



Full wwPDB EM Validation Report ⓘ

Jun 26, 2025 – 01:18 AM JST

PDB ID : 7V3U / pdb_00007v3u
EMDB ID : EMD-31684
Title : Cryo-EM structure of MCM double hexamer with structured Mcm4-NSD
Authors : Cheng, J.; Li, N.; Huo, Y.; Dang, S.; Tye, B.; Gao, N.; Zhai, Y.
Deposited on : 2021-08-11
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

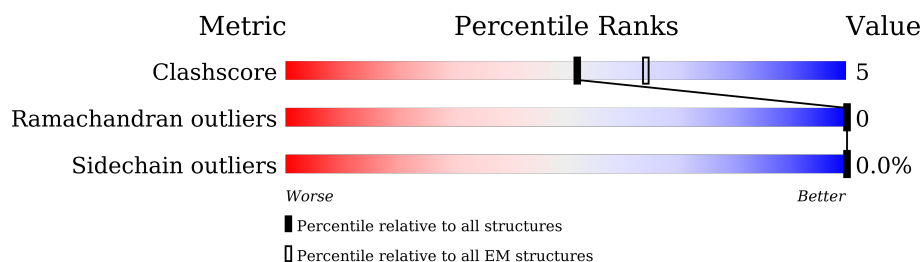
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	<div> <div>13%</div> <div>62%</div> <div>10%</div> <div>28%</div> </div>
1	B	868	<div> <div>13%</div> <div>61%</div> <div>12%</div> <div>28%</div> </div>
2	3	971	<div> <div>9%</div> <div>58%</div> <div>7%</div> <div>34%</div> </div>
2	C	971	<div> <div>10%</div> <div>57%</div> <div>8%</div> <div>34%</div> </div>
3	4	933	<div> <div>7%</div> <div>63%</div> <div>11%</div> <div>26%</div> </div>
3	D	933	<div> <div>8%</div> <div>61%</div> <div>11%</div> <div>28%</div> </div>
4	5	775	<div> <div>15%</div> <div>72%</div> <div>13%</div> <div>15%</div> </div>
4	E	775	<div> <div>15%</div> <div>70%</div> <div>15%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
5	6	1017	<div><div></div><div>11%</div><div>54%</div><div>9%</div><div>36%</div></div>
5	F	1017	<div><div></div><div>13%</div><div>55%</div><div>8%</div><div>36%</div></div>
6	7	845	<div><div></div><div>9%</div><div>72%</div><div>11%</div><div>17%</div></div>
6	G	845	<div><div></div><div>12%</div><div>71%</div><div>11%</div><div>17%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 62646 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	628	Total	C	N	O	S	0	0
			4970	3133	883	935	19		
1	B	628	Total	C	N	O	S	0	0
			4970	3133	883	935	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	637	Total	C	N	O	S	0	0
			4987	3142	889	943	13		
2	C	637	Total	C	N	O	S	0	0
			4987	3142	889	943	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	692	Total	C	N	O	S	0	0
			5509	3450	957	1071	31		
3	D	670	Total	C	N	O	S	0	0
			5323	3339	918	1036	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	658	Total	C	N	O	S	0	0
			5143	3226	882	1010	25		
4	E	658	Total	C	N	O	S	0	0
			5143	3226	882	1010	25		

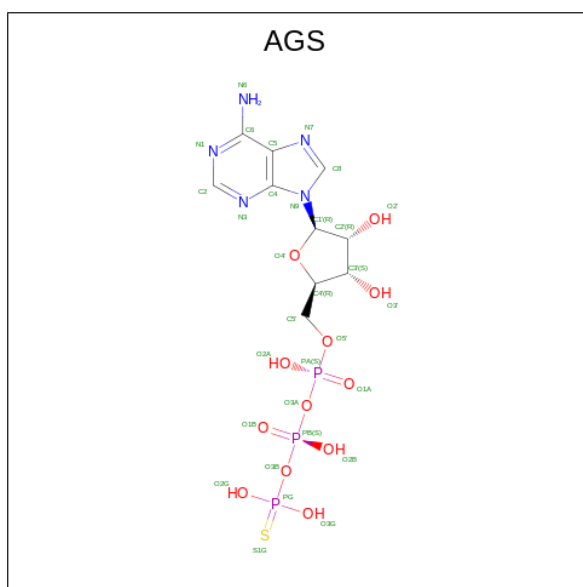
- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	646	Total	C	N	O	S	0	0
			5109	3215	892	977	25		
5	F	646	Total	C	N	O	S	0	0
			5109	3215	892	977	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	699	Total	C	N	O	S	0	0
			5505	3463	952	1059	31		
6	G	699	Total	C	N	O	S	0	0
			5505	3463	952	1059	31		

- Molecule 7 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
7	2	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	4	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	7	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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Mol	Chain	Residues	Atoms						AltConf
7	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
7	G	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

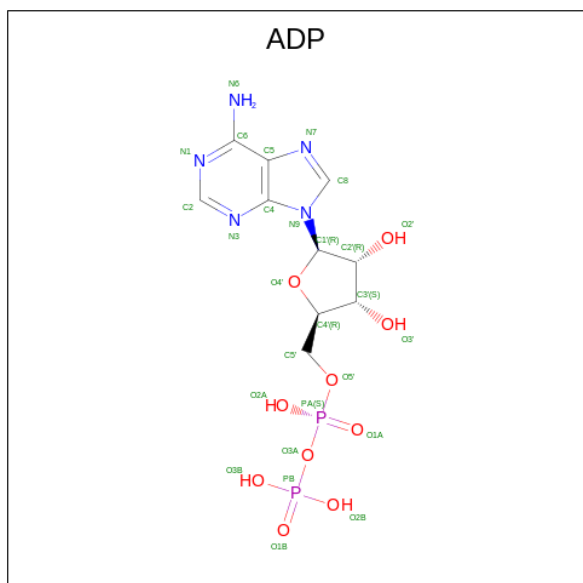
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	2	1	Total	Mg	0
			1	1	
8	3	1	Total	Mg	0
			1	1	
8	4	1	Total	Mg	0
			1	1	
8	5	1	Total	Mg	0
			1	1	
8	6	1	Total	Mg	0
			1	1	
8	7	1	Total	Mg	0
			1	1	
8	B	1	Total	Mg	0
			1	1	
8	C	1	Total	Mg	0
			1	1	
8	D	1	Total	Mg	0
			1	1	
8	E	1	Total	Mg	0
			1	1	
8	F	1	Total	Mg	0
			1	1	
8	G	1	Total	Mg	0
			1	1	

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	2	1	Total	Zn	0
			1	1	
9	4	1	Total	Zn	0
			1	1	
9	5	1	Total	Zn	0
			1	1	
9	6	1	Total	Zn	0
			1	1	
9	7	1	Total	Zn	0
			1	1	
9	B	1	Total	Zn	0
			1	1	
9	D	1	Total	Zn	0
			1	1	
9	E	1	Total	Zn	0
			1	1	
9	F	1	Total	Zn	0
			1	1	
9	G	1	Total	Zn	0
			1	1	

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



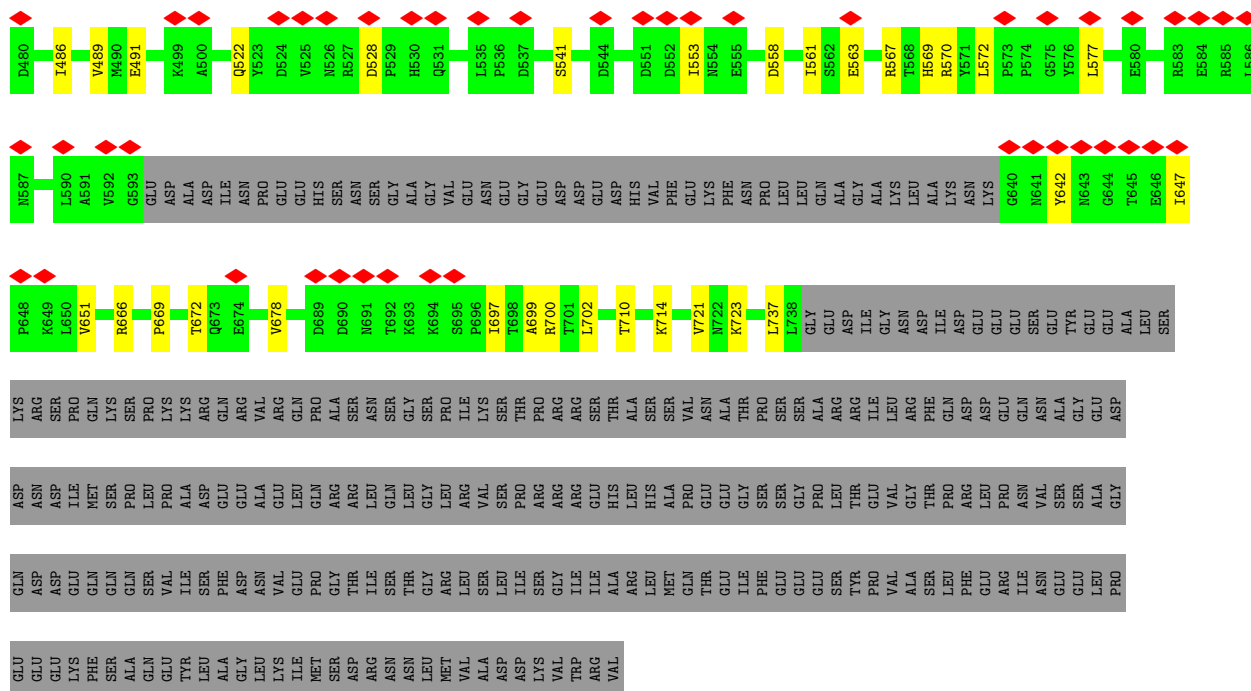
Mol	Chain	Residues	Atoms					AltConf
10	3	1	Total	C	N	O	P	0
			27	10	5	10	2	

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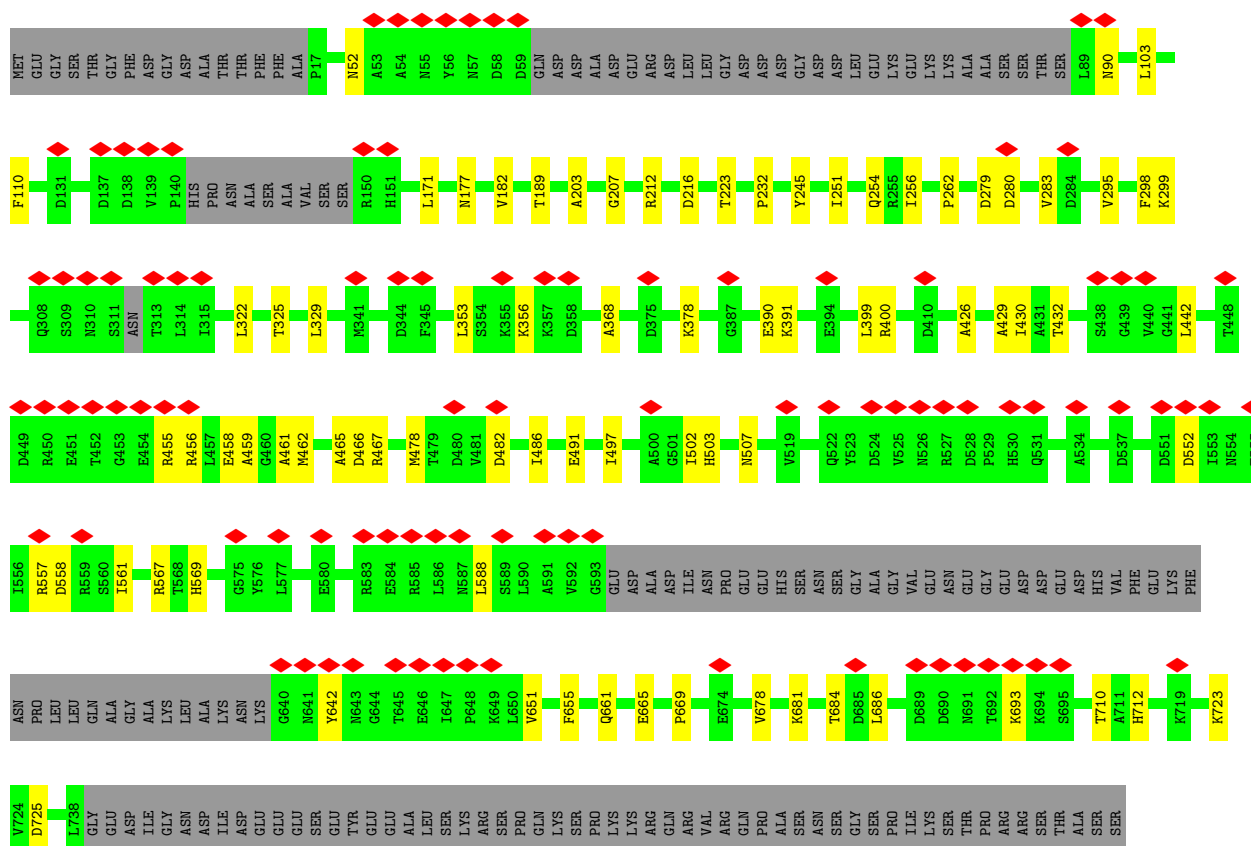
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	C	1	27	10	5	10	2	0





• Molecule 2: DNA replication licensing factor MCM3



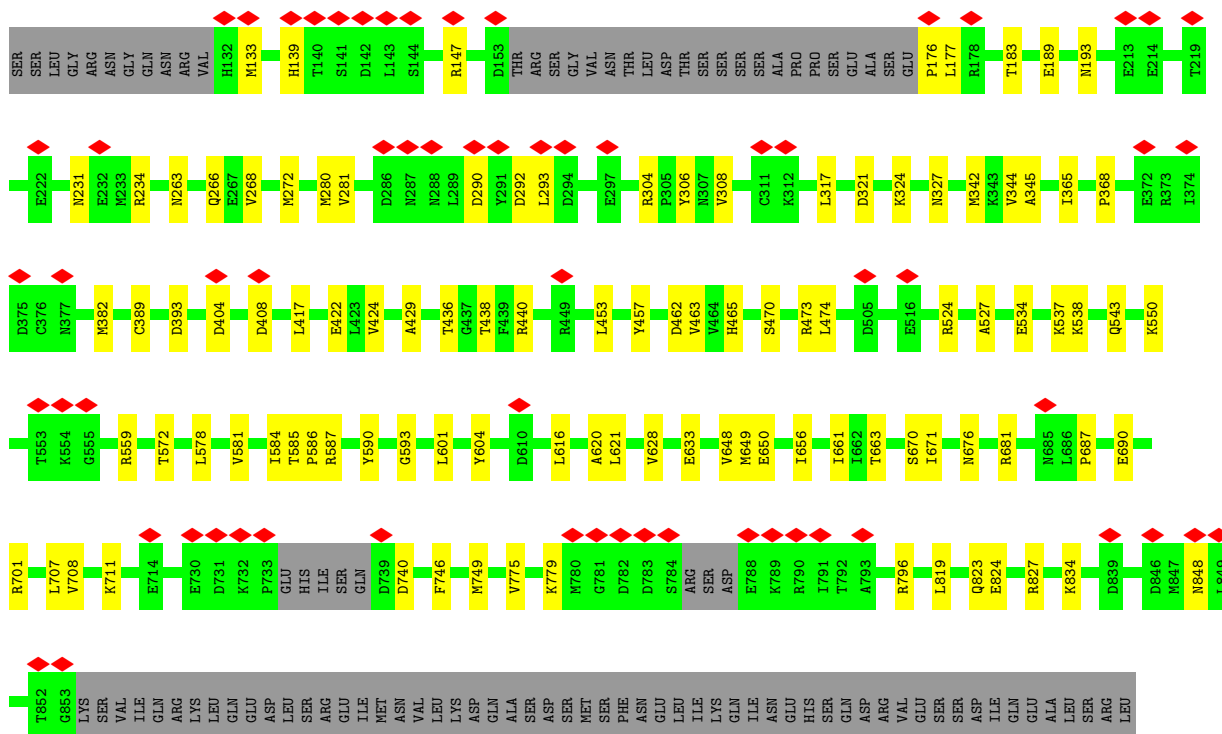
GLN	THR	GLU	THR	ILE	PHE	GLU	GLU	GLU	SER	TYR	PRO	VAL	ALA	SER	LEU	PHE	GLU	GLU	ARG	ILE	ASN	GLU	GLU	TYR	GLN	ALA	SER	SER	PHE	LYS	GLU	GLU	PRO	GLU	GLU	LEU	ALA	GLY	LEU	LYS	ILE	MET	SER	ASP	ASN	ASN	MET	LEU	VAL	VAL	TRP	ARG	VAL
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- Molecule 3: DNA replication licensing factor MCM4



MET	SER	GLN	GLN	SER	SER	PRO	THR	LYS	GLU	ASP	ASN	ASN	SER	SER	SER	PRO	VAL	VAL	VAL	ASN	ASN	ASP	SER	SER	PRO	PRO	PRO	PRO	GLN	LEU	SER	SER	PRO	ALA	ALA	PHE	TYR	SER	SER	SER	SER	SER	SER	GLN	GLY	ASP	ASP	ILE	ILE	TYR	GLY	ARG	ASN	ASN	GLN	ASN	LEU	SER	SER	GLN	GLY	GLY	GLU	GLU
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ASN	ILE	ARG	ALA	ALA	ILE	GLY	SER	SER	PRO	PRO	LEU	ASN	PHE	PRO	SER	SER	SER	GLN	ARG	GLN	ASN	ASP	VAL	PHE	GLN	SER	SER	GLY	GLY	ARG	GLN	GLY	ARG	ILE	ILE	ARG	SER	SER	ALA	ALA	SER	GLY	ARG	SER	ARG	ARG	TYR	HIS	SER	ASP	LEU	ARG	SER	ASP	ARG	ALA	LEU	PRO	THR	SER	SER
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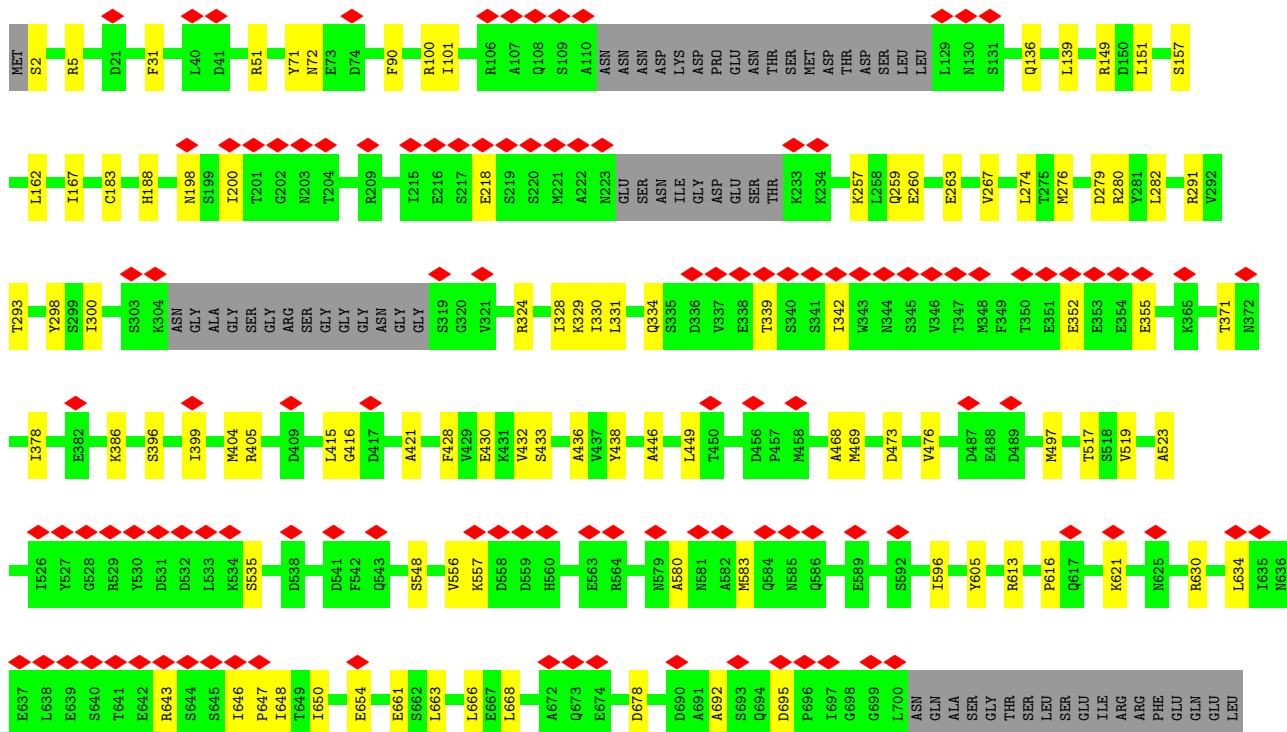
GLN	GLN	GLU	ASP	LYS	VAL	ILE	VAL	LEU	GLY	GLU	GLY	VAL	ARG	ARG	SER	VAL	ARG	LEU	ASN	ASN	ARG	VAL
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- Molecule 3: DNA replication licensing factor MCM4

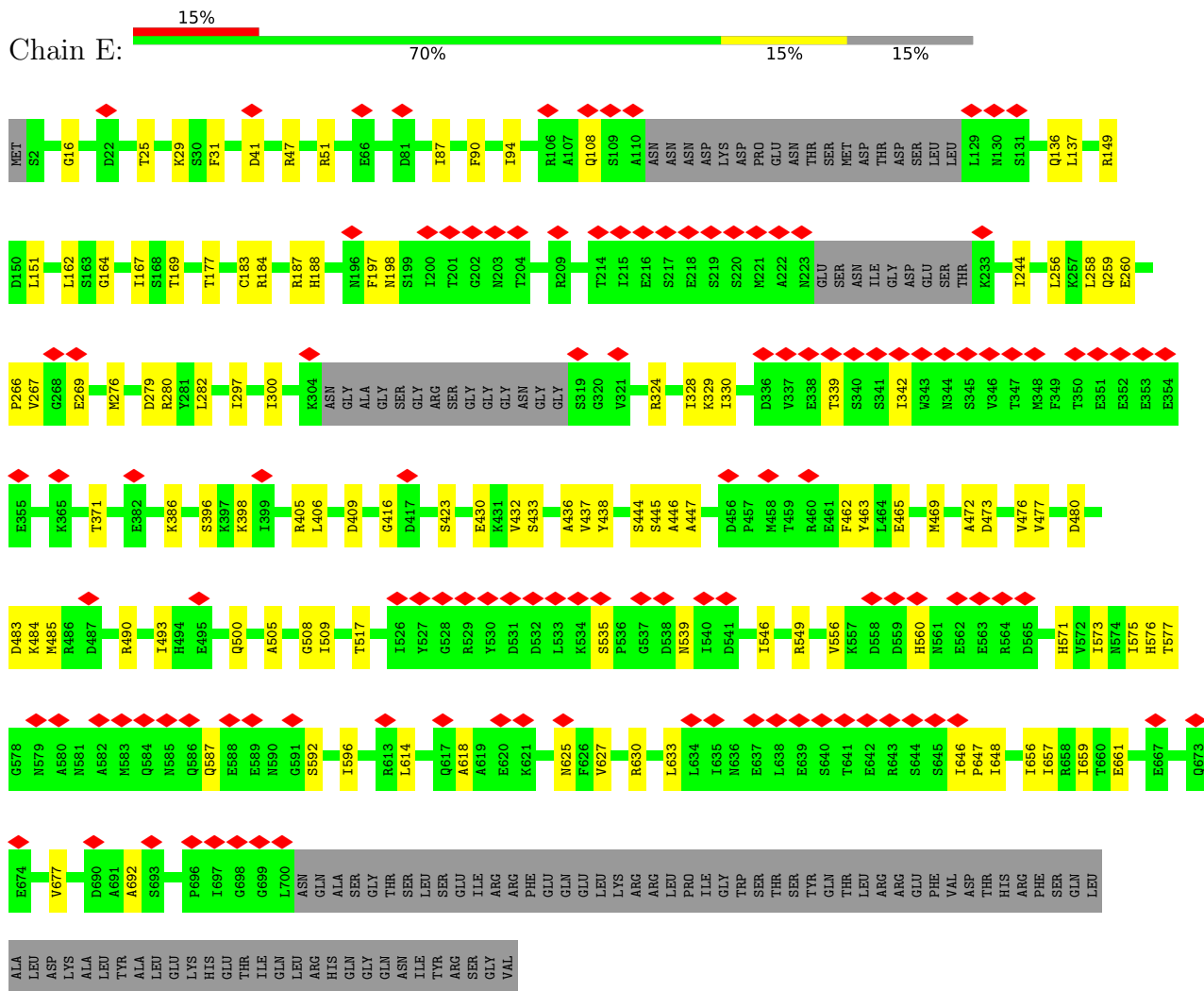


MET	SER	SER	GLN	GLN	SER	SER	SER	PRO	PRO	THR	LYS	GLU	ASP	ASN	ASN	SER	SER	SER	PRO	PRO	VAL	VAL	VAL	PRO	PRO	ASN	ASN	ASP	SER	SER	VAL	VAL	LEU	SER	SER	PRO	PRO	ALA	ALA	LEU	PHE	TYR	SER	SER	SER	SER	SER	SER	SER	GLN	GLY	ASP	ASP	ILE	TYR	TYR	GLY	ARG	ASN	ASN	ASN	SER	SER	GLN	ASN	ASN	LEU	SER	SER	GLN	GLY	GLY	GLU	TYR
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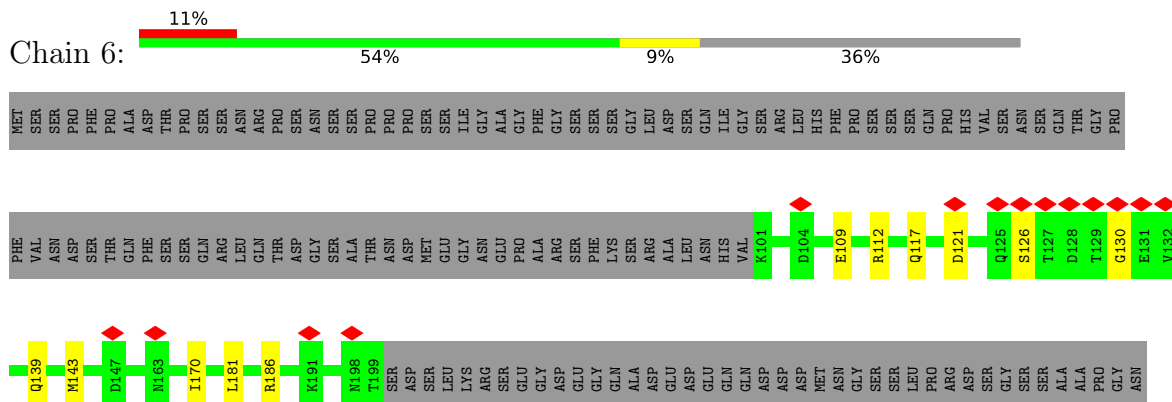
ASN ILE ARG ALA ALA ILE GLY SER SER PRO LEU PHE PRO SER SER GLN ARG GLN ASN ASN ASP VAL PHE GLN SER SER GLN ARG GLN GLY ARG ILE ILE ARG SER SER ALA ALA SER ALA GLY ARG SER SER ARG TYR HIS SER ASP ARG ALA LEU ARG SER ASP ARG ALA LEU PRO THR SER SER

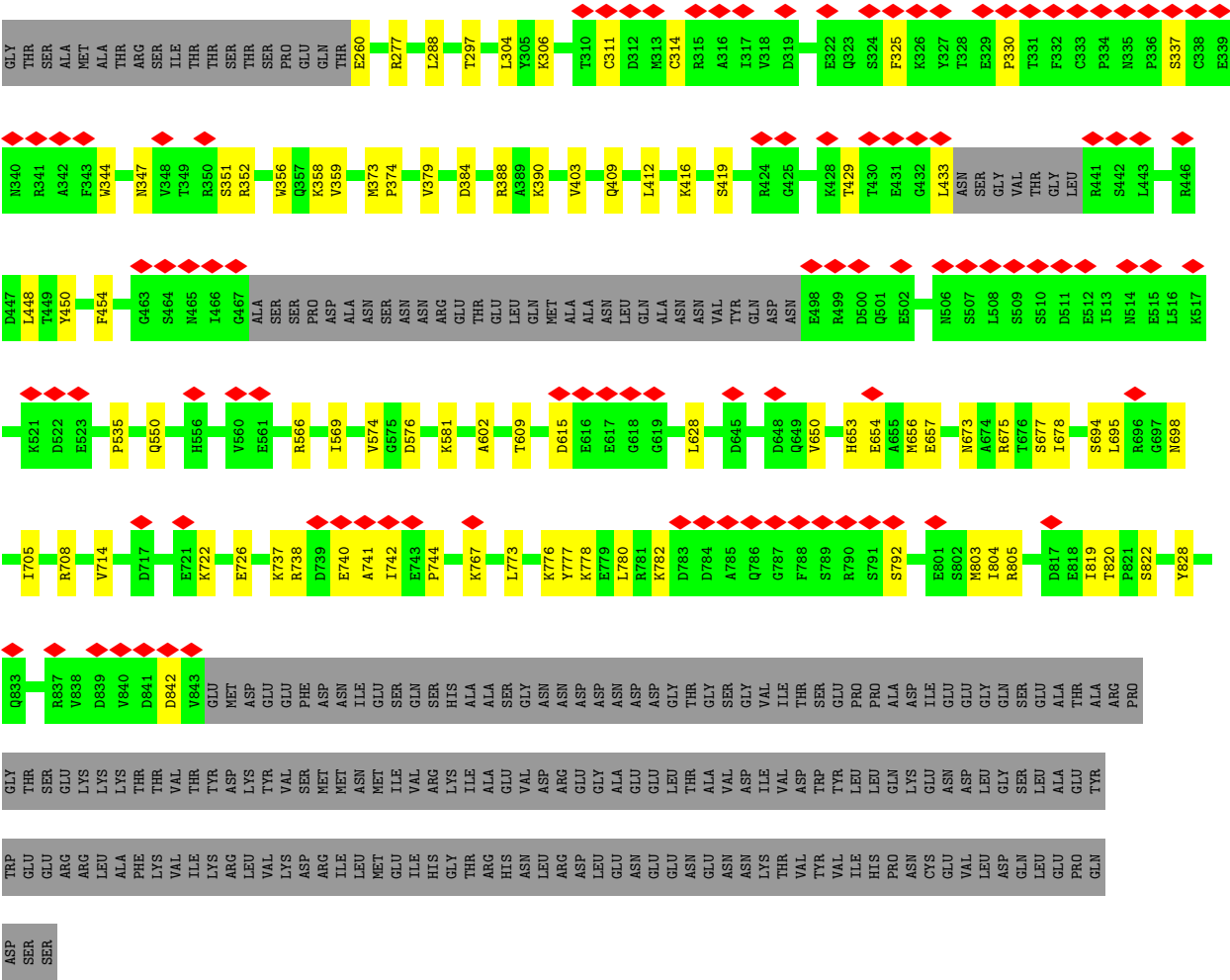


Chain E:

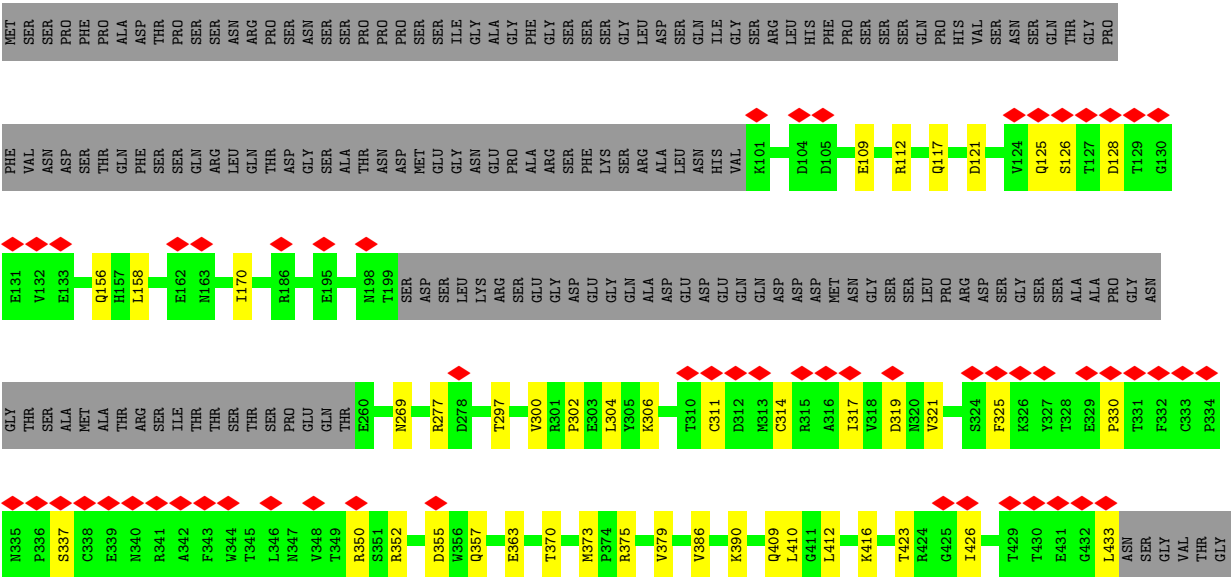


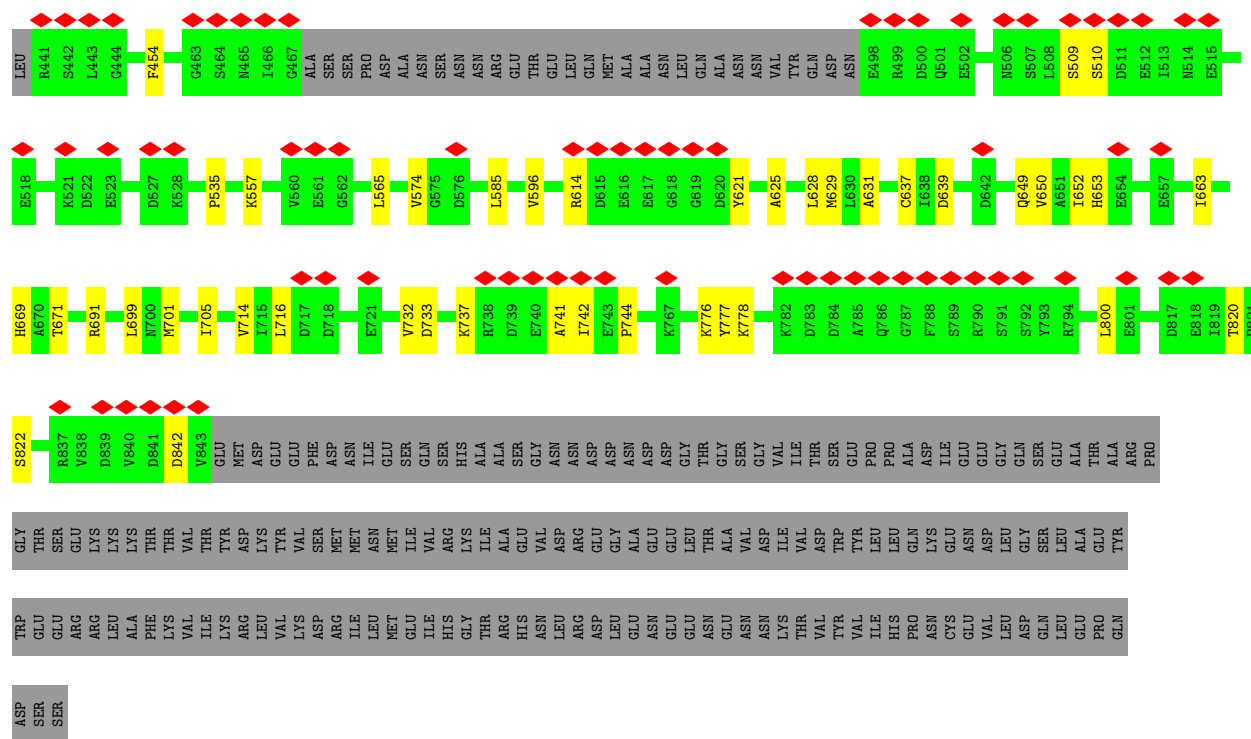
Chain 6:



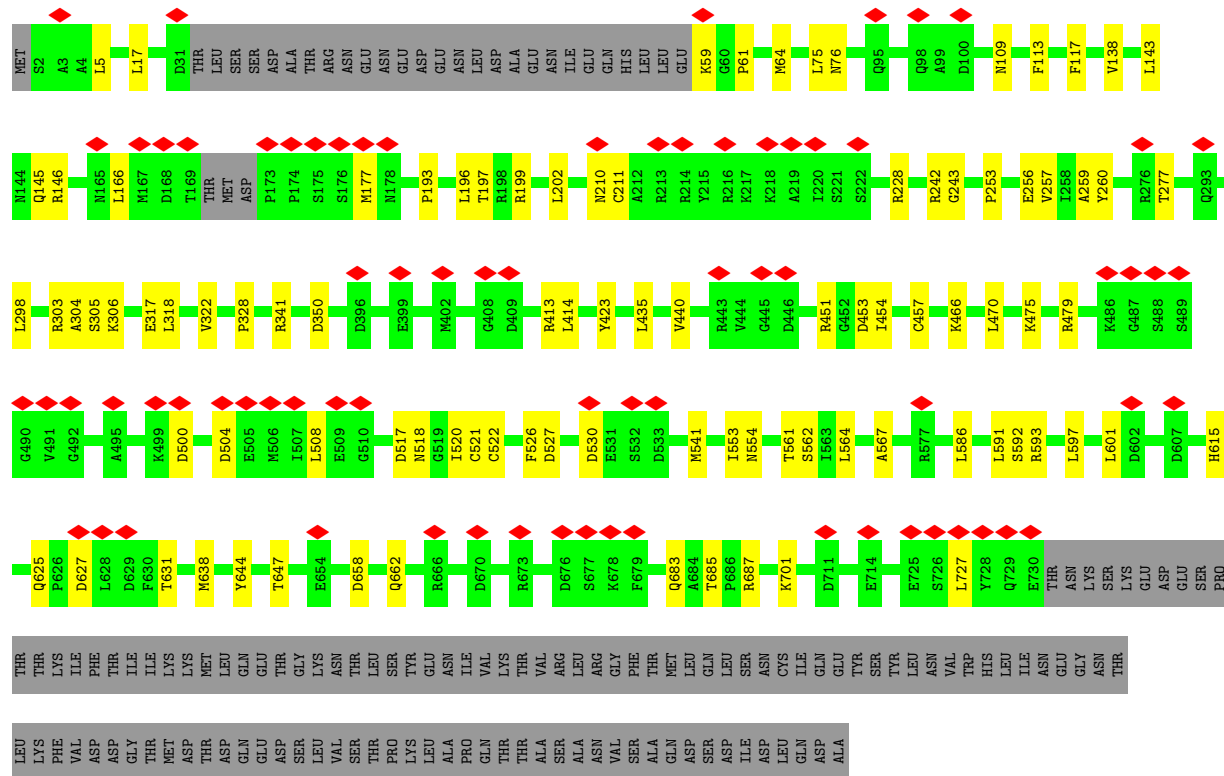
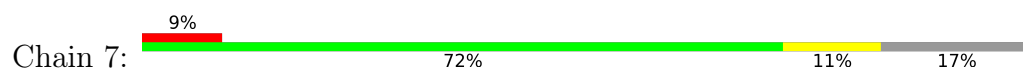


● Molecule 5: DNA replication licensing factor MCM6

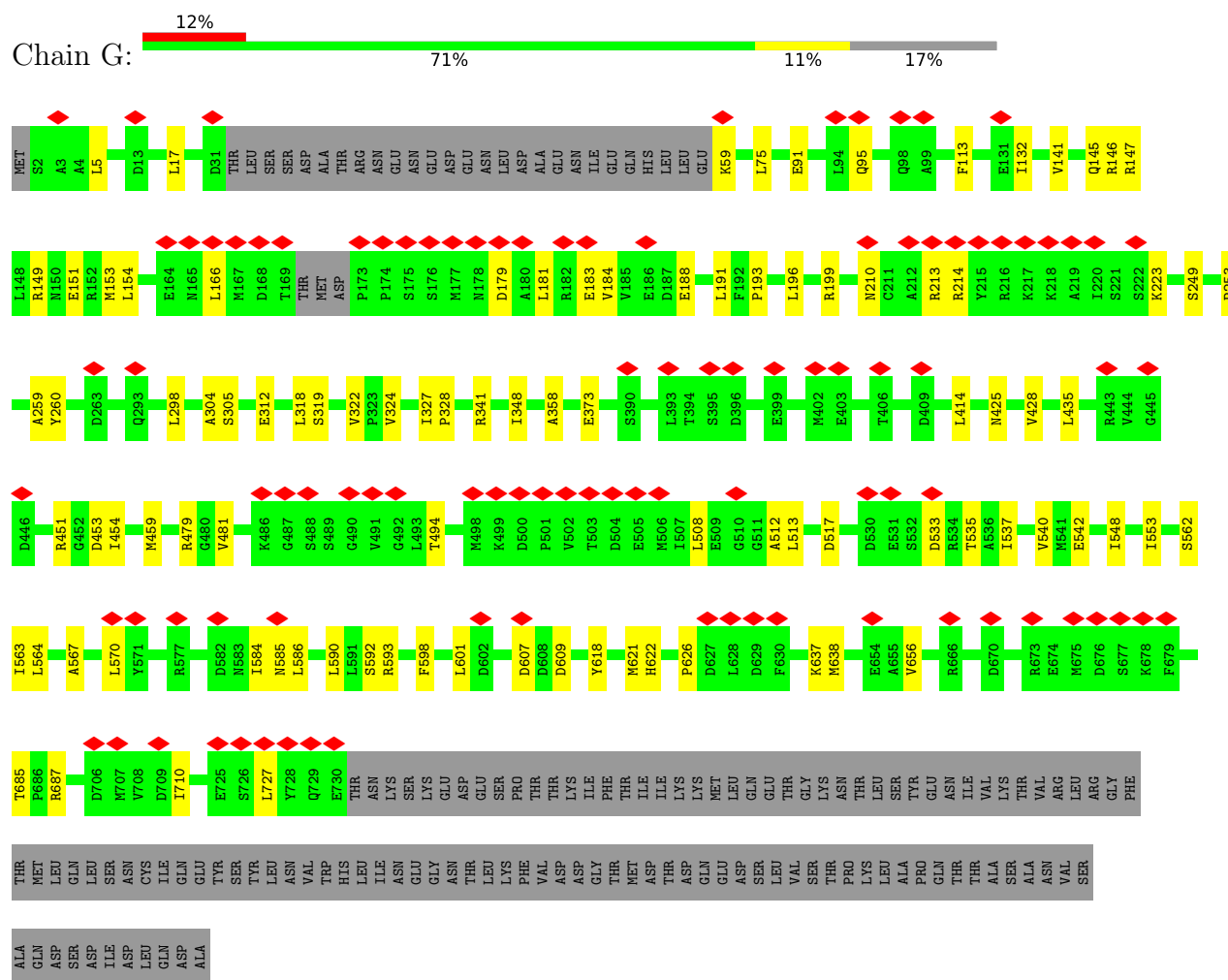




• Molecule 6: DNA replication licensing factor MCM7



• Molecule 6: DNA replication licensing factor MCM7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150000	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 ($e^-/\text{\AA}^2$)	46.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.307	Depositor
Minimum map value	-0.180	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	378.72003, 378.72003, 378.72003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.16	0/5057	0.41	0/6834
1	B	0.16	0/5057	0.40	0/6834
2	3	0.17	0/5073	0.39	2/6880 (0.0%)
2	C	0.17	0/5073	0.38	0/6880
3	4	0.17	0/5589	0.41	0/7553
3	D	0.16	0/5400	0.39	0/7300
4	5	0.16	0/5217	0.39	0/7054
4	E	0.18	0/5217	0.42	1/7054 (0.0%)
5	6	0.16	0/5190	0.39	2/7001 (0.0%)
5	F	0.15	0/5190	0.37	0/7001
6	7	0.17	0/5590	0.38	0/7554
6	G	0.17	0/5590	0.38	0/7554
All	All	0.17	0/63243	0.39	5/85499 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	647	PRO	CA-N-CD	-5.88	103.77	112.00
2	3	563	GLU	CA-CB-CG	5.47	125.04	114.10
2	3	563	GLU	N-CA-CB	5.33	118.54	110.28
5	6	819	ILE	CA-C-N	5.04	135.55	120.69
5	6	819	ILE	C-N-CA	5.04	135.55	120.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	4970	0	5026	55	0
1	B	4970	0	5026	68	0
2	3	4987	0	5049	47	0
2	C	4987	0	5050	50	0
3	4	5509	0	5549	66	0
3	D	5323	0	5373	60	0
4	5	5143	0	5191	64	0
4	E	5143	0	5191	72	0
5	6	5109	0	5134	64	0
5	F	5109	0	5134	60	0
6	7	5505	0	5563	62	0
6	G	5505	0	5565	61	0
7	2	31	0	12	0	0
7	4	31	0	12	4	0
7	5	31	0	12	1	0
7	6	31	0	12	1	0
7	7	31	0	12	1	0
7	B	31	0	12	1	0
7	D	31	0	12	4	0
7	E	31	0	12	0	0
7	F	31	0	12	1	0
7	G	31	0	12	0	0
8	2	1	0	0	0	0
8	3	1	0	0	0	0
8	4	1	0	0	0	0
8	5	1	0	0	0	0
8	6	1	0	0	0	0
8	7	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
9	2	1	0	0	0	0
9	4	1	0	0	0	0
9	5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	6	1	0	0	0	0
9	7	1	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
10	3	27	0	12	0	0
10	C	27	0	12	0	0
All	All	62646	0	62995	657	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 5.

All (657) 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)
4:E:167:ILE:HD11	4:E:259:GLN:HB2	1.63	0.81
4:E:276:MET:HG2	4:E:328:ILE:HB	1.66	0.77
4:E:198:ASN:HB3	4:E:329:LYS:HG2	1.71	0.73
4:5:167:ILE:HD11	4:5:259:GLN:HB2	1.69	0.72
4:E:398:LYS:HD2	4:E:406:LEU:HB2	1.74	0.70
6:G:685:THR:HG22	6:G:687:ARG:H	1.58	0.68
2:3:396:GLY:HA3	6:7:475:LYS:HE3	1.76	0.67
4:5:276:MET:HG2	4:5:328:ILE:HB	1.78	0.66
3:4:593:GLY:H	3:4:633:GLU:HB2	1.61	0.65
4:5:342:ILE:HD11	4:5:473:ASP:HB3	1.79	0.65
1:2:296:ARG:HH21	1:2:413:ASP:HB3	1.62	0.65
3:4:621:LEU:HD13	3:4:648:VAL:HG21	1.78	0.64
6:7:414:LEU:HD22	6:7:638:MET:HG3	1.79	0.64
7:4:2001:AGS:O3G	6:7:593:ARG:NH2	2.31	0.64
7:D:2001:AGS:O3G	6:G:593:ARG:NH2	2.31	0.63
3:D:594:LYS:HB3	6:G:535:THR:HG21	1.78	0.63
3:4:234:ARG:HB2	3:4:280:MET:HE1	1.80	0.63
2:C:368:ALA:HB3	2:C:378:LYS:HE2	1.81	0.63
4:5:548:SER:HB3	4:5:647:PRO:HG2	1.80	0.62
1:2:485:ARG:HB3	1:2:489:ARG:HH21	1.64	0.62
5:F:699:LEU:HD13	5:F:701:MET:HE2	1.81	0.62
2:3:368:ALA:HB3	2:3:378:LYS:HE2	1.81	0.62
1:B:400:GLY:HA3	5:F:390:LYS:HD3	1.82	0.61
6:G:586:LEU:HD11	6:G:590:LEU:HD22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:478:MET:HE1	2:3:486:ILE:HD12	1.82	0.61
3:4:281:VAL:HG13	3:4:293:LEU:HD11	1.82	0.61
5:6:314:CYS:SG	5:6:337:SER:OG	2.58	0.61
1:B:337:VAL:HA	1:B:380:THR:HG23	1.82	0.61
2:3:251:ILE:HG23	2:3:280:ASP:HB3	1.81	0.61
3:4:304:ARG:NH2	3:4:422:GLU:OE2	2.35	0.60
2:3:647:ILE:HG22	2:3:651:VAL:HG22	1.82	0.60
4:5:469:MET:HE3	4:5:517:THR:HB	1.84	0.60
2:C:567:ARG:O	2:C:642:TYR:OH	2.19	0.60
4:E:342:ILE:HD11	4:E:473:ASP:HB3	1.83	0.59
4:5:100:ARG:NH2	6:G:188:GLU:OE2	2.35	0.59
2:C:329:LEU:HD23	2:C:588:LEU:HB3	1.84	0.59
3:4:681:ARG:NH1	6:7:683:GLN:OE1	2.35	0.59
1:2:495:ASP:OD1	1:2:509:ARG:NH2	2.34	0.59
5:6:384:ASP:O	5:6:388:ARG:NH1	2.36	0.59
4:E:136:GLN:HB2	4:E:280:ARG:HE	1.68	0.59
3:4:417:LEU:HD13	3:4:463:VAL:HG21	1.85	0.59
6:7:138:VAL:HG11	6:7:303:ARG:HH21	1.67	0.59
1:2:384:ASN:HB2	1:2:412:ALA:HA	1.84	0.58
2:C:262:PRO:HG3	4:E:509:ILE:HD11	1.85	0.58
2:3:553:ILE:HG13	4:5:634:LEU:HD13	1.85	0.58
5:6:306:LYS:HB2	5:6:352:ARG:HB2	1.86	0.58
5:6:820:THR:HG22	5:6:822:SER:H	1.69	0.58
3:D:304:ARG:HB3	3:D:465:HIS:HB2	1.86	0.58
3:D:621:LEU:HD13	3:D:648:VAL:HG21	1.84	0.58
4:E:177:THR:HA	4:E:197:PHE:HZ	1.69	0.58
6:7:451:ARG:NH1	6:7:453:ASP:O	2.37	0.58
2:C:251:ILE:HG23	2:C:280:ASP:HB3	1.85	0.58
5:F:156:GLN:OE1	5:F:269:ASN:ND2	2.37	0.58
1:B:811:GLU:OE2	4:E:576:HIS:NE2	2.37	0.58
1:2:337:VAL:HA	1:2:380:THR:HG23	1.85	0.58
2:3:697:ILE:HD11	2:3:737:LEU:HD21	1.86	0.58
5:6:737:LYS:HB3	5:6:740:GLU:HB2	1.86	0.58
5:6:742:ILE:HG22	5:6:744:PRO:HD3	1.86	0.58
4:5:167:ILE:HD13	4:5:257:LYS:HG3	1.86	0.57
2:3:370:SER:OG	4:5:404:MET:SD	2.62	0.57
5:6:780:LEU:HD11	5:6:803:MET:HE1	1.86	0.57
4:5:198:ASN:HB3	4:5:329:LYS:HG2	1.86	0.57
5:6:186:ARG:HH22	5:6:260:GLU:HB3	1.69	0.57
5:F:314:CYS:SG	5:F:337:SER:OG	2.62	0.57
1:2:786:VAL:HA	1:2:789:VAL:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:231:ASN:OD1	3:4:234:ARG:NH2	2.38	0.57
6:G:414:LEU:HD22	6:G:638:MET:HG2	1.86	0.57
3:4:408:ASP:OD1	6:7:518:ASN:ND2	2.32	0.57
4:5:621:LYS:NZ	4:5:678:ASP:OD1	2.33	0.57
5:6:311:CYS:HB3	5:6:314:CYS:HB2	1.87	0.57
3:D:601:LEU:HD23	3:D:620:ALA:HB3	1.86	0.57
6:7:177:MET:SD	4:E:108:GLN:NE2	2.70	0.57
1:B:772:THR:HG23	1:B:773:LYS:HG2	1.85	0.57
6:7:508:LEU:HD22	6:7:553:ILE:HD13	1.87	0.57
1:B:386:GLN:HB2	1:B:415:VAL:HG12	1.87	0.57
3:D:428:ARG:HD2	5:F:370:THR:HG22	1.87	0.57
4:E:282:LEU:HD13	4:E:330:ILE:HG22	1.87	0.57
3:D:618:SER:HA	5:F:373:MET:HE3	1.87	0.56
1:2:562:ARG:NH1	1:2:598:LEU:O	2.36	0.56
4:E:409:ASP:OD2	4:E:500:GLN:NE2	2.38	0.56
1:B:384:ASN:HB2	1:B:412:ALA:HA	1.86	0.56
2:C:558:ASP:OD1	4:E:630:ARG:NE	2.34	0.56
6:G:508:LEU:HD22	6:G:553:ILE:HD13	1.86	0.56
1:2:400:GLY:HA3	5:6:390:LYS:HD3	1.87	0.56
3:D:592:SER:OG	3:D:633:GLU:OE2	2.23	0.56
1:2:760:GLN:NE2	1:2:764:MET:SD	2.79	0.56
5:F:311:CYS:HB3	5:F:314:CYS:HB2	1.86	0.56
3:D:183:THR:O	6:G:145:GLN:NE2	2.39	0.56
5:6:109:GLU:OE1	5:6:112:ARG:NH1	2.39	0.55
2:C:52:ASN:ND2	2:C:90:ASN:O	2.39	0.55
4:E:587:GLN:HE21	4:E:592:SER:HB2	1.72	0.55
3:D:842:THR:HG23	3:D:844:LYS:H	1.70	0.55
6:G:621:MET:HE3	6:G:622:HIS:CE1	2.42	0.55
3:4:578:LEU:HB3	3:4:590:TYR:HE2	1.70	0.55
2:C:552:ASP:HB3	2:C:557:ARG:HH12	1.71	0.55
6:7:75:LEU:O	6:7:199:ARG:NH1	2.39	0.55
2:C:569:HIS:HA	4:E:398:LYS:HZ1	1.70	0.55
5:F:412:LEU:O	5:F:416:LYS:NZ	2.37	0.55
1:2:659:SER:OG	1:2:684:ARG:NH1	2.39	0.55
5:6:773:LEU:HD21	5:6:804:ILE:HG12	1.89	0.55
3:4:183:THR:O	6:7:145:GLN:NE2	2.39	0.55
5:6:117:GLN:O	5:6:121:ASP:HB2	2.07	0.55
1:B:406:ARG:NH1	1:B:430:TYR:OH	2.40	0.55
3:4:601:LEU:HD23	3:4:620:ALA:HB3	1.89	0.54
4:5:433:SER:HB2	4:5:436:ALA:HB2	1.88	0.54
6:7:413:ARG:NH1	6:7:631:THR:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:391:GLN:HE21	1:2:403:PRO:HG2	1.72	0.54
1:2:772:THR:HG23	1:2:773:LYS:HG3	1.88	0.54
3:4:543:GLN:HE21	3:4:670:SER:HB3	1.71	0.54
3:D:794:THR:HG22	3:D:796:ARG:H	1.73	0.54
4:E:477:VAL:HG23	4:E:517:THR:HG21	1.88	0.54
5:F:663:ILE:O	5:F:669:HIS:HA	2.07	0.54
3:4:345:ALA:HB2	3:4:365:ILE:HD13	1.89	0.54
3:4:616:LEU:HD21	3:4:661:ILE:HD11	1.88	0.54
4:5:630:ARG:NH1	4:5:648:ILE:O	2.40	0.54
5:6:576:ASP:O	5:6:581:LYS:NZ	2.40	0.54
1:B:511:ILE:HG22	1:B:681:CYS:HB3	1.89	0.54
1:2:824:ARG:NH1	1:2:830:SER:OG	2.39	0.54
5:6:777:TYR:HA	5:6:780:LEU:HD12	1.90	0.54
2:C:459:ALA:HB2	6:G:327:ILE:HD11	1.89	0.54
3:D:487:GLN:NE2	3:D:491:ASP:OD1	2.41	0.54
4:E:432:VAL:HG23	4:E:596:ILE:HG13	1.90	0.54
1:2:406:ARG:NH1	1:2:430:TYR:OH	2.41	0.54
2:3:386:MET:HE2	2:3:714:LYS:HB3	1.90	0.54
4:5:51:ARG:NH2	6:G:166:LEU:O	2.40	0.54
4:5:149:ARG:NH1	4:5:260:GLU:OE1	2.41	0.54
4:E:656:ILE:HA	4:E:659:ILE:HD12	1.89	0.54
6:G:451:ARG:NH1	6:G:453:ASP:O	2.38	0.54
2:3:567:ARG:O	2:3:642:TYR:OH	2.25	0.54
3:4:524:ARG:NH1	3:4:740:ASP:O	2.41	0.54
4:5:136:GLN:HG3	4:5:280:ARG:HH21	1.72	0.54
6:7:260:TYR:HB3	6:7:298:LEU:HB3	1.90	0.54
5:6:694:SER:O	5:6:698:ASN:ND2	2.41	0.53
1:B:562:ARG:NH1	1:B:598:LEU:O	2.40	0.53
2:3:244:GLU:OE1	6:7:109:ASN:ND2	2.36	0.53
4:5:136:GLN:HB2	4:5:280:ARG:HE	1.74	0.53
4:5:263:GLU:OE1	4:5:291:ARG:NH2	2.39	0.53
1:2:498:ILE:HD12	1:2:513:THR:HA	1.91	0.53
1:2:849:GLN:HB2	1:2:854:ARG:HG3	1.90	0.53
4:5:663:LEU:HA	4:5:666:LEU:HD12	1.91	0.53
5:6:550:GLN:NE2	5:6:569:ILE:O	2.41	0.53
2:C:203:ALA:O	2:C:207:GLY:N	2.40	0.53
5:F:574:VAL:O	5:F:714:VAL:HA	2.08	0.53
6:G:260:TYR:HB3	6:G:298:LEU:HB3	1.89	0.53
4:5:399:ILE:HD13	4:5:405:ARG:HG3	1.91	0.53
1:B:519:LEU:HD21	1:B:556:VAL:HG13	1.91	0.53
4:E:485:MET:SD	4:E:490:ARG:NH1	2.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:342:LEU:HB3	5:F:433:LEU:HD13	1.91	0.53
1:2:560:ALA:HB3	1:2:563:ALA:HB2	1.91	0.53
3:4:133:MET:SD	3:4:133:MET:N	2.82	0.53
3:4:306:TYR:HA	3:4:436:THR:HG21	1.91	0.53
3:D:317:LEU:O	6:G:341:ARG:NH2	2.40	0.53
4:E:184:ARG:O	4:E:187:ARG:NH1	2.42	0.53
5:F:109:GLU:OE1	5:F:112:ARG:NH1	2.42	0.53
3:D:224:LEU:HD13	3:D:227:ILE:HD12	1.90	0.52
2:3:672:THR:OG1	2:3:721:VAL:O	2.27	0.52
5:F:277:ARG:NH2	5:F:373:MET:O	2.42	0.52
5:6:379:VAL:HG23	5:6:454:PHE:HB3	1.92	0.52
1:B:537:ILE:HG23	1:B:678:ASP:HB2	1.91	0.52
4:5:2:SER:HB2	2:C:245:TYR:HE1	1.74	0.52
6:7:454:ILE:O	6:7:562:SER:OG	2.23	0.52
2:3:432:THR:HG21	2:3:442:LEU:HD21	1.92	0.52
4:5:378:ILE:HD12	4:5:421:ALA:HB1	1.90	0.52
6:7:466:LYS:NZ	7:7:2001:AGS:S1G	2.77	0.52
1:2:519:LEU:HD21	1:2:556:VAL:HG13	1.91	0.52
2:C:442:LEU:HD13	2:C:486:ILE:HD11	1.92	0.52
2:C:558:ASP:HB3	4:E:627:VAL:HG23	1.90	0.52
4:E:463:TYR:OH	4:E:465:GLU:OE1	2.22	0.52
4:E:614:LEU:HD11	4:E:657:ILE:HG23	1.92	0.52
6:7:166:LEU:O	4:E:51:ARG:NH2	2.40	0.52
2:C:390:GLU:OE2	2:C:467:ARG:NH2	2.42	0.52
5:F:691:ARG:HE	5:F:716:LEU:HD22	1.75	0.52
5:6:170:ILE:HD12	5:6:181:LEU:HD11	1.91	0.52
5:F:277:ARG:NE	5:F:363:GLU:OE2	2.43	0.52
2:3:541:SER:HB2	2:3:700:ARG:HD2	1.93	0.51
1:B:576:LEU:HD23	1:B:595:ALA:HB3	1.92	0.51
2:3:678:VAL:HG21	2:3:723:LYS:HG3	1.91	0.51
4:5:282:LEU:HD13	4:5:330:ILE:HG22	1.91	0.51
2:C:223:THR:HG21	4:E:244:ILE:HA	1.93	0.51
3:D:830:ARG:NH1	3:D:835:ASP:OD1	2.43	0.51
5:F:509:SER:OG	5:F:510:SER:N	2.42	0.51
6:G:494:THR:HB	6:G:548:ILE:HD11	1.92	0.51
2:C:432:THR:HG21	2:C:442:LEU:HD21	1.92	0.51
4:E:618:ALA:HB1	4:E:677:VAL:HG21	1.92	0.51
6:G:149:ARG:HG3	6:G:153:MET:HE2	1.92	0.51
2:3:295:VAL:HB	2:3:325:THR:HB	1.92	0.51
6:7:228:ARG:NH1	6:7:317:GLU:OE1	2.36	0.51
3:D:676:ASN:ND2	7:D:2001:AGS:S1G	2.80	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:197:ILE:HB	2:3:249:THR:HG23	1.92	0.51
4:5:300:ILE:HG23	4:5:324:ARG:HB3	1.93	0.51
3:D:231:ASN:OD1	3:D:234:ARG:NH2	2.44	0.51
3:4:775:VAL:HG12	3:4:779:LYS:HE3	1.93	0.51
2:C:426:ALA:HB3	2:C:429:ALA:HB2	1.93	0.51
3:D:345:ALA:HB2	3:D:365:ILE:HD13	1.93	0.51
2:3:522:GLN:OE1	4:5:643:ARG:NH2	2.44	0.51
3:4:317:LEU:O	6:7:341:ARG:NH2	2.44	0.51
3:D:417:LEU:HD13	3:D:463:VAL:HG21	1.93	0.51
6:G:259:ALA:H	6:G:305:SER:HB3	1.76	0.51
5:6:737:LYS:HB2	5:6:741:ALA:HB2	1.92	0.50
3:4:550:LYS:HG2	5:6:738:ARG:HH21	1.76	0.50
3:4:656:ILE:HD13	5:6:602:ALA:HB1	1.92	0.50
5:6:535:PRO:HB2	5:6:742:ILE:HD12	1.94	0.50
4:5:646:ILE:HG21	4:5:692:ALA:HA	1.93	0.50
1:B:501:MET:HE1	1:B:767:ILE:HD11	1.94	0.50
1:B:693:GLU:OE1	5:F:778:LYS:NZ	2.45	0.50
5:F:306:LYS:HB2	5:F:352:ARG:HB2	1.93	0.50
3:4:534:GLU:HG3	3:4:538:LYS:HE3	1.93	0.50
3:D:206:ARG:NH1	3:D:247:ASN:OD1	2.43	0.50
3:D:434:GLU:HB3	3:D:467:LYS:HB3	1.94	0.50
3:D:569:ASP:O	3:D:574:LYS:NZ	2.45	0.50
1:2:576:LEU:HD23	1:2:595:ALA:HB3	1.94	0.50
3:4:701:ARG:NH2	7:6:2001:AGS:S1G	2.84	0.50
5:F:379:VAL:HG23	5:F:454:PHE:HB3	1.93	0.50
1:B:779:HIS:CD2	1:B:781:MET:HG3	2.47	0.49
2:C:212:ARG:HD2	2:C:232:PRO:HD3	1.92	0.49
3:D:581:VAL:HA	3:D:584:ILE:HG22	1.94	0.49
3:4:321:ASP:HA	3:4:324:LYS:HD2	1.93	0.49
3:D:217:ASN:HD21	3:D:220:THR:HB	1.77	0.49
7:D:2001:AGS:O3A	6:G:687:ARG:NH2	2.45	0.49
6:G:75:LEU:O	6:G:199:ARG:NH1	2.45	0.49
6:G:428:VAL:HA	6:G:598:PHE:CE2	2.46	0.49
2:C:661:GLN:O	2:C:665:GLU:HG2	2.12	0.49
2:C:686:LEU:O	2:C:693:LYS:NZ	2.45	0.49
3:D:616:LEU:HD22	3:D:661:ILE:HD11	1.94	0.49
2:3:528:ASP:OD1	2:3:528:ASP:N	2.44	0.49
3:4:628:VAL:HG22	3:4:670:SER:HB2	1.93	0.49
6:7:526:PHE:HB3	6:7:567:ALA:HB2	1.93	0.49
2:3:216:ASP:OD1	2:3:216:ASP:N	2.45	0.49
2:3:426:ALA:HB3	2:3:429:ALA:HB2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:569:HIS:NE2	4:5:654:GLU:OE1	2.37	0.49
5:F:777:TYR:CG	5:F:800:LEU:HD12	2.48	0.49
6:G:210:ASN:OD1	6:G:213:ARG:NH2	2.46	0.49
7:4:2001:AGS:O2B	7:4:2001:AGS:O2A	2.31	0.49
7:D:2001:AGS:O2A	7:D:2001:AGS:O2B	2.31	0.49
3:4:527:ALA:HB3	3:4:537:LYS:HE2	1.94	0.49
2:C:507:ASN:ND2	6:G:319:SER:O	2.46	0.49
2:C:669:PRO:HG2	2:C:710:THR:HG23	1.93	0.49
5:F:126:SER:OG	5:F:128:ASP:OD1	2.31	0.49
5:F:317:ILE:HD13	5:F:350:ARG:HD3	1.94	0.49
3:D:543:GLN:HE21	3:D:670:SER:HB3	1.78	0.49
2:C:299:LYS:HD3	2:C:322:LEU:HD22	1.95	0.49
1:2:211:LEU:HD13	1:2:271:PHE:HB2	1.95	0.48
5:F:557:LYS:HB2	5:F:565:LEU:HD12	1.95	0.48
6:G:601:LEU:HD12	6:G:727:LEU:HG	1.94	0.48
1:2:596:LEU:HD11	1:2:620:ILE:HD13	1.95	0.48
1:2:790:TYR:CZ	1:2:794:ARG:HD2	2.48	0.48
3:4:585:THR:HG21	3:4:628:VAL:HB	1.95	0.48
6:7:435:LEU:HD21	6:7:564:LEU:HB2	1.95	0.48
6:7:451:ARG:NE	6:7:541:MET:O	2.46	0.48
1:B:688:ASP:HB3	1:B:691:ALA:HB3	1.95	0.48
1:B:779:HIS:HD2	1:B:781:MET:HG3	1.78	0.48
1:2:300:PHE:O	1:2:319:ARG:NH1	2.47	0.48
2:3:353:LEU:HD22	2:3:647:ILE:HG21	1.95	0.48
5:6:842:ASP:N	5:6:842:ASP:OD1	2.47	0.48
1:B:633:LYS:NZ	4:E:446:ALA:O	2.45	0.48
5:6:277:ARG:NH2	5:6:373:MET:O	2.46	0.48
5:6:650:VAL:O	5:6:654:GLU:HG3	2.13	0.48
2:C:400:ARG:HD2	2:C:491:GLU:HA	1.96	0.48
4:E:416:GLY:HA3	4:E:556:VAL:HB	1.95	0.48
5:6:126:SER:HB3	5:6:130:GLY:H	1.79	0.48
1:B:636:ILE:HD11	4:E:167:ILE:HG23	1.95	0.48
3:D:328:LEU:HD11	3:D:461:VAL:HG21	1.94	0.48
4:E:462:PHE:HE2	4:E:508:GLY:H	1.61	0.48
5:F:535:PRO:HB2	5:F:742:ILE:HG23	1.95	0.48
1:2:621:HIS:NE2	1:2:625:GLU:OE2	2.46	0.48
2:3:101:ASP:O	2:3:105:GLU:HG3	2.14	0.48
3:4:470:SER:HB3	3:4:473:ARG:HG2	1.95	0.48
4:5:396:SER:OG	4:5:661:GLU:OE1	2.29	0.48
5:6:673:ASN:HB3	5:6:675:ARG:NH1	2.28	0.48
5:6:403:VAL:HG22	5:6:450:TYR:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:550:GLN:HE21	5:6:677:SER:HB3	1.78	0.48
1:B:560:ALA:HB3	1:B:563:ALA:HB2	1.96	0.48
5:F:125:GLN:NE2	5:F:126:SER:O	2.47	0.48
5:F:820:THR:HG22	5:F:822:SER:H	1.79	0.48
1:B:484:PHE:HZ	1:B:765:LYS:HB2	1.78	0.48
5:F:409:GLN:HG2	5:F:412:LEU:HD12	1.95	0.48
2:3:430:ILE:HD12	2:3:465:ALA:HB2	1.96	0.47
3:4:572:THR:HG21	3:4:708:VAL:HB	1.95	0.47
6:7:257:VAL:HG22	6:7:306:LYS:HB3	1.95	0.47
6:7:500:ASP:O	6:7:504:ASP:N	2.46	0.47
5:F:733:ASP:OD1	5:F:737:LYS:NZ	2.47	0.47
6:7:76:ASN:OD1	6:7:199:ARG:NH2	2.47	0.47
6:7:196:LEU:HD21	6:7:257:VAL:HG21	1.96	0.47
6:7:625:GLN:NE2	6:7:627:ASP:O	2.46	0.47
4:E:183:CYS:HB3	4:E:188:HIS:H	1.79	0.47
1:2:537:ILE:HG23	1:2:678:ASP:HB2	1.96	0.47
5:6:139:GLN:O	5:6:143:MET:HG3	2.14	0.47
2:C:712:HIS:ND1	2:C:725:ASP:OD1	2.43	0.47
5:F:653:HIS:HB3	5:F:705:ILE:HD13	1.95	0.47
5:F:691:ARG:HH21	5:F:716:LEU:HB3	1.78	0.47
1:B:824:ARG:NH2	1:B:833:ASP:OD1	2.48	0.47
1:2:406:ARG:NH1	1:2:449:THR:OG1	2.48	0.47
1:2:631:ILE:HG13	4:5:446:ALA:HB3	1.97	0.47
3:4:474:LEU:HB2	3:4:586:PRO:HD3	1.96	0.47
6:7:521:CYS:HB2	6:7:561:THR:HG21	1.96	0.47
1:B:306:LEU:HB2	1:B:392:GLU:HG3	1.97	0.47
1:B:447:PHE:HB2	5:F:302:PRO:HG2	1.96	0.47
1:B:598:LEU:HD21	4:E:267:VAL:HA	1.95	0.47
1:B:690:GLU:HB3	1:B:694:ARG:HH12	1.79	0.47
3:D:306:TYR:HA	3:D:436:THR:HG21	1.96	0.47
3:D:628:VAL:HG22	3:D:670:SER:HB2	1.96	0.47
5:F:277:ARG:HG2	5:F:375:ARG:HD2	1.97	0.47
3:4:189:GLU:OE2	3:4:193:ASN:ND2	2.48	0.47
5:6:650:VAL:HA	5:6:653:HIS:ND1	2.30	0.47
6:7:322:VAL:HG21	6:7:328:PRO:HG3	1.97	0.47
3:D:292:ASP:OD1	3:D:292:ASP:N	2.48	0.47
6:G:435:LEU:HD21	6:G:564:LEU:HB2	1.96	0.47
1:2:800:THR:HG21	1:2:853:VAL:HG13	1.96	0.47
5:F:117:GLN:O	5:F:121:ASP:HB2	2.15	0.47
5:F:742:ILE:HG22	5:F:744:PRO:HD3	1.96	0.47
1:B:391:GLN:NE2	5:F:671:THR:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:178:ARG:HA	3:D:178:ARG:HD2	1.77	0.47
3:D:585:THR:HG21	3:D:628:VAL:HB	1.96	0.47
4:E:433:SER:HB2	4:E:436:ALA:HB2	1.97	0.47
5:F:423:THR:HA	5:F:426:ILE:HD13	1.97	0.47
1:2:383:ARG:HB2	1:2:412:ALA:HB2	1.97	0.46
4:5:31:PHE:CG	4:5:90:PHE:HD1	2.33	0.46
4:5:415:LEU:HA	4:5:523:ALA:O	2.14	0.46
6:7:117:PHE:HB3	6:7:202:LEU:HD11	1.96	0.46
1:B:406:ARG:NH1	1:B:449:THR:OG1	2.48	0.46
1:B:783:MET:HG3	4:E:573:ILE:HG21	1.96	0.46
1:2:598:LEU:HD21	4:5:267:VAL:HA	1.97	0.46
1:B:536:ASP:HB2	1:B:645:SER:HB2	1.97	0.46
1:2:594:GLY:O	1:2:598:LEU:HB2	2.16	0.46
1:2:850:LYS:O	1:2:854:ARG:N	2.44	0.46
2:3:314:LEU:HD11	4:5:200:ILE:HA	1.96	0.46
1:B:786:VAL:HA	1:B:789:VAL:HG12	1.98	0.46
4:E:31:PHE:CG	4:E:90:PHE:HD1	2.33	0.46
5:F:321:VAL:HG11	5:F:330:PRO:HD3	1.96	0.46
6:G:542:GLU:OE2	6:G:687:ARG:NE	2.48	0.46
3:4:604:TYR:OH	6:7:554:ASN:ND2	2.49	0.46
1:B:410:LEU:HD22	1:B:456:ILE:HD11	1.97	0.46
6:G:454:ILE:O	6:G:562:SER:OG	2.30	0.46
6:G:570:LEU:HD23	6:G:585:ASN:HD21	1.79	0.46
1:B:790:TYR:CZ	1:B:794:ARG:HD2	2.50	0.46
4:E:25:THR:HG22	4:E:29:LYS:HE2	1.96	0.46
4:E:625:ASN:O	4:E:625:ASN:ND2	2.46	0.46
5:F:585:LEU:HD23	5:F:637:CYS:HB3	1.97	0.46
5:6:433:LEU:HD13	1:B:342:LEU:HB3	1.97	0.46
5:6:694:SER:OG	5:6:792:SER:O	2.32	0.46
3:D:356:MET:HE3	3:D:368:PRO:HG3	1.96	0.46
4:E:444:SER:HB2	4:E:447:ALA:HB3	1.96	0.46
4:E:535:SER:O	4:E:539:ASN:ND2	2.46	0.46
1:2:530:LYS:HB3	4:5:428:PHE:HE1	1.80	0.46
3:4:581:VAL:HA	3:4:584:ILE:HG22	1.97	0.46
4:5:5:ARG:HG2	4:5:218:GLU:HB2	1.97	0.46
4:5:430:GLU:HG3	4:5:438:TYR:HB2	1.98	0.46
6:7:61:PRO:HB2	6:7:64:MET:HB2	1.98	0.46
1:B:505:ILE:O	1:B:512:LYS:NZ	2.46	0.46
6:G:91:GLU:O	6:G:95:GLN:OE1	2.33	0.46
6:G:459:MET:HE1	6:G:584:ILE:HG23	1.98	0.46
3:4:304:ARG:HB3	3:4:465:HIS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:409:GLN:HG2	5:6:412:LEU:HD12	1.97	0.46
5:6:412:LEU:O	5:6:416:LYS:NZ	2.37	0.46
1:B:447:PHE:HE1	5:F:304:LEU:HB2	1.81	0.46
1:B:610:ASP:OD1	1:B:610:ASP:N	2.46	0.46
2:C:478:MET:HE2	2:C:482:ASP:HB3	1.98	0.46
6:G:17:LEU:HD13	6:G:113:PHE:HZ	1.80	0.46
6:G:537:ILE:HG23	6:G:563:ILE:HD13	1.97	0.46
1:2:534:ARG:O	1:2:815:ARG:NH1	2.48	0.46
3:D:812:LYS:HE3	3:D:814:LYS:HE2	1.98	0.46
6:G:656:VAL:HG12	6:G:710:ILE:HD13	1.98	0.46
3:4:290:ASP:OD1	3:4:290:ASP:N	2.49	0.45
4:5:151:LEU:HD11	4:5:162:LEU:HD22	1.97	0.45
4:5:157:SER:N	4:5:298:TYR:O	2.43	0.45
2:C:295:VAL:HB	2:C:325:THR:HB	1.97	0.45
4:E:149:ARG:NH1	4:E:260:GLU:OE2	2.49	0.45
1:B:267:MET:HB2	1:B:267:MET:HE2	1.64	0.45
1:B:324:VAL:HG21	1:B:418:SER:HB2	1.99	0.45
4:E:571:HIS:O	4:E:575:ILE:HG12	2.17	0.45
5:F:628:LEU:HD11	5:F:652:ILE:HG13	1.97	0.45
1:2:763:LEU:O	1:2:767:ILE:HG13	2.17	0.45
3:4:263:ASN:OD1	3:4:324:LYS:NZ	2.50	0.45
3:4:457:TYR:HB2	6:7:253:PRO:HG2	1.98	0.45
3:4:824:GLU:OE2	3:4:827:ARG:NH2	2.49	0.45
6:7:644:TYR:O	6:7:647:THR:OG1	2.33	0.45
1:B:622:GLU:OE1	4:E:445:SER:N	2.48	0.45
6:G:318:LEU:HD21	6:G:348:ILE:HD12	1.98	0.45
2:3:572:LEU:HD13	4:5:613:ARG:HH11	1.81	0.45
3:4:650:GLU:OE2	3:4:796:ARG:NH2	2.49	0.45
5:6:722:LYS:O	5:6:726:GLU:HG2	2.17	0.45
1:B:376:ASN:O	1:B:380:THR:OG1	2.29	0.45
1:B:661:LEU:HD12	1:B:662:PRO:HD2	1.99	0.45
1:B:770:ALA:HA	1:B:774:ILE:HG12	1.99	0.45
3:D:290:ASP:OD1	3:D:290:ASP:N	2.49	0.45
5:6:615:ASP:OD1	5:6:615:ASP:N	2.49	0.45
1:B:798:ILE:HD11	4:E:560:HIS:CE1	2.51	0.45
3:4:393:ASP:HB3	3:4:424:VAL:HG21	1.98	0.45
5:6:574:VAL:O	5:6:714:VAL:HA	2.17	0.45
5:F:355:ASP:HB3	5:F:386:VAL:HG21	1.99	0.45
4:5:580:ALA:HA	4:5:583:MET:HE2	1.99	0.45
1:B:651:ASN:ND2	7:B:2001:AGS:S1G	2.74	0.45
2:3:177:ASN:N	2:3:298:PHE:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:699:ALA:O	2:3:702:LEU:HB3	2.17	0.45
3:4:266:GLN:HE21	3:4:440:ARG:HH22	1.64	0.45
4:E:396:SER:OG	4:E:661:GLU:OE1	2.34	0.45
4:E:546:ILE:HA	4:E:549:ARG:HG2	1.98	0.45
5:F:650:VAL:HA	5:F:653:HIS:NE2	2.32	0.45
4:5:293:THR:HG23	4:5:334:GLN:HB2	1.99	0.45
4:5:497:MET:HG2	4:5:519:VAL:HG21	1.99	0.45
6:7:586:LEU:HD23	6:7:591:LEU:HD13	1.98	0.45
6:7:593:ARG:HG3	6:7:593:ARG:HH11	1.82	0.45
1:B:486:LYS:HA	1:B:489:ARG:HH21	1.81	0.45
4:E:258:LEU:HD13	4:E:276:MET:HE1	1.98	0.45
5:F:357:GLN:HB2	5:F:386:VAL:HG13	1.98	0.45
1:2:550:SER:O	1:2:554:LYS:HG3	2.16	0.44
2:3:203:ALA:O	2:3:207:GLY:N	2.50	0.44
5:6:656:MET:HB3	5:6:708:ARG:HD3	1.99	0.44
3:D:474:LEU:HB2	3:D:586:PRO:HD3	1.99	0.44
4:E:405:ARG:NH2	4:E:500:GLN:OE1	2.51	0.44
3:4:308:VAL:HG22	3:4:327:ASN:HB2	1.99	0.44
7:4:2001:AGS:O3A	6:7:687:ARG:NH2	2.50	0.44
6:7:440:VAL:HG22	6:7:701:LYS:HE3	1.98	0.44
2:C:353:LEU:HD13	2:C:356:LYS:HE3	1.98	0.44
3:D:694:LEU:HD22	3:D:698:LEU:HD23	1.97	0.44
3:D:746:PHE:HA	3:D:749:MET:HG2	1.99	0.44
5:F:842:ASP:OD1	5:F:842:ASP:N	2.47	0.44
1:B:481:GLU:O	1:B:485:ARG:HG2	2.17	0.44
1:B:597:VAL:HG23	1:B:629:ILE:HD12	1.99	0.44
2:C:681:LYS:HE2	2:C:681:LYS:HB3	1.67	0.44
3:D:429:ALA:O	3:D:587:ARG:NH2	2.45	0.44
4:5:535:SER:OG	4:5:695:ASP:OD1	2.36	0.44
1:B:511:ILE:O	1:B:515:VAL:HG23	2.17	0.44
1:B:785:LYS:NZ	1:B:831:SER:OG	2.49	0.44
2:C:391:LYS:HB2	2:C:399:LEU:HB2	1.99	0.44
3:D:758:ILE:HG22	3:D:760:PRO:HD3	1.98	0.44
4:E:41:ASP:OD1	4:E:41:ASP:N	2.50	0.44
5:F:776:LYS:HA	5:F:776:LYS:HD3	1.71	0.44
4:5:183:CYS:HB3	4:5:188:HIS:H	1.82	0.44
5:6:419:SER:HB2	5:6:448:LEU:HD11	2.00	0.44
4:E:300:ILE:HG23	4:E:324:ARG:HB3	1.98	0.44
6:G:193:PRO:HD2	6:G:196:LEU:HD12	1.98	0.44
6:G:513:LEU:HD13	6:G:540:VAL:HG21	1.98	0.44
2:3:570:ARG:NH2	4:5:613:ARG:HH21	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:2001:AGS:S1G	7:5:2001:AGS:O2B	2.75	0.44
5:6:297:THR:HG22	5:6:359:VAL:HG23	1.99	0.44
6:7:210:ASN:OD1	6:7:211:CYS:N	2.51	0.44
6:7:520:ILE:HA	6:7:562:SER:O	2.18	0.44
5:F:297:THR:OG1	5:F:357:GLN:NE2	2.50	0.44
3:4:707:LEU:O	3:4:834:LYS:NZ	2.47	0.44
6:7:146:ARG:NH2	6:7:304:ALA:O	2.44	0.44
4:E:430:GLU:HG3	4:E:438:TYR:HB2	2.00	0.44
2:3:198:ARG:HB3	2:3:249:THR:HG22	1.99	0.44
4:5:71:TYR:HD1	4:5:72:ASN:HB2	1.82	0.44
4:5:352:GLU:HA	4:5:355:GLU:HG2	2.00	0.44
5:6:776:LYS:HD3	5:6:776:LYS:HA	1.80	0.44
5:6:803:MET:HE2	5:6:828:TYR:HA	1.99	0.44
2:C:430:ILE:HD12	2:C:465:ALA:HB2	1.99	0.44
4:E:164:GLY:HA3	4:E:258:LEU:HD21	1.99	0.44
6:G:322:VAL:HG21	6:G:328:PRO:HG3	1.99	0.44
2:C:461:ALA:HB2	4:E:505:ALA:HB1	2.00	0.43
6:G:533:ASP:O	6:G:537:ILE:HG12	2.18	0.43
1:2:662:PRO:O	1:2:666:ASN:ND2	2.51	0.43
2:3:182:VAL:HG11	2:3:274:ILE:HD11	2.00	0.43
4:E:90:PHE:CE2	4:E:137:LEU:HD13	2.53	0.43
4:E:437:VAL:HG23	4:E:472:ALA:HB2	1.99	0.43
4:E:469:MET:HE3	4:E:469:MET:HB3	1.95	0.43
2:3:196:LEU:HD21	2:3:199:SER:HB3	2.00	0.43
3:4:139:HIS:H	3:4:266:GLN:HE22	1.65	0.43
3:4:819:LEU:HD23	3:4:823:GLN:HG3	1.99	0.43
1:B:676:ARG:HA	1:B:676:ARG:HD2	1.79	0.43
2:C:651:VAL:HG13	2:C:655:PHE:HD2	1.83	0.43
4:E:266:PRO:HG2	4:E:269:GLU:HB2	1.99	0.43
5:F:629:MET:HE2	5:F:629:MET:HB3	1.79	0.43
6:G:223:LYS:HA	6:G:223:LYS:HD2	1.81	0.43
5:6:288:LEU:HD23	5:6:454:PHE:HE1	1.83	0.43
5:6:429:THR:HG23	1:B:347:ILE:HD11	2.00	0.43
2:C:456:ARG:NH1	2:C:458:GLU:OE1	2.51	0.43
5:F:319:ASP:OD2	5:F:350:ARG:NH2	2.51	0.43
1:2:690:GLU:HG3	1:2:694:ARG:NE	2.34	0.43
5:6:566:ARG:O	5:6:805:ARG:NE	2.49	0.43
3:D:284:ILE:HD11	3:D:293:LEU:HD13	1.99	0.43
4:E:297:ILE:HB	4:E:329:LYS:HB2	2.00	0.43
6:7:166:LEU:HA	4:E:47:ARG:HH11	1.84	0.43
1:B:459:ARG:HD2	1:B:459:ARG:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:646:ILE:HG21	4:E:692:ALA:HA	2.00	0.43
6:G:147:ARG:O	6:G:151:GLU:HG2	2.18	0.43
6:G:425:ASN:HB3	6:G:428:VAL:HB	2.01	0.43
6:G:637:LYS:HD3	6:G:637:LYS:HA	1.82	0.43
3:4:147:ARG:HH22	4:E:16:GLY:HA2	1.83	0.43
3:4:453:LEU:O	6:7:277:THR:OG1	2.31	0.43
3:4:649:MET:HE2	3:4:671:ILE:HG21	2.01	0.43
5:6:347:ASN:O	5:6:351:SER:OG	2.34	0.43
3:D:265:PRO:HB3	3:D:325:LEU:HG	2.01	0.43
3:D:470:SER:HB3	3:D:473:ARG:HG2	2.01	0.43
5:F:625:ALA:HB1	5:F:629:MET:HB2	2.01	0.43
6:G:358:ALA:N	6:G:373:GLU:O	2.50	0.43
1:2:195:SER:O	1:2:199:THR:OG1	2.27	0.43
1:2:542:LEU:HD22	1:2:682:VAL:HG23	2.01	0.43
4:5:371:THR:HG21	4:5:386:LYS:HG2	2.01	0.43
1:B:220:ASP:OD1	1:B:220:ASP:N	2.45	0.43
1:B:778:LEU:HD12	4:E:577:THR:HG22	2.01	0.43
2:C:216:ASP:N	2:C:216:ASP:OD1	2.51	0.43
1:2:850:LYS:HE3	1:2:852:SER:HB2	2.01	0.43
2:3:462:MET:HE3	2:3:489:VAL:HG11	2.00	0.43
2:3:577:LEU:HD12	2:3:577:LEU:HA	1.91	0.43
3:4:268:VAL:O	3:4:272:MET:HG3	2.19	0.43
6:7:470:LEU:HD23	6:7:522:CYS:HB3	2.01	0.43
1:B:474:PHE:CE1	1:B:764:MET:HE2	2.54	0.43
1:B:552:ILE:O	1:B:556:VAL:HG23	2.19	0.43
2:C:189:THR:HG23	2:C:256:ILE:HG22	1.99	0.43
3:D:635:ASP:OD1	3:D:635:ASP:N	2.52	0.43
5:F:300:VAL:HG13	5:F:386:VAL:HG11	1.99	0.43
6:G:146:ARG:NH2	6:G:304:ALA:O	2.48	0.43
2:3:417:GLN:HE21	4:5:404:MET:HE3	1.84	0.43
3:4:559:ARG:HE	3:4:559:ARG:HB3	1.59	0.43
5:6:778:LYS:O	5:6:782:LYS:HG3	2.19	0.43
3:D:527:ALA:HB3	3:D:537:LYS:HE2	2.00	0.43
6:G:479:ARG:NE	6:G:517:ASP:O	2.52	0.43
1:2:445:PRO:HD3	5:6:325:PHE:O	2.18	0.42
1:2:510:ASP:OD2	1:2:510:ASP:N	2.51	0.42
2:3:558:ASP:CG	4:5:630:ARG:HE	2.27	0.42
3:4:292:ASP:OD1	3:4:292:ASP:N	2.51	0.42
3:4:344:VAL:O	3:4:389:CYS:HB2	2.19	0.42
2:C:177:ASN:N	2:C:298:PHE:O	2.45	0.42
3:D:404:ASP:OD1	3:D:405:PHE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:132:ILE:HD11	6:G:141:VAL:HG12	2.01	0.42
3:D:176:PRO:HB2	3:D:177:LEU:H	1.66	0.42
3:D:578:LEU:HB3	3:D:590:TYR:HE2	1.84	0.42
2:3:666:ARG:HD3	2:3:666:ARG:HA	1.86	0.42
1:B:628:SER:OG	1:B:639:THR:OG1	2.37	0.42
6:G:59:LYS:HB2	6:G:59:LYS:HE2	1.87	0.42
2:3:570:ARG:HH21	4:5:616:PRO:HD3	1.83	0.42
4:5:139:LEU:HD21	4:5:331:LEU:HD13	2.01	0.42
4:5:279:ASP:OD2	4:5:279:ASP:N	2.51	0.42
5:6:657:GLU:OE1	5:6:708:ARG:NH1	2.52	0.42
2:C:455:ARG:HB2	2:C:502:ILE:HD11	2.01	0.42
3:D:524:ARG:NH1	3:D:740:ASP:O	2.53	0.42
4:E:423:SER:OG	4:E:480:ASP:OD2	2.37	0.42
6:G:181:LEU:HA	6:G:184:VAL:HG12	2.02	0.42
6:G:592:SER:OG	6:G:687:ARG:NH1	2.53	0.42
4:5:436:ALA:HA	4:5:476:VAL:O	2.19	0.42
6:7:479:ARG:NE	6:7:517:ASP:O	2.51	0.42
2:C:171:LEU:HD11	2:C:182:VAL:HG21	2.00	0.42
2:C:497:ILE:O	2:C:503:HIS:HA	2.19	0.42
3:D:824:GLU:OE2	3:D:827:ARG:NH2	2.49	0.42
4:E:279:ASP:N	4:E:279:ASP:OD1	2.52	0.42
1:B:259:PHE:HB3	1:B:267:MET:HE3	2.00	0.42
1:B:323:VAL:HG22	1:B:423:GLU:HG2	2.01	0.42
4:E:483:ASP:OD1	4:E:484:LYS:N	2.53	0.42
6:G:607:ASP:OD1	6:G:607:ASP:N	2.52	0.42
2:3:400:ARG:HD2	2:3:491:GLU:HA	2.02	0.42
5:6:356:TRP:CH2	5:6:358:LYS:HB2	2.55	0.42
4:E:169:THR:HG22	4:E:256:LEU:HD22	2.01	0.42
2:3:280:ASP:OD2	2:3:280:ASP:N	2.51	0.42
3:4:687:PRO:HD2	3:4:690:GLU:HG3	2.00	0.42
6:7:193:PRO:HD2	6:7:196:LEU:HD12	2.02	0.42
6:7:457:CYS:HB3	6:7:597:LEU:HG	2.01	0.42
5:F:158:LEU:HD21	5:F:170:ILE:HD12	2.01	0.42
5:6:330:PRO:O	5:6:344:TRP:NE1	2.53	0.42
1:B:224:ARG:HE	1:B:224:ARG:HB3	1.64	0.42
4:E:633:LEU:HD13	4:E:648:ILE:HG22	2.02	0.42
2:3:669:PRO:HG2	2:3:710:THR:HG23	2.02	0.41
3:4:746:PHE:HA	3:4:749:MET:HG2	2.02	0.41
5:6:650:VAL:HA	5:6:653:HIS:CE1	2.55	0.41
6:7:143:LEU:HG	6:7:197:THR:HA	2.01	0.41
2:C:557:ARG:O	2:C:561:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:151:LEU:HD11	4:E:162:LEU:HD22	2.02	0.41
4:E:371:THR:HG21	4:E:386:LYS:HG2	2.02	0.41
4:E:436:ALA:HA	4:E:476:VAL:O	2.20	0.41
6:G:179:ASP:O	6:G:183:GLU:HG2	2.20	0.41
2:3:363:LEU:HD23	2:3:651:VAL:HG21	2.02	0.41
3:4:342:MET:HE2	3:4:389:CYS:SG	2.60	0.41
4:5:101:ILE:HG12	6:G:166:LEU:HD13	2.01	0.41
6:7:256:GLU:OE1	6:7:306:LYS:NZ	2.36	0.41
6:7:527:ASP:OD1	6:7:527:ASP:N	2.53	0.41
2:C:678:VAL:HG21	2:C:723:LYS:HG2	2.01	0.41
3:D:604:TYR:CE1	3:D:617:GLU:HB3	2.55	0.41
5:F:596:VAL:HG12	5:F:631:ALA:HB2	2.02	0.41
5:F:737:LYS:HB2	5:F:741:ALA:HB2	2.03	0.41
3:4:676:ASN:ND2	7:4:2001:AGS:S1G	2.93	0.41
5:6:656:MET:SD	5:6:678:ILE:HD12	2.60	0.41
6:7:685:THR:HG22	6:7:687:ARG:H	1.85	0.41
1:B:596:LEU:HD11	1:B:620:ILE:HD13	2.01	0.41
1:B:789:VAL:HG23	1:B:864:TYR:CZ	2.56	0.41
2:C:684:THR:HG22	6:G:609:ASP:HB3	2.01	0.41
3:D:445:ARG:HB2	5:F:410:LEU:HD11	2.02	0.41
1:2:306:LEU:HB2	1:2:392:GLU:HG3	2.02	0.41
3:4:616:LEU:HD23	3:4:616:LEU:HA	1.85	0.41
4:5:449:LEU:HD12	4:5:468:ALA:HB3	2.02	0.41
6:7:17:LEU:HD13	6:7:113:PHE:HZ	1.85	0.41
6:7:530:ASP:N	6:7:530:ASP:OD1	2.47	0.41
2:C:279:ASP:OD1	2:C:279:ASP:N	2.52	0.41
2:C:478:MET:HE1	2:C:486:ILE:HD12	2.02	0.41
3:D:701:ARG:NH1	7:F:2001:AGS:S1G	2.89	0.41
1:2:203:VAL:O	1:2:207:ILE:HG12	2.19	0.41
1:2:315:SER:N	1:2:430:TYR:O	2.48	0.41
1:2:376:ASN:O	1:2:380:THR:OG1	2.29	0.41
4:5:580:ALA:HA	4:5:583:MET:HG2	2.01	0.41
1:B:383:ARG:HB2	1:B:412:ALA:HB2	2.02	0.41
5:F:585:LEU:HD22	5:F:639:ASP:OD1	2.20	0.41
6:G:618:TYR:CG	6:G:626:PRO:HB3	2.55	0.41
1:2:220:ASP:OD1	1:2:220:ASP:N	2.44	0.41
4:5:557:LYS:HD2	4:5:557:LYS:HA	1.70	0.41
5:6:359:VAL:HG13	5:6:379:VAL:HG13	2.02	0.41
3:4:368:PRO:HG2	3:4:382:MET:HG3	2.03	0.41
2:C:254:GLN:HB2	2:C:283:VAL:HG12	2.01	0.41
1:2:530:LYS:HB3	4:5:428:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:846:VAL:HA	1:2:849:GLN:HG2	2.02	0.41
2:3:210:HIS:HB3	6:7:5:LEU:HG	2.03	0.41
3:4:176:PRO:HB2	3:4:177:LEU:H	1.61	0.41
3:4:650:GLU:HB2	3:4:701:ARG:HH11	1.86	0.41
4:5:605:TYR:HE2	4:5:668:LEU:HD11	1.85	0.41
3:D:802:ILE:HD11	5:F:732:VAL:HG22	2.01	0.41
6:G:249:SER:HB3	6:G:312:GLU:H	1.85	0.41
6:G:481:VAL:HG11	6:G:512:ALA:HB1	2.02	0.41
1:2:685:ASP:OD1	1:2:685:ASP:N	2.46	0.41
1:2:693:GLU:HG3	5:6:778:LYS:HD2	2.01	0.41
3:4:663:THR:HG21	5:6:374:PRO:HG3	2.03	0.41
4:5:274:LEU:HD23	4:5:274:LEU:HA	1.94	0.41
4:5:416:GLY:HA3	4:5:556:VAL:HB	2.02	0.41
4:5:432:VAL:HG23	4:5:596:ILE:HG13	2.03	0.41
5:6:609:THR:HG22	5:6:628:LEU:HD12	2.03	0.41
5:6:653:HIS:HB3	5:6:705:ILE:HD13	2.03	0.41
5:6:694:SER:OG	5:6:695:LEU:N	2.54	0.41
5:6:767:LYS:HB3	5:6:767:LYS:HE3	1.72	0.41
6:7:59:LYS:HE2	6:7:59:LYS:HB2	1.85	0.41
3:D:195:ARG:O	3:D:199:MET:HG2	2.21	0.41
1:2:447:PHE:HE1	5:6:304:LEU:HB2	1.85	0.41
2:3:561:ILE:HG21	4:5:650:ILE:HG12	2.02	0.41
6:7:243:GLY:HA2	6:7:318:LEU:HG	2.03	0.41
6:7:423:TYR:HB2	6:7:615:HIS:CG	2.56	0.41
1:B:495:ASP:O	1:B:499:SER:N	2.52	0.41
4:E:493:ILE:HD13	4:E:493:ILE:HA	1.94	0.41
3:4:429:ALA:O	3:4:587:ARG:NH2	2.52	0.40
5:6:412:LEU:HD23	5:6:412:LEU:HA	1.97	0.40
6:7:259:ALA:H	6:7:305:SER:HB3	1.85	0.40
6:7:658:ASP:O	6:7:662:GLN:HG2	2.21	0.40
2:C:462:MET:HE2	2:C:486:ILE:HG12	2.02	0.40
2:C:466:ASP:HB3	6:G:324:VAL:HG13	2.02	0.40
5:F:614:ARG:HB2	5:F:621:TYR:CE1	2.56	0.40
6:G:5:LEU:HD12	6:G:5:LEU:HA	1.90	0.40
3:4:438:THR:HG23	3:4:462:ASP:HB3	2.03	0.40
6:7:592:SER:OG	6:7:687:ARG:NH1	2.55	0.40
1:B:324:VAL:HG13	1:B:388:VAL:HG13	2.04	0.40
1:B:793:LEU:HD11	1:B:805:ILE:HG21	2.03	0.40
3:D:457:TYR:HB2	6:G:253:PRO:HG2	2.03	0.40
3:D:719:GLU:HA	3:D:722:LYS:HE2	2.03	0.40
6:G:210:ASN:O	6:G:214:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:459:MET:HA	6:G:567:ALA:O	2.22	0.40
2:3:442:LEU:HD13	2:3:486:ILE:HD11	2.02	0.40
3:4:404:ASP:OD1	3:4:404:ASP:N	2.51	0.40
3:4:711:LYS:HE3	3:4:848:ASN:HA	2.02	0.40
3:D:276:ILE:HD13	3:D:276:ILE:HA	1.91	0.40
4:E:87:ILE:HG23	4:E:137:LEU:HD23	2.03	0.40
5:F:574:VAL:HG21	5:F:699:LEU:HD11	2.04	0.40
5:F:649:GLN:HA	5:F:652:ILE:HG22	2.03	0.40
1:2:271:PHE:CD2	1:2:295:VAL:HG21	2.56	0.40
6:7:601:LEU:HD12	6:7:727:LEU:HG	2.03	0.40
1:B:445:PRO:HD3	5:F:325:PHE:O	2.20	0.40
3:D:212:ARG:HB3	3:D:215:PHE:HD1	1.87	0.40
3:D:435:VAL:HG13	3:D:463:VAL:HG13	2.04	0.40
3:D:456:LEU:HD12	3:D:456:LEU:HA	1.88	0.40
6:7:242:ARG:HB3	6:7:350:ASP:OD1	2.22	0.40
2:C:103:LEU:HD11	2:C:110:PHE:HD2	1.86	0.40
4:E:90:PHE:CE2	4:E:94:ILE:HD11	2.57	0.40
6:G:154:LEU:HD21	6:G:191:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	622/868 (72%)	602 (97%)	20 (3%)	0	100	100
1	B	622/868 (72%)	608 (98%)	14 (2%)	0	100	100
2	3	627/971 (65%)	612 (98%)	15 (2%)	0	100	100
2	C	627/971 (65%)	606 (97%)	21 (3%)	0	100	100
3	4	684/933 (73%)	668 (98%)	16 (2%)	0	100	100
3	D	664/933 (71%)	649 (98%)	15 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	5	650/775 (84%)	630 (97%)	20 (3%)	0	100	100
4	E	650/775 (84%)	633 (97%)	17 (3%)	0	100	100
5	6	638/1017 (63%)	615 (96%)	23 (4%)	0	100	100
5	F	638/1017 (63%)	620 (97%)	18 (3%)	0	100	100
6	7	693/845 (82%)	684 (99%)	9 (1%)	0	100	100
6	G	693/845 (82%)	682 (98%)	11 (2%)	0	100	100
All	All	7808/10818 (72%)	7609 (98%)	199 (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	552/770 (72%)	552 (100%)	0	100	100
1	B	552/770 (72%)	552 (100%)	0	100	100
2	3	550/835 (66%)	550 (100%)	0	100	100
2	C	550/835 (66%)	550 (100%)	0	100	100
3	4	628/848 (74%)	628 (100%)	0	100	100
3	D	606/848 (72%)	606 (100%)	0	100	100
4	5	588/688 (86%)	587 (100%)	1 (0%)	92	97
4	E	588/688 (86%)	587 (100%)	1 (0%)	92	97
5	6	565/886 (64%)	565 (100%)	0	100	100
5	F	565/886 (64%)	565 (100%)	0	100	100
6	7	618/753 (82%)	618 (100%)	0	100	100
6	G	618/753 (82%)	618 (100%)	0	100	100
All	All	6980/9560 (73%)	6978 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	5	339	THR
4	E	339	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	526	ASN
2	3	293	ASN
2	3	374	HIS
2	3	376	HIS
2	3	417	GLN
2	3	530	HIS
2	3	673	GLN
2	3	682	ASN
3	4	253	GLN
3	4	377	ASN
3	4	543	GLN
3	4	646	HIS
4	5	15	GLN
4	5	454	GLN
4	5	579	ASN
4	5	581	ASN
4	5	636	ASN
5	6	340	ASN
5	6	409	GLN
5	6	583	GLN
5	6	669	HIS
5	6	673	ASN
5	6	799	GLN
5	6	814	ASN
6	7	159	ASN
6	7	291	GLN
6	7	297	GLN
6	7	554	ASN
6	7	620	HIS
1	B	200	GLN
1	B	238	ASN
1	B	356	ASN
1	B	626	GLN
2	C	29	GLN
2	C	210	HIS
2	C	293	ASN
2	C	324	ASN

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Mol	Chain	Res	Type
2	C	351	ASN
2	C	374	HIS
2	C	682	ASN
3	D	240	ASN
3	D	350	ASN
3	D	377	ASN
3	D	400	GLN
4	E	524	ASN
4	E	579	ASN
4	E	632	GLN
4	E	636	ASN
4	E	673	GLN
5	F	269	ASN
5	F	362	GLN
5	F	540	HIS
5	F	814	ASN
6	G	16	ASN
6	G	19	ASN
6	G	332	ASN
6	G	518	ASN
6	G	622	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 22 are monoatomic - leaving 12 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
7	AGS	6	2001	8	26,33,33	0.69	1 (3%)	26,52,52	0.89	2 (7%)
10	ADP	C	2001	8	24,29,29	0.93	1 (4%)	29,45,45	1.43	4 (13%)
10	ADP	3	2001	8	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
7	AGS	D	2001	8	26,33,33	0.70	0	26,52,52	1.08	2 (7%)
7	AGS	5	2001	8	26,33,33	0.72	1 (3%)	26,52,52	1.17	2 (7%)
7	AGS	E	2001	8	26,33,33	0.72	1 (3%)	26,52,52	1.15	2 (7%)
7	AGS	F	2001	8	26,33,33	0.70	1 (3%)	26,52,52	1.06	2 (7%)
7	AGS	2	2001	8	26,33,33	0.71	1 (3%)	26,52,52	1.04	2 (7%)
7	AGS	G	2001	8	26,33,33	0.72	1 (3%)	26,52,52	1.06	2 (7%)
7	AGS	B	2001	8	26,33,33	0.69	1 (3%)	26,52,52	1.03	2 (7%)
7	AGS	4	2001	8	26,33,33	0.69	0	26,52,52	1.10	2 (7%)
7	AGS	7	2001	8	26,33,33	0.72	1 (3%)	26,52,52	1.05	2 (7%)

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
7	AGS	6	2001	8	-	3/17/38/38	0/3/3/3
10	ADP	C	2001	8	-	3/12/32/32	0/3/3/3
10	ADP	3	2001	8	-	3/12/32/32	0/3/3/3
7	AGS	D	2001	8	-	7/17/38/38	0/3/3/3
7	AGS	5	2001	8	-	6/17/38/38	0/3/3/3
7	AGS	E	2001	8	-	6/17/38/38	0/3/3/3
7	AGS	F	2001	8	-	2/17/38/38	0/3/3/3
7	AGS	2	2001	8	-	7/17/38/38	0/3/3/3
7	AGS	G	2001	8	-	7/17/38/38	0/3/3/3
7	AGS	B	2001	8	-	4/17/38/38	0/3/3/3
7	AGS	4	2001	8	-	7/17/38/38	0/3/3/3
7	AGS	7	2001	8	-	6/17/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	2001	ADP	C5-C4	2.46	1.47	1.40
10	C	2001	ADP	C5-C4	2.39	1.47	1.40
7	G	2001	AGS	PG-S1G	2.13	1.95	1.90
7	E	2001	AGS	PG-S1G	2.12	1.95	1.90
7	7	2001	AGS	PG-S1G	2.11	1.95	1.90
7	5	2001	AGS	PG-S1G	2.11	1.95	1.90
7	2	2001	AGS	PG-S1G	2.08	1.95	1.90
7	6	2001	AGS	PG-S1G	2.04	1.95	1.90
7	F	2001	AGS	PG-S1G	2.01	1.95	1.90
7	B	2001	AGS	PG-S1G	2.00	1.95	1.90

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	5	2001	AGS	PA-O3A-PB	-4.64	116.92	132.83
7	E	2001	AGS	PA-O3A-PB	-4.46	117.51	132.83
7	D	2001	AGS	PA-O3A-PB	-4.07	118.85	132.83
7	4	2001	AGS	PA-O3A-PB	-4.05	118.93	132.83
7	7	2001	AGS	PA-O3A-PB	-3.86	119.59	132.83
7	G	2001	AGS	PA-O3A-PB	-3.85	119.62	132.83
7	F	2001	AGS	PA-O3A-PB	-3.83	119.67	132.83
7	2	2001	AGS	PA-O3A-PB	-3.82	119.73	132.83
7	B	2001	AGS	PA-O3A-PB	-3.79	119.83	132.83
10	3	2001	ADP	C3'-C2'-C1'	3.58	106.36	100.98
10	C	2001	ADP	PA-O3A-PB	-3.39	121.20	132.83
10	3	2001	ADP	PA-O3A-PB	-3.19	121.87	132.83
10	C	2001	ADP	N3-C2-N1	-3.18	123.70	128.68
10	C	2001	ADP	C3'-C2'-C1'	3.14	105.70	100.98
10	3	2001	ADP	N3-C2-N1	-3.13	123.79	128.68
7	6	2001	AGS	PA-O3A-PB	-2.72	123.51	132.83
10	C	2001	ADP	C4-C5-N7	-2.60	106.69	109.40
10	3	2001	ADP	C4-C5-N7	-2.56	106.73	109.40
7	4	2001	AGS	C5-C6-N6	2.31	123.87	120.35
7	F	2001	AGS	C5-C6-N6	2.31	123.86	120.35
7	2	2001	AGS	C5-C6-N6	2.28	123.82	120.35
7	D	2001	AGS	C5-C6-N6	2.28	123.81	120.35
7	B	2001	AGS	C5-C6-N6	2.26	123.78	120.35
7	E	2001	AGS	C5-C6-N6	2.25	123.77	120.35
7	6	2001	AGS	C5-C6-N6	2.25	123.77	120.35
7	5	2001	AGS	C5-C6-N6	2.25	123.77	120.35
7	7	2001	AGS	C5-C6-N6	2.23	123.74	120.35
7	G	2001	AGS	C5-C6-N6	2.22	123.73	120.35

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	2	2001	AGS	PB-O3B-PG-O2G
7	2	2001	AGS	PB-O3B-PG-O3G
7	2	2001	AGS	C5'-O5'-PA-O3A
7	2	2001	AGS	O4'-C4'-C5'-O5'
7	4	2001	AGS	PB-O3B-PG-O2G
7	4	2001	AGS	PB-O3B-PG-O3G
7	5	2001	AGS	C5'-O5'-PA-O1A
7	5	2001	AGS	C5'-O5'-PA-O2A
7	6	2001	AGS	PB-O3B-PG-O2G
7	7	2001	AGS	C5'-O5'-PA-O1A
7	7	2001	AGS	C5'-O5'-PA-O2A
7	7	2001	AGS	C5'-O5'-PA-O3A
7	7	2001	AGS	O4'-C4'-C5'-O5'
7	B	2001	AGS	PB-O3B-PG-O3G
7	D	2001	AGS	PB-O3B-PG-O2G
7	D	2001	AGS	PB-O3B-PG-O3G
7	D	2001	AGS	C5'-O5'-PA-O2A
7	E	2001	AGS	C5'-O5'-PA-O1A
7	E	2001	AGS	C5'-O5'-PA-O2A
7	G	2001	AGS	C5'-O5'-PA-O1A
7	G	2001	AGS	C5'-O5'-PA-O2A
7	G	2001	AGS	C5'-O5'-PA-O3A
7	G	2001	AGS	O4'-C4'-C5'-O5'
7	4	2001	AGS	O4'-C4'-C5'-O5'
7	5	2001	AGS	O4'-C4'-C5'-O5'
7	5	2001	AGS	C3'-C4'-C5'-O5'
7	6	2001	AGS	O4'-C4'-C5'-O5'
7	D	2001	AGS	O4'-C4'-C5'-O5'
7	E	2001	AGS	O4'-C4'-C5'-O5'
10	3	2001	ADP	O4'-C4'-C5'-O5'
7	4	2001	AGS	C3'-C4'-C5'-O5'
7	E	2001	AGS	C3'-C4'-C5'-O5'
10	C	2001	ADP	O4'-C4'-C5'-O5'
10	C	2001	ADP	C3'-C4'-C5'-O5'
7	5	2001	AGS	PG-O3B-PB-O1B
7	E	2001	AGS	PG-O3B-PB-O1B
7	D	2001	AGS	C3'-C4'-C5'-O5'
10	3	2001	ADP	C3'-C4'-C5'-O5'
7	G	2001	AGS	PA-O3A-PB-O1B
7	6	2001	AGS	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
7	B	2001	AGS	O4'-C4'-C5'-O5'
7	5	2001	AGS	C5'-O5'-PA-O3A
7	B	2001	AGS	C5'-O5'-PA-O3A
7	D	2001	AGS	C5'-O5'-PA-O3A
7	E	2001	AGS	C5'-O5'-PA-O3A
7	F	2001	AGS	C5'-O5'-PA-O3A
7	2	2001	AGS	C5'-O5'-PA-O1A
7	2	2001	AGS	C5'-O5'-PA-O2A
7	4	2001	AGS	C5'-O5'-PA-O1A
7	4	2001	AGS	C5'-O5'-PA-O2A
7	D	2001	AGS	C5'-O5'-PA-O1A
7	G	2001	AGS	C3'-C4'-C5'-O5'
10	C	2001	ADP	C4'-C5'-O5'-PA
7	7	2001	AGS	PA-O3A-PB-O2B
7	F	2001	AGS	O4'-C4'-C5'-O5'
7	B	2001	AGS	PB-O3B-PG-O2G
7	7	2001	AGS	PA-O3A-PB-O1B
7	2	2001	AGS	C3'-C4'-C5'-O5'
7	4	2001	AGS	C5'-O5'-PA-O3A
7	G	2001	AGS	PA-O3A-PB-O2B
10	3	2001	ADP	C5'-O5'-PA-O1A

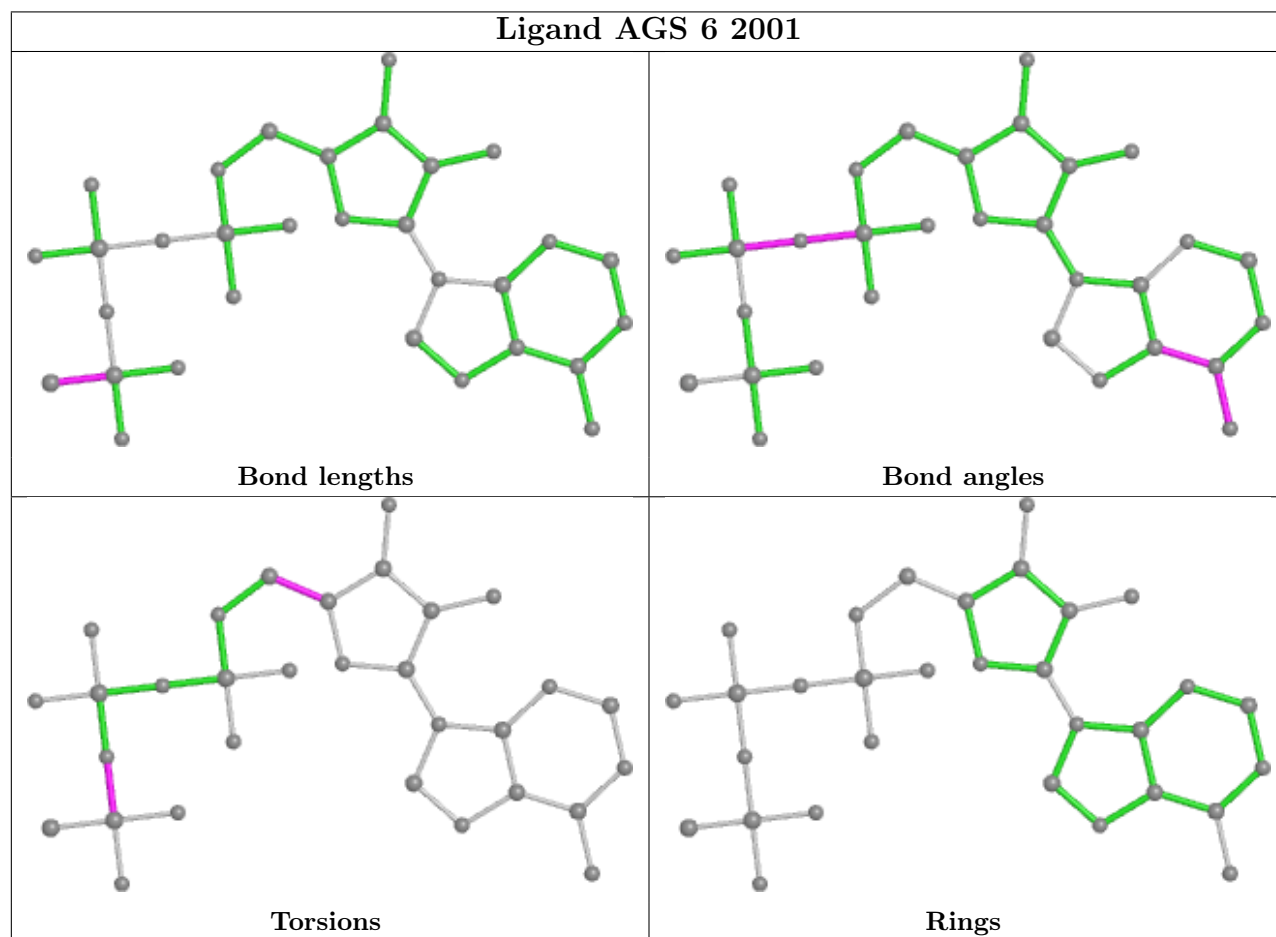
There are no ring outliers.

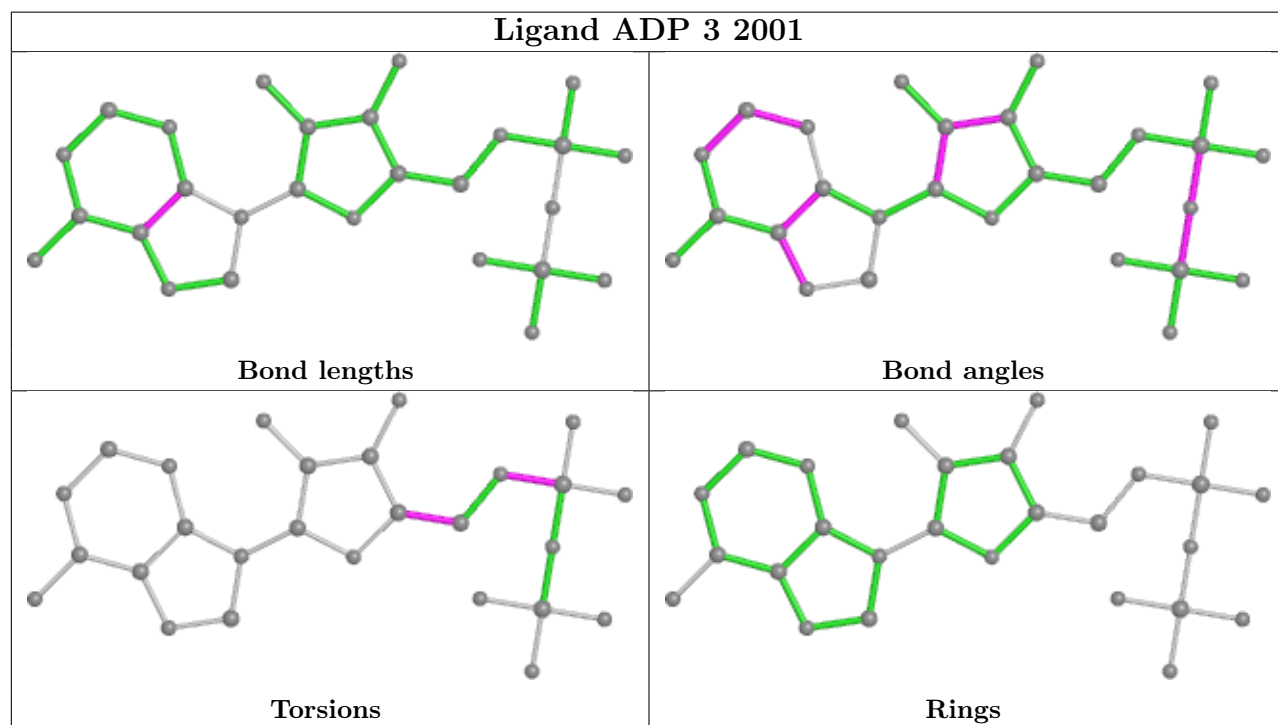
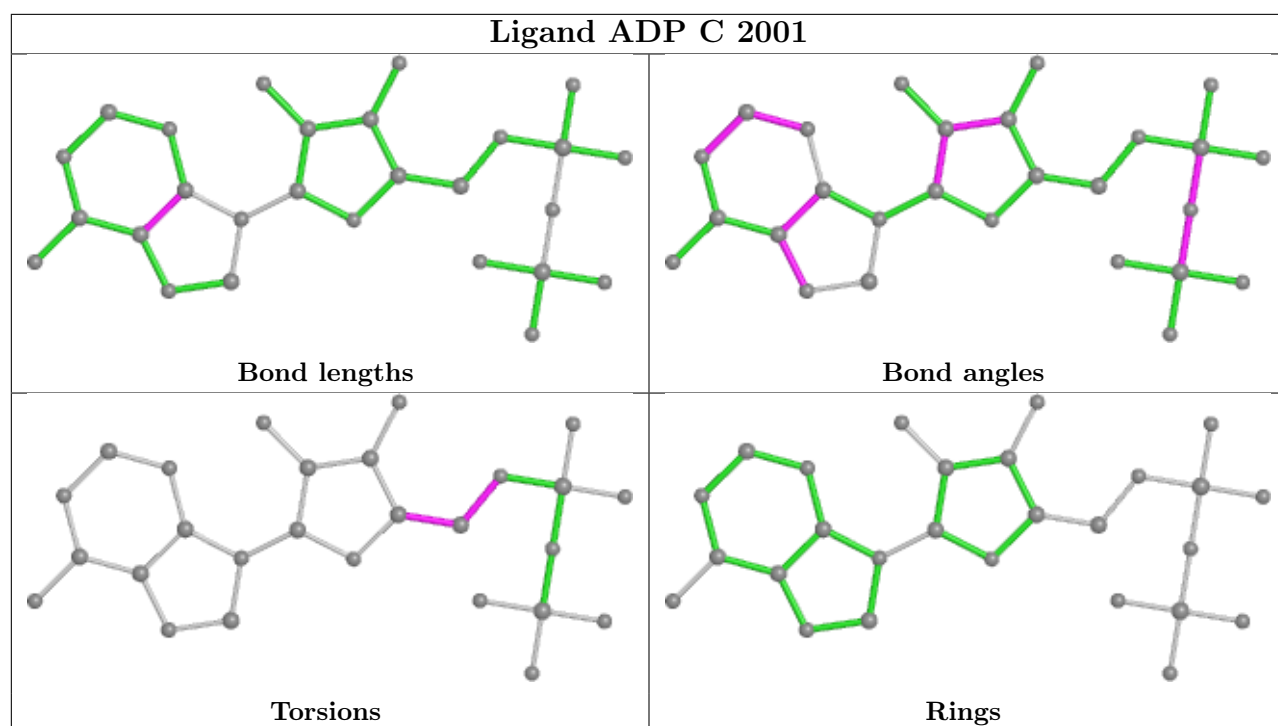
7 monomers are involved in 13 short contacts:

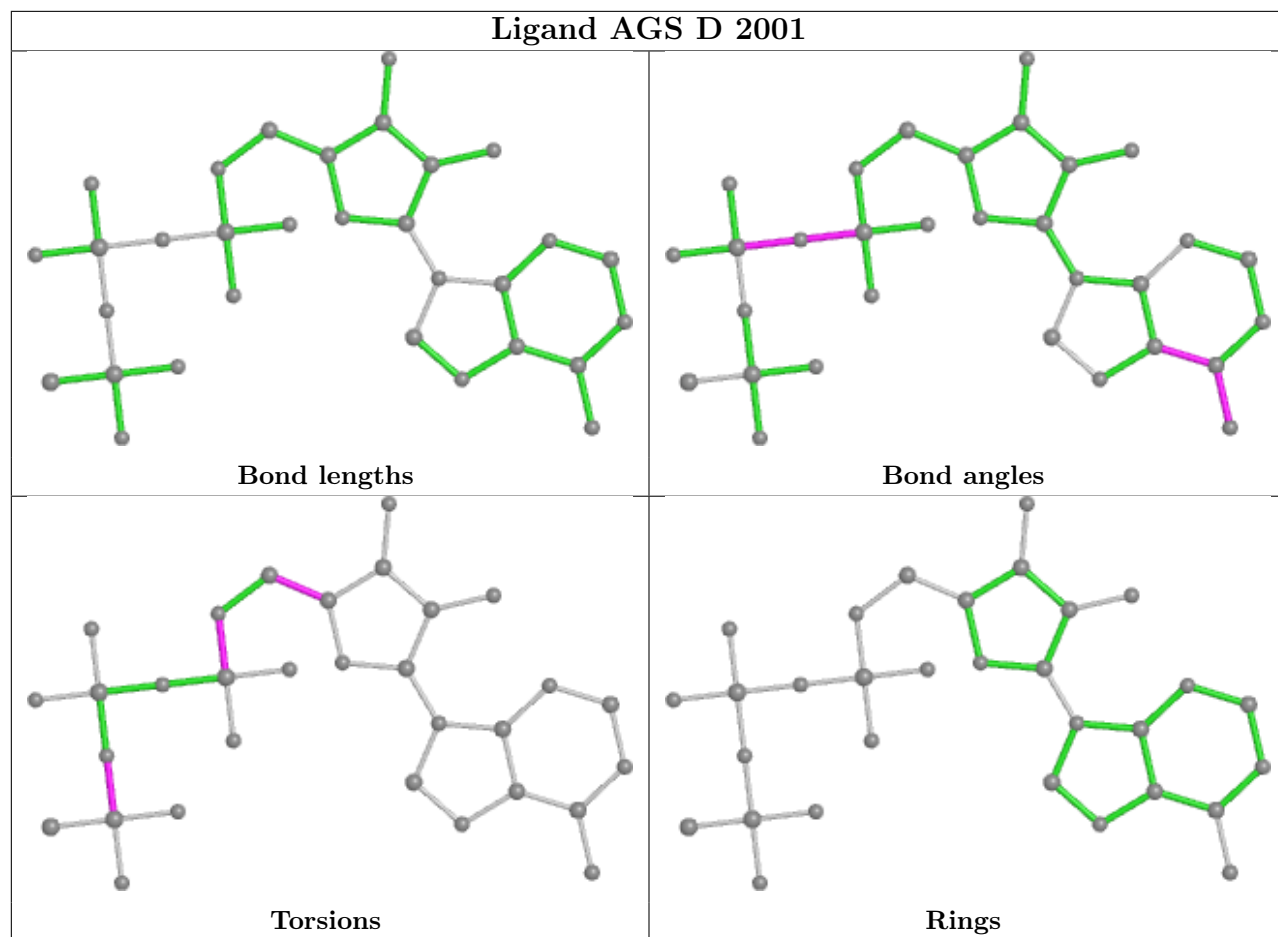
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	6	2001	AGS	1	0
7	D	2001	AGS	4	0
7	5	2001	AGS	1	0
7	F	2001	AGS	1	0
7	B	2001	AGS	1	0
7	4	2001	AGS	4	0
7	7	2001	AGS	1	0

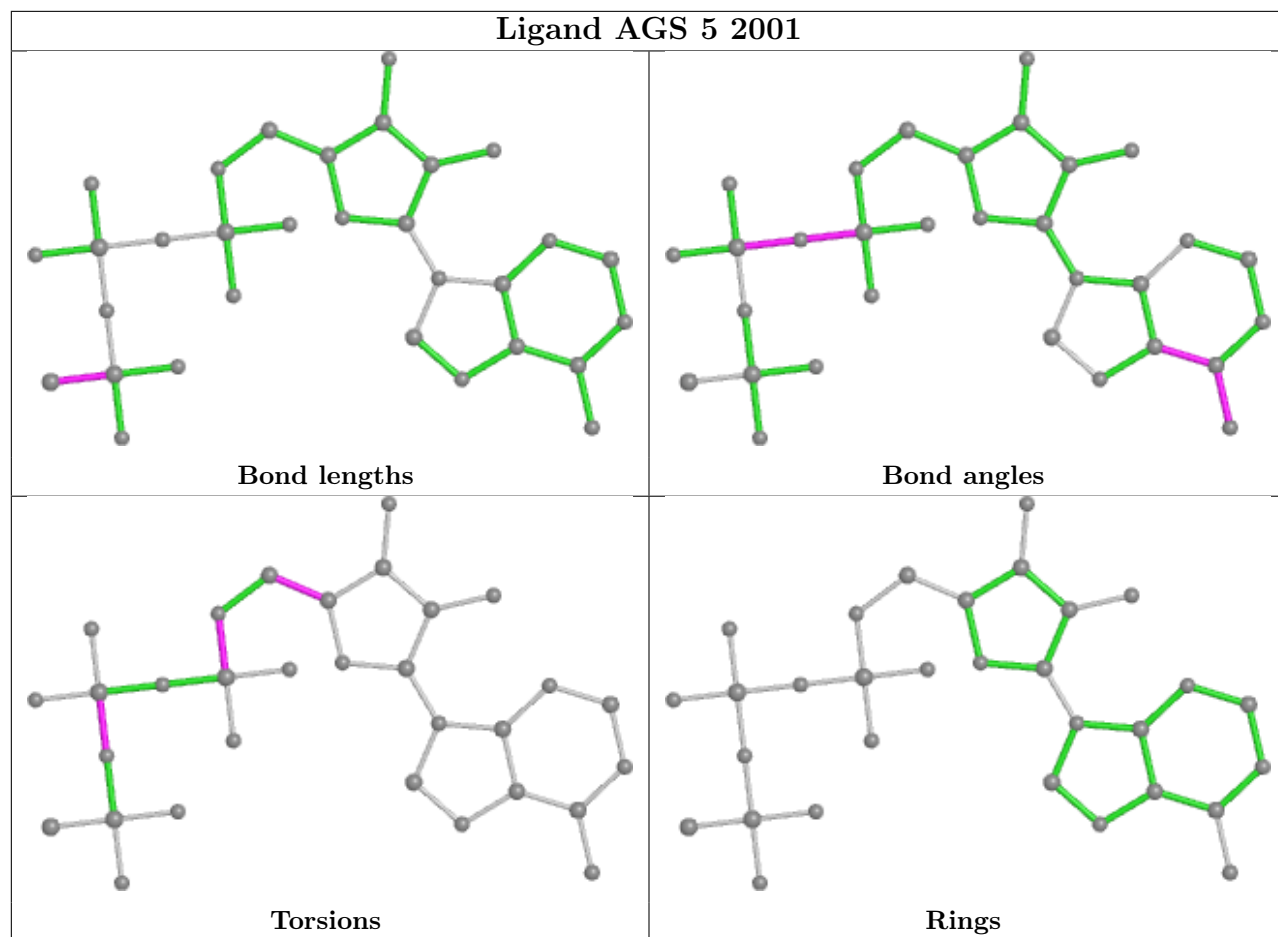
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

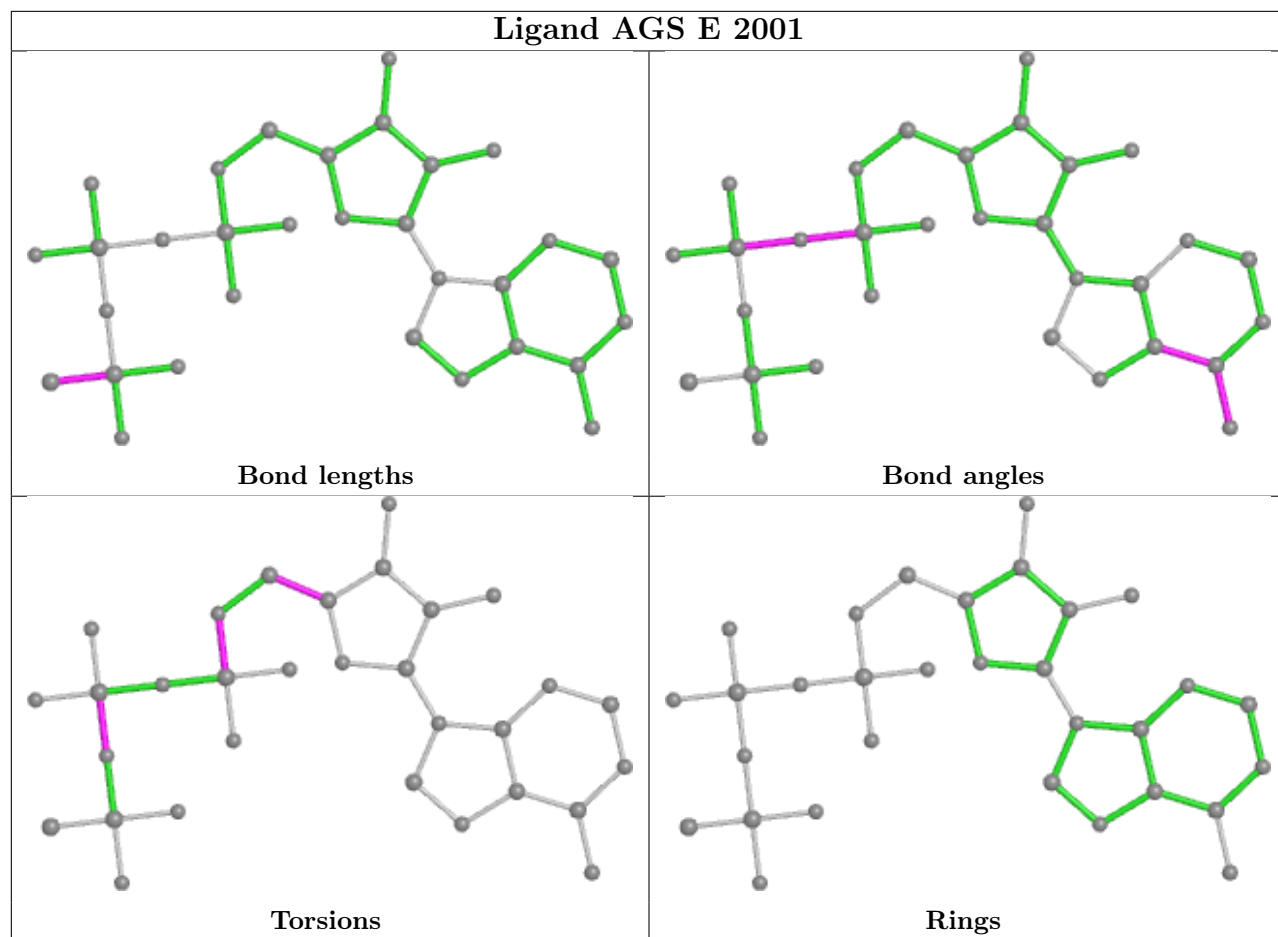
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

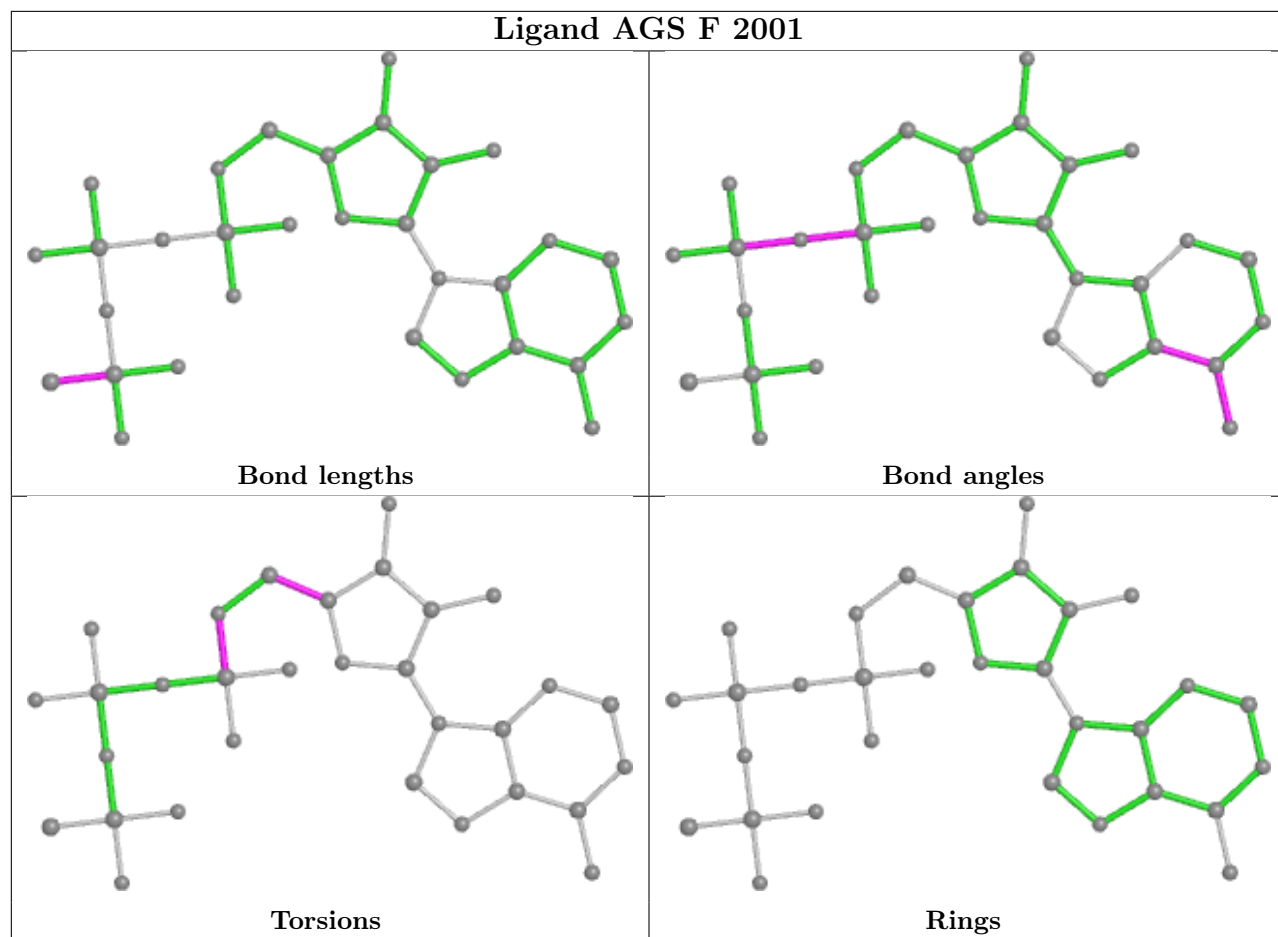


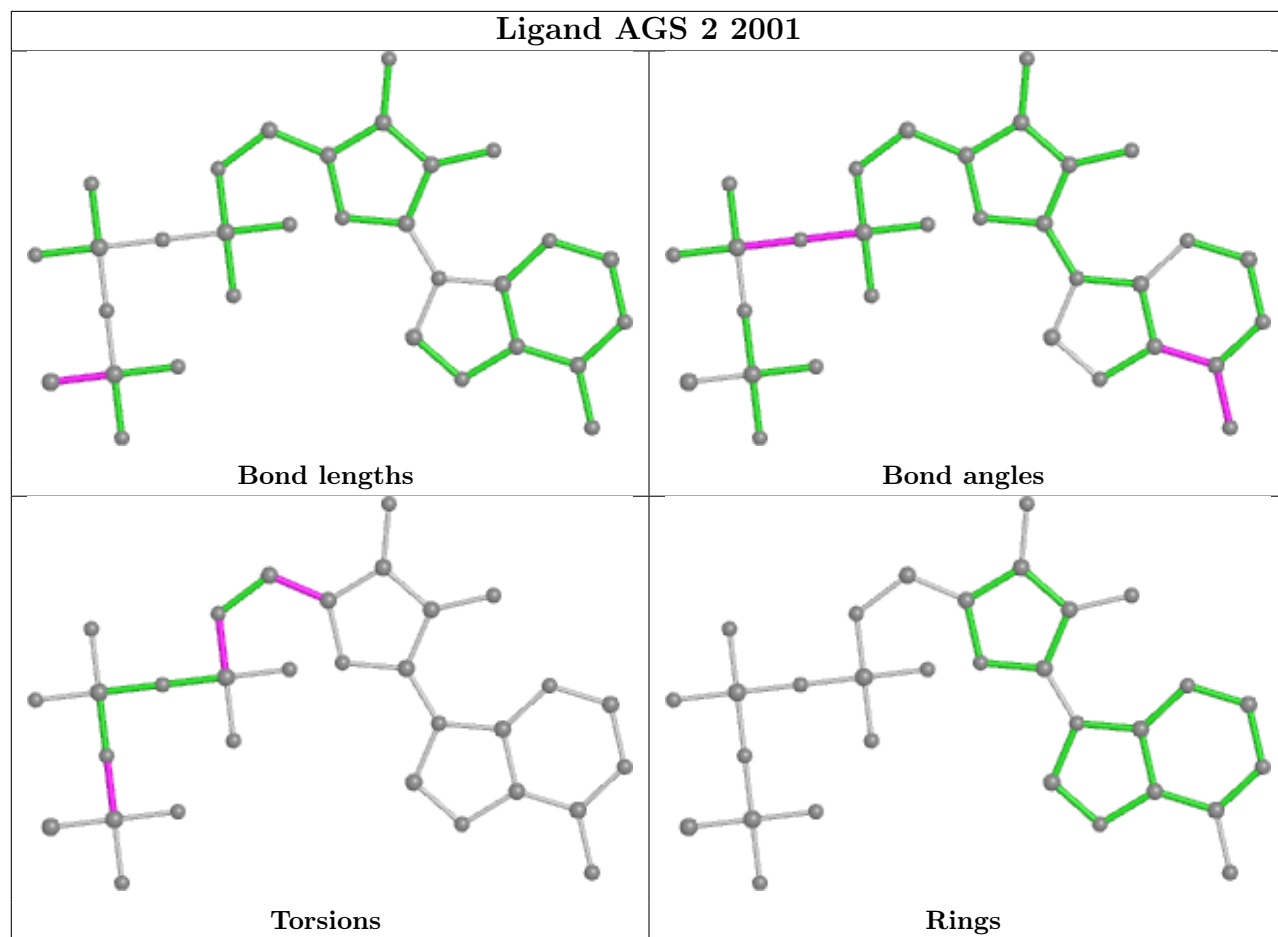


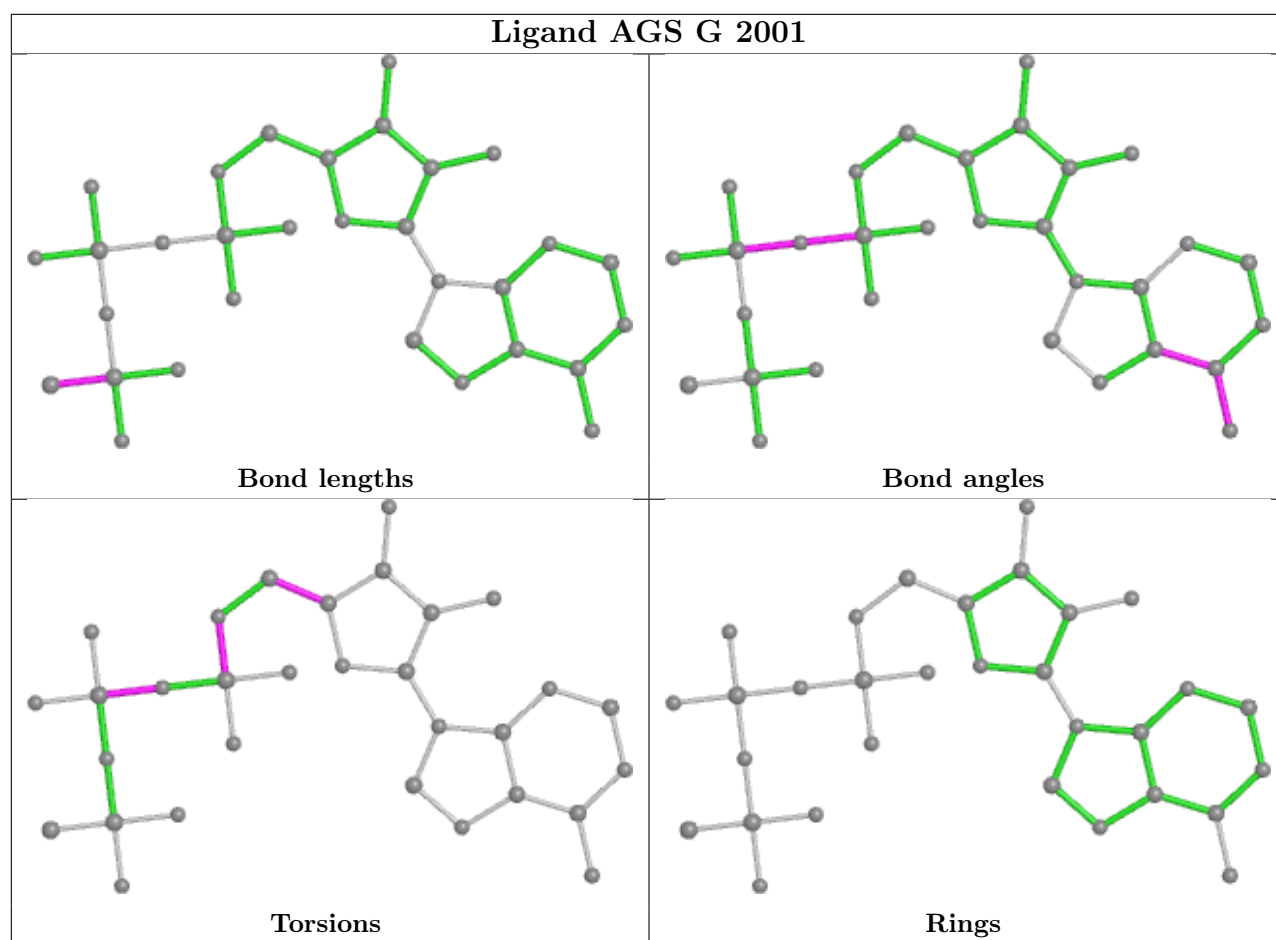


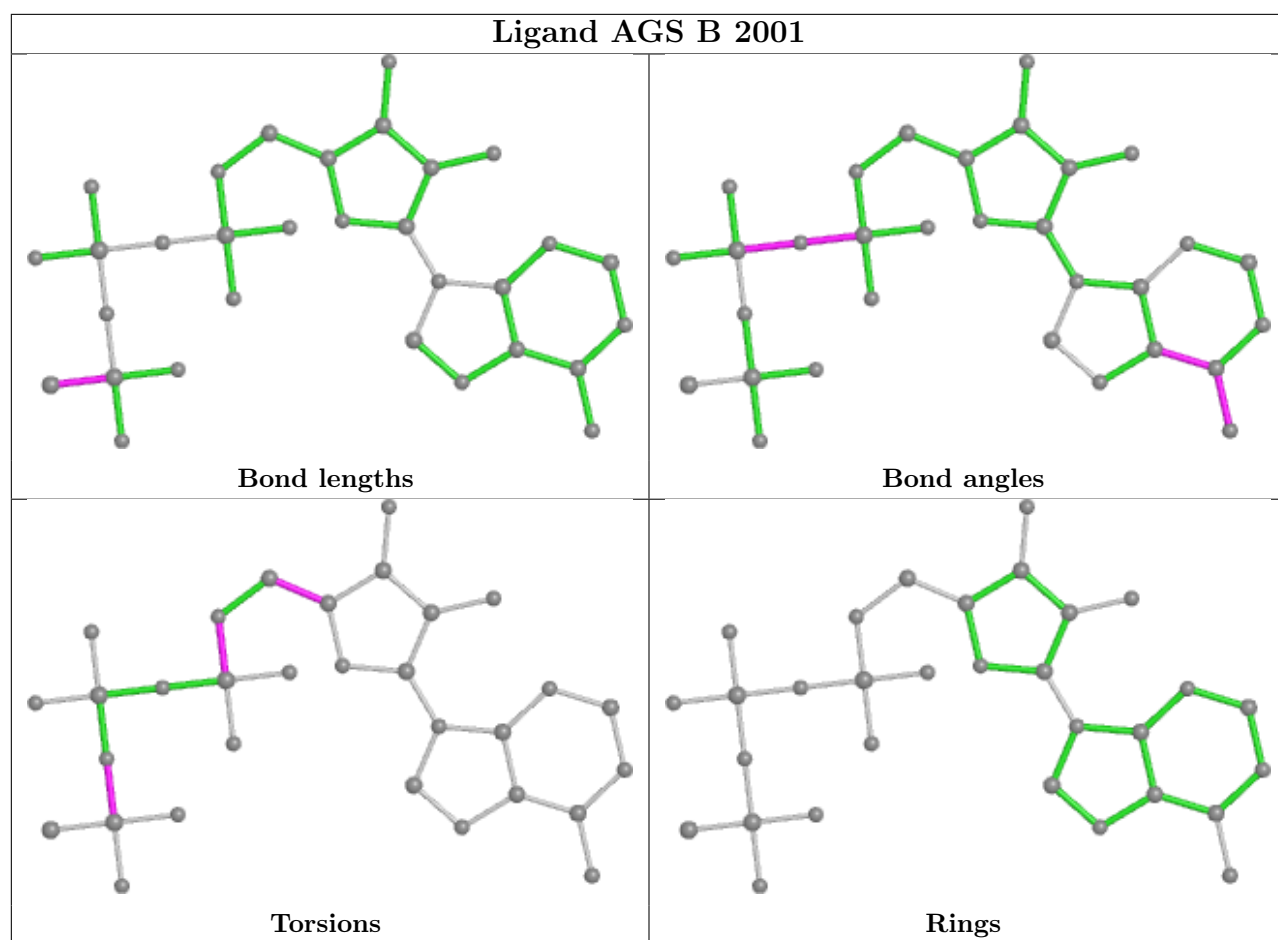


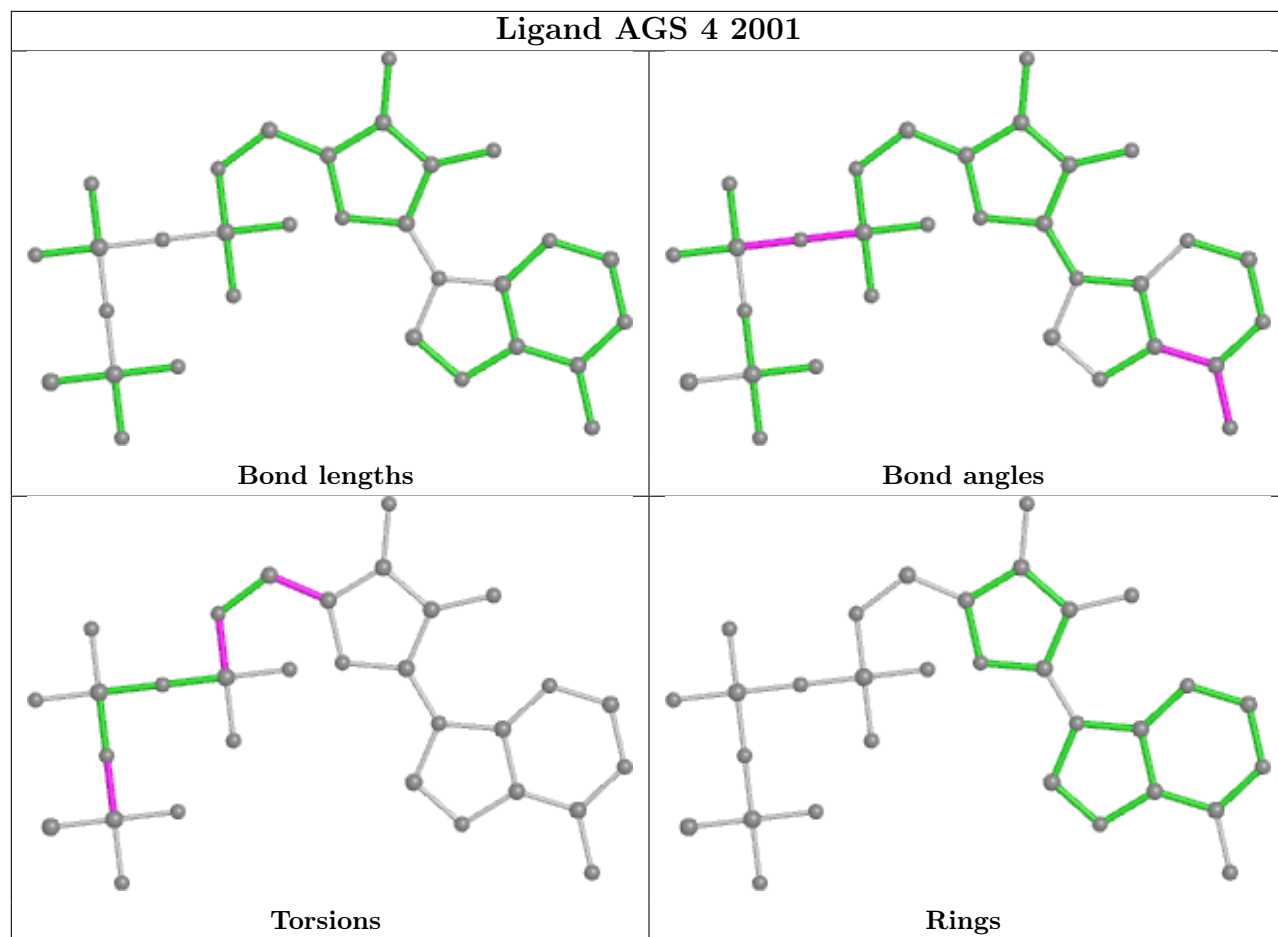


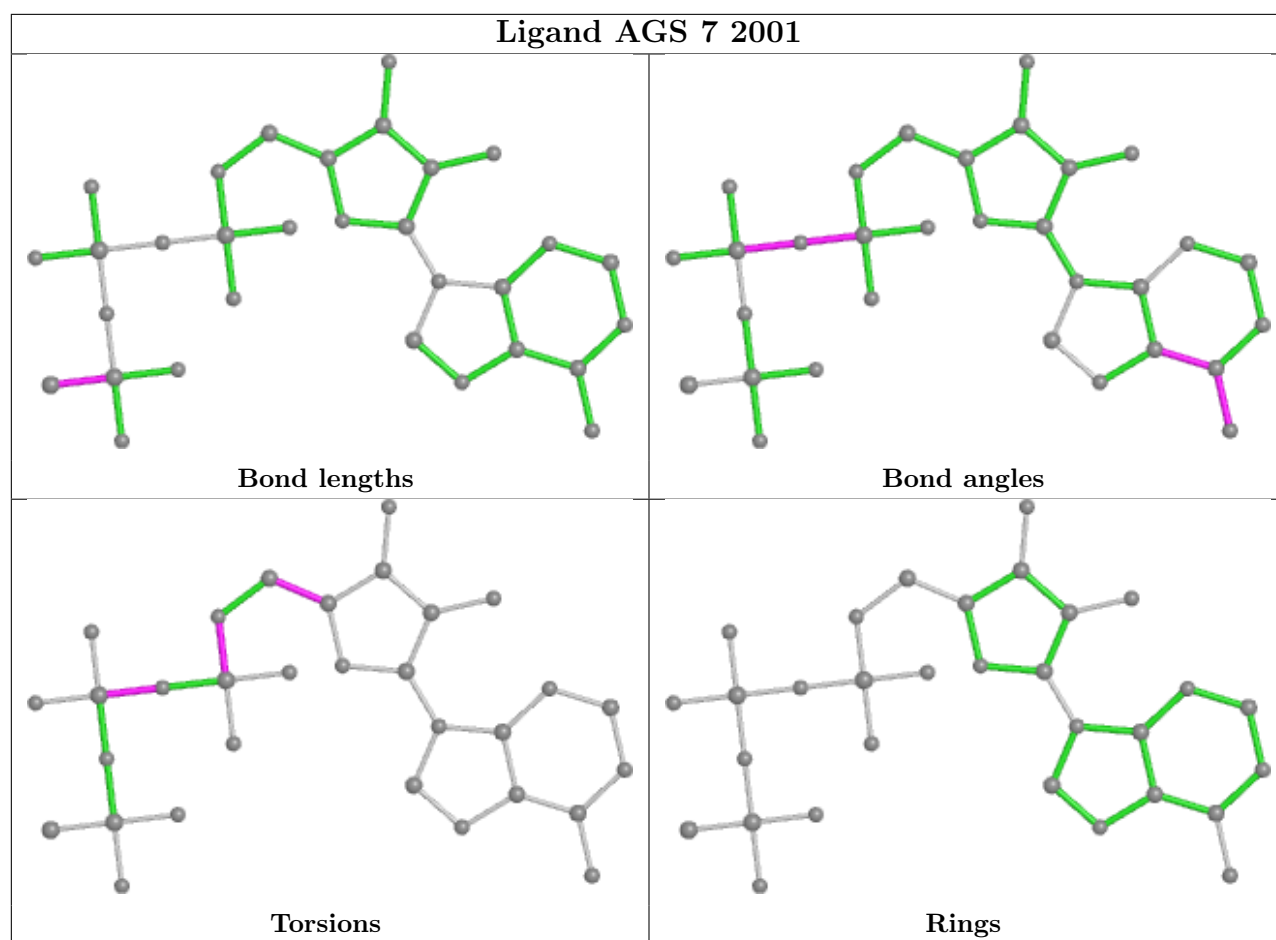












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

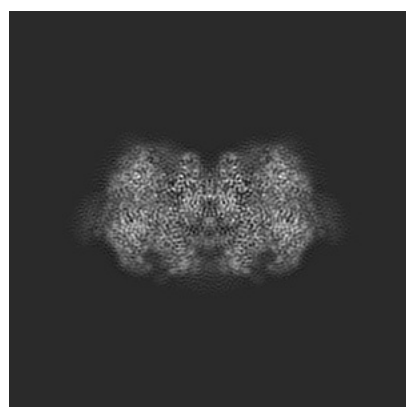
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31684. These allow visual inspection of the internal detail of the map and identification of artifacts.

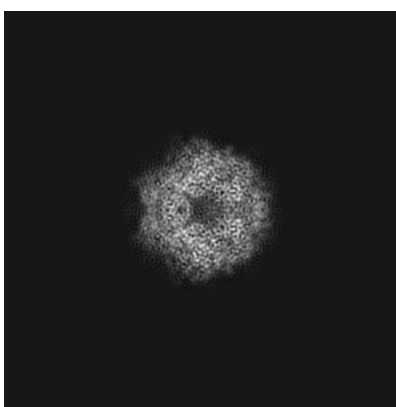
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

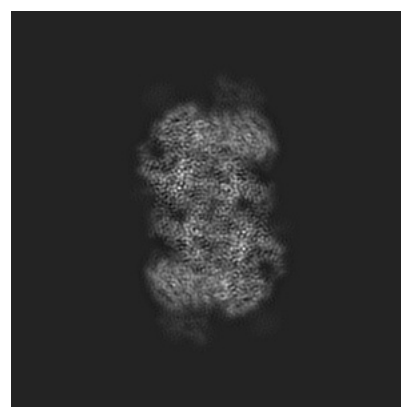
6.1.1 Primary map



X



Y

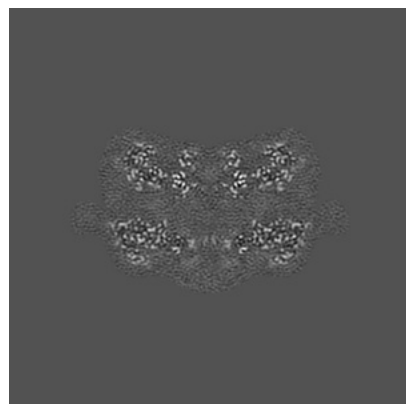


Z

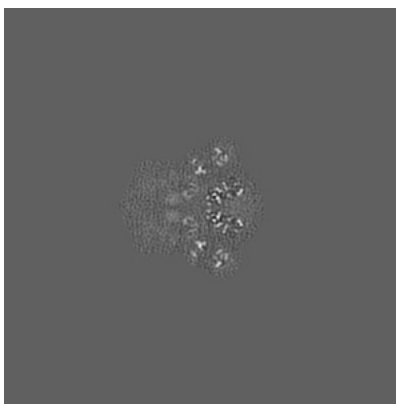
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

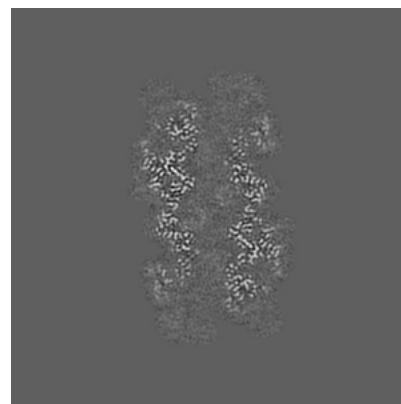
6.2.1 Primary map



X Index: 180



Y Index: 180

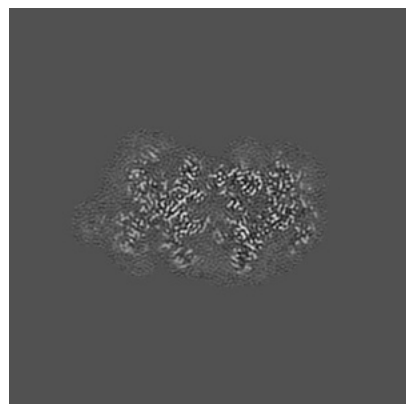


Z Index: 180

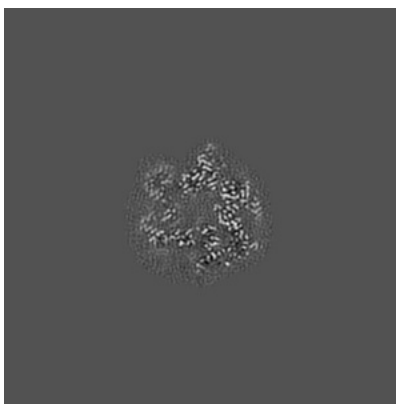
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

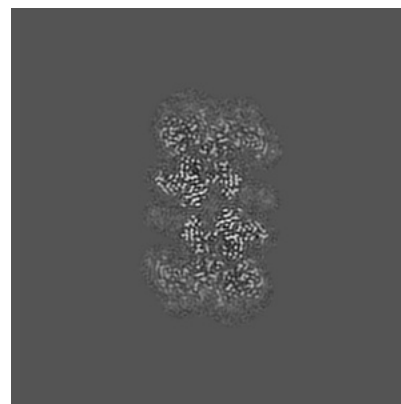
6.3.1 Primary map



X Index: 159



Y Index: 203

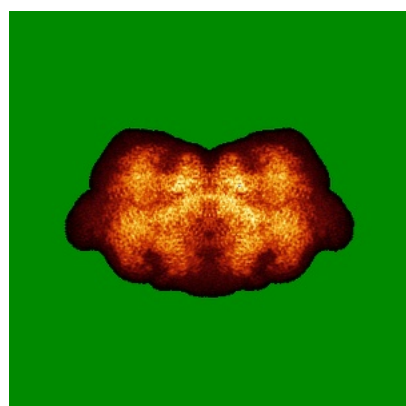


Z Index: 206

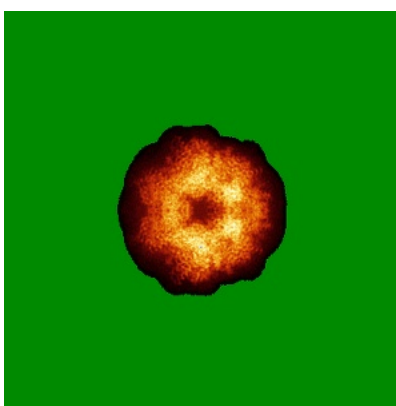
The images above show the largest variance slices of the map in three orthogonal directions.

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

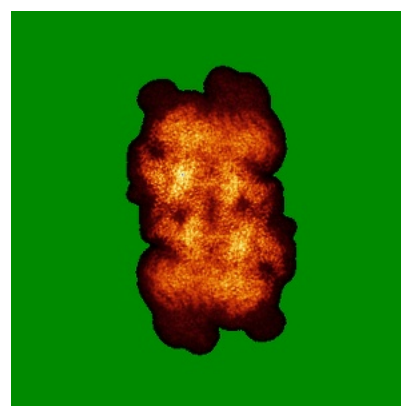
6.4.1 Primary map



X



Y

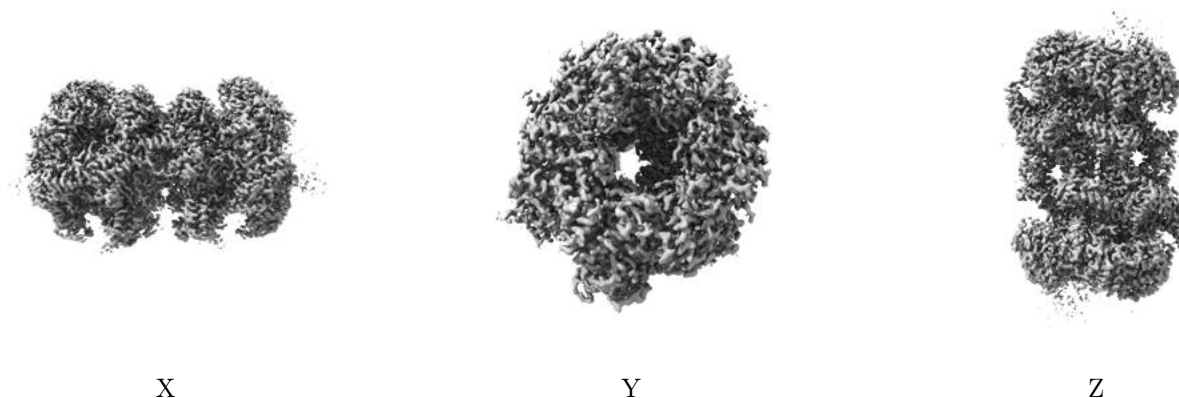


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

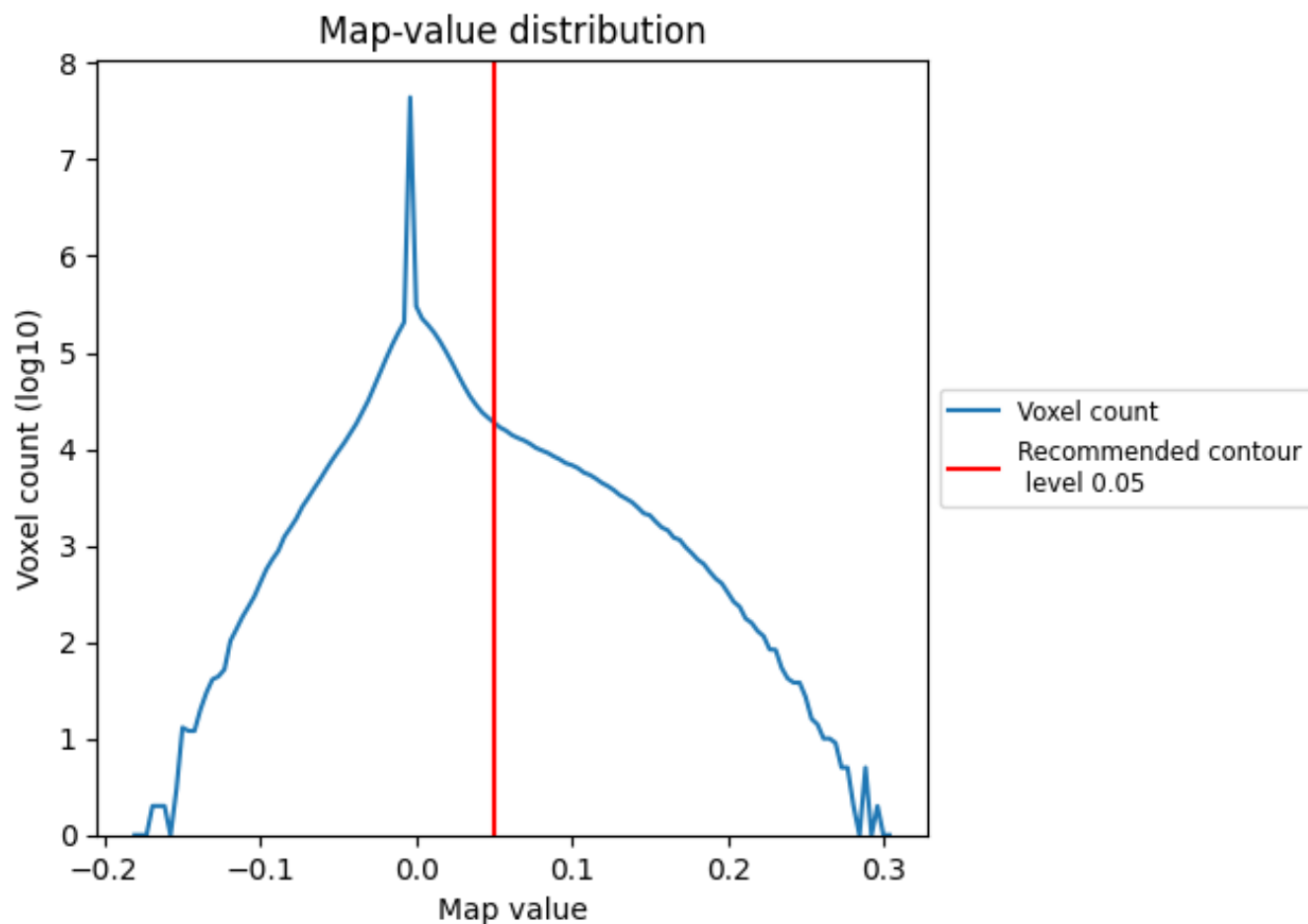
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

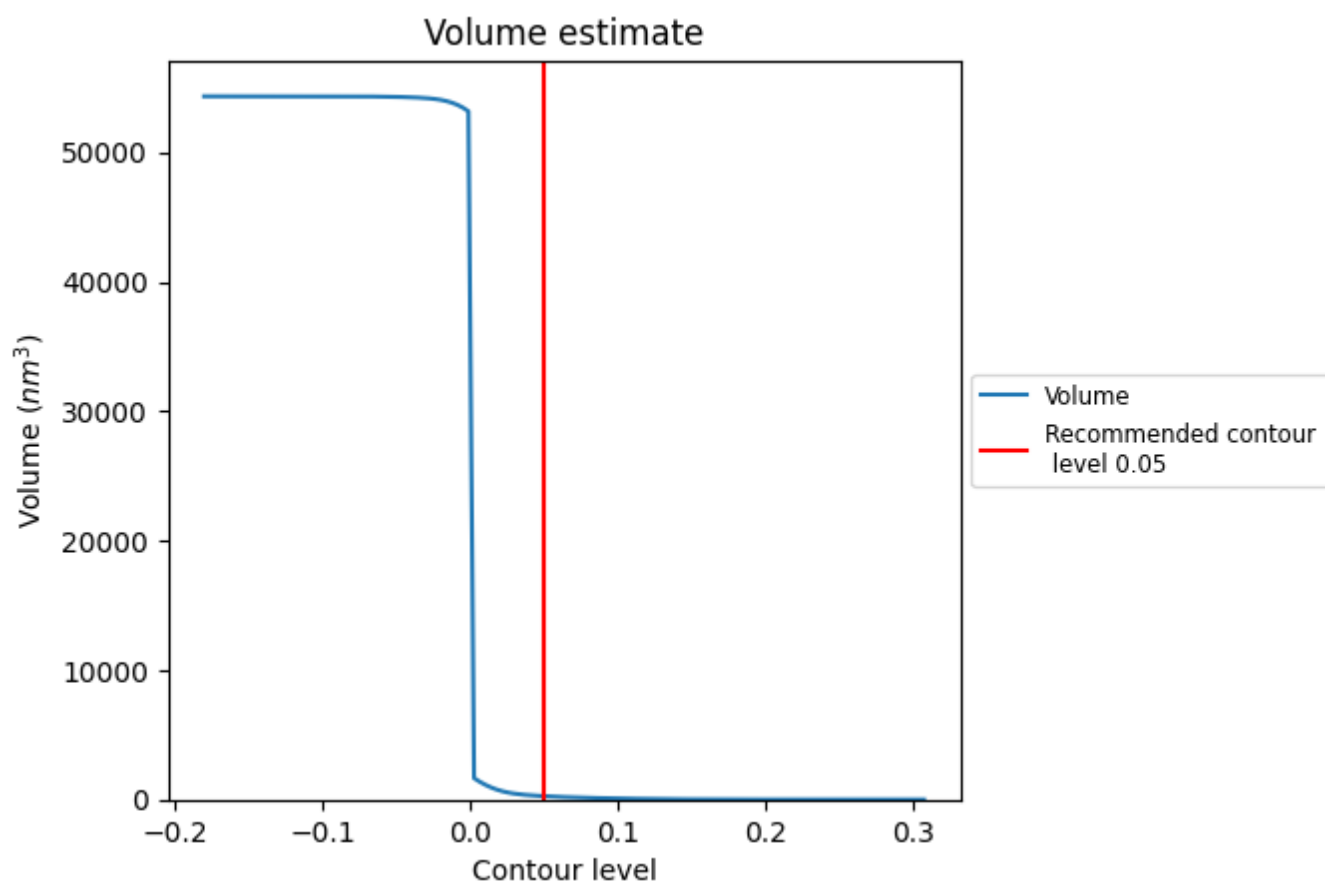
This section contains the results of statistical analysis of the map.

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.

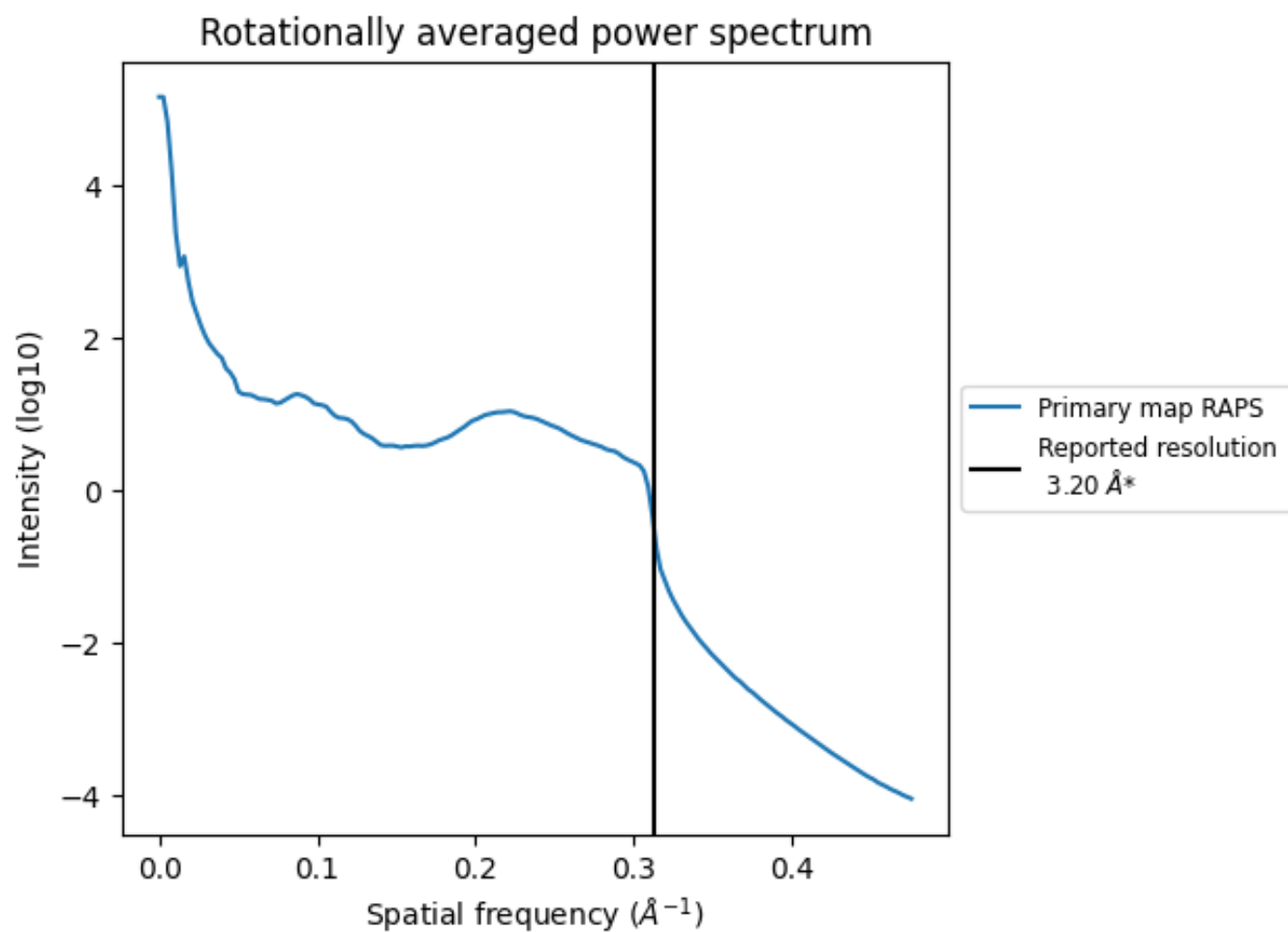
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 262 nm³; this corresponds to an approximate mass of 237 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 0.312 Å⁻¹

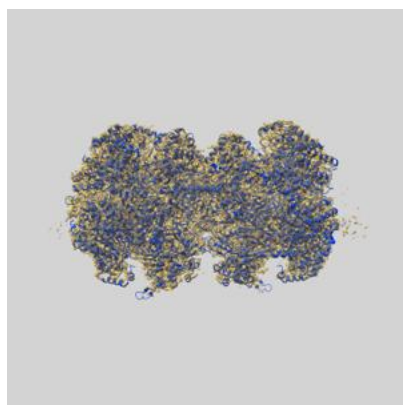
8 Fourier-Shell correlation ⓘ

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

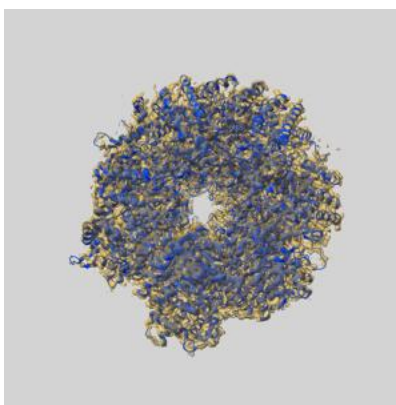
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31684 and PDB model 7V3U. Per-residue inclusion information can be found in section [3](#) on page [9](#).

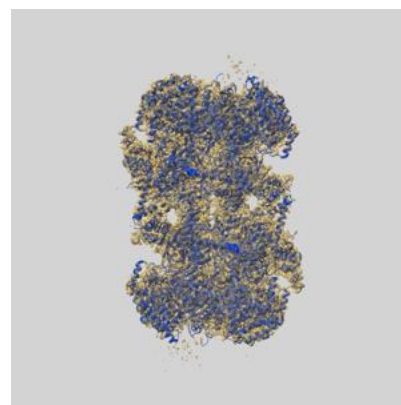
9.1 Map-model overlay [i](#)



X



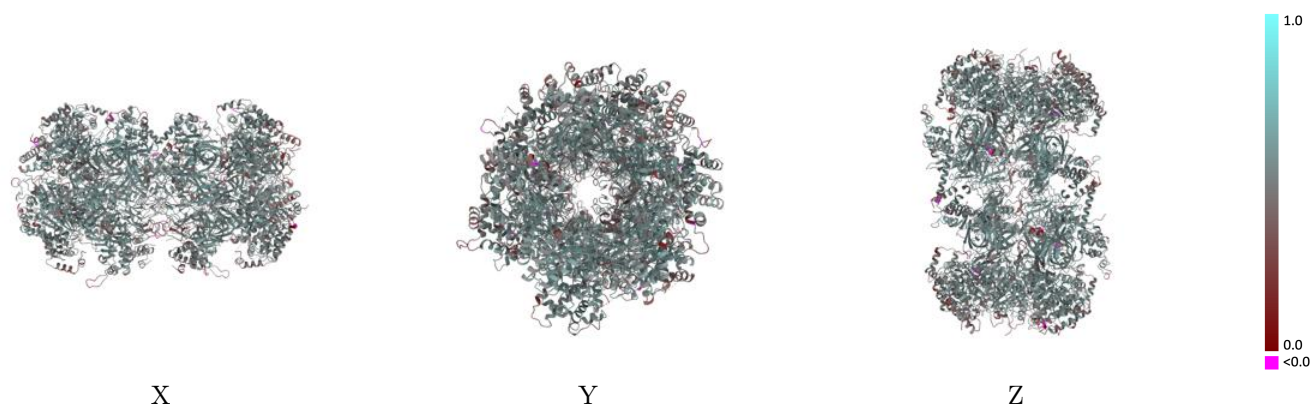
Y



Z

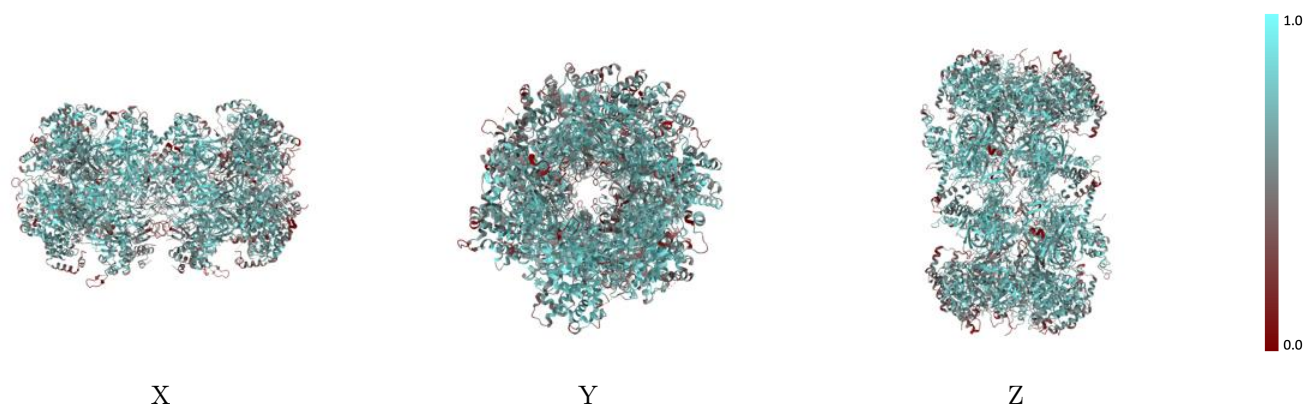
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



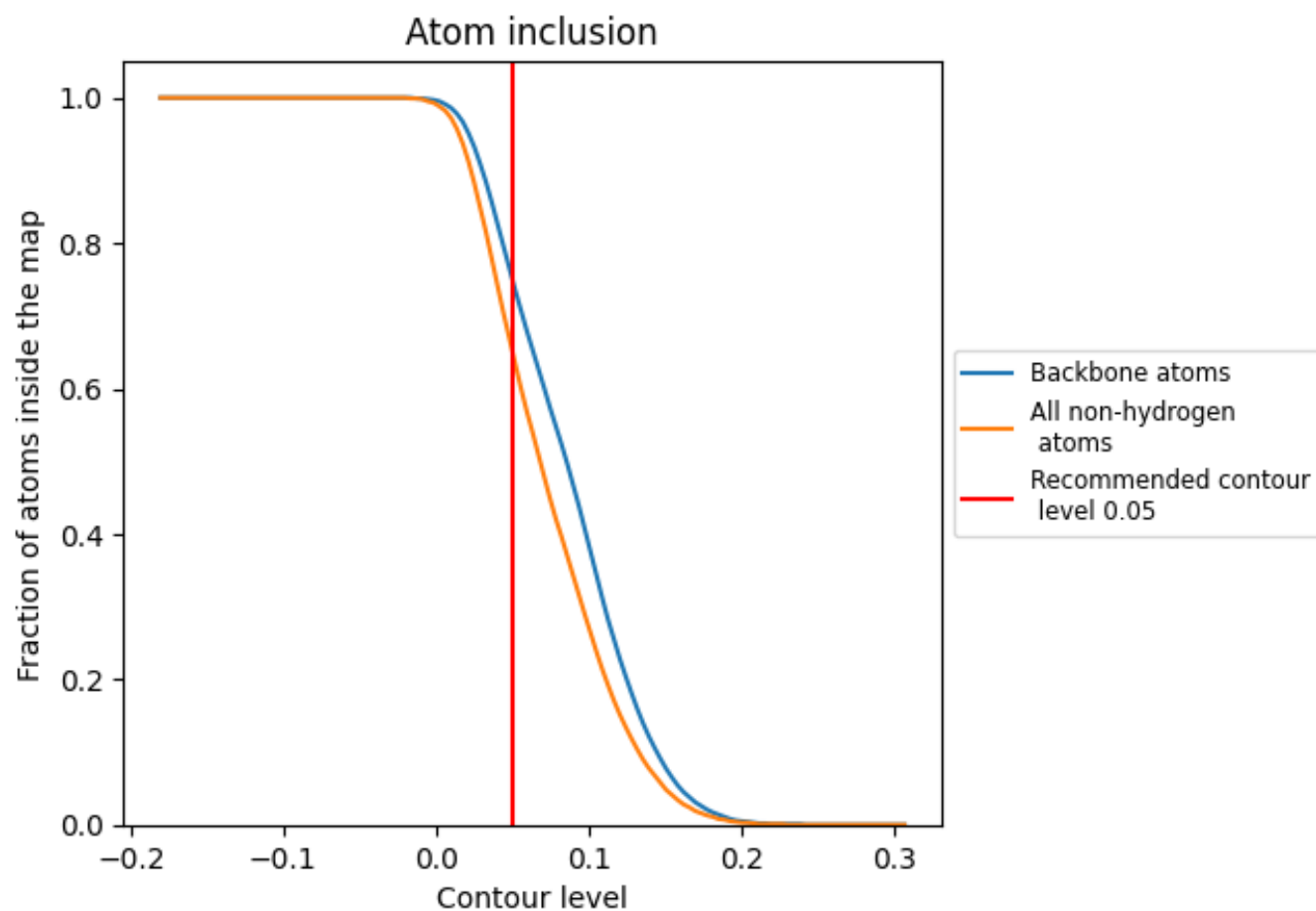
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 65% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.6530</div>	<div><div></div>0.5140</div>
2	<div><div></div>0.6140</div>	<div><div></div>0.5000</div>
3	<div><div></div>0.6770</div>	<div><div></div>0.5260</div>
4	<div><div></div>0.7020</div>	<div><div></div>0.5320</div>
5	<div><div></div>0.6350</div>	<div><div></div>0.5030</div>
6	<div><div></div>0.6270</div>	<div><div></div>0.5030</div>
7	<div><div></div>0.6990</div>	<div><div></div>0.5290</div>
B	<div><div></div>0.6060</div>	<div><div></div>0.5000</div>
C	<div><div></div>0.6680</div>	<div><div></div>0.5190</div>
D	<div><div></div>0.6890</div>	<div><div></div>0.5290</div>
E	<div><div></div>0.6280</div>	<div><div></div>0.5040</div>
F	<div><div></div>0.6020</div>	<div><div></div>0.4970</div>
G	<div><div></div>0.6810</div>	<div><div></div>0.5250</div>

1.0

0.0

<0.0