



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:15 PM UTC

PDB ID : 7W8G / pdb_00007w8g
EMDB ID : EMD-32355
Title : Cryo-EM structure of MCM double hexamer
Authors : Cheng, J.; Li, N.; Tye, B.; Zhai, Y.; Gao, N.
Deposited on : 2021-12-07
Resolution : 2.52 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

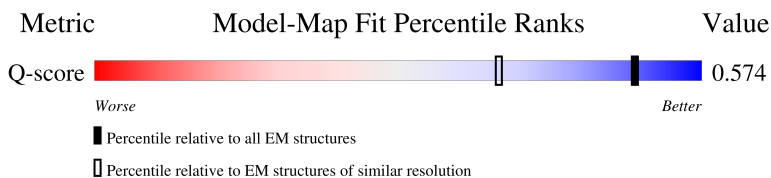
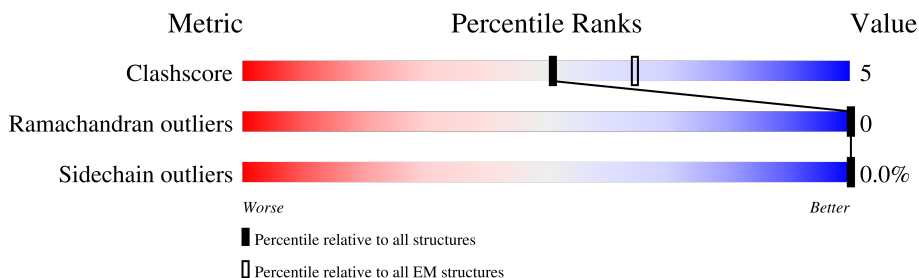
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.52 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.



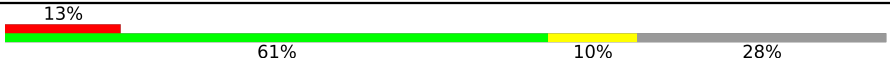
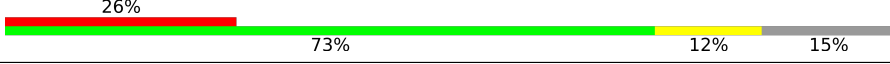
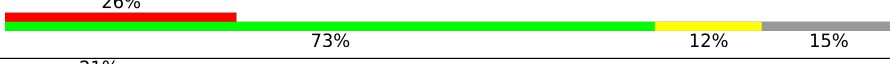
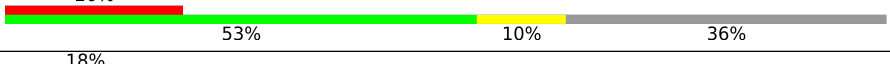
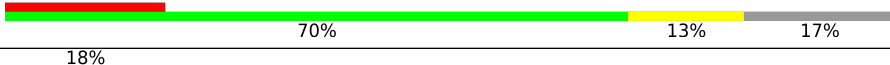
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7226 (2.02 - 3.02)

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	27% 62% 11% 28%
1	B	868	28% 59% 13% 28%
2	3	971	15% 57% 9% 34%
2	C	971	14% 57% 9% 34%

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Mol	Chain	Length	Quality of chain
3	4	933	
3	D	933	
4	5	775	
4	E	775	
5	6	1017	
5	F	1017	
6	7	845	
6	G	845	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 62460 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	670	Total	C	N	O	S	0	0
			5323	3339	918	1036	30		
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		

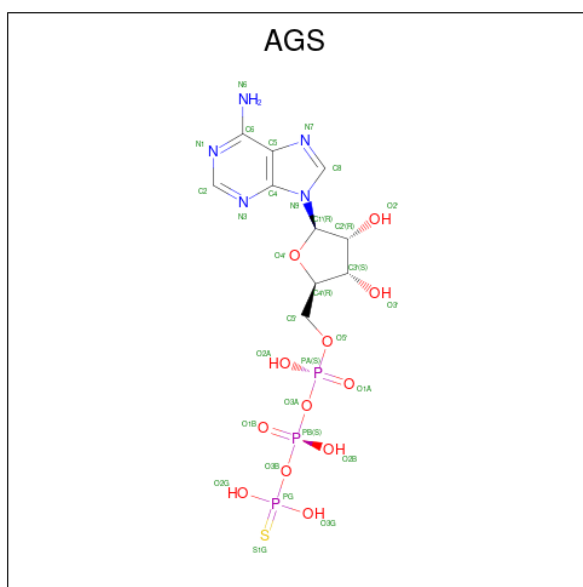
- Molecule 5 is a protein called DNA replication licensing factor MCM6.

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	

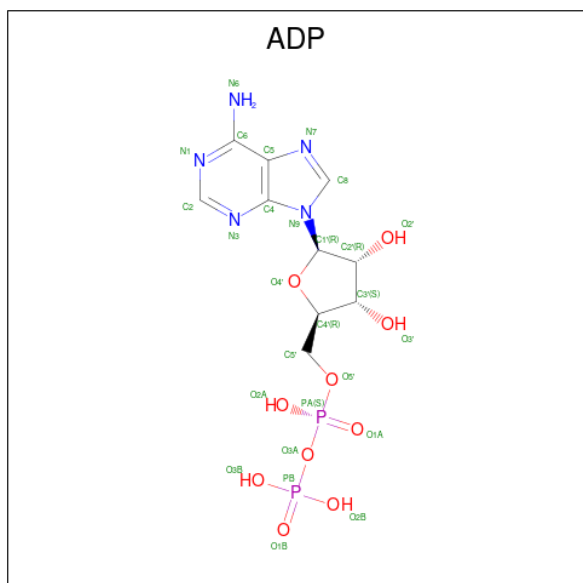
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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).

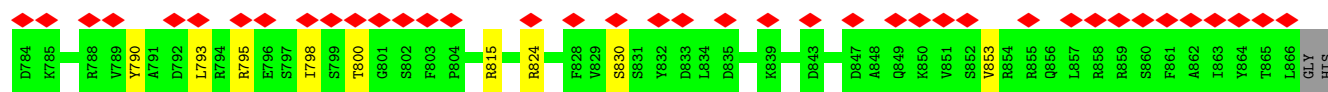


Mol	Chain	Residues	Atoms					AltConf
10	3	1	Total	C	N	O	P	0
			27	10	5	10	2	

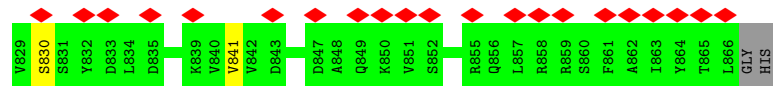
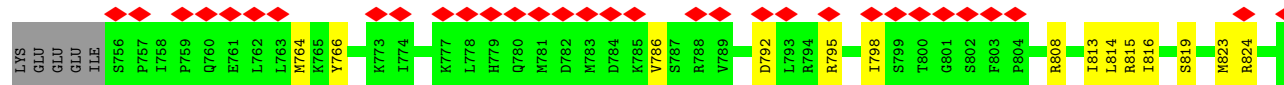
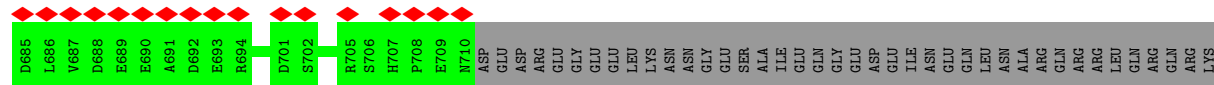
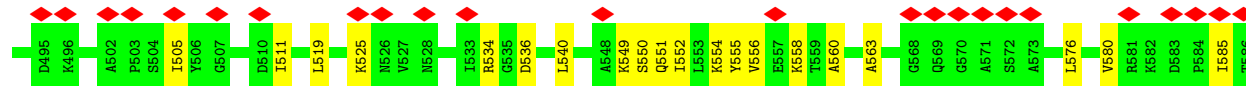
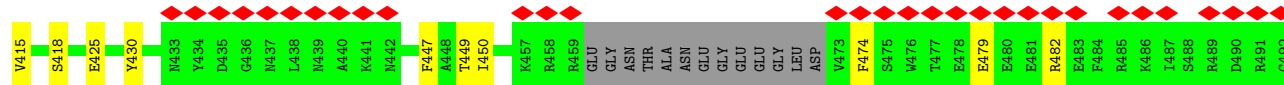
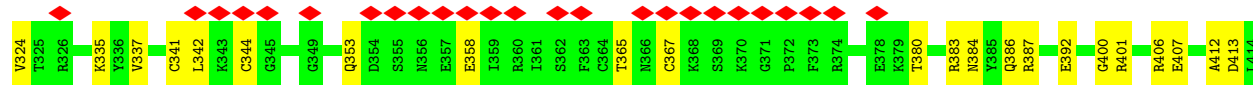
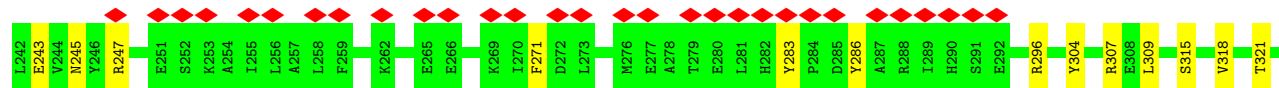
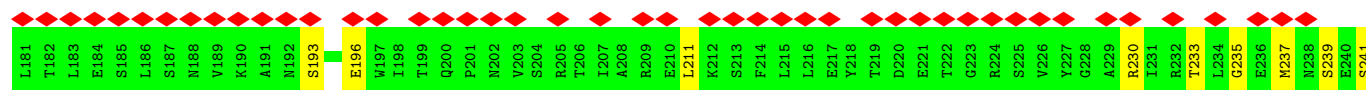
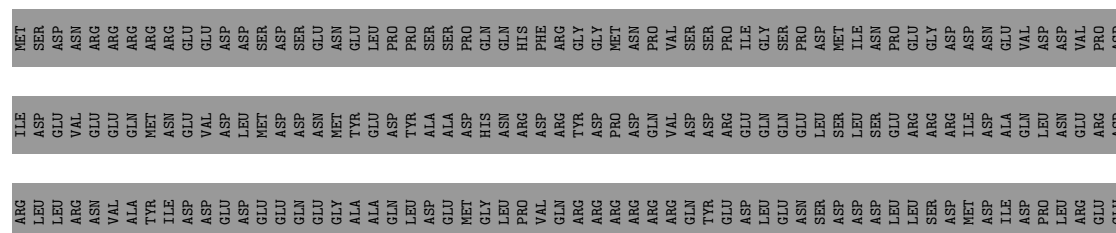
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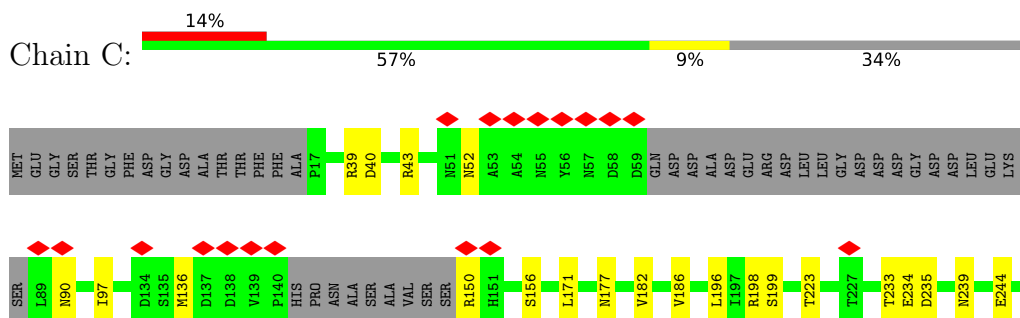
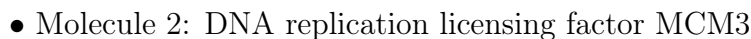
Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

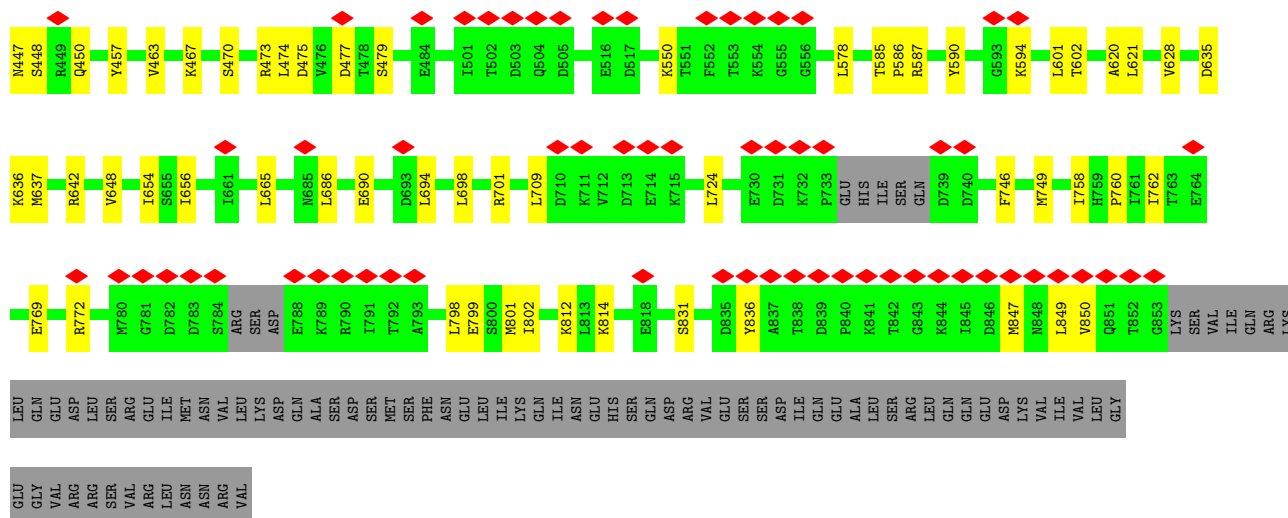


• Molecule 1: DNA replication licensing factor MCM2

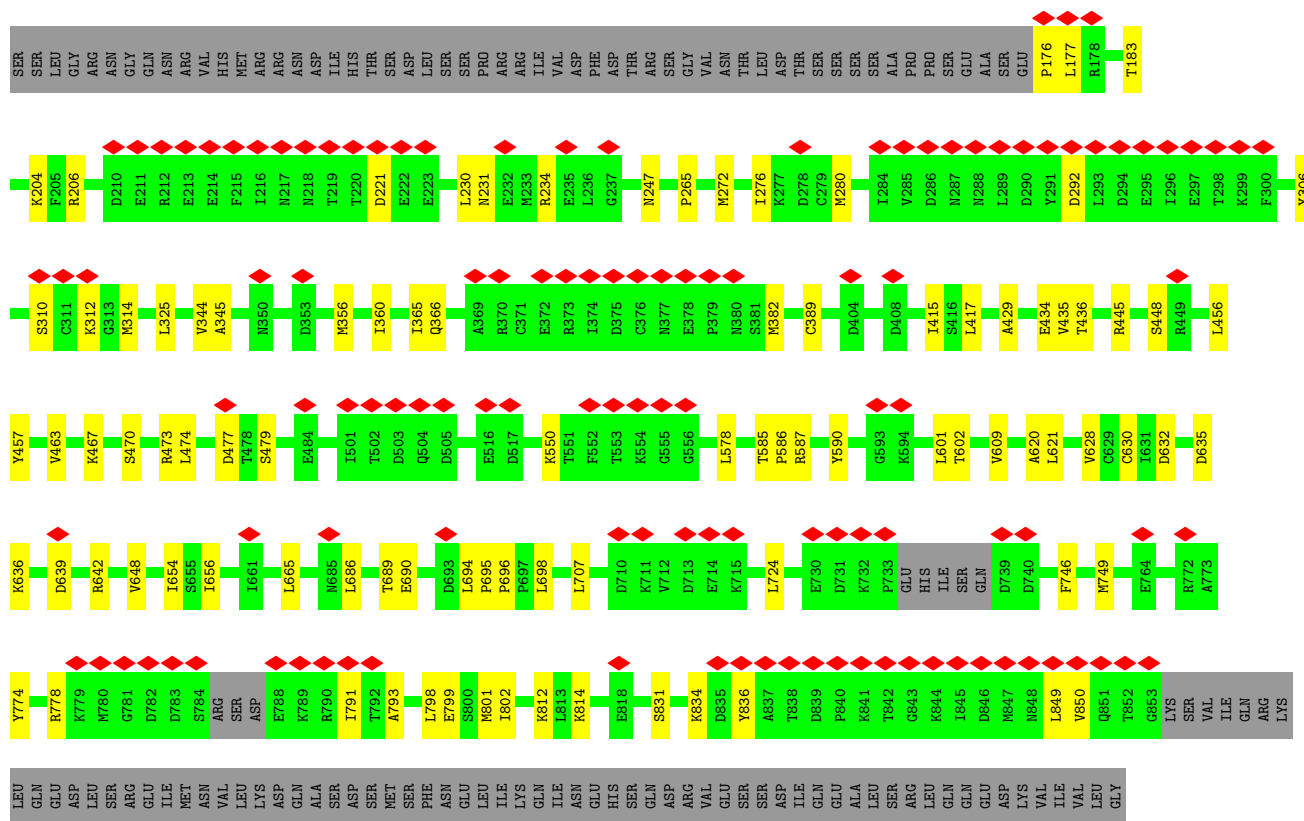
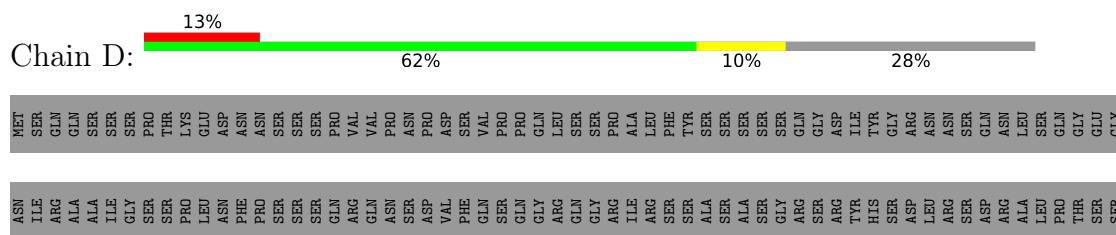


• Molecule 2: DNA replication licensing factor MCM3

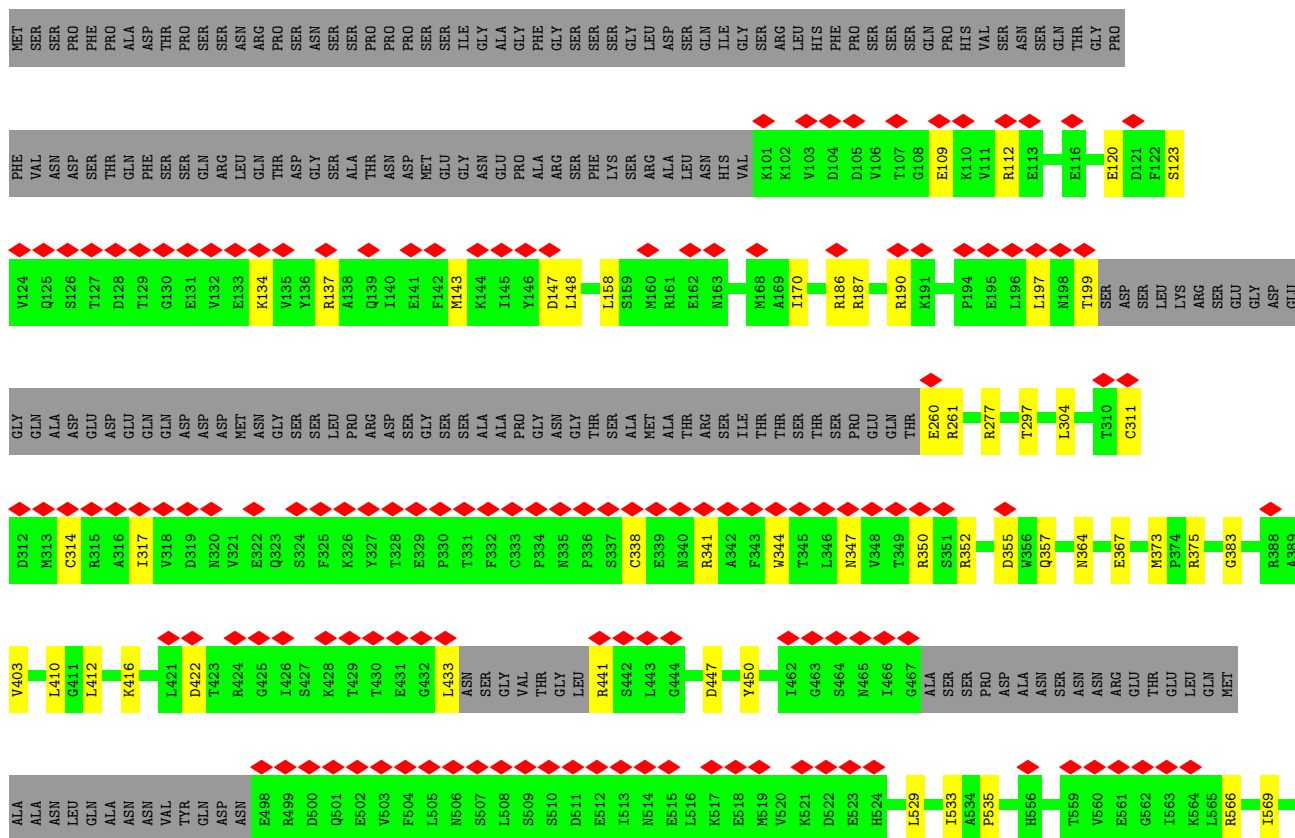


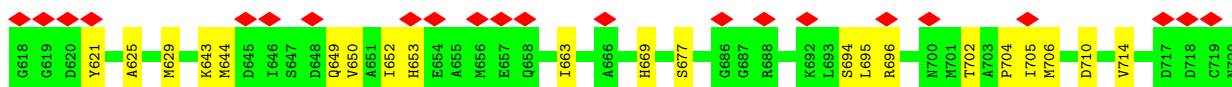


• Molecule 3: DNA replication licensing factor MCM4

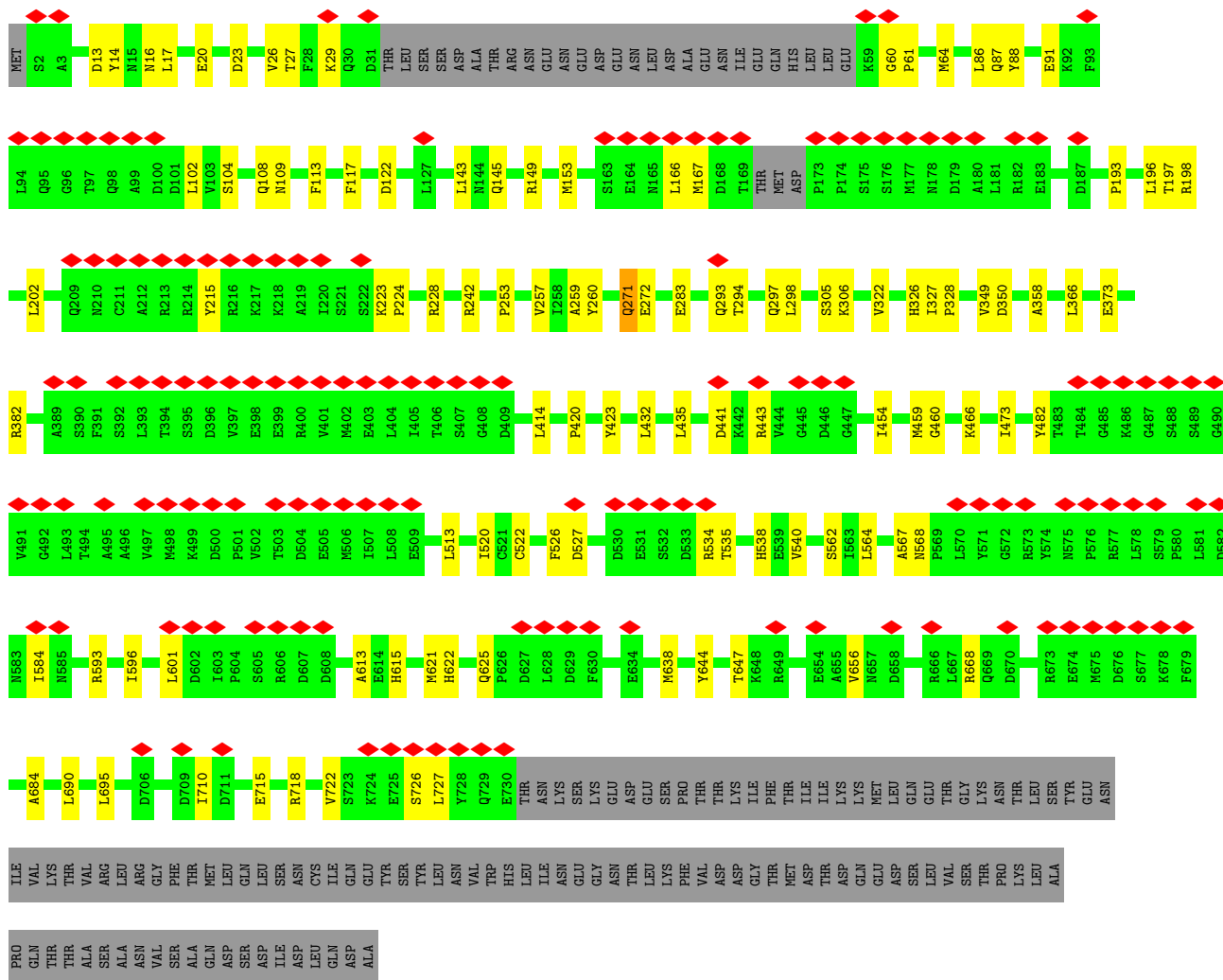


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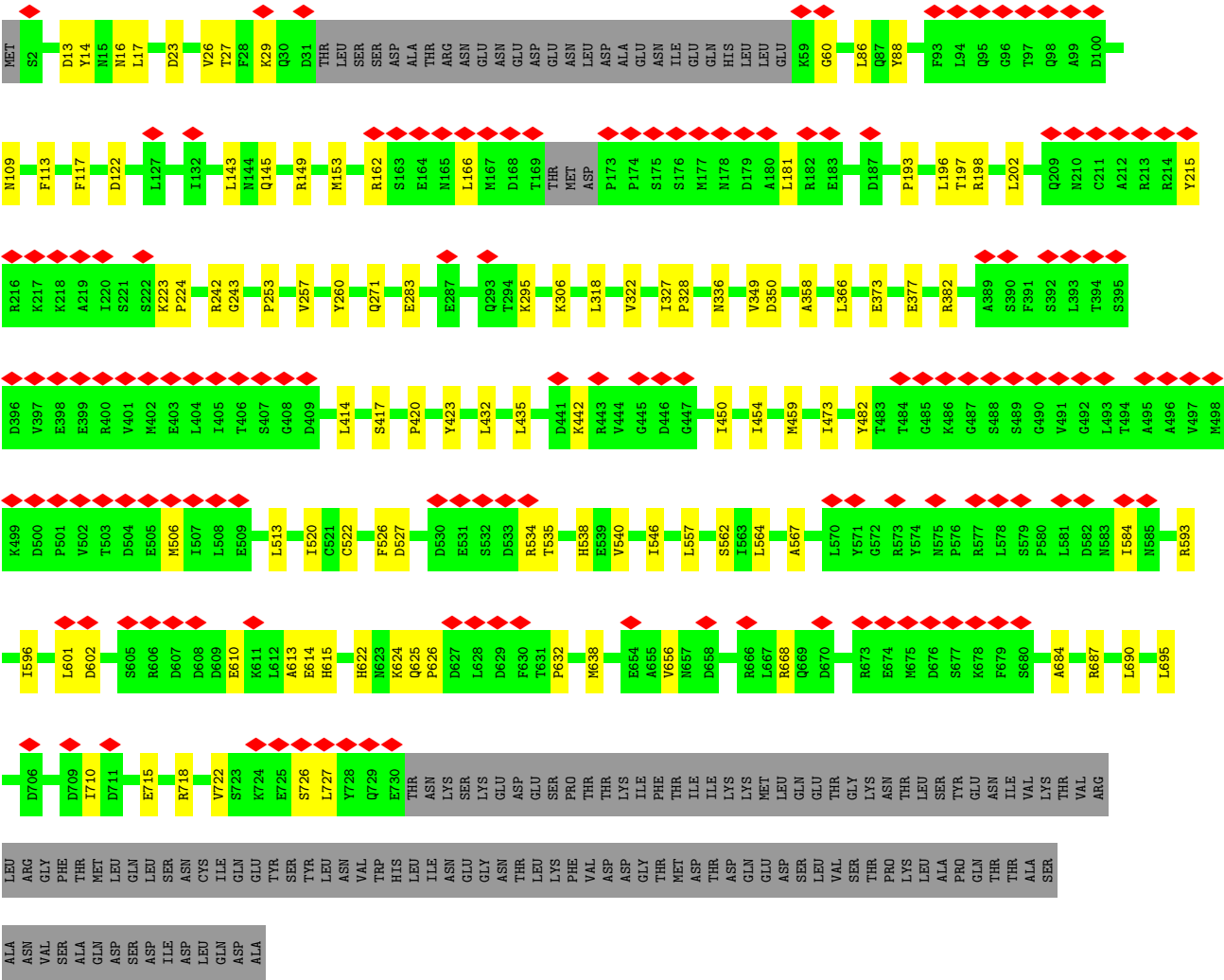




- Molecule 6: DNA replication licensing factor MCM7



- 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	94859	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)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.287	Depositor
Minimum map value	-0.158	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.045	Depositor
Map size ($\text{\AA}$)	378.72003, 378.72003, 378.72003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.052, 1.052, 1.052	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: AGS, MG, ADP, ZN

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	0.18	0/5057	0.47	0/6834
1	B	0.17	0/5057	0.46	0/6834
2	3	0.19	0/5073	0.47	0/6880
2	C	0.19	0/5073	0.46	0/6880
3	4	0.17	0/5400	0.44	0/7300
3	D	0.18	0/5400	0.44	0/7300
4	5	0.19	0/5217	0.47	0/7054
4	E	0.18	0/5217	0.47	0/7054
5	6	0.18	0/5190	0.46	0/7001
5	F	0.19	0/5190	0.49	1/7001 (0.0%)
6	7	0.18	0/5590	0.42	0/7554
6	G	0.19	0/5590	0.44	1/7554 (0.0%)
All	All	0.18	0/63054	0.46	2/85246 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	745	PRO	N-CD-CG	-5.98	94.23	103.20
6	G	632	PRO	CA-N-CD	-5.43	104.40	112.00

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	4970	0	5026	63	0
1	B	4970	0	5026	73	0
2	3	4987	0	5049	54	0
2	C	4987	0	5049	52	0
3	4	5323	0	5373	62	0
3	D	5323	0	5373	58	0
4	5	5143	0	5191	60	0
4	E	5143	0	5191	61	0
5	6	5109	0	5134	65	0
5	F	5109	0	5134	68	0
6	7	5505	0	5563	74	0
6	G	5505	0	5563	67	0
7	2	31	0	12	2	0
7	4	31	0	12	1	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	2	0
7	E	31	0	12	3	0
7	F	31	0	12	0	0
7	G	31	0	12	1	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	62460	0	62816	684	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 (684) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:CYS:HB3	1:B:367:CYS:SG	1.99	1.02
1:2:344:CYS:HB3	1:2:367:CYS:SG	1.99	1.01
6:7:482:TYR:HA	6:7:522:CYS:HB2	1.65	0.79
6:G:482:TYR:HA	6:G:522:CYS:HB2	1.66	0.76
5:F:702:THR:HG22	5:F:704:PRO:HD2	1.69	0.75
1:2:670:THR:HG22	1:2:672:PRO:HD2	1.70	0.73
1:B:670:THR:HG22	1:B:672:PRO:HD2	1.70	0.73
3:4:356:MET:HE3	3:4:382:MET:HE2	1.72	0.72
3:D:356:MET:HE3	3:D:382:MET:HE2	1.72	0.71
1:2:384:ASN:HB2	1:2:412:ALA:HA	1.73	0.70
5:6:657:GLU:HG3	5:6:708:ARG:HE	1.55	0.70
2:3:478:MET:HB2	2:3:483:ARG:HE	1.55	0.70
6:7:166:LEU:HA	4:E:47:ARG:HH11	1.57	0.70
5:6:773:LEU:HD21	5:6:804:ILE:HG12	1.75	0.69
1:B:384:ASN:HB2	1:B:412:ALA:HA	1.75	0.69
3:4:637:MET:O	3:4:642:ARG:NH1	2.26	0.68
1:2:341:CYS:HB3	1:2:344:CYS:SG	2.34	0.67
5:F:773:LEU:HD21	5:F:804:ILE:HG12	1.76	0.67
2:C:478:MET:HB2	2:C:483:ARG:HE	1.59	0.66
3:D:849:LEU:HD12	3:D:850:VAL:HG23	1.76	0.66
4:E:65:MET:HE1	4:E:159:ILE:HG21	1.76	0.66
1:B:341:CYS:HB3	1:B:344:CYS:SG	2.35	0.66
2:3:234:GLU:OE2	4:E:5:ARG:NH1	2.29	0.66
3:4:849:LEU:HD12	3:4:850:VAL:HG23	1.77	0.66
1:2:400:GLY:HA3	5:6:390:LYS:HD3	1.78	0.66
4:E:464:LEU:HD21	4:E:470:VAL:HG11	1.77	0.65
4:5:493:ILE:HG22	4:5:497:MET:HE2	1.77	0.65
6:G:26:VAL:HG23	6:G:27:THR:HG23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:307:ARG:NH1	1:2:392:GLU:OE2	2.28	0.65
3:4:434:GLU:HB3	3:4:467:LYS:HB3	1.78	0.65
3:4:417:LEU:HD13	3:4:463:VAL:HG21	1.79	0.65
5:6:364:ASN:HB2	5:6:367:GLU:HG3	1.78	0.64
2:C:40:ASP:OD2	2:C:43:ARG:NH2	2.30	0.64
3:D:434:GLU:HB3	3:D:467:LYS:HB3	1.79	0.64
6:7:166:LEU:HD12	6:7:167:MET:HG3	1.80	0.64
3:D:417:LEU:HD13	3:D:463:VAL:HG21	1.79	0.64
5:F:364:ASN:HB2	5:F:367:GLU:HG3	1.78	0.64
6:G:420:PRO:HB2	6:G:625:GLN:HG2	1.77	0.64
2:C:266:PRO:HB2	2:C:269:GLN:HG3	1.78	0.64
5:F:650:VAL:HA	5:F:653:HIS:CE1	2.33	0.64
6:G:435:LEU:HD21	6:G:564:LEU:HB2	1.80	0.63
6:7:420:PRO:HB2	6:7:625:GLN:HG2	1.81	0.63
6:7:435:LEU:HD21	6:7:564:LEU:HB2	1.81	0.63
1:2:511:ILE:HD11	1:2:683:VAL:HG21	1.81	0.63
2:3:368:ALA:HB3	2:3:378:LYS:HE2	1.80	0.63
7:D:2001:AGS:H5'2	6:G:687:ARG:HE	1.63	0.62
1:B:307:ARG:NH1	1:B:392:GLU:OE2	2.31	0.62
3:D:445:ARG:HD3	5:F:410:LEU:HD11	1.81	0.62
2:C:368:ALA:HB3	2:C:378:LYS:HE2	1.79	0.62
3:4:445:ARG:HD3	5:6:410:LEU:HD11	1.82	0.62
2:C:223:THR:HG21	4:E:244:ILE:HA	1.81	0.62
3:D:621:LEU:HD13	3:D:648:VAL:HG21	1.81	0.62
6:G:162:ARG:HE	6:G:181:LEU:HD21	1.65	0.62
3:D:798:LEU:HA	3:D:801:MET:HE3	1.81	0.62
5:F:737:LYS:HB2	5:F:741:ALA:HB2	1.82	0.62
5:F:109:GLU:OE1	5:F:112:ARG:NH1	2.33	0.62
3:D:445:ARG:NH1	5:F:447:ASP:OD2	2.33	0.62
2:3:567:ARG:O	2:3:642:TYR:OH	2.18	0.62
4:E:398:LYS:NZ	4:E:661:GLU:OE1	2.33	0.62
2:3:266:PRO:HB2	2:3:269:GLN:HG3	1.82	0.61
5:F:403:VAL:HG22	5:F:450:TYR:HB3	1.80	0.61
6:7:26:VAL:HG23	6:7:27:THR:HG23	1.82	0.61
2:C:567:ARG:O	2:C:642:TYR:OH	2.18	0.61
4:E:198:ASN:HA	4:E:329:LYS:HD3	1.82	0.61
3:D:314:MET:HE2	3:D:415:ILE:HG12	1.80	0.61
5:6:710:ASP:OD2	5:6:805:ARG:NH1	2.33	0.61
1:B:576:LEU:HD13	1:B:620:ILE:HD11	1.83	0.61
4:E:72:ASN:HB3	4:E:75:ILE:HG12	1.83	0.61
2:3:223:THR:HG21	4:5:244:ILE:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:656:ILE:HD13	5:6:602:ALA:HB1	1.83	0.61
6:7:166:LEU:HD13	4:E:101:ILE:HG12	1.82	0.61
1:B:406:ARG:NH1	1:B:449:THR:OG1	2.34	0.61
5:6:109:GLU:OE1	5:6:112:ARG:NH1	2.34	0.60
5:6:314:CYS:SG	5:6:338:CYS:HB3	2.41	0.60
3:4:314:MET:HG2	3:4:415:ILE:HG21	1.83	0.60
3:4:621:LEU:HD13	3:4:648:VAL:HG21	1.82	0.60
1:2:406:ARG:NH1	1:2:449:THR:OG1	2.34	0.60
6:7:350:ASP:OD2	6:7:382:ARG:NH2	2.35	0.60
2:3:712:HIS:ND1	2:3:725:ASP:OD1	2.33	0.60
1:B:400:GLY:HA3	5:F:390:LYS:HD3	1.83	0.60
2:C:712:HIS:ND1	2:C:725:ASP:OD1	2.34	0.60
2:3:647:ILE:HG22	2:3:651:VAL:HG12	1.82	0.60
5:6:403:VAL:HG22	5:6:450:TYR:HB3	1.81	0.60
6:G:414:LEU:HD22	6:G:638:MET:HG3	1.83	0.60
5:6:829:ASP:O	5:6:833:GLN:NE2	2.34	0.60
4:5:433:SER:HB3	4:5:436:ALA:HB2	1.82	0.60
2:3:295:VAL:HB	2:3:325:THR:HB	1.84	0.60
5:F:710:ASP:OD2	5:F:805:ARG:NH1	2.35	0.60
4:5:101:ILE:HG12	6:G:166:LEU:HD13	1.84	0.59
4:E:433:SER:HB3	4:E:436:ALA:HB2	1.82	0.59
4:E:152:ASP:HB3	4:E:154:GLU:HG2	1.83	0.59
1:2:321:THR:HG22	1:2:425:GLU:HG2	1.84	0.59
1:2:519:LEU:HD21	1:2:556:VAL:HG13	1.85	0.59
4:5:464:LEU:HD21	4:5:470:VAL:HG11	1.85	0.59
1:B:519:LEU:HD21	1:B:556:VAL:HG13	1.85	0.59
4:5:152:ASP:HB3	4:5:154:GLU:HG2	1.83	0.59
5:6:143:MET:HG2	5:6:148:LEU:HB2	1.84	0.59
5:F:311:CYS:HB3	5:F:314:CYS:HB2	1.82	0.59
5:F:314:CYS:SG	5:F:338:CYS:HB3	2.42	0.59
6:G:350:ASP:OD2	6:G:382:ARG:NH2	2.36	0.59
2:C:390:GLU:OE1	2:C:467:ARG:NH1	2.35	0.58
3:4:310:SER:HB2	3:4:312:LYS:HE3	1.85	0.58
5:6:650:VAL:HA	5:6:653:HIS:CE1	2.38	0.58
6:G:432:LEU:HD22	6:G:473:ILE:HG13	1.85	0.58
5:6:601:LYS:HG2	5:6:643:LYS:HB3	1.85	0.58
5:6:737:LYS:HB2	5:6:741:ALA:HB2	1.85	0.58
1:B:321:THR:HG22	1:B:425:GLU:HG2	1.85	0.58
2:3:244:GLU:OE1	6:7:109:ASN:ND2	2.36	0.58
5:F:742:ILE:HG22	5:F:744:PRO:HD3	1.84	0.58
6:G:14:TYR:OH	6:G:109:ASN:ND2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:2001:AGS:O2G	5:F:798:ARG:NH2	2.34	0.58
5:6:311:CYS:HB3	5:6:314:CYS:HB2	1.85	0.58
6:7:14:TYR:OH	6:7:109:ASN:ND2	2.36	0.58
6:7:414:LEU:HD22	6:7:638:MET:HG3	1.85	0.58
2:C:483:ARG:HD2	2:C:539:LEU:HD11	1.85	0.57
4:E:392:LEU:O	4:E:607:ARG:NH2	2.36	0.57
3:4:345:ALA:HB2	3:4:365:ILE:HD13	1.87	0.57
1:B:616:ASP:O	1:B:620:ILE:HD12	2.05	0.57
2:C:647:ILE:HG22	2:C:651:VAL:HG12	1.86	0.57
7:E:2001:AGS:S1G	7:E:2001:AGS:O2B	2.62	0.57
1:2:659:SER:OG	1:2:684:ARG:NH1	2.37	0.57
2:3:177:ASN:ND2	4:5:245:HIS:O	2.37	0.57
6:7:432:LEU:HD22	6:7:473:ILE:HG13	1.85	0.57
2:3:541:SER:HB2	2:3:700:ARG:HD2	1.86	0.57
3:D:601:LEU:HD23	3:D:620:ALA:HB3	1.87	0.57
2:C:244:GLU:OE1	6:G:109:ASN:ND2	2.36	0.57
3:4:429:ALA:O	3:4:587:ARG:NH2	2.38	0.57
5:6:147:ASP:OD1	5:6:261:ARG:NH1	2.38	0.57
6:7:466:LYS:NZ	7:7:2001:AGS:S1G	2.71	0.57
6:7:596:ILE:HD11	6:7:695:LEU:HD21	1.87	0.56
2:C:177:ASN:ND2	4:E:245:HIS:O	2.38	0.56
5:F:663:ILE:O	5:F:669:HIS:HA	2.04	0.56
4:5:206:SER:OG	4:5:209:ARG:NH2	2.38	0.56
1:2:598:LEU:HD21	4:5:267:VAL:HA	1.86	0.56
5:6:696:ARG:HA	5:6:706:MET:HE1	1.87	0.56
3:D:345:ALA:HB2	3:D:365:ILE:HD13	1.87	0.56
5:F:696:ARG:HA	5:F:706:MET:HE1	1.86	0.56
5:F:777:TYR:OH	5:F:781:ARG:NH1	2.38	0.56
5:F:820:THR:HG22	5:F:822:SER:H	1.71	0.56
6:G:593:ARG:NH1	6:G:687:ARG:HH12	2.03	0.56
3:D:310:SER:HB2	3:D:312:LYS:HE3	1.86	0.56
1:2:419:LYS:HD2	1:2:420:PRO:HD2	1.87	0.56
3:4:445:ARG:NH1	5:6:447:ASP:OD2	2.39	0.56
2:C:295:VAL:HB	2:C:325:THR:HB	1.87	0.56
1:2:596:LEU:HD11	1:2:620:ILE:HG13	1.88	0.56
1:B:505:ILE:HD11	1:B:551:GLN:HB2	1.86	0.56
1:B:511:ILE:HD11	1:B:683:VAL:HG21	1.88	0.56
3:D:639:ASP:OD1	3:D:642:ARG:NH2	2.36	0.56
3:4:798:LEU:HA	3:4:801:MET:HE3	1.87	0.56
6:7:260:TYR:HE2	6:7:271:GLN:HG2	1.70	0.56
1:B:612:MET:O	1:B:617:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:LEU:HD21	4:E:267:VAL:HA	1.88	0.55
6:G:149:ARG:O	6:G:153:MET:HG3	2.07	0.55
2:3:196:LEU:HD21	2:3:199:SER:HB3	1.89	0.55
4:E:432:VAL:HG23	4:E:596:ILE:HG13	1.88	0.55
1:2:342:LEU:HB3	5:F:433:LEU:HD13	1.88	0.55
3:4:601:LEU:HD23	3:4:620:ALA:HB3	1.89	0.55
4:5:398:LYS:HB2	4:5:406:LEU:HB2	1.88	0.55
7:2:2001:AGS:O2G	5:6:798:ARG:NH2	2.36	0.55
5:6:433:LEU:HD13	1:B:342:LEU:HB3	1.88	0.55
6:7:441:ASP:OD2	6:7:443:ARG:NH1	2.39	0.55
3:D:656:ILE:HD13	5:F:602:ALA:HB1	1.88	0.55
1:2:527:VAL:HG23	4:5:581:ASN:HB2	1.88	0.55
3:4:470:SER:HB3	3:4:473:ARG:HG2	1.88	0.55
3:D:470:SER:HB3	3:D:473:ARG:HG2	1.89	0.55
1:2:337:VAL:HA	1:2:380:THR:HG23	1.89	0.54
2:C:196:LEU:HD21	2:C:199:SER:HB3	1.88	0.54
1:B:230:ARG:NH1	1:B:243:GLU:O	2.40	0.54
6:7:272:GLU:HB2	4:E:7:GLU:H	1.72	0.54
2:C:680:VAL:HG22	6:G:613:ALA:HB1	1.90	0.54
3:D:477:ASP:OD2	3:D:479:SER:OG	2.25	0.54
6:G:596:ILE:HD11	6:G:695:LEU:HD21	1.90	0.54
6:G:260:TYR:HE2	6:G:271:GLN:HG2	1.72	0.54
3:4:799:GLU:OE1	5:6:735:HIS:NE2	2.41	0.54
4:5:5:ARG:HG2	4:5:218:GLU:HB3	1.90	0.54
2:C:459:ALA:HB2	6:G:327:ILE:HD11	1.90	0.54
1:B:337:VAL:HA	1:B:380:THR:HG23	1.90	0.54
6:G:336:ASN:ND2	6:G:377:GLU:OE2	2.41	0.54
3:4:769:GLU:OE2	3:4:772:ARG:NH2	2.41	0.54
4:5:481:GLU:OE1	4:5:484:LYS:NZ	2.41	0.54
2:C:542:ARG:NH1	7:G:2001:AGS:O3G	2.40	0.54
4:E:36:LEU:O	4:E:47:ARG:NH2	2.41	0.54
1:2:419:LYS:NZ	1:2:420:PRO:O	2.38	0.54
3:4:230:LEU:HD22	3:4:280:MET:HE3	1.90	0.54
3:D:429:ALA:O	3:D:587:ARG:NH2	2.38	0.54
6:G:513:LEU:HD13	6:G:540:VAL:HG21	1.89	0.54
6:G:526:PHE:HB3	6:G:567:ALA:HB2	1.90	0.54
2:3:491:GLU:OE1	2:3:700:ARG:NH1	2.41	0.53
3:D:707:LEU:O	3:D:834:LYS:NZ	2.37	0.53
1:2:534:ARG:O	1:2:815:ARG:NH1	2.39	0.53
3:4:709:LEU:HD13	3:4:847:MET:HE1	1.89	0.53
3:D:774:TYR:OH	3:D:778:ARG:NH1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:569:ILE:O	5:6:677:SER:OG	2.26	0.53
5:F:277:ARG:NH2	5:F:373:MET:O	2.41	0.53
3:4:206:ARG:NH1	3:4:247:ASN:OD1	2.40	0.53
4:5:216:GLU:HB3	4:5:218:GLU:HG2	1.90	0.53
5:6:820:THR:HG22	5:6:822:SER:H	1.74	0.53
1:B:795:ARG:HA	1:B:798:ILE:HD12	1.89	0.53
3:D:231:ASN:OD1	3:D:234:ARG:NH2	2.41	0.53
5:F:569:ILE:O	5:F:677:SER:OG	2.27	0.53
1:B:813:ILE:HG12	1:B:841:VAL:HG11	1.90	0.53
3:4:724:LEU:HD12	6:7:690:LEU:HD21	1.90	0.53
4:5:358:LEU:HB3	4:5:362:ARG:HH12	1.74	0.53
1:B:659:SER:OG	1:B:684:ARG:NH1	2.42	0.53
1:2:384:ASN:ND2	4:5:152:ASP:OD2	2.42	0.53
6:7:23:ASP:OD2	6:7:88:TYR:OH	2.23	0.53
4:E:481:GLU:OE1	4:E:484:LYS:NZ	2.42	0.53
5:6:260:GLU:O	5:6:352:ARG:NH2	2.41	0.52
1:B:474:PHE:HE1	1:B:764:MET:HE3	1.74	0.52
4:E:524:ASN:ND2	7:E:2001:AGS:O2G	2.41	0.52
4:5:432:VAL:HG23	4:5:596:ILE:HG13	1.90	0.52
1:2:505:ILE:HD11	1:2:551:GLN:HB2	1.92	0.52
3:4:694:LEU:HD22	3:4:698:LEU:HD23	1.91	0.52
4:5:370:LEU:HD22	4:5:599:MET:HE2	1.91	0.52
4:E:358:LEU:HB3	4:E:362:ARG:HH12	1.74	0.52
4:E:495:GLU:O	4:E:499:GLN:HB2	2.10	0.52
3:4:636:LYS:HD3	6:7:535:THR:HG22	1.91	0.52
4:5:198:ASN:HA	4:5:329:LYS:HD3	1.90	0.52
1:B:824:ARG:NH1	1:B:830:SER:OG	2.43	0.52
3:D:204:LYS:HB3	3:D:221:ASP:HB3	1.92	0.52
3:D:306:TYR:HA	3:D:436:THR:HG21	1.91	0.52
6:G:715:GLU:HA	6:G:718:ARG:HG2	1.91	0.52
4:5:486:ARG:NH2	4:5:489:ASP:OD1	2.43	0.52
2:3:366:SER:HB3	2:3:650:LEU:HB2	1.92	0.52
5:6:277:ARG:HG2	5:6:375:ARG:HD2	1.92	0.52
3:4:231:ASN:OD1	3:4:234:ARG:NH2	2.43	0.52
5:6:277:ARG:NH2	5:6:373:MET:O	2.42	0.52
1:2:335:LYS:HE3	1:2:383:ARG:HB3	1.91	0.51
5:6:186:ARG:HE	5:6:197:LEU:HD22	1.74	0.51
3:4:183:THR:O	6:7:145:GLN:NE2	2.43	0.51
6:G:117:PHE:HB3	6:G:202:LEU:HD11	1.91	0.51
6:7:513:LEU:HD13	6:7:540:VAL:HG21	1.91	0.51
3:D:636:LYS:HD3	6:G:535:THR:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:401:GLU:OE1	3:4:413:HIS:NE2	2.40	0.51
6:7:122:ASP:OD1	6:7:198:ARG:NE	2.42	0.51
2:C:672:THR:OG1	2:C:721:VAL:O	2.28	0.51
3:D:183:THR:O	6:G:145:GLN:NE2	2.43	0.51
5:F:123:SER:HB3	5:F:134:LYS:HG2	1.91	0.51
6:7:149:ARG:O	6:7:153:MET:HG3	2.11	0.51
3:D:445:ARG:NH2	3:D:448:SER:O	2.43	0.51
4:E:398:LYS:HB2	4:E:406:LEU:HB2	1.92	0.51
6:G:23:ASP:OD2	6:G:88:TYR:OH	2.26	0.51
3:4:477:ASP:OD2	3:4:479:SER:OG	2.27	0.51
6:7:117:PHE:HB3	6:7:202:LEU:HD11	1.91	0.51
2:C:263:GLU:OE2	4:E:511:THR:OG1	2.29	0.51
6:G:534:ARG:O	6:G:538:HIS:HB2	2.09	0.51
3:4:445:ARG:NH2	3:4:448:SER:O	2.43	0.51
1:B:383:ARG:HB2	1:B:412:ALA:HB2	1.93	0.51
3:4:364:VAL:HG11	6:7:297:GLN:HE22	1.75	0.51
5:6:742:ILE:HG22	5:6:744:PRO:HD3	1.92	0.51
2:C:422:VAL:HA	2:C:425:THR:HG22	1.93	0.51
1:2:824:ARG:NH1	1:2:830:SER:OG	2.42	0.51
4:5:614:LEU:HA	4:5:672:ALA:HB3	1.93	0.51
6:7:228:ARG:HH21	6:7:326:HIS:HB3	1.76	0.50
6:7:526:PHE:HB3	6:7:567:ALA:HB2	1.93	0.50
4:E:396:SER:OG	4:E:661:GLU:OE1	2.29	0.50
4:E:169:THR:HG22	4:E:256:LEU:HD22	1.92	0.50
4:E:216:GLU:HB3	4:E:218:GLU:HG2	1.93	0.50
2:3:255:ARG:NH2	6:7:366:LEU:O	2.45	0.50
2:3:661:GLN:O	2:3:665:GLU:HG2	2.11	0.50
1:B:309:LEU:HD21	1:B:318:VAL:HG21	1.93	0.50
1:B:384:ASN:ND2	4:E:152:ASP:OD2	2.43	0.50
1:B:792:ASP:OD1	1:B:795:ARG:NH1	2.43	0.50
3:D:206:ARG:NH1	3:D:247:ASN:OD1	2.40	0.50
6:G:596:ILE:HD11	6:G:695:LEU:HD11	1.94	0.50
3:4:306:TYR:HA	3:4:436:THR:HG21	1.92	0.50
1:2:605:LEU:HD23	1:2:647:ILE:HB	1.94	0.50
2:3:459:ALA:HB2	6:7:327:ILE:HD11	1.92	0.50
6:G:122:ASP:OD1	6:G:198:ARG:NE	2.42	0.50
1:2:239:SER:O	1:2:286:TYR:OH	2.29	0.50
2:3:39:ARG:HH12	2:3:136:MET:HB2	1.77	0.50
2:3:391:LYS:HB2	2:3:399:LEU:HB2	1.94	0.50
5:6:777:TYR:OH	5:6:781:ARG:NH1	2.41	0.50
2:C:661:GLN:O	2:C:665:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:277:ARG:HG2	5:F:375:ARG:HD2	1.93	0.50
2:3:235:ASP:OD1	2:3:239:ASN:N	2.45	0.50
4:5:169:THR:HG22	4:5:256:LEU:HD22	1.94	0.50
6:7:13:ASP:OD2	6:7:16:ASN:ND2	2.45	0.50
5:F:297:THR:OG1	5:F:357:GLN:NE2	2.44	0.49
1:2:309:LEU:HD21	1:2:318:VAL:HG21	1.94	0.49
2:3:52:ASN:ND2	2:3:90:ASN:O	2.44	0.49
4:5:570:ASN:O	4:5:574:ASN:ND2	2.45	0.49
1:B:534:ARG:O	1:B:815:ARG:NH1	2.41	0.49
3:D:292:ASP:OD1	3:D:292:ASP:N	2.43	0.49
3:4:594:LYS:HD2	6:7:535:THR:HG21	1.93	0.49
3:D:474:LEU:HB2	3:D:586:PRO:HD3	1.94	0.49
2:3:570:ARG:O	4:5:613:ARG:NH2	2.46	0.49
7:5:2001:AGS:S1G	7:5:2001:AGS:O2B	2.70	0.49
2:C:52:ASN:ND2	2:C:90:ASN:O	2.45	0.49
2:C:366:SER:HB3	2:C:650:LEU:HB2	1.95	0.49
3:D:799:GLU:OE2	5:F:735:HIS:NE2	2.46	0.49
6:G:459:MET:HA	6:G:567:ALA:O	2.13	0.49
1:2:495:ASP:OD1	1:2:509:ARG:NH2	2.45	0.49
2:3:672:THR:OG1	2:3:721:VAL:O	2.29	0.49
3:4:360:ILE:HG13	3:4:365:ILE:HG13	1.95	0.49
3:D:585:THR:HG21	3:D:628:VAL:HB	1.95	0.49
1:B:239:SER:O	1:B:286:TYR:OH	2.29	0.49
1:2:474:PHE:HE1	1:2:764:MET:HE3	1.78	0.49
3:4:585:THR:HG21	3:4:628:VAL:HB	1.94	0.49
3:4:701:ARG:NH2	7:6:2001:AGS:S1G	2.86	0.49
6:G:454:ILE:O	6:G:562:SER:OG	2.27	0.49
1:2:662:PRO:O	1:2:666:ASN:ND2	2.46	0.48
5:F:615:ASP:OD1	5:F:615:ASP:N	2.45	0.48
6:G:13:ASP:OD2	6:G:16:ASN:ND2	2.46	0.48
6:7:193:PRO:HD2	6:7:196:LEU:HD12	1.95	0.48
2:C:400:ARG:HB2	2:C:707:ARG:HH21	1.79	0.48
2:C:426:ALA:HB3	2:C:429:ALA:HB2	1.95	0.48
5:6:535:PRO:HB2	5:6:742:ILE:HG23	1.95	0.48
1:B:479:GLU:OE2	1:B:482:ARG:NH2	2.38	0.48
2:C:255:ARG:NH2	6:G:366:LEU:O	2.47	0.48
2:C:440:VAL:HB	2:C:445:ALA:HB2	1.95	0.48
3:D:665:LEU:HD13	5:F:373:MET:HE1	1.96	0.48
3:D:812:LYS:HD3	3:D:814:LYS:HE2	1.94	0.48
2:3:669:PRO:HG2	2:3:710:THR:HG23	1.95	0.48
5:6:199:THR:OG1	5:6:261:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:360:ILE:HG13	3:D:365:ILE:HG13	1.95	0.48
5:F:733:ASP:OD2	5:F:737:LYS:NZ	2.40	0.48
3:4:474:LEU:HB2	3:4:586:PRO:HD3	1.94	0.48
3:4:665:LEU:HD13	5:6:373:MET:HE1	1.96	0.48
5:6:441:ARG:HH22	6:7:283:GLU:HG3	1.79	0.48
1:B:296:ARG:HH21	1:B:413:ASP:HB3	1.78	0.48
1:2:555:TYR:HA	1:2:558:LYS:HE2	1.96	0.48
3:4:212:ARG:HB3	3:4:215:PHE:HD1	1.78	0.48
2:3:430:ILE:HD12	2:3:465:ALA:HB2	1.95	0.48
1:2:795:ARG:HA	1:2:798:ILE:HD12	1.95	0.48
1:B:335:LYS:HE3	1:B:383:ARG:HB3	1.95	0.48
3:D:457:TYR:HB2	6:G:253:PRO:HG2	1.96	0.48
5:F:601:LYS:HG2	5:F:643:LYS:HB3	1.95	0.48
1:2:386:GLN:HB2	1:2:415:VAL:HG12	1.96	0.48
4:5:685:GLN:HA	4:5:689:MET:HB2	1.95	0.48
2:C:669:PRO:HG2	2:C:710:THR:HG23	1.95	0.48
4:5:99:LYS:HG3	4:5:132:LEU:HD23	1.96	0.48
6:7:715:GLU:HA	6:7:718:ARG:HG2	1.96	0.48
4:E:282:LEU:HD13	4:E:330:ILE:HG22	1.96	0.48
1:2:296:ARG:HH21	1:2:413:ASP:HB3	1.79	0.47
4:5:469:MET:HA	4:5:477:VAL:HG21	1.96	0.47
5:6:123:SER:HB3	5:6:134:LYS:HG2	1.95	0.47
6:7:621:MET:HE3	6:7:622:HIS:NE2	2.29	0.47
3:4:602:THR:HG22	3:4:654:ILE:HD13	1.96	0.47
1:B:605:LEU:HD23	1:B:647:ILE:HB	1.95	0.47
5:F:653:HIS:HB3	5:F:705:ILE:HD13	1.96	0.47
6:7:656:VAL:HG12	6:7:710:ILE:HD13	1.96	0.47
6:G:656:VAL:HG12	6:G:710:ILE:HD13	1.96	0.47
1:B:315:SER:N	1:B:430:TYR:O	2.46	0.47
2:C:198:ARG:HB3	2:C:249:THR:HG22	1.96	0.47
3:D:435:VAL:HG13	3:D:463:VAL:HG13	1.96	0.47
4:E:497:MET:HG2	4:E:519:VAL:HG21	1.97	0.47
2:3:171:LEU:HD11	2:3:182:VAL:HG21	1.96	0.47
7:4:2001:AGS:O3G	6:7:593:ARG:NH2	2.36	0.47
4:5:646:ILE:HG21	4:5:692:ALA:HA	1.96	0.47
2:C:171:LEU:HD11	2:C:182:VAL:HG21	1.95	0.47
3:D:230:LEU:HD22	3:D:280:MET:HE3	1.96	0.47
5:6:615:ASP:OD1	5:6:615:ASP:N	2.45	0.47
6:7:242:ARG:HB3	6:7:350:ASP:OD1	2.15	0.47
6:7:322:VAL:HG21	6:7:328:PRO:HG3	1.96	0.47
1:B:596:LEU:HD11	1:B:620:ILE:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:746:PHE:HA	3:D:749:MET:HG2	1.97	0.47
6:G:193:PRO:HD2	6:G:196:LEU:HD12	1.97	0.47
4:E:32:LYS:HD3	4:E:100:ARG:HH12	1.79	0.47
2:3:198:ARG:HB3	2:3:249:THR:HG22	1.96	0.47
1:B:241:SER:OG	1:B:413:ASP:OD2	2.32	0.47
6:G:257:VAL:HG12	6:G:306:LYS:HB3	1.97	0.47
1:B:629:ILE:HG23	4:E:445:SER:HB3	1.97	0.47
2:C:235:ASP:OD2	2:C:239:ASN:N	2.48	0.47
2:3:251:ILE:HG23	2:3:280:ASP:HB2	1.96	0.46
3:4:292:ASP:OD1	3:4:292:ASP:N	2.43	0.46
4:5:182:MET:HE3	4:5:244:ILE:HD11	1.96	0.46
1:B:576:LEU:HD23	1:B:595:ALA:HB3	1.96	0.46
5:F:139:GLN:O	5:F:143:MET:HG3	2.15	0.46
5:F:186:ARG:HE	5:F:197:LEU:HD22	1.80	0.46
6:G:29:LYS:HE3	6:G:60:GLY:HA2	1.97	0.46
4:E:82:GLU:OE2	4:E:84:SER:OG	2.33	0.46
4:E:614:LEU:HA	4:E:672:ALA:HB3	1.98	0.46
6:G:223:LYS:HD2	6:G:224:PRO:HD2	1.97	0.46
3:4:457:TYR:HB2	6:7:253:PRO:HG2	1.97	0.46
3:4:578:LEU:HB3	3:4:590:TYR:HE2	1.79	0.46
2:C:39:ARG:HG2	2:C:136:MET:HE1	1.97	0.46
4:E:182:MET:HE3	4:E:244:ILE:HD11	1.96	0.46
5:F:330:PRO:O	5:F:344:TRP:NE1	2.48	0.46
5:F:535:PRO:HB2	5:F:742:ILE:HG23	1.97	0.46
5:6:187:ARG:HG2	5:6:190:ARG:HH22	1.80	0.46
6:7:293:GLN:HG2	6:7:294:THR:HG23	1.97	0.46
2:C:251:ILE:HG23	2:C:280:ASP:HB2	1.97	0.46
4:E:40:LEU:HB2	4:E:45:ILE:HD13	1.97	0.46
3:4:812:LYS:HD3	3:4:814:LYS:HE2	1.98	0.46
1:2:576:LEU:HD13	1:2:620:ILE:HD11	1.97	0.46
2:3:279:ASP:OD1	2:3:279:ASP:N	2.48	0.46
3:4:746:PHE:HA	3:4:749:MET:HG2	1.97	0.46
1:B:580:VAL:HG12	1:B:589:TRP:HE3	1.79	0.46
1:B:609:PHE:HB3	1:B:650:ALA:HB2	1.98	0.46
5:F:187:ARG:HG2	5:F:190:ARG:HH22	1.81	0.46
1:2:406:ARG:NH1	1:2:430:TYR:OH	2.47	0.46
5:F:396:LYS:HB2	5:F:462:ILE:HD11	1.98	0.46
3:D:344:VAL:O	3:D:389:CYS:HB2	2.16	0.46
3:4:366:GLN:HB3	5:6:422:ASP:HB2	1.98	0.46
5:6:341:ARG:O	5:6:344:TRP:NE1	2.49	0.46
3:D:272:MET:O	3:D:276:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:469:MET:HA	4:E:477:VAL:HG21	1.98	0.46
5:F:837:ARG:HA	5:F:837:ARG:HD2	1.80	0.46
1:2:629:ILE:HG23	4:5:445:SER:HB3	1.97	0.45
6:7:223:LYS:HD2	6:7:224:PRO:HD2	1.97	0.45
2:C:354:SER:HB3	2:C:717:LEU:HD12	1.98	0.45
5:F:441:ARG:HH22	6:G:283:GLU:HG2	1.81	0.45
1:2:423:GLU:OE1	1:2:459:ARG:NH1	2.50	0.45
3:4:435:VAL:HG13	3:4:463:VAL:HG13	1.97	0.45
3:4:686:LEU:HD12	3:4:690:GLU:HG2	1.98	0.45
2:C:97:ILE:HD13	2:C:156:SER:HB2	1.99	0.45
2:C:279:ASP:OD1	2:C:279:ASP:N	2.48	0.45
3:D:694:LEU:HD22	3:D:698:LEU:HD23	1.98	0.45
6:7:596:ILE:HD11	6:7:695:LEU:HD11	1.97	0.45
6:G:143:LEU:HG	6:G:197:THR:HA	1.99	0.45
2:3:400:ARG:NH2	2:3:544:ASP:OD1	2.44	0.45
2:3:400:ARG:HB2	2:3:707:ARG:HH21	1.82	0.45
2:3:680:VAL:HG22	6:7:613:ALA:HB1	1.98	0.45
4:5:90:PHE:CE2	4:5:137:LEU:HD13	2.51	0.45
1:B:324:VAL:HG21	1:B:418:SER:HB2	1.99	0.45
3:D:265:PRO:HB3	3:D:325:LEU:HG	1.99	0.45
1:2:230:ARG:NH1	1:2:243:GLU:O	2.50	0.45
4:5:87:ILE:HG12	4:5:137:LEU:HD23	1.98	0.45
4:E:90:PHE:CE2	4:E:137:LEU:HD13	2.52	0.45
6:G:283:GLU:OE2	6:G:295:LYS:HB2	2.16	0.45
1:2:224:ARG:HE	1:2:224:ARG:HB3	1.67	0.45
6:7:143:LEU:HG	6:7:197:THR:HA	1.98	0.45
6:7:257:VAL:HG12	6:7:306:LYS:HB3	1.99	0.45
6:7:460:GLY:O	6:7:568:ASN:ND2	2.48	0.45
1:B:550:SER:O	1:B:554:LYS:HG2	2.17	0.45
5:F:569:ILE:HD13	5:F:806:LEU:HD23	1.99	0.45
5:F:782:LYS:HB3	5:F:782:LYS:HE3	1.83	0.45
4:5:5:ARG:NE	2:C:234:GLU:OE2	2.49	0.45
6:7:644:TYR:O	6:7:647:THR:OG1	2.34	0.45
3:D:686:LEU:HD12	3:D:690:GLU:HG2	1.98	0.45
4:5:626:PHE:CG	4:5:653:LEU:HD12	2.51	0.45
5:6:663:ILE:O	5:6:669:HIS:HA	2.17	0.45
6:7:454:ILE:O	6:7:562:SER:OG	2.26	0.45
5:F:260:GLU:O	5:F:352:ARG:NH2	2.48	0.45
6:G:610:GLU:O	6:G:614:GLU:HG3	2.17	0.45
5:6:574:VAL:O	5:6:714:VAL:HA	2.17	0.45
5:6:699:LEU:HD22	5:6:701:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:216:ASP:O	2:3:219:THR:OG1	2.33	0.44
2:3:354:SER:HB3	2:3:717:LEU:HD12	1.99	0.44
2:3:384:MET:HE1	2:3:513:ILE:HD11	1.99	0.44
5:6:297:THR:OG1	5:6:357:GLN:NE2	2.50	0.44
6:7:534:ARG:O	6:7:538:HIS:HB2	2.17	0.44
1:B:447:PHE:HE1	5:F:304:LEU:HB2	1.83	0.44
3:D:366:GLN:HB3	5:F:422:ASP:HB2	2.00	0.44
1:2:511:ILE:HG21	1:2:552:ILE:HD13	1.99	0.44
4:5:140:ASN:OD1	4:5:334:GLN:NE2	2.50	0.44
4:5:453:VAL:HG21	4:5:504:ILE:HG21	1.99	0.44
1:B:407:GLU:HB2	1:B:450:ILE:HG22	1.98	0.44
1:B:560:ALA:HB3	1:B:563:ALA:HB2	2.00	0.44
2:3:97:ILE:HD13	2:3:156:SER:HB2	1.98	0.44
5:6:569:ILE:HD13	5:6:806:LEU:HD23	1.99	0.44
5:6:707:SER:OG	5:6:708:ARG:NH1	2.49	0.44
1:B:474:PHE:CE1	1:B:764:MET:HB3	2.52	0.44
2:C:430:ILE:HD12	2:C:465:ALA:HB2	1.98	0.44
4:E:263:GLU:OE2	4:E:291:ARG:NH2	2.40	0.44
1:2:582:LYS:HE3	1:2:587:LYS:HD3	1.98	0.44
1:B:211:LEU:HD13	1:B:271:PHE:HB2	1.99	0.44
6:G:546:ILE:HD12	6:G:557:LEU:HD11	2.00	0.44
3:4:344:VAL:O	3:4:389:CYS:HB2	2.17	0.44
6:7:20:GLU:HG2	6:7:102:LEU:HD22	1.99	0.44
2:3:264:MET:HE3	2:3:586:LEU:HD13	2.00	0.44
2:3:314:LEU:HD11	4:5:200:ILE:HA	2.00	0.44
4:5:149:ARG:NH2	4:5:260:GLU:OE2	2.43	0.44
6:7:104:SER:O	6:7:108:GLN:HG2	2.17	0.44
1:B:245:ASN:HD21	1:B:247:ARG:HH21	1.66	0.44
1:2:193:SER:HB3	1:2:196:GLU:OE1	2.18	0.44
2:3:52:ASN:HD22	2:3:90:ASN:H	1.66	0.44
1:B:406:ARG:NH1	1:B:430:TYR:OH	2.51	0.44
1:B:525:LYS:HB3	1:B:525:LYS:HE3	1.86	0.44
6:G:358:ALA:HB3	6:G:373:GLU:HB2	2.00	0.44
1:2:474:PHE:CE1	1:2:764:MET:HB3	2.52	0.44
1:2:676:ARG:HA	1:2:676:ARG:HD2	1.87	0.44
4:5:82:GLU:OE2	4:5:84:SER:OG	2.35	0.44
4:5:415:LEU:HD23	4:5:523:ALA:HB3	1.99	0.44
4:5:677:VAL:O	4:5:681:ILE:HG12	2.17	0.44
1:B:816:ILE:O	1:B:819:SER:OG	2.33	0.44
4:E:31:PHE:CE1	4:E:75:ILE:HD12	2.53	0.44
5:6:355:ASP:HB2	5:6:383:GLY:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:653:HIS:HB3	5:6:705:ILE:HD13	1.99	0.43
1:B:555:TYR:HA	1:B:558:LYS:HE2	2.00	0.43
3:D:778:ARG:HD2	3:D:793:ALA:HB3	1.99	0.43
5:F:158:LEU:HD21	5:F:170:ILE:HD12	1.99	0.43
5:F:694:SER:OG	5:F:695:LEU:N	2.51	0.43
5:6:777:TYR:HB2	5:6:800:LEU:HD13	2.00	0.43
5:F:412:LEU:O	5:F:416:LYS:NZ	2.48	0.43
2:3:43:ARG:O	2:3:47:VAL:HG13	2.18	0.43
6:7:601:LEU:H	6:7:727:LEU:HD21	1.82	0.43
4:E:266:PRO:HG2	4:E:269:GLU:HB2	2.00	0.43
1:B:193:SER:HB3	1:B:196:GLU:OE1	2.19	0.43
4:E:618:ALA:HB1	4:E:677:VAL:HG21	2.00	0.43
5:F:625:ALA:HB1	5:F:629:MET:HB2	2.00	0.43
5:F:842:ASP:OD1	5:F:842:ASP:N	2.50	0.43
6:G:520:ILE:HA	6:G:562:SER:O	2.19	0.43
1:2:663:LEU:HD12	1:2:663:LEU:HA	1.83	0.43
2:3:400:ARG:HD2	2:3:491:GLU:HA	1.99	0.43
6:7:17:LEU:HD13	6:7:113:PHE:HZ	1.84	0.43
6:7:459:MET:HA	6:7:567:ALA:O	2.18	0.43
6:7:527:ASP:OD1	6:7:527:ASP:N	2.52	0.43
6:7:722:VAL:HA	6:7:726:SER:HB3	2.01	0.43
1:B:304:TYR:HD2	1:B:318:VAL:HG23	1.84	0.43
1:2:527:VAL:HG11	4:5:575:ILE:HG23	2.00	0.43
6:7:668:ARG:NH1	6:7:684:ALA:O	2.43	0.43
1:B:386:GLN:HB2	1:B:415:VAL:HG12	2.00	0.43
5:6:566:ARG:O	5:6:805:ARG:NE	2.52	0.43
2:C:400:ARG:HD2	2:C:491:GLU:HA	2.00	0.43
4:E:132:LEU:HD12	4:E:133:PRO:HD2	2.01	0.43
5:F:772:TYR:HE1	5:F:825:ALA:HB2	1.83	0.43
1:2:651:ASN:ND2	7:2:2001:AGS:S1G	2.82	0.43
5:6:694:SER:OG	5:6:695:LEU:N	2.52	0.43
6:G:322:VAL:HG21	6:G:328:PRO:HG3	2.01	0.43
6:G:668:ARG:NH1	6:G:684:ALA:O	2.44	0.43
1:2:447:PHE:HE1	5:6:304:LEU:HB2	1.83	0.43
4:E:685:GLN:HA	4:E:689:MET:HB2	2.00	0.43
1:2:241:SER:OG	1:2:413:ASP:OD2	2.31	0.43
1:2:323:VAL:HG22	1:2:423:GLU:HB2	2.01	0.43
1:2:387:ARG:NH1	4:5:319:SER:OG	2.50	0.43
1:2:790:TYR:HA	1:2:793:LEU:HD12	2.01	0.43
3:4:635:ASP:OD1	3:4:635:ASP:N	2.50	0.43
4:5:132:LEU:HD12	4:5:133:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:282:LEU:HD13	4:5:330:ILE:HG22	2.00	0.43
5:6:625:ALA:HB1	5:6:629:MET:HB2	2.01	0.43
1:B:401:ARG:NH2	5:F:387:GLU:O	2.52	0.43
6:7:358:ALA:HB3	6:7:373:GLU:HB2	2.01	0.42
3:D:176:PRO:HB2	3:D:177:LEU:H	1.63	0.42
5:F:777:TYR:HB2	5:F:800:LEU:HD13	2.00	0.42
6:G:615:HIS:CD2	6:G:626:PRO:HG2	2.54	0.42
1:2:315:SER:N	1:2:430:TYR:O	2.45	0.42
1:2:407:GLU:HB2	1:2:450:ILE:HG22	2.01	0.42
1:2:800:THR:HG21	1:2:853:VAL:HG13	2.01	0.42
3:4:831:SER:HA	3:4:836:TYR:HE1	1.85	0.42
6:7:224:PRO:HB2	6:7:242:ARG:HG2	2.01	0.42
6:7:242:ARG:HA	6:7:349:VAL:O	2.19	0.42
6:7:520:ILE:HA	6:7:562:SER:O	2.19	0.42
1:B:766:TYR:OH	1:B:823:MET:O	2.32	0.42
2:C:446:VAL:HG21	2:C:502:ILE:HG21	2.01	0.42
2:C:687:ARG:NH1	6:G:602:ASP:OD1	2.44	0.42
4:E:87:ILE:HG12	4:E:137:LEU:HD23	2.01	0.42
5:F:109:GLU:O	5:F:113:GLU:HG3	2.18	0.42
6:G:527:ASP:OD1	6:G:527:ASP:N	2.52	0.42
2:3:299:LYS:HD2	2:3:299:LYS:HA	1.81	0.42
5:F:317:ILE:HD12	5:F:350:ARG:NH2	2.35	0.42
4:5:266:PRO:HG2	4:5:269:GLU:HB2	2.00	0.42
6:7:29:LYS:HE3	6:7:60:GLY:HA2	2.01	0.42
1:B:235:GLY:HA3	1:B:283:TYR:CE1	2.54	0.42
1:B:536:ASP:HB2	1:B:645:SER:HB2	2.00	0.42
3:D:635:ASP:OD1	3:D:635:ASP:N	2.51	0.42
3:D:724:LEU:HD22	6:G:690:LEU:HD21	2.02	0.42
5:F:644:MET:HE1	5:F:652:ILE:HD13	2.00	0.42
1:2:304:TYR:HD2	1:2:318:VAL:HG23	1.85	0.42
6:7:259:ALA:H	6:7:305:SER:HB3	1.85	0.42
2:C:478:MET:HE3	2:C:482:ASP:HB3	2.01	0.42
3:D:550:LYS:HG2	5:F:738:ARG:HH21	1.84	0.42
3:D:578:LEU:HD23	3:D:630:CYS:HB3	2.00	0.42
5:F:347:ASN:HD21	5:F:350:ARG:HD3	1.85	0.42
6:G:601:LEU:H	6:G:727:LEU:HD21	1.85	0.42
6:G:722:VAL:HA	6:G:726:SER:HB3	2.02	0.42
1:B:610:ASP:OD1	1:B:610:ASP:N	2.53	0.42
3:D:609:VAL:HG11	6:G:506:MET:H	1.84	0.42
6:G:17:LEU:HD13	6:G:113:PHE:HZ	1.85	0.42
3:4:326:ILE:O	3:4:436:THR:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:90:PHE:CE2	4:5:94:ILE:HD11	2.54	0.42
1:B:540:LEU:HB3	1:B:680:LEU:HD23	2.02	0.42
3:D:802:ILE:HD11	5:F:732:VAL:HG22	2.02	0.42
4:E:32:LYS:HE3	4:E:32:LYS:HB2	1.84	0.42
4:5:5:ARG:HG3	2:C:233:THR:HB	2.02	0.42
5:6:120:GLU:HB3	5:6:137:ARG:HH21	1.84	0.42
6:G:423:TYR:HB2	6:G:615:HIS:CG	2.55	0.42
1:2:347:ILE:HD11	5:F:429:THR:HG23	2.02	0.42
2:3:233:THR:HB	4:E:5:ARG:HG3	2.01	0.42
3:4:265:PRO:HB3	3:4:325:LEU:HG	2.01	0.42
3:D:590:TYR:OH	3:D:632:ASP:OD2	2.38	0.42
4:E:90:PHE:CE2	4:E:94:ILE:HD11	2.55	0.42
4:E:565:ASP:HA	4:E:568:ILE:HG22	2.02	0.42
3:4:229:GLN:HA	3:4:232:GLU:HG2	2.02	0.41
3:4:550:LYS:HG2	5:6:738:ARG:HH21	1.84	0.41
3:4:762:ILE:HB	5:6:736:MET:HG2	2.02	0.41
5:6:158:LEU:HD21	5:6:170:ILE:HD12	2.02	0.41
5:6:317:ILE:HD12	5:6:350:ARG:NH2	2.34	0.41
5:6:842:ASP:N	5:6:842:ASP:OD1	2.50	0.41
1:B:808:ARG:NH2	7:E:2001:AGS:S1G	2.81	0.41
6:G:459:MET:SD	6:G:584:ILE:HG12	2.60	0.41
4:5:31:PHE:CE1	4:5:75:ILE:HD12	2.55	0.41
4:5:31:PHE:CG	4:5:90:PHE:HD1	2.38	0.41
4:5:405:ARG:HH12	4:5:500:GLN:HG3	1.85	0.41
1:B:353:GLN:HE22	1:B:358:GLU:HA	1.85	0.41
1:B:600:ASP:OD2	1:B:643:ARG:NH2	2.40	0.41
2:C:724:VAL:HA	2:C:727:LYS:HG2	2.00	0.41
3:D:602:THR:HG22	3:D:654:ILE:HD13	2.01	0.41
3:D:831:SER:HA	3:D:836:TYR:HE1	1.85	0.41
4:E:83:PRO:HG3	4:E:159:ILE:HG13	2.02	0.41
4:E:149:ARG:NH2	4:E:260:GLU:OE2	2.43	0.41
5:F:574:VAL:O	5:F:714:VAL:HA	2.20	0.41
6:G:417:SER:HA	6:G:420:PRO:HG3	2.02	0.41
3:4:802:ILE:HD11	5:6:732:VAL:HG22	2.00	0.41
2:C:150:ARG:HD3	2:C:150:ARG:HA	1.91	0.41
4:E:31:PHE:CG	4:E:90:PHE:HD1	2.39	0.41
6:G:242:ARG:HA	6:G:349:VAL:O	2.20	0.41
3:4:315:ARG:NH2	3:4:411:THR:O	2.35	0.41
4:5:65:MET:HG2	4:5:139:LEU:HD12	2.01	0.41
2:C:186:VAL:HG12	2:C:288:PRO:HA	2.02	0.41
3:D:689:THR:HG22	3:D:791:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:211:LEU:HD13	1:2:271:PHE:HB2	2.01	0.41
1:B:387:ARG:NH1	4:E:319:SER:OG	2.48	0.41
1:B:558:LYS:HE3	1:B:558:LYS:HB2	1.81	0.41
2:C:666:ARG:HA	2:C:666:ARG:HD3	1.87	0.41
3:D:456:LEU:HD12	3:D:456:LEU:HA	1.95	0.41
7:D:2001:AGS:O3A	6:G:687:ARG:NH2	2.53	0.41
4:E:450:THR:HA	4:E:469:MET:HB2	2.02	0.41
5:F:333:CYS:HB2	5:F:344:TRP:CZ2	2.56	0.41
6:G:442:LYS:HB3	6:G:450:ILE:HB	2.03	0.41
2:3:276:VAL:HG11	2:3:294:VAL:HG11	2.02	0.41
1:B:563:ALA:HA	1:B:603:VAL:O	2.21	0.41
1:B:585:ILE:HD11	5:F:621:TYR:HE2	1.84	0.41
3:D:707:LEU:HD23	3:D:707:LEU:HA	1.95	0.41
4:E:685:GLN:OE1	4:E:689:MET:HG3	2.21	0.41
6:G:86:LEU:HG	6:G:215:TYR:HD2	1.86	0.41
1:2:540:LEU:HB3	1:2:680:LEU:HD23	2.03	0.41
3:4:447:ASN:HB2	3:4:450:GLN:HB2	2.03	0.41
3:4:475:ASP:OD1	3:4:475:ASP:N	2.51	0.41
4:5:565:ASP:HA	4:5:568:ILE:HG22	2.03	0.41
6:7:459:MET:SD	6:7:584:ILE:HG12	2.61	0.41
2:3:386:MET:HE3	2:3:715:VAL:HG22	2.02	0.41
5:6:347:ASN:HD21	5:6:350:ARG:HD3	1.85	0.41
2:C:452:THR:HG21	2:C:456:ARG:HH22	1.85	0.41
3:D:695:PRO:HA	3:D:696:PRO:HD3	1.98	0.41
5:F:784:ASP:OD2	5:F:795:ILE:HG12	2.20	0.41
1:2:558:LYS:HE3	1:2:558:LYS:HB2	1.81	0.41
3:4:380:ASN:ND2	1:B:365:THR:O	2.54	0.41
4:5:32:LYS:HB2	4:5:32:LYS:HE3	1.83	0.41
4:5:494:HIS:HA	4:5:497:MET:HE3	2.03	0.41
4:5:572:VAL:HA	4:5:575:ILE:HD12	2.02	0.41
5:6:684:PRO:HB3	5:6:698:ASN:HB3	2.03	0.41
6:7:61:PRO:HB2	6:7:64:MET:HB2	2.02	0.41
6:7:260:TYR:HB3	6:7:298:LEU:HB3	2.02	0.41
6:7:432:LEU:HB3	6:7:473:ILE:HD11	2.03	0.41
6:7:621:MET:HE3	6:7:622:HIS:CD2	2.56	0.41
2:C:393:LEU:HD12	2:C:397:SER:HB3	2.03	0.41
2:C:538:SER:O	2:C:542:ARG:HG2	2.21	0.41
4:E:137:LEU:HG	4:E:139:LEU:HD22	2.03	0.41
5:F:180:PHE:HA	5:F:183:LYS:HE2	2.03	0.41
4:5:389:VAL:O	4:5:393:MET:HG2	2.21	0.41
4:5:618:ALA:HB1	4:5:677:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:649:THR:H	4:5:652:GLN:HG2	1.86	0.41
1:B:233:THR:O	1:B:237:MET:HG2	2.21	0.41
5:F:649:GLN:HA	5:F:652:ILE:HG12	2.02	0.41
1:2:342:LEU:HD12	1:2:372:PRO:HB2	2.03	0.40
2:3:645:THR:H	2:3:648:PRO:HG3	1.86	0.40
1:B:549:LYS:HB2	1:B:549:LYS:HE2	1.92	0.40
2:C:262:PRO:HG3	4:E:509:ILE:HD11	2.02	0.40
5:F:300:VAL:HG13	5:F:386:VAL:HG11	2.03	0.40
6:G:243:GLY:HA2	6:G:318:LEU:HG	2.03	0.40
2:3:349:ASN:HA	2:3:352:LYS:HG2	2.04	0.40
5:6:816:VAL:HG21	5:6:823:PHE:HE2	1.86	0.40
4:E:405:ARG:HH12	4:E:500:GLN:HG3	1.86	0.40
4:E:440:SER:OG	4:E:443:GLY:O	2.31	0.40
6:G:622:HIS:O	6:G:624:LYS:NZ	2.54	0.40
1:2:383:ARG:HD2	1:2:411:LEU:HD12	2.04	0.40
2:3:150:ARG:HD3	2:3:150:ARG:HA	1.91	0.40
2:3:343:THR:OG1	2:3:346:ASP:OD2	2.30	0.40
3:4:315:ARG:NH2	3:4:413:HIS:HD2	2.19	0.40
4:5:270:MET:SD	4:5:271:PRO:HD2	2.62	0.40
5:6:412:LEU:O	5:6:416:LYS:NZ	2.49	0.40
5:6:742:ILE:HD13	5:6:742:ILE:HA	1.88	0.40
1:B:511:ILE:HG21	1:B:552:ILE:HD13	2.03	0.40
2:C:400:ARG:NH2	2:C:544:ASP:OD1	2.44	0.40
4:E:393:MET:HE2	4:E:666:LEU:HD23	2.02	0.40
2:3:333:SER:HB2	2:3:423:LEU:HD11	2.04	0.40
2:3:426:ALA:HB3	2:3:429:ALA:HB2	2.03	0.40
1:B:786:VAL:HG11	1:B:814:LEU:HD11	2.04	0.40
4:E:256:LEU:HB2	4:E:276:MET:HE3	2.04	0.40
5:F:816:VAL:HG21	5:F:823:PHE:HE2	1.86	0.40
6:G:432:LEU:HB3	6:G:473:ILE:HD11	2.02	0.40
1:2:343:LYS:HE3	1:2:371:GLY:HA3	2.04	0.40
2:3:281:ASP:OD1	2:3:281:ASP:N	2.50	0.40
2:3:452:THR:HG21	2:3:456:ARG:HH22	1.85	0.40
3:4:758:ILE:HG22	3:4:760:PRO:HD3	2.02	0.40
5:6:529:LEU:O	5:6:533:ILE:HG12	2.21	0.40
6:7:86:LEU:HG	6:7:215:TYR:HD2	1.87	0.40
6:7:87:GLN:NE2	6:7:91:GLU:OE2	2.48	0.40
6:7:271:GLN:HE21	6:7:271:GLN:HB2	1.64	0.40
6:7:423:TYR:HB2	6:7:615:HIS:CG	2.57	0.40
4:E:444:SER:HB2	4:E:447:ALA:HB3	2.04	0.40
6:G:224:PRO:HB2	6:G:242:ARG:HG2	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%)	609 (98%)	13 (2%)	0	100	100
1	B	622/868 (72%)	607 (98%)	15 (2%)	0	100	100
2	3	627/971 (65%)	607 (97%)	20 (3%)	0	100	100
2	C	627/971 (65%)	603 (96%)	24 (4%)	0	100	100
3	4	664/933 (71%)	650 (98%)	14 (2%)	0	100	100
3	D	664/933 (71%)	649 (98%)	15 (2%)	0	100	100
4	5	650/775 (84%)	637 (98%)	13 (2%)	0	100	100
4	E	650/775 (84%)	637 (98%)	13 (2%)	0	100	100
5	6	638/1017 (63%)	621 (97%)	17 (3%)	0	100	100
5	F	638/1017 (63%)	621 (97%)	17 (3%)	0	100	100
6	7	693/845 (82%)	685 (99%)	8 (1%)	0	100	100
6	G	693/845 (82%)	683 (99%)	10 (1%)	0	100	100
All	All	7788/10818 (72%)	7609 (98%)	179 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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	606/848 (72%)	606 (100%)	0	100	100
3	D	606/848 (72%)	606 (100%)	0	100	100
4	5	588/688 (86%)	587 (100%)	1 (0%)	87	95
4	E	588/688 (86%)	587 (100%)	1 (0%)	87	95
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%)	617 (100%)	1 (0%)	87	95
6	G	618/753 (82%)	618 (100%)	0	100	100
All	All	6958/9560 (73%)	6955 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	5	339	THR
6	7	271	GLN
4	E	339	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	200	GLN
1	2	353	GLN
1	2	526	ASN
1	2	528	ASN
1	2	569	GLN
1	2	621	HIS
1	2	641	GLN
2	3	239	ASN
2	3	253	HIS
2	3	293	ASN
2	3	330	HIS
2	3	424	ASN
2	3	673	GLN
3	4	229	GLN

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Mol	Chain	Res	Type
3	4	259	HIS
3	4	354	HIS
3	4	450	GLN
3	4	646	HIS
3	4	651	GLN
4	5	43	GLN
4	5	454	GLN
4	5	574	ASN
4	5	579	ASN
4	5	581	ASN
4	5	584	GLN
4	5	625	ASN
4	5	636	ASN
5	6	139	GLN
5	6	149	ASN
5	6	347	ASN
5	6	362	GLN
5	6	364	ASN
5	6	366	ASN
5	6	540	HIS
5	6	583	GLN
5	6	653	HIS
5	6	669	HIS
5	6	700	ASN
6	7	16	ASN
6	7	68	GLN
6	7	178	ASN
6	7	264	GLN
6	7	271	GLN
6	7	568	ASN
6	7	615	HIS
6	7	729	GLN
1	B	353	GLN
1	B	526	ASN
1	B	528	ASN
1	B	621	HIS
1	B	641	GLN
1	B	779	HIS
2	C	239	ASN
2	C	293	ASN
2	C	307	ASN
2	C	330	HIS

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Mol	Chain	Res	Type
2	C	351	ASN
2	C	392	ASN
2	C	417	GLN
2	C	424	ASN
2	C	673	GLN
3	D	259	HIS
3	D	350	ASN
3	D	450	GLN
3	D	483	GLN
3	D	651	GLN
3	D	823	GLN
4	E	499	GLN
4	E	576	HIS
4	E	584	GLN
4	E	625	ASN
4	E	636	ASN
5	F	139	GLN
5	F	347	ASN
5	F	362	GLN
5	F	364	ASN
5	F	366	ASN
5	F	540	HIS
6	G	16	ASN
6	G	68	GLN
6	G	87	GLN
6	G	159	ASN
6	G	264	GLN
6	G	568	ASN
6	G	615	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	F	2001	8	32,33,33	0.47	0	45,52,52	0.62	1 (2%)
7	AGS	D	2001	8	32,33,33	0.49	1 (3%)	45,52,52	0.69	1 (2%)
7	AGS	E	2001	8	32,33,33	0.54	1 (3%)	45,52,52	0.64	1 (2%)
7	AGS	5	2001	8	32,33,33	0.54	1 (3%)	45,52,52	0.68	1 (2%)
7	AGS	B	2001	8	32,33,33	0.47	0	45,52,52	0.70	1 (2%)
7	AGS	G	2001	8	32,33,33	0.49	1 (3%)	45,52,52	0.61	1 (2%)
7	AGS	2	2001	8	32,33,33	0.47	0	45,52,52	0.68	1 (2%)
7	AGS	6	2001	8	32,33,33	0.49	1 (3%)	45,52,52	0.62	1 (2%)
10	ADP	3	2001	8	28,29,29	1.43	4 (14%)	43,45,45	1.82	9 (20%)
7	AGS	7	2001	8	32,33,33	0.48	1 (3%)	45,52,52	0.63	1 (2%)
7	AGS	4	2001	8	32,33,33	0.49	1 (3%)	45,52,52	0.72	1 (2%)
10	ADP	C	2001	8	28,29,29	1.42	4 (14%)	43,45,45	1.83	10 (23%)

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	F	2001	8	-	6/21/38/38	0/3/3/3
7	AGS	D	2001	8	-	6/21/38/38	0/3/3/3
7	AGS	E	2001	8	-	3/21/38/38	0/3/3/3
7	AGS	5	2001	8	-	3/21/38/38	0/3/3/3
7	AGS	B	2001	8	-	5/21/38/38	0/3/3/3
7	AGS	G	2001	8	-	6/21/38/38	0/3/3/3
7	AGS	2	2001	8	-	5/21/38/38	0/3/3/3
7	AGS	6	2001	8	-	6/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	3	2001	8	-	4/16/32/32	0/3/3/3
7	AGS	7	2001	8	-	6/21/38/38	0/3/3/3
7	AGS	4	2001	8	-	6/21/38/38	0/3/3/3
10	ADP	C	2001	8	-	4/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	2001	ADP	C5-C4	4.73	1.47	1.39
10	C	2001	ADP	C5-C4	4.66	1.47	1.39
10	3	2001	ADP	C5-C6	2.74	1.48	1.41
10	C	2001	ADP	C5-C6	2.68	1.48	1.41
10	3	2001	ADP	C8-N7	2.35	1.36	1.31
10	C	2001	ADP	C8-N7	2.34	1.36	1.31
10	3	2001	ADP	C5-N7	-2.29	1.34	1.39
10	C	2001	ADP	C5-N7	-2.29	1.34	1.39
7	G	2001	AGS	PG-S1G	2.12	1.95	1.90
7	E	2001	AGS	PG-S1G	2.12	1.95	1.90
7	7	2001	AGS	PG-S1G	2.10	1.95	1.90
7	4	2001	AGS	PG-S1G	2.09	1.95	1.90
7	5	2001	AGS	PG-S1G	2.08	1.95	1.90
7	D	2001	AGS	PG-S1G	2.07	1.95	1.90
7	6	2001	AGS	PG-S1G	2.05	1.95	1.90

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	2001	ADP	C5-C4-N3	-5.76	118.79	126.72
10	C	2001	ADP	C5-C4-N3	-5.68	118.89	126.72
10	C	2001	ADP	N3-C4-N9	4.47	134.77	127.17
10	3	2001	ADP	N3-C4-N9	4.46	134.76	127.17
7	B	2001	AGS	PB-O3B-PG	-3.79	119.30	133.17
7	4	2001	AGS	PB-O3B-PG	-3.78	119.35	133.17
10	3	2001	ADP	C2-N3-C4	3.68	120.82	111.83
10	C	2001	ADP	C2-N3-C4	3.66	120.78	111.83
7	2	2001	AGS	PB-O3B-PG	-3.61	119.94	133.17
7	5	2001	AGS	PB-O3B-PG	-3.59	120.04	133.17
10	3	2001	ADP	C4-C5-N7	-3.58	106.49	110.58
7	D	2001	AGS	PB-O3B-PG	-3.57	120.10	133.17
10	C	2001	ADP	C4-C5-N7	-3.52	106.56	110.58
10	C	2001	ADP	N3-C2-N1	-3.32	123.56	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	7	2001	AGS	PB-O3B-PG	-3.29	121.14	133.17
10	3	2001	ADP	N3-C2-N1	-3.27	123.64	128.58
7	E	2001	AGS	PB-O3B-PG	-3.25	121.28	133.17
7	G	2001	AGS	PB-O3B-PG	-3.25	121.29	133.17
7	6	2001	AGS	PB-O3B-PG	-3.16	121.61	133.17
7	F	2001	AGS	PB-O3B-PG	-3.15	121.65	133.17
10	C	2001	ADP	C4-N9-C8	2.72	108.59	105.74
10	C	2001	ADP	C5-N7-C8	2.58	107.50	103.45
10	3	2001	ADP	C4-N9-C8	2.55	108.42	105.74
10	3	2001	ADP	C5-N7-C8	2.54	107.44	103.45
10	C	2001	ADP	C3'-C2'-C1'	2.30	105.81	101.46
10	3	2001	ADP	C3'-C2'-C1'	2.27	105.75	101.46
10	3	2001	ADP	C6-C5-N7	2.18	136.30	132.09
10	C	2001	ADP	C6-C5-N7	2.18	136.29	132.09
10	C	2001	ADP	N9-C8-N7	-2.06	111.02	113.94

There are no chirality outliers.

All (60) 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	4	2001	AGS	C5'-O5'-PA-O2A
7	4	2001	AGS	C5'-O5'-PA-O3A
7	6	2001	AGS	C5'-O5'-PA-O1A
7	6	2001	AGS	C5'-O5'-PA-O2A
7	7	2001	AGS	C5'-O5'-PA-O1A
7	7	2001	AGS	C5'-O5'-PA-O2A
7	B	2001	AGS	PB-O3B-PG-O2G
7	B	2001	AGS	PB-O3B-PG-O3G
7	D	2001	AGS	C5'-O5'-PA-O2A
7	E	2001	AGS	O4'-C4'-C5'-O5'
7	F	2001	AGS	PB-O3B-PG-O2G
7	F	2001	AGS	C5'-O5'-PA-O2A
7	G	2001	AGS	C5'-O5'-PA-O1A
7	G	2001	AGS	C5'-O5'-PA-O2A
10	3	2001	ADP	O4'-C4'-C5'-O5'
10	C	2001	ADP	C5'-O5'-PA-O2A
10	C	2001	ADP	O4'-C4'-C5'-O5'
7	E	2001	AGS	C3'-C4'-C5'-O5'
10	3	2001	ADP	C3'-C4'-C5'-O5'
10	C	2001	ADP	C3'-C4'-C5'-O5'

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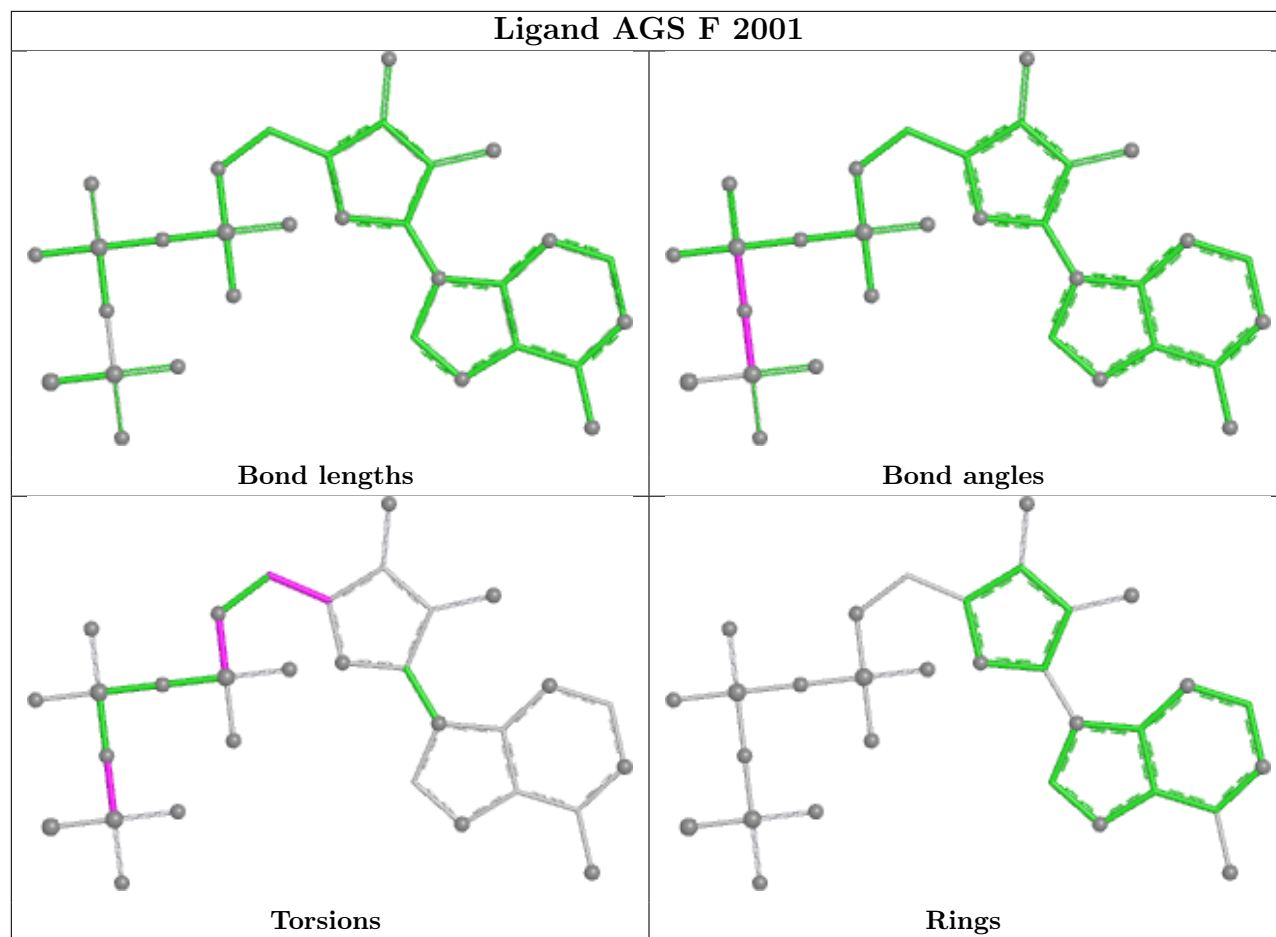
Mol	Chain	Res	Type	Atoms
7	4	2001	AGS	O4'-C4'-C5'-O5'
7	5	2001	AGS	O4'-C4'-C5'-O5'
7	5	2001	AGS	C3'-C4'-C5'-O5'
7	6	2001	AGS	O4'-C4'-C5'-O5'
7	F	2001	AGS	O4'-C4'-C5'-O5'
7	D	2001	AGS	O4'-C4'-C5'-O5'
7	7	2001	AGS	O4'-C4'-C5'-O5'
7	4	2001	AGS	C3'-C4'-C5'-O5'
7	G	2001	AGS	O4'-C4'-C5'-O5'
7	7	2001	AGS	PA-O3A-PB-O1B
7	G	2001	AGS	PA-O3A-PB-O1B
7	6	2001	AGS	C3'-C4'-C5'-O5'
7	D	2001	AGS	C3'-C4'-C5'-O5'
7	4	2001	AGS	C5'-O5'-PA-O1A
7	6	2001	AGS	C5'-O5'-PA-O3A
7	7	2001	AGS	C5'-O5'-PA-O3A
7	D	2001	AGS	C5'-O5'-PA-O1A
7	D	2001	AGS	C5'-O5'-PA-O3A
7	F	2001	AGS	C5'-O5'-PA-O1A
7	F	2001	AGS	C5'-O5'-PA-O3A
7	G	2001	AGS	C5'-O5'-PA-O3A
10	3	2001	ADP	C5'-O5'-PA-O2A
7	F	2001	AGS	C3'-C4'-C5'-O5'
7	B	2001	AGS	PB-O3A-PA-O2A
7	B	2001	AGS	O4'-C4'-C5'-O5'
7	5	2001	AGS	PG-O3B-PB-O2B
7	E	2001	AGS	PG-O3B-PB-O2B
7	6	2001	AGS	PB-O3B-PG-O2G
10	3	2001	ADP	C4'-C5'-O5'-PA
10	C	2001	ADP	C4'-C5'-O5'-PA
7	2	2001	AGS	O4'-C4'-C5'-O5'
7	4	2001	AGS	C4'-C5'-O5'-PA
7	2	2001	AGS	PB-O3A-PA-O2A
7	D	2001	AGS	C4'-C5'-O5'-PA
7	2	2001	AGS	PB-O3A-PA-O1A
7	7	2001	AGS	PA-O3A-PB-O2B
7	B	2001	AGS	PB-O3A-PA-O1A
7	G	2001	AGS	PA-O3A-PB-O2B

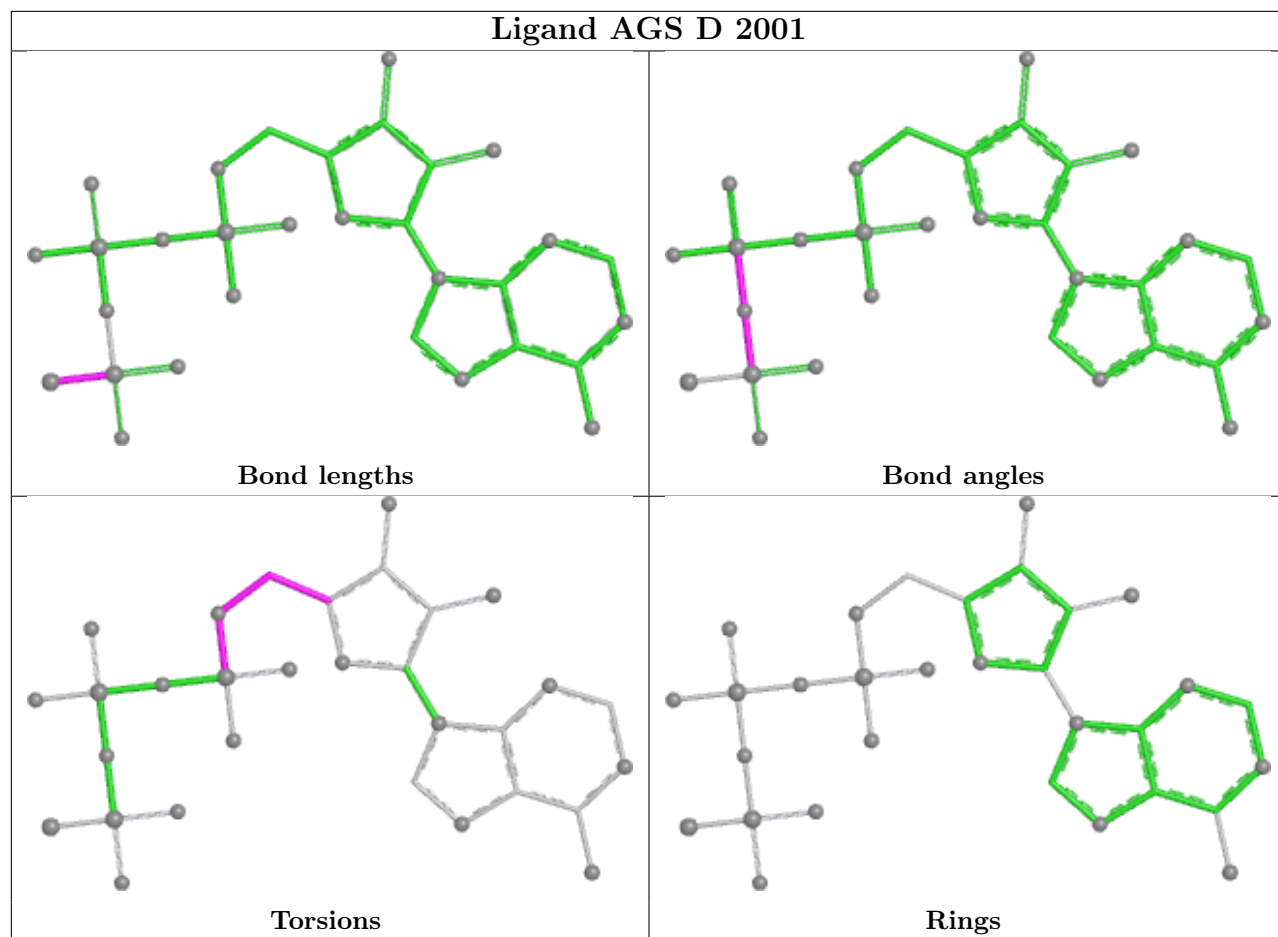
There are no ring outliers.

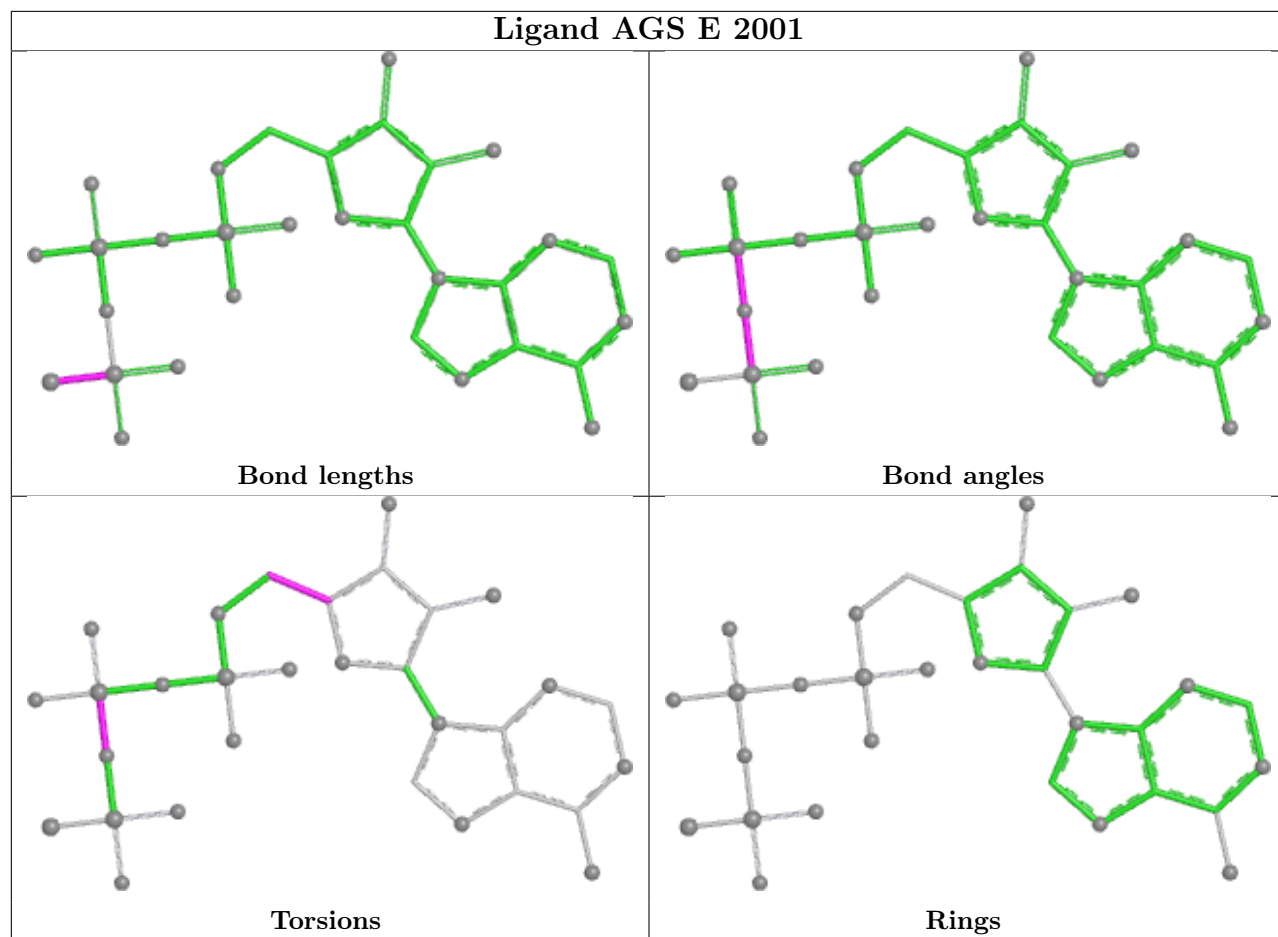
9 monomers are involved in 13 short contacts:

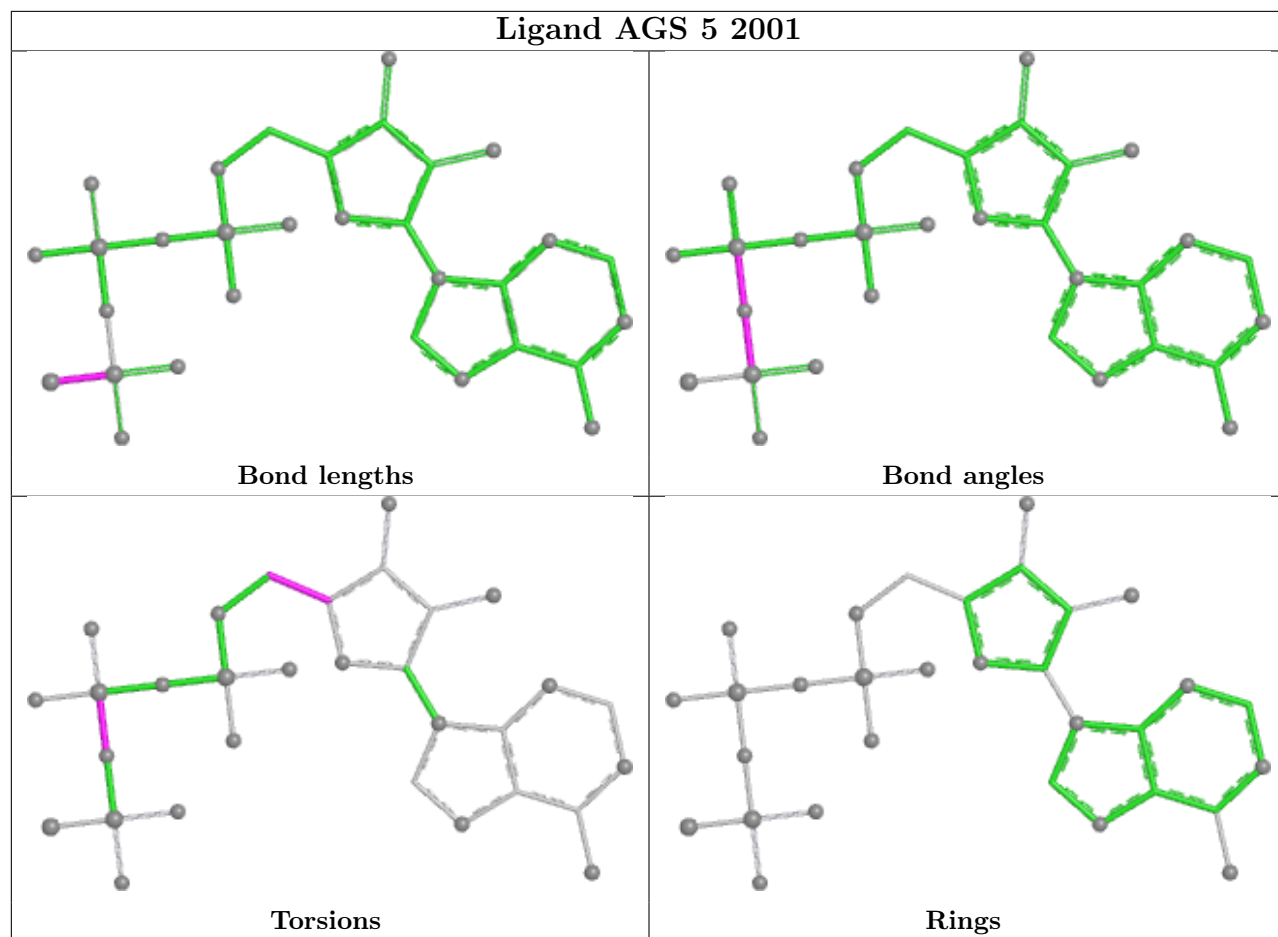
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	2001	AGS	2	0
7	E	2001	AGS	3	0
7	5	2001	AGS	1	0
7	B	2001	AGS	1	0
7	G	2001	AGS	1	0
7	2	2001	AGS	2	0
7	6	2001	AGS	1	0
7	7	2001	AGS	1	0
7	4	2001	AGS	1	0

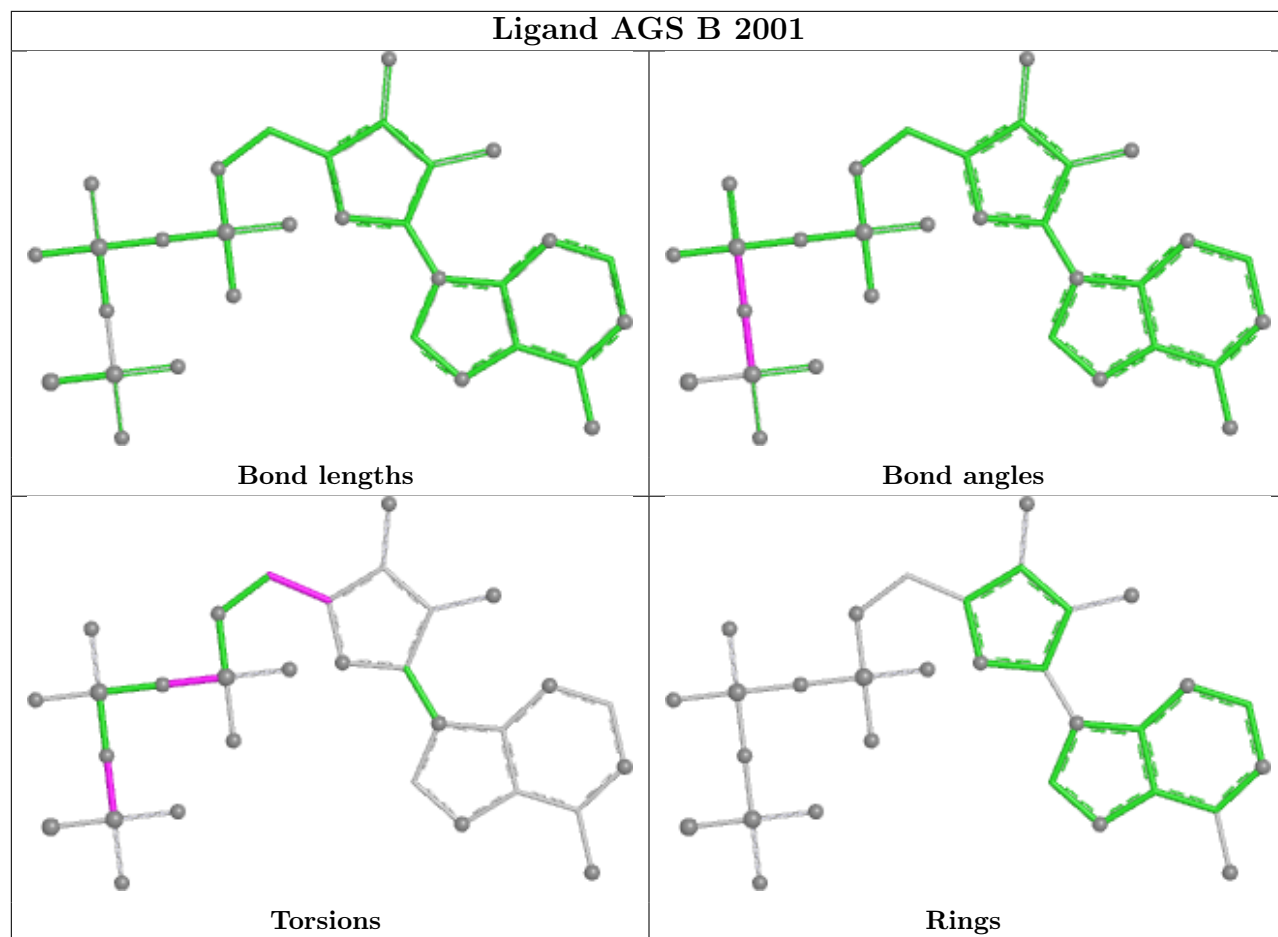
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

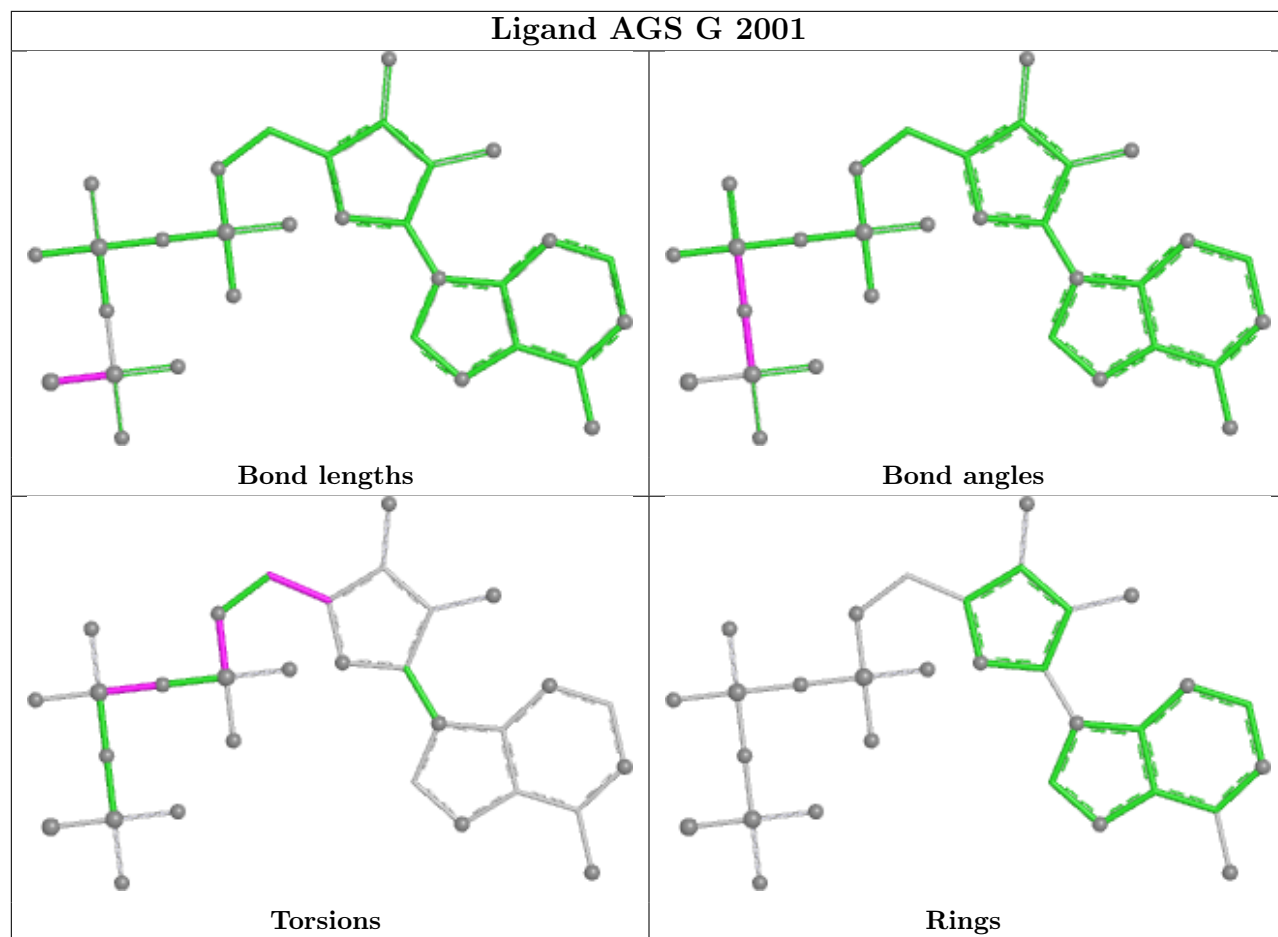


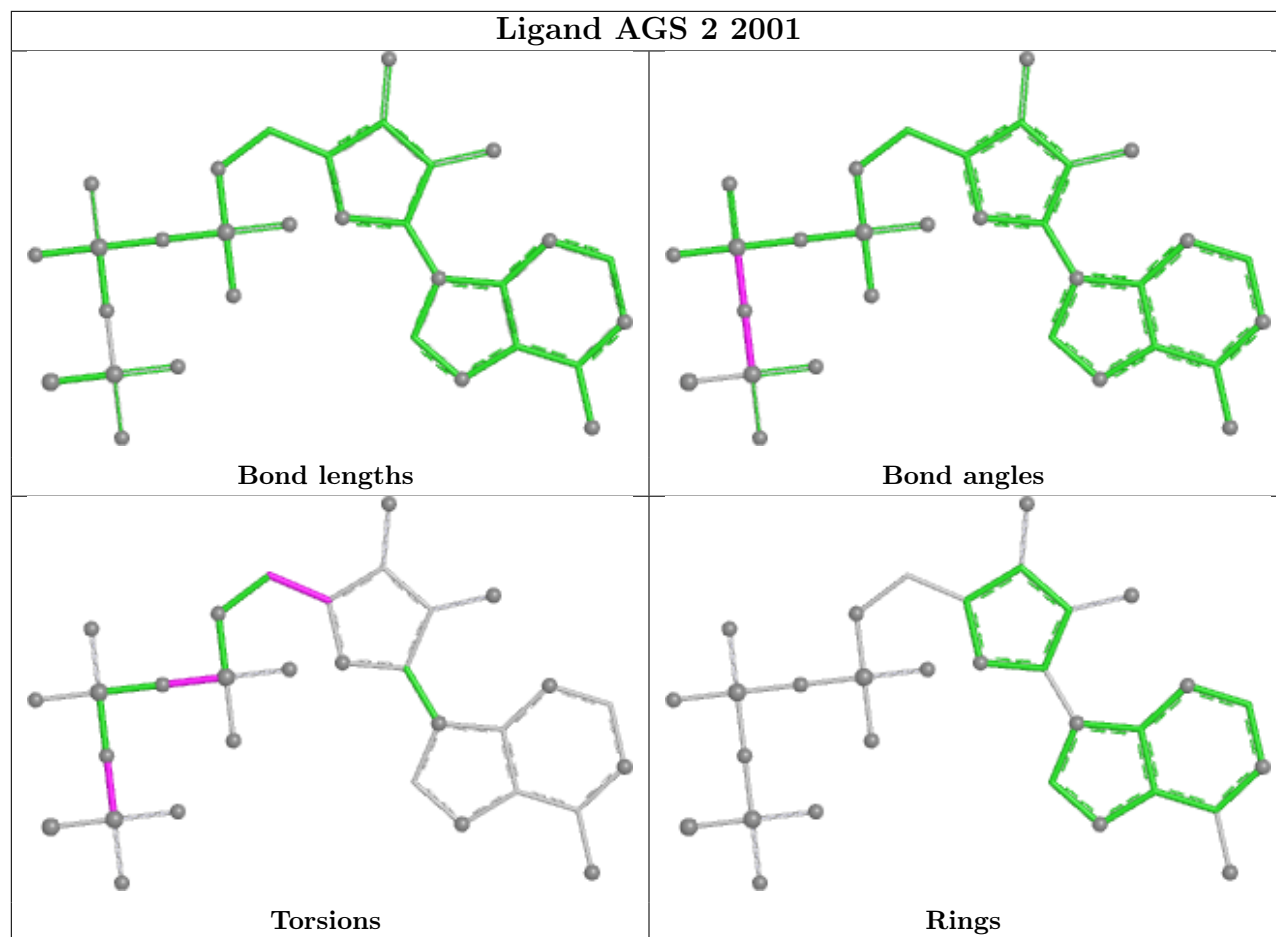


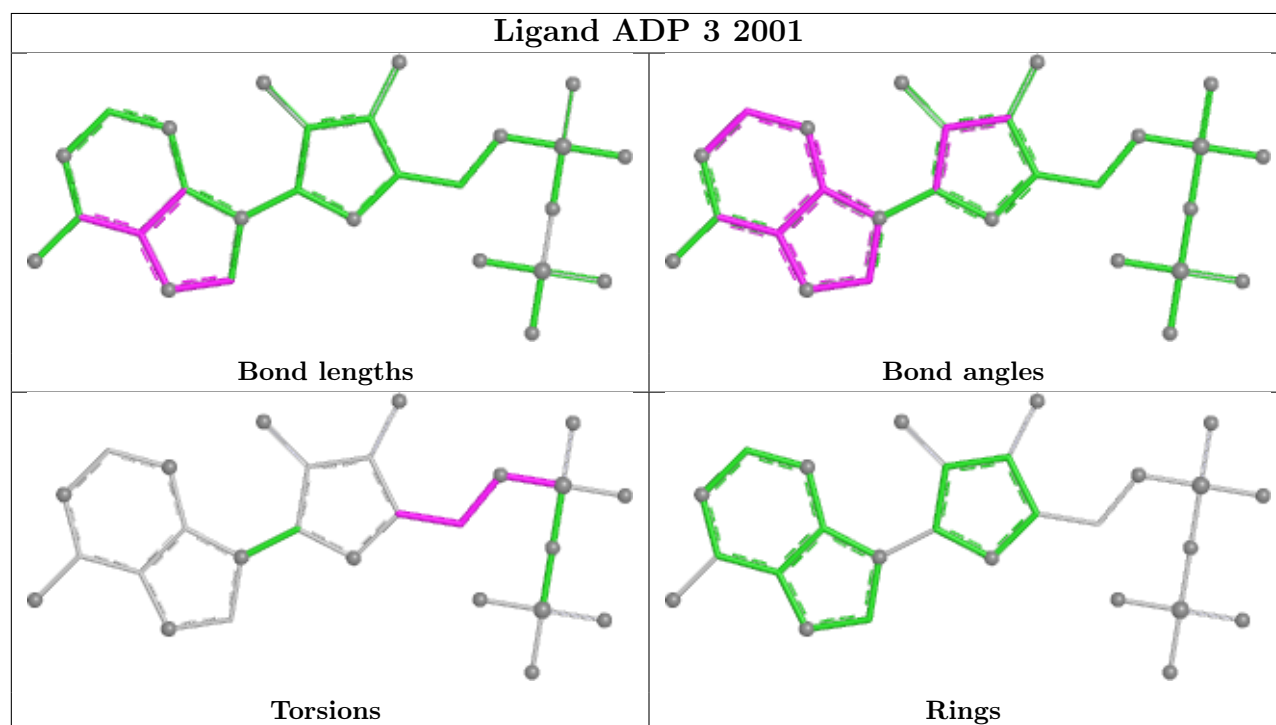
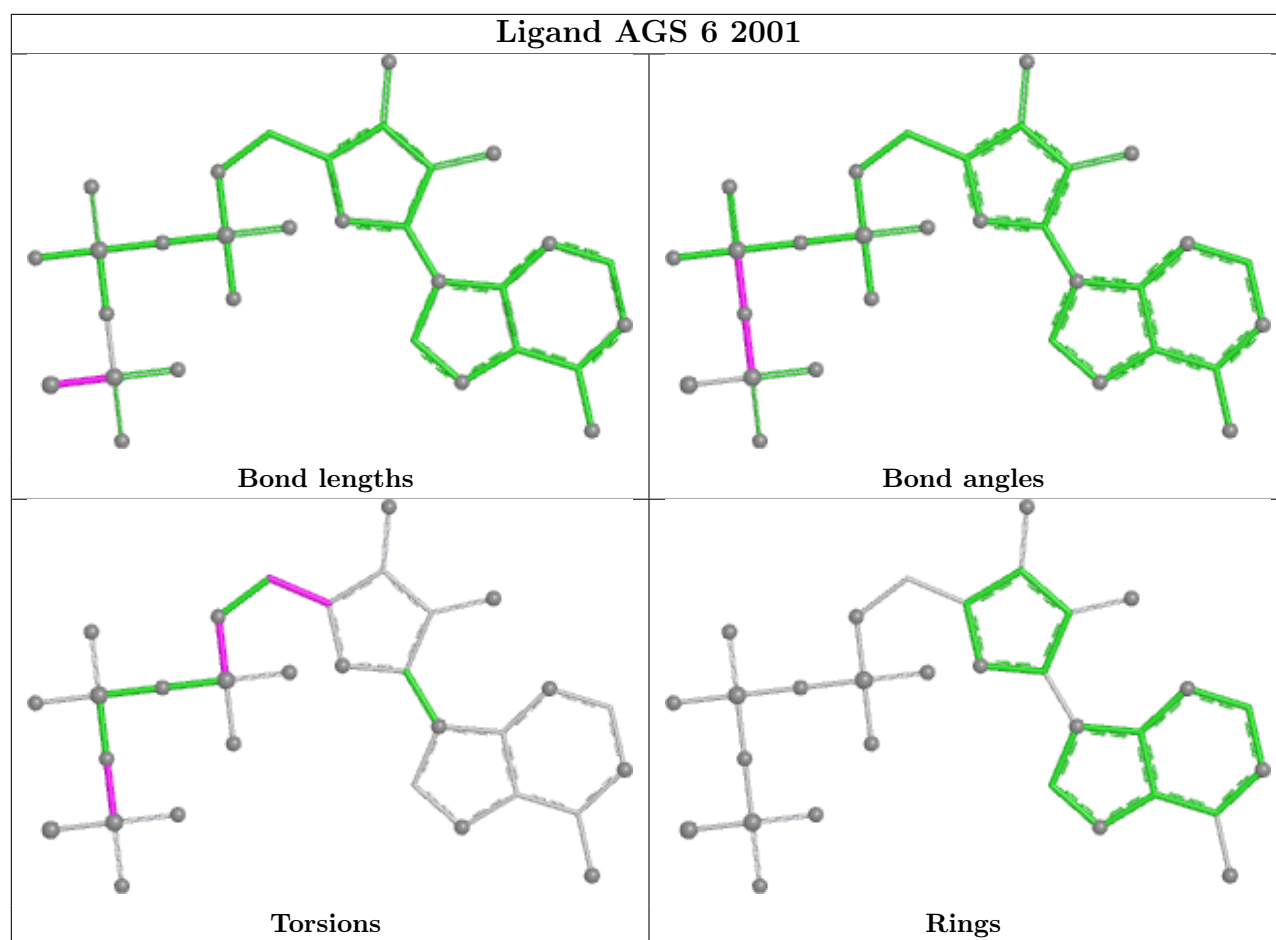


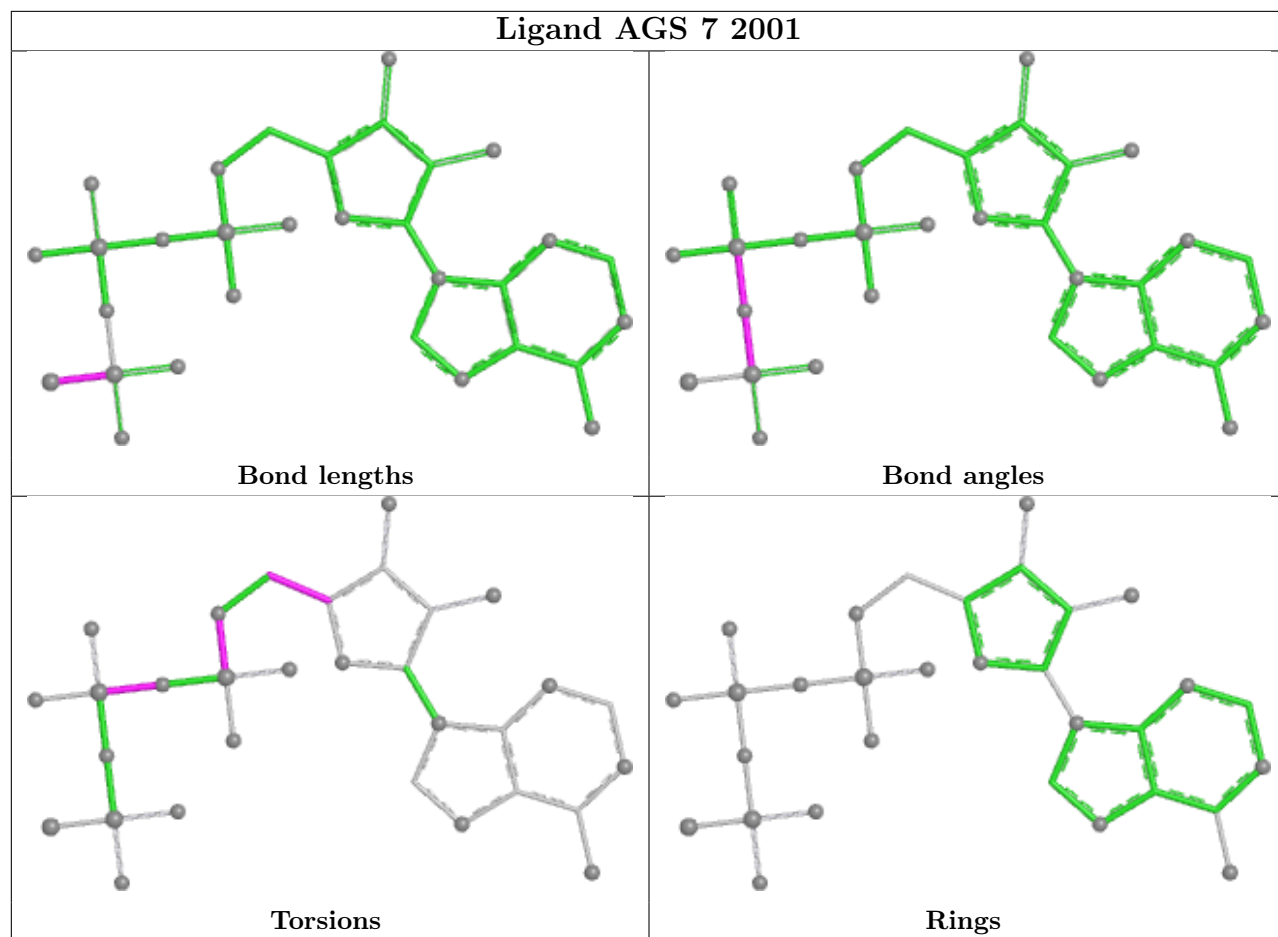


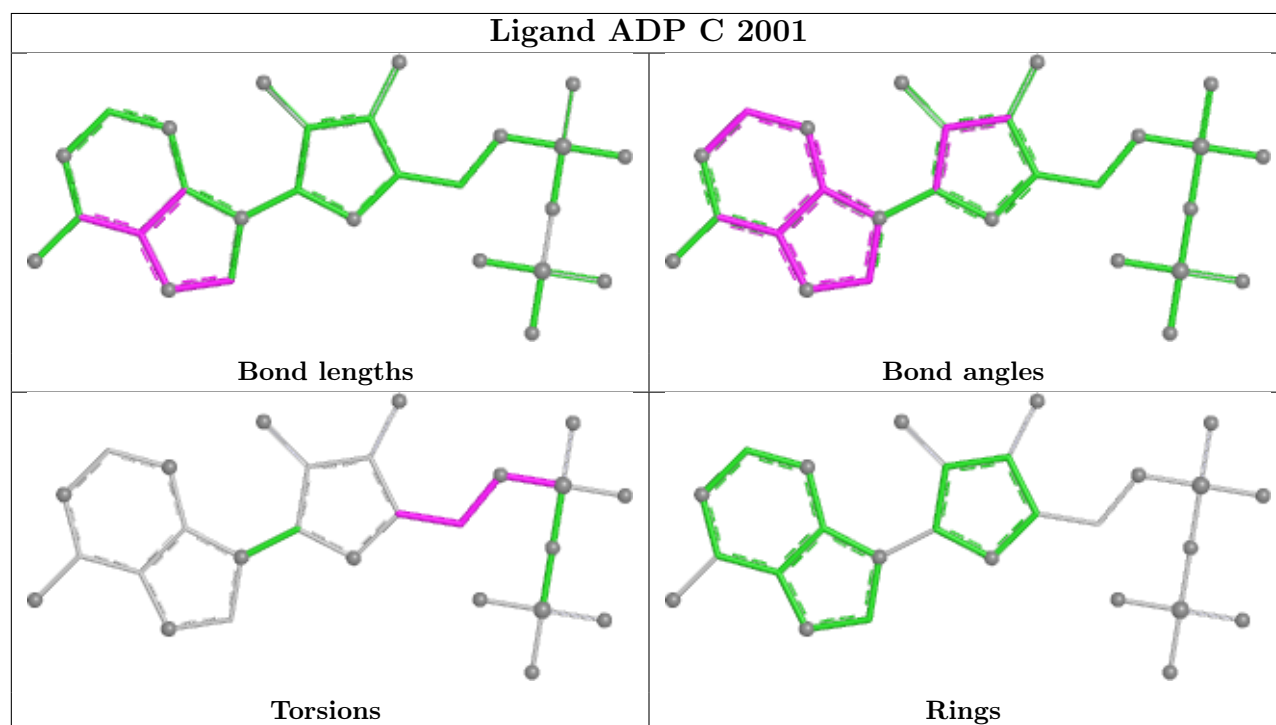
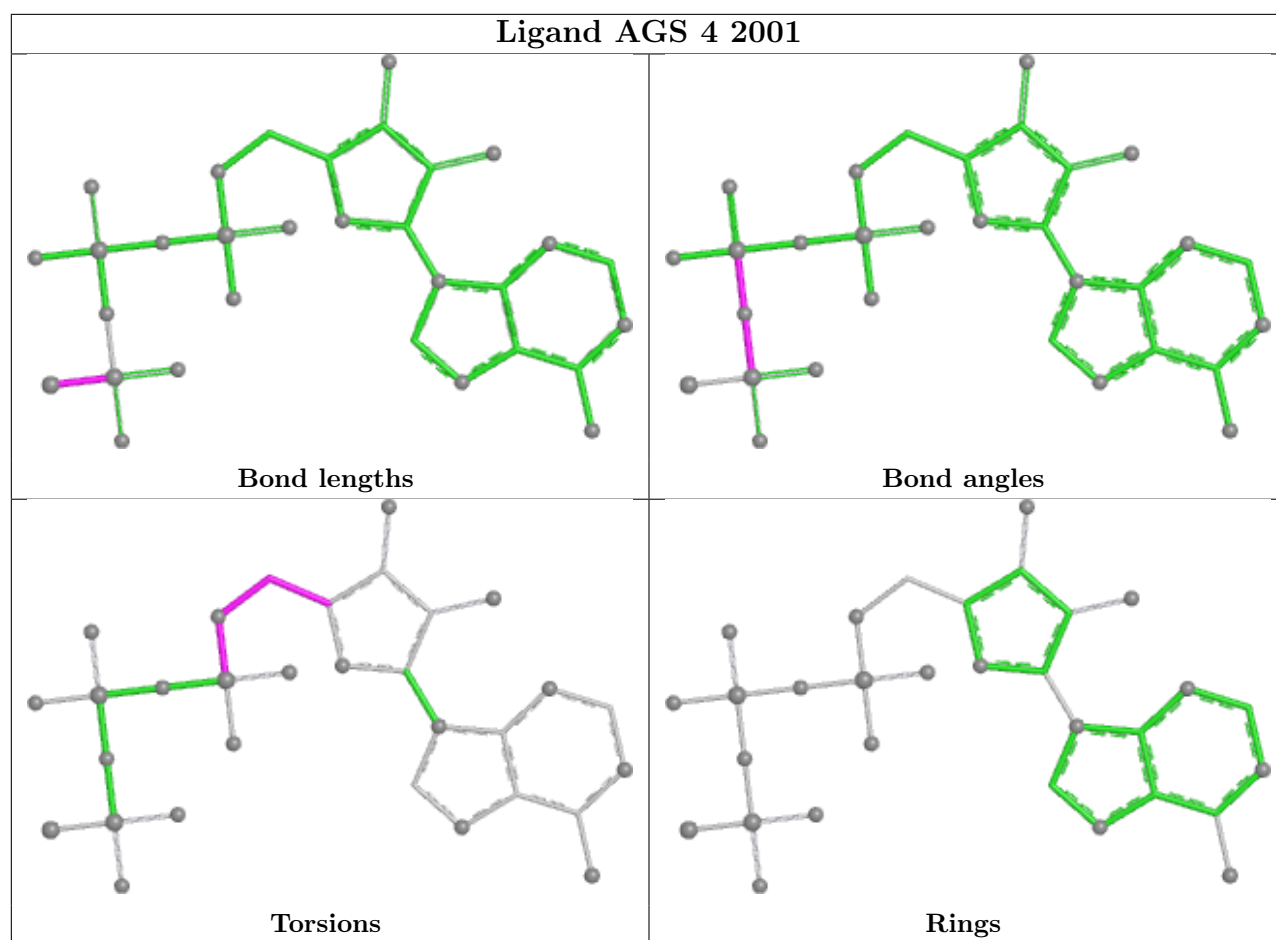












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

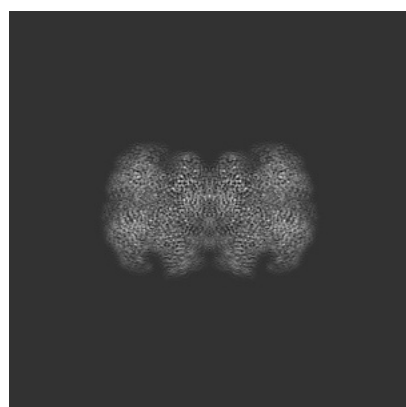
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32355. These allow visual inspection of the internal detail of the map and identification of artifacts.

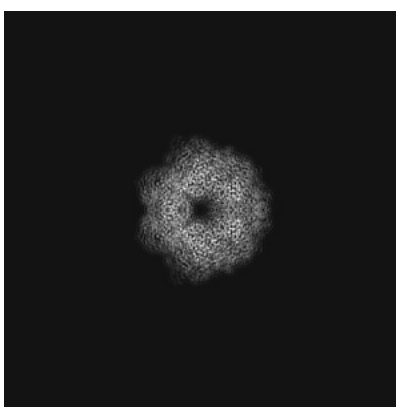
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

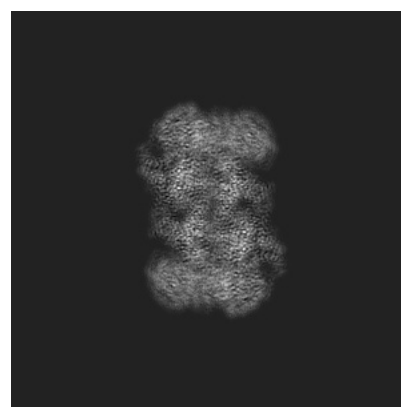
6.1.1 Primary map



X



Y



Z

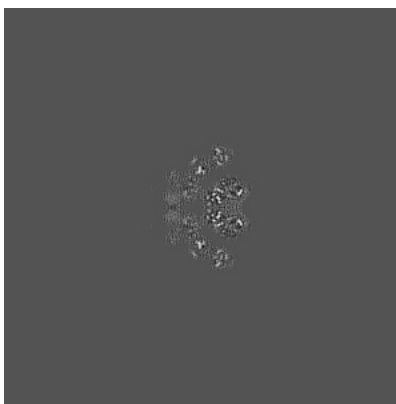
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180



Y Index: 180

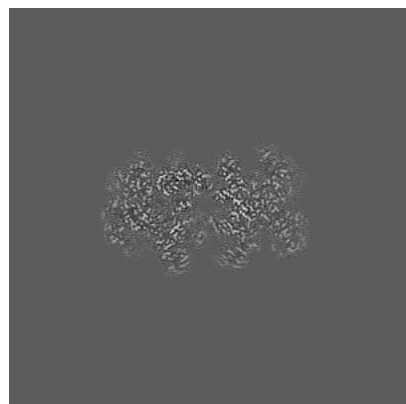


Z Index: 180

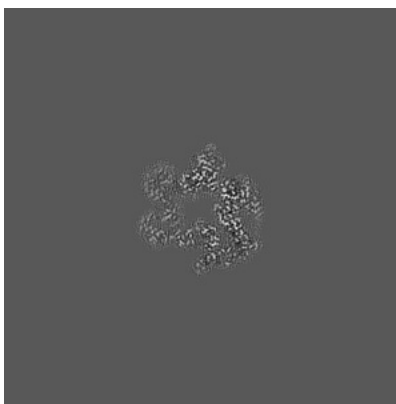
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

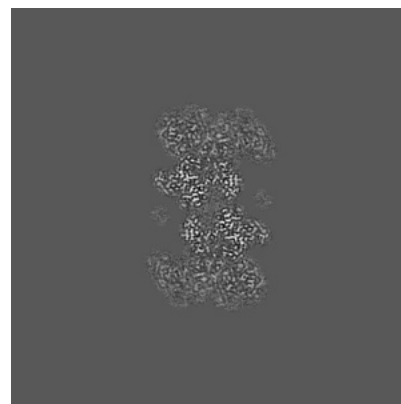
6.3.1 Primary map



X Index: 201



Y Index: 203

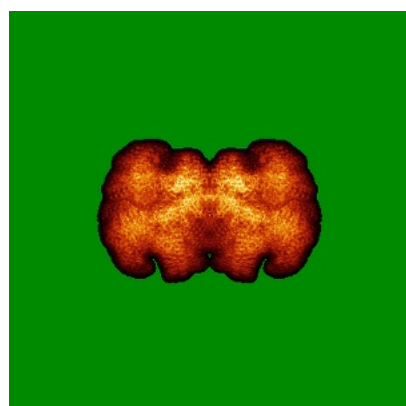


Z Index: 206

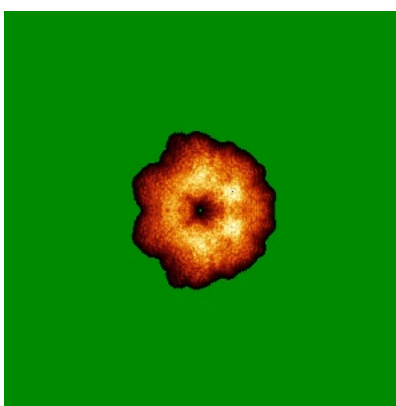
The images above show the largest variance slices of the map in three orthogonal directions.

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

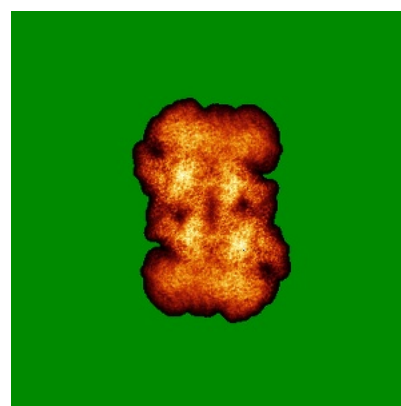
6.4.1 Primary map



X



Y

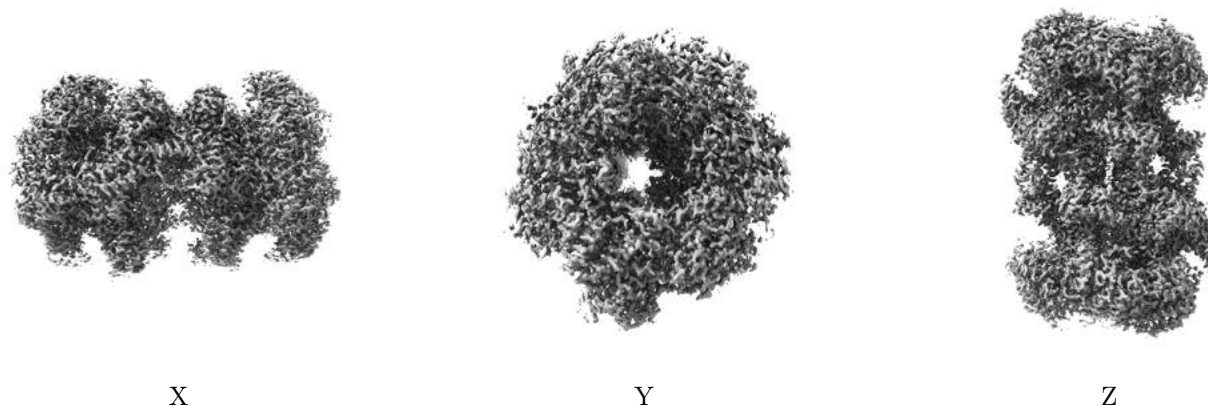


Z

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

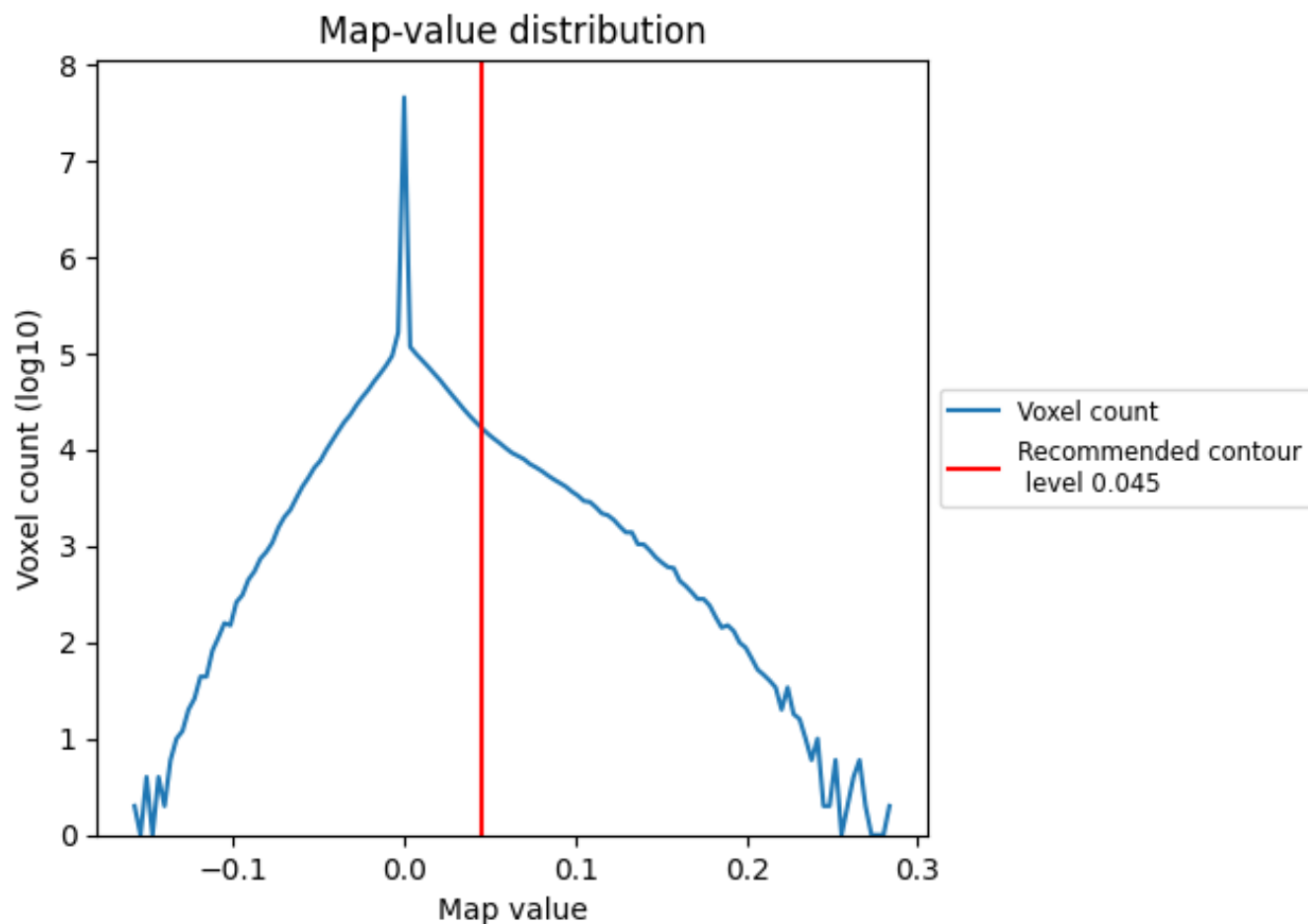
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

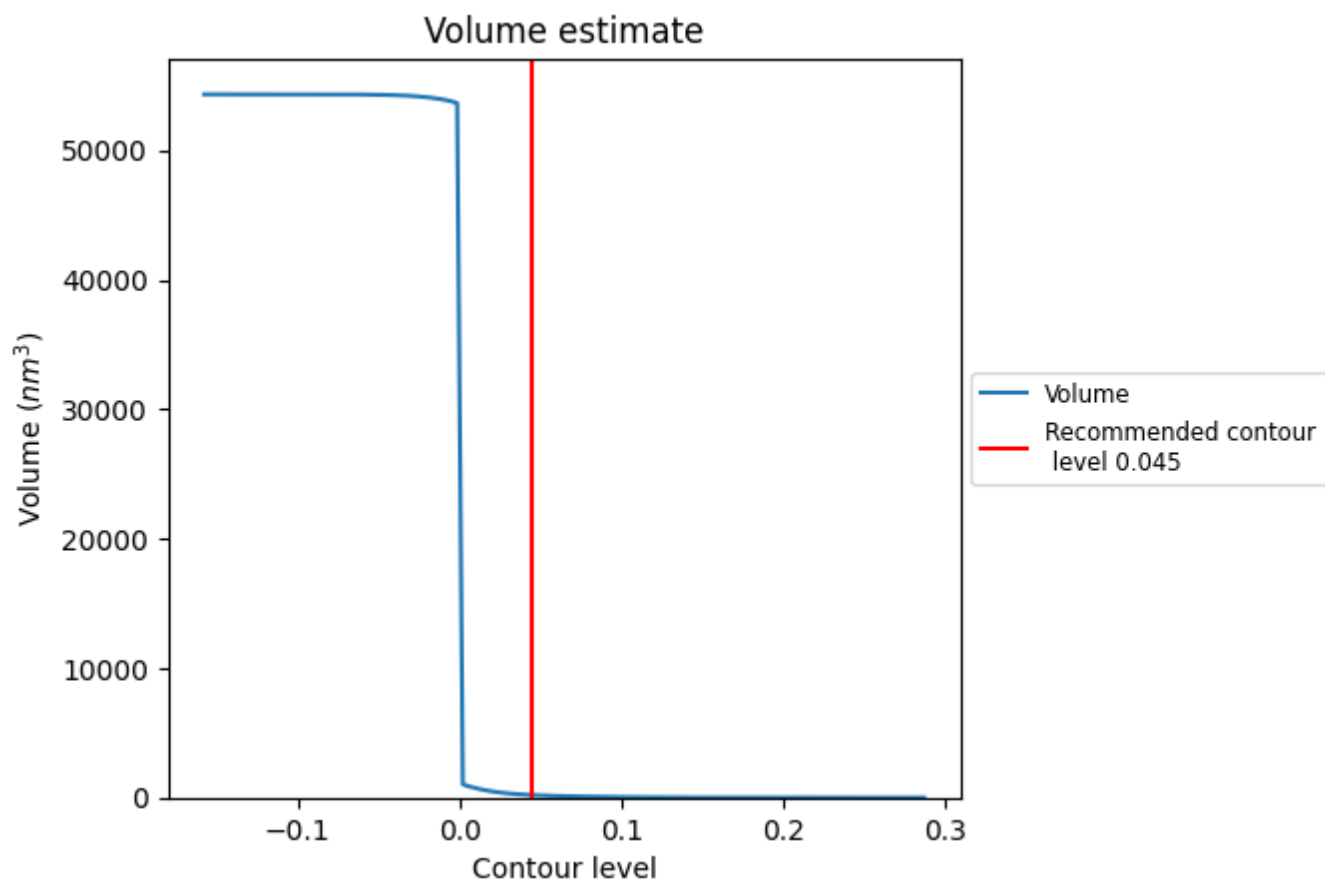
This section contains the results of statistical analysis of the map.

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.

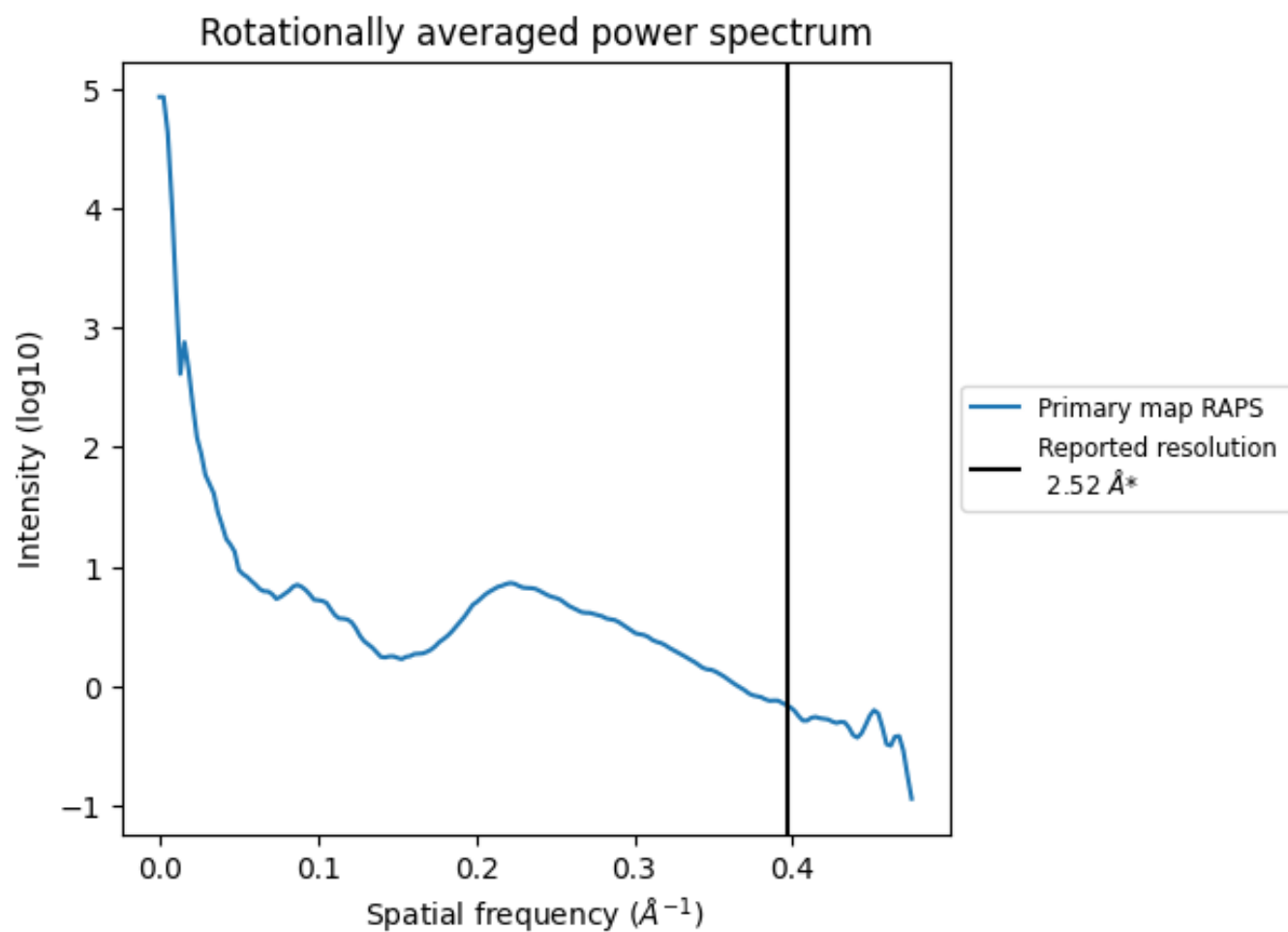
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194 nm³; this corresponds to an approximate mass of 176 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 0.397 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

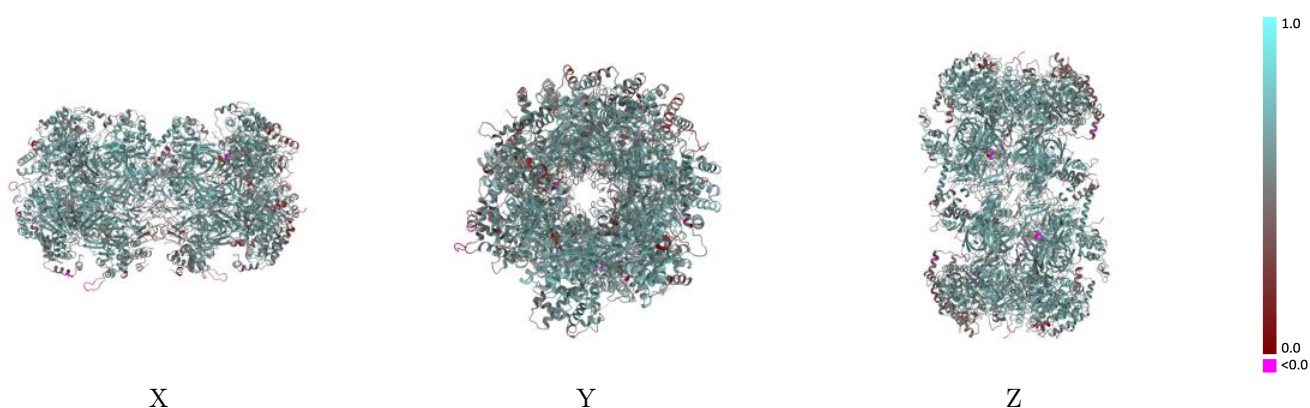
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32355 and PDB model 7W8G. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)

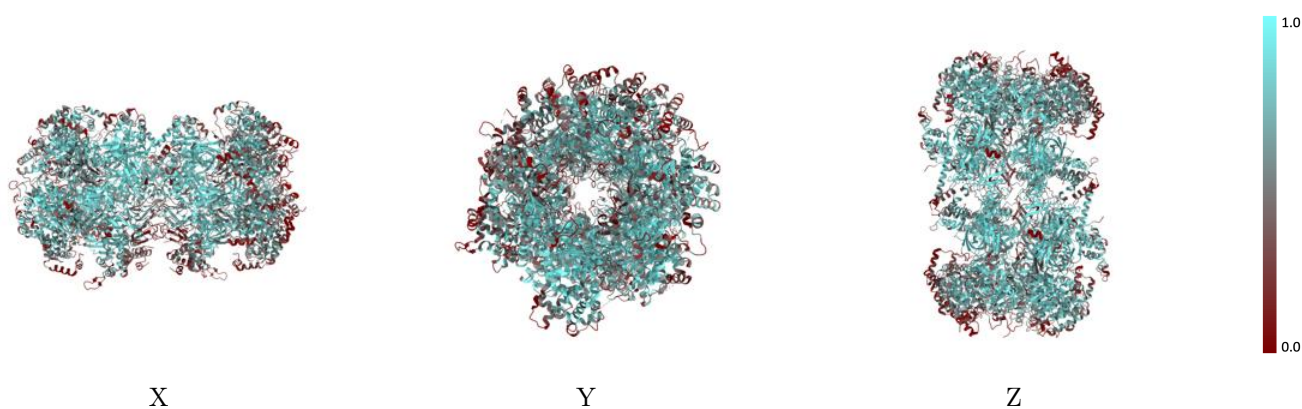
This section was not generated.

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



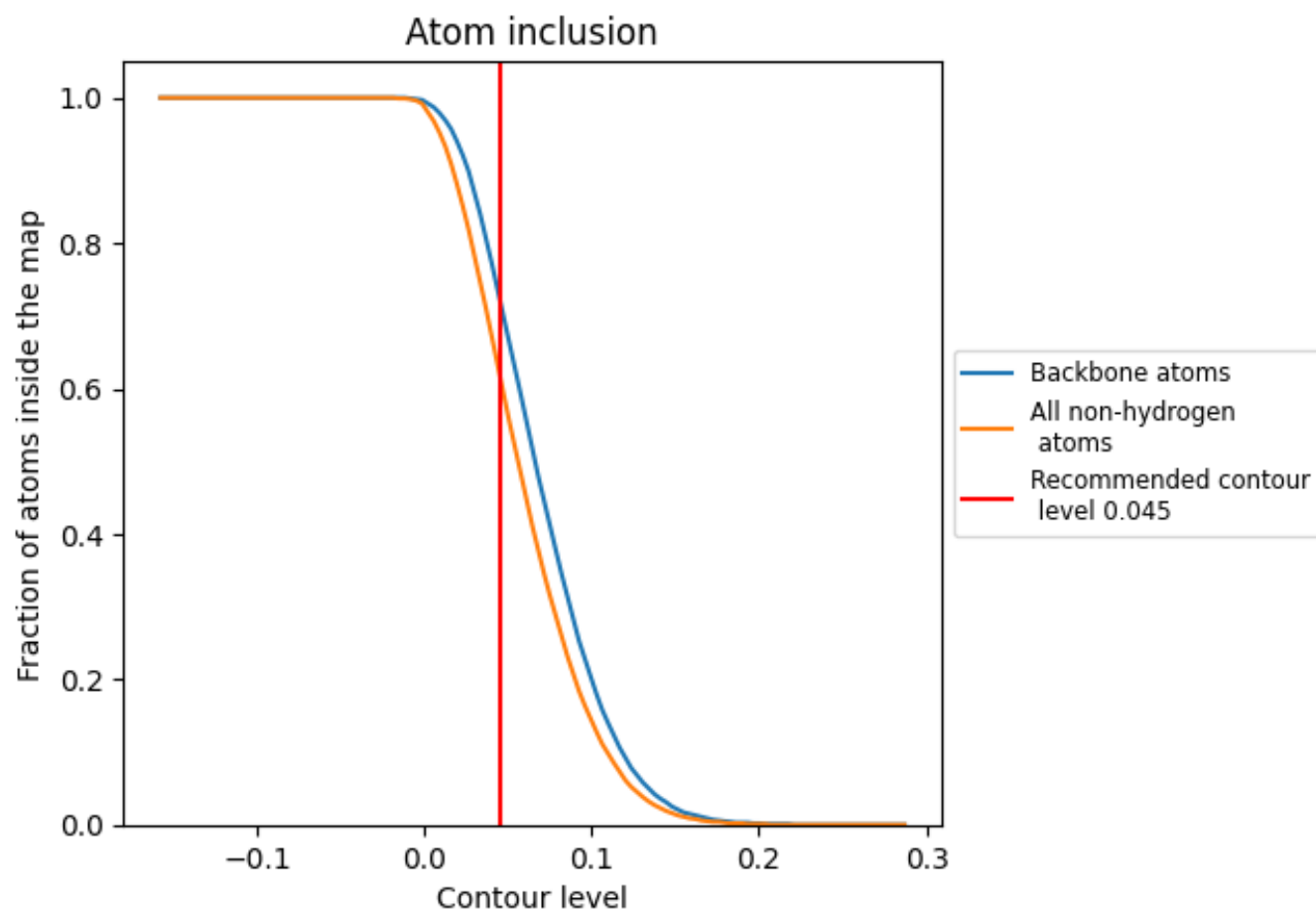
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 62% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6190	0.5740
2	0.5180	0.5420
3	0.6680	0.5940
4	0.6920	0.6030
5	0.5940	0.5640
6	0.5530	0.5360
7	0.6820	0.6010
B	0.5160	0.5430
C	0.6650	0.5950
D	0.6910	0.6030
E	0.5920	0.5610
F	0.5540	0.5360
G	0.6820	0.6040

1.0

0.0

<0.0