



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 07:55 PM UTC

PDB ID : 7V3V / pdb_00007v3v
EMDB ID : EMD-31685
Title : Cryo-EM structure of MCM double hexamer bound with DDK in State I
Authors : Cheng, J.; Li, N.; Huo, Y.; Dang, S.; Tye, B.; Gao, N.; Zhai, Y.
Deposited on : 2021-08-11
Resolution : 2.90 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:

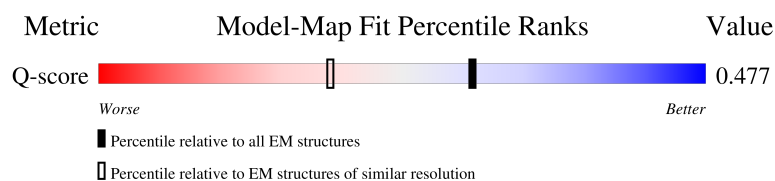
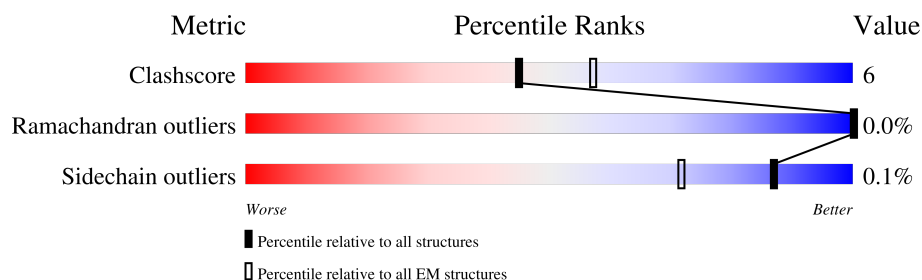
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.90 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.



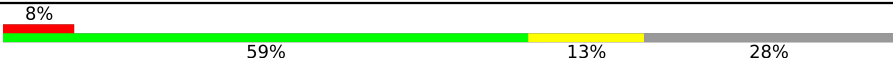
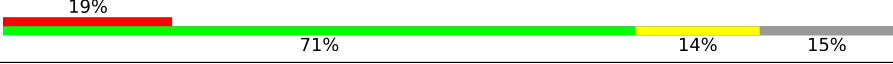
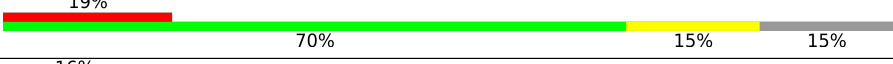
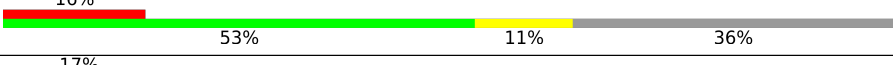
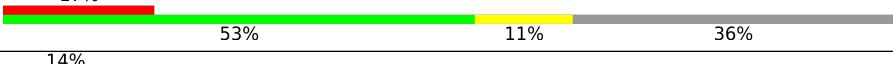
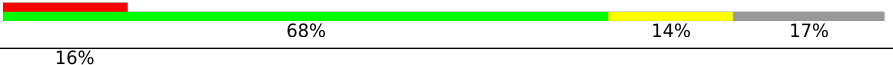
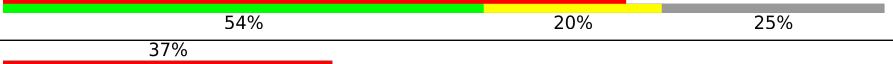
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	21% 62% 11% 28%
1	B	868	21% 59% 13% 28%
2	3	971	11% 56% 10% 34%
2	C	971	11% 56% 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	
7	H	507	
8	I	704	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 68356 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	659	Total	C	N	O	S	0	0
			5148	3229	883	1011	25		
4	E	659	Total	C	N	O	S	0	0
			5148	3229	883	1011	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		

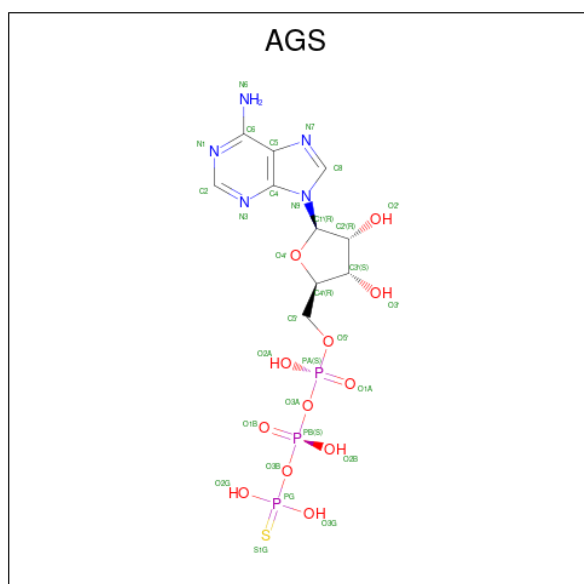
- Molecule 7 is a protein called Cell division control protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	381	Total	C	N	O	S	0	0
			3109	2014	520	562	13		

- Molecule 8 is a protein called DDK kinase regulatory subunit DBF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	328	Total	C	N	O	S	0	0
			2745	1756	478	499	12		

- Molecule 9 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
9	2	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	4	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	7	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	G	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
9	H	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	2	1	Total	Mg	0
			1	1	
10	3	1	Total	Mg	0
			1	1	
10	4	2	Total	Mg	0
			2	2	
10	5	1	Total	Mg	0
			1	1	
10	7	1	Total	Mg	0
			1	1	
10	B	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	
10	D	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
10	E	1	Total 1	Mg 1	0
10	G	1	Total 1	Mg 1	0

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

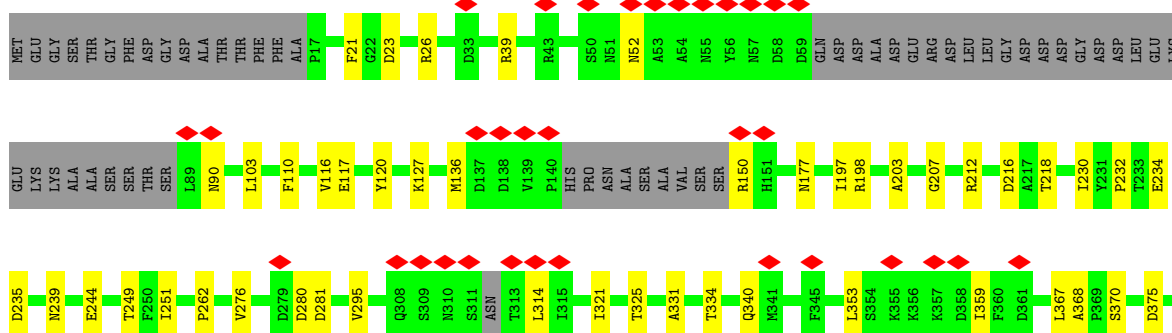
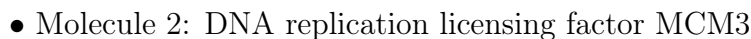
Mol	Chain	Residues	Atoms		AltConf
11	2	1	Total 1	Zn 1	0
11	4	1	Total 1	Zn 1	0
11	5	1	Total 1	Zn 1	0
11	6	1	Total 1	Zn 1	0
11	7	1	Total 1	Zn 1	0
11	B	1	Total 1	Zn 1	0
11	D	1	Total 1	Zn 1	0
11	E	1	Total 1	Zn 1	0
11	F	1	Total 1	Zn 1	0
11	G	1	Total 1	Zn 1	0
11	I	1	Total 1	Zn 1	0

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



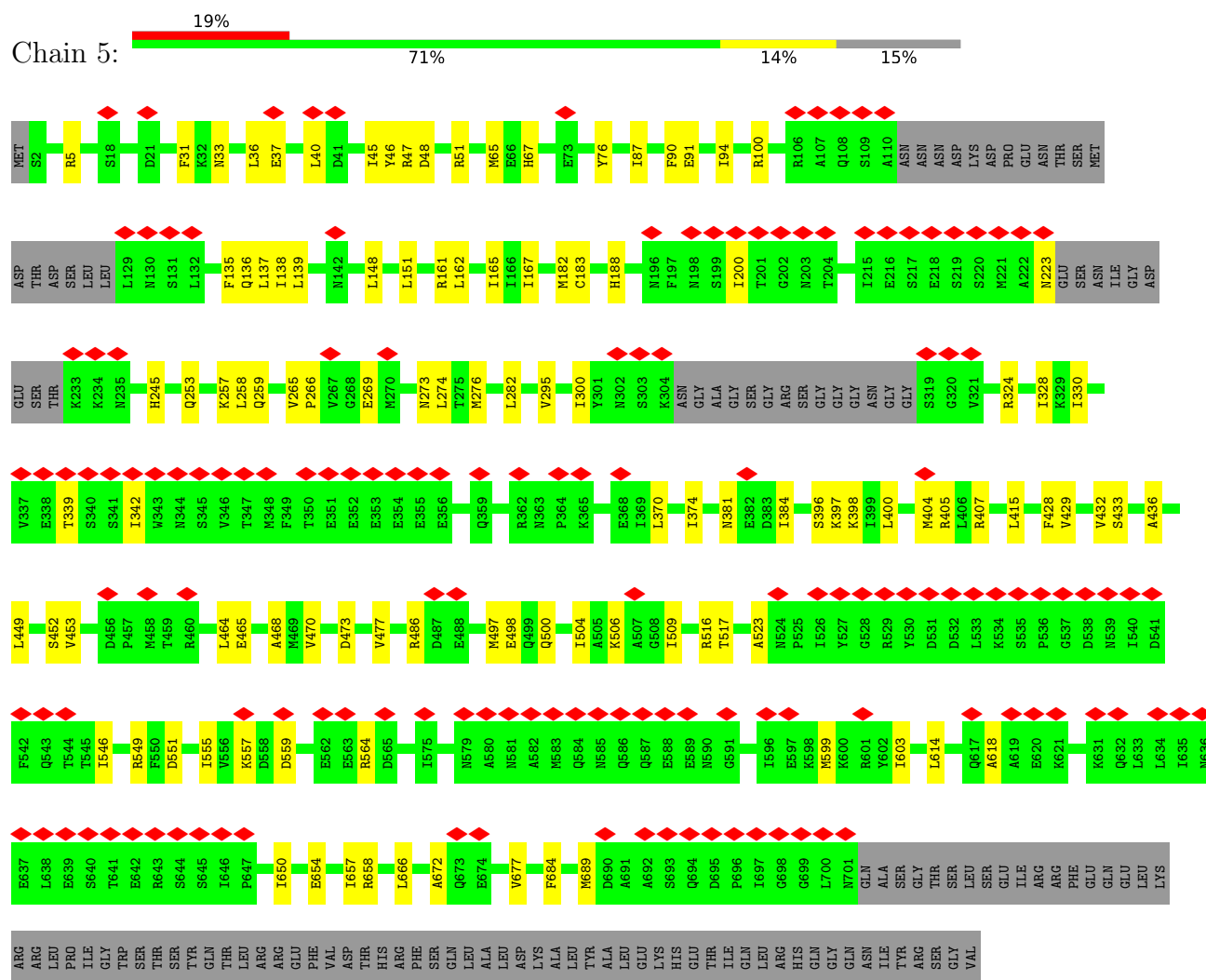
Mol	Chain	Residues	Atoms					AltConf
12	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	C	1	Total	C	N	O	P	0
			27	10	5	10	2	





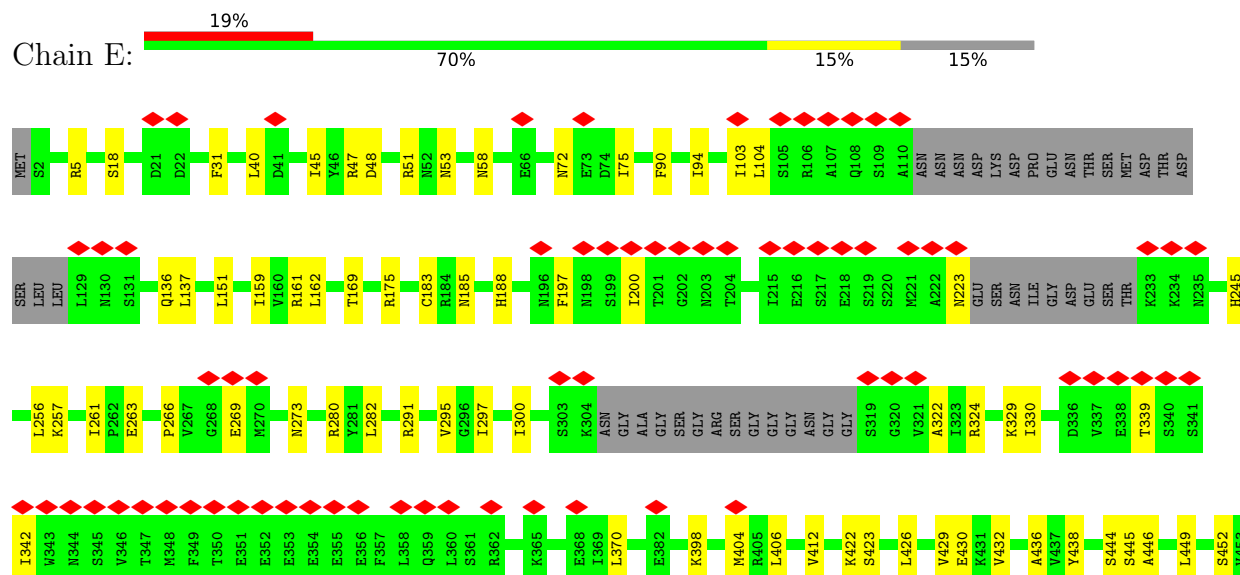
• Molecule 4: Minichromosome maintenance protein 5

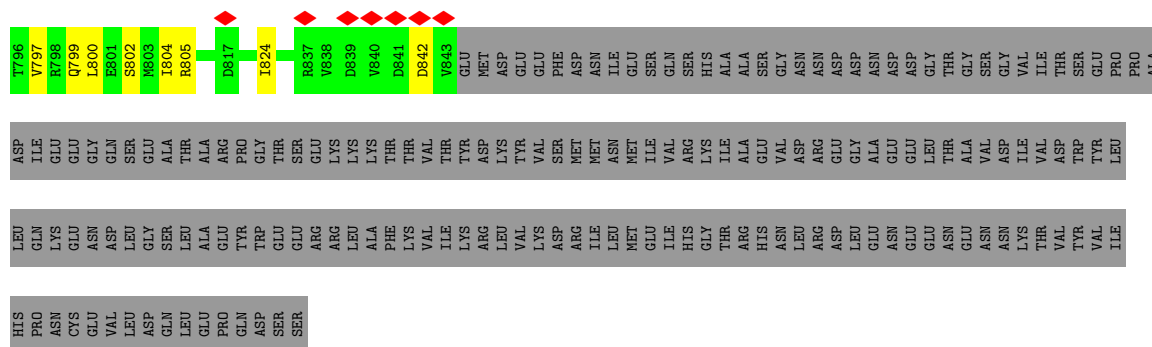
Chain 5:



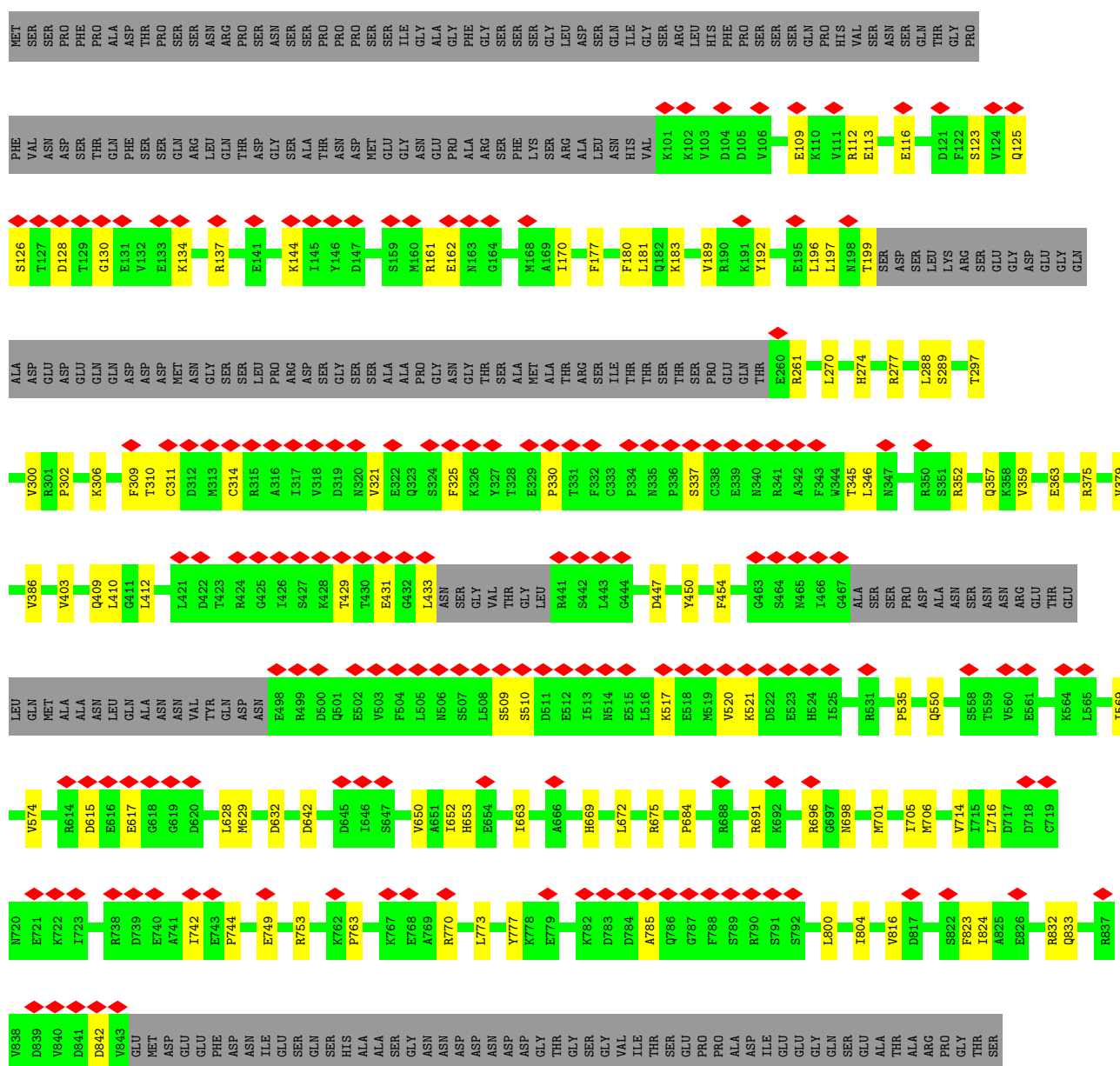
• Molecule 4: Minichromosome maintenance protein 5

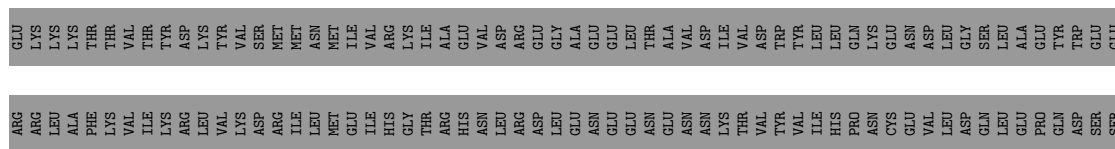
Chain E:



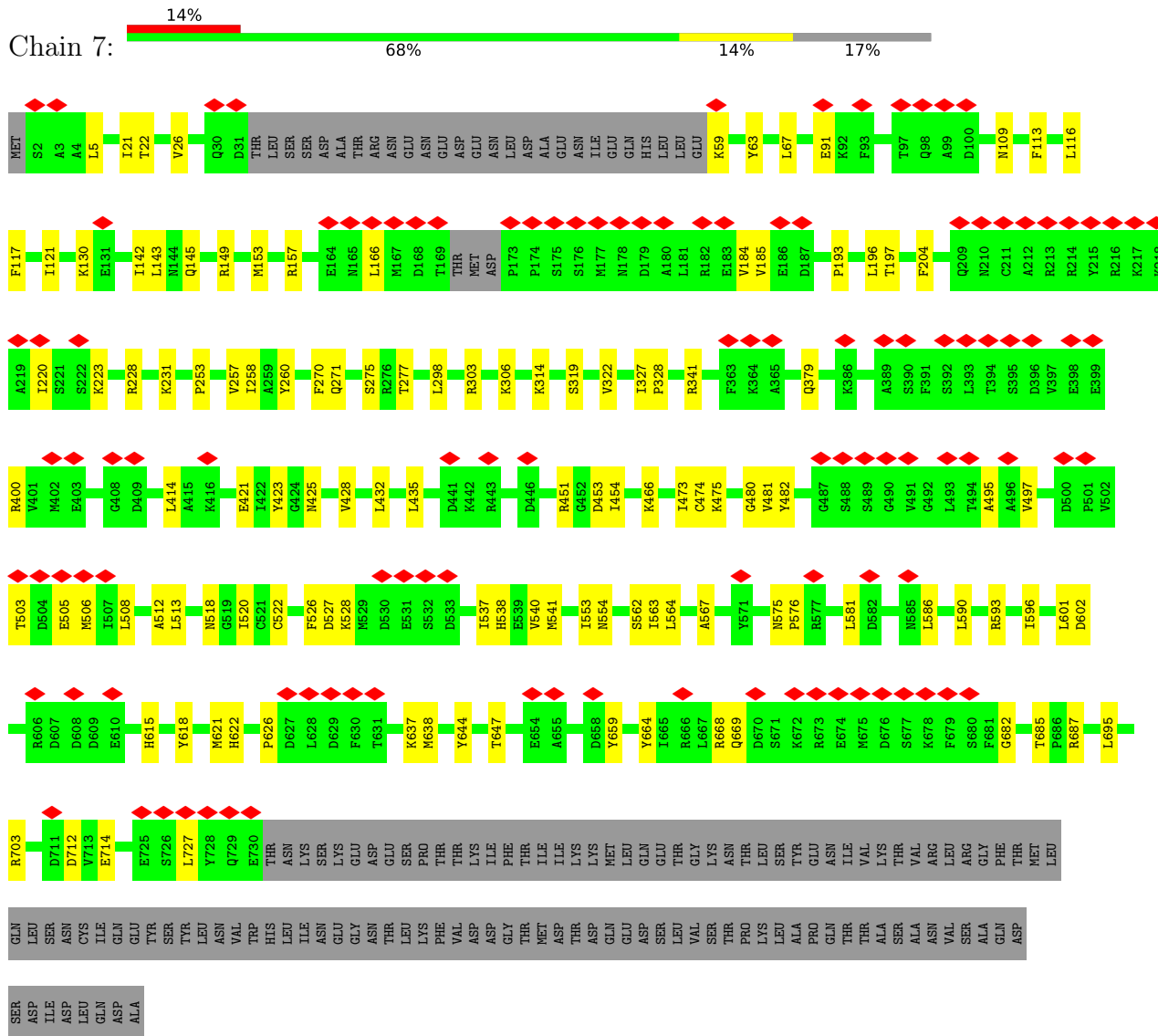


• Molecule 5: DNA replication licensing factor MCM6

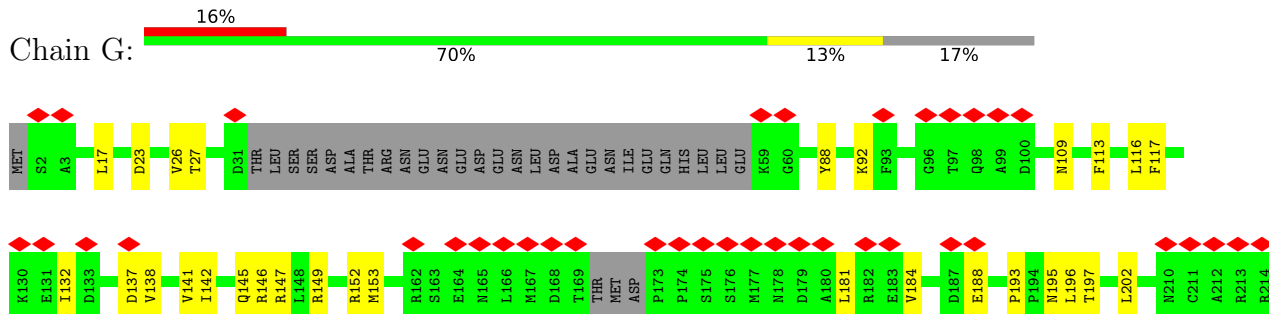




- Molecule 6: DNA replication licensing factor MCM7



- Molecule 6: DNA replication licensing factor MCM7





E698	N699	L700	R701	F702	Q703	IIE
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	258000	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 K3 (6k x 4k)	Depositor
Maximum map value	0.562	Depositor
Minimum map value	-0.321	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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	0.17	0/5057	0.42	0/6834
1	B	0.17	0/5057	0.45	0/6834
2	3	0.18	0/5073	0.41	0/6880
2	C	0.18	0/5073	0.41	0/6880
3	4	0.18	0/5400	0.45	0/7300
3	D	0.18	0/5400	0.42	0/7300
4	5	0.18	0/5222	0.44	2/7061 (0.0%)
4	E	0.19	0/5222	0.44	0/7061
5	6	0.18	0/5190	0.45	0/7001
5	F	0.17	0/5190	0.44	1/7001 (0.0%)
6	7	0.18	0/5590	0.45	1/7554 (0.0%)
6	G	0.19	0/5590	0.43	0/7554
7	H	0.27	0/3186	0.73	6/4298 (0.1%)
8	I	0.24	0/2805	0.66	1/3776 (0.0%)
All	All	0.19	0/69055	0.46	11/93334 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	316	ARG	CB-CG-CD	6.76	126.86	111.30
7	H	402	GLU	N-CA-CB	6.28	119.46	110.16
5	F	116	GLU	N-CA-CB	5.67	119.06	110.28
7	H	126	GLU	CA-CB-CG	5.59	125.27	114.10
6	7	91	GLU	N-CA-CB	5.35	119.13	110.40
8	I	199	MET	CB-CG-SD	5.33	128.70	112.70
7	H	126	GLU	CB-CA-C	5.28	120.62	109.79
4	5	497	MET	CA-C-N	-5.25	112.38	120.88
4	5	497	MET	C-N-CA	-5.25	112.38	120.88
7	H	19	MET	CB-CG-SD	5.23	128.40	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	402	GLU	CB-CG-CD	5.07	121.22	112.60

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	61	0
1	B	4970	0	5026	75	0
2	3	4987	0	5049	62	0
2	C	4987	0	5050	58	0
3	4	5323	0	5373	83	0
3	D	5323	0	5373	62	0
4	5	5148	0	5193	65	0
4	E	5148	0	5193	79	0
5	6	5109	0	5134	74	0
5	F	5109	0	5134	68	0
6	7	5505	0	5563	77	0
6	G	5505	0	5563	69	0
7	H	3109	0	3090	74	0
8	I	2745	0	2746	55	0
9	2	31	0	12	0	0
9	4	31	0	12	2	0
9	5	31	0	12	1	0
9	6	31	0	12	2	0
9	7	31	0	12	1	0
9	B	31	0	12	0	0
9	D	31	0	12	4	0
9	E	31	0	12	1	0
9	F	31	0	12	1	0
9	G	31	0	12	1	0
9	H	31	0	12	6	0
10	2	1	0	0	0	0
10	3	1	0	0	0	0
10	4	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	5	1	0	0	0	0
10	7	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	2	0	0	0	0
10	E	1	0	0	0	0
10	G	1	0	0	0	0
11	2	1	0	0	0	0
11	4	1	0	0	0	0
11	5	1	0	0	0	0
11	6	1	0	0	0	0
11	7	1	0	0	0	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	F	1	0	0	0	0
11	G	1	0	0	0	0
11	I	1	0	0	0	0
12	3	27	0	12	1	0
12	C	27	0	12	0	0
All	All	68356	0	68669	867	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (867) 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)
5:6:311:CYS:HB3	5:6:314:CYS:SG	2.12	0.90
4:5:167:ILE:HD11	4:5:259:GLN:HB2	1.62	0.81
3:D:650:GLU:HG3	3:D:651:GLN:HG3	1.62	0.80
8:I:194:ALA:HA	8:I:199:MET:HE2	1.63	0.80
7:H:292:LYS:HZ1	8:I:278:ILE:HG21	1.50	0.75
6:7:586:LEU:HD11	6:7:590:LEU:HD22	1.68	0.74
5:F:270:LEU:HD12	5:F:289:SER:HB2	1.70	0.74
8:I:125:ARG:NH2	8:I:161:GLN:O	2.18	0.73
7:H:138:LYS:HB2	8:I:344:PHE:HB3	1.72	0.72
2:3:353:LEU:HD21	2:3:647:ILE:HG21	1.72	0.71
8:I:200:LYS:HD2	8:I:202:TRP:HE1	1.53	0.71
1:2:676:ARG:HA	1:2:808:ARG:HH22	1.54	0.71
5:6:313:MET:HE3	5:6:338:CYS:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:251:ILE:HG23	2:C:280:ASP:HB3	1.73	0.70
3:D:445:ARG:HD3	5:F:410:LEU:HD11	1.72	0.70
6:7:685:THR:HG22	6:7:687:ARG:H	1.57	0.69
3:4:726:ASN:HA	3:4:729:LEU:HD23	1.75	0.68
7:H:142:LYS:NZ	7:H:176:GLY:O	2.27	0.67
8:I:126:ILE:HG21	8:I:155:PHE:HE2	1.59	0.67
1:B:624:MET:O	1:B:676:ARG:NH2	2.28	0.67
3:4:434:GLU:HB2	3:4:467:LYS:HB3	1.76	0.67
5:6:589:VAL:HG21	5:6:597:TYR:HB2	1.75	0.67
7:H:457:ARG:HH12	7:H:463:LEU:HD21	1.61	0.66
6:G:685:THR:HG22	6:G:687:ARG:H	1.59	0.66
4:5:477:VAL:HG23	4:5:517:THR:HG21	1.76	0.66
2:3:570:ARG:NH1	4:5:614:LEU:O	2.27	0.66
6:G:228:ARG:NH2	6:G:327:ILE:O	2.29	0.66
2:C:459:ALA:HB2	6:G:327:ILE:HD11	1.79	0.65
4:E:548:SER:HB3	4:E:647:PRO:HG2	1.78	0.65
3:4:445:ARG:NH1	5:6:447:ASP:OD1	2.29	0.65
4:E:161:ARG:HG3	4:E:295:VAL:HG22	1.79	0.64
6:G:513:LEU:HD13	6:G:540:VAL:HG21	1.79	0.64
7:H:16:LYS:HA	7:H:19:MET:HE2	1.79	0.64
4:E:630:ARG:NH1	4:E:648:ILE:O	2.31	0.64
3:4:650:GLU:HG3	3:4:651:GLN:HG3	1.80	0.64
5:6:699:LEU:HB3	5:6:701:MET:HG2	1.79	0.64
4:E:342:ILE:HD11	4:E:473:ASP:HB3	1.79	0.64
7:H:111:ARG:NH1	8:I:694:ASP:OD1	2.31	0.64
1:B:701:ASP:OD2	1:B:705:ARG:NH1	2.31	0.64
5:6:296:ARG:NH2	5:6:624:GLU:OE2	2.30	0.64
4:E:430:GLU:HG3	4:E:438:TYR:HB2	1.80	0.64
5:6:773:LEU:HD13	5:6:824:ILE:HD12	1.80	0.63
4:E:458:MET:HG3	4:E:459:THR:HG23	1.81	0.63
3:4:777:MET:SD	3:4:797:GLN:NE2	2.71	0.63
7:H:395:THR:HA	7:H:439:HIS:HE1	1.62	0.63
5:F:125:GLN:HE21	5:F:130:GLY:HA2	1.64	0.63
5:F:311:CYS:HB3	5:F:314:CYS:HB2	1.79	0.62
3:4:417:LEU:HD13	3:4:463:VAL:HG21	1.81	0.62
1:B:384:ASN:HB2	1:B:412:ALA:HA	1.81	0.62
3:D:621:LEU:HD13	3:D:648:VAL:HG21	1.80	0.62
7:H:155:HIS:NE2	7:H:301:ASP:OD2	2.24	0.62
5:F:773:LEU:HD21	5:F:804:ILE:HG12	1.81	0.62
2:3:244:GLU:OE1	6:7:109:ASN:ND2	2.28	0.62
3:D:780:MET:HG2	3:D:790:ARG:HH22	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:5:ARG:NH1	2:C:234:GLU:OE2	2.33	0.62
2:C:367:LEU:HD23	2:C:656:LEU:HD21	1.80	0.62
3:D:431:ASP:OD2	3:D:468:LYS:NZ	2.33	0.62
2:3:424:ASN:O	2:3:657:ARG:NH2	2.33	0.61
3:D:230:LEU:HD22	3:D:280:MET:HE2	1.82	0.61
4:5:87:ILE:HG23	4:5:137:LEU:HD13	1.83	0.61
3:4:204:LYS:HB3	3:4:221:ASP:HB3	1.82	0.61
5:6:169:ALA:HB2	8:I:238:LEU:HD11	1.82	0.61
5:6:123:SER:HB3	5:6:134:LYS:HG2	1.83	0.61
5:6:611:ALA:HB3	5:6:624:GLU:HB2	1.81	0.61
3:D:268:VAL:HG12	3:D:272:MET:HE2	1.82	0.61
7:H:61:PHE:O	7:H:63:SER:N	2.33	0.61
2:3:52:ASN:ND2	2:3:90:ASN:O	2.33	0.60
6:7:260:TYR:HE2	6:7:271:GLN:HG2	1.66	0.60
1:B:488:SER:HB3	1:B:825:LEU:HD12	1.82	0.60
3:4:769:GLU:OE2	3:4:772:ARG:NH2	2.33	0.60
3:D:189:GLU:OE2	3:D:193:ASN:ND2	2.34	0.60
3:4:621:LEU:HD13	3:4:648:VAL:HG21	1.83	0.60
1:B:353:GLN:NE2	1:B:357:GLU:O	2.34	0.60
4:5:654:GLU:HA	4:5:657:ILE:HD12	1.83	0.60
3:4:445:ARG:HB2	5:6:410:LEU:HD21	1.82	0.60
3:4:601:LEU:HD23	3:4:620:ALA:HB3	1.83	0.60
2:C:567:ARG:O	2:C:642:TYR:OH	2.16	0.60
3:D:701:ARG:NH2	9:F:2001:AGS:S1G	2.75	0.60
6:7:621:MET:HE3	6:7:622:HIS:CE1	2.37	0.60
1:2:300:PHE:O	1:2:319:ARG:NH1	2.35	0.60
3:D:758:ILE:HG22	3:D:760:PRO:HD3	1.84	0.60
4:E:40:LEU:HB2	4:E:45:ILE:HD13	1.84	0.60
2:C:368:ALA:HB3	2:C:378:LYS:HE2	1.83	0.59
6:G:26:VAL:HG23	6:G:27:THR:HG23	1.83	0.59
5:6:306:LYS:HB2	5:6:352:ARG:HB2	1.84	0.59
1:2:307:ARG:NH1	1:2:392:GLU:OE2	2.35	0.59
4:E:136:GLN:HG3	4:E:280:ARG:HH21	1.68	0.59
6:G:149:ARG:HH11	6:G:152:ARG:HH21	1.51	0.59
7:H:144:ILE:HG13	7:H:309:LEU:HD13	1.85	0.59
8:I:278:ILE:HG22	8:I:279:ILE:HG13	1.85	0.59
1:2:624:MET:O	1:2:676:ARG:NH2	2.35	0.59
2:3:390:GLU:OE1	2:3:467:ARG:NH1	2.34	0.59
3:4:458:LYS:NZ	5:6:411:GLY:O	2.36	0.59
7:H:161:HIS:NE2	7:H:182:ASP:O	2.36	0.59
7:H:268:ASN:HD21	8:I:522:LYS:HD3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:701:THR:O	2:3:704:THR:HB	2.03	0.58
5:6:773:LEU:HD21	5:6:804:ILE:HG12	1.85	0.58
8:I:177:ARG:HH21	8:I:191:LEU:HD23	1.68	0.58
8:I:126:ILE:HG21	8:I:155:PHE:CE2	2.38	0.58
1:2:384:ASN:HB2	1:2:412:ALA:HA	1.83	0.58
4:5:551:ASP:OD2	4:5:658:ARG:NH1	2.36	0.58
3:4:656:ILE:HD13	5:6:602:ALA:HB1	1.86	0.58
6:G:428:VAL:HA	6:G:598:PHE:CE2	2.39	0.58
3:4:686:LEU:HD22	3:4:690:GLU:HG2	1.86	0.58
1:B:347:ILE:HD13	1:B:379:LYS:HZ3	1.69	0.58
5:F:161:ARG:HG3	5:F:162:GLU:HG3	1.85	0.57
6:7:451:ARG:NH1	6:7:453:ASP:O	2.37	0.57
1:B:549:LYS:NZ	1:B:650:ALA:O	2.37	0.57
2:C:262:PRO:HG3	4:E:509:ILE:HD11	1.86	0.57
3:D:445:ARG:NH1	5:F:447:ASP:OD2	2.37	0.57
4:E:282:LEU:HD13	4:E:330:ILE:HG22	1.86	0.57
7:H:276:ALA:HB2	7:H:292:LYS:HB3	1.86	0.57
9:E:2001:AGS:S1G	9:E:2001:AGS:O2B	2.62	0.57
2:C:52:ASN:ND2	2:C:90:ASN:O	2.37	0.57
2:C:340:GLN:HE22	2:C:657:ARG:HG3	1.69	0.57
6:7:482:TYR:HA	6:7:522:CYS:HB2	1.86	0.57
1:B:654:GLY:O	5:F:696:ARG:NH1	2.38	0.57
2:C:177:ASN:ND2	4:E:245:HIS:O	2.38	0.57
9:D:2001:AGS:O3G	6:G:593:ARG:NH2	2.37	0.57
3:D:628:VAL:HG22	3:D:670:SER:HB2	1.87	0.57
5:F:306:LYS:HB2	5:F:352:ARG:HB2	1.87	0.57
5:F:650:VAL:HA	5:F:653:HIS:CE1	2.40	0.57
1:B:511:ILE:HG22	1:B:681:CYS:HB3	1.86	0.56
2:C:370:SER:OG	4:E:404:MET:SD	2.63	0.56
2:3:457:LEU:HD21	2:3:502:ILE:HG21	1.86	0.56
1:B:498:ILE:HD12	1:B:513:THR:HA	1.86	0.56
2:C:353:LEU:HB3	2:C:359:ILE:HD13	1.87	0.56
3:4:345:ALA:HB2	3:4:365:ILE:HD13	1.87	0.56
3:4:474:LEU:HB2	3:4:586:PRO:HD3	1.87	0.56
5:6:170:ILE:HD12	5:6:181:LEU:HD11	1.88	0.56
5:6:653:HIS:HB3	5:6:705:ILE:HD13	1.87	0.56
3:D:474:LEU:HB2	3:D:586:PRO:HD3	1.87	0.56
6:G:605:SER:OG	6:G:608:ASP:OD1	2.23	0.56
1:2:406:ARG:NH1	1:2:449:THR:OG1	2.38	0.56
3:4:645:LEU:HB3	3:4:649:MET:HE2	1.86	0.56
1:B:534:ARG:O	1:B:815:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:311:CYS:SG	3:4:329:LYS:NZ	2.79	0.56
5:6:357:GLN:HB2	5:6:386:VAL:HG13	1.87	0.56
1:2:347:ILE:HD11	5:F:429:THR:HG23	1.88	0.56
3:D:306:TYR:HA	3:D:436:THR:HG21	1.86	0.56
8:I:268:LEU:HD13	8:I:279:ILE:HD12	1.88	0.56
6:G:534:ARG:O	6:G:538:HIS:HB2	2.04	0.56
7:H:137:ILE:HD13	7:H:140:ILE:HD12	1.88	0.56
1:B:588:GLU:OE2	4:E:273:ASN:ND2	2.38	0.56
3:D:183:THR:O	6:G:145:GLN:NE2	2.39	0.56
4:E:654:GLU:HA	4:E:657:ILE:HD12	1.88	0.56
3:4:758:ILE:HG22	3:4:760:PRO:HD3	1.88	0.56
3:D:601:LEU:HD23	3:D:620:ALA:HB3	1.86	0.56
1:2:406:ARG:NH1	1:2:430:TYR:OH	2.39	0.56
5:6:379:VAL:HG23	5:6:454:PHE:HB3	1.88	0.56
4:5:433:SER:HB2	4:5:436:ALA:HB2	1.88	0.55
2:C:457:LEU:HD11	2:C:504:THR:HG21	1.87	0.55
8:I:268:LEU:HD22	8:I:278:ILE:HB	1.89	0.55
4:5:464:LEU:HD21	4:5:470:VAL:HG11	1.88	0.55
5:6:691:ARG:HH12	5:6:716:LEU:HD22	1.70	0.55
6:7:414:LEU:HD22	6:7:638:MET:HG2	1.88	0.55
1:B:305:SER:OG	1:B:392:GLU:OE2	2.25	0.55
3:D:321:ASP:HA	3:D:324:LYS:HE3	1.89	0.55
7:H:39:ILE:HG13	7:H:47:VAL:HG13	1.87	0.55
5:6:661:ILE:HB	5:6:672:LEU:HB2	1.88	0.55
4:E:605:TYR:HE2	4:E:668:LEU:HD21	1.71	0.55
1:B:343:LYS:HE3	1:B:372:PRO:HD2	1.88	0.55
2:3:177:ASN:ND2	4:5:245:HIS:O	2.39	0.55
2:3:39:ARG:HG2	2:3:132:LEU:HD21	1.88	0.55
1:B:704:VAL:HG11	5:F:770:ARG:HH21	1.72	0.55
4:E:48:ASP:OD1	4:E:51:ARG:NH2	2.39	0.55
4:E:266:PRO:HG2	4:E:269:GLU:HB3	1.88	0.55
8:I:306:ARG:NH2	8:I:317:GLU:OE2	2.38	0.55
6:7:21:ILE:HG12	6:7:117:PHE:HE1	1.71	0.55
7:H:126:GLU:OE1	7:H:130:THR:OG1	2.23	0.55
4:5:100:ARG:NH2	6:G:188:GLU:OE2	2.40	0.55
5:6:710:ASP:OD1	5:6:805:ARG:NH1	2.40	0.55
2:C:244:GLU:OE1	6:G:109:ASN:ND2	2.28	0.55
3:D:459:THR:OG1	6:G:252:LYS:NZ	2.39	0.55
6:G:132:ILE:HD11	6:G:141:VAL:HG12	1.87	0.55
1:2:498:ILE:HD12	1:2:513:THR:HA	1.89	0.55
3:4:189:GLU:OE2	3:4:193:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:372:GLU:OE1	8:I:249:ARG:NH2	2.40	0.55
3:4:408:ASP:OD1	6:7:518:ASN:ND2	2.40	0.55
4:E:297:ILE:HB	4:E:329:LYS:HB2	1.89	0.54
7:H:182:ASP:OD2	9:H:2001:AGS:O2A	2.25	0.54
7:H:326:ALA:HB2	8:I:279:ILE:HG21	1.88	0.54
8:I:129:ASP:HB3	8:I:175:THR:HA	1.88	0.54
2:C:686:LEU:O	2:C:693:LYS:NZ	2.40	0.54
3:D:345:ALA:HB2	3:D:365:ILE:HD13	1.88	0.54
6:G:508:LEU:HD22	6:G:553:ILE:HD13	1.88	0.54
2:3:565:VAL:HG21	4:5:650:ILE:HD11	1.89	0.54
1:B:790:TYR:HE1	4:E:565:ASP:HB2	1.72	0.54
6:G:466:LYS:NZ	9:G:2001:AGS:S1G	2.72	0.54
3:D:429:ALA:O	3:D:587:ARG:NH2	2.39	0.54
5:F:277:ARG:NE	5:F:363:GLU:OE2	2.40	0.54
5:6:409:GLN:NE2	5:6:450:TYR:O	2.41	0.54
1:2:612:MET:HE1	1:2:620:ILE:HG13	1.89	0.54
1:B:337:VAL:HA	1:B:380:THR:HG23	1.88	0.54
8:I:132:ASP:OD2	8:I:141:LYS:NZ	2.40	0.54
7:H:266:PRO:HA	8:I:258:ILE:HA	1.90	0.53
4:E:482:PHE:O	4:E:490:ARG:NH2	2.41	0.53
2:3:95:ARG:NH1	2:3:156:SER:OG	2.39	0.53
1:B:576:LEU:HD23	1:B:595:ALA:HB3	1.88	0.53
2:3:368:ALA:HB3	2:3:378:LYS:HE2	1.89	0.53
7:H:352:PHE:CE1	8:I:268:LEU:HG	2.44	0.53
1:2:562:ARG:NH2	4:5:265:VAL:O	2.42	0.53
4:5:65:MET:HB3	4:5:76:TYR:HE1	1.74	0.53
7:H:350:LEU:HB2	8:I:269:TYR:O	2.09	0.53
3:4:692:ILE:HG22	3:4:694:LEU:HD13	1.91	0.53
4:5:40:LEU:HB2	4:5:45:ILE:HD13	1.91	0.53
1:B:271:PHE:HD2	1:B:295:VAL:HG21	1.74	0.53
3:D:313:GLY:N	3:D:316:GLU:OE2	2.41	0.53
5:F:170:ILE:HD12	5:F:181:LEU:HD11	1.89	0.53
6:G:195:ASN:OD1	6:G:306:LYS:NZ	2.41	0.53
3:4:317:LEU:O	6:7:341:ARG:NH2	2.42	0.53
7:H:90:GLU:HB2	7:H:184:GLY:HA2	1.91	0.53
7:H:182:ASP:OD2	9:H:2001:AGS:O2B	2.27	0.53
2:3:314:LEU:HD11	4:5:200:ILE:HA	1.91	0.53
3:D:569:ASP:O	3:D:574:LYS:NZ	2.42	0.53
5:F:742:ILE:HG22	5:F:744:PRO:HD3	1.90	0.53
2:3:396:GLY:HA3	6:7:475:LYS:HE3	1.89	0.53
5:6:386:VAL:HG12	5:6:387:GLU:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:535:PRO:HB2	5:F:742:ILE:HG23	1.91	0.53
7:H:273:ILE:HD11	7:H:292:LYS:HE3	1.91	0.53
5:6:571:ILE:HG12	5:6:711:LEU:HB2	1.89	0.53
6:7:508:LEU:HD22	6:7:553:ILE:HD13	1.91	0.53
9:H:2001:AGS:O2B	9:H:2001:AGS:O3G	2.26	0.53
1:2:337:VAL:HA	1:2:380:THR:HG23	1.91	0.52
1:2:560:ALA:HB3	1:2:563:ALA:HB2	1.91	0.52
2:3:669:PRO:HG2	2:3:710:THR:HG23	1.91	0.52
5:6:144:LYS:HG3	5:6:193:ALA:HB1	1.91	0.52
6:7:513:LEU:HD13	6:7:540:VAL:HG21	1.90	0.52
4:E:444:SER:OG	4:E:445:SER:N	2.43	0.52
5:F:137:ARG:NH2	5:F:192:TYR:OH	2.42	0.52
7:H:22:LEU:HD13	7:H:77:LYS:HD2	1.91	0.52
3:4:183:THR:O	6:7:145:GLN:NE2	2.42	0.52
6:7:497:VAL:HG12	6:7:506:MET:HE3	1.90	0.52
2:3:391:LYS:HB2	2:3:399:LEU:HB2	1.92	0.52
6:7:659:TYR:OH	6:7:714:GLU:OE2	2.26	0.52
2:C:216:ASP:OD2	2:C:218:THR:OG1	2.25	0.52
6:G:228:ARG:NH1	6:G:317:GLU:OE1	2.43	0.52
1:2:534:ARG:O	1:2:815:ARG:NH1	2.41	0.52
5:6:663:ILE:O	5:6:669:HIS:HA	2.10	0.52
2:C:39:ARG:HG3	2:C:136:MET:HE1	1.91	0.52
1:2:353:GLN:NE2	1:2:357:GLU:O	2.41	0.52
1:B:501:MET:HE3	1:B:555:TYR:HE2	1.74	0.52
5:F:109:GLU:O	5:F:113:GLU:HG2	2.10	0.52
2:3:203:ALA:O	2:3:207:GLY:N	2.42	0.52
4:5:36:LEU:O	4:5:47:ARG:NH2	2.34	0.52
3:D:204:LYS:HB3	3:D:221:ASP:HB3	1.92	0.52
3:D:842:THR:HG23	3:D:844:LYS:H	1.74	0.52
1:B:605:LEU:HD23	1:B:647:ILE:HB	1.92	0.52
3:D:487:GLN:HA	3:D:490:VAL:HG12	1.92	0.52
3:D:794:THR:HG22	3:D:796:ARG:H	1.74	0.52
4:E:261:ILE:HD12	4:E:291:ARG:HH11	1.74	0.52
6:G:459:MET:HE1	6:G:584:ILE:HG12	1.92	0.52
4:5:167:ILE:HD13	4:5:257:LYS:HG3	1.92	0.52
5:F:629:MET:HE3	5:F:672:LEU:HB3	1.90	0.52
7:H:115:GLN:NE2	7:H:116:VAL:O	2.42	0.52
7:H:149:ARG:HD3	7:H:152:LYS:HE3	1.92	0.52
3:4:265:PRO:HB3	3:4:325:LEU:HG	1.92	0.52
3:4:628:VAL:HG22	3:4:670:SER:HB2	1.92	0.52
2:C:276:VAL:HG22	2:C:321:ILE:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:295:VAL:HB	2:C:325:THR:HB	1.92	0.52
2:3:455:ARG:HB2	2:3:502:ILE:HD11	1.92	0.51
3:4:778:ARG:NH1	5:6:719:CYS:SG	2.83	0.51
5:F:574:VAL:O	5:F:714:VAL:HA	2.11	0.51
6:G:147:ARG:NH2	6:G:197:THR:O	2.43	0.51
1:B:241:SER:OG	1:B:413:ASP:OD2	2.28	0.51
3:D:199:MET:HA	3:D:227:ILE:HD11	1.91	0.51
4:E:72:ASN:HB3	4:E:75:ILE:HG12	1.92	0.51
4:E:300:ILE:HG23	4:E:324:ARG:HB3	1.92	0.51
7:H:291:MET:HE2	7:H:350:LEU:HD21	1.92	0.51
2:3:584:GLU:OE2	4:5:516:ARG:NH1	2.42	0.51
3:4:604:TYR:OH	6:7:554:ASN:ND2	2.41	0.51
6:7:664:TYR:CZ	6:7:668:ARG:HD2	2.45	0.51
5:6:574:VAL:HG21	5:6:699:LEU:HD11	1.92	0.51
6:7:481:VAL:HG11	6:7:512:ALA:HB1	1.92	0.51
6:7:644:TYR:O	6:7:647:THR:OG1	2.27	0.51
1:B:218:TYR:OH	1:B:251:GLU:OE2	2.29	0.51
6:G:425:ASN:HB3	6:G:428:VAL:HB	1.92	0.51
4:5:300:ILE:HG23	4:5:324:ARG:HB3	1.93	0.51
1:B:690:GLU:HB2	1:B:694:ARG:HH12	1.76	0.51
6:G:146:ARG:NH2	6:G:304:ALA:O	2.44	0.51
5:F:126:SER:OG	5:F:128:ASP:OD1	2.24	0.51
5:F:379:VAL:HG23	5:F:454:PHE:HB3	1.93	0.51
6:G:88:TYR:CZ	6:G:92:LYS:HD2	2.46	0.51
5:6:710:ASP:HB3	5:6:802:SER:HB2	1.93	0.51
7:H:344:CYS:SG	7:H:452:MET:HB3	2.50	0.51
2:3:524:ASP:OD2	2:3:527:ARG:NH1	2.38	0.51
3:D:585:THR:HG21	3:D:628:VAL:HB	1.93	0.51
4:E:464:LEU:HD21	4:E:470:VAL:HG11	1.92	0.50
5:F:691:ARG:HE	5:F:716:LEU:HD22	1.75	0.50
6:G:350:ASP:HB2	6:G:382:ARG:HG3	1.93	0.50
5:F:357:GLN:HB2	5:F:386:VAL:HG13	1.93	0.50
8:I:270:ASP:O	8:I:273:GLN:NE2	2.44	0.50
5:6:509:SER:OG	5:6:510:SER:N	2.45	0.50
4:E:473:ASP:OD1	4:E:516:ARG:N	2.43	0.50
7:H:326:ALA:HB2	8:I:279:ILE:HD13	1.93	0.50
8:I:321:LYS:HB3	8:I:325:LYS:HZ2	1.77	0.50
1:B:406:ARG:NH1	1:B:430:TYR:OH	2.43	0.50
2:C:487:HIS:CE1	2:C:539:LEU:HD13	2.47	0.50
4:E:18:SER:HG	8:I:284:LYS:HZ3	1.59	0.50
4:E:455:ARG:NH2	4:E:460:ARG:O	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:559:ASP:N	4:E:564:ARG:HH22	2.09	0.50
2:3:529:PRO:HA	2:3:532:ASN:HB2	1.93	0.50
1:B:537:ILE:HG23	1:B:678:ASP:HB2	1.92	0.50
2:3:251:ILE:HG23	2:3:280:ASP:HB3	1.94	0.50
2:3:276:VAL:HG22	2:3:321:ILE:HB	1.94	0.50
4:E:559:ASP:H	4:E:564:ARG:HH22	1.59	0.50
6:G:589:ALA:HB1	6:G:593:ARG:HH12	1.77	0.50
2:C:314:LEU:HD11	4:E:200:ILE:HA	1.93	0.50
5:6:277:ARG:NH2	5:6:373:MET:O	2.44	0.50
6:7:538:HIS:HE1	6:7:593:ARG:NH1	2.10	0.50
1:B:597:VAL:HG23	1:B:629:ILE:HD12	1.94	0.50
5:F:125:GLN:NE2	5:F:126:SER:O	2.45	0.50
6:G:634:GLU:HB3	6:G:637:LYS:HE2	1.94	0.50
1:2:385:TYR:OH	1:2:387:ARG:NH2	2.44	0.50
3:4:493:ASN:OD1	3:4:494:GLU:N	2.45	0.50
6:7:220:ILE:HD12	6:7:223:LYS:HD3	1.93	0.50
1:2:296:ARG:HH21	1:2:413:ASP:HB3	1.77	0.49
5:6:433:LEU:HD13	1:B:342:LEU:HB3	1.94	0.49
6:7:526:PHE:HB3	6:7:567:ALA:HB2	1.94	0.49
5:F:550:GLN:NE2	5:F:569:ILE:O	2.45	0.49
6:G:451:ARG:NH1	6:G:453:ASP:O	2.43	0.49
3:4:812:LYS:HE3	3:4:814:LYS:HE2	1.93	0.49
1:B:625:GLU:HA	1:B:676:ARG:HH12	1.78	0.49
7:H:52:ASP:OD1	7:H:52:ASP:N	2.45	0.49
1:2:701:ASP:HA	1:2:704:VAL:HG22	1.94	0.49
3:4:432:ARG:NH1	3:4:585:THR:O	2.45	0.49
4:5:276:MET:HG2	4:5:328:ILE:HB	1.94	0.49
6:G:181:LEU:HA	6:G:184:VAL:HG12	1.93	0.49
6:G:432:LEU:HB3	6:G:473:ILE:HD11	1.94	0.49
2:3:667:VAL:HG23	2:3:719:LYS:HD2	1.95	0.49
5:F:297:THR:HA	5:F:359:VAL:HG12	1.94	0.49
7:H:375:ASP:HA	7:H:378:ASN:HB2	1.95	0.49
1:2:676:ARG:HA	1:2:808:ARG:NH2	2.26	0.49
4:E:412:VAL:HG22	4:E:552:MET:HB2	1.94	0.49
5:F:310:THR:HG1	5:F:345:THR:HG1	1.57	0.49
5:F:701:MET:HE3	5:F:706:MET:HG2	1.94	0.49
1:B:658:ASN:H	1:B:666:ASN:HD21	1.60	0.49
3:D:607:ARG:NH2	5:F:617:GLU:OE2	2.46	0.49
3:D:616:LEU:HD22	3:D:661:ILE:HD11	1.94	0.49
4:E:532:ASP:OD1	4:E:557:LYS:NZ	2.44	0.49
7:H:56:LYS:HE3	7:H:60:LYS:HZ2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:115:GLN:HE22	7:H:117:ILE:HD13	1.78	0.49
8:I:320:TYR:HE1	8:I:382:MET:HE1	1.77	0.49
3:4:263:ASN:OD1	3:4:324:LYS:NZ	2.45	0.49
5:6:403:VAL:HG22	5:6:450:TYR:HB3	1.94	0.49
6:7:166:LEU:HA	4:E:47:ARG:HH11	1.78	0.49
1:B:690:GLU:HB2	1:B:694:ARG:NH1	2.28	0.49
5:F:842:ASP:OD1	5:F:842:ASP:N	2.46	0.49
6:G:350:ASP:OD2	6:G:382:ARG:NH1	2.46	0.49
1:2:342:LEU:HB3	5:F:433:LEU:HD13	1.95	0.49
2:3:528:ASP:OD1	2:3:528:ASP:N	2.44	0.49
4:E:663:LEU:HA	4:E:666:LEU:HD12	1.93	0.49
6:G:227:VAL:HA	6:G:230:ILE:HD12	1.94	0.49
7:H:127:GLU:O	7:H:130:THR:OG1	2.31	0.49
7:H:291:MET:HE1	7:H:345:ALA:HA	1.94	0.49
3:4:457:TYR:HB2	6:7:253:PRO:HG2	1.94	0.49
4:5:374:ILE:HD13	4:5:428:PHE:HE2	1.78	0.49
5:F:300:VAL:HG13	5:F:386:VAL:HG11	1.95	0.49
6:G:525:GLU:OE1	6:G:528:LYS:NZ	2.32	0.49
7:H:169:PHE:CZ	7:H:178:GLY:HA3	2.48	0.49
3:4:204:LYS:O	3:4:208:ILE:HG13	2.13	0.48
3:4:393:ASP:HB3	3:4:424:VAL:HG21	1.94	0.48
5:F:314:CYS:SG	5:F:337:SER:OG	2.70	0.48
6:G:521:CYS:HB2	6:G:561:THR:HG21	1.95	0.48
3:4:238:THR:HG22	3:4:240:ASN:H	1.78	0.48
4:E:452:SER:HB3	4:E:454:GLN:HE22	1.77	0.48
1:2:334:LEU:HB3	1:2:337:VAL:HG22	1.94	0.48
2:3:212:ARG:HD2	2:3:232:PRO:HD3	1.95	0.48
1:B:608:GLU:OE2	1:B:611:LYS:NZ	2.39	0.48
3:4:370:ARG:NH2	3:4:377:ASN:O	2.40	0.48
3:4:774:TYR:HD2	5:6:728:ALA:HB2	1.78	0.48
4:5:48:ASP:OD1	4:5:51:ARG:NH2	2.46	0.48
4:5:137:LEU:HD21	4:5:139:LEU:HD23	1.96	0.48
2:C:395:ASN:ND2	6:G:421:GLU:OE1	2.44	0.48
2:3:419:LEU:HD12	2:3:471:CYS:HB3	1.95	0.48
2:3:482:ASP:O	2:3:486:ILE:HG12	2.13	0.48
6:7:260:TYR:HB3	6:7:298:LEU:HB3	1.94	0.48
4:E:136:GLN:HB2	4:E:280:ARG:HE	1.78	0.48
7:H:339:LYS:HB3	7:H:343:LYS:NZ	2.28	0.48
8:I:341:ARG:O	8:I:345:GLN:HG2	2.14	0.48
3:4:395:GLN:NE2	3:4:425:ASP:OD1	2.42	0.48
4:5:453:VAL:HG21	4:5:504:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:581:LEU:HD11	6:7:682:GLY:HA2	1.96	0.48
1:B:633:LYS:HE2	4:E:446:ALA:HB1	1.96	0.48
4:5:370:LEU:HG	4:5:666:LEU:HD11	1.96	0.48
6:7:322:VAL:HG21	6:7:328:PRO:HG3	1.96	0.48
1:B:560:ALA:HB3	1:B:563:ALA:HB2	1.96	0.48
6:G:142:ILE:HD11	6:G:303:ARG:HG3	1.96	0.48
7:H:260:ASP:OD2	7:H:263:LYS:NZ	2.43	0.48
1:2:553:LEU:HD22	1:2:605:LEU:HD23	1.96	0.48
3:D:676:ASN:ND2	9:D:2001:AGS:S1G	2.81	0.48
7:H:321:GLN:NE2	8:I:309:PHE:HB2	2.29	0.48
1:2:255:ILE:HG23	1:2:256:LEU:HD12	1.95	0.48
1:2:537:ILE:O	1:2:645:SER:OG	2.31	0.48
6:7:503:THR:HG23	6:7:505:GLU:HG2	1.96	0.48
1:B:328:THR:HG22	1:B:387:ARG:H	1.79	0.48
1:B:334:LEU:HD13	4:E:322:ALA:HB1	1.95	0.47
1:B:406:ARG:NH1	1:B:449:THR:OG1	2.47	0.47
1:B:625:GLU:OE2	1:B:676:ARG:NH1	2.46	0.47
3:D:231:ASN:OD1	3:D:234:ARG:NH2	2.46	0.47
6:G:575:ASN:C	6:G:575:ASN:HD22	2.20	0.47
6:G:637:LYS:HA	6:G:640:GLU:HG2	1.96	0.47
8:I:115:ASN:O	8:I:119:ILE:HG13	2.14	0.47
2:3:235:ASP:OD1	2:3:239:ASN:N	2.45	0.47
6:7:193:PRO:HD2	6:7:196:LEU:HD12	1.95	0.47
1:B:339:PHE:HB2	1:B:348:LEU:HD12	1.94	0.47
2:C:426:ALA:HB3	2:C:429:ALA:HB2	1.97	0.47
7:H:160:ILE:HG12	7:H:298:THR:HA	1.96	0.47
2:3:678:VAL:HG21	2:3:723:LYS:HG3	1.96	0.47
6:7:157:ARG:HG3	6:7:185:VAL:HG22	1.95	0.47
1:B:501:MET:HG3	1:B:516:ALA:HB2	1.95	0.47
2:C:572:LEU:HD21	4:E:613:ARG:HD2	1.95	0.47
6:G:318:LEU:HD21	6:G:348:ILE:HD12	1.96	0.47
8:I:373:ASP:H	8:I:376:LYS:HG2	1.78	0.47
3:4:581:VAL:HA	3:4:584:ILE:HG22	1.97	0.47
4:5:449:LEU:HD12	4:5:468:ALA:HB3	1.97	0.47
6:7:435:LEU:HD21	6:7:564:LEU:HB2	1.97	0.47
6:7:466:LYS:NZ	9:7:2001:AGS:S1G	2.80	0.47
5:F:628:LEU:HD11	5:F:652:ILE:HG13	1.96	0.47
2:3:388:GLY:O	2:3:714:LYS:NZ	2.44	0.47
4:5:148:LEU:HD11	4:5:274:LEU:HD12	1.97	0.47
5:6:673:ASN:HB3	5:6:675:ARG:HH11	1.80	0.47
6:7:149:ARG:O	6:7:153:MET:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:PRO:HB2	1:B:429:ILE:HG12	1.97	0.47
1:B:814:LEU:HD21	4:E:573:ILE:HD13	1.96	0.47
1:2:260:LEU:HD21	1:2:297:ILE:HG13	1.97	0.47
2:3:567:ARG:O	2:3:642:TYR:OH	2.27	0.47
3:4:308:VAL:HG22	3:4:327:ASN:HB2	1.97	0.47
3:4:508:LYS:HG2	3:4:746:PHE:CE1	2.50	0.47
3:4:543:GLN:HE21	3:4:670:SER:HB3	1.78	0.47
6:7:400:ARG:HB3	6:7:637:LYS:HE3	1.97	0.47
1:B:795:ARG:HA	1:B:798:ILE:HD12	1.96	0.47
5:F:509:SER:OG	5:F:510:SER:N	2.48	0.47
6:G:117:PHE:HB3	6:G:202:LEU:HD11	1.97	0.47
8:I:268:LEU:O	8:I:278:ILE:N	2.48	0.47
3:4:578:LEU:HB3	3:4:590:TYR:HE2	1.80	0.47
1:B:707:HIS:NE2	5:F:763:PRO:O	2.37	0.47
2:C:235:ASP:OD1	2:C:239:ASN:N	2.48	0.47
2:C:672:THR:OG1	2:C:721:VAL:O	2.27	0.47
3:D:842:THR:OG1	3:D:844:LYS:NZ	2.40	0.47
7:H:370:LYS:NZ	7:H:447:GLU:OE2	2.33	0.47
8:I:303:SER:OG	8:I:312:ASP:OD2	2.27	0.47
2:3:484:VAL:HG22	6:7:528:LYS:HD2	1.96	0.47
4:5:614:LEU:HA	4:5:672:ALA:HB3	1.97	0.47
4:E:31:PHE:CG	4:E:90:PHE:HD1	2.33	0.47
5:F:109:GLU:OE1	5:F:112:ARG:NH2	2.48	0.47
7:H:187:GLU:OE2	7:H:277:ASN:ND2	2.48	0.47
7:H:367:ASN:HB2	7:H:371:GLU:OE2	2.14	0.47
9:H:2001:AGS:O2A	9:H:2001:AGS:O2B	2.32	0.47
1:2:387:ARG:HG2	1:2:407:GLU:OE2	2.15	0.47
2:3:97:ILE:HD13	2:3:156:SER:HB2	1.97	0.47
5:6:742:ILE:HG22	5:6:744:PRO:HD3	1.96	0.47
6:7:454:ILE:O	6:7:562:SER:OG	2.30	0.47
1:B:607:ASP:OD2	1:B:608:GLU:N	2.48	0.47
2:C:203:ALA:O	2:C:207:GLY:N	2.48	0.47
3:D:366:GLN:NE2	6:G:297:GLN:OE1	2.43	0.47
5:F:632:ASP:OD1	5:F:675:ARG:N	2.47	0.47
1:2:608:GLU:OE1	1:2:611:LYS:NZ	2.37	0.46
1:B:523:VAL:HG11	1:B:775:TYR:HA	1.96	0.46
3:D:635:ASP:OD1	3:D:635:ASP:N	2.48	0.46
4:E:151:LEU:HD11	4:E:162:LEU:HD22	1.97	0.46
7:H:151:LEU:HA	7:H:154:VAL:HG22	1.97	0.46
7:H:157:LYS:HA	7:H:157:LYS:HD3	1.75	0.46
4:5:223:ASN:HD21	2:C:230:ILE:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:257:LYS:HD2	4:5:273:ASN:HD22	1.80	0.46
5:6:305:TYR:HB2	5:6:354:LEU:HG	1.96	0.46
2:C:430:ILE:HD12	2:C:465:ALA:HB2	1.96	0.46
7:H:291:MET:HE3	7:H:352:PHE:CE2	2.50	0.46
2:3:129:LEU:HD23	2:3:153:TRP:HB3	1.96	0.46
2:3:280:ASP:OD1	2:3:280:ASP:N	2.49	0.46
3:4:585:THR:HG21	3:4:628:VAL:HB	1.96	0.46
1:2:400:GLY:HA2	5:6:594:ARG:HH22	1.81	0.46
2:3:417:GLN:NE2	4:5:404:MET:HE2	2.31	0.46
3:4:645:LEU:O	3:4:649:MET:HG3	2.16	0.46
4:5:46:TYR:OH	4:5:67:HIS:ND1	2.42	0.46
1:B:519:LEU:HD11	1:B:556:VAL:HG13	1.98	0.46
3:D:344:VAL:O	3:D:389:CYS:HB2	2.15	0.46
3:4:304:ARG:HB3	3:4:465:HIS:HB2	1.97	0.46
3:4:647:GLU:HA	3:4:650:GLU:HG2	1.96	0.46
4:5:555:ILE:HG22	4:5:557:LYS:HE3	1.97	0.46
6:7:495:ALA:HB1	6:7:508:LEU:HD11	1.97	0.46
6:G:481:VAL:HG12	6:G:516:ALA:HB2	1.98	0.46
6:G:542:GLU:HG3	6:G:687:ARG:HH21	1.81	0.46
6:G:621:MET:HE3	6:G:622:HIS:CE1	2.50	0.46
3:4:344:VAL:O	3:4:389:CYS:HB2	2.16	0.46
3:4:559:ARG:HE	3:4:559:ARG:HB3	1.57	0.46
3:4:746:PHE:HA	3:4:749:MET:HG2	1.98	0.46
5:6:795:ILE:HG23	5:6:799:GLN:HB2	1.98	0.46
2:C:507:ASN:ND2	6:G:319:SER:O	2.47	0.46
3:D:564:ILE:HG12	3:D:704:LEU:HB2	1.98	0.46
3:D:581:VAL:HA	3:D:584:ILE:HG22	1.96	0.46
6:G:137:ASP:OD1	6:G:138:VAL:N	2.48	0.46
4:5:136:GLN:HG2	4:5:138:ILE:HG13	1.98	0.46
5:6:412:LEU:O	5:6:416:LYS:NZ	2.40	0.46
5:6:842:ASP:N	5:6:842:ASP:OD1	2.45	0.46
2:C:280:ASP:OD1	2:C:281:ASP:N	2.49	0.46
1:2:556:VAL:HB	1:2:605:LEU:HD21	1.97	0.46
2:3:197:ILE:HB	2:3:249:THR:HG23	1.97	0.46
4:5:407:ARG:HB2	4:5:500:GLN:NE2	2.31	0.46
6:7:618:TYR:HB3	6:7:626:PRO:HG3	1.98	0.46
1:B:588:GLU:OE2	4:E:257:LYS:NZ	2.47	0.46
2:C:396:GLY:HA3	6:G:475:LYS:HE2	1.96	0.46
3:D:548:THR:OG1	3:D:806:GLU:OE2	2.27	0.46
5:F:777:TYR:CG	5:F:800:LEU:HD12	2.51	0.46
8:I:693:ILE:O	8:I:697:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:306:TYR:HA	3:4:436:THR:HG21	1.97	0.46
2:C:340:GLN:NE2	2:C:658:LYS:HG3	2.31	0.46
2:3:218:THR:HG21	2:3:277:ILE:HG21	1.98	0.46
3:D:527:ALA:HB3	3:D:537:LYS:HE2	1.97	0.46
4:E:398:LYS:HZ1	4:E:406:LEU:HD22	1.81	0.46
4:E:473:ASP:OD2	4:E:516:ARG:NH2	2.46	0.46
6:G:584:ILE:HD13	6:G:597:LEU:HD21	1.98	0.46
7:H:302:ILE:HA	7:H:305:VAL:HG12	1.98	0.46
1:2:708:PRO:HD3	5:6:557:LYS:HG2	1.98	0.45
3:4:373:ARG:HA	8:I:253:THR:HG21	1.96	0.45
6:7:703:ARG:NH2	6:7:712:ASP:OD2	2.43	0.45
6:G:193:PRO:HD2	6:G:196:LEU:HD12	1.97	0.45
1:2:519:LEU:HD21	1:2:556:VAL:HG13	1.98	0.45
2:C:459:ALA:HB1	2:C:463:VAL:HB	1.98	0.45
7:H:15:ILE:HG13	7:H:19:MET:HE1	1.98	0.45
7:H:43:THR:N	9:H:2001:AGS:O1B	2.47	0.45
3:4:470:SER:HB3	3:4:473:ARG:HG2	1.98	0.45
6:7:257:VAL:HG12	6:7:306:LYS:HB3	1.99	0.45
1:B:476:TRP:HZ3	1:B:768:HIS:HD2	1.64	0.45
5:F:321:VAL:HG11	5:F:330:PRO:HD3	1.97	0.45
7:H:59:LYS:HE3	7:H:59:LYS:HB2	1.81	0.45
4:5:151:LEU:HD11	4:5:162:LEU:HD22	1.98	0.45
5:6:701:MET:HE3	5:6:705:ILE:HG22	1.98	0.45
2:C:117:GLU:HB3	2:C:120:TYR:HD2	1.81	0.45
5:F:177:PHE:HA	5:F:180:PHE:HD2	1.82	0.45
7:H:35:LEU:HA	7:H:50:ALA:HA	1.97	0.45
7:H:80:VAL:O	8:I:663:ASN:ND2	2.49	0.45
5:6:566:ARG:O	5:6:805:ARG:NE	2.47	0.45
5:6:650:VAL:HA	5:6:653:HIS:ND1	2.32	0.45
4:E:498:GLU:CD	4:E:549:ARG:HH11	2.25	0.45
1:2:394:PRO:O	5:6:673:ASN:ND2	2.47	0.45
4:5:452:SER:O	4:5:465:GLU:N	2.48	0.45
5:6:429:THR:HG23	1:B:347:ILE:HD11	1.98	0.45
5:6:535:PRO:HB2	5:6:742:ILE:HD12	1.98	0.45
3:D:265:PRO:HB3	3:D:325:LEU:HG	1.99	0.45
3:D:637:MET:HE3	3:D:641:THR:HG22	1.98	0.45
6:G:537:ILE:HG23	6:G:563:ILE:HD13	1.97	0.45
4:5:599:MET:O	4:5:603:ILE:HG12	2.16	0.45
2:C:533:ILE:HG21	2:C:540:LEU:HD11	1.98	0.45
4:E:423:SER:HA	4:E:426:LEU:HD12	1.98	0.45
5:F:663:ILE:O	5:F:669:HIS:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:383:ARG:HB2	1:2:412:ALA:HB2	1.99	0.45
2:3:687:ARG:NH2	6:7:602:ASP:OD1	2.43	0.45
3:4:714:GLU:OE2	6:7:669:GLN:NE2	2.50	0.45
4:5:161:ARG:HG2	4:5:295:VAL:HG22	1.99	0.45
6:7:142:ILE:HD11	6:7:303:ARG:HG3	1.99	0.45
3:D:846:ASP:HB3	3:D:849:LEU:HB2	1.99	0.45
3:4:433:ILE:HG22	3:4:468:LYS:HG2	1.99	0.45
3:4:530:ILE:HA	9:4:2001:AGS:H2	1.97	0.45
4:5:618:ALA:HB1	4:5:677:VAL:HG21	1.99	0.45
3:D:435:VAL:HG13	3:D:463:VAL:HG13	1.99	0.45
3:D:647:GLU:HA	3:D:650:GLU:HG2	1.98	0.45
4:E:547:LEU:HD23	4:E:646:ILE:HD12	1.98	0.45
5:F:642:ASP:OD2	5:F:642:ASP:N	2.46	0.45
8:I:324:VAL:HG22	8:I:378:PHE:HE1	1.82	0.45
1:2:703:HIS:CE1	5:6:565:LEU:HD22	2.51	0.45
1:2:820:PHE:HA	1:2:823:MET:HE3	1.99	0.45
3:4:701:ARG:NH2	9:6:2001:AGS:S1G	2.90	0.45
9:4:2001:AGS:O2B	9:4:2001:AGS:O2A	2.35	0.45
4:5:342:ILE:HD11	4:5:473:ASP:HB3	1.99	0.45
4:5:506:LYS:HB2	4:5:509:ILE:HG22	1.99	0.45
6:7:67:LEU:HD21	6:7:121:ILE:HG23	2.00	0.45
4:E:625:ASN:C	4:E:625:ASN:HD22	2.25	0.45
5:F:403:VAL:HG22	5:F:450:TYR:HB3	1.98	0.45
6:G:113:PHE:HA	6:G:116:LEU:HB2	1.98	0.45
7:H:181:VAL:HG22	7:H:182:ASP:H	1.82	0.45
1:2:676:ARG:HD2	1:2:808:ARG:HH12	1.82	0.44
3:4:794:THR:HG22	3:4:796:ARG:H	1.82	0.44
1:B:790:TYR:CZ	1:B:794:ARG:HD2	2.53	0.44
4:E:618:ALA:HB1	4:E:677:VAL:HG21	1.98	0.44
4:5:282:LEU:HD13	4:5:330:ILE:HG22	1.99	0.44
5:F:773:LEU:HD13	5:F:824:ILE:HD12	1.99	0.44
8:I:327:TYR:HE1	8:I:375:THR:HG22	1.82	0.44
6:7:5:LEU:HD12	6:7:5:LEU:HA	1.88	0.44
6:7:258:ILE:O	6:7:270:PHE:HA	2.17	0.44
6:7:527:ASP:OD1	6:7:527:ASP:N	2.50	0.44
2:C:197:ILE:HB	2:C:249:THR:HG23	1.99	0.44
5:F:517:LYS:HA	5:F:520:VAL:HG22	1.99	0.44
6:G:497:VAL:HG12	6:G:506:MET:HE3	2.00	0.44
7:H:127:GLU:OE1	7:H:129:ARG:NH1	2.51	0.44
7:H:388:GLU:OE2	8:I:373:ASP:HB3	2.17	0.44
7:H:401:GLN:HB3	7:H:436:TRP:HH2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:526:TYR:O	5:6:530:VAL:HG23	2.17	0.44
3:D:775:VAL:HG12	3:D:779:LYS:NZ	2.33	0.44
1:2:374:ARG:NE	5:F:431:GLU:OE2	2.51	0.44
1:2:610:ASP:OD1	1:2:611:LYS:N	2.51	0.44
6:7:143:LEU:HG	6:7:197:THR:HA	1.99	0.44
6:7:537:ILE:HG23	6:7:563:ILE:HD13	1.99	0.44
1:2:474:PHE:HE1	1:2:764:MET:HE2	1.82	0.44
1:2:537:ILE:HG23	1:2:678:ASP:HB2	1.99	0.44
2:3:295:VAL:HB	2:3:325:THR:HB	1.99	0.44
4:5:266:PRO:HG2	4:5:269:GLU:HB2	1.99	0.44
5:6:608:LEU:HD13	5:6:627:ALA:HB3	1.99	0.44
6:7:423:TYR:HB2	6:7:615:HIS:CG	2.52	0.44
6:7:537:ILE:HG22	6:7:541:MET:HE2	1.99	0.44
2:C:680:VAL:HG22	6:G:613:ALA:HB1	1.99	0.44
4:E:436:ALA:HA	4:E:476:VAL:O	2.17	0.44
6:G:23:ASP:O	6:G:27:THR:OG1	2.25	0.44
6:G:260:TYR:HB3	6:G:298:LEU:HB3	1.99	0.44
8:I:117:LYS:HG3	8:I:214:LEU:HD11	2.00	0.44
8:I:268:LEU:HB3	8:I:279:ILE:H	1.83	0.44
1:2:795:ARG:HA	1:2:798:ILE:HD12	1.99	0.44
1:B:474:PHE:CE1	1:B:764:MET:HE2	2.53	0.44
6:G:322:VAL:HG21	6:G:328:PRO:HG3	1.99	0.44
2:3:443:THR:HB	2:3:495:VAL:HG11	2.00	0.44
3:4:458:LYS:NZ	3:4:610:ASP:OD1	2.47	0.44
4:5:415:LEU:HA	4:5:523:ALA:O	2.17	0.44
4:E:159:ILE:HG22	4:E:161:ARG:HH11	1.83	0.44
4:E:169:THR:HG22	4:E:256:LEU:HD22	1.98	0.44
4:E:535:SER:O	4:E:539:ASN:ND2	2.49	0.44
1:2:338:LYS:HD2	1:2:379:LYS:HB3	1.99	0.44
1:2:505:ILE:O	1:2:512:LYS:NZ	2.45	0.44
2:3:240:LYS:NZ	4:E:5:ARG:O	2.50	0.44
5:6:574:VAL:O	5:6:714:VAL:HA	2.17	0.44
6:7:59:LYS:HE2	6:7:59:LYS:HB2	1.89	0.44
6:7:596:ILE:HD11	6:7:695:LEU:HD11	2.00	0.44
1:B:445:PRO:HD3	5:F:325:PHE:O	2.18	0.44
2:3:557:ARG:O	2:3:561:ILE:HG12	2.18	0.43
4:5:546:ILE:HD12	4:5:546:ILE:H	1.82	0.43
5:6:105:ASP:O	5:6:109:GLU:HG2	2.18	0.43
1:B:432:ASN:OD1	1:B:447:PHE:HB3	2.18	0.43
2:C:558:ASP:HB3	4:E:627:VAL:HG12	2.00	0.43
5:F:277:ARG:HG2	5:F:375:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:653:HIS:HB3	5:F:705:ILE:HD13	2.00	0.43
8:I:155:PHE:HD2	8:I:162:ILE:HD11	1.82	0.43
1:2:386:GLN:HB2	1:2:415:VAL:HG12	1.99	0.43
1:2:508:HIS:O	1:2:512:LYS:HG3	2.17	0.43
4:5:165:ILE:O	4:5:258:LEU:HD12	2.18	0.43
1:B:484:PHE:HZ	1:B:765:LYS:HB2	1.83	0.43
3:D:456:LEU:HD12	3:D:456:LEU:HA	1.91	0.43
3:D:563:ASN:ND2	3:D:649:MET:SD	2.92	0.43
6:G:454:ILE:O	6:G:562:SER:OG	2.29	0.43
1:2:614:ASP:OD2	4:5:486:ARG:NH2	2.43	0.43
1:2:850:LYS:HE3	1:2:852:SER:HB3	2.00	0.43
2:3:182:VAL:HG11	2:3:274:ILE:HD11	2.00	0.43
3:4:401:GLU:HG2	3:4:403:PRO:HD3	1.99	0.43
4:5:396:SER:O	4:5:398:LYS:NZ	2.49	0.43
4:E:398:LYS:NZ	4:E:406:LEU:HD22	2.33	0.43
5:6:294:VAL:HG21	5:6:389:ALA:HB1	1.99	0.43
2:C:536:PRO:HG2	2:C:539:LEU:HB2	2.00	0.43
3:D:716:ASN:ND2	3:D:853:GLY:O	2.51	0.43
7:H:375:ASP:HA	7:H:378:ASN:HD22	1.83	0.43
2:3:358:ASP:O	2:3:362:ILE:HG13	2.19	0.43
3:4:224:LEU:HD13	3:4:227:ILE:HG13	2.00	0.43
1:B:486:LYS:HA	1:B:489:ARG:HH21	1.83	0.43
1:B:789:VAL:HG23	1:B:864:TYR:CZ	2.53	0.43
6:G:520:ILE:HA	6:G:562:SER:O	2.19	0.43
7:H:23:TYR:HA	7:H:29:ILE:HD11	2.01	0.43
4:5:559:ASP:H	4:5:564:ARG:NH1	2.16	0.43
2:C:198:ARG:HB3	2:C:249:THR:HG22	2.01	0.43
3:D:629:CYS:HB3	3:D:671:ILE:HD13	2.01	0.43
3:D:639:ASP:OD1	3:D:642:ARG:NH2	2.51	0.43
5:F:199:THR:OG1	5:F:261:ARG:NH1	2.51	0.43
6:G:149:ARG:HG3	6:G:153:MET:HE2	1.99	0.43
7:H:302:ILE:HD12	7:H:457:ARG:CZ	2.49	0.43
7:H:399:LEU:HD12	7:H:399:LEU:HA	1.90	0.43
1:2:326:ARG:NH1	1:2:389:THR:OG1	2.51	0.43
2:3:230:ILE:HA	4:E:223:ASN:HD21	1.84	0.43
5:6:525:ILE:HG13	5:6:529:LEU:HD23	2.01	0.43
5:6:144:LYS:HA	5:6:196:LEU:HD11	2.00	0.43
6:7:474:CYS:HB2	6:7:480:GLY:HA3	2.00	0.43
6:G:537:ILE:HG22	6:G:541:MET:HE3	2.00	0.43
1:2:212:LYS:HE3	1:2:274:VAL:HG13	2.01	0.43
3:4:590:TYR:OH	3:4:632:ASP:OD2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:473:ILE:HD13	6:7:473:ILE:HA	1.87	0.43
3:D:432:ARG:O	3:D:473:ARG:NH2	2.52	0.43
4:E:498:GLU:OE2	4:E:651:ARG:NH1	2.52	0.43
6:G:530:ASP:N	6:G:530:ASP:OD1	2.51	0.43
5:6:303:GLU:O	5:6:353:PHE:HA	2.18	0.42
5:6:694:SER:O	5:6:698:ASN:ND2	2.52	0.42
5:6:797:VAL:O	5:6:800:LEU:N	2.51	0.42
6:7:113:PHE:HA	6:7:116:LEU:HB2	2.01	0.42
1:B:562:ARG:NE	1:B:598:LEU:O	2.49	0.42
4:E:622:LEU:HD23	4:E:622:LEU:HA	1.82	0.42
5:F:123:SER:HB3	5:F:134:LYS:HG2	2.01	0.42
1:2:628:SER:OG	1:2:639:THR:OG1	2.37	0.42
4:5:257:LYS:HD2	4:5:273:ASN:ND2	2.34	0.42
4:5:684:PHE:CE2	4:5:689:MET:HE3	2.54	0.42
5:6:431:GLU:OE2	1:B:374:ARG:NE	2.52	0.42
6:7:601:LEU:HD12	6:7:727:LEU:HG	2.00	0.42
2:C:116:VAL:HG12	2:C:117:GLU:HG3	2.01	0.42
5:F:409:GLN:HG2	5:F:412:LEU:HD12	2.01	0.42
6:G:428:VAL:HA	6:G:598:PHE:HE2	1.83	0.42
8:I:126:ILE:HD12	8:I:172:ILE:O	2.19	0.42
8:I:150:LEU:HD13	8:I:153:ARG:HE	1.83	0.42
8:I:300:LYS:NZ	8:I:309:PHE:O	2.45	0.42
1:2:510:ASP:OD2	1:2:511:ILE:N	2.52	0.42
3:4:178:ARG:NH1	8:I:533:ASP:OD1	2.52	0.42
3:4:688:VAL:O	3:4:692:ILE:HG12	2.19	0.42
5:6:298:SER:HB2	5:6:301:ARG:HH12	1.83	0.42
6:7:166:LEU:HD12	4:E:104:LEU:HD12	2.00	0.42
1:B:763:LEU:O	1:B:767:ILE:HG13	2.20	0.42
7:H:163:ASP:O	7:H:168:ASN:ND2	2.51	0.42
7:H:339:LYS:HB3	7:H:343:LYS:HZ3	1.83	0.42
3:4:356:MET:HE3	3:4:382:MET:HE2	2.00	0.42
6:7:520:ILE:HA	6:7:562:SER:O	2.19	0.42
1:B:537:ILE:O	1:B:645:SER:OG	2.36	0.42
1:B:785:LYS:NZ	1:B:831:SER:OG	2.49	0.42
1:2:253:LYS:HB3	1:2:256:LEU:HD13	2.02	0.42
1:2:494:ILE:O	1:2:498:ILE:HG12	2.20	0.42
1:2:849:GLN:HB3	1:2:853:VAL:HB	2.01	0.42
2:3:487:HIS:CE1	6:7:528:LYS:HE3	2.55	0.42
2:C:375:ASP:O	2:C:379:LYS:HG2	2.19	0.42
3:D:694:LEU:HG	3:D:698:LEU:HD23	2.01	0.42
4:E:261:ILE:HG22	4:E:263:GLU:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:182:ILE:HA	8:I:185:LEU:HD12	2.01	0.42
1:2:195:SER:O	1:2:199:THR:OG1	2.30	0.42
1:B:336:TYR:HB2	1:B:381:VAL:HB	2.01	0.42
2:C:390:GLU:CD	2:C:467:ARG:HH12	2.28	0.42
2:C:566:LEU:HD23	2:C:566:LEU:HA	1.87	0.42
9:D:2001:AGS:O2A	9:D:2001:AGS:O2B	2.38	0.42
4:E:90:PHE:CE2	4:E:137:LEU:HD13	2.54	0.42
6:G:17:LEU:HD13	6:G:113:PHE:HZ	1.85	0.42
8:I:125:ARG:NH2	8:I:162:ILE:HA	2.35	0.42
2:3:408:VAL:O	2:3:548:VAL:HA	2.19	0.42
4:5:429:VAL:HA	4:5:432:VAL:HG12	2.01	0.42
2:C:528:ASP:N	2:C:528:ASP:OD1	2.53	0.42
7:H:123:TYR:CG	7:H:179:VAL:HG11	2.54	0.42
7:H:359:TRP:NE1	7:H:361:LYS:O	2.52	0.42
2:3:430:ILE:HD12	2:3:465:ALA:HB2	2.01	0.42
3:4:665:LEU:HD13	5:6:373:MET:HE1	2.02	0.42
4:5:90:PHE:CE2	4:5:94:ILE:HD11	2.54	0.42
4:5:498:GLU:OE2	4:5:549:ARG:HG3	2.20	0.42
5:6:354:LEU:HD12	5:6:382:ARG:HH21	1.84	0.42
3:D:292:ASP:N	3:D:292:ASP:OD1	2.48	0.42
3:D:323:ASP:OD1	3:D:440:ARG:NH1	2.51	0.42
4:E:185:ASN:OD1	4:E:185:ASN:N	2.50	0.42
4:E:677:VAL:O	4:E:681:ILE:HG12	2.19	0.42
2:3:535:LEU:HB3	2:3:540:LEU:HD11	2.02	0.42
5:F:144:LYS:HA	5:F:196:LEU:HD21	2.02	0.42
5:F:180:PHE:HA	5:F:183:LYS:HG2	2.00	0.42
5:F:684:PRO:HB3	5:F:698:ASN:HB3	2.01	0.42
6:G:503:THR:HG23	6:G:505:GLU:HG2	2.01	0.42
7:H:66:TRP:NE1	7:H:123:TYR:HD1	2.17	0.42
7:H:76:LYS:NZ	9:H:2001:AGS:S1G	2.91	0.42
7:H:287:PRO:O	7:H:291:MET:HG3	2.20	0.42
7:H:300:ILE:HD12	7:H:300:ILE:H	1.85	0.42
7:H:435:ILE:O	7:H:439:HIS:CB	2.68	0.42
1:2:667:VAL:HG12	1:2:669:LEU:H	1.84	0.42
3:4:234:ARG:HB2	3:4:280:MET:HE1	2.01	0.42
5:6:538:PHE:H	9:6:2001:AGS:H2	1.85	0.42
5:6:642:ASP:OD1	5:6:643:LYS:N	2.53	0.42
1:B:366:ASN:C	1:B:366:ASN:HD22	2.27	0.42
4:E:429:VAL:HA	4:E:432:VAL:HG12	2.01	0.42
2:3:225:ILE:HD11	4:5:182:MET:HE3	2.01	0.41
2:3:459:ALA:HB2	6:7:327:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:538:HIS:CE1	6:7:593:ARG:CZ	3.03	0.41
1:B:485:ARG:O	1:B:488:SER:OG	2.29	0.41
1:B:494:ILE:O	1:B:498:ILE:HG12	2.20	0.41
2:C:331:ALA:HB3	2:C:334:THR:HG21	2.02	0.41
2:C:476:ASP:N	2:C:476:ASP:OD2	2.52	0.41
5:F:274:HIS:ND1	5:F:288:LEU:HD11	2.35	0.41
5:F:615:ASP:OD1	5:F:615:ASP:N	2.52	0.41
1:2:497:ILE:HD13	1:2:823:MET:HB3	2.02	0.41
1:2:793:LEU:HD21	1:2:842:VAL:HG22	2.01	0.41
2:3:538:SER:O	2:3:542:ARG:HG2	2.20	0.41
3:D:435:VAL:HG22	3:D:466:VAL:HG22	2.02	0.41
6:G:435:LEU:HD21	6:G:564:LEU:HB2	2.01	0.41
6:G:722:VAL:HA	6:G:726:SER:HB3	2.02	0.41
3:4:422:GLU:HB3	3:4:493:ASN:HA	2.02	0.41
3:4:650:GLU:HB3	3:4:701:ARG:NH1	2.35	0.41
3:4:824:GLU:OE2	3:4:827:ARG:NH2	2.52	0.41
4:5:397:LYS:HE2	4:5:405:ARG:HH21	1.85	0.41
5:6:612:VAL:HB	5:6:665:LYS:HD2	2.01	0.41
1:B:508:HIS:HB3	1:B:511:ILE:HG12	2.02	0.41
2:C:23:ASP:OD1	2:C:26:ARG:NH2	2.53	0.41
2:C:561:ILE:HG21	4:E:650:ILE:HG12	2.02	0.41
7:H:290:LEU:HD23	7:H:329:LEU:HD22	2.01	0.41
7:H:371:GLU:H	7:H:371:GLU:CD	2.29	0.41
8:I:125:ARG:NH1	8:I:163:THR:HG23	2.35	0.41
4:5:91:GLU:HG3	4:5:135:PHE:O	2.20	0.41
4:5:183:CYS:HB3	4:5:188:HIS:H	1.85	0.41
6:7:63:TYR:O	6:7:67:LEU:HD13	2.20	0.41
6:7:130:LYS:HB3	6:7:130:LYS:HE3	1.85	0.41
6:7:275:SER:OG	6:7:277:THR:O	2.36	0.41
1:B:434:TYR:HE1	5:F:346:LEU:HD23	1.85	0.41
3:D:203:TYR:CE2	3:D:207:LYS:HE3	2.55	0.41
7:H:26:LEU:HA	7:H:27:PRO:HD3	1.96	0.41
8:I:265:HIS:HA	8:I:282:GLU:HA	2.02	0.41
3:4:767:LYS:HD2	5:6:736:MET:HE1	2.00	0.41
5:6:528:LYS:HD2	5:6:745:PRO:HB3	2.01	0.41
1:B:687:VAL:HG11	5:F:785:ALA:HB2	2.02	0.41
4:E:422:LYS:HB2	4:E:422:LYS:HE2	1.92	0.41
4:E:564:ARG:O	4:E:567:SER:OG	2.34	0.41
1:2:438:LEU:HD13	1:2:445:PRO:HA	2.02	0.41
2:3:198:ARG:HB3	2:3:249:THR:HG22	2.03	0.41
4:E:183:CYS:HB3	4:E:188:HIS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:203:ALA:O	2:3:207:GLY:CA	2.68	0.41
3:4:445:ARG:HH21	3:4:450:GLN:C	2.29	0.41
5:6:653:HIS:O	5:6:657:GLU:HG2	2.20	0.41
8:I:330:ASP:O	8:I:334:LYS:HD2	2.21	0.41
12:3:2001:ADP:C4	4:5:650:ILE:HD13	2.56	0.41
2:C:569:HIS:HA	4:E:398:LYS:HE2	2.02	0.41
4:E:370:LEU:HD23	4:E:370:LEU:HA	1.90	0.41
5:F:521:LYS:HA	5:F:521:LYS:HD2	1.89	0.41
5:F:832:ARG:HH22	5:F:833:GLN:HE22	1.68	0.41
1:2:511:ILE:O	1:2:515:VAL:HG23	2.21	0.41
2:3:369:PRO:HB3	2:3:650:LEU:HD11	2.03	0.41
2:3:507:ASN:ND2	6:7:319:SER:O	2.48	0.41
3:4:325:LEU:HD23	3:4:325:LEU:HA	1.97	0.41
3:4:429:ALA:O	3:4:587:ARG:NH2	2.46	0.41
3:4:517:ASP:OD1	3:4:517:ASP:N	2.51	0.41
4:5:31:PHE:CG	4:5:90:PHE:HD1	2.39	0.41
4:5:381:ASN:HB3	4:5:384:ILE:HD12	2.03	0.41
5:6:694:SER:OG	5:6:792:SER:O	2.34	0.41
6:7:204:PHE:H	6:7:379:GLN:HB3	1.86	0.41
6:7:425:ASN:HB3	6:7:428:VAL:HB	2.03	0.41
1:B:318:VAL:O	1:B:427:THR:HA	2.20	0.41
1:B:505:ILE:O	1:B:512:LYS:NZ	2.44	0.41
2:C:21:PHE:HE1	2:C:127:LYS:HD3	1.86	0.41
2:C:571:TYR:HB2	2:C:642:TYR:CZ	2.56	0.41
2:C:701:THR:HG23	2:C:733:LEU:HD21	2.03	0.41
2:C:712:HIS:ND1	2:C:725:ASP:OD1	2.43	0.41
3:D:530:ILE:HA	9:D:2001:AGS:H2	2.03	0.41
3:D:637:MET:HG2	3:D:642:ARG:HG3	2.03	0.41
3:D:645:LEU:O	3:D:649:MET:HG2	2.21	0.41
5:F:749:GLU:OE1	5:F:753:ARG:NH2	2.52	0.41
6:G:439:GLY:O	6:G:701:LYS:NZ	2.46	0.41
6:G:526:PHE:HE2	6:G:590:LEU:HD21	1.84	0.41
8:I:190:ILE:HG13	8:I:191:LEU:HD22	2.03	0.41
8:I:327:TYR:CE2	8:I:331:LYS:HE3	2.56	0.41
2:3:457:LEU:HD11	2:3:504:THR:HG21	2.03	0.41
6:7:432:LEU:HB3	6:7:473:ILE:HD11	2.03	0.41
2:C:212:ARG:HD2	2:C:232:PRO:HD3	2.02	0.41
3:D:642:ARG:HH11	3:D:698:LEU:HD22	1.86	0.41
4:E:53:ASN:HB3	4:E:58:ASN:O	2.21	0.41
2:3:393:LEU:HD13	6:7:421:GLU:HG2	2.03	0.40
3:4:434:GLU:HG3	3:4:467:LYS:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:798:LEU:HA	3:4:801:MET:HE2	2.03	0.40
4:5:400:LEU:HD12	4:5:404:MET:SD	2.61	0.40
6:7:184:VAL:HB	4:E:103:ILE:HG21	2.03	0.40
6:7:228:ARG:O	6:7:231:LYS:NZ	2.54	0.40
4:E:175:ARG:NH1	4:E:197:PHE:O	2.54	0.40
4:E:684:PHE:CE2	4:E:689:MET:HE3	2.56	0.40
5:F:816:VAL:HG21	5:F:823:PHE:HE2	1.86	0.40
3:4:508:LYS:HA	3:4:511:GLU:HG3	2.03	0.40
6:7:575:ASN:HA	6:7:576:PRO:HD3	1.96	0.40
1:B:271:PHE:CD2	1:B:295:VAL:HG21	2.54	0.40
5:F:189:VAL:HG13	5:F:197:LEU:HD11	2.02	0.40
7:H:365:TYR:HB3	7:H:371:GLU:OE2	2.22	0.40
1:2:215:LEU:HD12	1:2:215:LEU:HA	1.96	0.40
3:4:277:LYS:NZ	3:4:299:LYS:O	2.39	0.40
3:4:557:ARG:NH1	3:4:666:ASN:OD1	2.48	0.40
5:6:649:GLN:HA	5:6:652:ILE:HG22	2.03	0.40
1:B:376:ASN:O	1:B:380:THR:OG1	2.27	0.40
2:C:150:ARG:HD3	2:C:150:ARG:HA	1.92	0.40
2:3:454:GLU:OE1	6:7:314:LYS:NZ	2.54	0.40
4:5:33:ASN:O	4:5:37:GLU:HB2	2.21	0.40
5:6:399:GLY:HA3	5:6:456:ALA:HA	2.04	0.40
5:6:699:LEU:HD13	5:6:701:MET:SD	2.62	0.40
2:C:103:LEU:HD11	2:C:110:PHE:HD2	1.85	0.40
3:D:332:VAL:HG12	3:D:429:ALA:HA	2.04	0.40
4:E:90:PHE:CE2	4:E:94:ILE:HD11	2.56	0.40
4:E:449:LEU:HD12	4:E:468:ALA:HB3	2.03	0.40
5:F:309:PHE:CD2	5:F:330:PRO:HD2	2.57	0.40
8:I:327:TYR:CE1	8:I:375:THR:HG22	2.57	0.40
3:4:354:HIS:CE1	8:I:249:ARG:HB2	2.57	0.40
9:5:2001:AGS:S1G	9:5:2001:AGS:O2B	2.79	0.40
6:7:22:THR:O	6:7:26:VAL:HG23	2.21	0.40
1:B:447:PHE:HB2	5:F:302:PRO:HG2	2.03	0.40
1:B:849:GLN:HB2	1:B:854:ARG:HG3	2.03	0.40
6:G:661:VAL:O	6:G:665:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	622/868 (72%)	605 (97%)	17 (3%)	0	100	100
1	B	622/868 (72%)	608 (98%)	14 (2%)	0	100	100
2	3	627/971 (65%)	611 (97%)	16 (3%)	0	100	100
2	C	627/971 (65%)	609 (97%)	17 (3%)	1 (0%)	43	72
3	4	664/933 (71%)	647 (97%)	17 (3%)	0	100	100
3	D	664/933 (71%)	648 (98%)	16 (2%)	0	100	100
4	5	651/775 (84%)	632 (97%)	19 (3%)	0	100	100
4	E	651/775 (84%)	632 (97%)	19 (3%)	0	100	100
5	6	638/1017 (63%)	619 (97%)	19 (3%)	0	100	100
5	F	638/1017 (63%)	623 (98%)	15 (2%)	0	100	100
6	7	693/845 (82%)	678 (98%)	15 (2%)	0	100	100
6	G	693/845 (82%)	681 (98%)	12 (2%)	0	100	100
7	H	375/507 (74%)	351 (94%)	22 (6%)	2 (0%)	24	54
8	I	318/704 (45%)	311 (98%)	6 (2%)	1 (0%)	36	65
All	All	8483/12029 (70%)	8255 (97%)	224 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	62	ALA
7	H	53	ILE
8	I	301	ILE
2	C	648	PRO

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%)	549 (100%)	1 (0%)	87	96
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%)	586 (100%)	2 (0%)	86	96
4	E	588/688 (86%)	587 (100%)	1 (0%)	87	96
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%)	617 (100%)	1 (0%)	87	96
7	H	334/454 (74%)	334 (100%)	0	100	100
8	I	303/639 (47%)	303 (100%)	0	100	100
All	All	7595/10653 (71%)	7590 (100%)	5 (0%)	87	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	5	253	GLN
4	5	339	THR
2	C	487	HIS
4	E	339	THR
6	G	575	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	200	GLN
1	2	528	ASN
1	2	666	ASN
2	3	175	HIS
2	3	259	GLN

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Mol	Chain	Res	Type
2	3	307	ASN
2	3	376	HIS
2	3	417	GLN
2	3	424	ASN
2	3	492	GLN
2	3	517	ASN
2	3	673	GLN
2	3	682	ASN
2	3	722	ASN
3	4	229	GLN
3	4	259	HIS
3	4	350	ASN
3	4	447	ASN
3	4	450	GLN
3	4	582	HIS
4	5	195	ASN
4	5	253	GLN
4	5	363	ASN
4	5	454	GLN
4	5	499	GLN
4	5	584	GLN
4	5	625	ASN
5	6	182	GLN
5	6	340	ASN
5	6	550	GLN
5	6	556	HIS
5	6	814	ASN
6	7	9	GLN
6	7	178	ASN
6	7	538	HIS
6	7	543	GLN
6	7	620	HIS
6	7	669	GLN
1	B	238	ASN
1	B	760	GLN
2	C	175	HIS
2	C	340	GLN
2	C	351	ASN
2	C	376	HIS
2	C	522	GLN
3	D	274	GLN
3	D	350	ASN

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Mol	Chain	Res	Type
3	D	410	GLN
3	D	716	ASN
4	E	43	GLN
4	E	454	GLN
4	E	571	HIS
5	F	125	GLN
5	F	156	GLN
5	F	182	GLN
5	F	269	ASN
5	F	362	GLN
5	F	550	GLN
5	F	833	GLN
6	G	9	GLN
6	G	19	ASN
6	G	68	GLN
6	G	111	ASN
6	G	264	GLN
6	G	336	ASN
6	G	425	ASN
7	H	115	GLN
7	H	268	ASN
7	H	378	ASN
7	H	400	GLN
7	H	439	HIS
7	H	448	GLN
8	I	197	ASN
8	I	239	HIS
8	I	657	ASN

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 36 ligands modelled in this entry, 23 are monoatomic - leaving 13 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
9	AGS	2	2001	10	32,33,33	0.48	1 (3%)	45,52,52	0.61	1 (2%)
9	AGS	D	2001	10	32,33,33	0.48	1 (3%)	45,52,52	0.66	1 (2%)
9	AGS	6	2001	10	32,33,33	0.47	1 (3%)	45,52,52	0.65	1 (2%)
9	AGS	7	2001	10	32,33,33	0.56	1 (3%)	45,52,52	0.60	1 (2%)
9	AGS	F	2001	10	32,33,33	0.47	1 (3%)	45,52,52	0.65	1 (2%)
9	AGS	4	2001	10	32,33,33	0.48	1 (3%)	45,52,52	0.68	1 (2%)
9	AGS	H	2001	-	32,33,33	0.46	1 (3%)	45,52,52	0.63	1 (2%)
9	AGS	5	2001	10	32,33,33	0.66	2 (6%)	45,52,52	0.75	1 (2%)
9	AGS	G	2001	10	32,33,33	0.49	1 (3%)	45,52,52	0.62	1 (2%)
12	ADP	3	2001	10	28,29,29	1.39	4 (14%)	43,45,45	1.80	9 (20%)
12	ADP	C	2001	10	28,29,29	1.40	4 (14%)	43,45,45	1.80	9 (20%)
9	AGS	B	2001	10	32,33,33	0.53	1 (3%)	45,52,52	0.66	1 (2%)
9	AGS	E	2001	10	32,33,33	0.53	1 (3%)	45,52,52	0.66	1 (2%)

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
9	AGS	2	2001	10	-	6/21/38/38	0/3/3/3
9	AGS	D	2001	10	-	8/21/38/38	0/3/3/3
9	AGS	6	2001	10	-	3/21/38/38	0/3/3/3
9	AGS	7	2001	10	-	4/21/38/38	0/3/3/3
9	AGS	F	2001	10	-	4/21/38/38	0/3/3/3
9	AGS	4	2001	10	-	5/21/38/38	0/3/3/3
9	AGS	H	2001	-	-	5/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	AGS	5	2001	10	-	4/21/38/38	0/3/3/3
9	AGS	G	2001	10	-	5/21/38/38	0/3/3/3
12	ADP	3	2001	10	-	2/16/32/32	0/3/3/3
12	ADP	C	2001	10	-	2/16/32/32	0/3/3/3
9	AGS	B	2001	10	-	6/21/38/38	0/3/3/3
9	AGS	E	2001	10	-	6/21/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	2001	ADP	C5-C4	4.59	1.47	1.39
12	3	2001	ADP	C5-C4	4.55	1.47	1.39
12	C	2001	ADP	C5-C6	2.63	1.48	1.41
12	3	2001	ADP	C5-C6	2.62	1.48	1.41
12	C	2001	ADP	C5-N7	-2.44	1.34	1.39
12	3	2001	ADP	C5-N7	-2.39	1.34	1.39
12	3	2001	ADP	C8-N7	2.27	1.36	1.31
12	C	2001	ADP	C8-N7	2.21	1.35	1.31
9	5	2001	AGS	PA-O3A	-2.19	1.57	1.59
9	5	2001	AGS	PG-S1G	2.17	1.95	1.90
9	7	2001	AGS	PG-S1G	2.14	1.95	1.90
9	D	2001	AGS	PG-S1G	2.12	1.95	1.90
9	H	2001	AGS	PG-S1G	2.12	1.95	1.90
9	B	2001	AGS	PG-S1G	2.11	1.95	1.90
9	G	2001	AGS	PG-S1G	2.11	1.95	1.90
9	4	2001	AGS	PG-S1G	2.11	1.95	1.90
9	2	2001	AGS	PG-S1G	2.10	1.95	1.90
9	E	2001	AGS	PG-S1G	2.08	1.95	1.90
9	6	2001	AGS	PG-S1G	2.07	1.95	1.90
9	F	2001	AGS	PG-S1G	2.06	1.95	1.90

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	3	2001	ADP	C5-C4-N3	-5.76	118.78	126.72
12	C	2001	ADP	C5-C4-N3	-5.66	118.93	126.72
12	C	2001	ADP	N3-C4-N9	4.54	134.89	127.17
12	3	2001	ADP	N3-C4-N9	4.44	134.72	127.17
9	5	2001	AGS	PB-O3B-PG	-3.90	118.90	133.17
9	4	2001	AGS	PB-O3B-PG	-3.83	119.15	133.17
12	3	2001	ADP	C2-N3-C4	3.73	120.95	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	2001	AGS	PB-O3B-PG	-3.61	119.97	133.17
12	C	2001	ADP	C2-N3-C4	3.60	120.62	111.83
9	B	2001	AGS	PB-O3B-PG	-3.60	120.00	133.17
9	E	2001	AGS	PB-O3B-PG	-3.55	120.16	133.17
12	3	2001	ADP	C4-C5-N7	-3.46	106.62	110.58
9	H	2001	AGS	PB-O3B-PG	-3.36	120.86	133.17
12	C	2001	ADP	C4-C5-N7	-3.36	106.75	110.58
12	3	2001	ADP	N3-C2-N1	-3.34	123.52	128.58
9	F	2001	AGS	PB-O3B-PG	-3.34	120.93	133.17
9	6	2001	AGS	PB-O3B-PG	-3.33	120.99	133.17
9	G	2001	AGS	PB-O3B-PG	-3.27	121.19	133.17
9	2	2001	AGS	PB-O3B-PG	-3.20	121.44	133.17
12	C	2001	ADP	N3-C2-N1	-3.17	123.78	128.58
9	7	2001	AGS	PB-O3B-PG	-3.13	121.72	133.17
12	C	2001	ADP	C4-N9-C8	2.71	108.58	105.74
12	C	2001	ADP	C5-N7-C8	2.48	107.34	103.45
12	3	2001	ADP	C5-N7-C8	2.44	107.29	103.45
12	3	2001	ADP	C3'-C2'-C1'	2.34	105.89	101.46
12	3	2001	ADP	C4-N9-C8	2.34	108.19	105.74
12	C	2001	ADP	C3'-C2'-C1'	2.33	105.87	101.46
12	3	2001	ADP	C6-C5-N7	2.11	136.15	132.09
12	C	2001	ADP	C6-C5-N7	2.04	136.01	132.09

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	2	2001	AGS	C5'-O5'-PA-O1A
9	2	2001	AGS	C5'-O5'-PA-O2A
9	4	2001	AGS	C5'-O5'-PA-O2A
9	5	2001	AGS	C5'-O5'-PA-O2A
9	5	2001	AGS	C5'-O5'-PA-O3A
9	6	2001	AGS	PB-O3B-PG-O2G
9	7	2001	AGS	C5'-O5'-PA-O2A
9	7	2001	AGS	C5'-O5'-PA-O3A
9	B	2001	AGS	PB-O3B-PG-O2G
9	B	2001	AGS	PB-O3B-PG-O3G
9	B	2001	AGS	C5'-O5'-PA-O2A
9	D	2001	AGS	PB-O3B-PG-O2G
9	D	2001	AGS	PB-O3B-PG-O3G
9	D	2001	AGS	C5'-O5'-PA-O2A
9	E	2001	AGS	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
9	E	2001	AGS	C5'-O5'-PA-O3A
9	F	2001	AGS	PB-O3B-PG-O2G
9	F	2001	AGS	C5'-O5'-PA-O3A
9	G	2001	AGS	C5'-O5'-PA-O2A
9	G	2001	AGS	C5'-O5'-PA-O3A
9	H	2001	AGS	C5'-O5'-PA-O3A
12	C	2001	ADP	O4'-C4'-C5'-O5'
9	E	2001	AGS	O4'-C4'-C5'-O5'
12	C	2001	ADP	C3'-C4'-C5'-O5'
9	4	2001	AGS	O4'-C4'-C5'-O5'
9	D	2001	AGS	O4'-C4'-C5'-O5'
9	D	2001	AGS	C3'-C4'-C5'-O5'
9	E	2001	AGS	C3'-C4'-C5'-O5'
12	3	2001	ADP	O4'-C4'-C5'-O5'
12	3	2001	ADP	C3'-C4'-C5'-O5'
9	2	2001	AGS	O4'-C4'-C5'-O5'
9	4	2001	AGS	C3'-C4'-C5'-O5'
9	F	2001	AGS	O4'-C4'-C5'-O5'
9	G	2001	AGS	O4'-C4'-C5'-O5'
9	B	2001	AGS	PA-O3A-PB-O1B
9	2	2001	AGS	C5'-O5'-PA-O3A
9	4	2001	AGS	C5'-O5'-PA-O1A
9	4	2001	AGS	C5'-O5'-PA-O3A
9	5	2001	AGS	C5'-O5'-PA-O1A
9	7	2001	AGS	C5'-O5'-PA-O1A
9	B	2001	AGS	C5'-O5'-PA-O1A
9	B	2001	AGS	C5'-O5'-PA-O3A
9	D	2001	AGS	C5'-O5'-PA-O1A
9	D	2001	AGS	C5'-O5'-PA-O3A
9	E	2001	AGS	C5'-O5'-PA-O1A
9	F	2001	AGS	C5'-O5'-PA-O2A
9	H	2001	AGS	C5'-O5'-PA-O1A
9	E	2001	AGS	PG-O3B-PB-O2B
9	G	2001	AGS	PA-O3A-PB-O2B
9	H	2001	AGS	PA-O3A-PB-O2B
9	5	2001	AGS	PG-O3B-PB-O2B
9	H	2001	AGS	PG-O3B-PB-O2B
9	6	2001	AGS	PB-O3B-PG-O3G
9	D	2001	AGS	C4'-C5'-O5'-PA
9	2	2001	AGS	PA-O3A-PB-O1B
9	G	2001	AGS	PA-O3A-PB-O1B
9	6	2001	AGS	O4'-C4'-C5'-O5'

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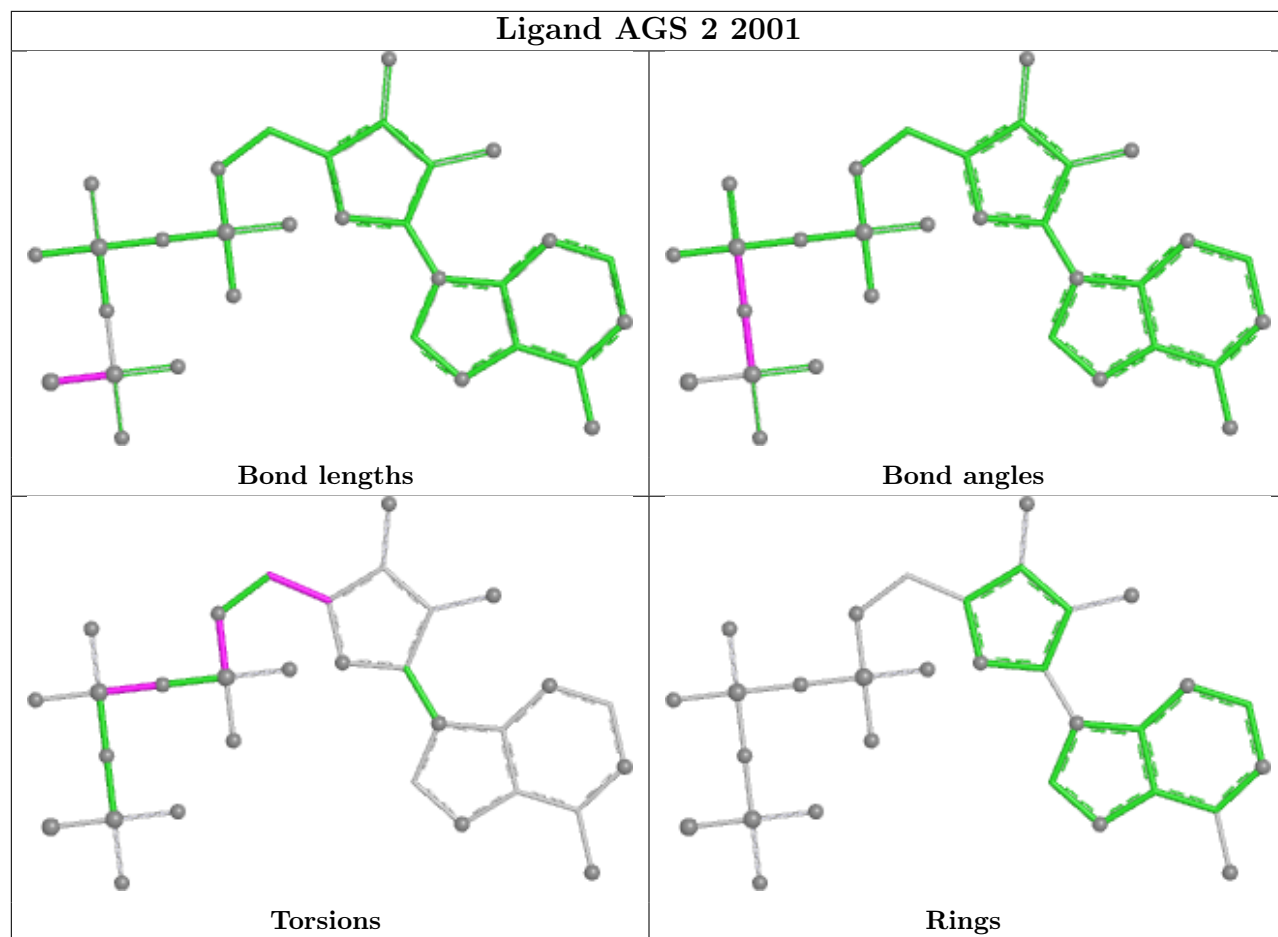
Mol	Chain	Res	Type	Atoms
9	2	2001	AGS	PA-O3A-PB-O2B
9	H	2001	AGS	PA-O3A-PB-O1B
9	7	2001	AGS	O4'-C4'-C5'-O5'

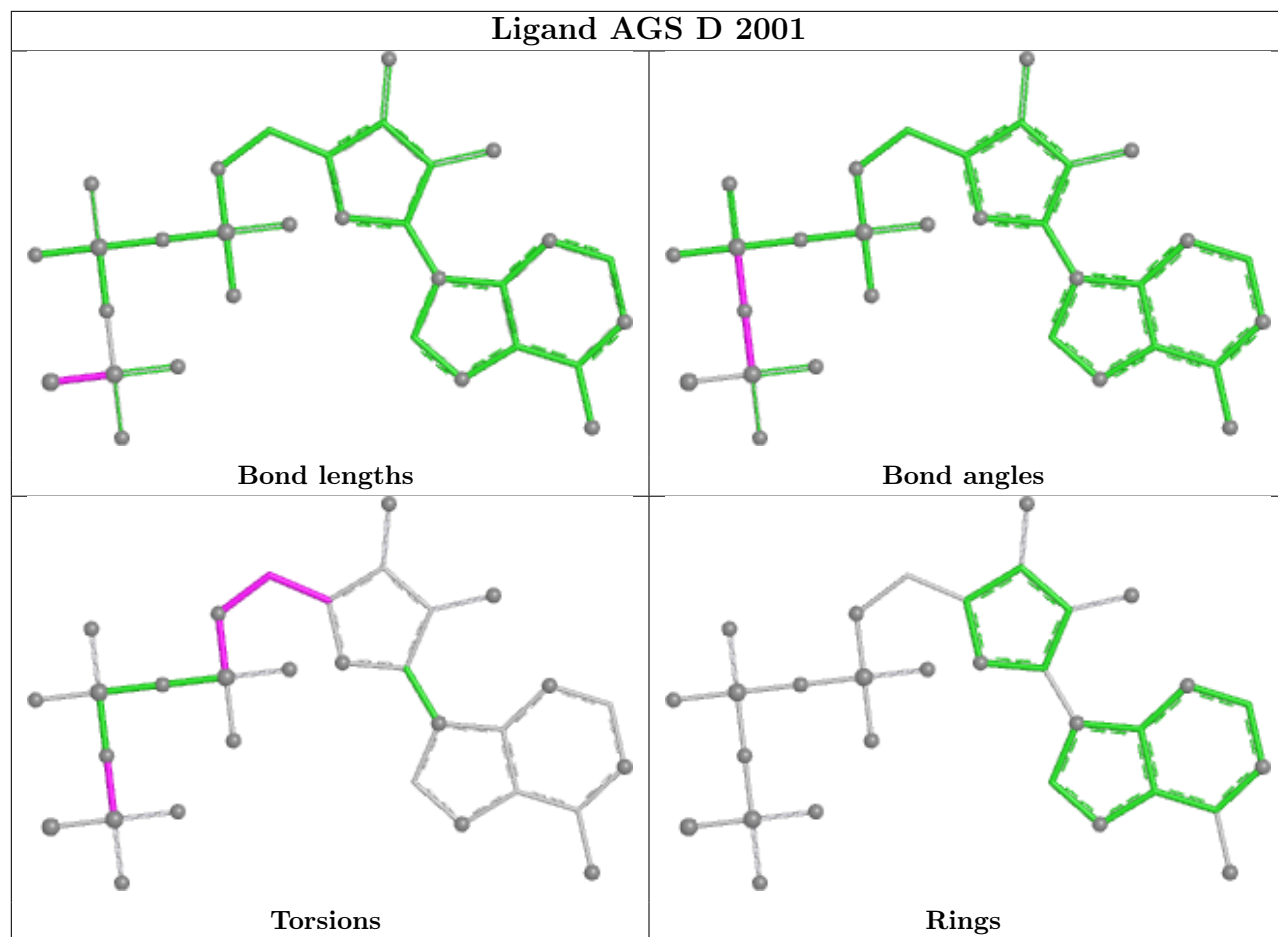
There are no ring outliers.

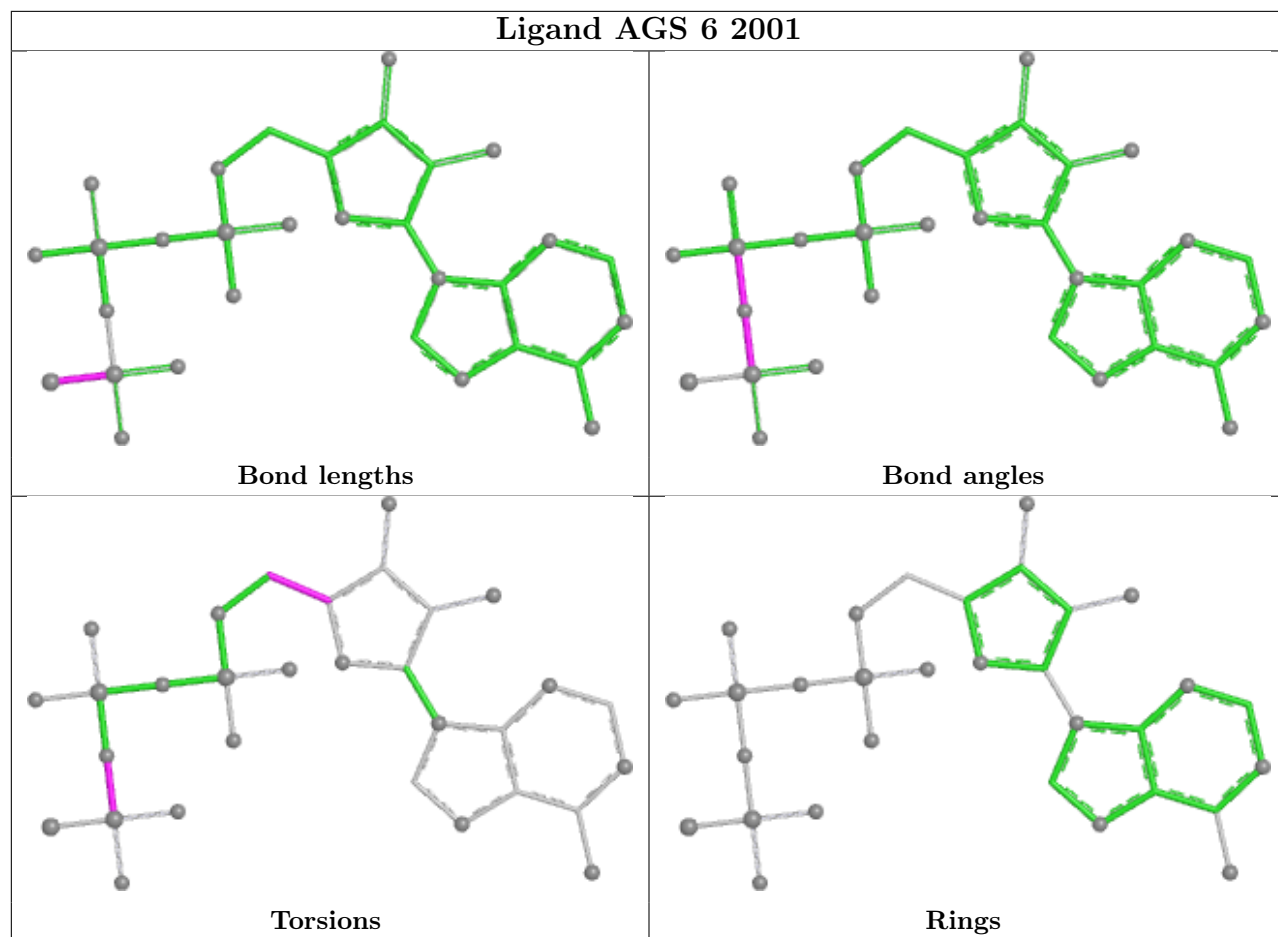
10 monomers are involved in 20 short contacts:

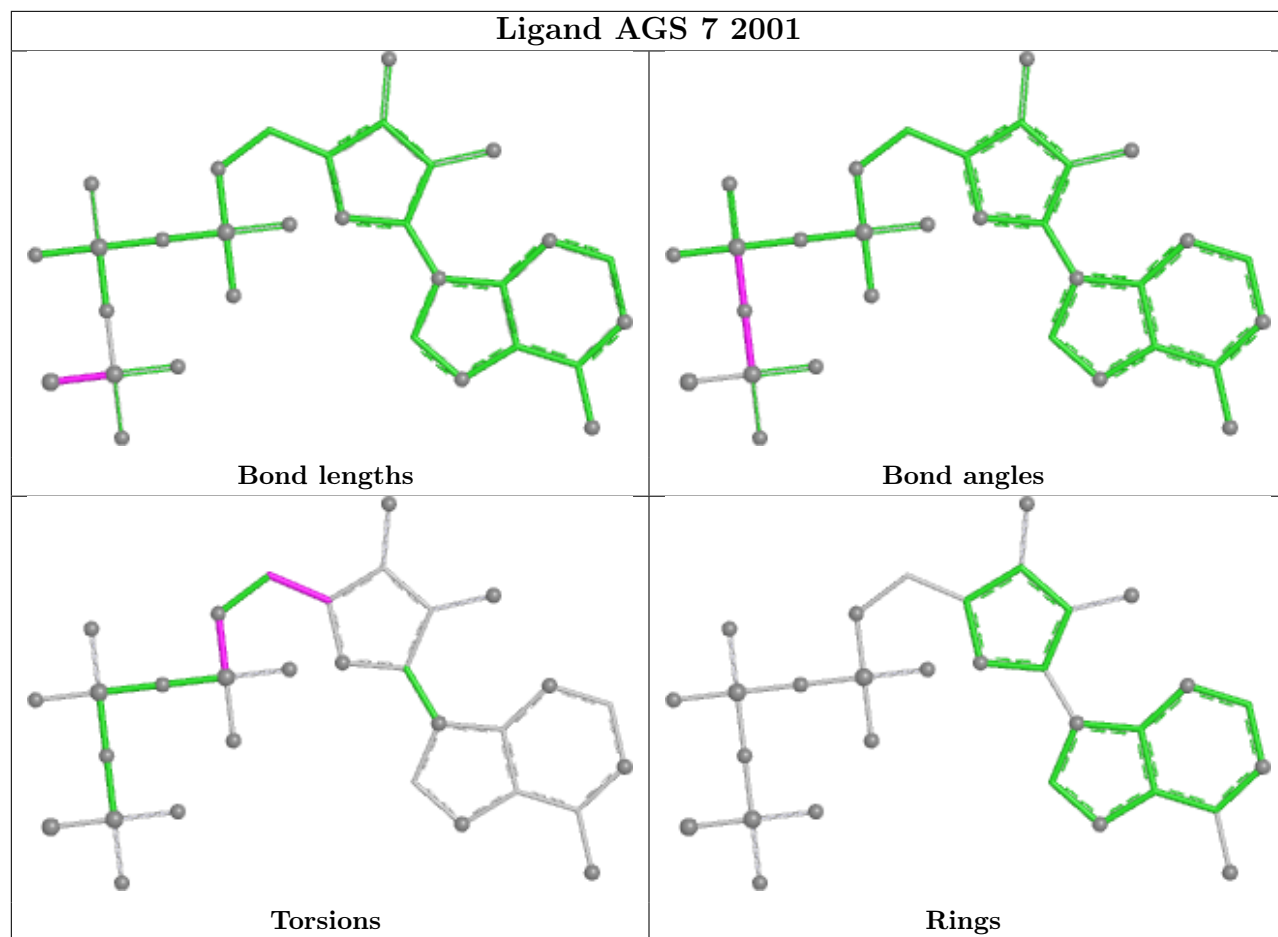
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	2001	AGS	4	0
9	6	2001	AGS	2	0
9	7	2001	AGS	1	0
9	F	2001	AGS	1	0
9	4	2001	AGS	2	0
9	H	2001	AGS	6	0
9	5	2001	AGS	1	0
9	G	2001	AGS	1	0
12	3	2001	ADP	1	0
9	E	2001	AGS	1	0

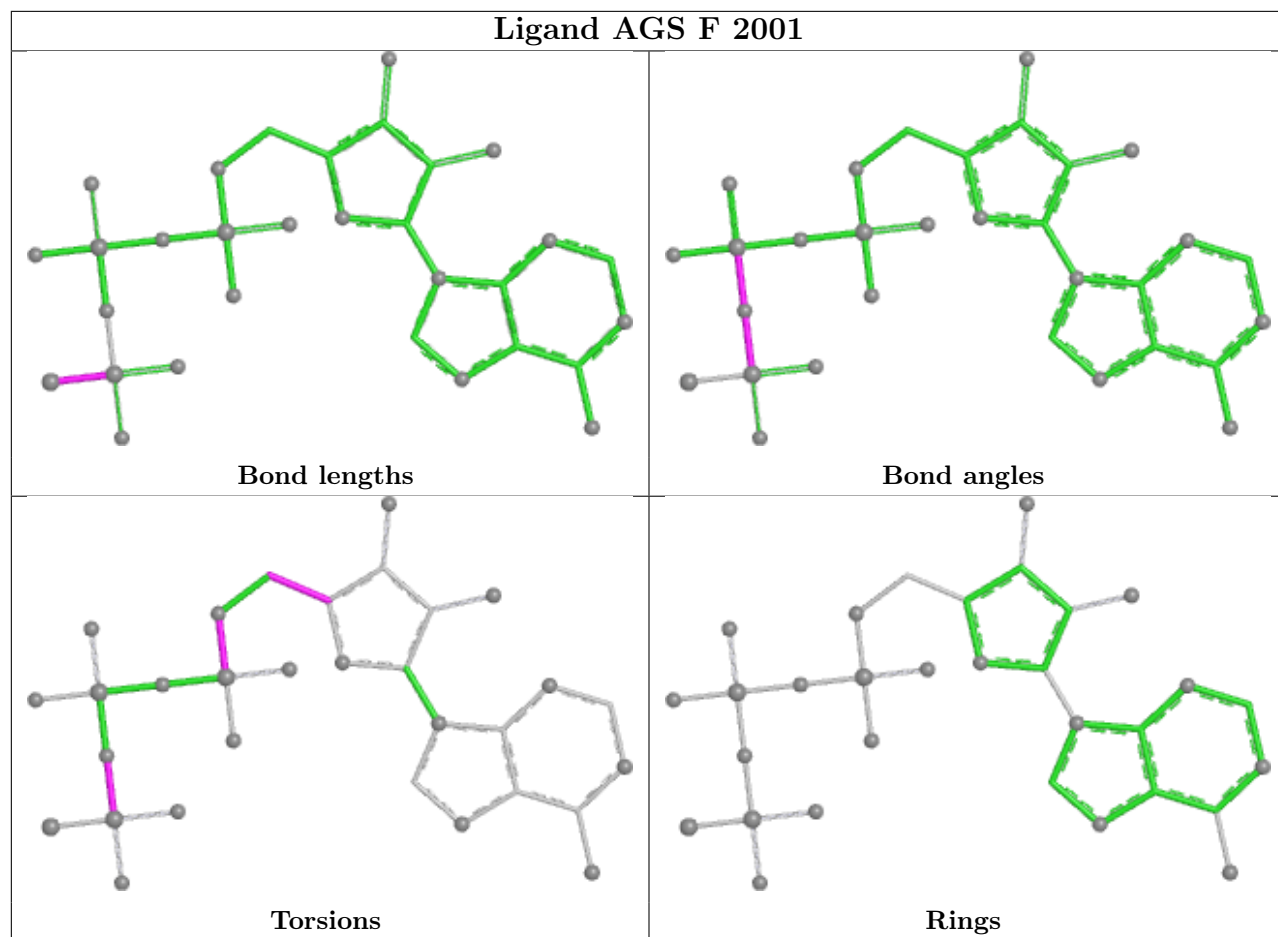
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

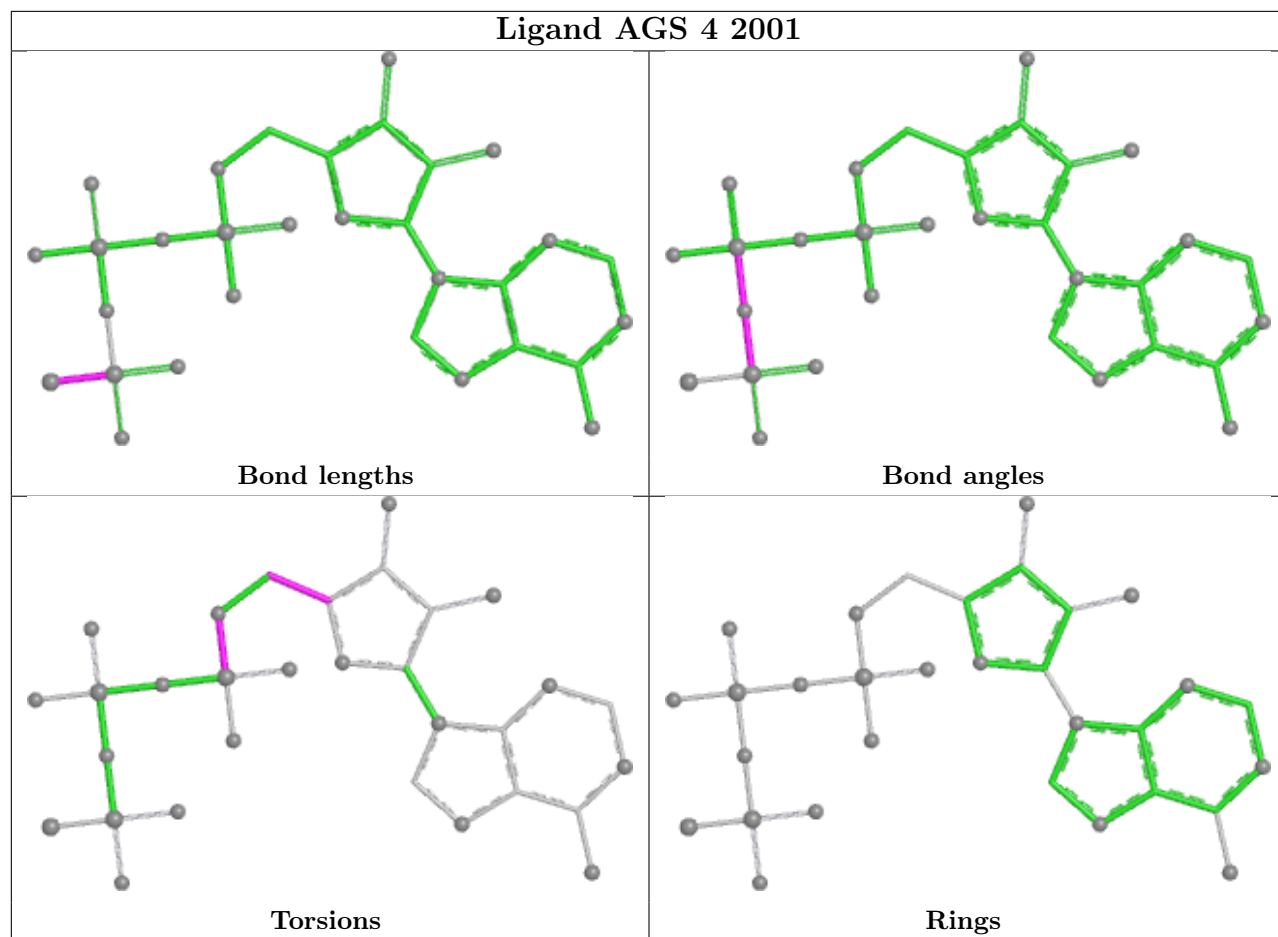


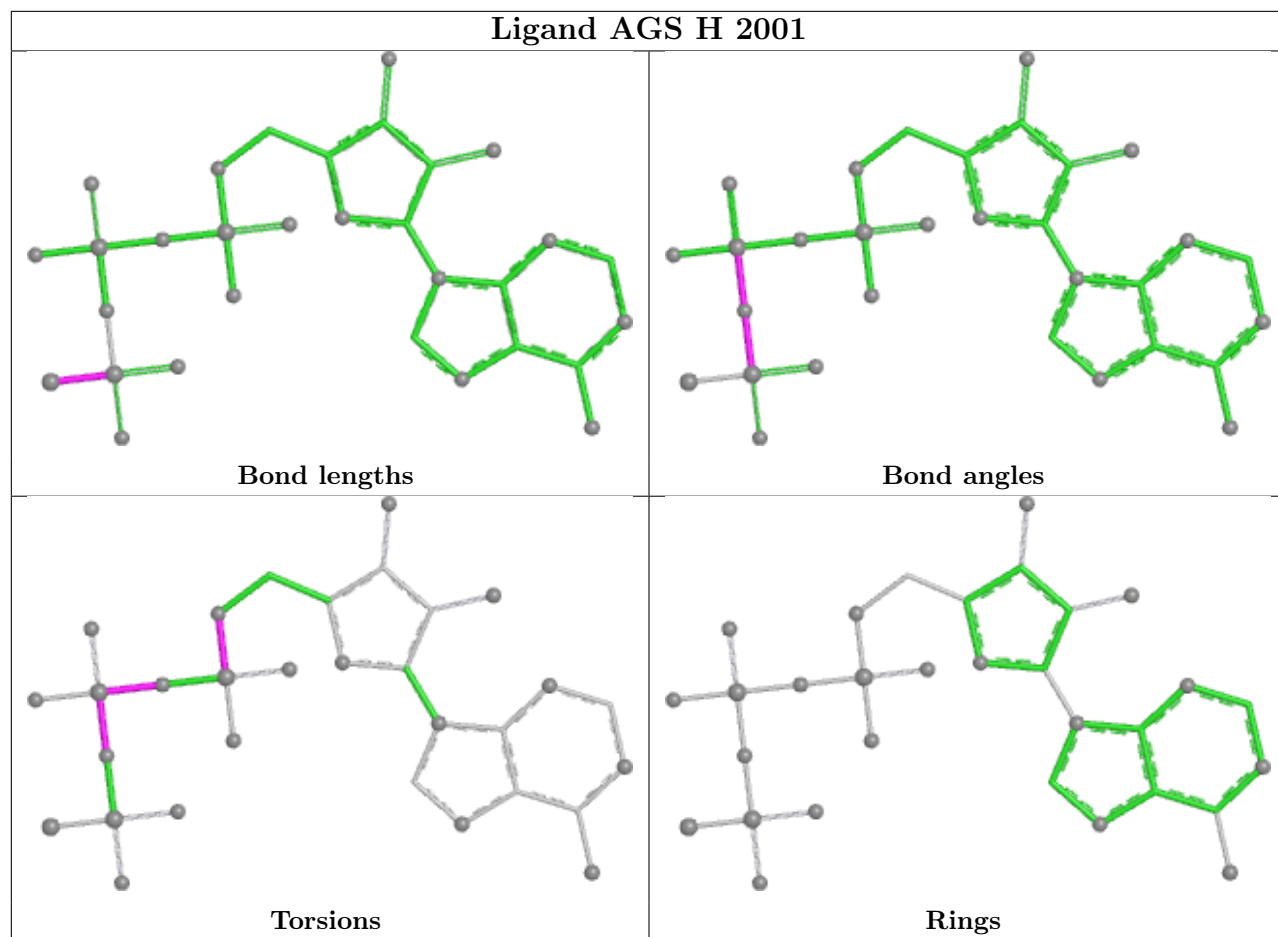


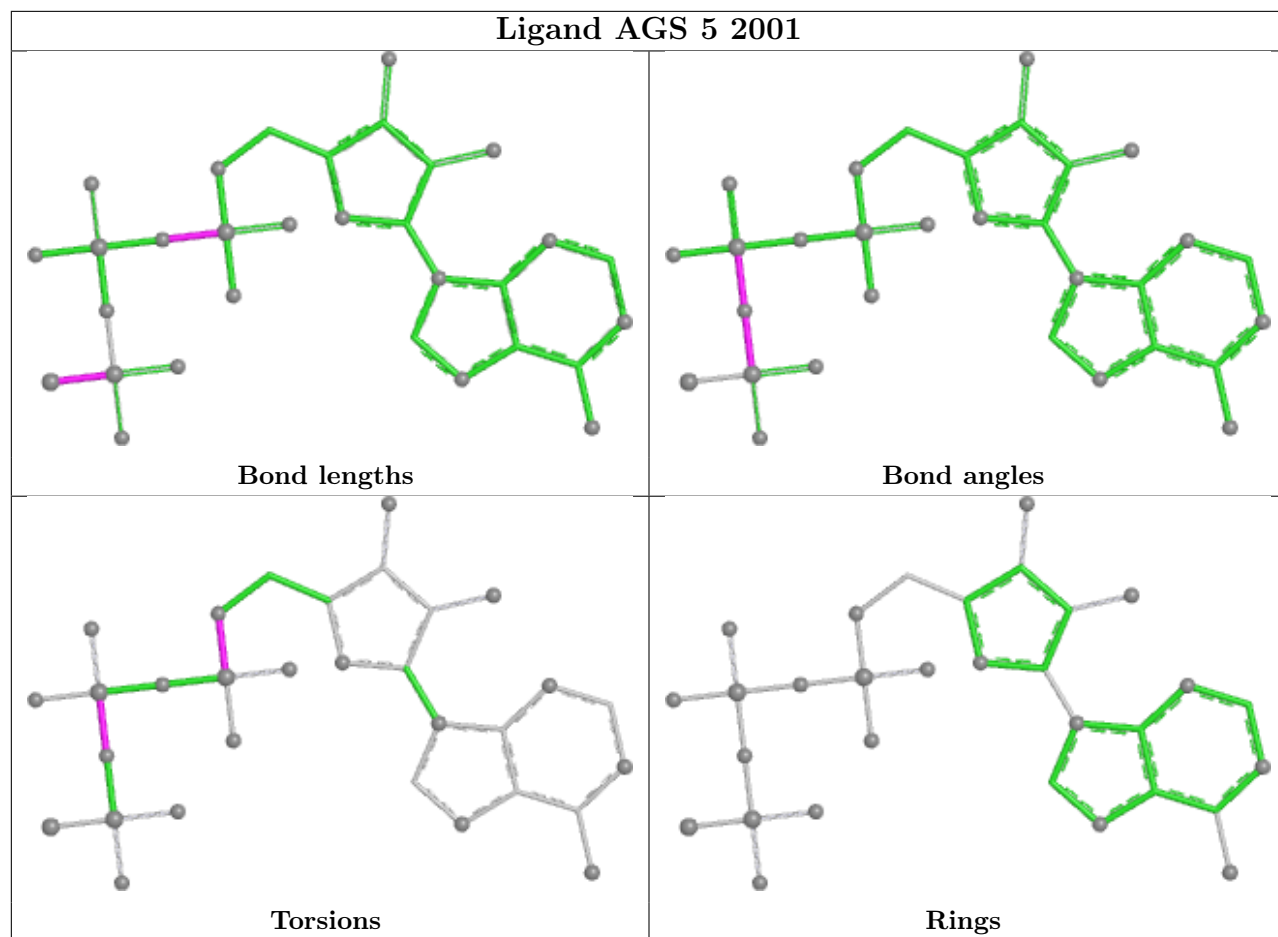




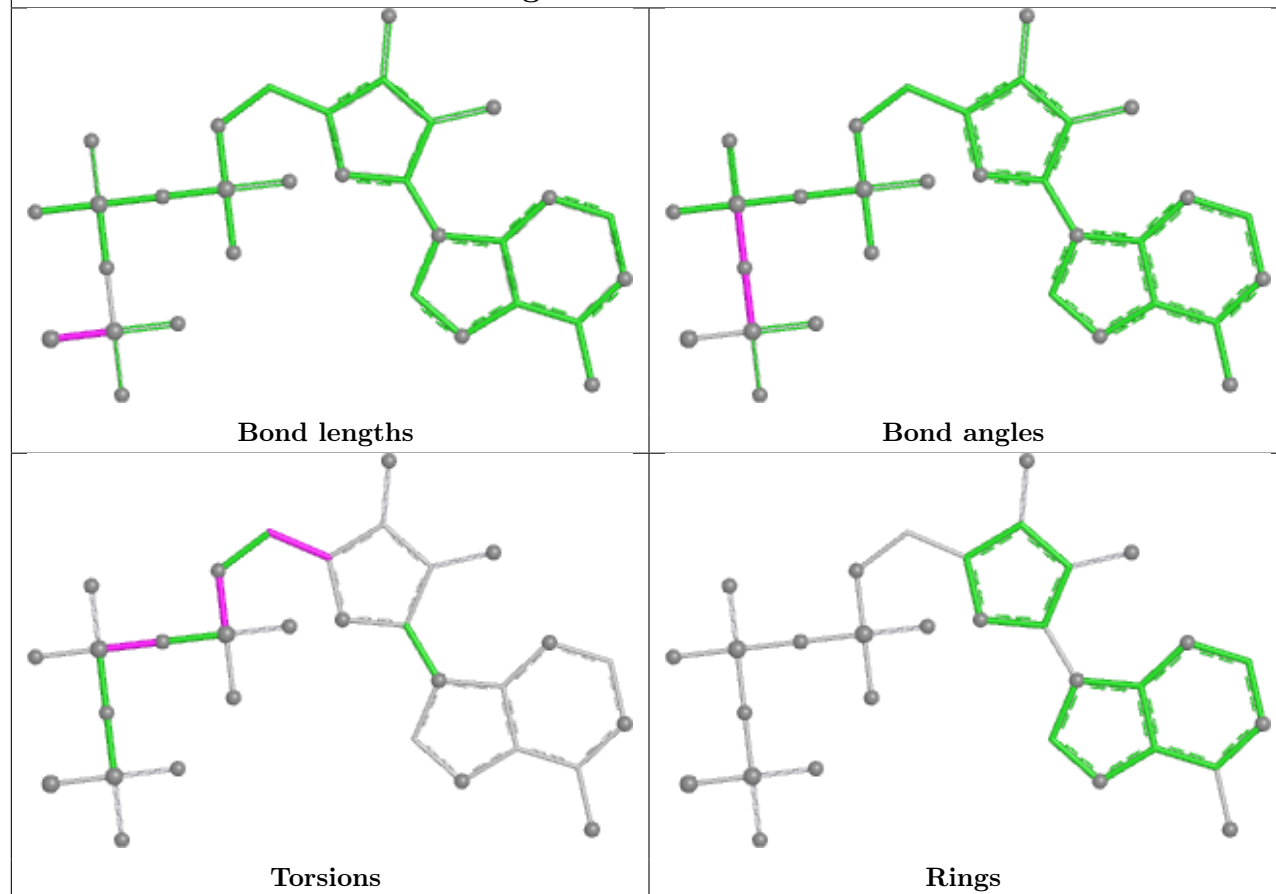




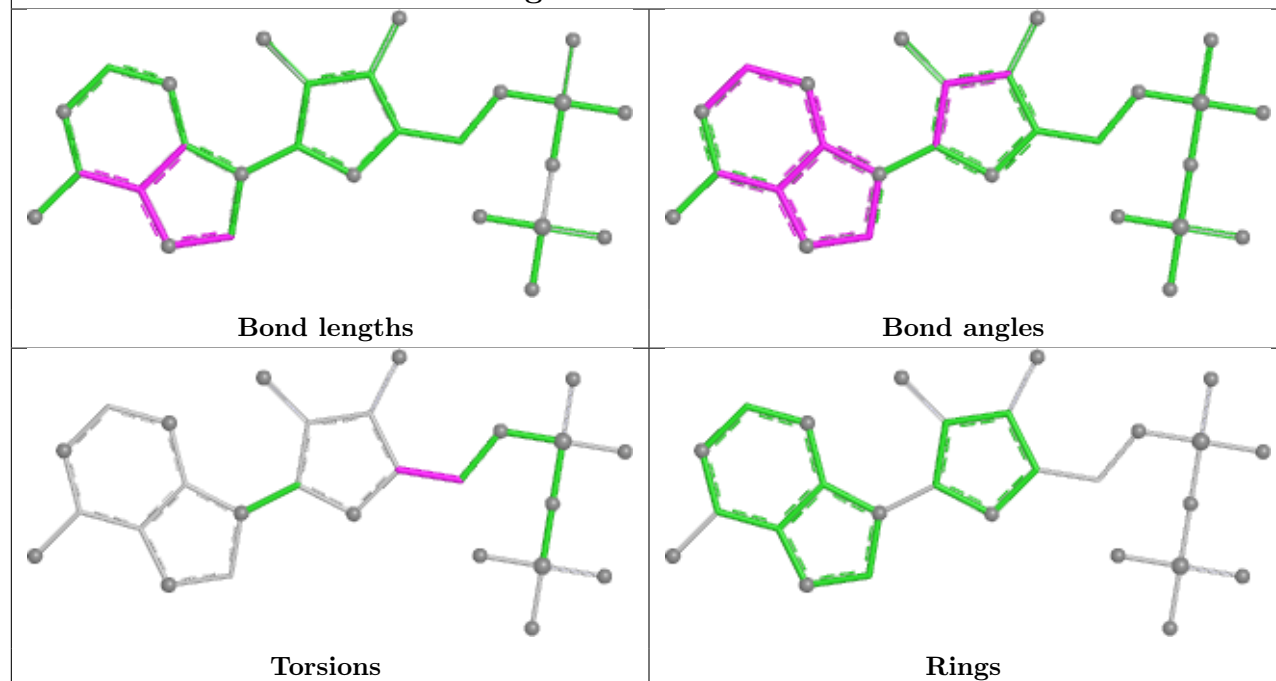


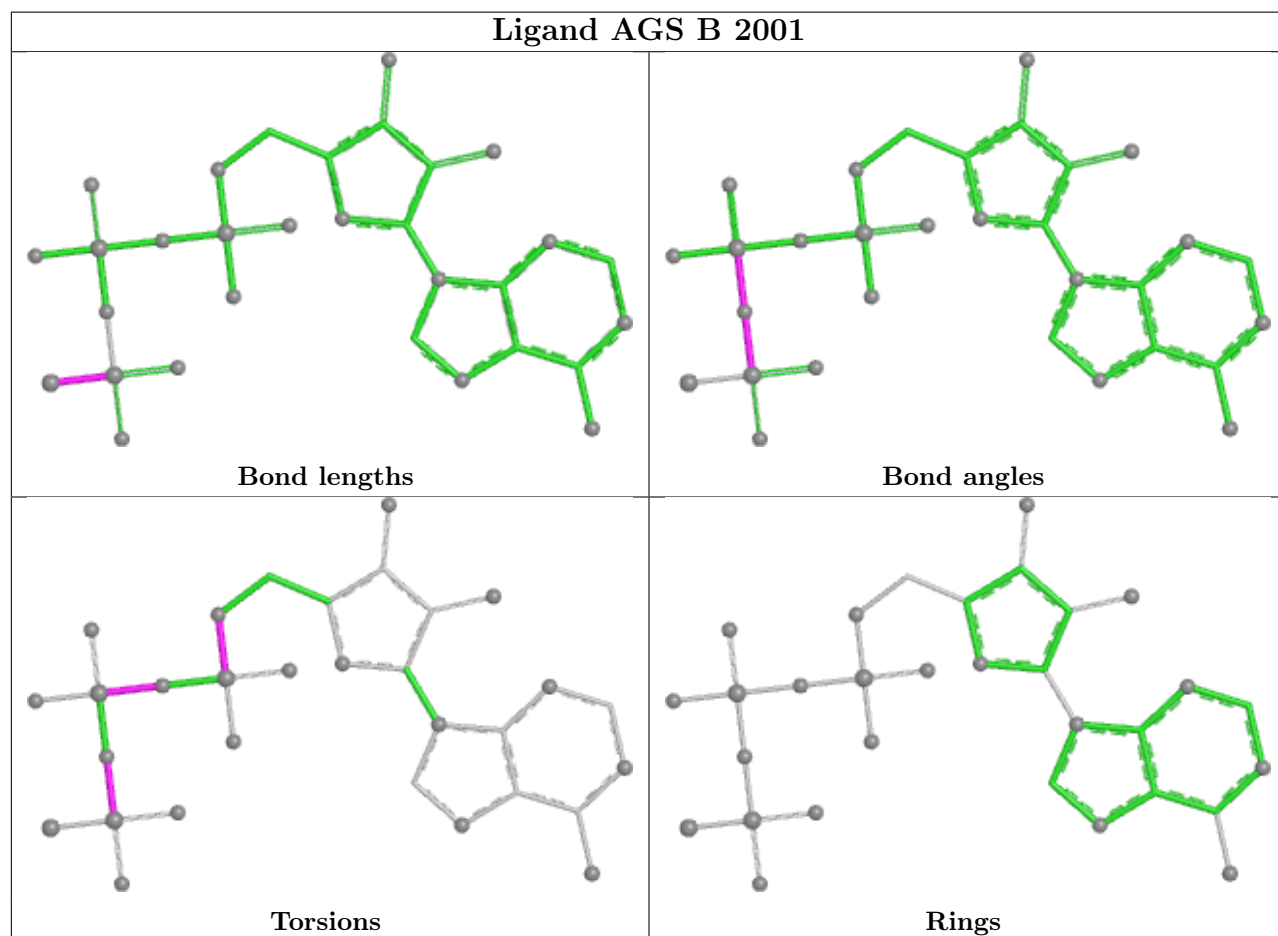
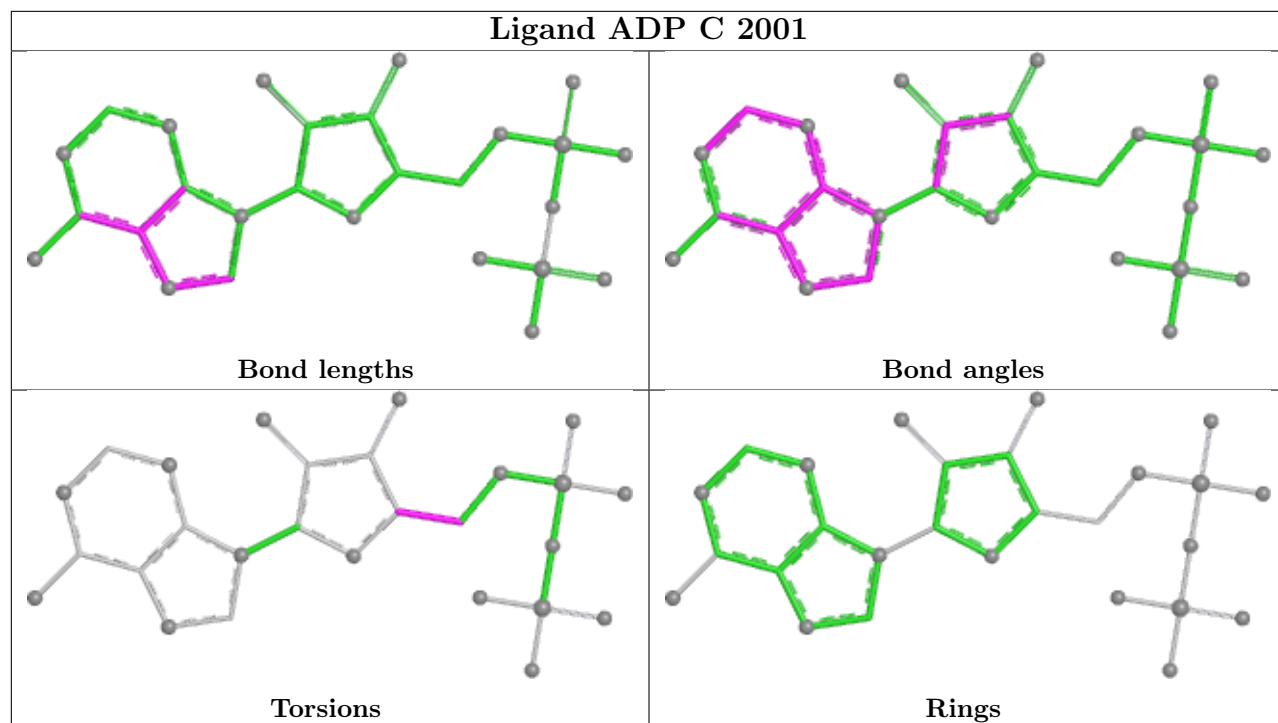


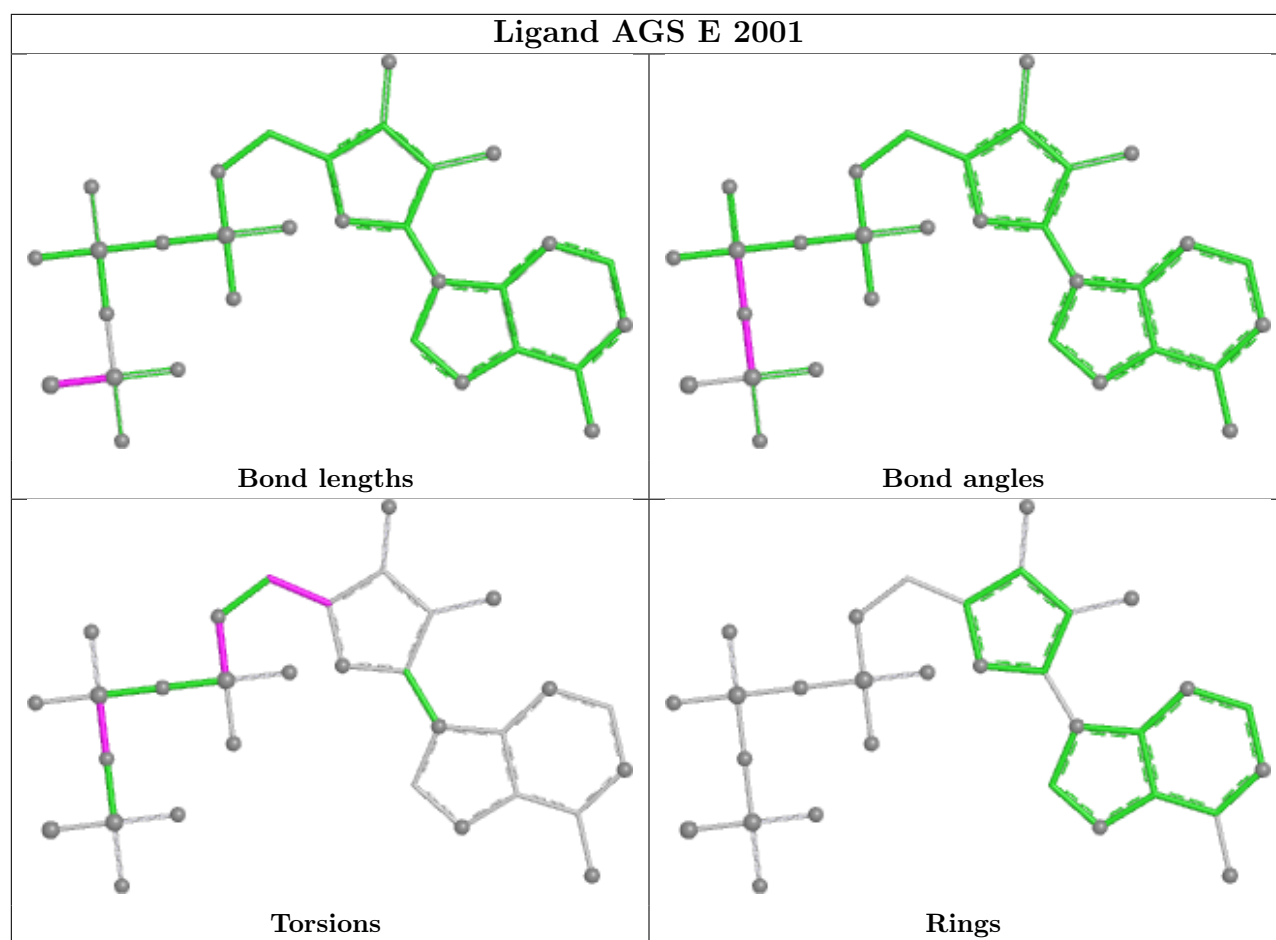
Ligand AGS G 2001



Ligand ADP 3 2001







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.

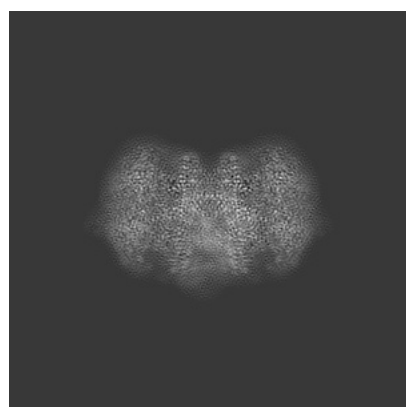
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31685. These allow visual inspection of the internal detail of the map and identification of artifacts.

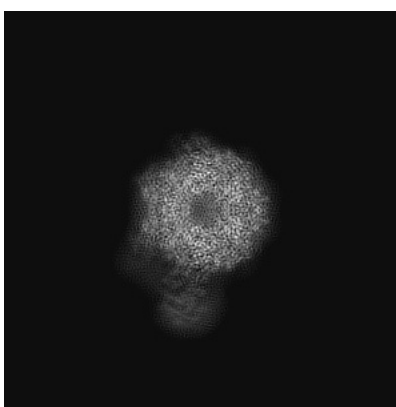
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

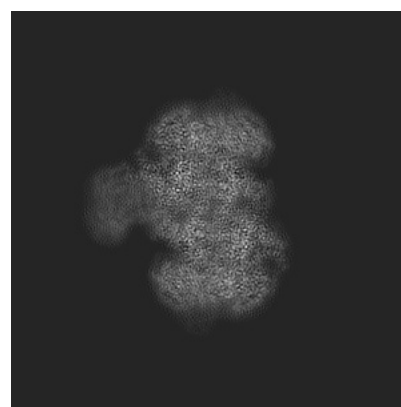
6.1.1 Primary map



X



Y

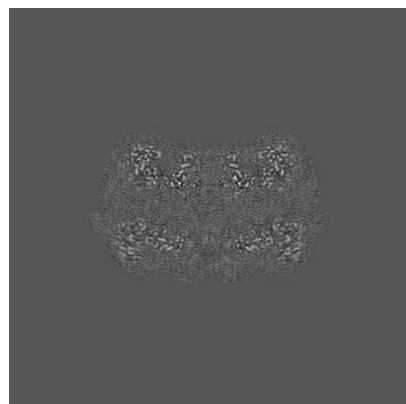


Z

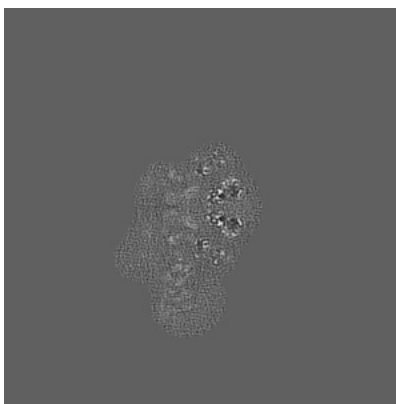
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

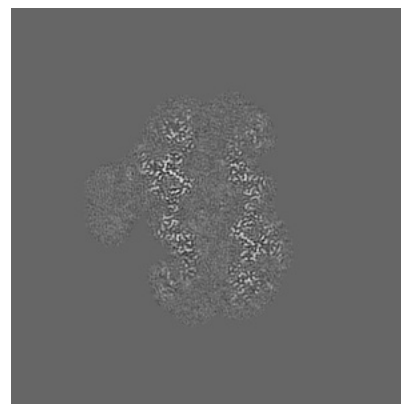
6.2.1 Primary map



X Index: 180



Y Index: 180

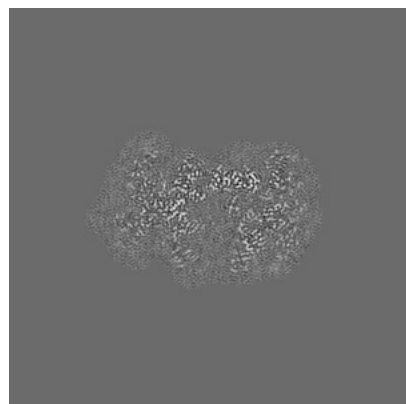


Z Index: 180

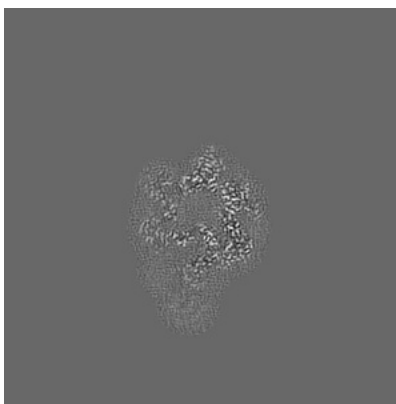
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

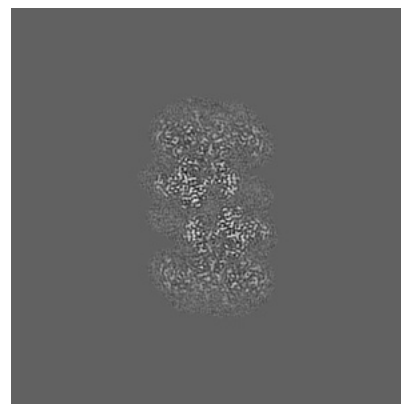
6.3.1 Primary map



X Index: 161



Y Index: 204

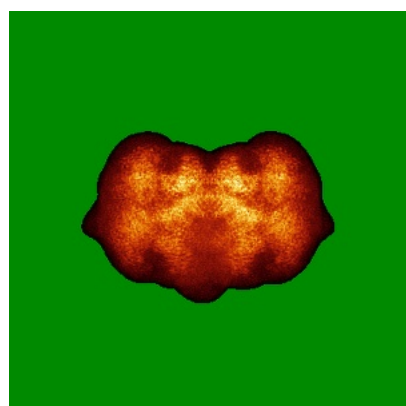


Z Index: 206

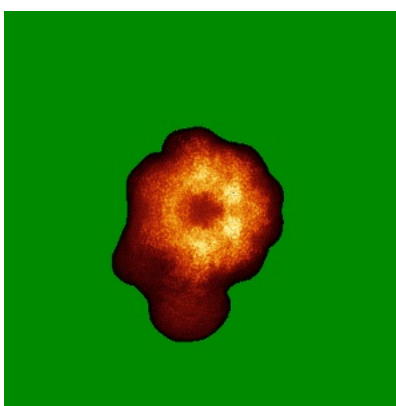
The images above show the largest variance slices of the map in three orthogonal directions.

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

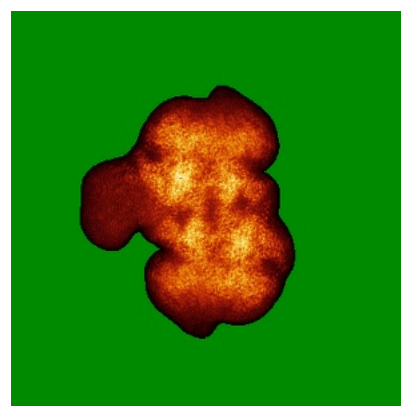
6.4.1 Primary map



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

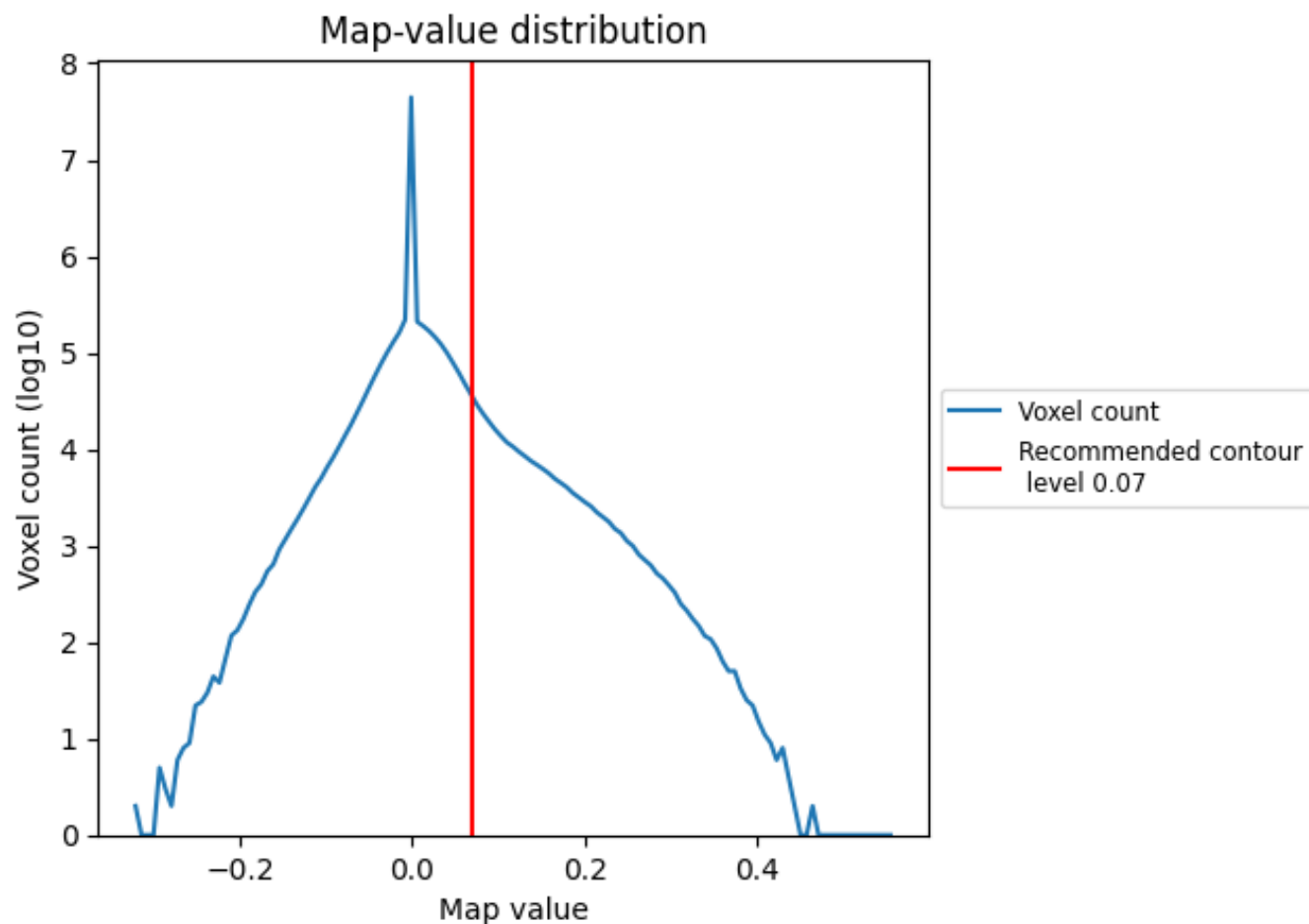
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

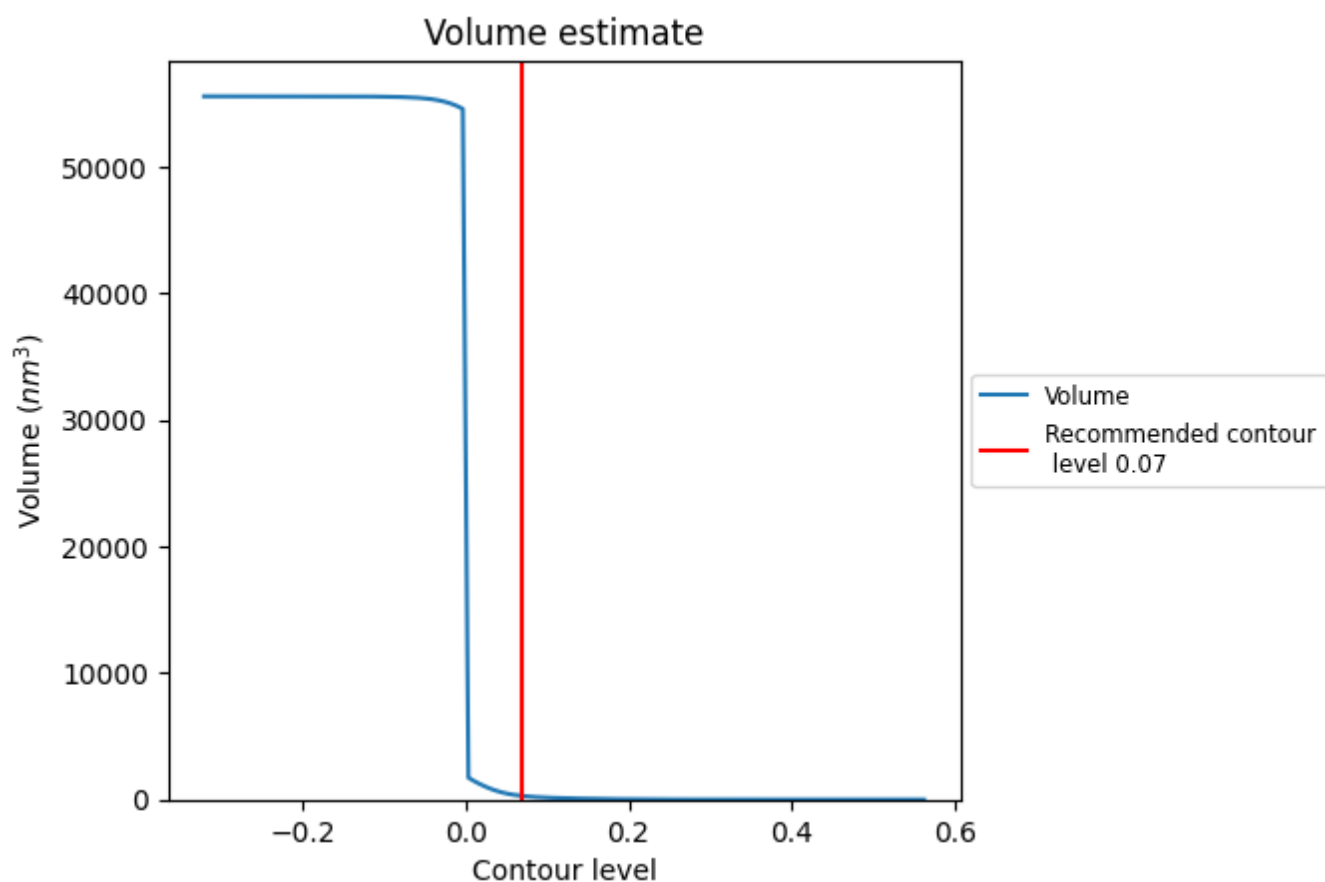
This section contains the results of statistical analysis of the map.

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.

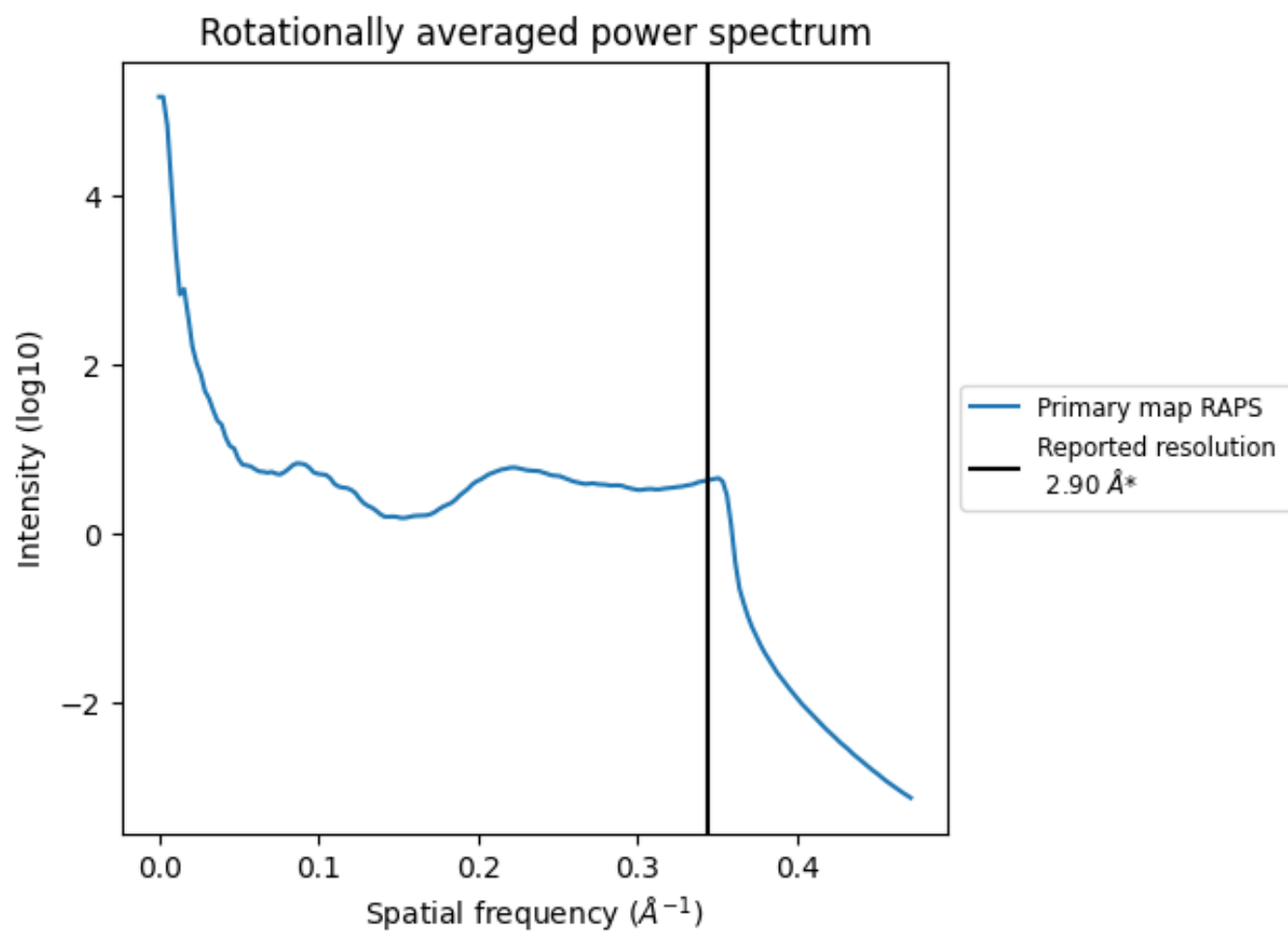
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 284 nm³; this corresponds to an approximate mass of 257 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 0.345 Å⁻¹

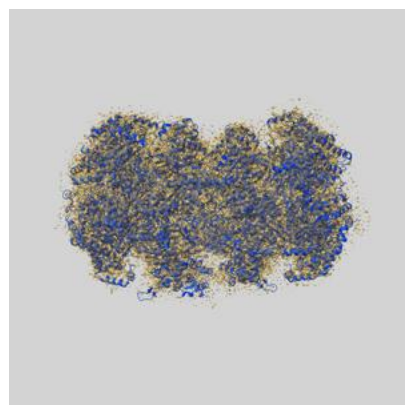
8 Fourier-Shell correlation ⓘ

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

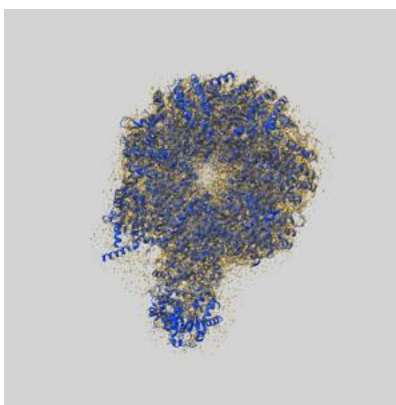
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31685 and PDB model 7V3V. Per-residue inclusion information can be found in section [3](#) on page [9](#).

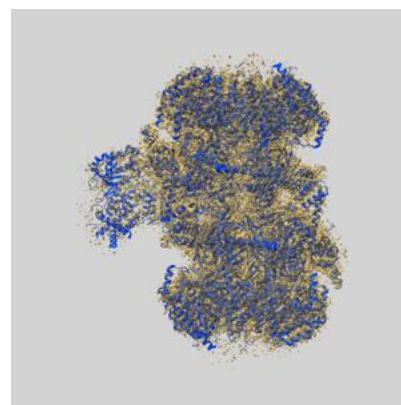
9.1 Map-model overlay [i](#)



X



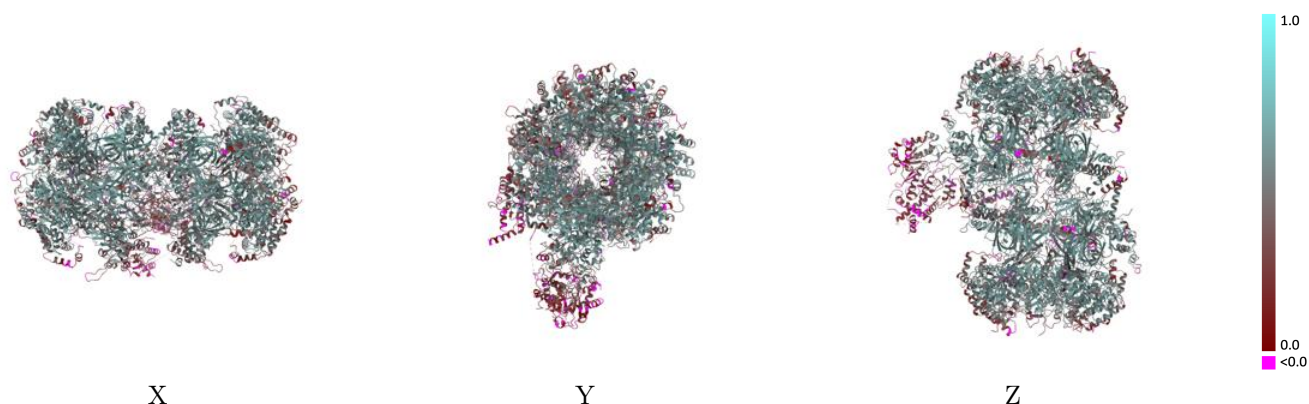
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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](#)

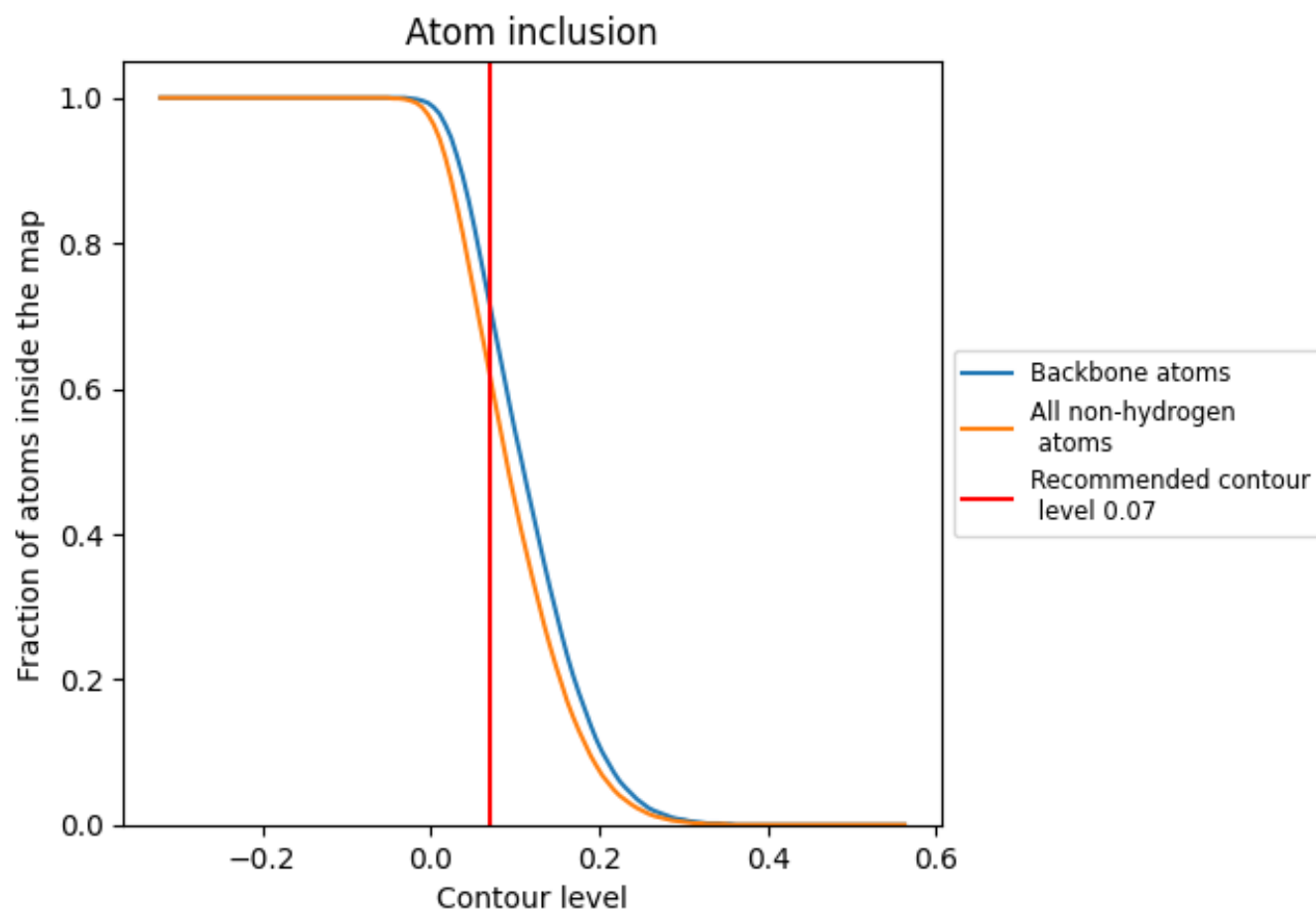


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6190	0.4770
2	0.5770	0.4640
3	0.7200	0.5300
4	0.7470	0.5450
5	0.6450	0.4940
6	0.6110	0.4710
7	0.7210	0.5310
B	0.5720	0.4580
C	0.7240	0.5360
D	0.7010	0.5250
E	0.6490	0.4970
F	0.5880	0.4610
G	0.6950	0.5190
H	0.1200	0.1960
I	0.1840	0.2110

