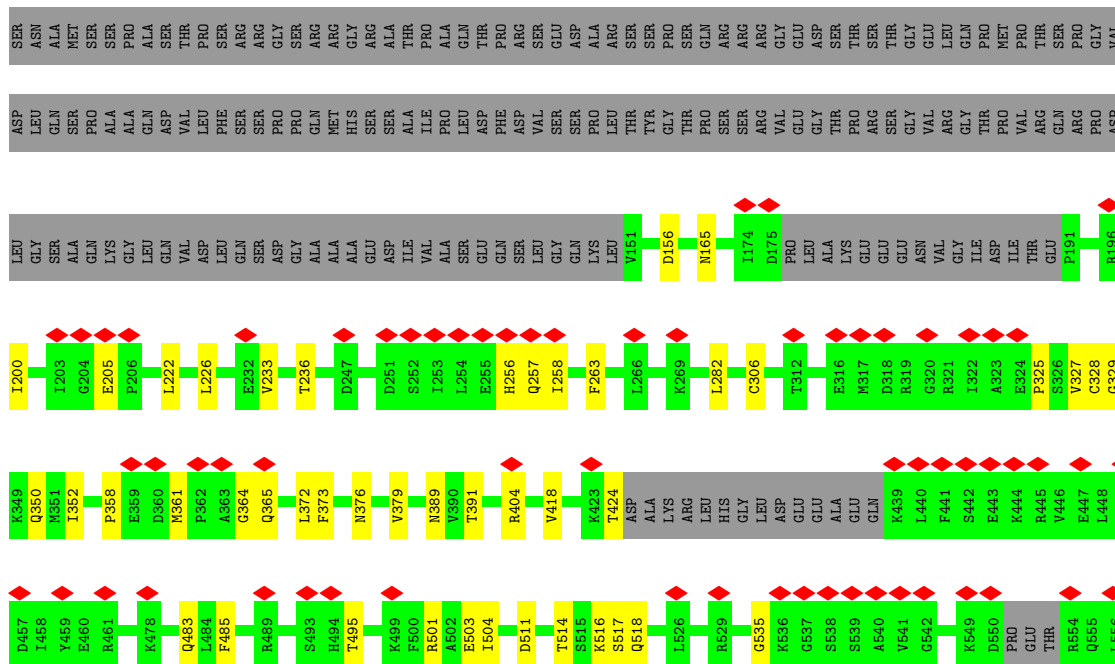
Position 307: THR

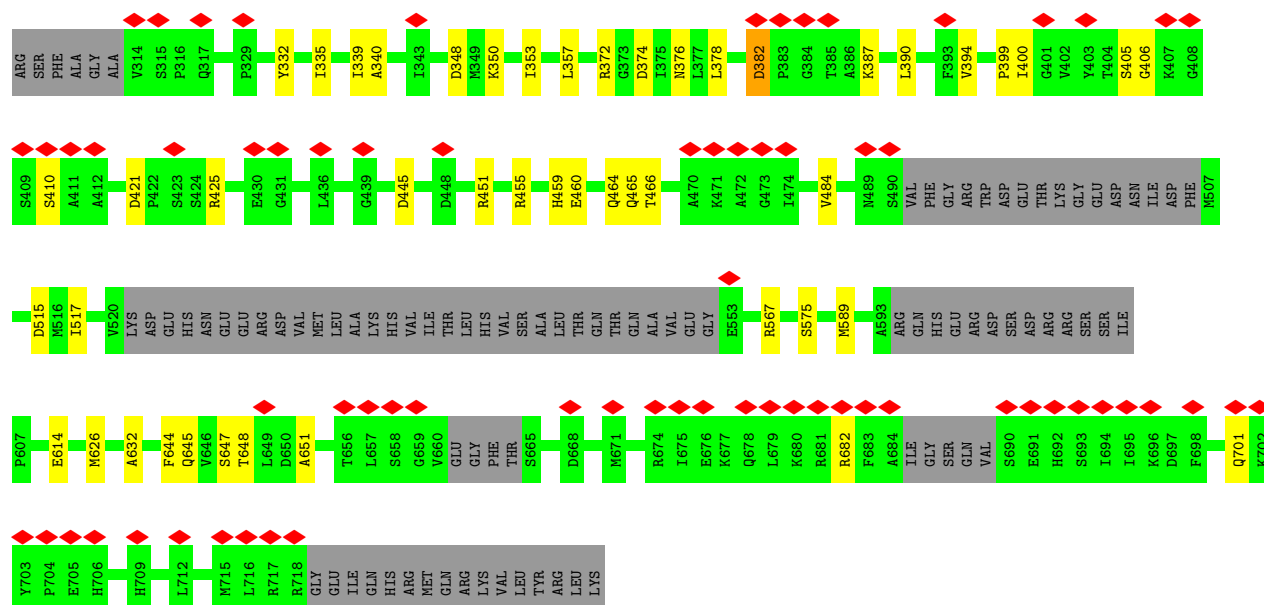
Position 308: THR

Position 309: THR

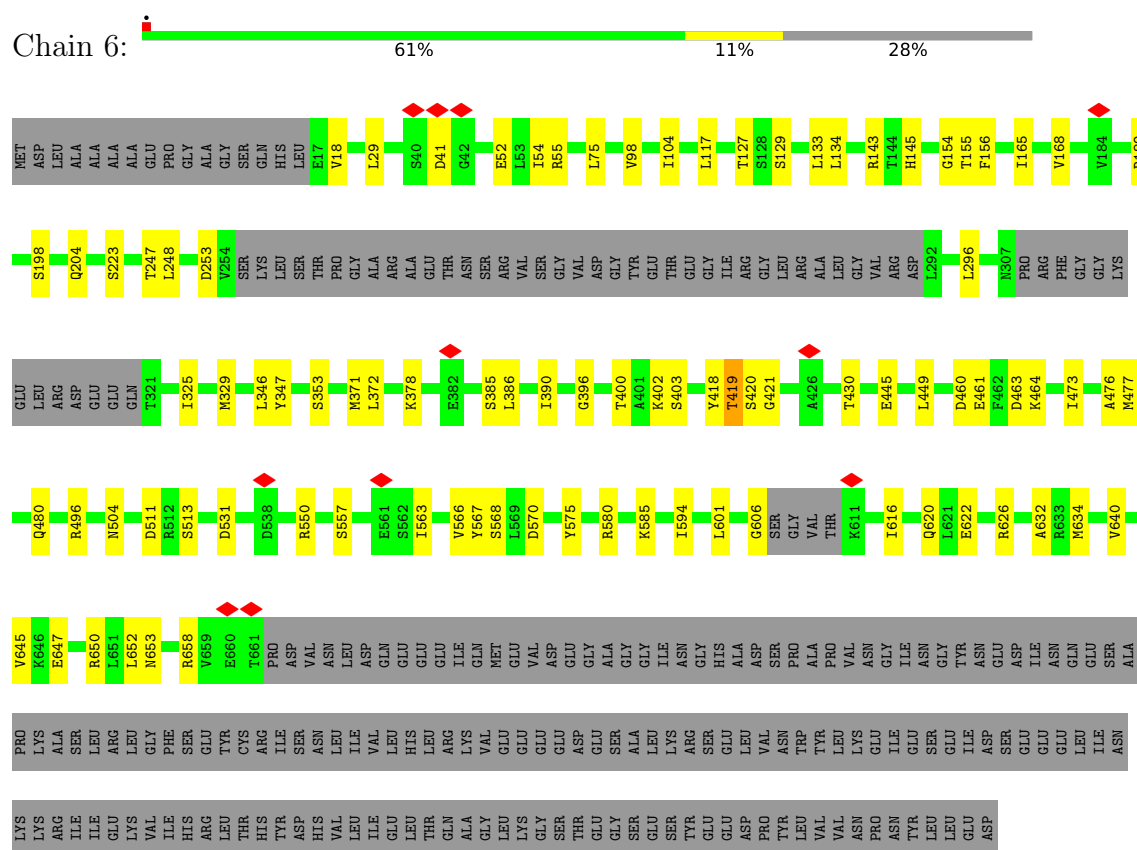
Position 310:

Chain 4:



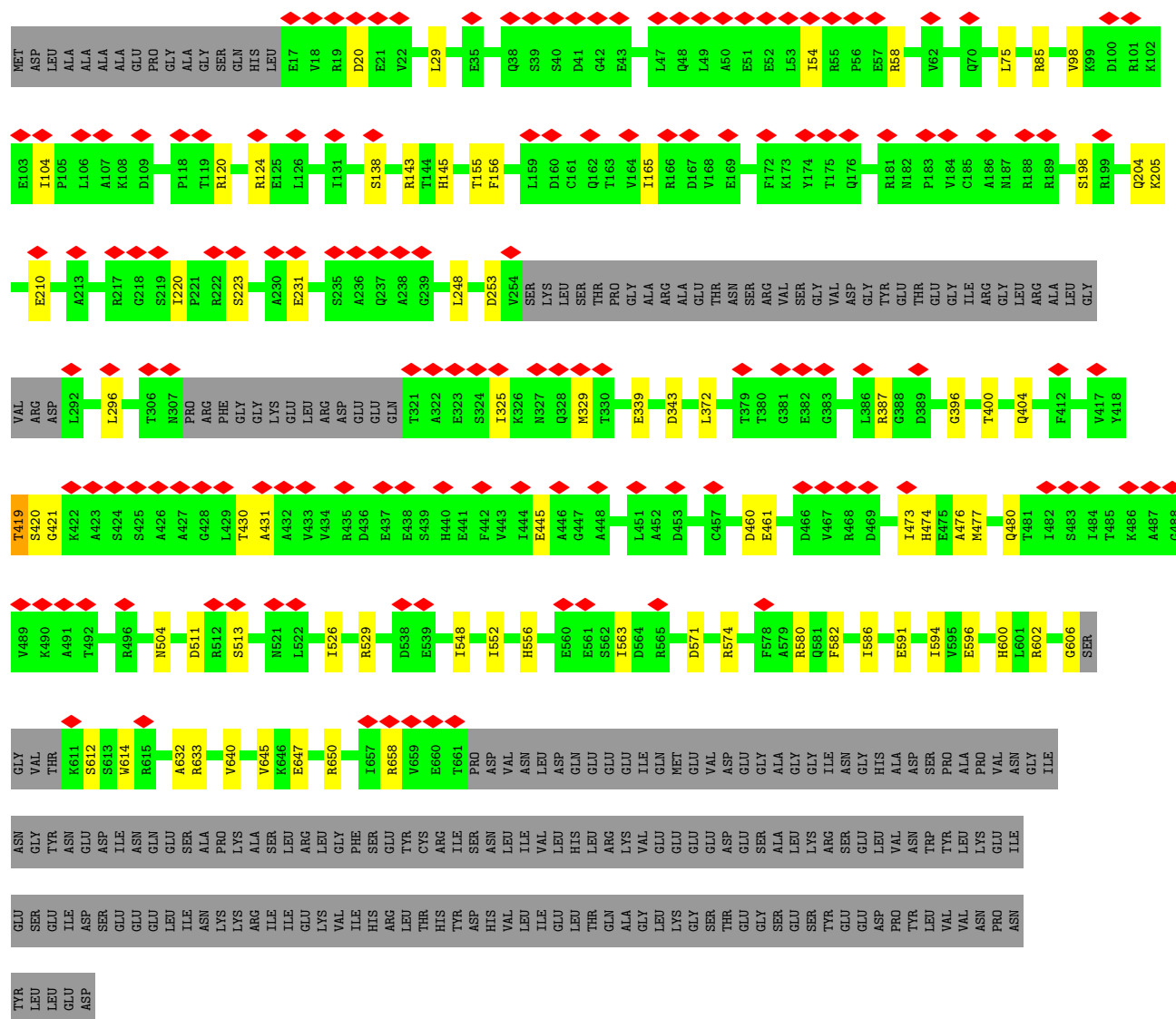


- Molecule 5: DNA replication licensing factor MCM6



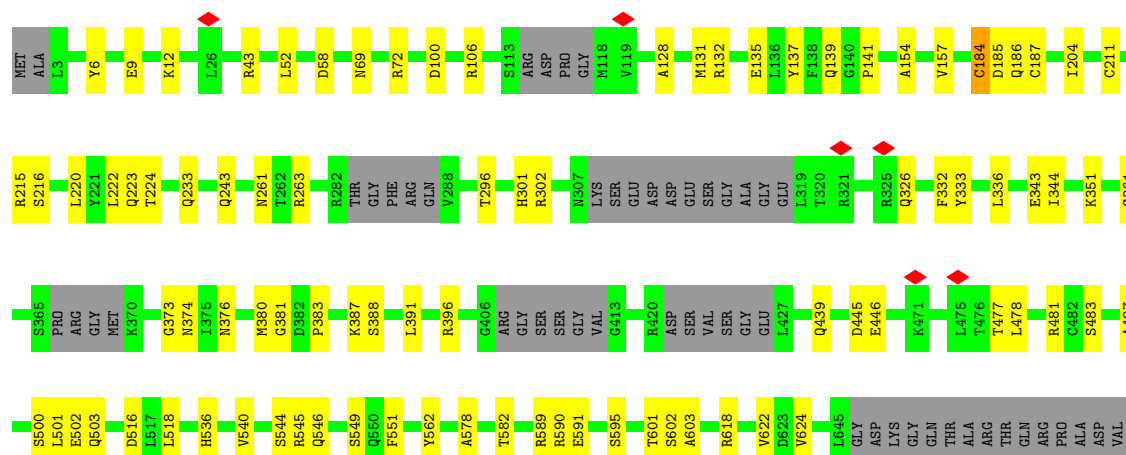
- Molecule 5: DNA replication licensing factor MCM6





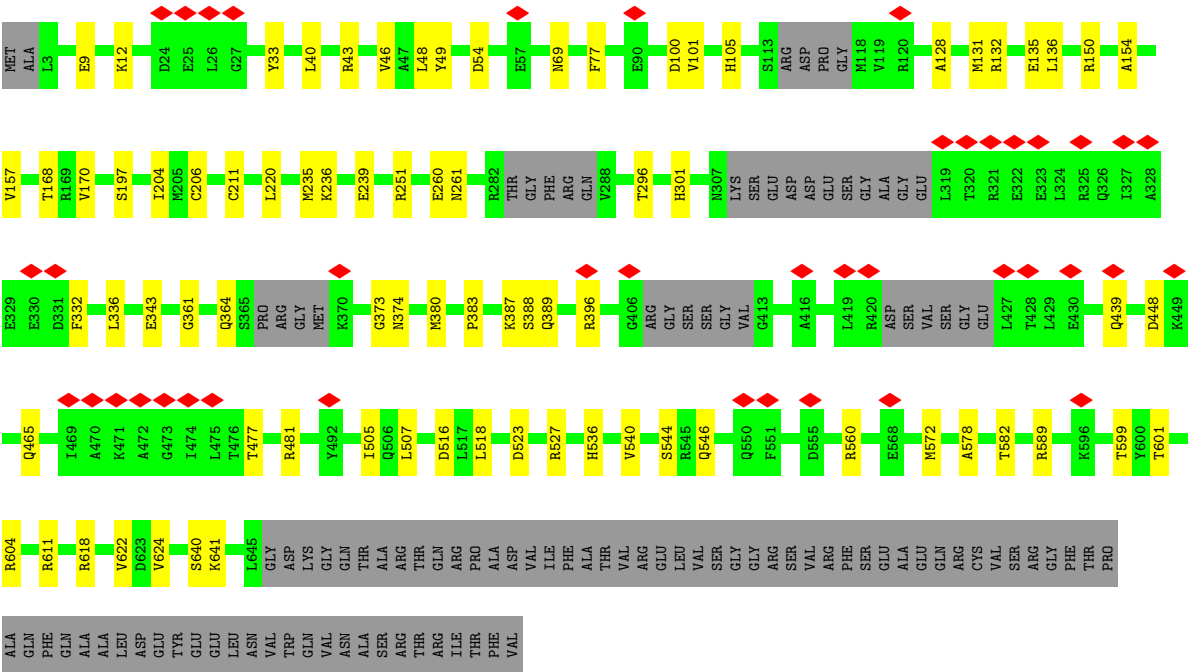
• Molecule 6: DNA replication licensing factor MCM7

Chain 7: 72% 12% 16%



ILE	PHE	ALA	THR	VAL	ARG	GLU	LEU	VAL	SER	GLY	GLY	ARG	SER	VAL	ARG	PHE	SER	SER	GLU	ALA	GLU	GLN	ARG	CYS	VAL	SER	ARG	GLY	PHE	THR	THR	PRO	ALA	GLN	GLN	ALA	ALA	LEU	ASP	GLU	TYR	GLU	GLU	LEU	ASN	VAL	TRP	GLN	VAL	ASN	ALA	SER	ARG	THR	ARG	ILE	THR	PHE	VAL
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● Molecule 6: DNA replication licensing factor MCM7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	101722	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 ($e^-/\text{\AA}^2$)	50.96	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.754	Depositor
Minimum map value	-0.266	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	499.2, 499.2, 499.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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: MG, ATP, ZN, ADP

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	0.13	0/4818	0.32	0/6501
1	A	0.13	0/4818	0.31	0/6501
2	3	0.15	0/4731	0.31	0/6385
2	B	0.14	0/4731	0.31	0/6385
3	4	0.14	0/4718	0.32	0/6372
3	C	0.13	0/4718	0.31	0/6372
4	5	0.14	0/4754	0.32	0/6381
4	D	0.13	0/4754	0.32	0/6381
5	6	0.13	0/4814	0.32	0/6494
5	E	0.13	0/4814	0.30	0/6494
6	7	0.15	0/4917	0.32	0/6634
6	F	0.14	0/4917	0.32	0/6634
All	All	0.14	0/57504	0.32	0/77534

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	4732	4740	4740	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4732	4740	4740	55	0
2	3	4663	4691	4691	44	0
2	B	4663	4691	4691	40	0
3	4	4636	4675	4675	66	0
3	C	4636	4677	4676	52	0
4	5	4686	4783	4782	68	0
4	D	4686	4783	4782	49	0
5	6	4737	4759	4759	57	0
5	E	4737	4760	4759	62	0
6	7	4845	4904	4904	55	0
6	F	4845	4905	4905	57	0
7	2	1	0	0	0	0
7	4	1	0	0	0	0
7	5	1	0	0	0	0
7	6	1	0	0	0	0
7	7	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
8	2	1	0	0	0	0
8	3	1	0	0	0	0
8	4	2	0	0	0	0
8	7	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	1	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
9	2	31	12	12	14	0
9	4	31	12	12	7	0
9	6	31	12	12	5	0
9	7	31	12	12	2	0
9	A	31	12	12	8	0
9	C	31	12	12	6	0
9	E	31	12	12	8	0
9	F	31	12	12	7	0
10	3	27	12	12	5	0
10	B	27	12	12	5	0
All	All	56920	57228	57224	642	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

All (642) 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)
9:A:1002:ATP:PG	5:E:529:ARG:HH22	1.80	1.04
9:A:1002:ATP:O2G	5:E:529:ARG:NH2	1.93	1.01
6:F:383:PRO:HB3	9:F:1002:ATP:O3G	1.64	0.97
3:C:514:THR:N	9:C:1002:ATP:O2B	1.98	0.94
3:C:517:SER:HG	8:C:1001:MG:MG	0.55	0.93
10:3:1002:ADP:O2'	4:5:614:GLU:OE2	1.94	0.84
3:4:282:LEU:HD11	3:4:391:THR:HG22	1.60	0.83
1:2:525:PRO:HB3	9:2:1002:ATP:O1G	1.81	0.80
3:4:514:THR:N	9:4:903:ATP:O2B	2.15	0.79
3:4:658:TYR:OH	9:4:903:ATP:N6	2.21	0.74
1:2:675:LEU:HD22	9:2:1002:ATP:C6	2.23	0.73
3:4:328:CYS:SG	3:4:329:GLY:N	2.62	0.72
2:B:571:TYR:OH	2:B:631:ALA:O	2.08	0.72
5:6:372:LEU:O	5:6:580:ARG:NH2	2.23	0.71
2:3:331:ASN:O	6:7:396:ARG:NH1	2.23	0.71
1:A:503:GLU:OE1	1:A:779:ARG:NH2	2.23	0.71
5:E:372:LEU:O	5:E:580:ARG:NH2	2.23	0.71
3:4:473:HIS:NE2	9:4:903:ATP:N6	2.39	0.71
3:4:708:GLN:OE1	5:6:550:ARG:NH2	2.23	0.71
5:E:552:ILE:HD11	9:E:1002:ATP:H1'	1.72	0.71
6:7:43:ARG:NH1	6:7:100:ASP:OD2	2.24	0.70
10:B:1002:ADP:O2'	4:D:614:GLU:OE2	2.05	0.70
2:B:466:MET:O	2:B:470:GLY:N	2.25	0.70
1:2:377:ARG:NE	1:2:395:ASP:OD1	2.23	0.70
1:2:642:THR:O	1:2:646:ASN:ND2	2.25	0.70
1:2:414:LEU:HD13	1:2:444:VAL:HG22	1.73	0.70
1:2:351:SER:N	1:2:357:SER:O	2.24	0.69
4:5:34:ARG:NH1	4:5:83:ASP:OD2	2.25	0.69
4:5:111:THR:O	4:5:114:ARG:NH1	2.24	0.69
1:A:377:ARG:NE	1:A:395:ASP:OD1	2.25	0.69
4:D:357:LEU:O	4:D:567:ARG:NH1	2.25	0.69
5:E:387:ARG:NH2	5:E:477:MET:O	2.25	0.69
6:F:168:THR:OG1	6:F:236:LYS:O	2.09	0.69
3:C:328:CYS:SG	3:C:329:GLY:N	2.65	0.68
2:3:157:ARG:NH1	2:3:173:VAL:O	2.25	0.68
4:5:60:LYS:NZ	4:5:110:VAL:O	2.27	0.68
6:F:204:ILE:O	6:F:220:LEU:N	2.27	0.68
5:6:143:ARG:NH2	5:6:445:GLU:OE1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:43:ARG:NH1	6:F:100:ASP:OD2	2.27	0.68
1:2:328:ASN:N	1:2:362:GLU:O	2.26	0.68
3:C:568:ASN:OD1	3:C:610:ARG:NH1	2.27	0.67
1:A:351:SER:N	1:A:357:SER:O	2.28	0.67
2:B:83:PHE:O	2:B:86:SER:OG	2.11	0.67
3:C:732:ARG:NH2	9:E:1002:ATP:O3G	2.27	0.67
6:7:545:ARG:NH1	6:7:546:GLN:O	2.28	0.66
6:7:590:ARG:NH1	6:7:591:GLU:OE2	2.28	0.66
6:7:106:ARG:NH2	6:7:131:MET:SD	2.68	0.66
4:D:575:SER:OG	4:D:632:ALA:O	2.13	0.66
6:7:326:GLN:OE1	6:7:562:TYR:OH	2.13	0.66
6:7:361:GLY:O	6:7:618:ARG:NH1	2.28	0.66
5:6:511:ASP:OD1	5:6:513:SER:OG	2.10	0.66
4:D:353:ILE:HD11	4:D:390:LEU:HD21	1.78	0.66
5:E:54:ILE:HG22	5:E:104:ILE:HD11	1.76	0.66
1:A:296:SER:O	1:A:298:ARG:NH1	2.27	0.66
4:D:682:ARG:NH2	4:D:701:GLN:OE1	2.28	0.66
4:D:378:LEU:HD23	4:D:517:ILE:HD12	1.77	0.66
6:F:388:SER:HB2	9:F:1002:ATP:O1B	1.95	0.65
1:2:316:THR:O	1:2:374:GLN:NE2	2.29	0.65
1:2:402:LEU:HD13	1:2:444:VAL:HG23	1.76	0.65
2:3:4:THR:N	2:B:156:GLU:O	2.29	0.65
4:5:104:LYS:NZ	4:5:123:ASP:OD1	2.27	0.65
2:3:466:MET:O	2:3:470:GLY:N	2.29	0.65
1:A:642:THR:O	1:A:646:ASN:ND2	2.29	0.65
2:3:83:PHE:O	2:3:86:SER:OG	2.12	0.64
3:C:592:GLU:OE1	3:C:643:ARG:NE	2.28	0.64
3:C:282:LEU:HD11	3:C:391:THR:HG22	1.78	0.64
5:E:552:ILE:HG23	5:E:556:HIS:HE2	1.62	0.64
5:E:571:ASP:OD1	5:E:574:ARG:NH1	2.30	0.64
3:C:306:CYS:SG	3:C:336:SER:OG	2.52	0.64
1:2:675:LEU:HD22	9:2:1002:ATP:N1	2.12	0.64
5:E:552:ILE:HG22	5:E:556:HIS:CD2	2.32	0.64
9:2:1002:ATP:H4'	5:6:622:GLU:OE2	1.97	0.64
3:C:348:ASP:O	3:C:376:ASN:N	2.31	0.64
3:C:501:ARG:O	3:C:739:ARG:NE	2.29	0.64
2:3:49:VAL:N	2:3:101:GLY:O	2.30	0.64
6:7:135:GLU:OE1	6:7:137:TYR:OH	2.16	0.64
4:D:162:ARG:O	4:D:224:PHE:N	2.31	0.64
6:F:343:GLU:O	6:F:536:HIS:NE2	2.31	0.63
5:6:145:HIS:O	5:6:204:GLN:NE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:333:ASN:OD1	5:6:189:ARG:NE	2.32	0.63
1:A:621:GLN:OE1	1:A:623:ARG:NH2	2.31	0.63
5:6:156:PHE:O	5:6:165:ILE:N	2.32	0.63
9:A:1002:ATP:O3G	5:E:529:ARG:NH1	2.30	0.63
3:4:639:THR:O	3:4:642:SER:OG	2.14	0.63
6:7:376:ASN:N	6:7:516:ASP:OD2	2.31	0.63
1:2:525:PRO:CB	9:2:1002:ATP:O1G	2.47	0.63
5:E:145:HIS:O	5:E:204:GLN:NE2	2.31	0.62
1:A:402:LEU:HD13	1:A:444:VAL:HG23	1.80	0.62
5:6:606:GLY:O	5:6:658:ARG:NE	2.33	0.62
3:4:156:ASP:OD1	3:4:224:ARG:NH2	2.32	0.62
5:6:568:SER:OG	5:6:570:ASP:OD1	2.14	0.62
2:B:427:GLU:OE1	2:B:478:ARG:NE	2.32	0.62
4:5:225:GLN:OE1	4:5:255:ASP:N	2.33	0.62
1:A:323:SER:OG	1:A:366:GLU:OE2	2.18	0.62
2:B:187:GLU:OE1	6:F:69:ASN:ND2	2.33	0.62
2:B:49:VAL:N	2:B:101:GLY:O	2.33	0.62
3:4:710:LEU:HD13	3:4:738:ILE:HG22	1.82	0.61
3:4:568:ASN:OD1	3:4:610:ARG:NH1	2.34	0.61
6:7:374:ASN:OD1	6:7:483:SER:N	2.34	0.61
2:3:522:SER:OG	4:5:302:ASP:O	2.15	0.61
1:A:316:THR:O	1:A:374:GLN:NE2	2.34	0.61
4:5:357:LEU:HD21	4:5:394:VAL:CG2	2.31	0.61
4:5:138:ARG:NH2	4:5:231:GLU:OE1	2.33	0.61
5:6:575:TYR:OH	5:6:634:MET:O	2.08	0.61
3:C:769:LEU:O	3:C:773:ALA:N	2.33	0.61
2:B:352:SER:HB2	10:B:1002:ADP:PA	2.41	0.60
5:E:552:ILE:HG23	5:E:556:HIS:NE2	2.16	0.60
1:2:319:LEU:N	1:2:373:TYR:O	2.33	0.60
6:F:128:ALA:O	6:F:132:ARG:NH1	2.34	0.60
6:F:239:GLU:OE1	6:F:251:ARG:N	2.33	0.60
5:6:531:ASP:OD2	5:6:626:ARG:NH2	2.34	0.60
1:A:675:LEU:HD22	9:A:1002:ATP:C6	2.36	0.60
3:C:581:GLU:OE2	3:C:584:ARG:NH1	2.34	0.60
5:E:552:ILE:O	5:E:556:HIS:CD2	2.55	0.60
1:2:303:ASN:N	1:2:418:TYR:O	2.34	0.60
4:5:372:ARG:NH2	4:5:515:ASP:OD1	2.34	0.60
2:B:352:SER:HB2	10:B:1002:ADP:O1A	2.02	0.60
6:F:361:GLY:O	6:F:618:ARG:NH1	2.35	0.60
2:3:467:GLU:O	4:5:718:ARG:NH2	2.35	0.59
1:2:675:LEU:CD2	9:2:1002:ATP:C6	2.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:483:GLN:NE2	3:4:504:ILE:O	2.35	0.59
4:5:253:LEU:HD11	4:5:299:ILE:HG12	1.83	0.59
2:B:595:SER:OG	6:F:527:ARG:NH1	2.34	0.59
4:D:376:ASN:OD1	4:D:484:VAL:N	2.36	0.59
4:5:167:ARG:NH2	4:5:181:ASN:O	2.35	0.59
4:5:58:GLU:O	4:5:62:HIS:ND1	2.35	0.59
2:B:218:ASP:OD1	2:B:218:ASP:N	2.33	0.59
6:F:9:GLU:OE1	6:F:12:LYS:NZ	2.35	0.59
3:4:501:ARG:NH1	3:4:503:GLU:O	2.36	0.59
6:7:184:CYS:SG	6:7:185:ASP:N	2.76	0.59
3:4:732:ARG:NH2	9:6:902:ATP:O3B	2.36	0.58
1:A:300:LEU:O	1:A:304:GLN:NE2	2.37	0.58
3:4:291:ARG:NH2	3:4:550:ASP:OD1	2.37	0.58
6:F:374:ASN:ND2	6:F:465:GLN:OE1	2.36	0.58
4:D:374:ASP:OD2	4:D:465:GLN:NE2	2.35	0.58
4:D:72:VAL:O	4:D:129:LYS:N	2.36	0.58
2:3:47:LEU:O	2:3:101:GLY:N	2.36	0.58
6:7:9:GLU:OE1	6:7:12:LYS:NZ	2.31	0.58
1:A:230:LEU:HD23	1:A:283:VAL:HG22	1.85	0.58
6:7:445:ASP:OD1	6:7:446:GLU:N	2.36	0.58
3:4:518:GLN:HG3	9:4:903:ATP:O2A	2.03	0.58
5:6:248:LEU:HD11	5:6:296:LEU:HB3	1.85	0.58
5:6:594:ILE:HD13	5:6:645:VAL:HG13	1.86	0.58
4:D:225:GLN:OE1	4:D:255:ASP:N	2.36	0.58
1:A:421:ASN:O	1:A:436:ALA:N	2.36	0.58
1:A:528:ALA:HB2	9:A:1002:ATP:C8	2.39	0.58
1:2:503:GLU:N	1:2:775:GLU:OE1	2.37	0.58
3:4:733:GLN:O	3:4:736:SER:OG	2.20	0.58
4:5:339:ILE:HD11	4:5:350:LYS:HB3	1.84	0.58
5:6:54:ILE:HG22	5:6:104:ILE:HD11	1.86	0.58
3:C:373:PHE:O	3:C:418:VAL:HG12	2.04	0.58
2:3:466:MET:SD	2:3:473:ASP:N	2.77	0.58
3:4:769:LEU:O	3:4:773:ALA:N	2.36	0.57
3:C:518:GLN:HG3	9:C:1002:ATP:O2A	2.04	0.57
6:F:388:SER:CB	9:F:1002:ATP:O1B	2.52	0.57
4:5:360:GLY:O	4:5:625:LYS:NZ	2.29	0.57
3:C:667:VAL:HG11	6:F:578:ALA:HB2	1.86	0.57
4:5:572:PRO:O	4:5:573:ARG:NH1	2.37	0.57
6:F:261:ASN:ND2	6:F:301:HIS:O	2.38	0.57
1:A:524:ASP:OD2	1:A:636:ARG:NH1	2.38	0.57
1:2:329:CYS:SG	1:2:330:ASN:N	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:3:1002:ADP:PA	4:5:611:ARG:HH22	2.28	0.57
3:C:483:GLN:NE2	3:C:504:ILE:O	2.38	0.57
2:3:521:GLY:O	4:5:481:ARG:NH2	2.38	0.57
10:3:1002:ADP:O5'	4:5:611:ARG:NH2	2.38	0.57
1:A:323:SER:O	1:A:341:GLN:N	2.38	0.57
1:2:675:LEU:HD21	9:2:1002:ATP:N6	2.19	0.56
1:2:397:ILE:HD12	1:2:438:VAL:HG21	1.87	0.56
1:2:589:PHE:HZ	1:2:600:ILE:HD13	1.69	0.56
3:4:555:GLN:OE1	3:4:555:GLN:N	2.38	0.56
5:E:156:PHE:N	5:E:165:ILE:O	2.39	0.56
3:4:311:HIS:HA	5:6:18:VAL:HG21	1.87	0.56
2:3:232:GLY:O	2:3:270:LYS:NZ	2.38	0.56
6:7:243:GLN:N	6:7:243:GLN:OE1	2.39	0.56
2:B:409:ASP:N	2:B:409:ASP:OD1	2.37	0.56
1:2:603:ALA:O	1:2:607:GLN:N	2.37	0.56
3:4:361:MET:HE1	3:4:367:PRO:HG3	1.87	0.56
5:E:596:GLU:OE2	5:E:600:HIS:NE2	2.38	0.56
5:E:253:ASP:OD1	5:E:253:ASP:N	2.38	0.56
5:E:552:ILE:CG2	5:E:556:HIS:CD2	2.89	0.56
4:5:516:MET:HE1	4:5:643:LEU:HG	1.88	0.56
4:5:365:LEU:HD11	4:5:371:ARG:NE	2.21	0.56
1:A:247:PHE:O	1:A:251:ALA:N	2.38	0.56
1:2:505:LYS:O	1:2:513:VAL:N	2.38	0.55
1:A:260:ASP:OD1	1:A:283:VAL:N	2.38	0.55
6:7:52:LEU:HD12	6:7:141:PRO:HD3	1.87	0.55
5:E:473:ILE:HG22	5:E:477:MET:HE3	1.89	0.55
10:3:1002:ADP:PA	4:5:611:ARG:NH2	2.80	0.55
3:4:667:VAL:HG11	6:7:578:ALA:HB2	1.88	0.55
4:D:353:ILE:CD1	4:D:390:LEU:HD21	2.36	0.55
3:C:358:PRO:HA	3:C:361:MET:HE2	1.89	0.55
5:E:156:PHE:O	5:E:165:ILE:N	2.40	0.55
1:A:328:ASN:N	1:A:362:GLU:O	2.39	0.55
4:D:253:LEU:HD11	4:D:299:ILE:HG12	1.87	0.55
6:7:58:ASP:OD1	6:7:58:ASP:N	2.39	0.55
4:D:332:TYR:CG	4:D:626:MET:HE1	2.42	0.55
5:E:606:GLY:O	5:E:658:ARG:NE	2.39	0.55
5:E:120:ARG:NE	5:E:138:SER:OG	2.40	0.55
2:3:299:LEU:O	2:3:303:LEU:N	2.40	0.55
4:5:353:ILE:HD11	4:5:390:LEU:HD21	1.88	0.55
5:E:647:GLU:OE1	5:E:650:ARG:NE	2.40	0.55
6:F:77:PHE:HB3	6:F:136:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:187:GLU:OE1	6:7:69:ASN:ND2	2.40	0.55
5:6:647:GLU:OE1	5:6:650:ARG:NE	2.40	0.55
3:4:701:ARG:O	3:4:753:VAL:N	2.38	0.54
5:6:402:LYS:N	9:6:902:ATP:O2B	2.40	0.54
6:F:387:LYS:HE2	9:F:1002:ATP:O1G	2.08	0.54
1:A:593:ASN:ND2	1:A:596:ASP:OD2	2.39	0.54
6:7:391:LEU:HD11	6:7:487:ALA:HB3	1.90	0.54
1:A:682:SER:O	1:A:686:HIS:ND1	2.41	0.54
2:B:307:ILE:HG23	10:B:1002:ADP:C6	2.43	0.54
5:E:552:ILE:CG2	5:E:556:HIS:HE2	2.20	0.54
6:7:222:LEU:HD23	6:7:223:GLN:N	2.23	0.54
2:B:25:ASP:O	2:B:33:GLN:NE2	2.41	0.54
1:2:514:ARG:NH1	1:2:518:ASN:OD1	2.41	0.54
4:5:382:ASP:O	4:5:387:LYS:NZ	2.41	0.54
4:5:451:ARG:O	4:5:455:ARG:N	2.39	0.54
5:E:421:GLY:N	5:E:460:ASP:O	2.41	0.54
3:C:703:SER:OG	3:C:753:VAL:O	2.22	0.53
5:E:20:ASP:OD2	5:E:85:ARG:NE	2.41	0.53
6:F:170:VAL:HG12	6:F:235:MET:HB3	1.90	0.53
4:5:374:ASP:OD2	4:5:465:GLN:NE2	2.42	0.53
4:D:382:ASP:O	4:D:387:LYS:NZ	2.41	0.53
5:E:124:ARG:NH2	5:E:220:ILE:O	2.41	0.53
5:E:143:ARG:NH2	5:E:445:GLU:OE1	2.42	0.53
5:E:594:ILE:HD13	5:E:645:VAL:HG13	1.90	0.53
6:7:383:PRO:HB3	9:7:1002:ATP:O3G	2.09	0.53
6:7:211:CYS:O	6:7:215:ARG:N	2.42	0.53
2:B:385:ASP:N	2:B:390:GLU:O	2.41	0.53
3:C:732:ARG:NH2	9:E:1002:ATP:O3B	2.41	0.53
5:E:124:ARG:NE	5:E:210:GLU:OE2	2.41	0.53
6:7:128:ALA:O	6:7:132:ARG:NH1	2.42	0.53
2:3:571:TYR:OH	2:3:631:ALA:O	2.24	0.53
6:F:383:PRO:CB	9:F:1002:ATP:O3G	2.49	0.53
1:2:247:PHE:O	1:2:251:ALA:N	2.41	0.53
1:2:777:HIS:HA	1:2:780:ILE:HD12	1.91	0.53
2:3:324:GLY:O	2:3:630:LYS:NZ	2.29	0.53
5:6:378:LYS:O	5:6:386:LEU:N	2.41	0.53
6:7:391:LEU:HD11	6:7:487:ALA:CB	2.39	0.53
5:E:404:GLN:HB2	9:E:1002:ATP:O2A	2.09	0.53
6:F:448:ASP:HA	6:F:507:LEU:HD21	1.90	0.53
5:6:52:GLU:OE2	5:6:55:ARG:NE	2.40	0.53
4:5:421:ASP:O	4:5:425:ARG:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:253:ASP:OD1	5:6:253:ASP:N	2.42	0.52
5:6:460:ASP:OD1	5:6:461:GLU:N	2.41	0.52
1:A:315:CYS:O	1:A:571:LEU:N	2.41	0.52
4:5:5:ASP:OD1	2:B:186:THR:HG23	2.09	0.52
3:4:371:ILE:O	3:4:372:LEU:HD23	2.09	0.52
5:6:127:THR:HG1	5:6:129:SER:HG	1.55	0.52
3:C:503:GLU:N	3:C:503:GLU:OE1	2.42	0.52
3:C:710:LEU:HD13	3:C:738:ILE:HD13	1.91	0.52
1:2:675:LEU:CD2	9:2:1002:ATP:N1	2.73	0.52
5:E:552:ILE:CG2	5:E:556:HIS:NE2	2.73	0.52
5:E:552:ILE:HG22	5:E:556:HIS:HD2	1.75	0.52
3:4:278:ASP:OD1	3:4:278:ASP:N	2.42	0.52
1:A:297:LEU:HD12	1:A:297:LEU:O	2.10	0.52
4:5:263:VAL:HG12	4:5:301:VAL:HG12	1.91	0.52
3:4:592:GLU:OE1	3:4:643:ARG:NE	2.43	0.52
3:4:732:ARG:NH2	9:6:902:ATP:PB	2.83	0.52
4:5:304:ASP:OD1	4:5:304:ASP:N	2.39	0.52
2:3:187:GLU:OE2	6:7:6:TYR:OH	2.20	0.51
5:6:154:GLY:O	5:6:168:VAL:N	2.43	0.51
2:B:336:ARG:NH2	2:B:480:ASP:OD1	2.41	0.51
6:7:204:ILE:O	6:7:220:LEU:N	2.40	0.51
1:A:481:ILE:HG21	1:A:495:LEU:HB2	1.91	0.51
3:C:263:PHE:HA	3:C:391:THR:HG21	1.91	0.51
5:E:511:ASP:OD1	5:E:513:SER:OG	2.28	0.51
1:A:248:LEU:HA	1:A:255:LEU:HD12	1.92	0.51
3:4:701:ARG:NH2	5:6:557:SER:O	2.43	0.51
1:A:267:VAL:O	1:A:271:TYR:N	2.42	0.51
2:B:513:GLN:N	2:B:513:GLN:OE1	2.42	0.51
1:2:485:ILE:HG23	9:2:1002:ATP:C6	2.46	0.51
2:3:598:ARG:HD2	2:3:613:VAL:HG13	1.93	0.51
5:6:133:LEU:O	5:6:247:THR:OG1	2.25	0.51
5:6:396:GLY:O	5:6:504:ASN:OD1	2.29	0.51
3:C:721:GLY:O	3:C:728:SER:OG	2.18	0.51
4:5:353:ILE:CD1	4:5:390:LEU:HD21	2.42	0.50
1:2:313:THR:O	1:2:573:ALA:HB3	2.10	0.50
6:7:184:CYS:SG	6:7:186:GLN:N	2.80	0.50
9:A:1002:ATP:PG	5:E:529:ARG:NH2	2.65	0.50
4:D:382:ASP:N	4:D:382:ASP:OD1	2.43	0.50
1:2:221:ASP:O	1:2:227:ARG:NH1	2.44	0.50
1:A:329:CYS:SG	1:A:357:SER:OG	2.69	0.50
2:B:130:ILE:HD11	2:B:232:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:352:ILE:O	3:C:372:LEU:N	2.41	0.50
1:2:485:ILE:HG23	9:2:1002:ATP:N6	2.27	0.50
4:5:162:ARG:O	4:5:224:PHE:N	2.44	0.50
6:F:439:GLN:N	6:F:481:ARG:O	2.38	0.50
2:3:221:LEU:HD13	2:3:225:LEU:O	2.12	0.50
3:4:440:LEU:HD11	3:4:693:TYR:HD1	1.77	0.50
3:4:503:GLU:N	3:4:503:GLU:OE1	2.45	0.50
3:C:732:ARG:HH21	9:E:1002:ATP:PG	2.34	0.50
4:D:406:GLY:N	4:D:445:ASP:O	2.44	0.50
6:F:589:ARG:NH1	6:F:601:THR:O	2.44	0.50
1:2:222:MET:O	1:2:226:ASN:N	2.43	0.50
6:7:540:VAL:O	6:7:544:SER:N	2.44	0.50
1:2:421:ASN:O	1:2:436:ALA:N	2.45	0.50
2:3:378:LEU:O	2:3:397:ALA:N	2.45	0.50
3:4:768:ALA:O	3:4:772:SER:OG	2.19	0.50
4:5:575:SER:OG	4:5:632:ALA:O	2.14	0.50
4:D:301:VAL:HG23	4:D:303:THR:HG23	1.94	0.50
2:3:508:ARG:NH2	4:5:571:GLY:O	2.43	0.50
6:7:381:GLY:O	6:7:387:LYS:NZ	2.32	0.50
6:7:343:GLU:O	6:7:536:HIS:NE2	2.45	0.49
6:7:380:MET:HE1	6:7:501:LEU:HD11	1.93	0.49
6:7:589:ARG:NH1	6:7:601:THR:O	2.46	0.49
2:B:336:ARG:NH1	2:B:338:ASP:O	2.45	0.49
9:C:1002:ATP:O1A	6:F:604:ARG:NH2	2.43	0.49
6:F:364:GLN:NE2	6:F:572:MET:SD	2.86	0.49
1:2:297:LEU:HD12	1:2:297:LEU:O	2.13	0.49
3:4:193:TYR:OH	3:4:214:HIS:ND1	2.41	0.49
4:5:128:LEU:HD11	4:5:297:LEU:HB2	1.93	0.49
6:7:602:SER:OG	6:7:603:ALA:N	2.46	0.49
4:5:339:ILE:HD11	4:5:350:LYS:CB	2.42	0.49
1:A:684:VAL:HG11	5:E:591:GLU:CD	2.37	0.49
4:5:82:GLU:N	4:5:82:GLU:OE1	2.41	0.49
1:2:260:ASP:OD1	1:2:283:VAL:N	2.44	0.49
4:5:153:GLY:HA3	4:5:229:LEU:HD11	1.94	0.49
6:7:233:GLN:OE1	6:7:263:ARG:N	2.41	0.49
6:F:206:CYS:SG	6:F:211:CYS:SG	3.10	0.49
4:5:363:LYS:NZ	4:5:621:GLU:OE1	2.28	0.49
6:F:49:TYR:OH	6:F:260:GLU:OE1	2.20	0.49
3:C:233:VAL:O	3:C:236:THR:OG1	2.19	0.48
1:2:482:ALA:HB1	1:2:485:ILE:HB	1.95	0.48
4:5:250:ASP:OD1	4:5:250:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLU:O	1:A:243:VAL:N	2.45	0.48
1:A:319:LEU:N	1:A:373:TYR:O	2.45	0.48
3:4:196:ARG:NH1	3:4:209:ASN:O	2.46	0.48
5:E:419:THR:OG1	5:E:420:SER:N	2.47	0.48
5:E:476:ALA:O	5:E:480:GLN:N	2.43	0.48
5:6:476:ALA:O	5:6:480:GLN:N	2.45	0.48
6:F:516:ASP:OD2	6:F:611:ARG:NH1	2.46	0.48
1:2:776:ALA:O	1:2:780:ILE:N	2.44	0.48
3:C:165:ASN:ND2	3:C:222:LEU:HD22	2.28	0.48
5:E:396:GLY:O	5:E:504:ASN:OD1	2.30	0.48
6:F:40:LEU:HD11	6:F:48:LEU:HD22	1.95	0.48
6:7:211:CYS:SG	6:7:216:SER:OG	2.71	0.48
1:A:527:THR:OG1	1:A:529:LYS:NZ	2.45	0.48
2:B:174:TYR:OH	2:B:186:THR:HG21	2.13	0.48
1:2:590:ASP:O	1:2:597:ARG:NH2	2.44	0.48
1:2:525:PRO:HA	9:2:1002:ATP:O1G	2.13	0.48
6:F:33:TYR:OH	6:F:54:ASP:OD2	2.30	0.48
1:A:485:ILE:HG21	1:A:532:PHE:CZ	2.48	0.48
4:D:410:SER:O	4:D:451:ARG:NH2	2.46	0.48
2:3:18:ASP:OD2	2:3:58:ASN:ND2	2.46	0.47
3:4:667:VAL:HG11	6:7:578:ALA:CB	2.44	0.47
4:5:365:LEU:HD11	4:5:371:ARG:HE	1.78	0.47
6:7:549:SER:OG	6:7:551:PHE:O	2.32	0.47
3:C:667:VAL:HG11	6:F:578:ALA:CB	2.44	0.47
1:2:498:ALA:HB2	1:2:519:VAL:HG21	1.96	0.47
4:5:108:ASP:OD1	4:5:114:ARG:NH2	2.47	0.47
5:6:585:LYS:O	5:6:640:VAL:N	2.45	0.47
1:A:505:LYS:O	1:A:513:VAL:N	2.45	0.47
1:A:580:ASP:O	1:A:623:ARG:N	2.47	0.47
1:2:535:TYR:CE1	1:2:539:VAL:HG21	2.49	0.47
3:C:256:HIS:ND1	3:C:257:GLN:O	2.48	0.47
2:3:499:ASP:OD1	4:5:583:LYS:NZ	2.22	0.47
3:C:329:GLY:O	3:C:332:HIS:NE2	2.47	0.47
5:6:419:THR:OG1	5:6:420:SER:N	2.47	0.47
2:3:515:GLY:O	4:5:571:GLY:N	2.43	0.47
3:4:163:LYS:NZ	3:4:167:GLN:OE1	2.48	0.47
4:D:167:ARG:O	4:D:220:LYS:N	2.47	0.47
1:A:517:ILE:HD11	1:A:773:MET:HA	1.96	0.47
2:B:327:ARG:O	2:B:335:ILE:N	2.48	0.47
4:D:339:ILE:HD11	4:D:350:LYS:HB3	1.97	0.47
5:E:155:THR:OG1	5:E:198:SER:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:582:PHE:O	5:E:633:ARG:NH1	2.47	0.47
3:4:485:PHE:CD2	3:4:747:VAL:HG22	2.50	0.47
6:7:500:SER:N	6:7:503:GLN:OE1	2.45	0.47
5:E:98:VAL:HG22	5:E:104:ILE:HG12	1.96	0.47
5:E:387:ARG:NE	5:E:480:GLN:OE1	2.48	0.47
1:2:364:ASN:ND2	5:6:189:ARG:O	2.49	0.46
1:2:668:ASP:OD1	1:2:668:ASP:N	2.48	0.46
1:2:682:SER:O	1:2:686:HIS:ND1	2.48	0.46
3:4:313:THR:OG1	3:4:314:ARG:N	2.47	0.46
4:5:399:PRO:C	4:5:400:ILE:HD12	2.41	0.46
5:E:58:ARG:NH1	5:E:231:GLU:OE1	2.49	0.46
1:2:182:VAL:HG11	1:2:250:GLU:HB2	1.98	0.46
4:5:34:ARG:HB3	4:5:84:LEU:HD11	1.98	0.46
9:A:1002:ATP:O3G	5:E:529:ARG:NH2	2.49	0.46
4:D:82:GLU:OE1	4:D:82:GLU:N	2.45	0.46
5:E:339:GLU:O	5:E:343:ASP:N	2.46	0.46
6:F:46:VAL:O	6:F:135:GLU:N	2.44	0.46
1:A:498:ALA:HB2	1:A:519:VAL:HG21	1.97	0.46
4:D:108:ASP:OD2	4:D:112:ARG:NH2	2.48	0.46
4:5:145:MET:HE3	4:5:271:ILE:HG12	1.98	0.46
6:7:388:SER:OG	6:7:445:ASP:OD2	2.33	0.46
4:D:302:ASP:OD1	4:D:302:ASP:N	2.48	0.46
5:E:248:LEU:HD11	5:E:296:LEU:HB3	1.97	0.46
1:2:241:GLU:O	1:2:243:VAL:N	2.47	0.46
5:6:29:LEU:HB3	5:6:75:LEU:HD22	1.98	0.46
3:C:718:ARG:NH2	3:C:729:ALA:O	2.48	0.46
4:D:332:TYR:CD1	4:D:626:MET:HE1	2.51	0.46
4:D:644:PHE:O	4:D:648:THR:N	2.48	0.46
4:D:455:ARG:O	4:D:459:HIS:ND1	2.46	0.46
6:F:101:VAL:HG22	6:F:105:HIS:CD2	2.51	0.46
1:2:723:TYR:OH	1:2:780:ILE:O	2.23	0.46
2:3:223:ASP:N	2:3:223:ASP:OD1	2.48	0.46
3:4:485:PHE:O	3:4:695:HIS:NE2	2.47	0.46
5:6:347:TYR:HD1	5:6:634:MET:HE2	1.81	0.46
1:A:603:ALA:O	1:A:607:GLN:N	2.45	0.46
1:A:723:TYR:OH	1:A:780:ILE:O	2.25	0.46
3:4:263:PHE:HA	3:4:391:THR:HG21	1.97	0.46
4:D:399:PRO:HB2	4:D:400:ILE:HD12	1.97	0.46
5:6:117:LEU:HD22	5:6:134:LEU:HD23	1.98	0.45
6:7:380:MET:HE3	6:7:518:LEU:HD11	1.97	0.45
4:D:168:ILE:O	4:D:182:ILE:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:548:ILE:HG23	9:E:1002:ATP:C2	2.51	0.45
5:E:552:ILE:CD1	9:E:1002:ATP:H1'	2.43	0.45
5:E:632:ALA:HB2	5:E:640:VAL:HG22	1.98	0.45
1:2:329:CYS:SG	1:2:357:SER:OG	2.68	0.45
6:7:139:GLN:OE1	6:7:302:ARG:NE	2.49	0.45
5:E:460:ASP:OD1	5:E:461:GLU:N	2.48	0.45
2:3:12:LEU:CD1	2:3:75:ALA:HB2	2.46	0.45
3:4:350:GLN:HB2	3:4:379:VAL:HG13	1.99	0.45
5:6:353:SER:HB3	5:6:566:VAL:HG12	1.99	0.45
5:6:601:LEU:HG	5:6:616:ILE:HD13	1.97	0.45
5:6:616:ILE:HG23	5:6:620:GLN:HG3	1.98	0.45
1:A:536:ILE:CD1	1:A:627:ILE:HG21	2.47	0.45
9:C:1002:ATP:PA	6:F:604:ARG:NH2	2.90	0.45
6:7:261:ASN:ND2	6:7:301:HIS:O	2.49	0.45
4:5:143:ASP:OD1	4:5:144:MET:N	2.50	0.45
4:5:647:SER:O	4:5:651:ALA:N	2.45	0.45
5:6:325:ILE:O	5:6:329:MET:N	2.48	0.45
5:6:585:LYS:O	5:6:640:VAL:HG23	2.17	0.45
4:D:102:ALA:O	4:D:106:VAL:HG22	2.17	0.45
4:D:357:LEU:HD21	4:D:394:VAL:CG2	2.46	0.45
4:D:405:SER:OG	4:D:406:GLY:N	2.50	0.45
1:A:666:THR:O	5:E:602:ARG:NH2	2.49	0.45
1:A:675:LEU:CD2	9:A:1002:ATP:N6	2.80	0.45
4:5:128:LEU:HD12	4:5:128:LEU:O	2.16	0.45
2:B:598:ARG:NH2	6:F:523:ASP:OD1	2.50	0.45
4:D:372:ARG:NH2	4:D:515:ASP:OD1	2.49	0.45
5:E:29:LEU:HB3	5:E:75:LEU:HD22	1.98	0.45
1:2:200:LYS:O	1:2:204:ARG:NH1	2.48	0.45
3:4:718:ARG:O	3:4:722:SER:N	2.50	0.45
3:C:361:MET:HE3	3:C:364:GLY:HA2	1.99	0.45
4:D:335:ILE:O	4:D:339:ILE:HG23	2.17	0.45
3:4:603:ILE:HD13	5:6:223:SER:HB3	1.99	0.45
2:3:642:ALA:O	2:3:646:VAL:HG23	2.17	0.44
3:4:743:ALA:O	3:4:747:VAL:HG23	2.16	0.44
1:A:355:CYS:O	3:C:404:ARG:NH2	2.49	0.44
4:D:340:ALA:O	4:D:350:LYS:NZ	2.33	0.44
3:4:266:LEU:HG	3:4:268:THR:HG23	2.00	0.44
1:2:400:ALA:HA	1:2:403:VAL:HG13	2.00	0.44
3:4:511:ASP:O	3:4:516:LYS:NZ	2.50	0.44
5:6:473:ILE:HG22	5:6:477:MET:HE3	1.98	0.44
2:3:178:ASP:OD1	2:3:179:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:SER:O	2:B:295:ILE:HG22	2.18	0.44
2:B:333:SER:O	2:B:334:HIS:ND1	2.50	0.44
3:C:350:GLN:HB2	3:C:379:VAL:HG13	1.99	0.44
5:6:98:VAL:HG22	5:6:104:ILE:HG12	1.99	0.44
5:6:418:TYR:OH	5:6:460:ASP:OD2	2.33	0.44
1:A:297:LEU:HD13	1:A:418:TYR:CE1	2.52	0.44
6:F:77:PHE:CB	6:F:136:LEU:HD21	2.48	0.44
3:4:327:VAL:HG23	3:4:333:THR:O	2.18	0.44
3:4:466:LEU:HD13	3:4:467:ALA:N	2.33	0.44
1:2:332:CYS:SG	1:2:333:ASN:N	2.91	0.44
4:5:655:GLY:O	4:5:659:GLY:N	2.50	0.44
1:2:527:THR:OG1	1:2:529:LYS:NZ	2.51	0.44
6:7:332:PHE:CZ	6:7:336:LEU:HD11	2.53	0.44
1:A:406:CYS:SG	1:A:444:VAL:HG11	2.58	0.44
1:2:648:ASP:C	1:2:649:LEU:HD22	2.43	0.43
3:C:389:ASN:ND2	3:C:424:THR:OG1	2.51	0.43
5:E:612:SER:OG	5:E:614:TRP:O	2.21	0.43
2:B:148:CYS:O	2:B:152:LYS:N	2.51	0.43
2:B:195:ASP:OD1	2:B:195:ASP:N	2.50	0.43
3:C:485:PHE:CD1	3:C:747:VAL:HG22	2.52	0.43
3:C:639:THR:O	3:C:642:SER:OG	2.30	0.43
1:2:248:LEU:HA	1:2:255:LEU:HD12	1.99	0.43
2:3:25:ASP:OD2	2:3:31:ILE:N	2.51	0.43
2:3:590:ILE:HD11	2:3:621:LEU:HD13	2.00	0.43
10:3:1002:ADP:O3'	4:5:614:GLU:OE2	2.35	0.43
3:4:256:HIS:ND1	3:4:257:GLN:O	2.52	0.43
3:4:329:GLY:O	3:4:332:HIS:NE2	2.51	0.43
6:7:184:CYS:SG	6:7:187:CYS:N	2.91	0.43
1:A:297:LEU:HD11	1:A:394:LYS:HE3	2.00	0.43
6:F:389:GLN:NE2	9:F:1002:ATP:H2'	2.32	0.43
1:2:407:LYS:NZ	1:2:619:SER:O	2.31	0.43
1:2:413:GLU:N	1:2:445:ALA:O	2.45	0.43
1:2:675:LEU:CD2	9:2:1002:ATP:N6	2.82	0.43
3:4:348:ASP:O	3:4:376:ASN:N	2.48	0.43
2:B:638:ASP:N	2:B:641:ASP:OD2	2.50	0.43
1:2:618:THR:OG1	1:2:619:SER:N	2.52	0.43
3:C:327:VAL:O	3:C:337:MET:HE2	2.19	0.43
1:2:557:THR:HG21	1:2:599:SER:HB2	2.00	0.43
1:A:221:ASP:O	1:A:227:ARG:NH1	2.46	0.43
4:D:250:ASP:OD1	4:D:251:ARG:N	2.49	0.43
4:D:353:ILE:O	4:D:357:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:621:GLN:OE1	1:2:623:ARG:NH2	2.52	0.43
2:3:597:LEU:O	2:3:601:ASP:N	2.52	0.43
3:4:518:GLN:NE2	9:4:903:ATP:H3'	2.34	0.43
5:6:632:ALA:HB2	5:6:640:VAL:HG22	2.01	0.43
6:7:361:GLY:N	6:7:373:GLY:O	2.47	0.43
4:D:251:ARG:O	4:D:254:CYS:N	2.46	0.43
4:5:136:SER:OG	4:5:139:SER:OG	2.27	0.43
4:5:378:LEU:HD23	4:5:517:ILE:HD12	2.00	0.43
5:6:155:THR:OG1	5:6:198:SER:OG	2.25	0.43
6:7:344:ILE:O	6:7:351:LYS:NZ	2.36	0.43
3:C:365:GLN:O	6:F:477:THR:N	2.48	0.43
1:2:315:CYS:O	1:2:570:THR:OG1	2.22	0.43
1:2:633:ILE:N	1:2:646:ASN:O	2.50	0.43
4:5:108:ASP:OD2	4:5:112:ARG:NH2	2.52	0.43
5:E:155:THR:N	5:E:198:SER:OG	2.48	0.43
6:F:131:MET:SD	6:F:131:MET:N	2.92	0.43
3:4:280:ASP:OD2	6:7:224:THR:OG1	2.37	0.43
3:4:467:ALA:O	3:4:477:LYS:NZ	2.38	0.43
3:4:566:SER:O	3:4:566:SER:OG	2.34	0.43
4:5:489:ASN:OD1	4:5:489:ASN:N	2.51	0.43
6:7:477:THR:C	6:7:478:LEU:HD12	2.43	0.43
2:3:208:ALA:CB	4:5:474:ILE:HD13	2.49	0.42
5:6:403:SER:HB2	9:6:902:ATP:O1B	2.18	0.42
5:6:430:THR:HG22	5:6:449:LEU:HD23	2.02	0.42
4:D:130:SER:O	4:D:150:LYS:NZ	2.52	0.42
6:F:389:GLN:NE2	9:F:1002:ATP:C2'	2.82	0.42
1:2:501:GLY:O	1:2:776:ALA:HB2	2.18	0.42
4:5:439:GLY:O	4:5:567:ARG:NH2	2.51	0.42
1:A:684:VAL:HG12	5:E:586:ILE:HB	2.01	0.42
2:B:43:ASN:O	2:B:95:TYR:OH	2.15	0.42
1:2:423:ASP:OD1	1:2:424:GLY:N	2.50	0.42
1:2:500:PHE:HB2	1:2:776:ALA:HB1	2.01	0.42
1:2:802:PHE:O	1:2:806:GLN:NE2	2.48	0.42
3:4:358:PRO:HA	3:4:361:MET:HE2	2.00	0.42
3:4:473:HIS:CD2	9:4:903:ATP:N6	2.87	0.42
5:6:421:GLY:N	5:6:460:ASP:O	2.44	0.42
6:F:154:ALA:O	6:F:157:VAL:HG12	2.19	0.42
4:5:185:ARG:N	4:5:189:GLU:OE2	2.52	0.42
1:A:618:THR:OG1	1:A:619:SER:N	2.53	0.42
1:2:589:PHE:CZ	1:2:600:ILE:HD13	2.53	0.42
2:3:650:GLN:O	2:3:654:PHE:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:300:GLN:O	3:4:317:MET:N	2.53	0.42
5:6:594:ILE:CD1	5:6:645:VAL:HG13	2.48	0.42
2:B:352:SER:HB2	10:B:1002:ADP:O2A	2.20	0.42
4:D:421:ASP:O	4:D:425:ARG:N	2.45	0.42
2:3:638:ASP:OD1	2:3:639:LEU:N	2.52	0.42
3:4:732:ARG:HH21	9:6:902:ATP:PG	2.41	0.42
2:3:292:SER:O	2:3:295:ILE:HG22	2.19	0.42
3:C:200:ILE:HG21	3:C:258:ILE:HD12	2.01	0.42
2:3:593:GLU:HG3	2:3:646:VAL:HG21	2.01	0.42
3:4:658:TYR:HH	9:4:903:ATP:N6	2.15	0.42
6:F:332:PHE:CE2	6:F:336:LEU:HD11	2.55	0.42
6:F:361:GLY:N	6:F:373:GLY:O	2.51	0.42
6:F:396:ARG:O	6:F:560:ARG:NH2	2.53	0.42
6:7:591:GLU:O	6:7:595:SER:N	2.45	0.42
3:C:511:ASP:O	3:C:516:LYS:NZ	2.53	0.42
6:F:380:MET:HE3	6:F:518:LEU:HD11	2.01	0.42
1:2:525:PRO:CB	9:2:1002:ATP:PG	3.08	0.42
3:4:574:ASP:OD1	3:4:575:GLU:N	2.53	0.42
3:C:535:GLY:N	3:C:574:ASP:O	2.46	0.42
1:2:410:ASP:N	1:2:410:ASP:OD1	2.53	0.41
1:2:525:PRO:CA	9:2:1002:ATP:O1G	2.67	0.41
4:5:376:ASN:OD1	4:5:484:VAL:N	2.48	0.41
2:B:370:GLY:N	2:B:409:ASP:O	2.53	0.41
2:3:187:GLU:OE2	6:7:72:ARG:NE	2.49	0.41
1:A:633:ILE:N	1:A:646:ASN:O	2.50	0.41
3:C:495:THR:HA	5:E:563:ILE:HG21	2.02	0.41
4:D:155:ILE:O	4:D:260:GLY:N	2.48	0.41
4:D:647:SER:O	4:D:651:ALA:N	2.48	0.41
1:2:177:LEU:HD12	1:2:178:LYS:HG2	2.02	0.41
2:3:459:TYR:HB3	2:3:486:LEU:HD22	2.03	0.41
3:4:282:LEU:HD12	3:4:392:GLY:O	2.20	0.41
2:B:390:GLU:OE2	2:B:391:ARG:N	2.53	0.41
3:C:663:ALA:HB3	6:F:582:THR:HG23	2.03	0.41
5:6:652:LEU:HD12	5:6:653:ASN:N	2.36	0.41
2:B:299:LEU:O	2:B:303:LEU:N	2.53	0.41
3:C:156:ASP:OD1	3:C:156:ASP:N	2.54	0.41
6:F:150:ARG:NH1	6:F:239:GLU:OE2	2.53	0.41
2:B:232:GLY:O	2:B:270:LYS:NZ	2.35	0.41
2:B:439:HIS:O	2:B:439:HIS:ND1	2.54	0.41
5:E:98:VAL:O	5:E:104:ILE:HD13	2.21	0.41
3:4:495:THR:HA	5:6:563:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:32:GLN:NE2	4:5:105:GLU:OE2	2.53	0.41
5:6:117:LEU:HD22	5:6:134:LEU:CD2	2.51	0.41
5:6:371:MET:HA	5:6:390:ILE:HD11	2.02	0.41
5:6:385:SER:OG	5:6:496:ARG:NH2	2.53	0.41
2:B:157:ARG:NH1	2:B:173:VAL:O	2.54	0.41
3:C:200:ILE:HG23	3:C:205:GLU:O	2.21	0.41
3:C:222:LEU:O	3:C:226:LEU:N	2.48	0.41
5:E:145:HIS:ND1	5:E:205:LYS:O	2.53	0.41
5:E:325:ILE:O	5:E:329:MET:N	2.49	0.41
4:5:589:MET:SD	4:5:645:GLN:NE2	2.94	0.41
1:A:769:SER:OG	1:A:798:MET:SD	2.76	0.41
3:C:732:ARG:NH2	9:E:1002:ATP:PG	2.94	0.41
4:D:460:GLU:OE2	4:D:466:THR:OG1	2.30	0.41
2:3:390:GLU:OE2	2:3:391:ARG:N	2.54	0.41
2:3:412:ASP:OD1	2:3:413:LYS:N	2.53	0.41
1:A:536:ILE:HD12	1:A:627:ILE:HG21	2.03	0.41
2:B:378:LEU:HD12	2:B:418:ASP:HB3	2.02	0.41
1:2:536:ILE:HD12	1:2:627:ILE:HG21	2.02	0.41
2:3:49:VAL:O	2:3:103:GLU:N	2.53	0.41
3:4:603:ILE:HG21	5:6:223:SER:HB3	2.02	0.41
4:5:155:ILE:HD12	4:5:257:VAL:HG21	2.03	0.41
4:5:644:PHE:O	4:5:648:THR:N	2.52	0.41
1:A:222:MET:O	1:A:226:ASN:N	2.53	0.41
1:A:414:LEU:HD13	1:A:444:VAL:HG22	2.01	0.41
1:A:423:ASP:OD1	1:A:424:GLY:N	2.53	0.41
2:B:642:ALA:O	2:B:646:VAL:HG23	2.20	0.41
3:C:574:ASP:OD1	3:C:575:GLU:N	2.54	0.41
3:C:646:LEU:HD11	3:C:740:LEU:HD21	2.03	0.41
9:C:1002:ATP:O1A	6:F:604:ARG:NH1	2.53	0.41
9:C:1002:ATP:PA	6:F:604:ARG:HH22	2.43	0.41
4:D:348:ASP:OD1	4:D:348:ASP:N	2.54	0.41
5:E:474:HIS:HB2	5:E:526:ILE:HD11	2.03	0.41
6:F:343:GLU:OE1	6:F:343:GLU:N	2.50	0.41
6:F:540:VAL:O	6:F:544:SER:N	2.48	0.41
6:7:388:SER:HB2	9:7:1002:ATP:O1B	2.21	0.41
4:D:217:ASP:OD1	4:D:217:ASP:N	2.54	0.41
4:D:589:MET:SD	4:D:645:GLN:NE2	2.94	0.41
6:F:380:MET:HE2	6:F:505:ILE:HD13	2.03	0.41
6:F:518:LEU:O	6:F:640:SER:OG	2.37	0.41
6:F:622:VAL:HG12	6:F:624:VAL:H	1.85	0.41
1:2:414:LEU:HD12	1:2:415:THR:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:83:ASP:OD1	4:5:83:ASP:N	2.55	0.40
3:C:325:PRO:CB	3:C:337:MET:HE3	2.52	0.40
4:D:460:GLU:O	4:D:464:GLN:N	2.51	0.40
2:3:439:HIS:ND1	2:3:439:HIS:O	2.54	0.40
6:F:546:GLN:OE1	6:F:546:GLN:N	2.51	0.40
6:F:599:THR:O	6:F:641:LYS:NZ	2.55	0.40
1:2:232:VAL:O	1:2:286:SER:N	2.49	0.40
1:2:314:SER:OG	1:2:571:LEU:O	2.21	0.40
1:2:316:THR:HG22	1:2:375:ARG:O	2.21	0.40
6:7:154:ALA:O	6:7:157:VAL:HG12	2.21	0.40
6:7:622:VAL:HG12	6:7:624:VAL:H	1.86	0.40
2:B:480:ASP:O	2:B:481:LEU:HD22	2.21	0.40
3:C:603:ILE:HG21	5:E:223:SER:HB3	2.03	0.40
4:D:143:ASP:OD1	4:D:144:MET:N	2.55	0.40
2:3:50:ASN:OD1	2:3:53:ASP:N	2.48	0.40
2:3:385:ASP:OD2	2:3:388:THR:HG22	2.22	0.40
3:4:586:VAL:HG13	3:4:596:LEU:HD13	2.04	0.40
5:6:346:LEU:HD12	5:6:567:TYR:CZ	2.56	0.40
5:6:463:ASP:OD1	5:6:464:LYS:N	2.54	0.40
1:A:285:ILE:N	1:A:442:ASN:OD1	2.53	0.40
5:E:430:THR:OG1	5:E:431:ALA:N	2.54	0.40
3:4:484:LEU:HD23	3:4:570:ILE:HD12	2.03	0.40
3:4:590:VAL:O	3:4:594:GLN:N	2.50	0.40
3:4:663:ALA:HB3	6:7:582:THR:HG23	2.04	0.40
4:5:253:LEU:HD11	4:5:299:ILE:CG1	2.50	0.40
4:5:321:GLU:OE1	4:5:324:ARG:NE	2.47	0.40
6:7:439:GLN:N	6:7:481:ARG:O	2.51	0.40
2:B:371:ARG:NH2	2:B:410:GLU:OE1	2.55	0.40
4:D:69:TRP:O	4:D:70:ILE:HG23	2.21	0.40
6:F:40:LEU:CD1	6:F:48:LEU:HD22	2.51	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	584/904 (65%)	545 (93%)	39 (7%)	0	100	100
1	A	584/904 (65%)	548 (94%)	36 (6%)	0	100	100
2	3	584/810 (72%)	547 (94%)	37 (6%)	0	100	100
2	B	584/810 (72%)	540 (92%)	44 (8%)	0	100	100
3	4	568/866 (66%)	543 (96%)	25 (4%)	0	100	100
3	C	568/866 (66%)	537 (94%)	31 (6%)	0	100	100
4	5	577/734 (79%)	549 (95%)	28 (5%)	0	100	100
4	D	577/734 (79%)	559 (97%)	18 (3%)	0	100	100
5	6	583/821 (71%)	559 (96%)	24 (4%)	0	100	100
5	E	583/821 (71%)	566 (97%)	17 (3%)	0	100	100
6	7	593/719 (82%)	566 (95%)	27 (5%)	0	100	100
6	F	593/719 (82%)	567 (96%)	26 (4%)	0	100	100
All	All	6978/9708 (72%)	6626 (95%)	352 (5%)	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	524/781 (67%)	523 (100%)	1 (0%)	87	87
1	A	524/781 (67%)	522 (100%)	2 (0%)	84	83
2	3	513/708 (72%)	511 (100%)	2 (0%)	84	83
2	B	513/708 (72%)	508 (99%)	5 (1%)	68	74
3	4	515/755 (68%)	512 (99%)	3 (1%)	78	79
3	C	515/755 (68%)	512 (99%)	3 (1%)	78	79
4	5	512/625 (82%)	510 (100%)	2 (0%)	84	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	512/625 (82%)	509 (99%)	3 (1%)	78	79
5	6	530/724 (73%)	527 (99%)	3 (1%)	78	79
5	E	530/724 (73%)	528 (100%)	2 (0%)	84	83
6	7	530/619 (86%)	526 (99%)	4 (1%)	73	76
6	F	530/619 (86%)	528 (100%)	2 (0%)	84	83
All	All	6248/8424 (74%)	6216 (100%)	32 (0%)	78	81

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	403	VAL
2	3	196	HIS
2	3	408	ILE
3	4	275	ASN
3	4	278	ASP
3	4	567	ASP
4	5	265	ILE
4	5	463	GLU
5	6	41	ASP
5	6	400	THR
5	6	419	THR
6	7	184	CYS
6	7	296	THR
6	7	333	TYR
6	7	502	GLU
1	A	398	LEU
1	A	468	SER
2	B	196	HIS
2	B	218	ASP
2	B	366	ILE
2	B	409	ASP
2	B	448	VAL
3	C	348	ASP
3	C	595	THR
3	C	633	ASN
4	D	265	ILE
4	D	302	ASP
4	D	382	ASP
5	E	400	THR
5	E	419	THR

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Mol	Chain	Res	Type
6	F	197	SER
6	F	296	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	443	HIS
1	2	506	ASN
2	3	236	GLN
3	4	594	GLN
4	5	177	ASN
5	6	454	ASN
6	7	439	GLN
1	A	374	GLN
2	B	182	ASN
2	B	468	ASN
2	B	493	GLN
3	C	167	GLN
3	C	225	GLN
3	C	281	GLN
3	C	625	ASN
3	C	633	ASN
4	D	122	GLN
4	D	464	GLN
4	D	713	GLN
5	E	454	ASN
5	E	504	ASN
5	E	635	HIS
6	F	18	GLN
6	F	389	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 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	$\# Z > 2$
10	ADP	3	1002	8	28,29,29	1.36	5 (17%)	43,45,45	1.89	10 (23%)
9	ATP	7	1002	8	32,33,33	0.58	1 (3%)	48,52,52	0.74	1 (2%)
9	ATP	F	1002	8	32,33,33	0.59	1 (3%)	48,52,52	0.75	1 (2%)
10	ADP	B	1002	8	28,29,29	1.36	5 (17%)	43,45,45	1.88	10 (23%)
9	ATP	2	1002	8	32,33,33	0.45	0	48,52,52	0.78	2 (4%)
9	ATP	C	1002	8	32,33,33	0.32	0	48,52,52	0.69	0
9	ATP	6	902	8	32,33,33	0.49	0	48,52,52	0.76	1 (2%)
9	ATP	4	903	8	32,33,33	0.32	0	48,52,52	0.69	0
9	ATP	A	1002	8	32,33,33	0.44	0	48,52,52	0.78	2 (4%)
9	ATP	E	1002	8	32,33,33	0.47	0	48,52,52	0.76	0

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
10	ADP	3	1002	8	-	3/16/32/32	0/3/3/3
9	ATP	7	1002	8	-	5/22/38/38	0/3/3/3
9	ATP	F	1002	8	-	5/22/38/38	0/3/3/3
10	ADP	B	1002	8	-	3/16/32/32	0/3/3/3
9	ATP	2	1002	8	-	4/22/38/38	0/3/3/3
9	ATP	C	1002	8	-	3/22/38/38	0/3/3/3
9	ATP	6	902	8	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ATP	4	903	8	-	3/22/38/38	0/3/3/3
9	ATP	A	1002	8	-	4/22/38/38	0/3/3/3
9	ATP	E	1002	8	-	4/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	1002	ADP	C5-C4	4.29	1.46	1.39
10	B	1002	ADP	C5-C4	4.26	1.46	1.39
9	F	1002	ATP	PB-O3B	-2.61	1.56	1.59
9	7	1002	ATP	PB-O3B	-2.56	1.56	1.59
10	3	1002	ADP	C5-N7	-2.54	1.34	1.39
10	B	1002	ADP	C5-N7	-2.51	1.34	1.39
10	3	1002	ADP	C5-C6	2.49	1.47	1.41
10	B	1002	ADP	C5-C6	2.48	1.47	1.41
10	B	1002	ADP	C8-N7	2.25	1.36	1.31
10	3	1002	ADP	C8-N7	2.23	1.36	1.31
10	3	1002	ADP	C4-N9	-2.07	1.33	1.37
10	B	1002	ADP	C4-N9	-2.06	1.33	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1002	ADP	C5-C4-N3	-5.94	118.53	126.72
10	3	1002	ADP	C5-C4-N3	-5.94	118.54	126.72
10	3	1002	ADP	N3-C4-N9	4.67	135.11	127.17
10	B	1002	ADP	N3-C4-N9	4.65	135.07	127.17
10	3	1002	ADP	C2-N3-C4	3.91	121.38	111.83
10	B	1002	ADP	C2-N3-C4	3.90	121.34	111.83
10	3	1002	ADP	N3-C2-N1	-3.69	123.00	128.58
10	B	1002	ADP	N3-C2-N1	-3.67	123.03	128.58
10	3	1002	ADP	C4-C5-N7	-3.55	106.53	110.58
10	B	1002	ADP	C4-C5-N7	-3.54	106.53	110.58
10	3	1002	ADP	C4-N9-C8	2.85	108.73	105.74
10	B	1002	ADP	C4-N9-C8	2.81	108.69	105.74
10	3	1002	ADP	C5-N7-C8	2.67	107.65	103.45
10	B	1002	ADP	C5-N7-C8	2.65	107.61	103.45
9	7	1002	ATP	C4'-O4'-C1'	-2.52	103.90	109.47
9	F	1002	ATP	C4'-O4'-C1'	-2.52	103.90	109.47
9	A	1002	ATP	C4'-O4'-C1'	-2.44	104.07	109.47
9	2	1002	ATP	C4'-O4'-C1'	-2.44	104.09	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	1002	ADP	N9-C8-N7	-2.25	110.75	113.94
10	B	1002	ADP	N9-C8-N7	-2.23	110.77	113.94
10	3	1002	ADP	C6-C5-N7	2.11	136.16	132.09
10	B	1002	ADP	C6-C5-N7	2.10	136.13	132.09
9	2	1002	ATP	O3'-C3'-C4'	-2.05	105.19	111.08
10	B	1002	ADP	C3'-C2'-C1'	2.04	105.33	101.46
10	3	1002	ADP	C3'-C2'-C1'	2.03	105.31	101.46
9	A	1002	ATP	O3'-C3'-C4'	-2.02	105.27	111.08
9	6	902	ATP	O2'-C2'-C3'	-2.00	105.41	111.82

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	2	1002	ATP	C5'-O5'-PA-O1A
9	2	1002	ATP	C5'-O5'-PA-O3A
9	4	903	ATP	C5'-O5'-PA-O2A
9	6	902	ATP	PB-O3B-PG-O2G
9	6	902	ATP	C5'-O5'-PA-O2A
9	6	902	ATP	C5'-O5'-PA-O3A
9	7	1002	ATP	C5'-O5'-PA-O2A
9	7	1002	ATP	C5'-O5'-PA-O3A
9	A	1002	ATP	C5'-O5'-PA-O1A
9	A	1002	ATP	C5'-O5'-PA-O3A
9	C	1002	ATP	C5'-O5'-PA-O2A
9	E	1002	ATP	PB-O3B-PG-O2G
9	E	1002	ATP	C5'-O5'-PA-O2A
9	E	1002	ATP	C5'-O5'-PA-O3A
9	F	1002	ATP	C5'-O5'-PA-O2A
9	F	1002	ATP	C5'-O5'-PA-O3A
9	7	1002	ATP	O4'-C4'-C5'-O5'
9	F	1002	ATP	O4'-C4'-C5'-O5'
9	7	1002	ATP	C4'-C5'-O5'-PA
9	F	1002	ATP	C4'-C5'-O5'-PA
10	3	1002	ADP	PA-O3A-PB-O1B
10	B	1002	ADP	PA-O3A-PB-O1B
9	7	1002	ATP	C3'-C4'-C5'-O5'
9	F	1002	ATP	C3'-C4'-C5'-O5'
9	2	1002	ATP	PA-O3A-PB-O1B
9	A	1002	ATP	PA-O3A-PB-O1B
9	2	1002	ATP	C5'-O5'-PA-O2A
9	4	903	ATP	C5'-O5'-PA-O1A

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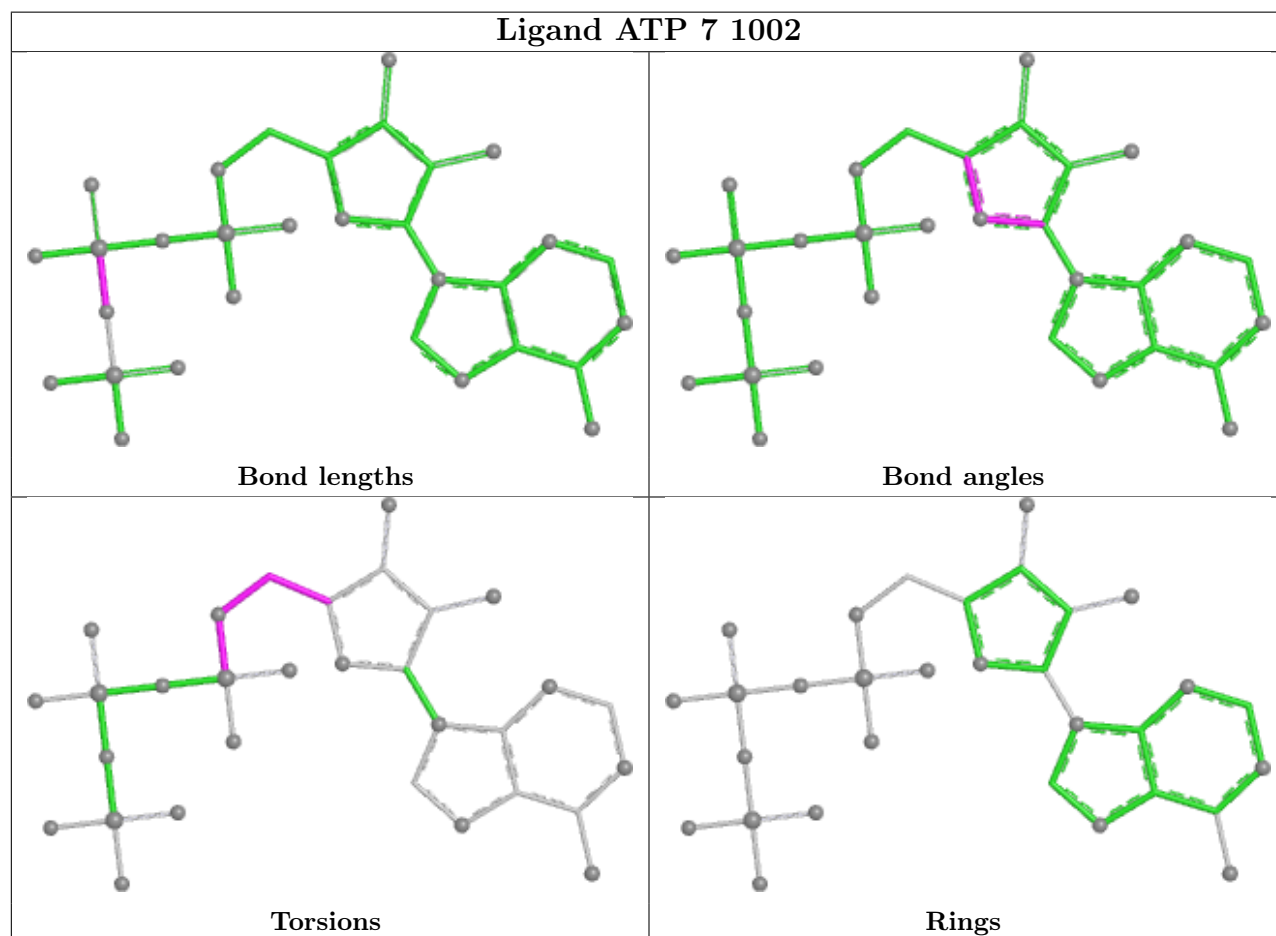
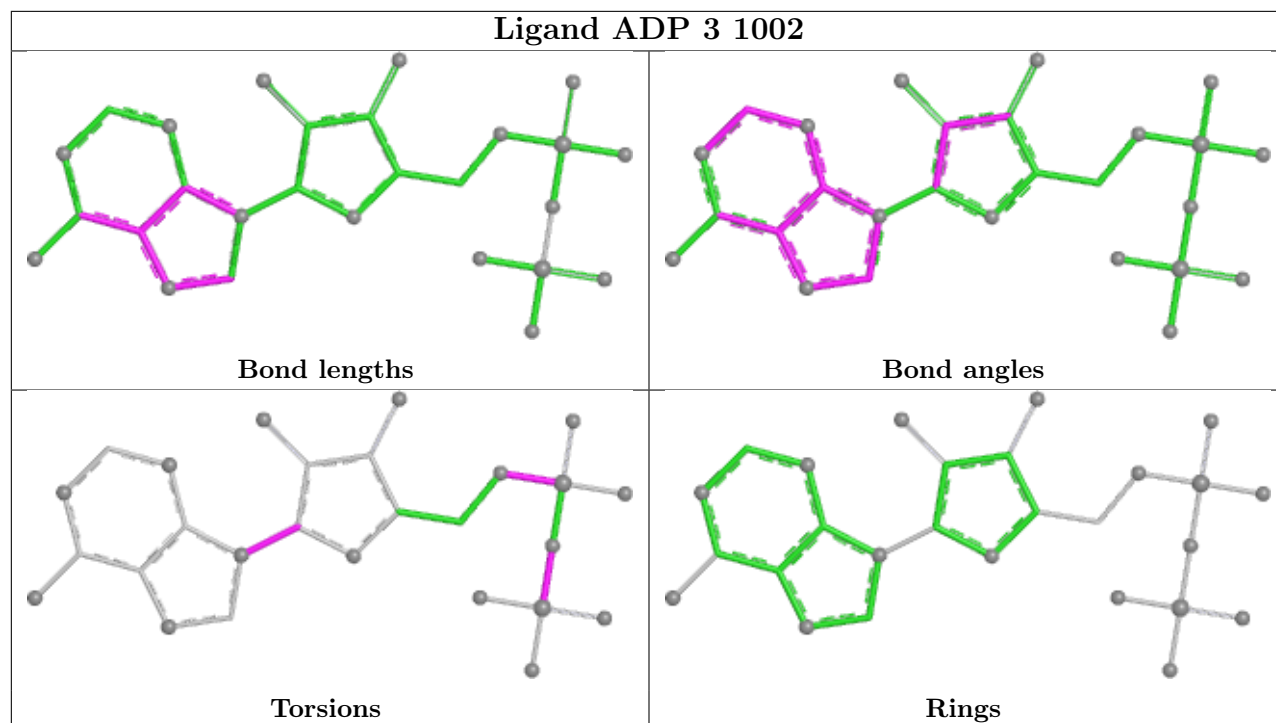
Mol	Chain	Res	Type	Atoms
9	4	903	ATP	C5'-O5'-PA-O3A
9	A	1002	ATP	C5'-O5'-PA-O2A
9	C	1002	ATP	C5'-O5'-PA-O1A
9	C	1002	ATP	C5'-O5'-PA-O3A
10	3	1002	ADP	C5'-O5'-PA-O1A
10	B	1002	ADP	C5'-O5'-PA-O1A
9	6	902	ATP	PB-O3B-PG-O1G
9	E	1002	ATP	PB-O3B-PG-O1G
10	3	1002	ADP	C2'-C1'-N9-C8
10	B	1002	ADP	C2'-C1'-N9-C8

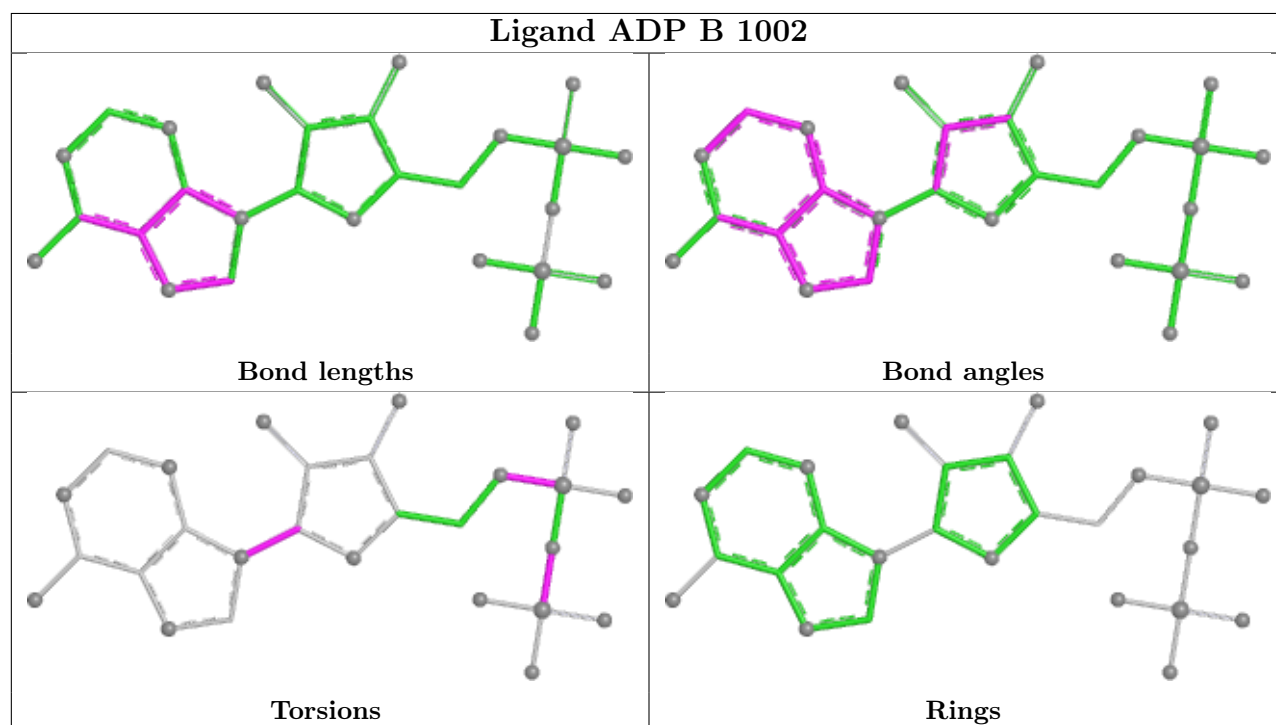
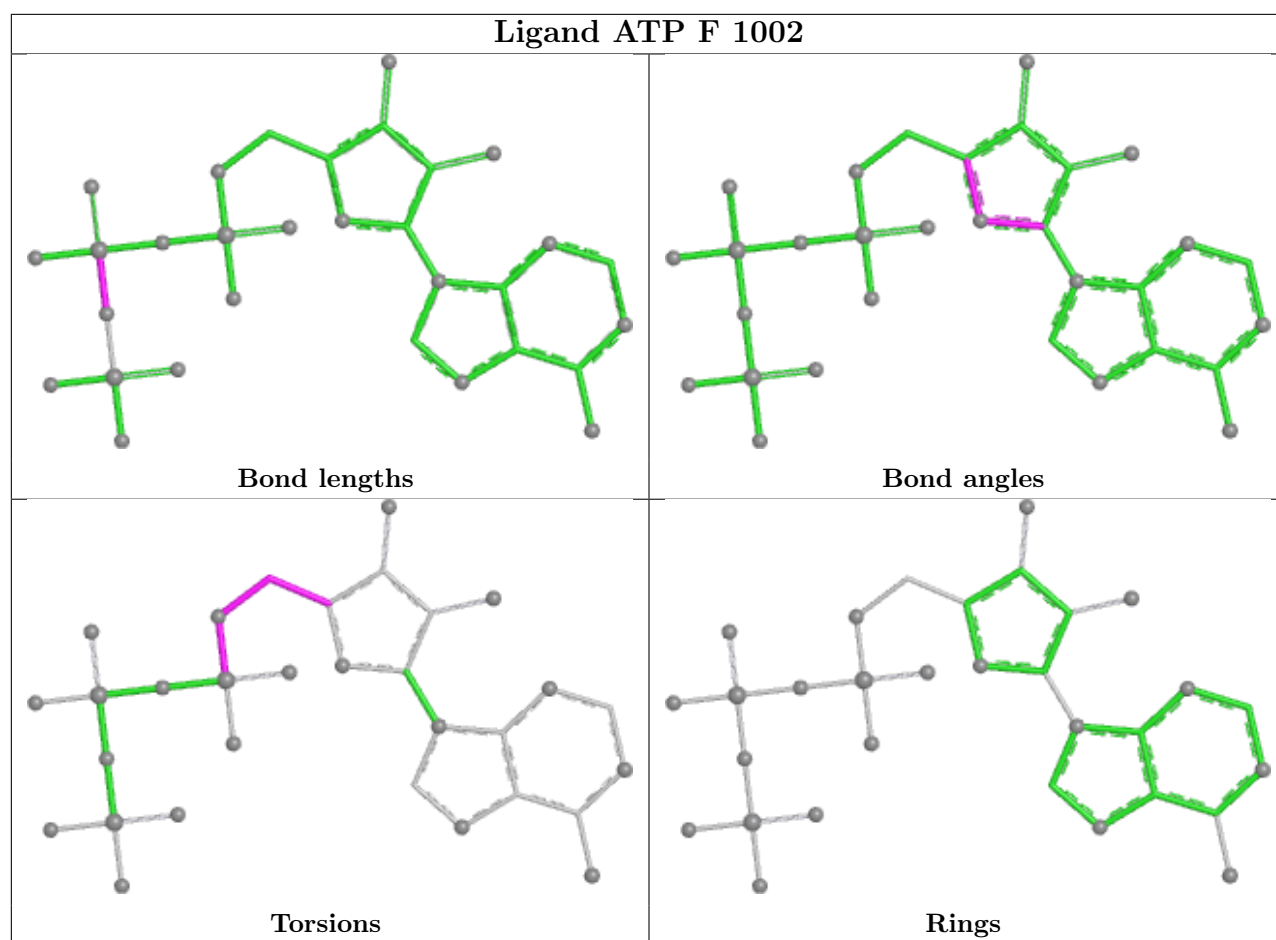
There are no ring outliers.

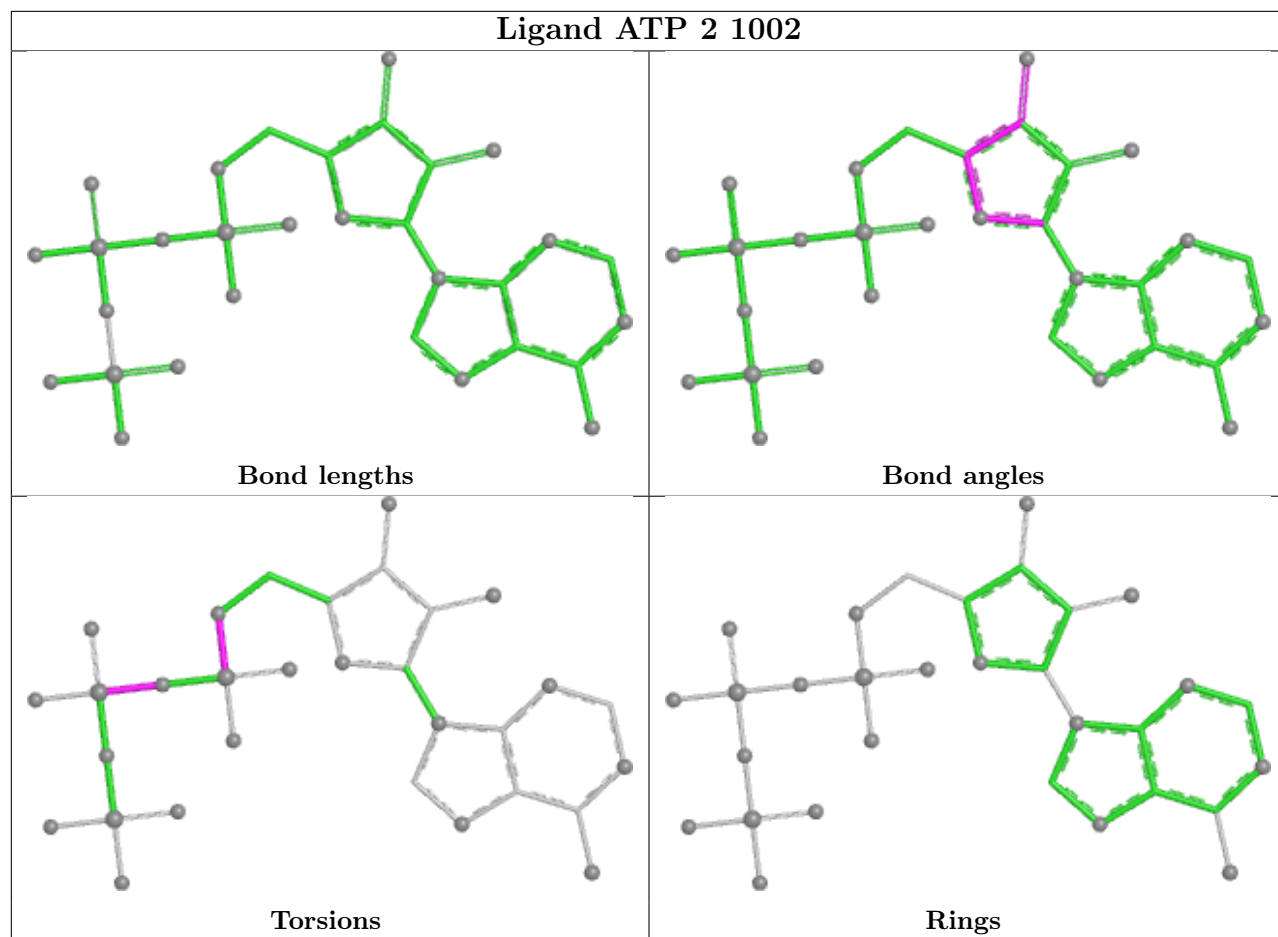
10 monomers are involved in 67 short contacts:

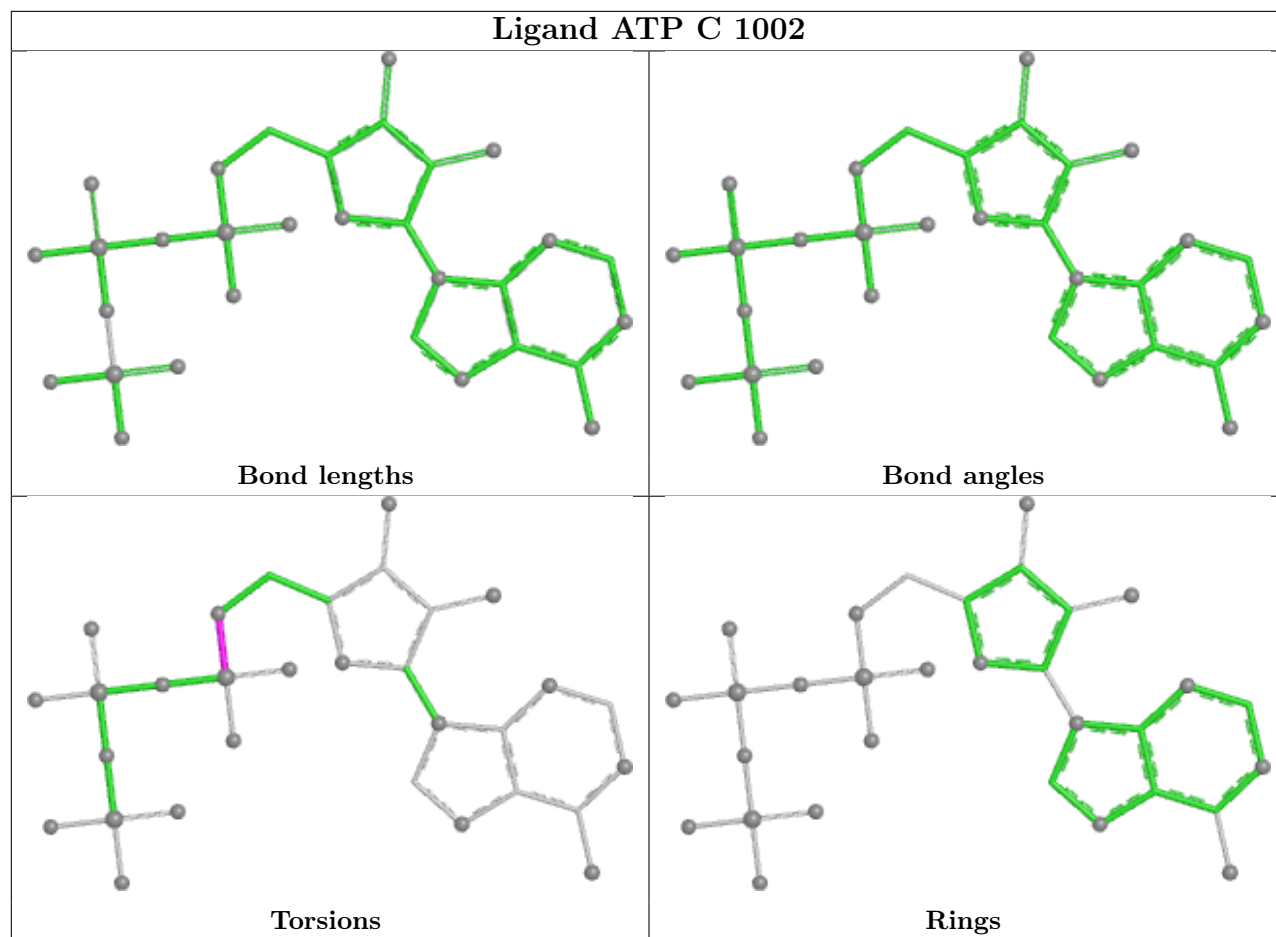
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	3	1002	ADP	5	0
9	7	1002	ATP	2	0
9	F	1002	ATP	7	0
10	B	1002	ADP	5	0
9	2	1002	ATP	14	0
9	C	1002	ATP	6	0
9	6	902	ATP	5	0
9	4	903	ATP	7	0
9	A	1002	ATP	8	0
9	E	1002	ATP	8	0

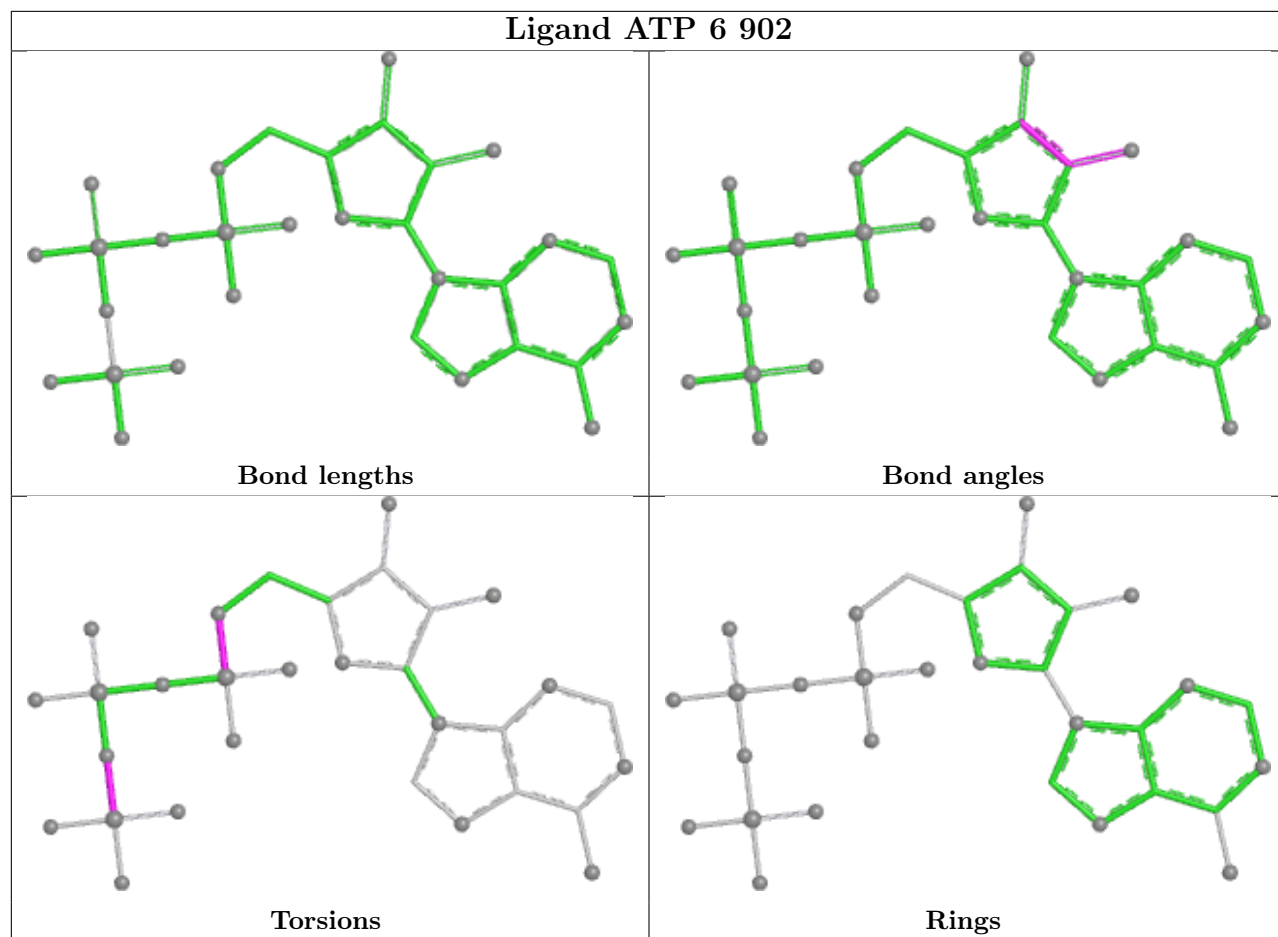
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

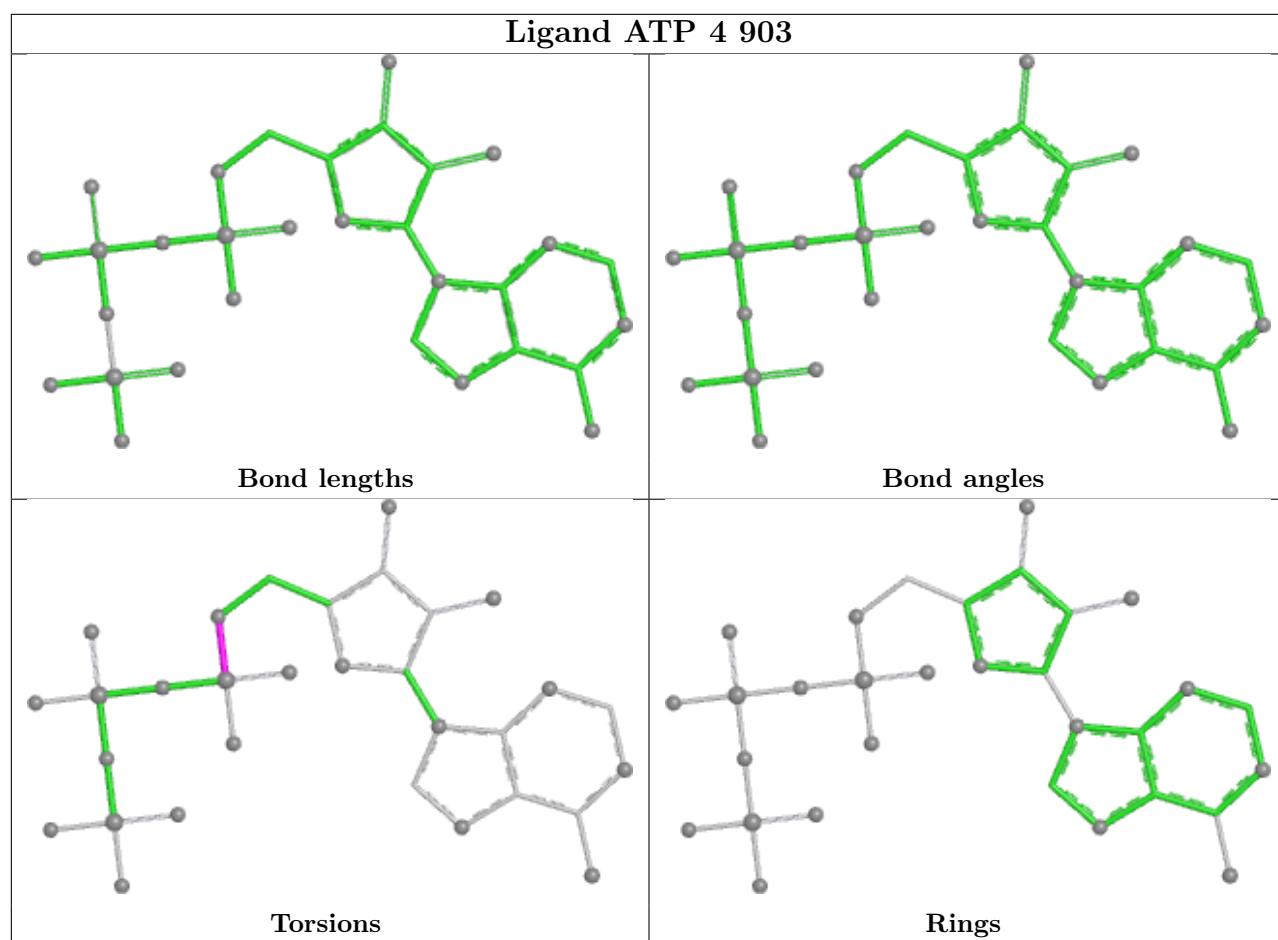


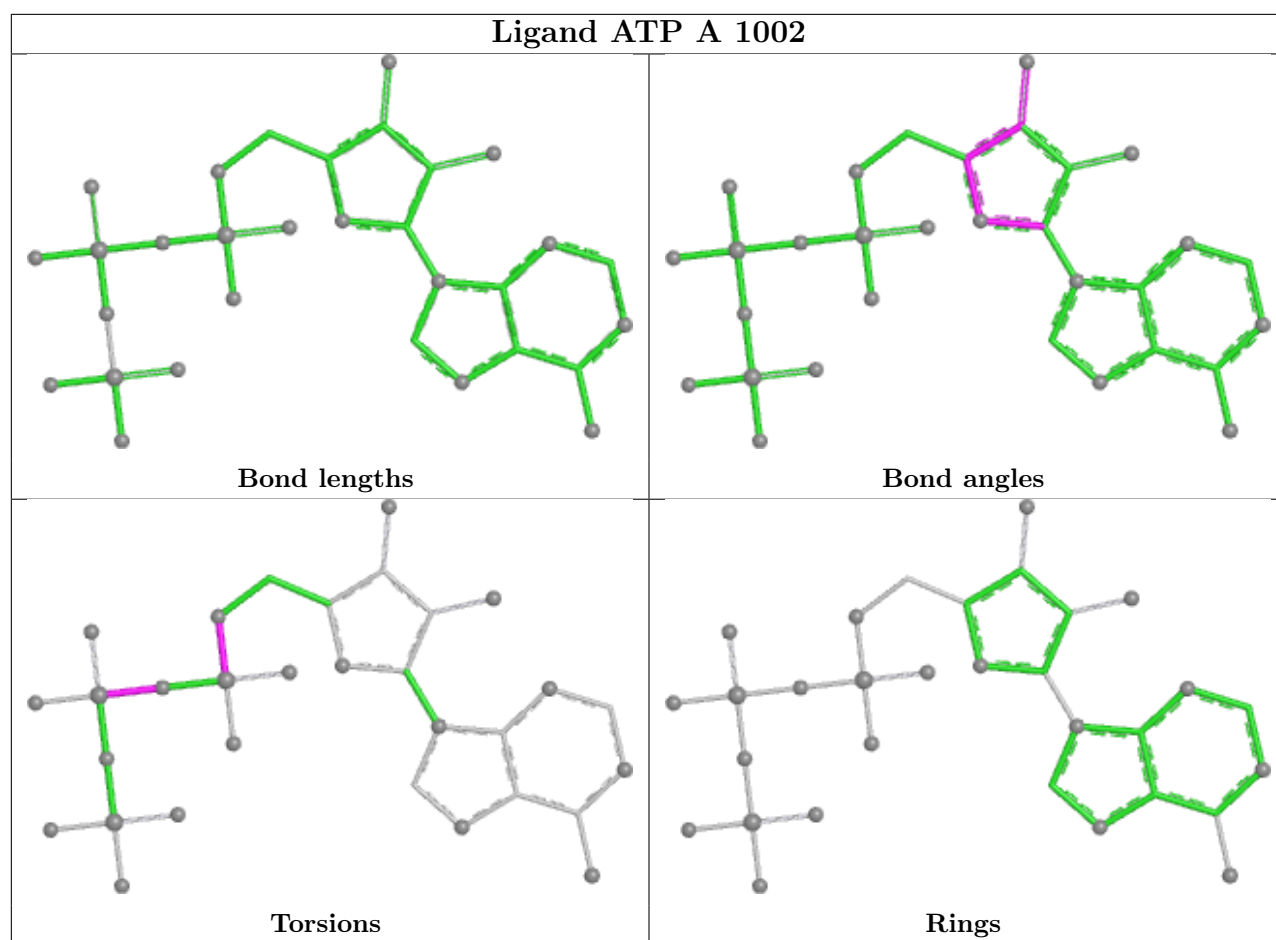


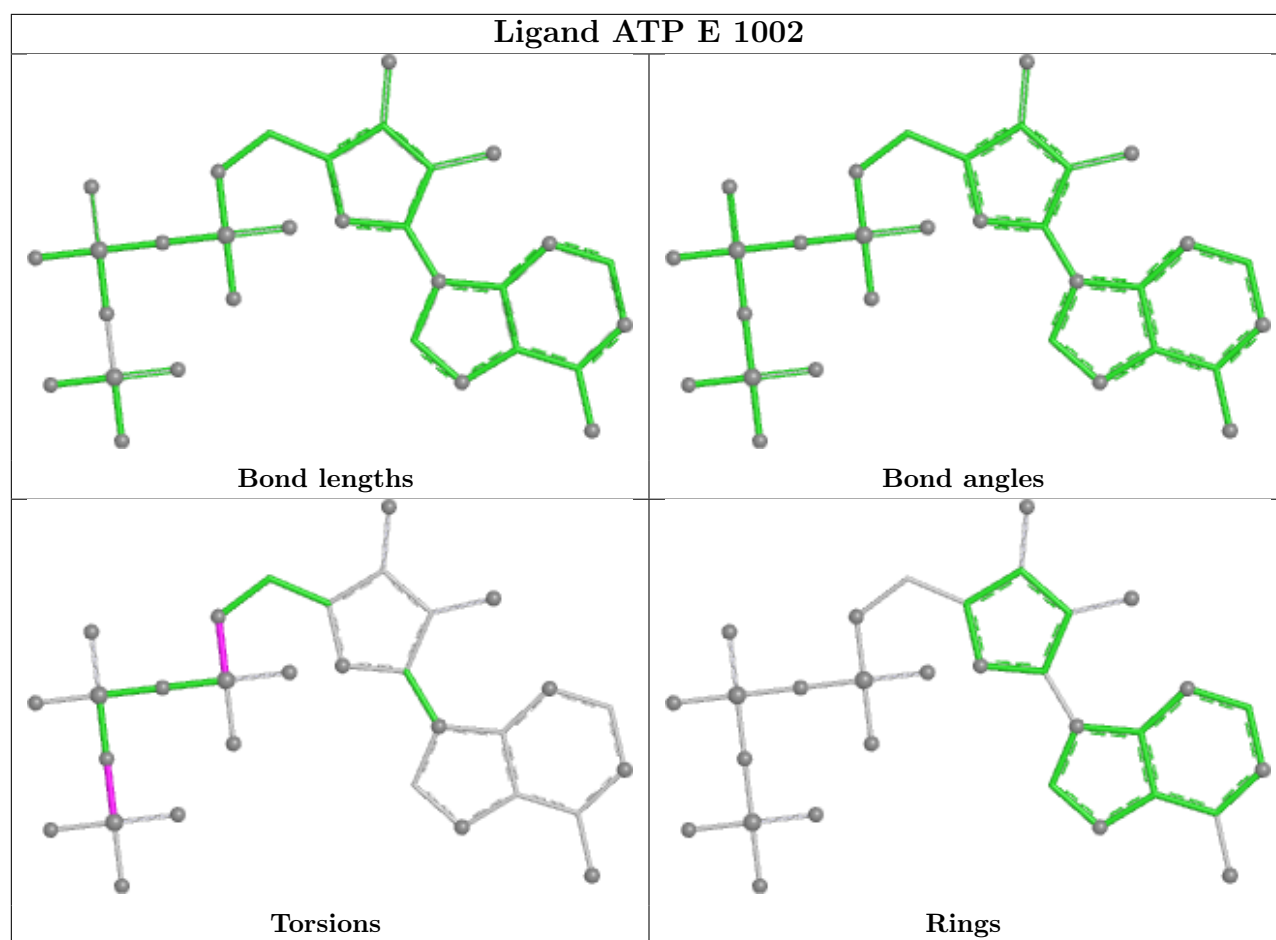












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

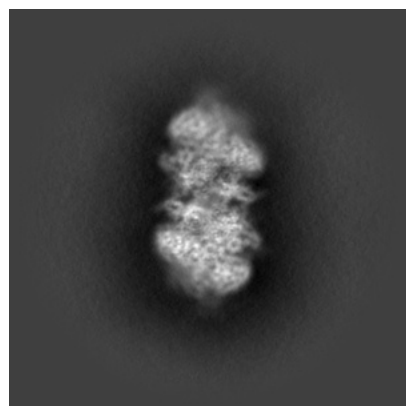
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43709. These allow visual inspection of the internal detail of the map and identification of artifacts.

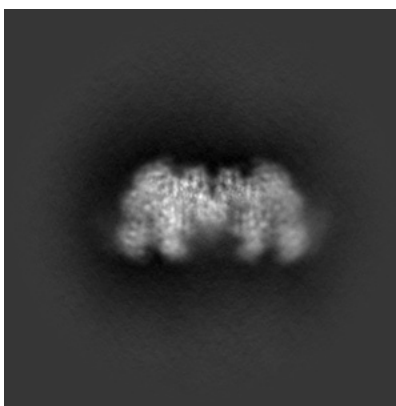
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

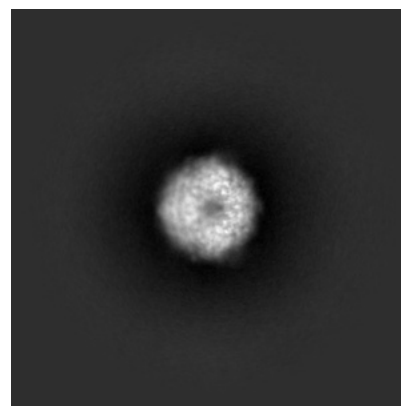
6.1.1 Primary map



X

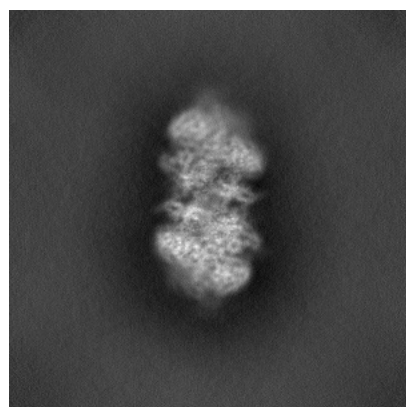


Y

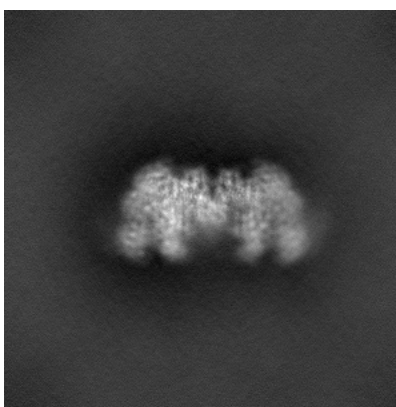


Z

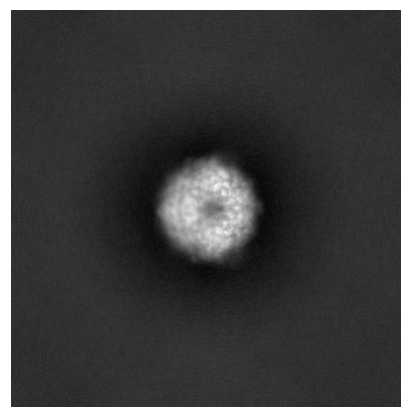
6.1.2 Raw map



X



Y

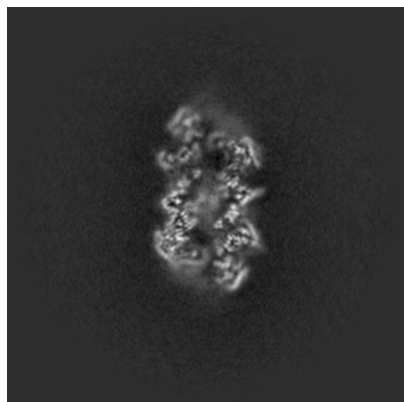


Z

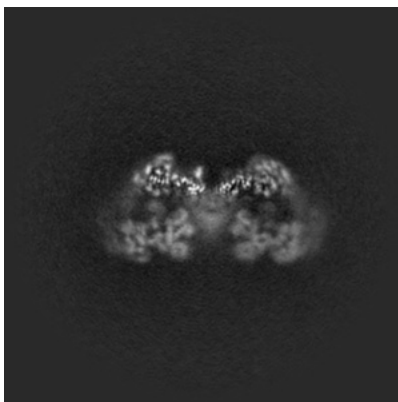
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

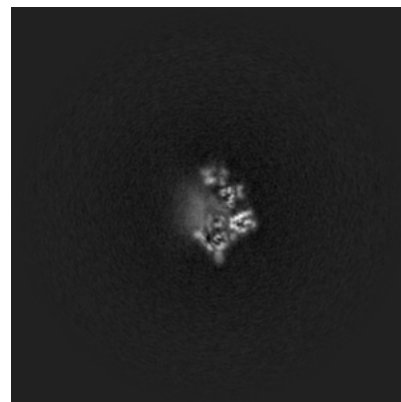
6.2.1 Primary map



X Index: 300

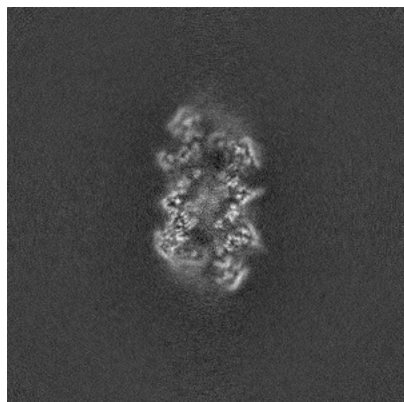


Y Index: 300

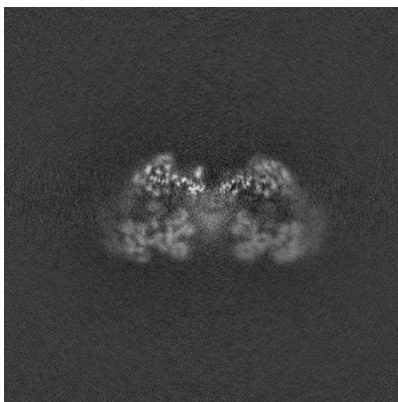


Z Index: 300

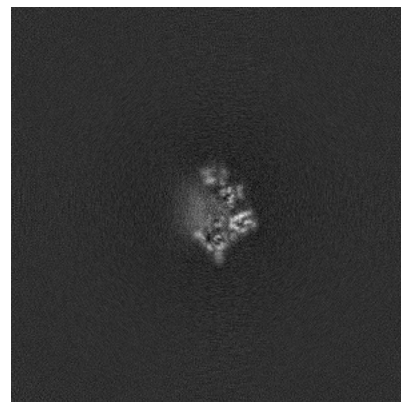
6.2.2 Raw map



X Index: 300



Y Index: 300

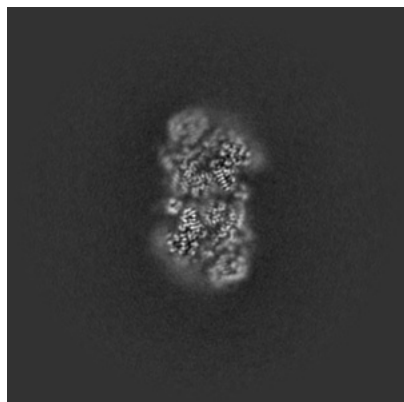


Z Index: 300

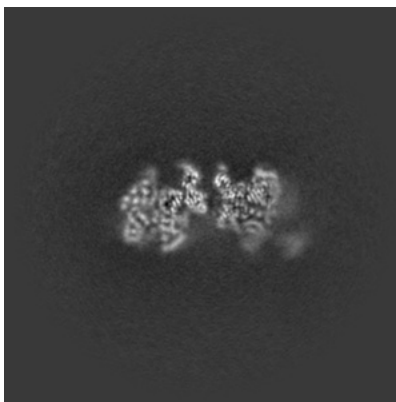
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

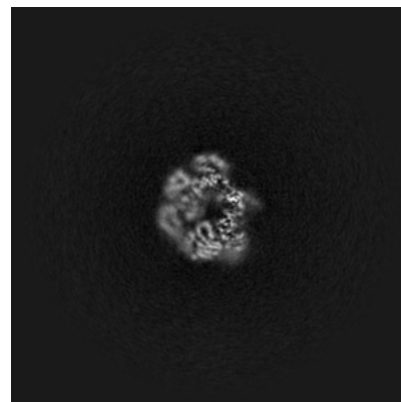
6.3.1 Primary map



X Index: 321

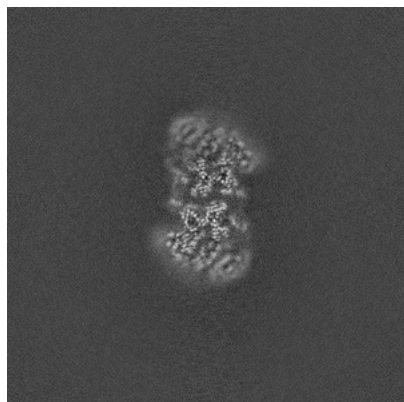


Y Index: 338

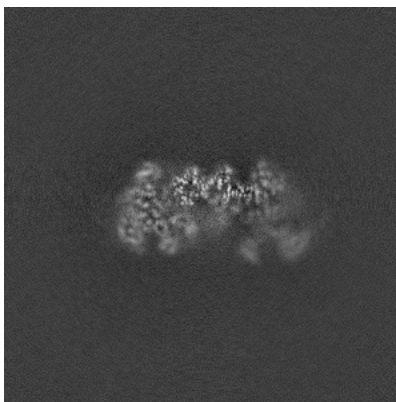


Z Index: 254

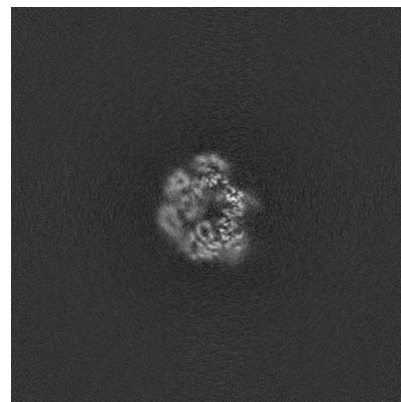
6.3.2 Raw map



X Index: 328



Y Index: 323

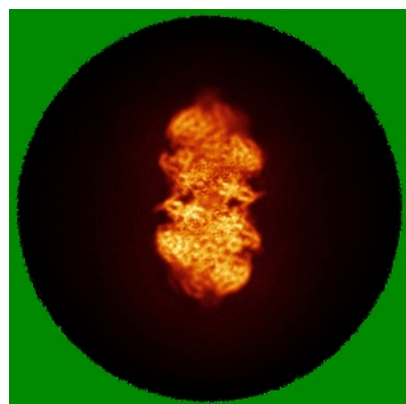


Z Index: 255

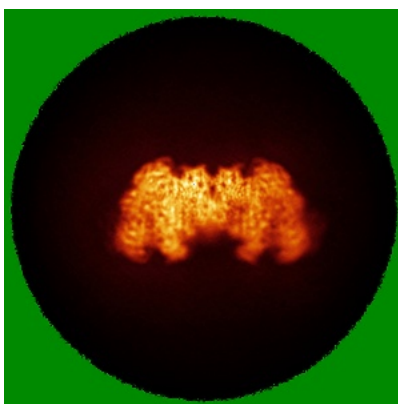
The images above show the largest variance slices of the map in three orthogonal directions.

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

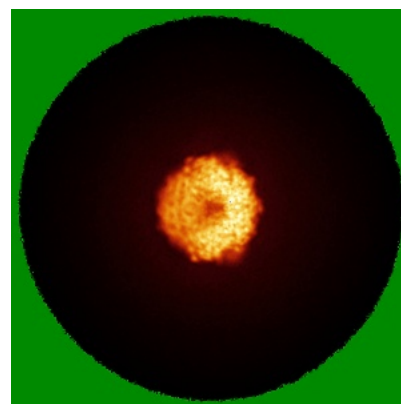
6.4.1 Primary map



X

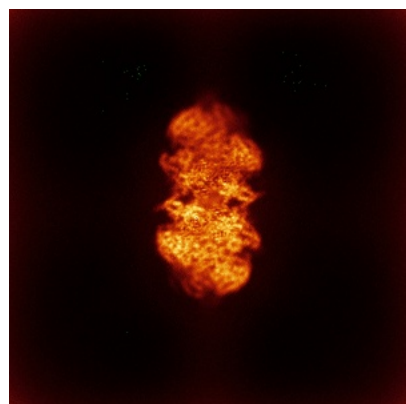


Y

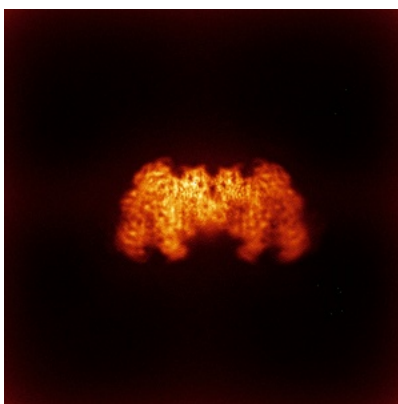


Z

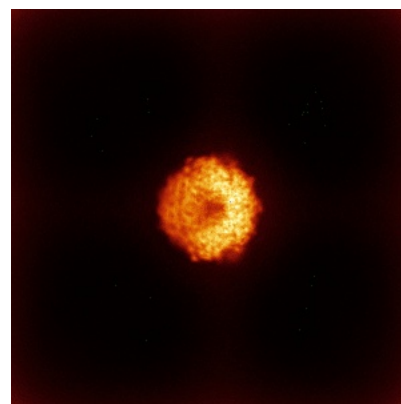
6.4.2 Raw map



X



Y

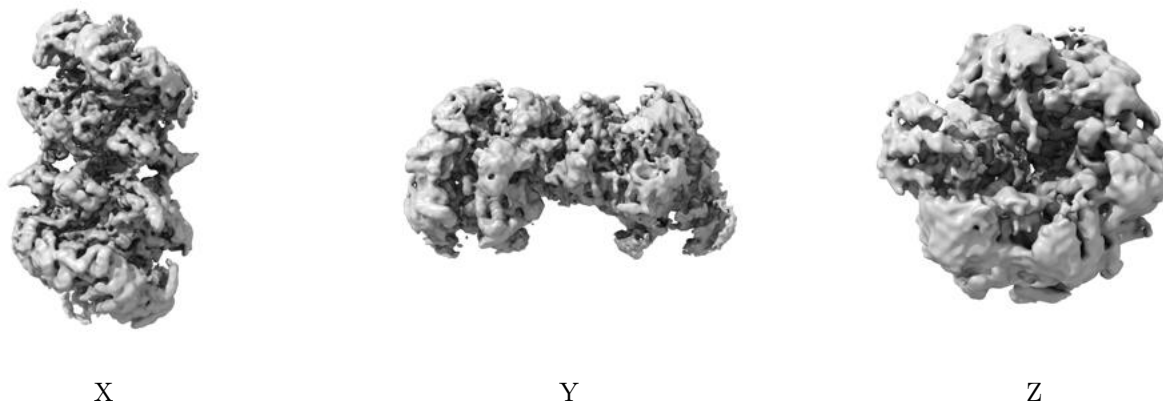


Z

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.

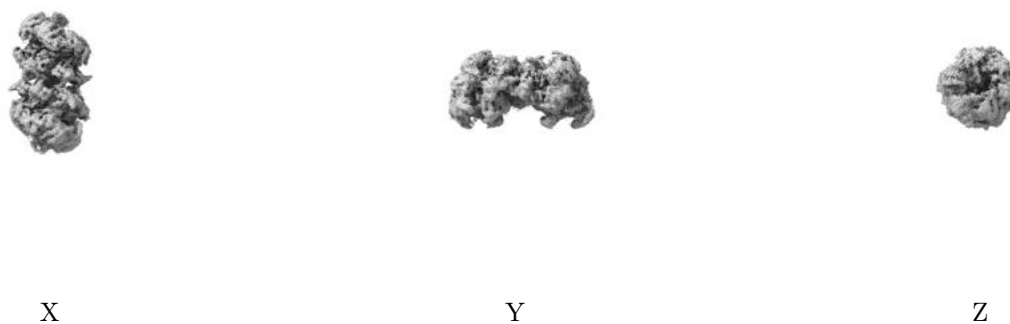
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

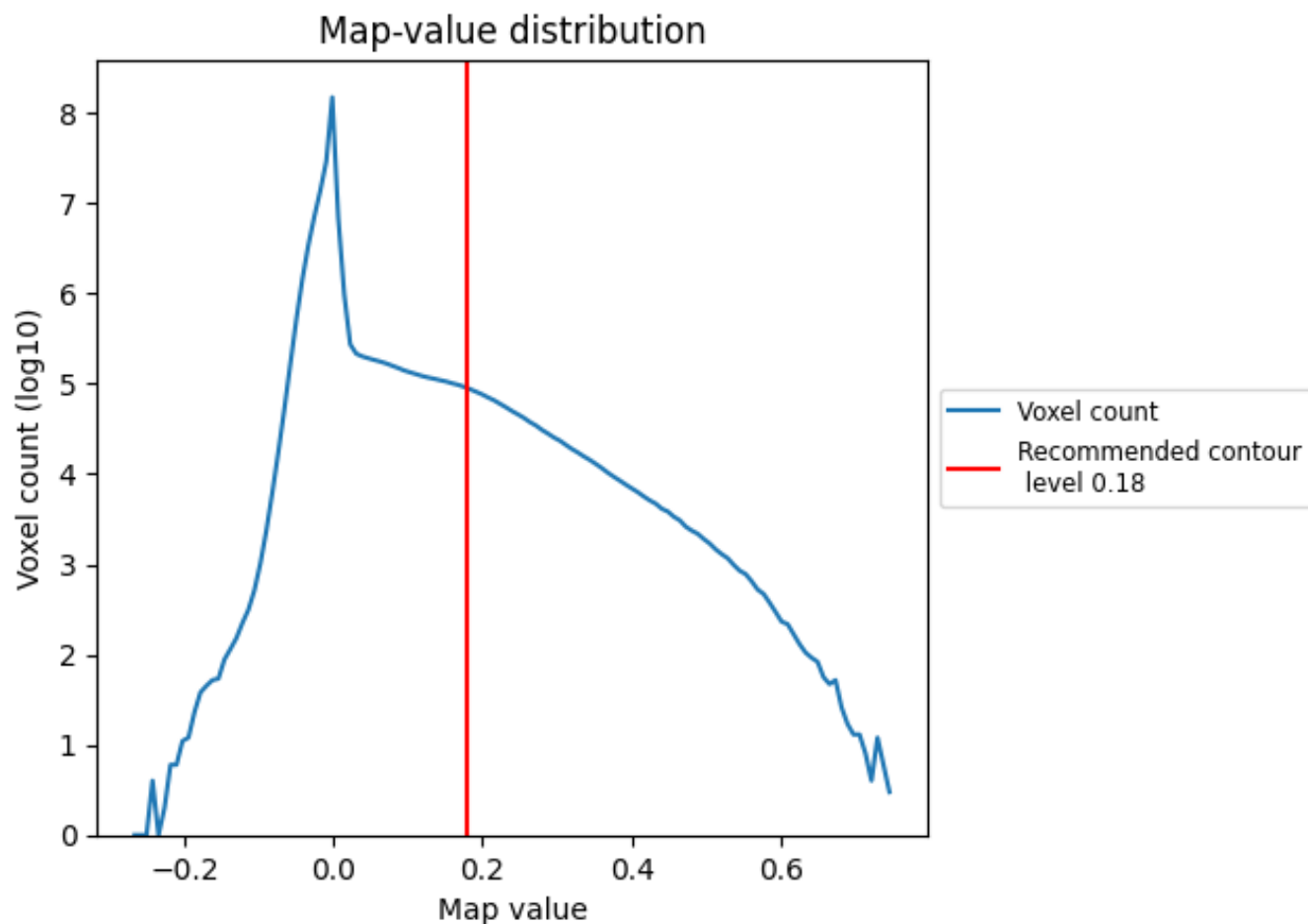
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

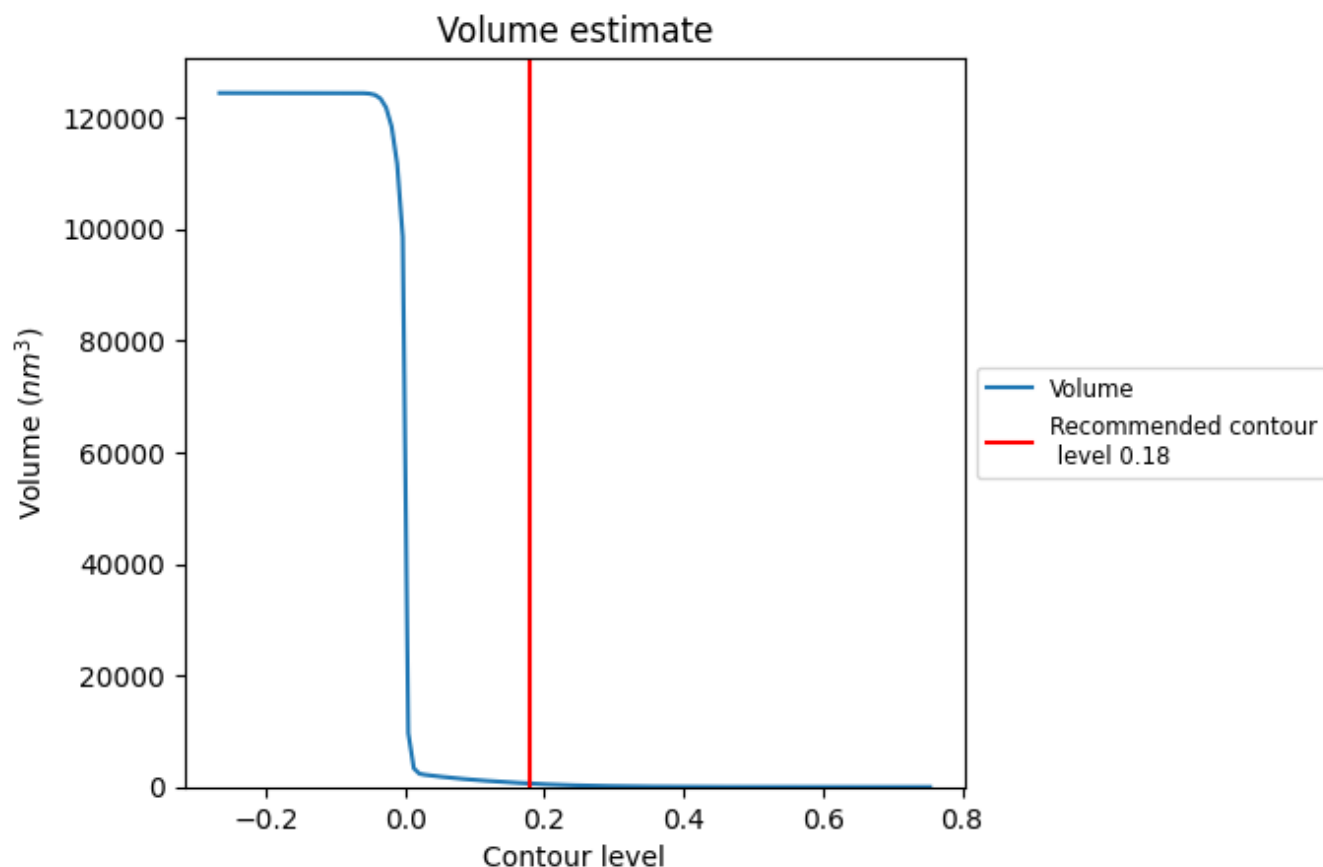
This section contains the results of statistical analysis of the map.

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.

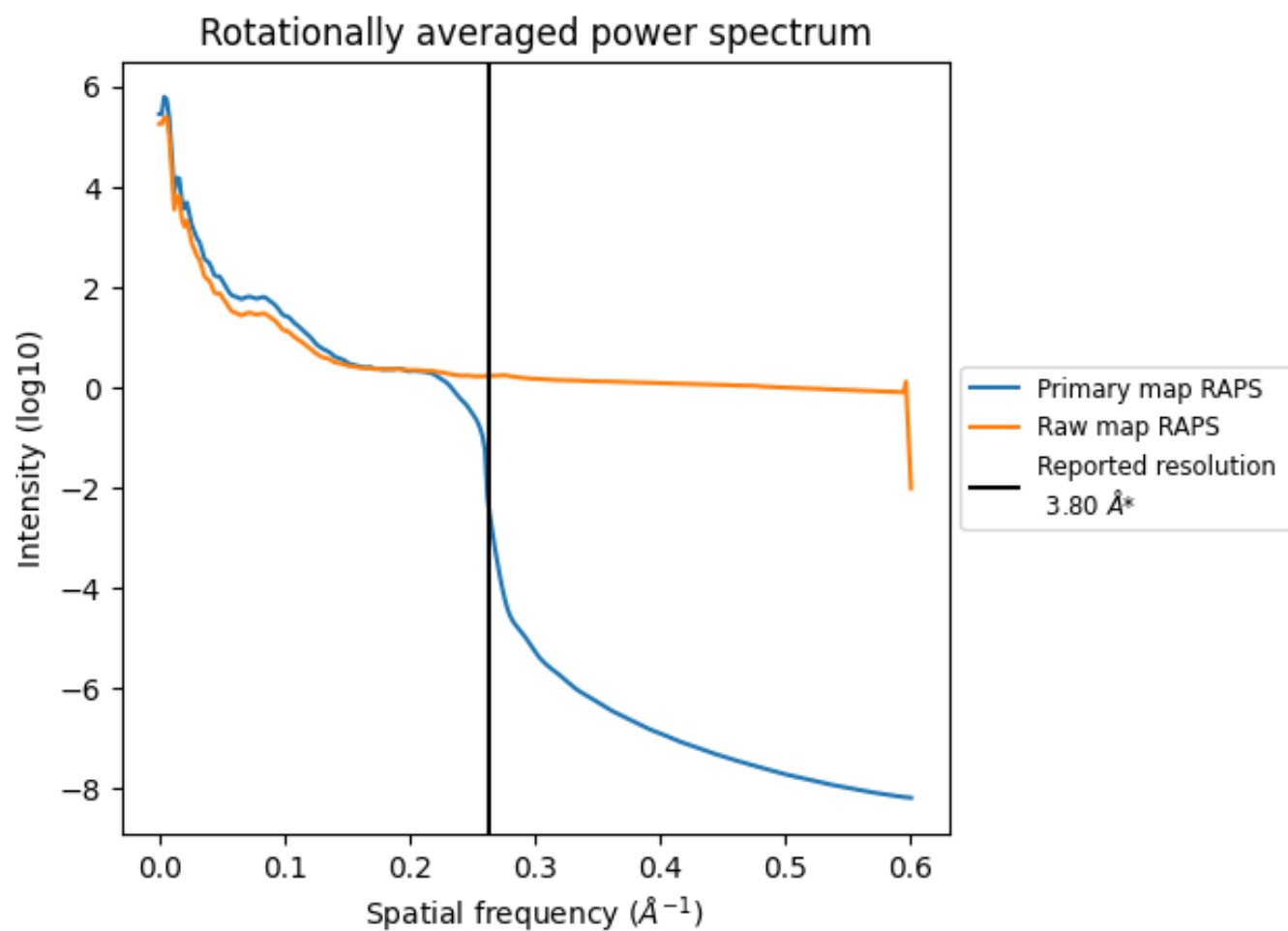
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 612 nm^3 ; this corresponds to an approximate mass of 553 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

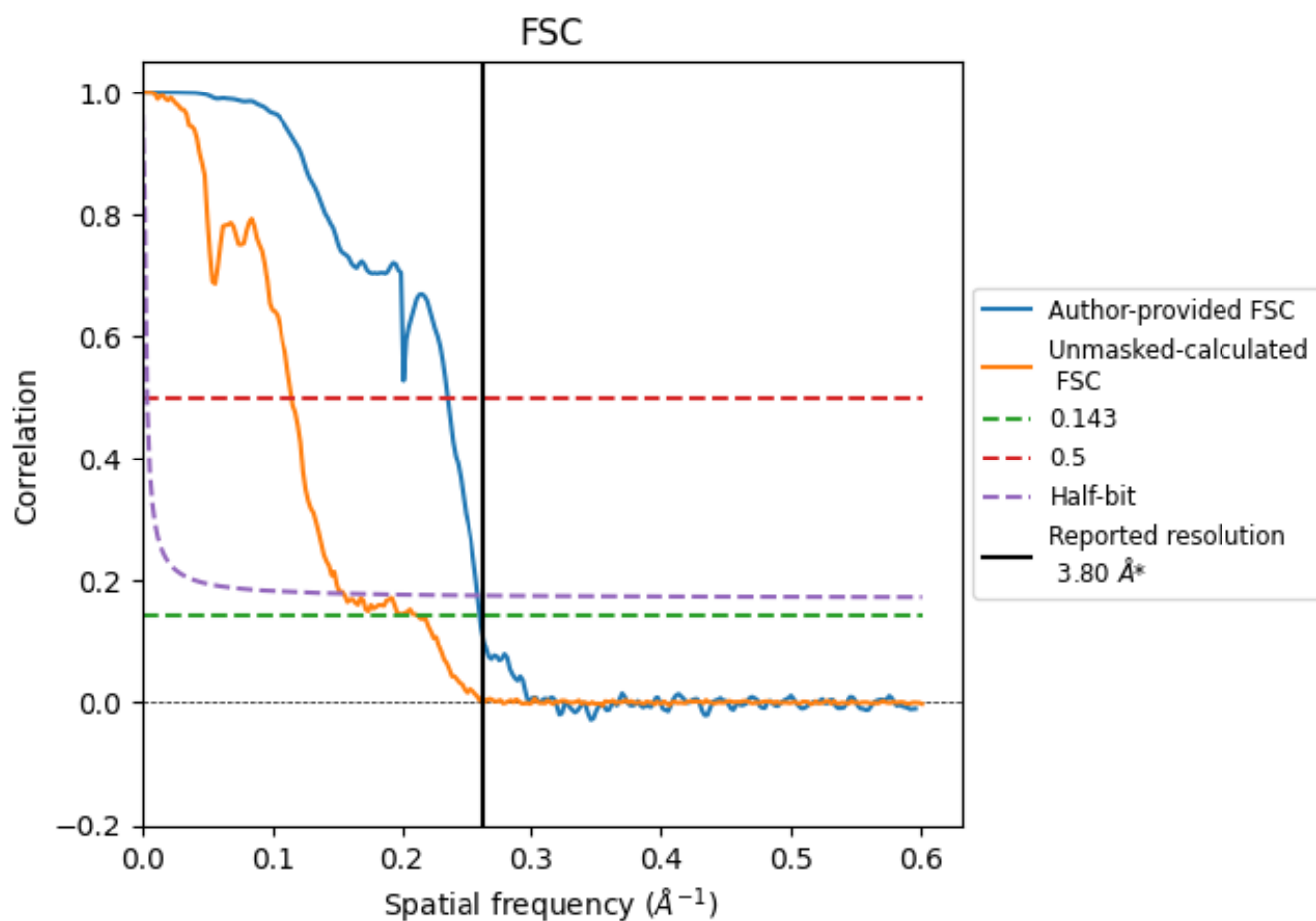


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

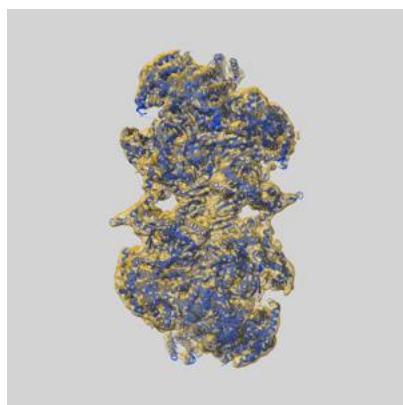
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.84	4.25	3.87
Unmasked-calculated*	4.71	8.67	6.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.71 differs from the reported value 3.8 by more than 10 %

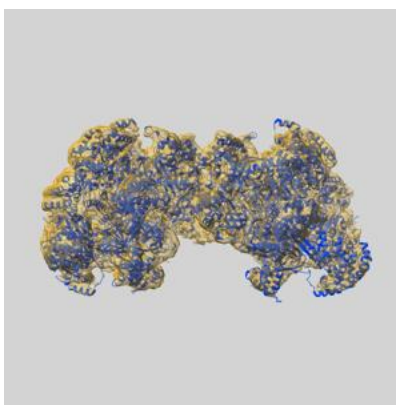
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43709 and PDB model 8W0G. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

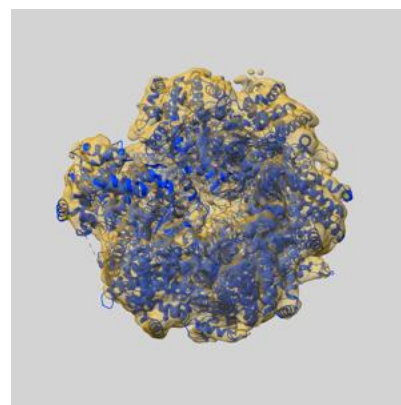
9.1 Map-model overlay [i](#)



X



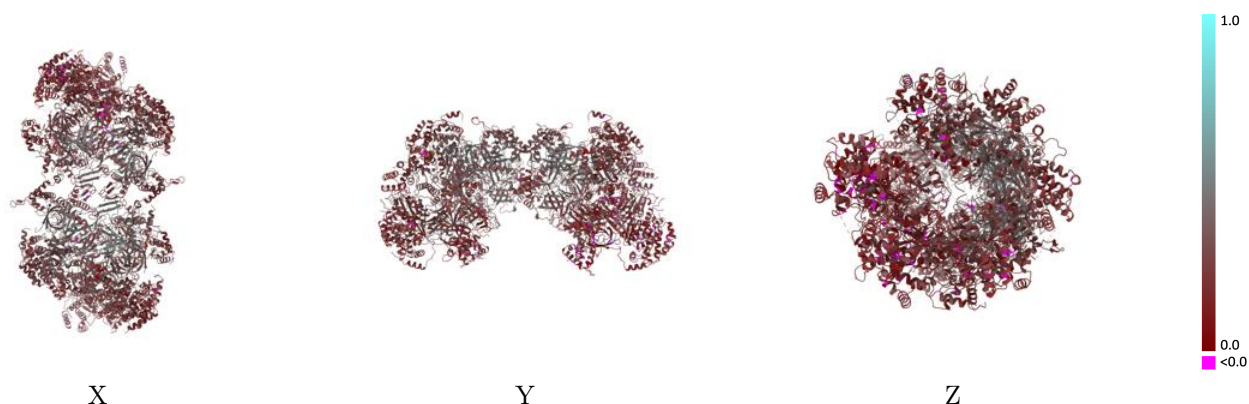
Y



Z

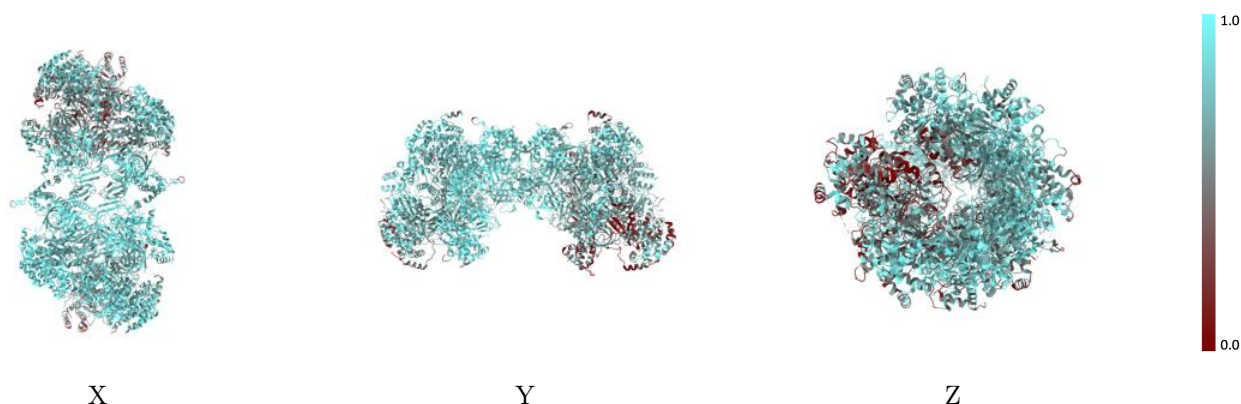
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



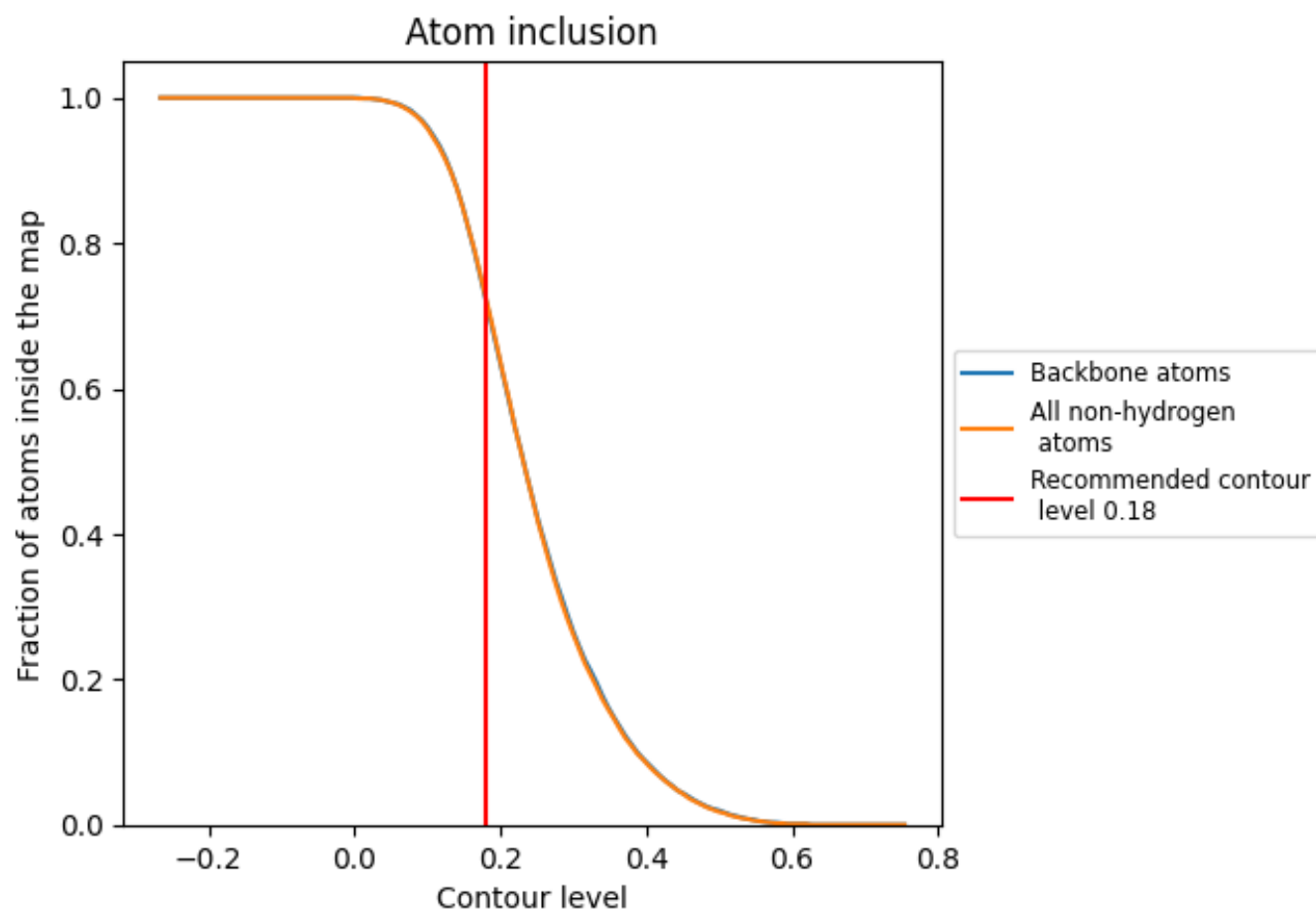
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7240	0.2680
2	0.6830	0.2100
3	0.8980	0.3640
4	0.8420	0.2780
5	0.8610	0.2930
6	0.7970	0.2350
7	0.8720	0.3430
A	0.4210	0.1630
B	0.7950	0.3390
C	0.6510	0.2320
D	0.7040	0.2610
E	0.5880	0.1870
F	0.7340	0.3070

