



Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 09:10 AM JST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

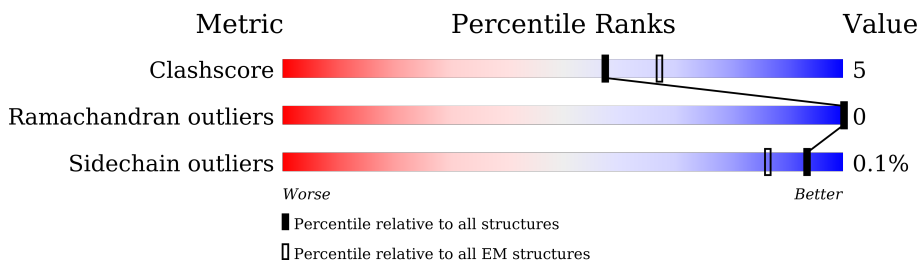
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



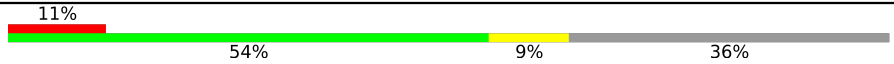

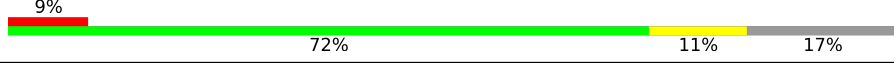

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	13% (red), 63% (green), 10% (yellow), 28% (grey)
1	B	868	13% (red), 62% (green), 11% (yellow), 28% (grey)
2	3	971	9% (red), 59% (green), 6% (yellow), 34% (grey)
2	C	971	10% (red), 58% (green), 8% (yellow), 34% (grey)
3	4	933	7% (red), 64% (green), 10% (yellow), 26% (grey)
3	D	933	8% (red), 61% (green), 11% (yellow), 28% (grey)
4	5	775	15% (red), 72% (green), 13% (yellow), 15% (grey)
4	E	775	15% (red), 71% (green), 14% (yellow), 15% (grey)

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	6	1017	
5	F	1017	
6	7	845	
6	G	845	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 62646 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA replication licensing factor MCM2.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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		

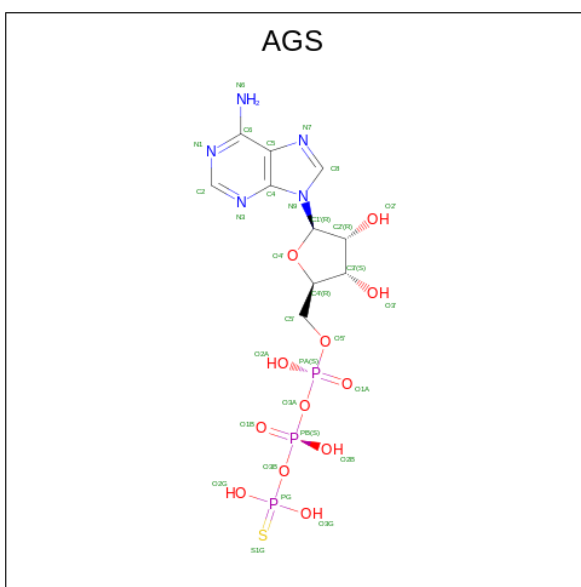
- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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 (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
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	

Continued on next page...

Continued from previous page...

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

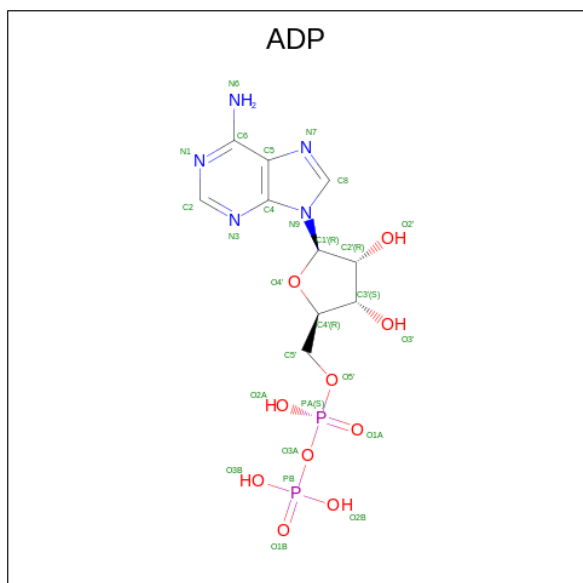
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 9 is ZINC ION (three-letter code: 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 (three-letter code: 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	

Continued on next page...

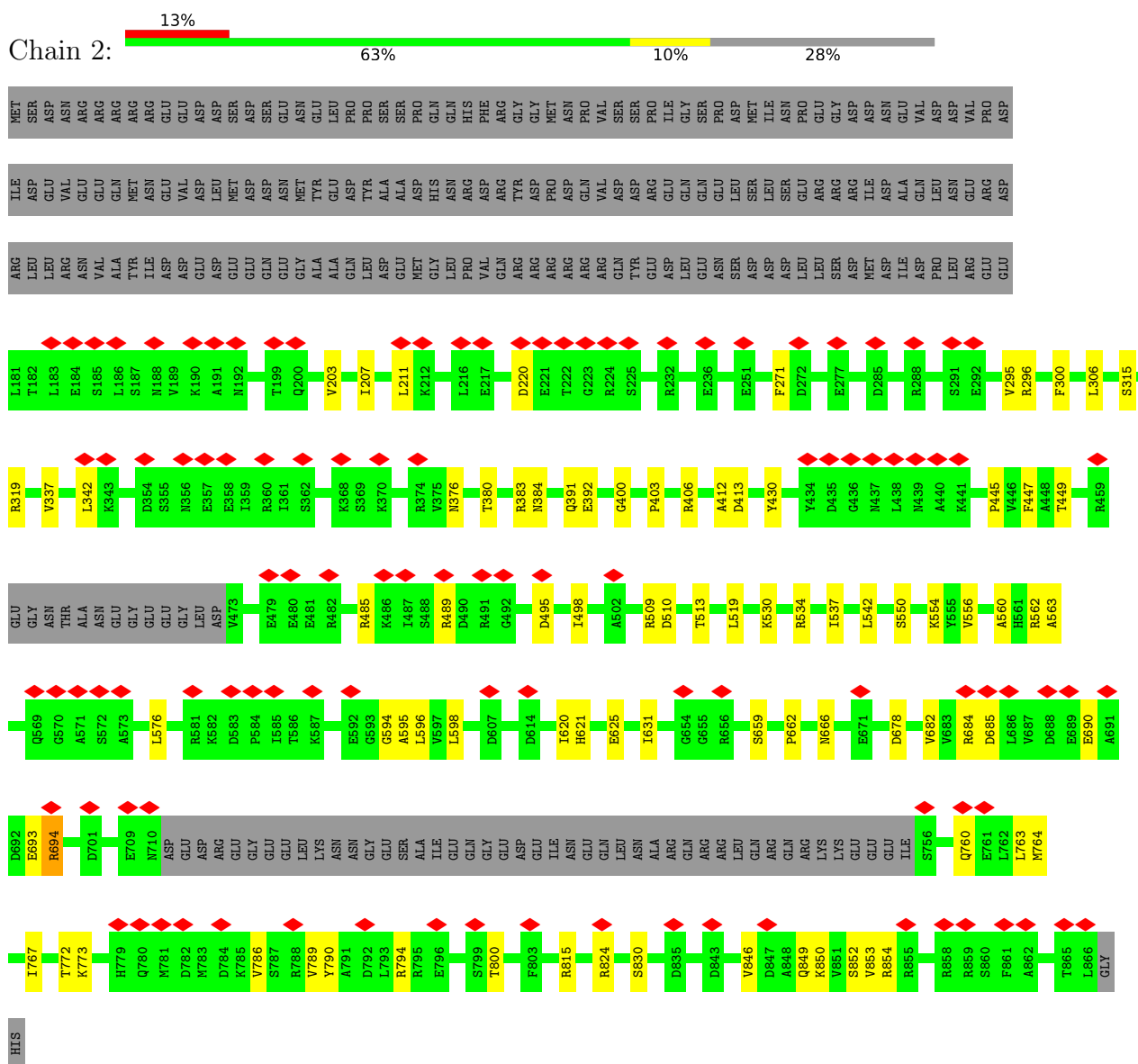
Continued from previous page...

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

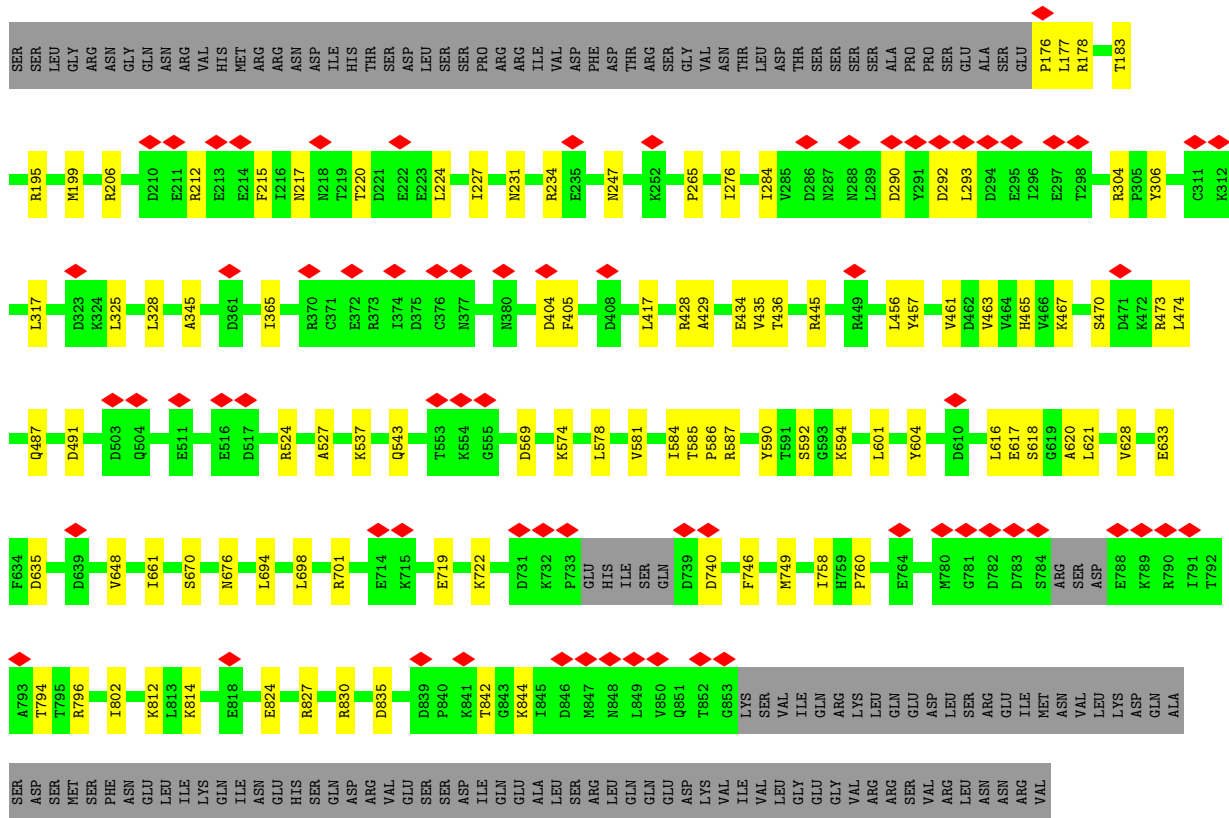
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

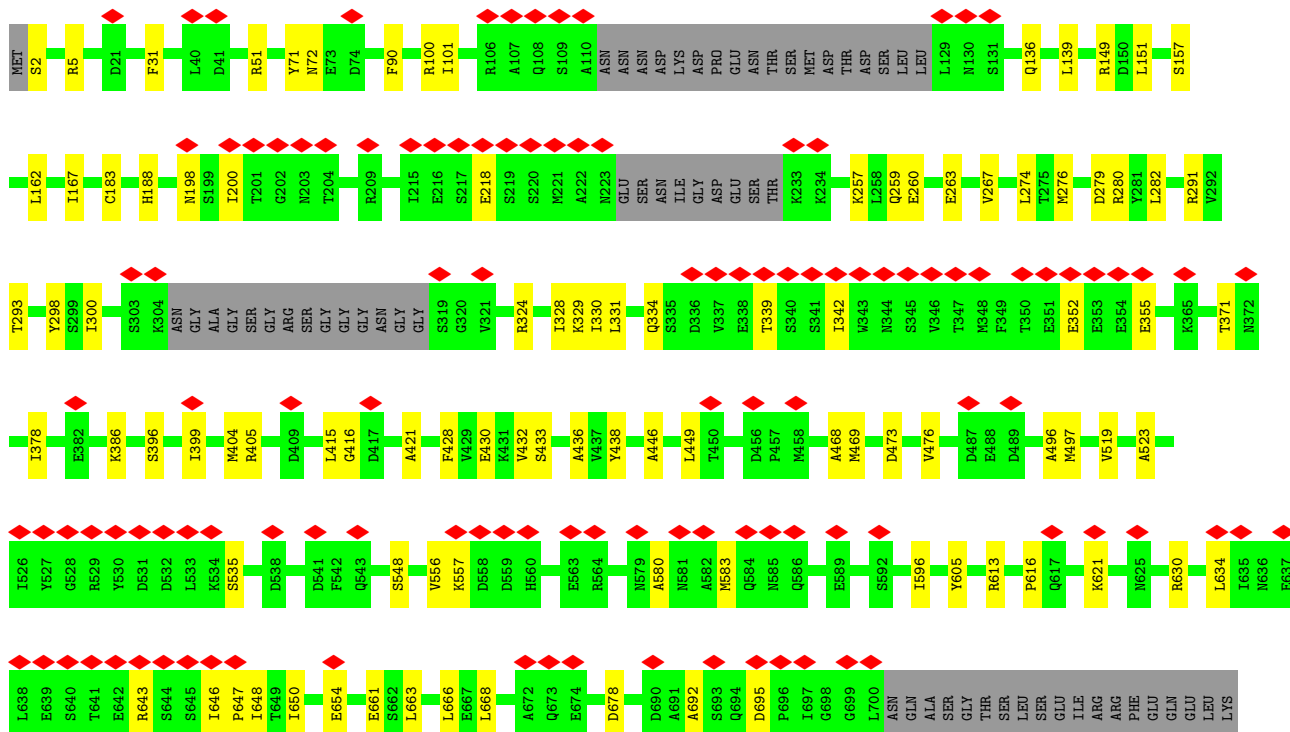
- Molecule 1: DNA replication licensing factor MCM2

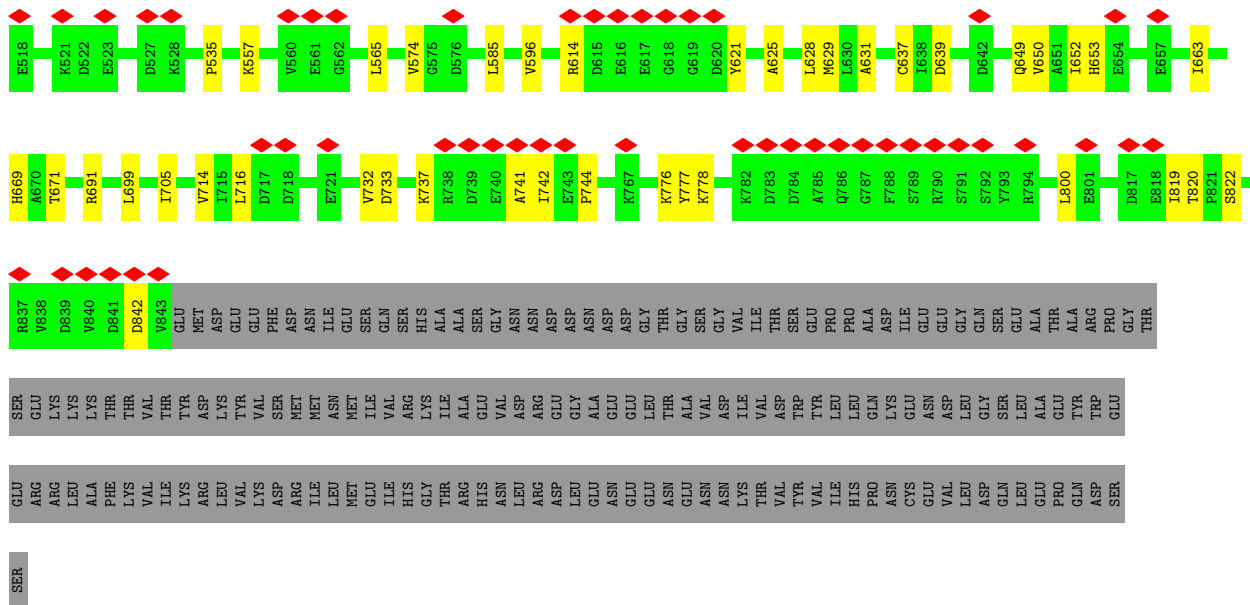


- Molecule 1: DNA replication licensing factor MCM2

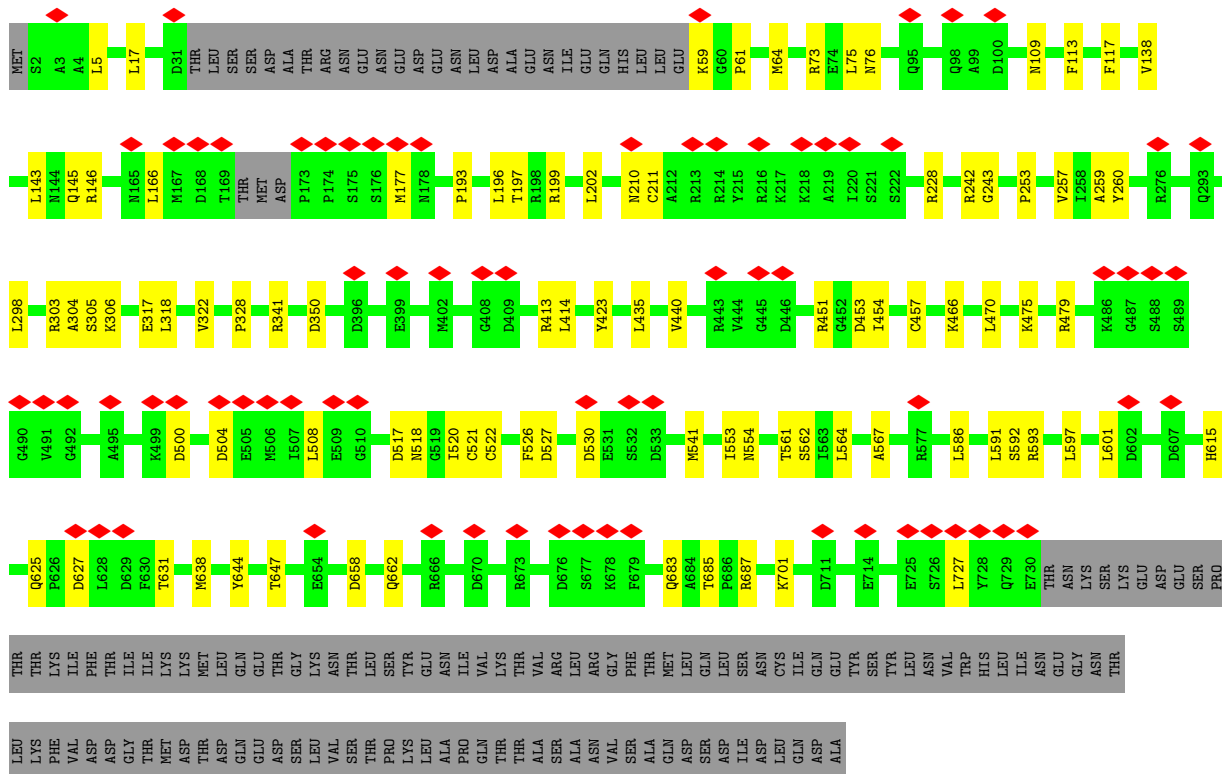


• Molecule 4: Minichromosome maintenance protein 5

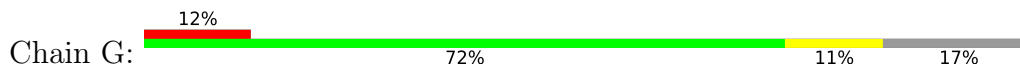


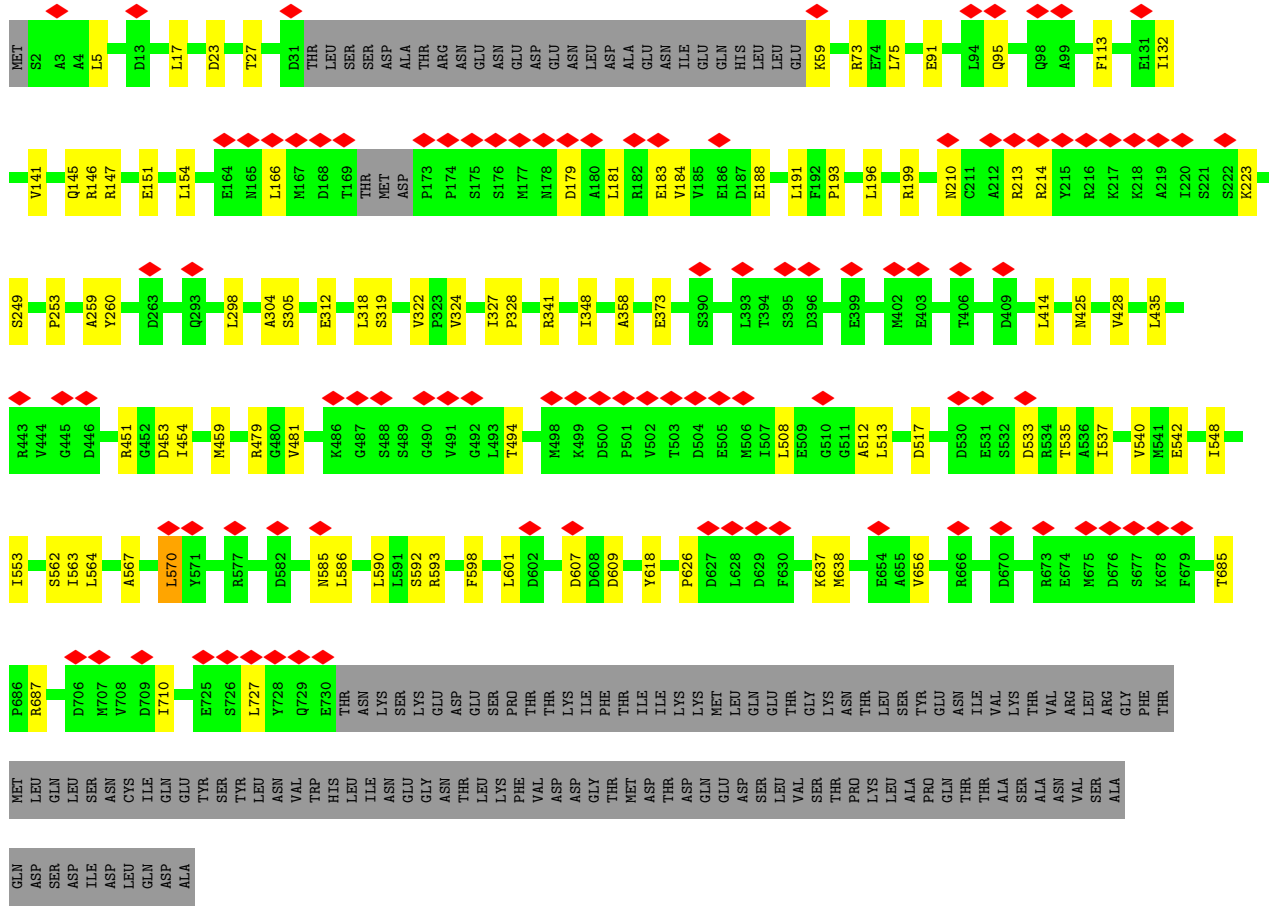


• Molecule 6: DNA replication licensing factor MCM7



• Molecule 6: DNA replication licensing factor MCM7





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.307	Depositor
Minimum map value	-0.180	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.05	Depositor
Map size (\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 (\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: MG, AGS, 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	0.27	0/5057	0.56	0/6834
1	B	0.27	0/5057	0.56	1/6834 (0.0%)
2	3	0.27	0/5073	0.54	1/6880 (0.0%)
2	C	0.27	0/5073	0.54	0/6880
3	4	0.28	0/5589	0.54	0/7553
3	D	0.27	0/5400	0.53	0/7300
4	5	0.27	0/5217	0.53	0/7054
4	E	0.28	0/5217	0.55	1/7054 (0.0%)
5	6	0.27	0/5190	0.54	1/7001 (0.0%)
5	F	0.27	0/5190	0.53	1/7001 (0.0%)
6	7	0.28	0/5590	0.54	0/7554
6	G	0.28	0/5590	0.53	1/7554 (0.0%)
All	All	0.27	0/63243	0.54	6/85499 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	570	LEU	CA-CB-CG	5.87	128.80	115.30
5	6	819	ILE	C-N-CA	5.54	135.55	121.70
4	E	647	PRO	CA-N-CD	-5.52	103.77	111.50
2	3	563	GLU	CA-CB-CG	5.29	125.04	113.40
1	B	792	ASP	CB-CG-OD2	5.15	122.93	118.30
5	F	819	ILE	C-N-CA	5.06	134.36	121.70

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	54	0
1	B	4970	0	5026	62	0
2	3	4987	0	5049	42	0
2	C	4987	0	5050	47	0
3	4	5509	0	5549	61	0
3	D	5323	0	5373	59	0
4	5	5143	0	5191	61	0
4	E	5143	0	5191	68	0
5	6	5109	0	5134	61	0
5	F	5109	0	5134	58	0
6	7	5505	0	5563	60	0
6	G	5505	0	5565	59	0
7	2	31	0	12	0	0
7	4	31	0	12	4	0
7	5	31	0	12	1	0
7	6	31	0	12	1	0
7	7	31	0	12	1	0
7	B	31	0	12	1	0
7	D	31	0	12	4	0
7	E	31	0	12	0	0
7	F	31	0	12	1	0
7	G	31	0	12	0	0
8	2	1	0	0	0	0
8	3	1	0	0	0	0
8	4	1	0	0	0	0
8	5	1	0	0	0	0
8	6	1	0	0	0	0
8	7	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
9	2	1	0	0	0	0
9	4	1	0	0	0	0
9	5	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	6	1	0	0	0	0
9	7	1	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
10	3	27	0	12	0	0
10	C	27	0	12	0	0
All	All	62646	0	62995	623	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 (623) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:167:ILE:HD11	4:E:259:GLN:HB2	1.63	0.81
4:E:276:MET:HG2	4:E:328:ILE:HB	1.66	0.77
4:E:198:ASN:HB3	4:E:329:LYS:HG2	1.71	0.73
4:5:167:ILE:HD11	4:5:259:GLN:HB2	1.69	0.72
4:E:398:LYS:HD2	4:E:406:LEU:HB2	1.74	0.70
6:G:685:THR:HG22	6:G:687:ARG:H	1.58	0.68
2:3:396:GLY:HA3	6:7:475:LYS:HE3	1.76	0.67
4:5:276:MET:HG2	4:5:328:ILE:HB	1.78	0.66
3:4:593:GLY:H	3:4:633:GLU:HB2	1.61	0.65
4:5:342:ILE:HD11	4:5:473:ASP:HB3	1.79	0.65
1:2:296:ARG:HH21	1:2:413:ASP:HB3	1.62	0.65
3:4:621:LEU:HD13	3:4:648:VAL:HG21	1.78	0.64
6:7:414:LEU:HD22	6:7:638:MET:HG3	1.79	0.64
7:4:2001:AGS:O3G	6:7:593:ARG:NH2	2.31	0.64
7:D:2001:AGS:O3G	6:G:593:ARG:NH2	2.31	0.63
3:D:594:LYS:HB3	6:G:535:THR:HG21	1.78	0.63
2:C:368:ALA:HB3	2:C:378:LYS:HE2	1.81	0.63
4:5:548:SER:HB3	4:5:647:PRO:HG2	1.80	0.62
1:2:485:ARG:HB3	1:2:489:ARG:HH21	1.64	0.62
2:3:368:ALA:HB3	2:3:378:LYS:HE2	1.81	0.62
1:B:400:GLY:HA3	5:F:390:LYS:HD3	1.82	0.61
6:G:586:LEU:HD11	6:G:590:LEU:HD22	1.82	0.61
3:4:281:VAL:HG13	3:4:293:LEU:HD11	1.82	0.61
5:6:314:CYS:SG	5:6:337:SER:OG	2.58	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:VAL:HA	1:B:380:THR:HG23	1.82	0.61
2:3:251:ILE:HG23	2:3:280:ASP:HB3	1.81	0.61
3:4:304:ARG:NH2	3:4:422:GLU:OE2	2.35	0.60
2:3:647:ILE:HG22	2:3:651:VAL:HG22	1.82	0.60
2:C:567:ARG:O	2:C:642:TYR:OH	2.19	0.60
4:E:342:ILE:HD11	4:E:473:ASP:HB3	1.83	0.59
4:5:100:ARG:NH2	6:G:188:GLU:OE2	2.35	0.59
2:C:329:LEU:HD23	2:C:588:LEU:HB3	1.84	0.59
3:4:681:ARG:NH1	6:7:683:GLN:OE1	2.35	0.59
1:2:495:ASP:OD1	1:2:509:ARG:NH2	2.34	0.59
5:6:384:ASP:O	5:6:388:ARG:NH1	2.36	0.59
4:E:136:GLN:HB2	4:E:280:ARG:HE	1.68	0.59
3:4:417:LEU:HD13	3:4:463:VAL:HG21	1.85	0.59
6:7:138:VAL:HG11	6:7:303:ARG:HH21	1.67	0.59
1:2:384:ASN:HB2	1:2:412:ALA:HA	1.84	0.58
2:C:262:PRO:HG3	4:E:509:ILE:HD11	1.85	0.58
2:3:553:ILE:HG13	4:5:634:LEU:HD13	1.85	0.58
5:6:306:LYS:HB2	5:6:352:ARG:HB2	1.86	0.58
5:6:820:THR:HG22	5:6:822:SER:H	1.69	0.58
3:D:304:ARG:HB3	3:D:465:HIS:HB2	1.86	0.58
3:D:621:LEU:HD13	3:D:648:VAL:HG21	1.84	0.58
4:E:177:THR:HA	4:E:197:PHE:HZ	1.69	0.58
6:7:451:ARG:NH1	6:7:453:ASP:O	2.37	0.58
2:C:251:ILE:HG23	2:C:280:ASP:HB3	1.85	0.58
5:F:156:GLN:OE1	5:F:269:ASN:ND2	2.37	0.58
1:B:811:GLU:OE2	4:E:576:HIS:NE2	2.37	0.58
1:2:337:VAL:HA	1:2:380:THR:HG23	1.85	0.58
2:3:697:ILE:HD11	2:3:737:LEU:HD21	1.86	0.58
5:6:737:LYS:HB3	5:6:740:GLU:HB2	1.86	0.58
5:6:742:ILE:HG22	5:6:744:PRO:HD3	1.86	0.58
4:5:167:ILE:HD13	4:5:257:LYS:HG3	1.86	0.57
2:3:370:SER:OG	4:5:404:MET:SD	2.62	0.57
4:5:198:ASN:HB3	4:5:329:LYS:HG2	1.86	0.57
5:6:186:ARG:HH22	5:6:260:GLU:HB3	1.69	0.57
5:F:314:CYS:SG	5:F:337:SER:OG	2.62	0.57
1:2:786:VAL:HA	1:2:789:VAL:HG12	1.87	0.57
3:4:231:ASN:OD1	3:4:234:ARG:NH2	2.38	0.57
6:G:414:LEU:HD22	6:G:638:MET:HG2	1.86	0.57
3:4:408:ASP:OD1	6:7:518:ASN:ND2	2.32	0.57
4:5:621:LYS:NZ	4:5:678:ASP:OD1	2.33	0.57
5:6:311:CYS:HB3	5:6:314:CYS:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:601:LEU:HD23	3:D:620:ALA:HB3	1.86	0.57
6:7:177:MET:SD	4:E:108:GLN:NE2	2.70	0.57
1:B:772:THR:HG23	1:B:773:LYS:HG2	1.85	0.57
6:7:508:LEU:HD22	6:7:553:ILE:HD13	1.87	0.57
1:B:386:GLN:HB2	1:B:415:VAL:HG12	1.87	0.57
3:D:428:ARG:HD2	5:F:370:THR:HG22	1.87	0.57
4:E:282:LEU:HD13	4:E:330:ILE:HG22	1.87	0.57
1:2:562:ARG:NH1	1:2:598:LEU:O	2.36	0.56
4:E:409:ASP:OD2	4:E:500:GLN:NE2	2.38	0.56
1:B:384:ASN:HB2	1:B:412:ALA:HA	1.86	0.56
2:C:558:ASP:OD1	4:E:630:ARG:NE	2.34	0.56
6:G:508:LEU:HD22	6:G:553:ILE:HD13	1.86	0.56
1:2:400:GLY:HA3	5:6:390:LYS:HD3	1.87	0.56
3:D:592:SER:OG	3:D:633:GLU:OE2	2.23	0.56
1:2:760:GLN:NE2	1:2:764:MET:SD	2.79	0.56
5:F:311:CYS:HB3	5:F:314:CYS:HB2	1.86	0.56
3:D:183:THR:O	6:G:145:GLN:NE2	2.39	0.56
5:6:109:GLU:OE1	5:6:112:ARG:NH1	2.39	0.55
5:6:412:LEU:O	5:6:416:LYS:NZ	2.37	0.55
2:C:52:ASN:ND2	2:C:90:ASN:O	2.39	0.55
4:E:587:GLN:HE21	4:E:592:SER:HB2	1.72	0.55
3:D:842:THR:HG23	3:D:844:LYS:H	1.70	0.55
3:4:578:LEU:HB3	3:4:590:TYR:HE2	1.70	0.55
2:C:552:ASP:HB3	2:C:557:ARG:HH12	1.71	0.55
6:7:75:LEU:O	6:7:199:ARG:NH1	2.39	0.55
2:C:569:HIS:HA	4:E:398:LYS:HZ1	1.70	0.55
1:2:659:SER:OG	1:2:684:ARG:NH1	2.39	0.55
5:6:773:LEU:HD21	5:6:804:ILE:HG12	1.89	0.55
3:4:183:THR:O	6:7:145:GLN:NE2	2.39	0.55
5:6:117:GLN:O	5:6:121:ASP:HB2	2.07	0.55
1:B:406:ARG:NH1	1:B:430:TYR:OH	2.40	0.55
3:4:601:LEU:HD23	3:4:620:ALA:HB3	1.89	0.54
4:5:433:SER:HB2	4:5:436:ALA:HB2	1.88	0.54
6:7:413:ARG:NH1	6:7:631:THR:O	2.39	0.54
1:2:391:GLN:HE21	1:2:403:PRO:HG2	1.72	0.54
1:2:772:THR:HG23	1:2:773:LYS:HG3	1.88	0.54
3:4:543:GLN:HE21	3:4:670:SER:HB3	1.71	0.54
3:D:794:THR:HG22	3:D:796:ARG:H	1.73	0.54
4:E:477:VAL:HG23	4:E:517:THR:HG21	1.88	0.54
5:F:663:ILE:O	5:F:669:HIS:HA	2.07	0.54
3:4:345:ALA:HB2	3:4:365:ILE:HD13	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:616:LEU:HD21	3:4:661:ILE:HD11	1.88	0.54
4:5:630:ARG:NH1	4:5:648:ILE:O	2.40	0.54
5:6:576:ASP:O	5:6:581:LYS:NZ	2.40	0.54
1:B:511:ILE:HG22	1:B:681:CYS:HB3	1.89	0.54
1:2:824:ARG:NH1	1:2:830:SER:OG	2.39	0.54
5:6:777:TYR:HA	5:6:780:LEU:HD12	1.90	0.54
2:C:459:ALA:HB2	6:G:327:ILE:HD11	1.89	0.54
3:D:487:GLN:NE2	3:D:491:ASP:OD1	2.41	0.54
4:E:432:VAL:HG23	4:E:596:ILE:HG13	1.90	0.54
1:2:406:ARG:NH1	1:2:430:TYR:OH	2.41	0.54
4:5:51:ARG:NH2	6:G:166:LEU:O	2.40	0.54
4:5:149:ARG:NH1	4:5:260:GLU:OE1	2.41	0.54
4:E:656:ILE:HA	4:E:659:ILE:HD12	1.89	0.54
6:G:451:ARG:NH1	6:G:453:ASP:O	2.38	0.54
2:3:567:ARG:O	2:3:642:TYR:OH	2.25	0.54
3:4:524:ARG:NH1	3:4:740:ASP:O	2.41	0.54
4:5:136:GLN:HG3	4:5:280:ARG:HH21	1.72	0.54
6:7:260:TYR:HB3	6:7:298:LEU:HB3	1.90	0.54
5:6:694:SER:O	5:6:698:ASN:ND2	2.41	0.53
1:B:562:ARG:NH1	1:B:598:LEU:O	2.40	0.53
2:3:244:GLU:OE1	6:7:109:ASN:ND2	2.36	0.53
4:5:136:GLN:HB2	4:5:280:ARG:HE	1.74	0.53
4:5:263:GLU:OE1	4:5:291:ARG:NH2	2.39	0.53
1:2:498:ILE:HD12	1:2:513:THR:HA	1.91	0.53
1:2:849:GLN:HB2	1:2:854:ARG:HG3	1.90	0.53
4:5:663:LEU:HA	4:5:666:LEU:HD12	1.91	0.53
5:6:550:GLN:NE2	5:6:569:ILE:O	2.41	0.53
2:C:203:ALA:O	2:C:207:GLY:N	2.40	0.53
5:F:574:VAL:O	5:F:714:VAL:HA	2.08	0.53
6:G:260:TYR:HB3	6:G:298:LEU:HB3	1.89	0.53
4:5:399:ILE:HD13	4:5:405:ARG:HG3	1.91	0.53
1:B:519:LEU:HD21	1:B:556:VAL:HG13	1.91	0.53
4:E:485:MET:SD	4:E:490:ARG:NH1	2.82	0.53
1:2:342:LEU:HB3	5:F:433:LEU:HD13	1.91	0.53
1:2:560:ALA:HB3	1:2:563:ALA:HB2	1.91	0.53
3:4:133:MET:SD	3:4:133:MET:N	2.82	0.53
3:4:306:TYR:HA	3:4:436:THR:HG21	1.91	0.53
3:D:317:LEU:O	6:G:341:ARG:NH2	2.40	0.53
4:E:184:ARG:O	4:E:187:ARG:NH1	2.42	0.53
5:F:109:GLU:OE1	5:F:112:ARG:NH1	2.42	0.53
6:7:466:LYS:NZ	7:7:2001:AGS:S1G	2.77	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:224:LEU:HD13	3:D:227:ILE:HD12	1.90	0.52
2:3:672:THR:OG1	2:3:721:VAL:O	2.27	0.52
5:F:277:ARG:NH2	5:F:373:MET:O	2.42	0.52
5:6:379:VAL:HG23	5:6:454:PHE:HB3	1.92	0.52
1:B:537:ILE:HG23	1:B:678:ASP:HB2	1.91	0.52
4:5:2:SER:HB2	2:C:245:TYR:HE1	1.74	0.52
6:7:454:ILE:O	6:7:562:SER:OG	2.23	0.52
2:3:432:THR:HG21	2:3:442:LEU:HD21	1.92	0.52
4:5:378:ILE:HD12	4:5:421:ALA:HB1	1.90	0.52
1:2:519:LEU:HD21	1:2:556:VAL:HG13	1.91	0.52
2:C:442:LEU:HD13	2:C:486:ILE:HD11	1.92	0.52
2:C:558:ASP:HB3	4:E:627:VAL:HG23	1.90	0.52
4:E:614:LEU:HD11	4:E:657:ILE:HG23	1.92	0.52
6:7:166:LEU:O	4:E:51:ARG:NH2	2.40	0.52
2:C:390:GLU:OE2	2:C:467:ARG:NH2	2.42	0.52
5:F:691:ARG:HE	5:F:716:LEU:HD22	1.75	0.52
5:6:170:ILE:HD12	5:6:181:LEU:HD11	1.91	0.52
5:F:277:ARG:NE	5:F:363:GLU:OE2	2.43	0.52
2:3:541:SER:HB2	2:3:700:ARG:HD2	1.93	0.51
1:B:576:LEU:HD23	1:B:595:ALA:HB3	1.92	0.51
2:3:678:VAL:HG21	2:3:723:LYS:HG3	1.91	0.51
4:5:282:LEU:HD13	4:5:330:ILE:HG22	1.91	0.51
2:C:223:THR:HG21	4:E:244:ILE:HA	1.93	0.51
3:D:830:ARG:NH1	3:D:835:ASP:OD1	2.43	0.51
5:F:509:SER:OG	5:F:510:SER:N	2.42	0.51
6:G:494:THR:HB	6:G:548:ILE:HD11	1.92	0.51
2:C:432:THR:HG21	2:C:442:LEU:HD21	1.92	0.51
4:E:618:ALA:HB1	4:E:677:VAL:HG21	1.92	0.51
2:3:295:VAL:HB	2:3:325:THR:HB	1.92	0.51
6:7:228:ARG:NH1	6:7:317:GLU:OE1	2.36	0.51
3:D:676:ASN:ND2	7:D:2001:AGS:S1G	2.80	0.51
2:3:197:ILE:HB	2:3:249:THR:HG23	1.92	0.51
4:5:300:ILE:HG23	4:5:324:ARG:HB3	1.93	0.51
3:D:231:ASN:OD1	3:D:234:ARG:NH2	2.44	0.51
3:4:775:VAL:HG12	3:4:779:LYS:HE3	1.93	0.51
2:C:426:ALA:HB3	2:C:429:ALA:HB2	1.93	0.51
3:D:345:ALA:HB2	3:D:365:ILE:HD13	1.93	0.51
2:3:522:GLN:OE1	4:5:643:ARG:NH2	2.44	0.51
3:4:317:LEU:O	6:7:341:ARG:NH2	2.44	0.51
3:D:417:LEU:HD13	3:D:463:VAL:HG21	1.93	0.51
6:G:259:ALA:H	6:G:305:SER:HB3	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:737:LYS:HB2	5:6:741:ALA:HB2	1.92	0.50
3:4:550:LYS:HG2	5:6:738:ARG:HH21	1.76	0.50
3:4:656:ILE:HD13	5:6:602:ALA:HB1	1.92	0.50
5:6:535:PRO:HB2	5:6:742:ILE:HD12	1.94	0.50
4:5:646:ILE:HG21	4:5:692:ALA:HA	1.93	0.50
5:F:306:LYS:HB2	5:F:352:ARG:HB2	1.93	0.50
3:4:534:GLU:HG3	3:4:538:LYS:HE3	1.93	0.50
3:D:206:ARG:NH1	3:D:247:ASN:OD1	2.43	0.50
3:D:434:GLU:HB3	3:D:467:LYS:HB3	1.94	0.50
3:D:569:ASP:O	3:D:574:LYS:NZ	2.45	0.50
1:2:576:LEU:HD23	1:2:595:ALA:HB3	1.94	0.50
3:4:701:ARG:NH2	7:6:2001:AGS:S1G	2.84	0.50
5:F:379:VAL:HG23	5:F:454:PHE:HB3	1.93	0.50
1:B:779:HIS:CD2	1:B:781:MET:HG3	2.47	0.49
2:C:212:ARG:HD2	2:C:232:PRO:HD3	1.92	0.49
3:D:581:VAL:HA	3:D:584:ILE:HG22	1.94	0.49
3:4:321:ASP:HA	3:4:324:LYS:HD2	1.93	0.49
3:D:217:ASN:HD21	3:D:220:THR:HB	1.77	0.49
7:D:2001:AGS:O3A	6:G:687:ARG:NH2	2.45	0.49
6:G:75:LEU:O	6:G:199:ARG:NH1	2.45	0.49
6:G:428:VAL:HA	6:G:598:PHE:CE2	2.46	0.49
2:C:661:GLN:O	2:C:665:GLU:HG2	2.12	0.49
2:C:686:LEU:O	2:C:693:LYS:NZ	2.45	0.49
3:D:616:LEU:HD22	3:D:661:ILE:HD11	1.94	0.49
2:3:528:ASP:OD1	2:3:528:ASP:N	2.44	0.49
3:4:628:VAL:HG22	3:4:670:SER:HB2	1.93	0.49
6:7:526:PHE:HB3	6:7:567:ALA:HB2	1.93	0.49
5:F:412:LEU:O	5:F:416:LYS:NZ	2.37	0.49
2:3:216:ASP:OD1	2:3:216:ASP:N	2.45	0.49
2:3:426:ALA:HB3	2:3:429:ALA:HB2	1.92	0.49
2:3:569:HIS:NE2	4:5:654:GLU:OE1	2.37	0.49
5:F:777:TYR:CG	5:F:800:LEU:HD12	2.48	0.49
6:G:210:ASN:OD1	6:G:213:ARG:NH2	2.46	0.49
7:4:2001:AGS:O2B	7:4:2001:AGS:O2A	2.31	0.49
7:D:2001:AGS:O2A	7:D:2001:AGS:O2B	2.31	0.49
3:4:527:ALA:HB3	3:4:537:LYS:HE2	1.94	0.49
2:C:507:ASN:ND2	6:G:319:SER:O	2.46	0.49
2:C:669:PRO:HG2	2:C:710:THR:HG23	1.93	0.49
5:F:126:SER:OG	5:F:128:ASP:OD1	2.31	0.49
5:F:317:ILE:HD13	5:F:350:ARG:HD3	1.94	0.49
3:D:543:GLN:HE21	3:D:670:SER:HB3	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:299:LYS:HD3	2:C:322:LEU:HD22	1.95	0.49
1:2:211:LEU:HD13	1:2:271:PHE:HB2	1.95	0.48
5:F:557:LYS:HB2	5:F:565:LEU:HD12	1.95	0.48
6:G:601:LEU:HD12	6:G:727:LEU:HG	1.94	0.48
1:2:596:LEU:HD11	1:2:620:ILE:HD13	1.95	0.48
1:2:790:TYR:CZ	1:2:794:ARG:HD2	2.48	0.48
3:4:585:THR:HG21	3:4:628:VAL:HB	1.95	0.48
6:7:435:LEU:HD21	6:7:564:LEU:HB2	1.95	0.48
6:7:451:ARG:NE	6:7:541:MET:O	2.46	0.48
1:B:688:ASP:HB3	1:B:691:ALA:HB3	1.95	0.48
1:B:779:HIS:HD2	1:B:781:MET:HG3	1.78	0.48
1:2:300:PHE:O	1:2:319:ARG:NH1	2.47	0.48
2:3:353:LEU:HD22	2:3:647:ILE:HG21	1.95	0.48
5:6:842:ASP:N	5:6:842:ASP:OD1	2.47	0.48
1:B:633:LYS:NZ	4:E:446:ALA:O	2.45	0.48
5:6:277:ARG:NH2	5:6:373:MET:O	2.46	0.48
5:6:650:VAL:O	5:6:654:GLU:HG3	2.13	0.48
2:C:400:ARG:HD2	2:C:491:GLU:HA	1.96	0.48
4:E:416:GLY:HA3	4:E:556:VAL:HB	1.95	0.48
5:6:126:SER:HB3	5:6:130:GLY:H	1.79	0.48
1:B:636:ILE:HD11	4:E:167:ILE:HG23	1.95	0.48
3:D:328:LEU:HD11	3:D:461:VAL:HG21	1.94	0.48
4:E:462:PHE:HE2	4:E:508:GLY:H	1.61	0.48
5:F:535:PRO:HB2	5:F:742:ILE:HG23	1.95	0.48
1:2:621:HIS:NE2	1:2:625:GLU:OE2	2.46	0.48
2:3:101:ASP:O	2:3:105:GLU:HG3	2.14	0.48
3:4:470:SER:HB3	3:4:473:ARG:HG2	1.95	0.48
4:5:396:SER:OG	4:5:661:GLU:OE1	2.29	0.48
5:6:673:ASN:HB3	5:6:675:ARG:NH1	2.28	0.48
5:6:403:VAL:HG22	5:6:450:TYR:HB3	1.95	0.48
5:6:550:GLN:HE21	5:6:677:SER:HB3	1.78	0.48
1:B:560:ALA:HB3	1:B:563:ALA:HB2	1.96	0.48
5:F:125:GLN:NE2	5:F:126:SER:O	2.47	0.48
5:F:820:THR:HG22	5:F:822:SER:H	1.79	0.48
1:B:484:PHE:HZ	1:B:765:LYS:HB2	1.78	0.48
5:F:409:GLN:HG2	5:F:412:LEU:HD12	1.95	0.48
2:3:430:ILE:HD12	2:3:465:ALA:HB2	1.96	0.47
3:4:572:THR:HG21	3:4:708:VAL:HB	1.95	0.47
6:7:257:VAL:HG22	6:7:306:LYS:HB3	1.95	0.47
6:7:500:ASP:O	6:7:504:ASP:N	2.46	0.47
6:7:76:ASN:OD1	6:7:199:ARG:NH2	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:196:LEU:HD21	6:7:257:VAL:HG21	1.96	0.47
6:7:625:GLN:NE2	6:7:627:ASP:O	2.46	0.47
4:E:183:CYS:HB3	4:E:188:HIS:H	1.79	0.47
1:2:537:ILE:HG23	1:2:678:ASP:HB2	1.96	0.47
5:6:139:GLN:O	5:6:143:MET:HG3	2.14	0.47
2:C:712:HIS:ND1	2:C:725:ASP:OD1	2.43	0.47
5:F:653:HIS:HB3	5:F:705:ILE:HD13	1.95	0.47
5:F:691:ARG:HH21	5:F:716:LEU:HB3	1.78	0.47
1:B:824:ARG:NH2	1:B:833:ASP:OD1	2.48	0.47
1:2:406:ARG:NH1	1:2:449:THR:OG1	2.48	0.47
1:2:631:ILE:HG13	4:5:446:ALA:HB3	1.97	0.47
3:4:474:LEU:HB2	3:4:586:PRO:HD3	1.96	0.47
6:7:521:CYS:HB2	6:7:561:THR:HG21	1.96	0.47
1:B:306:LEU:HB2	1:B:392:GLU:HG3	1.97	0.47
1:B:447:PHE:HB2	5:F:302:PRO:HG2	1.96	0.47
1:B:598:LEU:HD21	4:E:267:VAL:HA	1.95	0.47
1:B:690:GLU:HB3	1:B:694:ARG:HH12	1.79	0.47
3:D:306:TYR:HA	3:D:436:THR:HG21	1.96	0.47
3:D:628:VAL:HG22	3:D:670:SER:HB2	1.96	0.47
5:F:277:ARG:HG2	5:F:375:ARG:HD2	1.97	0.47
5:F:733:ASP:OD1	5:F:737:LYS:NZ	2.47	0.47
3:4:189:GLU:OE2	3:4:193:ASN:ND2	2.48	0.47
5:6:650:VAL:HA	5:6:653:HIS:ND1	2.30	0.47
6:7:322:VAL:HG21	6:7:328:PRO:HG3	1.97	0.47
3:D:292:ASP:OD1	3:D:292:ASP:N	2.48	0.47
6:G:435:LEU:HD21	6:G:564:LEU:HB2	1.96	0.47
1:2:800:THR:HG21	1:2:853:VAL:HG13	1.96	0.47
5:F:117:GLN:O	5:F:121:ASP:HB2	2.15	0.47
5:F:742:ILE:HG22	5:F:744:PRO:HD3	1.96	0.47
1:B:391:GLN:NE2	5:F:671:THR:O	2.46	0.47
3:D:178:ARG:HA	3:D:178:ARG:HD2	1.77	0.47
3:D:585:THR:HG21	3:D:628:VAL:HB	1.96	0.47
4:E:433:SER:HB2	4:E:436:ALA:HB2	1.97	0.47
5:F:423:THR:HA	5:F:426:ILE:HD13	1.97	0.47
1:2:383:ARG:HB2	1:2:412:ALA:HB2	1.97	0.46
4:5:31:PHE:CG	4:5:90:PHE:HD1	2.33	0.46
4:5:415:LEU:HA	4:5:523:ALA:O	2.14	0.46
6:7:117:PHE:HB3	6:7:202:LEU:HD11	1.96	0.46
1:B:406:ARG:NH1	1:B:449:THR:OG1	2.48	0.46
1:B:783:MET:HG3	4:E:573:ILE:HG21	1.96	0.46
1:2:598:LEU:HD21	4:5:267:VAL:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:ASP:HB2	1:B:645:SER:HB2	1.97	0.46
1:2:594:GLY:O	1:2:598:LEU:HB2	2.16	0.46
1:2:850:LYS:O	1:2:854:ARG:N	2.44	0.46
2:3:314:LEU:HD11	4:5:200:ILE:HA	1.96	0.46
1:B:786:VAL:HA	1:B:789:VAL:HG12	1.98	0.46
4:E:31:PHE:CG	4:E:90:PHE:HD1	2.33	0.46
5:F:321:VAL:HG11	5:F:330:PRO:HD3	1.96	0.46
6:G:542:GLU:OE2	6:G:687:ARG:NE	2.48	0.46
3:4:604:TYR:OH	6:7:554:ASN:ND2	2.49	0.46
1:B:410:LEU:HD22	1:B:456:ILE:HD11	1.97	0.46
6:G:454:ILE:O	6:G:562:SER:OG	2.30	0.46
6:G:570:LEU:HD23	6:G:585:ASN:HD21	1.79	0.46
1:B:790:TYR:CZ	1:B:794:ARG:HD2	2.50	0.46
4:E:25:THR:HG22	4:E:29:LYS:HE2	1.96	0.46
4:E:625:ASN:O	4:E:625:ASN:ND2	2.46	0.46
5:F:585:LEU:HD23	5:F:637:CYS:HB3	1.97	0.46
5:6:433:LEU:HD13	1:B:342:LEU:HB3	1.97	0.46
5:6:694:SER:OG	5:6:792:SER:O	2.32	0.46
4:E:444:SER:HB2	4:E:447:ALA:HB3	1.96	0.46
4:E:535:SER:O	4:E:539:ASN:ND2	2.46	0.46
1:2:530:LYS:HB3	4:5:428:PHE:HE1	1.80	0.46
3:4:581:VAL:HA	3:4:584:ILE:HG22	1.97	0.46
4:5:5:ARG:HG2	4:5:218:GLU:HB2	1.97	0.46
4:5:430:GLU:HG3	4:5:438:TYR:HB2	1.98	0.46
6:7:61:PRO:HB2	6:7:64:MET:HB2	1.98	0.46
6:G:91:GLU:O	6:G:95:GLN:OE1	2.33	0.46
3:4:304:ARG:HB3	3:4:465:HIS:HB2	1.97	0.46
5:6:409:GLN:HG2	5:6:412:LEU:HD12	1.97	0.46
1:B:447:PHE:HE1	5:F:304:LEU:HB2	1.81	0.46
1:B:610:ASP:OD1	1:B:610:ASP:N	2.46	0.46
6:G:17:LEU:HD13	6:G:113:PHE:HZ	1.80	0.46
6:G:537:ILE:HG23	6:G:563:ILE:HD13	1.97	0.46
1:2:534:ARG:O	1:2:815:ARG:NH1	2.48	0.46
3:D:812:LYS:HE3	3:D:814:LYS:HE2	1.98	0.46
6:G:656:VAL:HG12	6:G:710:ILE:HD13	1.98	0.46
3:4:290:ASP:OD1	3:4:290:ASP:N	2.49	0.45
4:5:151:LEU:HD11	4:5:162:LEU:HD22	1.97	0.45
4:5:157:SER:N	4:5:298:TYR:O	2.43	0.45
2:C:295:VAL:HB	2:C:325:THR:HB	1.97	0.45
4:E:149:ARG:NH1	4:E:260:GLU:OE2	2.49	0.45
1:B:324:VAL:HG21	1:B:418:SER:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:571:HIS:O	4:E:575:ILE:HG12	2.17	0.45
5:F:628:LEU:HD11	5:F:652:ILE:HG13	1.97	0.45
1:2:763:LEU:O	1:2:767:ILE:HG13	2.17	0.45
3:4:263:ASN:OD1	3:4:324:LYS:NZ	2.50	0.45
3:4:457:TYR:HB2	6:7:253:PRO:HG2	1.98	0.45
3:4:824:GLU:OE2	3:4:827:ARG:NH2	2.49	0.45
1:B:622:GLU:OE1	4:E:445:SER:N	2.48	0.45
6:G:318:LEU:HD21	6:G:348:ILE:HD12	1.98	0.45
2:3:572:LEU:HD13	4:5:613:ARG:HH11	1.81	0.45
3:4:650:GLU:OE2	3:4:796:ARG:NH2	2.49	0.45
5:6:722:LYS:O	5:6:726:GLU:HG2	2.17	0.45
1:B:661:LEU:HD12	1:B:662:PRO:HD2	1.99	0.45
1:B:770:ALA:HA	1:B:774:ILE:HG12	1.99	0.45
3:D:290:ASP:OD1	3:D:290:ASP:N	2.49	0.45
5:6:615:ASP:OD1	5:6:615:ASP:N	2.49	0.45
6:7:644:TYR:O	6:7:647:THR:OG1	2.33	0.45
1:B:798:ILE:HD11	4:E:560:HIS:CE1	2.51	0.45
3:4:393:ASP:HB3	3:4:424:VAL:HG21	1.98	0.45
5:6:574:VAL:O	5:6:714:VAL:HA	2.17	0.45
5:F:355:ASP:HB3	5:F:386:VAL:HG21	1.99	0.45
1:B:651:ASN:ND2	7:B:2001:AGS:S1G	2.74	0.45
2:3:177:ASN:N	2:3:298:PHE:O	2.43	0.45
2:3:699:ALA:O	2:3:702:LEU:HB3	2.17	0.45
3:4:266:GLN:HE21	3:4:440:ARG:HH22	1.64	0.45
4:E:546:ILE:HA	4:E:549:ARG:HG2	1.98	0.45
5:F:650:VAL:HA	5:F:653:HIS:NE2	2.32	0.45
4:5:293:THR:HG23	4:5:334:GLN:HB2	1.99	0.45
4:5:497:MET:HG2	4:5:519:VAL:HG21	1.99	0.45
6:7:586:LEU:HD23	6:7:591:LEU:HD13	1.98	0.45
6:7:593:ARG:HG3	6:7:593:ARG:HH11	1.82	0.45
1:B:486:LYS:HA	1:B:489:ARG:HH21	1.81	0.45
5:F:357:GLN:HB2	5:F:386:VAL:HG13	1.98	0.45
1:2:550:SER:O	1:2:554:LYS:HG3	2.16	0.44
2:3:203:ALA:O	2:3:207:GLY:N	2.50	0.44
5:6:656:MET:HB3	5:6:708:ARG:HD3	1.99	0.44
3:D:474:LEU:HB2	3:D:586:PRO:HD3	1.99	0.44
4:E:405:ARG:NH2	4:E:500:GLN:OE1	2.51	0.44
3:4:308:VAL:HG22	3:4:327:ASN:HB2	1.99	0.44
7:4:2001:AGS:O3A	6:7:687:ARG:NH2	2.50	0.44
6:7:440:VAL:HG22	6:7:701:LYS:HE3	1.98	0.44
2:C:353:LEU:HD13	2:C:356:LYS:HE3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:694:LEU:HD22	3:D:698:LEU:HD23	1.97	0.44
3:D:746:PHE:HA	3:D:749:MET:HG2	1.99	0.44
5:F:842:ASP:OD1	5:F:842:ASP:N	2.47	0.44
1:B:481:GLU:O	1:B:485:ARG:HG2	2.17	0.44
1:B:597:VAL:HG23	1:B:629:ILE:HD12	1.99	0.44
2:C:681:LYS:HE2	2:C:681:LYS:HB3	1.67	0.44
3:D:429:ALA:O	3:D:587:ARG:NH2	2.45	0.44
4:5:535:SER:OG	4:5:695:ASP:OD1	2.36	0.44
1:B:511:ILE:O	1:B:515:VAL:HG23	2.17	0.44
1:B:785:LYS:NZ	1:B:831:SER:OG	2.49	0.44
2:C:391:LYS:HB2	2:C:399:LEU:HB2	1.99	0.44
3:D:758:ILE:HG22	3:D:760:PRO:HD3	1.98	0.44
4:E:41:ASP:OD1	4:E:41:ASP:N	2.50	0.44
5:F:776:LYS:HA	5:F:776:LYS:HD3	1.71	0.44
4:5:183:CYS:HB3	4:5:188:HIS:H	1.82	0.44
5:6:419:SER:HB2	5:6:448:LEU:HD11	2.00	0.44
3:D:618:SER:HA	5:F:373:MET:HE3	1.99	0.44
4:E:300:ILE:HG23	4:E:324:ARG:HB3	1.98	0.44
6:G:193:PRO:HD2	6:G:196:LEU:HD12	1.98	0.44
6:G:513:LEU:HD13	6:G:540:VAL:HG21	1.98	0.44
2:3:570:ARG:NH2	4:5:613:ARG:HH21	2.15	0.44
7:5:2001:AGS:S1G	7:5:2001:AGS:O2B	2.75	0.44
5:6:297:THR:HG22	5:6:359:VAL:HG23	1.99	0.44
6:7:210:ASN:OD1	6:7:211:CYS:N	2.51	0.44
6:7:520:ILE:HA	6:7:562:SER:O	2.18	0.44
5:F:297:THR:OG1	5:F:357:GLN:NE2	2.50	0.44
6:7:146:ARG:NH2	6:7:304:ALA:O	2.44	0.44
4:E:430:GLU:HG3	4:E:438:TYR:HB2	2.00	0.44
2:3:198:ARG:HB3	2:3:249:THR:HG22	1.99	0.44
4:5:71:TYR:HD1	4:5:72:ASN:HB2	1.82	0.44
4:5:352:GLU:HA	4:5:355:GLU:HG2	2.00	0.44
5:6:776:LYS:HD3	5:6:776:LYS:HA	1.80	0.44
2:C:430:ILE:HD12	2:C:465:ALA:HB2	1.99	0.44
4:E:164:GLY:HA3	4:E:258:LEU:HD21	1.99	0.44
6:G:322:VAL:HG21	6:G:328:PRO:HG3	1.99	0.44
2:C:461:ALA:HB2	4:E:505:ALA:HB1	2.00	0.43
6:G:23:ASP:OD1	6:G:27:THR:OG1	2.36	0.43
6:G:533:ASP:O	6:G:537:ILE:HG12	2.18	0.43
1:2:662:PRO:O	1:2:666:ASN:ND2	2.51	0.43
2:3:182:VAL:HG11	2:3:274:ILE:HD11	2.00	0.43
4:E:90:PHE:CE2	4:E:137:LEU:HD13	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:437:VAL:HG23	4:E:472:ALA:HB2	1.99	0.43
2:3:196:LEU:HD21	2:3:199:SER:HB3	2.00	0.43
3:4:139:HIS:H	3:4:266:GLN:HE22	1.65	0.43
3:4:819:LEU:HD23	3:4:823:GLN:HG3	1.99	0.43
1:B:676:ARG:HA	1:B:676:ARG:HD2	1.79	0.43
1:B:693:GLU:OE1	5:F:778:LYS:NZ	2.45	0.43
2:C:651:VAL:HG13	2:C:655:PHE:HD2	1.83	0.43
4:E:266:PRO:HG2	4:E:269:GLU:HB2	1.99	0.43
6:G:223:LYS:HA	6:G:223:LYS:HD2	1.81	0.43
5:6:288:LEU:HD23	5:6:454:PHE:HE1	1.83	0.43
5:6:429:THR:HG23	1:B:347:ILE:HD11	2.00	0.43
2:C:456:ARG:NH1	2:C:458:GLU:OE1	2.51	0.43
5:F:319:ASP:OD2	5:F:350:ARG:NH2	2.51	0.43
1:2:690:GLU:HG3	1:2:694:ARG:NE	2.34	0.43
5:6:566:ARG:O	5:6:805:ARG:NE	2.49	0.43
3:D:284:ILE:HD11	3:D:293:LEU:HD13	1.99	0.43
4:E:297:ILE:HB	4:E:329:LYS:HB2	2.00	0.43
6:7:166:LEU:HA	4:E:47:ARG:HH11	1.84	0.43
1:B:459:ARG:HD2	1:B:459:ARG:HA	1.75	0.43
4:E:646:ILE:HG21	4:E:692:ALA:HA	2.00	0.43
6:G:147:ARG:O	6:G:151:GLU:HG2	2.18	0.43
6:G:425:ASN:HB3	6:G:428:VAL:HB	2.01	0.43
6:G:637:LYS:HD3	6:G:637:LYS:HA	1.82	0.43
3:4:147:ARG:HH22	4:E:16:GLY:HA2	1.83	0.43
3:D:265:PRO:HB3	3:D:325:LEU:HG	2.01	0.43
3:D:470:SER:HB3	3:D:473:ARG:HG2	2.01	0.43
5:F:625:ALA:HB1	5:F:629:MET:HB2	2.01	0.43
6:G:358:ALA:N	6:G:373:GLU:O	2.50	0.43
1:2:542:LEU:HD22	1:2:682:VAL:HG23	2.01	0.43
4:5:371:THR:HG21	4:5:386:LYS:HG2	2.01	0.43
1:B:220:ASP:OD1	1:B:220:ASP:N	2.45	0.43
1:B:778:LEU:HD12	4:E:577:THR:HG22	2.01	0.43
2:C:216:ASP:N	2:C:216:ASP:OD1	2.51	0.43
1:2:850:LYS:HE3	1:2:852:SER:HB2	2.01	0.43
2:3:577:LEU:HD12	2:3:577:LEU:HA	1.91	0.43
3:4:268:VAL:O	3:4:272:MET:HG3	2.19	0.43
6:7:470:LEU:HD23	6:7:522:CYS:HB3	2.01	0.43
1:B:552:ILE:O	1:B:556:VAL:HG23	2.19	0.43
2:C:189:THR:HG23	2:C:256:ILE:HG22	1.99	0.43
3:D:635:ASP:OD1	3:D:635:ASP:N	2.52	0.43
5:F:300:VAL:HG13	5:F:386:VAL:HG11	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:146:ARG:NH2	6:G:304:ALA:O	2.48	0.43
3:4:559:ARG:HE	3:4:559:ARG:HB3	1.59	0.43
5:6:778:LYS:O	5:6:782:LYS:HG3	2.19	0.43
3:D:527:ALA:HB3	3:D:537:LYS:HE2	2.00	0.43
6:G:479:ARG:NE	6:G:517:ASP:O	2.52	0.43
1:2:445:PRO:HD3	5:6:325:PHE:O	2.18	0.42
1:2:510:ASP:OD2	1:2:510:ASP:N	2.51	0.42
3:4:292:ASP:OD1	3:4:292:ASP:N	2.51	0.42
3:4:344:VAL:O	3:4:389:CYS:HB2	2.19	0.42
2:C:177:ASN:N	2:C:298:PHE:O	2.45	0.42
3:D:404:ASP:OD1	3:D:405:PHE:N	2.52	0.42
6:G:132:ILE:HD11	6:G:141:VAL:HG12	2.01	0.42
3:D:176:PRO:HB2	3:D:177:LEU:H	1.66	0.42
3:D:578:LEU:HB3	3:D:590:TYR:HE2	1.84	0.42
2:3:666:ARG:HD3	2:3:666:ARG:HA	1.86	0.42
1:B:628:SER:OG	1:B:639:THR:OG1	2.37	0.42
6:G:59:LYS:HB2	6:G:59:LYS:HE2	1.87	0.42
2:3:570:ARG:HH21	4:5:616:PRO:HD3	1.83	0.42
4:5:139:LEU:HD21	4:5:331:LEU:HD13	2.01	0.42
4:5:279:ASP:OD2	4:5:279:ASP:N	2.51	0.42
5:6:657:GLU:OE1	5:6:708:ARG:NH1	2.52	0.42
2:C:455:ARG:HB2	2:C:502:ILE:HD11	2.01	0.42
3:D:524:ARG:NH1	3:D:740:ASP:O	2.53	0.42
4:E:423:SER:OG	4:E:480:ASP:OD2	2.37	0.42
6:G:181:LEU:HA	6:G:184:VAL:HG12	2.02	0.42
6:G:592:SER:OG	6:G:687:ARG:NH1	2.53	0.42
4:5:436:ALA:HA	4:5:476:VAL:O	2.19	0.42
6:7:479:ARG:NE	6:7:517:ASP:O	2.51	0.42
2:C:171:LEU:HD11	2:C:182:VAL:HG21	2.00	0.42
2:C:497:ILE:O	2:C:503:HIS:HA	2.19	0.42
3:D:824:GLU:OE2	3:D:827:ARG:NH2	2.49	0.42
4:E:279:ASP:N	4:E:279:ASP:OD1	2.52	0.42
1:B:323:VAL:HG22	1:B:423:GLU:HG2	2.01	0.42
4:E:483:ASP:OD1	4:E:484:LYS:N	2.53	0.42
6:G:607:ASP:OD1	6:G:607:ASP:N	2.52	0.42
2:3:400:ARG:HD2	2:3:491:GLU:HA	2.02	0.42
5:6:356:TRP:CH2	5:6:358:LYS:HB2	2.55	0.42
4:E:169:THR:HG22	4:E:256:LEU:HD22	2.01	0.42
2:3:280:ASP:OD2	2:3:280:ASP:N	2.51	0.42
3:4:687:PRO:HD2	3:4:690:GLU:HG3	2.00	0.42
6:7:193:PRO:HD2	6:7:196:LEU:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:457:CYS:HB3	6:7:597:LEU:HG	2.01	0.42
5:F:158:LEU:HD21	5:F:170:ILE:HD12	2.01	0.42
5:6:330:PRO:O	5:6:344:TRP:NE1	2.53	0.42
1:B:224:ARG:HE	1:B:224:ARG:HB3	1.64	0.42
4:E:633:LEU:HD13	4:E:648:ILE:HG22	2.02	0.42
2:3:669:PRO:HG2	2:3:710:THR:HG23	2.02	0.41
3:4:746:PHE:HA	3:4:749:MET:HG2	2.02	0.41
4:5:469:MET:HE1	4:5:496:ALA:HB1	2.01	0.41
5:6:650:VAL:HA	5:6:653:HIS:CE1	2.55	0.41
6:7:143:LEU:HG	6:7:197:THR:HA	2.01	0.41
2:C:557:ARG:O	2:C:561:ILE:HG12	2.20	0.41
4:E:151:LEU:HD11	4:E:162:LEU:HD22	2.02	0.41
4:E:371:THR:HG21	4:E:386:LYS:HG2	2.02	0.41
4:E:436:ALA:HA	4:E:476:VAL:O	2.20	0.41
6:G:179:ASP:O	6:G:183:GLU:HG2	2.20	0.41
2:3:363:LEU:HD23	2:3:651:VAL:HG21	2.02	0.41
4:5:101:ILE:HG12	6:G:166:LEU:HD13	2.01	0.41
6:7:527:ASP:OD1	6:7:527:ASP:N	2.53	0.41
2:C:678:VAL:HG21	2:C:723:LYS:HG2	2.01	0.41
3:D:604:TYR:CE1	3:D:617:GLU:HB3	2.55	0.41
5:F:596:VAL:HG12	5:F:631:ALA:HB2	2.02	0.41
5:F:737:LYS:HB2	5:F:741:ALA:HB2	2.03	0.41
3:4:676:ASN:ND2	7:4:2001:AGS:S1G	2.93	0.41
5:6:656:MET:SD	5:6:678:ILE:HD12	2.60	0.41
6:7:685:THR:HG22	6:7:687:ARG:H	1.85	0.41
1:B:596:LEU:HD11	1:B:620:ILE:HD13	2.01	0.41
1:B:789:VAL:HG23	1:B:864:TYR:CZ	2.56	0.41
2:C:684:THR:HG22	6:G:609:ASP:HB3	2.01	0.41
3:D:445:ARG:HB2	5:F:410:LEU:HD11	2.02	0.41
1:2:306:LEU:HB2	1:2:392:GLU:HG3	2.02	0.41
3:4:616:LEU:HD23	3:4:616:LEU:HA	1.85	0.41
4:5:449:LEU:HD12	4:5:468:ALA:HB3	2.02	0.41
6:7:17:LEU:HD13	6:7:113:PHE:HZ	1.85	0.41
6:7:530:ASP:N	6:7:530:ASP:OD1	2.47	0.41
2:C:279:ASP:OD1	2:C:279:ASP:N	2.52	0.41
3:D:701:ARG:NH1	7:F:2001:AGS:S1G	2.89	0.41
1:2:203:VAL:O	1:2:207:ILE:HG12	2.19	0.41
1:2:315:SER:N	1:2:430:TYR:O	2.48	0.41
1:2:376:ASN:O	1:2:380:THR:OG1	2.29	0.41
4:5:580:ALA:HA	4:5:583:MET:HG2	2.01	0.41
1:B:383:ARG:HB2	1:B:412:ALA:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:585:LEU:HD22	5:F:639:ASP:OD1	2.20	0.41
6:G:618:TYR:CG	6:G:626:PRO:HB3	2.55	0.41
1:2:220:ASP:OD1	1:2:220:ASP:N	2.44	0.41
4:5:557:LYS:HD2	4:5:557:LYS:HA	1.70	0.41
5:6:359:VAL:HG13	5:6:379:VAL:HG13	2.02	0.41
3:4:368:PRO:HG2	3:4:382:MET:HG3	2.03	0.41
2:C:254:GLN:HB2	2:C:283:VAL:HG12	2.01	0.41
1:2:530:LYS:HB3	4:5:428:PHE:CE1	2.56	0.41
1:2:846:VAL:HA	1:2:849:GLN:HG2	2.02	0.41
2:3:210:HIS:HB3	6:7:5:LEU:HG	2.03	0.41
3:4:176:PRO:HB2	3:4:177:LEU:H	1.61	0.41
3:4:650:GLU:HB2	3:4:701:ARG:HH11	1.86	0.41
4:5:605:TYR:HE2	4:5:668:LEU:HD11	1.85	0.41
3:D:802:ILE:HD11	5:F:732:VAL:HG22	2.01	0.41
6:G:249:SER:HB3	6:G:312:GLU:H	1.85	0.41
6:G:481:VAL:HG11	6:G:512:ALA:HB1	2.02	0.41
1:2:685:ASP:OD1	1:2:685:ASP:N	2.46	0.41
1:2:693:GLU:HG3	5:6:778:LYS:HD2	2.01	0.41
3:4:663:THR:HG21	5:6:374:PRO:HG3	2.03	0.41
4:5:274:LEU:HD23	4:5:274:LEU:HA	1.94	0.41
4:5:416:GLY:HA3	4:5:556:VAL:HB	2.02	0.41
4:5:432:VAL:HG23	4:5:596:ILE:HG13	2.03	0.41
5:6:609:THR:HG22	5:6:628:LEU:HD12	2.03	0.41
5:6:653:HIS:HB3	5:6:705:ILE:HD13	2.03	0.41
5:6:694:SER:OG	5:6:695:LEU:N	2.54	0.41
5:6:767:LYS:HB3	5:6:767:LYS:HE3	1.72	0.41
6:7:59:LYS:HE2	6:7:59:LYS:HB2	1.85	0.41
3:D:195:ARG:O	3:D:199:MET:HG2	2.21	0.41
1:2:447:PHE:HE1	5:6:304:LEU:HB2	1.85	0.41
2:3:561:ILE:HG21	4:5:650:ILE:HG12	2.02	0.41
6:7:243:GLY:HA2	6:7:318:LEU:HG	2.03	0.41
6:7:423:TYR:HB2	6:7:615:HIS:CG	2.56	0.41
1:B:495:ASP:O	1:B:499:SER:N	2.52	0.41
4:E:493:ILE:HD13	4:E:493:ILE:HA	1.94	0.41
3:4:429:ALA:O	3:4:587:ARG:NH2	2.52	0.40
5:6:412:LEU:HD23	5:6:412:LEU:HA	1.97	0.40
6:7:259:ALA:H	6:7:305:SER:HB3	1.85	0.40
6:7:658:ASP:O	6:7:662:GLN:HG2	2.21	0.40
2:C:466:ASP:HB3	6:G:324:VAL:HG13	2.02	0.40
5:F:614:ARG:HB2	5:F:621:TYR:CE1	2.56	0.40
6:G:5:LEU:HD12	6:G:5:LEU:HA	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:438:THR:HG23	3:4:462:ASP:HB3	2.03	0.40
6:7:592:SER:OG	6:7:687:ARG:NH1	2.55	0.40
1:B:324:VAL:HG13	1:B:388:VAL:HG13	2.04	0.40
1:B:793:LEU:HD11	1:B:805:ILE:HG21	2.03	0.40
3:D:457:TYR:HB2	6:G:253:PRO:HG2	2.03	0.40
3:D:719:GLU:HA	3:D:722:LYS:HE2	2.03	0.40
6:G:210:ASN:O	6:G:214:ARG:HG3	2.21	0.40
6:G:459:MET:HA	6:G:567:ALA:O	2.22	0.40
2:3:442:LEU:HD13	2:3:486:ILE:HD11	2.02	0.40
3:4:404:ASP:OD1	3:4:404:ASP:N	2.51	0.40
3:4:711:LYS:HE3	3:4:848:ASN:HA	2.02	0.40
3:D:276:ILE:HD13	3:D:276:ILE:HA	1.91	0.40
4:E:87:ILE:HG23	4:E:137:LEU:HD23	2.03	0.40
5:F:574:VAL:HG21	5:F:699:LEU:HD11	2.04	0.40
5:F:649:GLN:HA	5:F:652:ILE:HG22	2.03	0.40
1:2:271:PHE:CD2	1:2:295:VAL:HG21	2.56	0.40
6:7:601:LEU:HD12	6:7:727:LEU:HG	2.03	0.40
1:B:445:PRO:HD3	5:F:325:PHE:O	2.20	0.40
3:D:212:ARG:HB3	3:D:215:PHE:HD1	1.87	0.40
3:D:435:VAL:HG13	3:D:463:VAL:HG13	2.04	0.40
3:D:456:LEU:HD12	3:D:456:LEU:HA	1.88	0.40
6:7:242:ARG:HB3	6:7:350:ASP:OD1	2.22	0.40
2:C:103:LEU:HD11	2:C:110:PHE:HD2	1.86	0.40
4:E:90:PHE:CE2	4:E:94:ILE:HD11	2.57	0.40
6:G:154:LEU:HD21	6:G:191:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	2	622/868 (72%)	602 (97%)	20 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	622/868 (72%)	608 (98%)	14 (2%)	0	100	100
2	3	627/971 (65%)	612 (98%)	15 (2%)	0	100	100
2	C	627/971 (65%)	606 (97%)	21 (3%)	0	100	100
3	4	684/933 (73%)	668 (98%)	16 (2%)	0	100	100
3	D	664/933 (71%)	649 (98%)	15 (2%)	0	100	100
4	5	650/775 (84%)	630 (97%)	20 (3%)	0	100	100
4	E	650/775 (84%)	633 (97%)	17 (3%)	0	100	100
5	6	638/1017 (63%)	615 (96%)	23 (4%)	0	100	100
5	F	638/1017 (63%)	620 (97%)	18 (3%)	0	100	100
6	7	693/845 (82%)	684 (99%)	9 (1%)	0	100	100
6	G	693/845 (82%)	682 (98%)	11 (2%)	0	100	100
All	All	7808/10818 (72%)	7609 (98%)	199 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [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%)	551 (100%)	1 (0%)	93	98
1	B	552/770 (72%)	551 (100%)	1 (0%)	93	98
2	3	550/835 (66%)	550 (100%)	0	100	100
2	C	550/835 (66%)	550 (100%)	0	100	100
3	4	628/848 (74%)	628 (100%)	0	100	100
3	D	606/848 (72%)	606 (100%)	0	100	100
4	5	588/688 (86%)	587 (100%)	1 (0%)	93	98
4	E	588/688 (86%)	586 (100%)	2 (0%)	92	96
5	6	565/886 (64%)	563 (100%)	2 (0%)	91	95
5	F	565/886 (64%)	565 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	7	618/753 (82%)	617 (100%)	1 (0%)	93	98
6	G	618/753 (82%)	617 (100%)	1 (0%)	93	98
All	All	6980/9560 (73%)	6971 (100%)	9 (0%)	93	98

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	694	ARG
4	5	339	THR
5	6	101	LYS
5	6	738	ARG
6	7	73	ARG
1	B	489	ARG
4	E	339	THR
4	E	625	ASN
6	G	73	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	5	499	GLN
4	E	574	ASN
4	E	636	ASN
5	F	269	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	E	2001	8	26,33,33	0.72	1 (3%)	26,52,52	1.15	2 (7%)
10	ADP	C	2001	8	24,29,29	0.93	1 (4%)	29,45,45	1.43	4 (13%)
10	ADP	3	2001	8	24,29,29	0.95	1 (4%)	29,45,45	1.48	4 (13%)
7	AGS	2	2001	8	26,33,33	0.71	1 (3%)	26,52,52	1.04	2 (7%)
7	AGS	6	2001	8	26,33,33	0.69	1 (3%)	26,52,52	0.89	2 (7%)
7	AGS	D	2001	8	26,33,33	0.70	0	26,52,52	1.08	2 (7%)
7	AGS	B	2001	8	26,33,33	0.69	1 (3%)	26,52,52	1.03	2 (7%)
7	AGS	4	2001	8	26,33,33	0.69	0	26,52,52	1.10	2 (7%)
7	AGS	G	2001	8	26,33,33	0.72	1 (3%)	26,52,52	1.06	2 (7%)
7	AGS	F	2001	8	26,33,33	0.70	1 (3%)	26,52,52	1.06	2 (7%)
7	AGS	5	2001	8	26,33,33	0.72	1 (3%)	26,52,52	1.17	2 (7%)
7	AGS	7	2001	8	26,33,33	0.72	1 (3%)	26,52,52	1.05	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	AGS	E	2001	8	-	6/17/38/38	0/3/3/3
10	ADP	C	2001	8	-	3/12/32/32	0/3/3/3
10	ADP	3	2001	8	-	3/12/32/32	0/3/3/3
7	AGS	2	2001	8	-	7/17/38/38	0/3/3/3
7	AGS	6	2001	8	-	3/17/38/38	0/3/3/3
7	AGS	D	2001	8	-	7/17/38/38	0/3/3/3
7	AGS	B	2001	8	-	4/17/38/38	0/3/3/3
7	AGS	4	2001	8	-	7/17/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	AGS	G	2001	8	-	7/17/38/38	0/3/3/3
7	AGS	F	2001	8	-	2/17/38/38	0/3/3/3
7	AGS	5	2001	8	-	6/17/38/38	0/3/3/3
7	AGS	7	2001	8	-	6/17/38/38	0/3/3/3

All (10) bond length outliers are listed below:

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

All (28) bond angle outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	2001	AGS	C5-C6-N6	2.31	123.86	120.35
7	2	2001	AGS	C5-C6-N6	2.28	123.82	120.35
7	D	2001	AGS	C5-C6-N6	2.28	123.81	120.35
7	B	2001	AGS	C5-C6-N6	2.26	123.78	120.35
7	E	2001	AGS	C5-C6-N6	2.25	123.77	120.35
7	6	2001	AGS	C5-C6-N6	2.25	123.77	120.35
7	5	2001	AGS	C5-C6-N6	2.25	123.77	120.35
7	7	2001	AGS	C5-C6-N6	2.23	123.74	120.35
7	G	2001	AGS	C5-C6-N6	2.22	123.73	120.35

There are no chirality outliers.

All (61) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

7 monomers are involved in 13 short contacts:

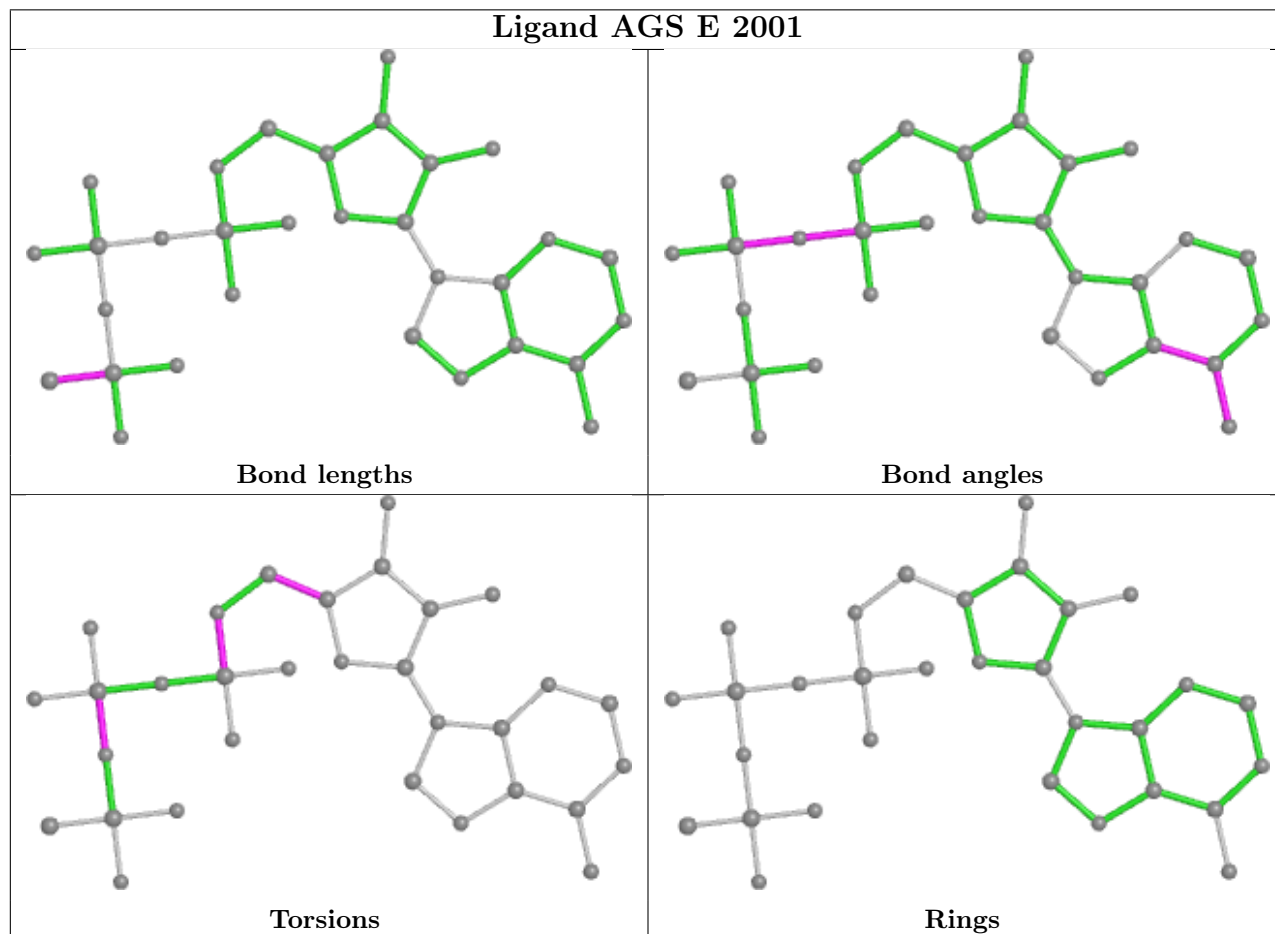
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	6	2001	AGS	1	0
7	D	2001	AGS	4	0
7	B	2001	AGS	1	0
7	4	2001	AGS	4	0

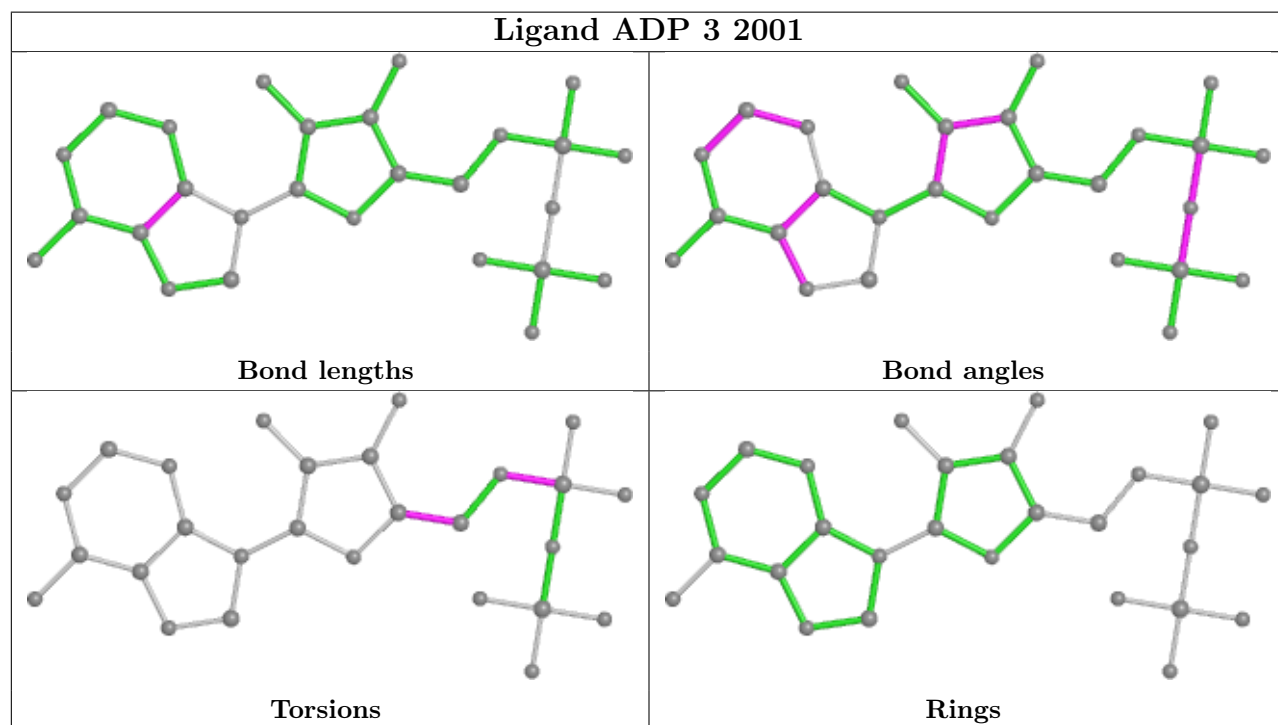
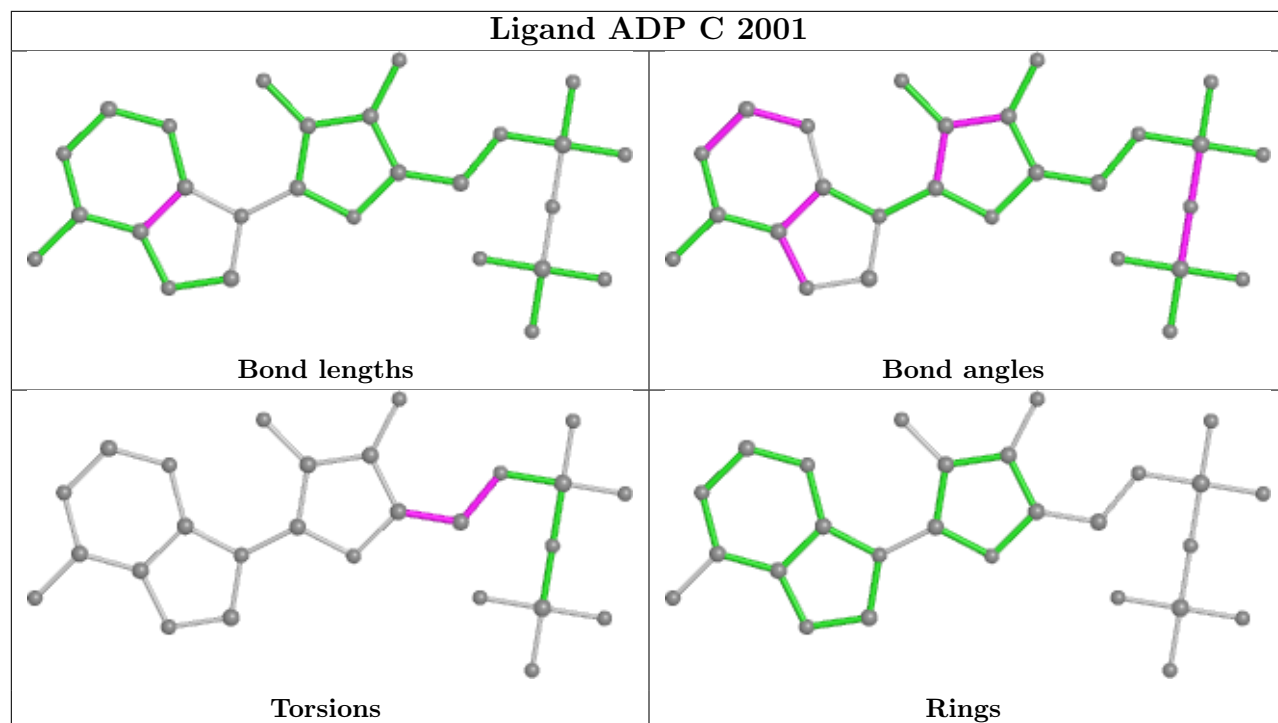
Continued on next page...

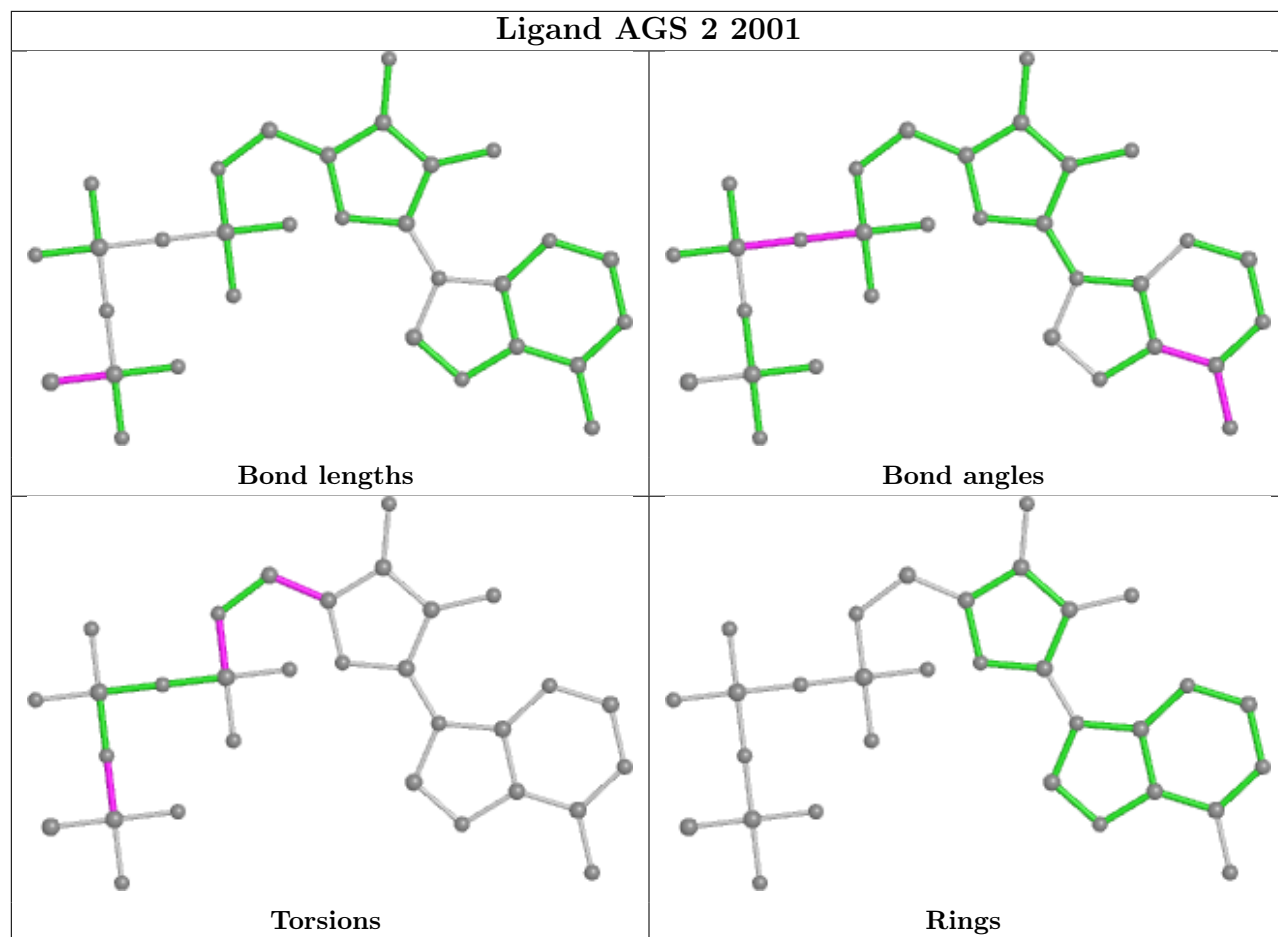
Continued from previous page...

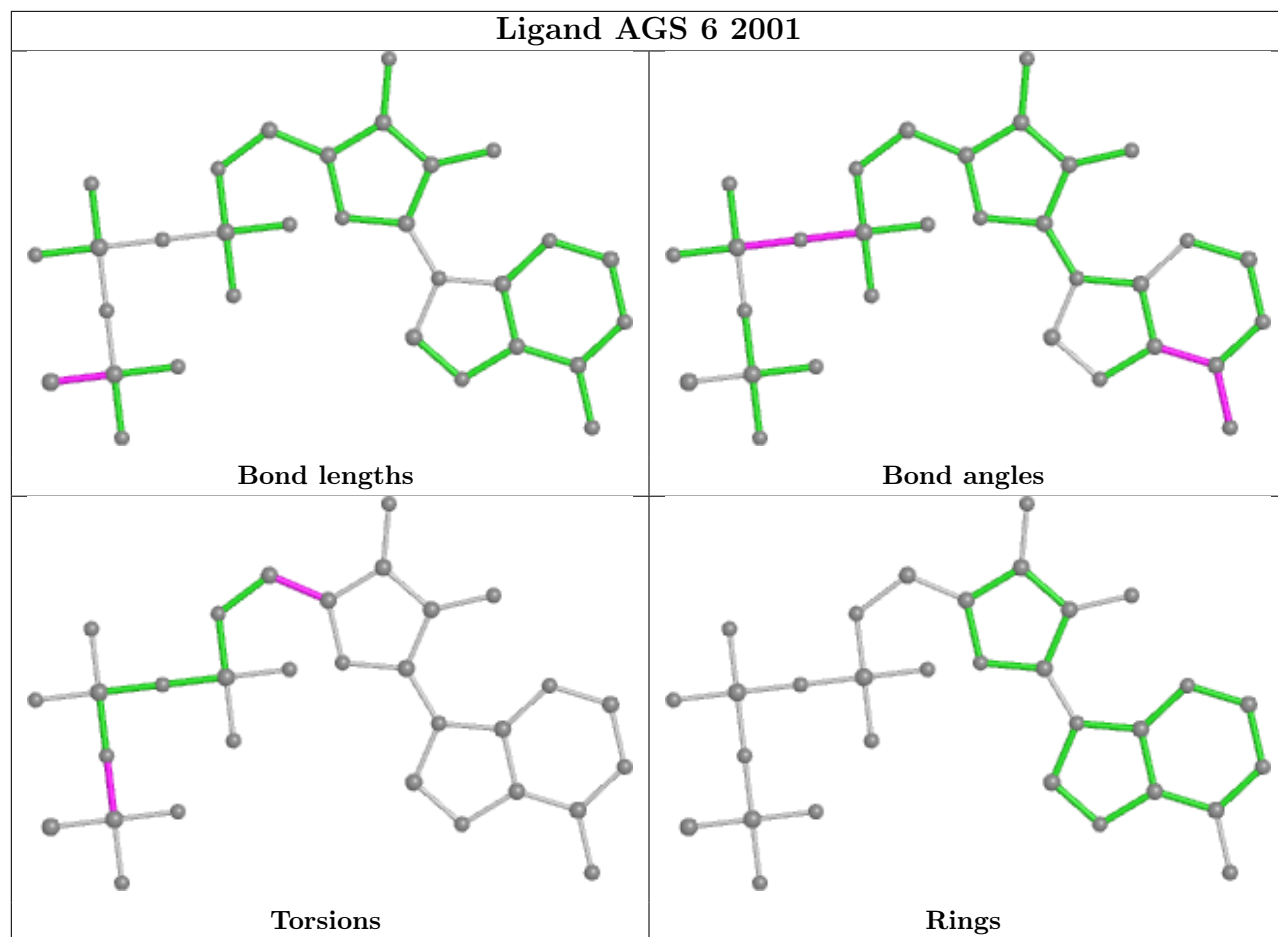
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	2001	AGS	1	0
7	5	2001	AGS	1	0
7	7	2001	AGS	1	0

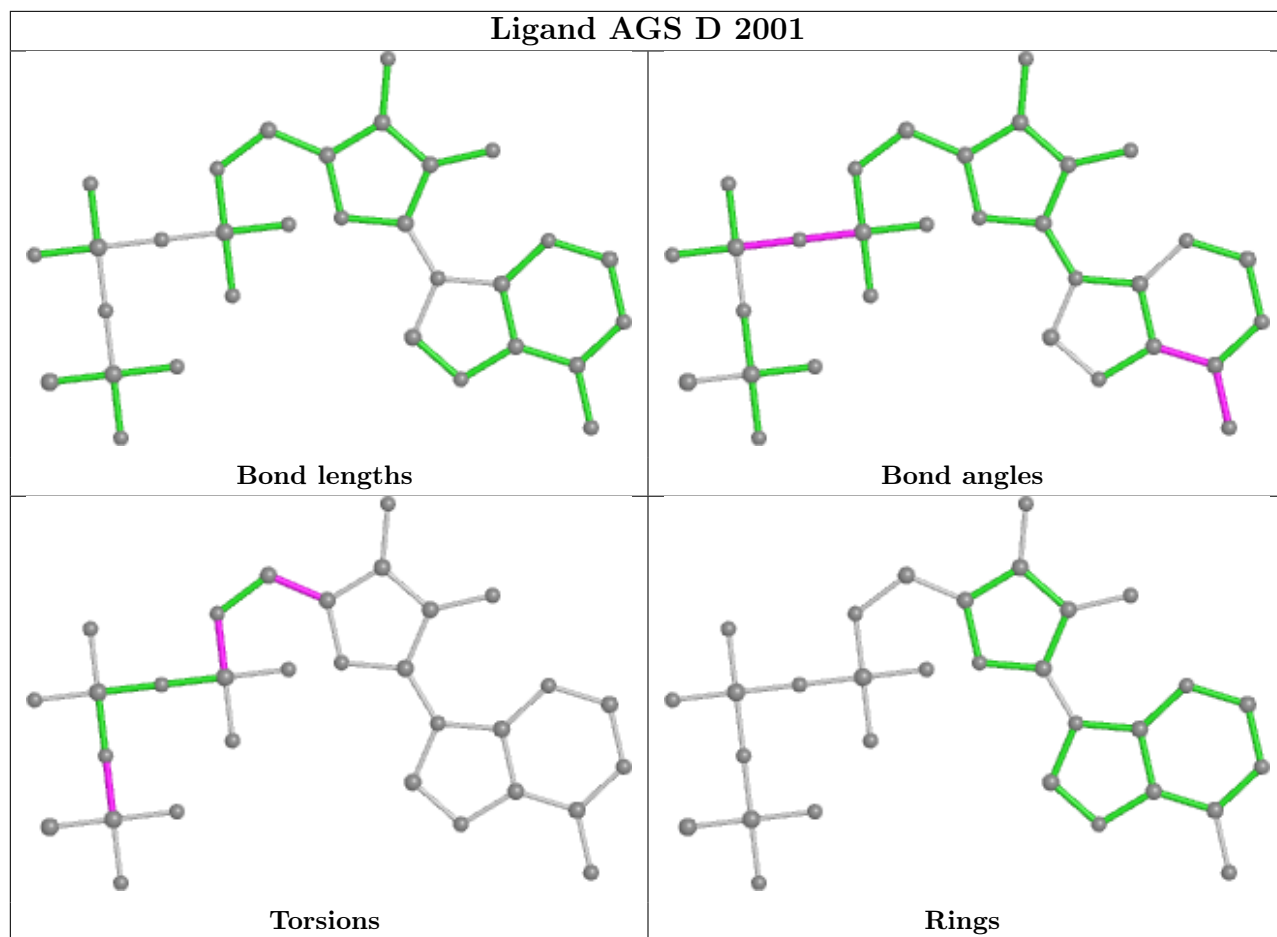
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

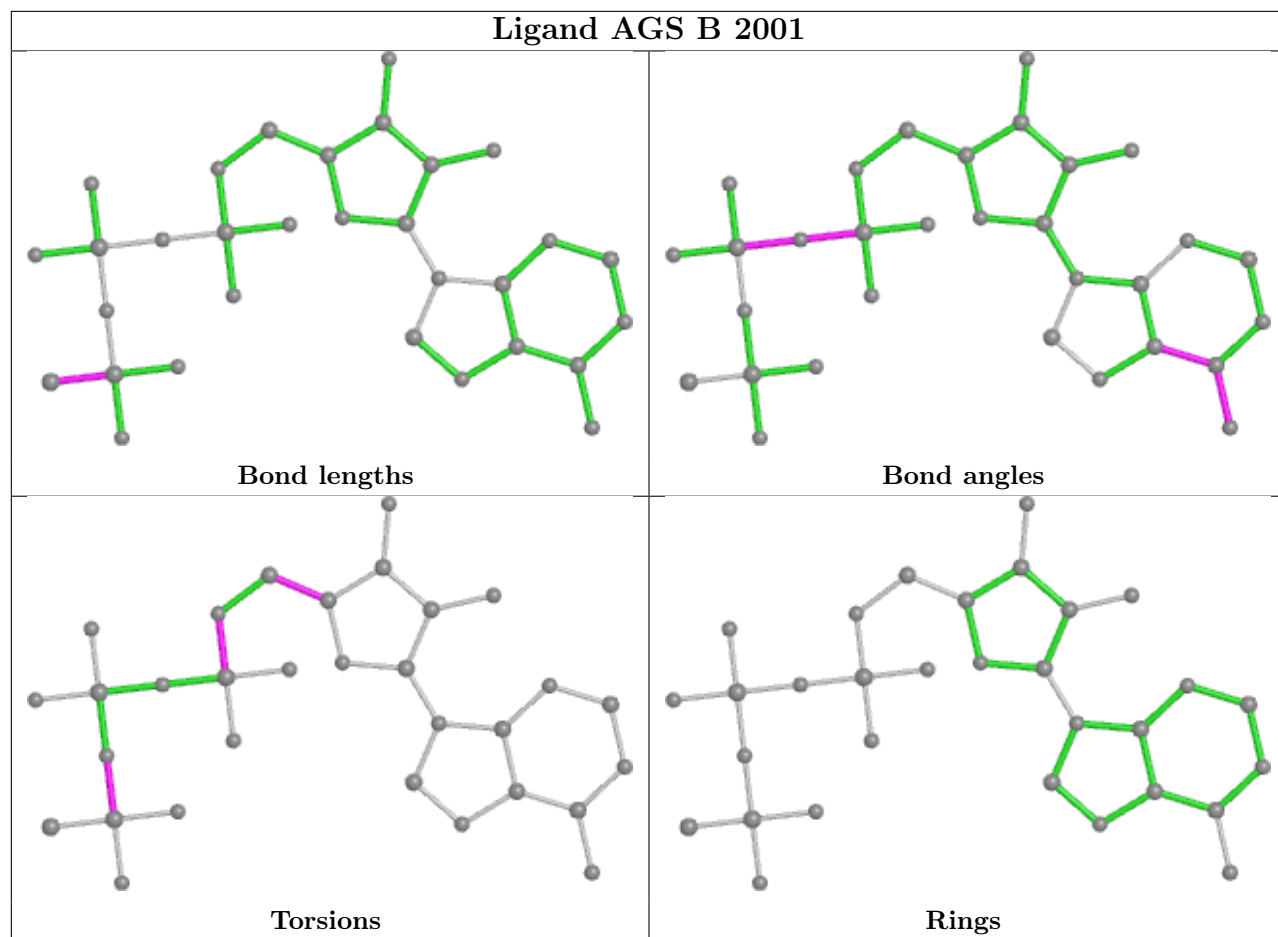


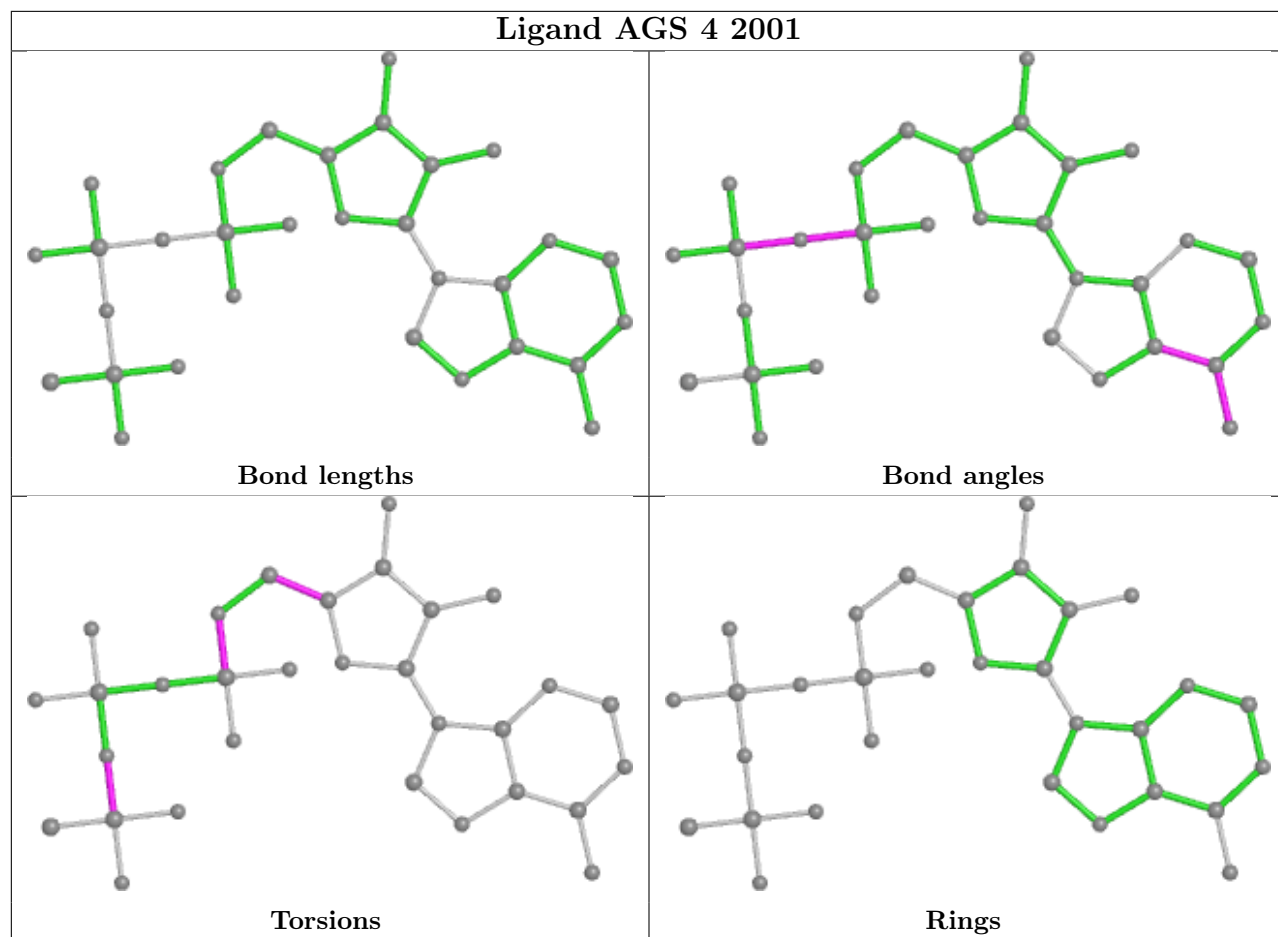


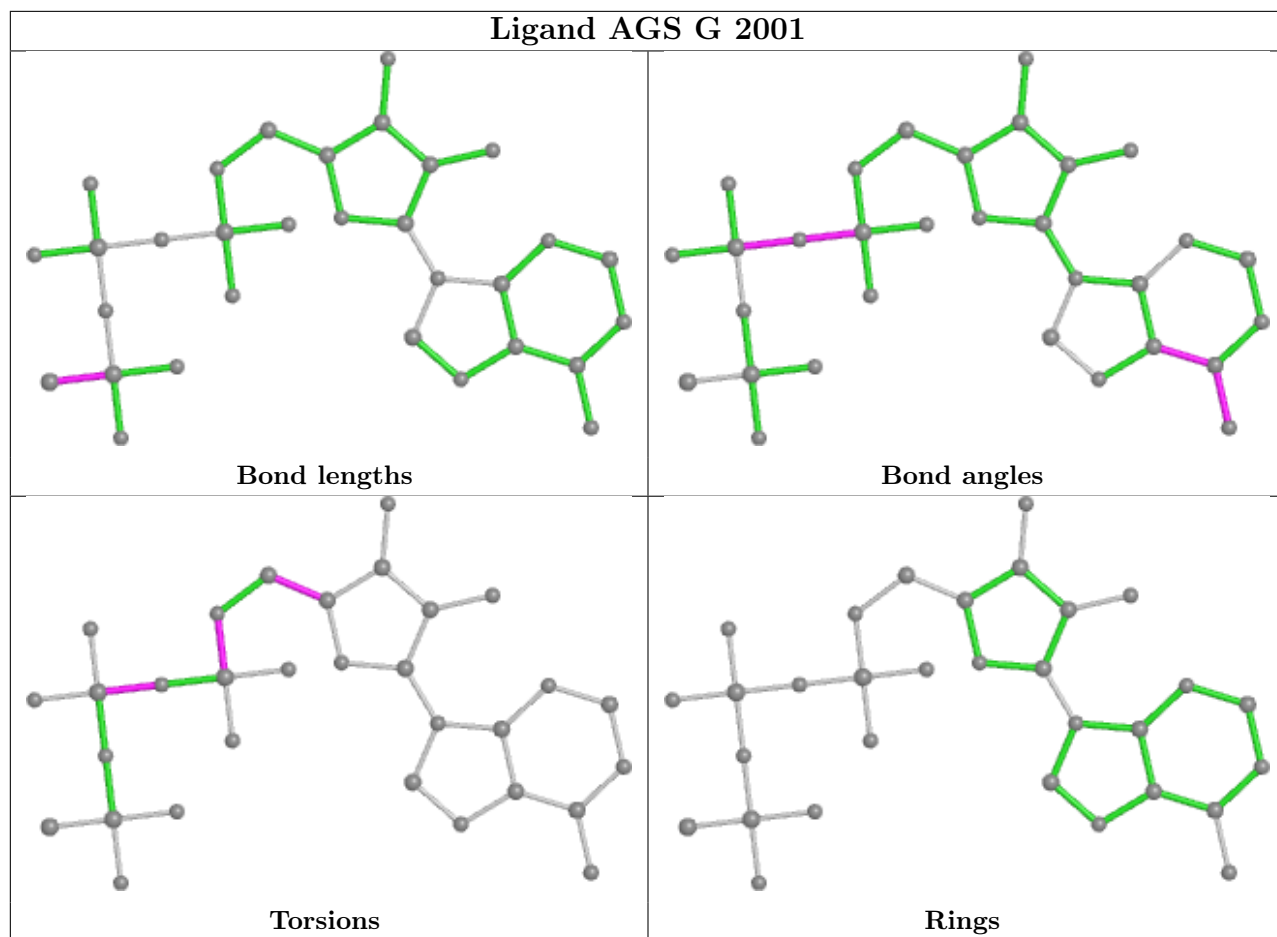


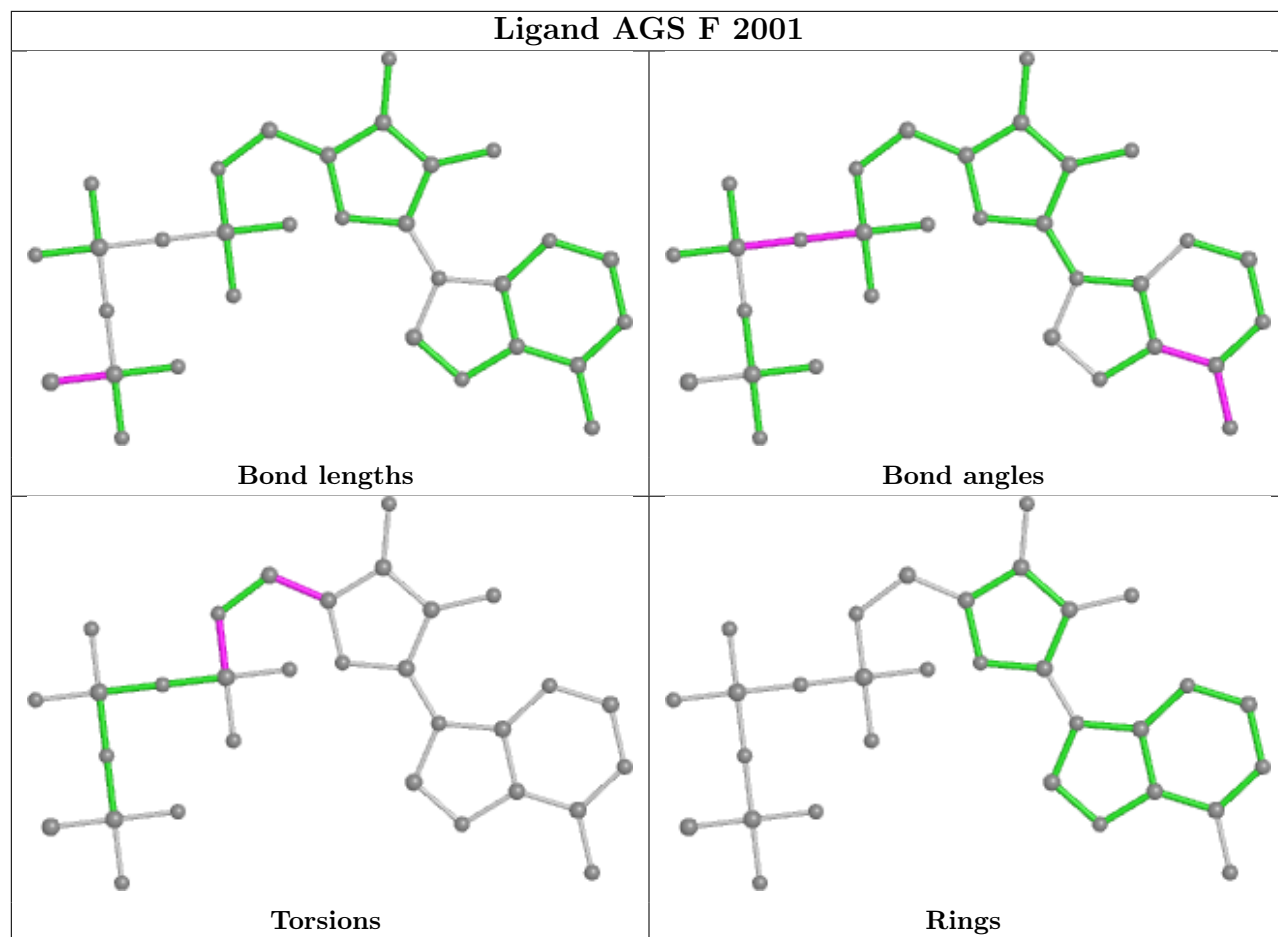


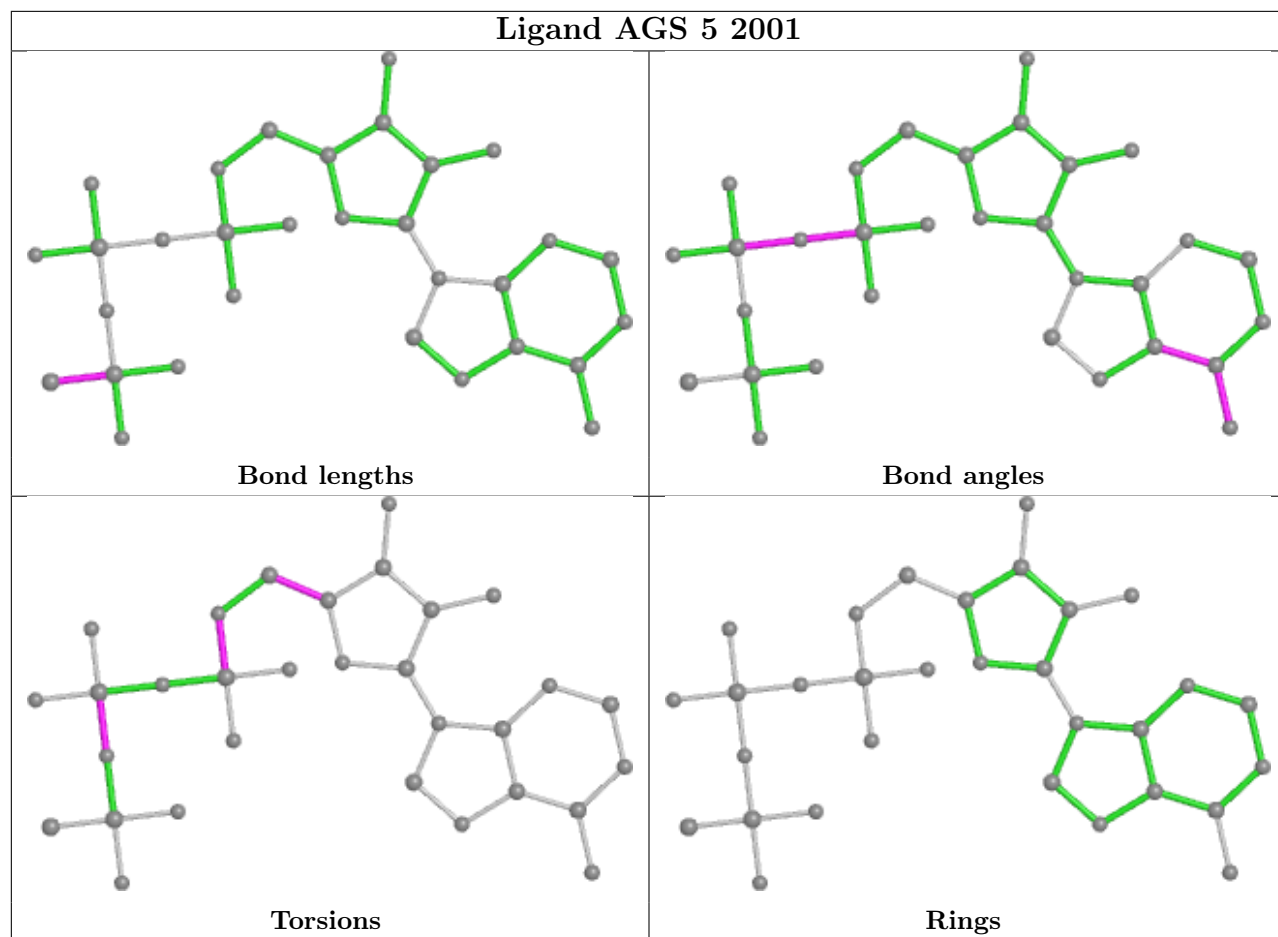


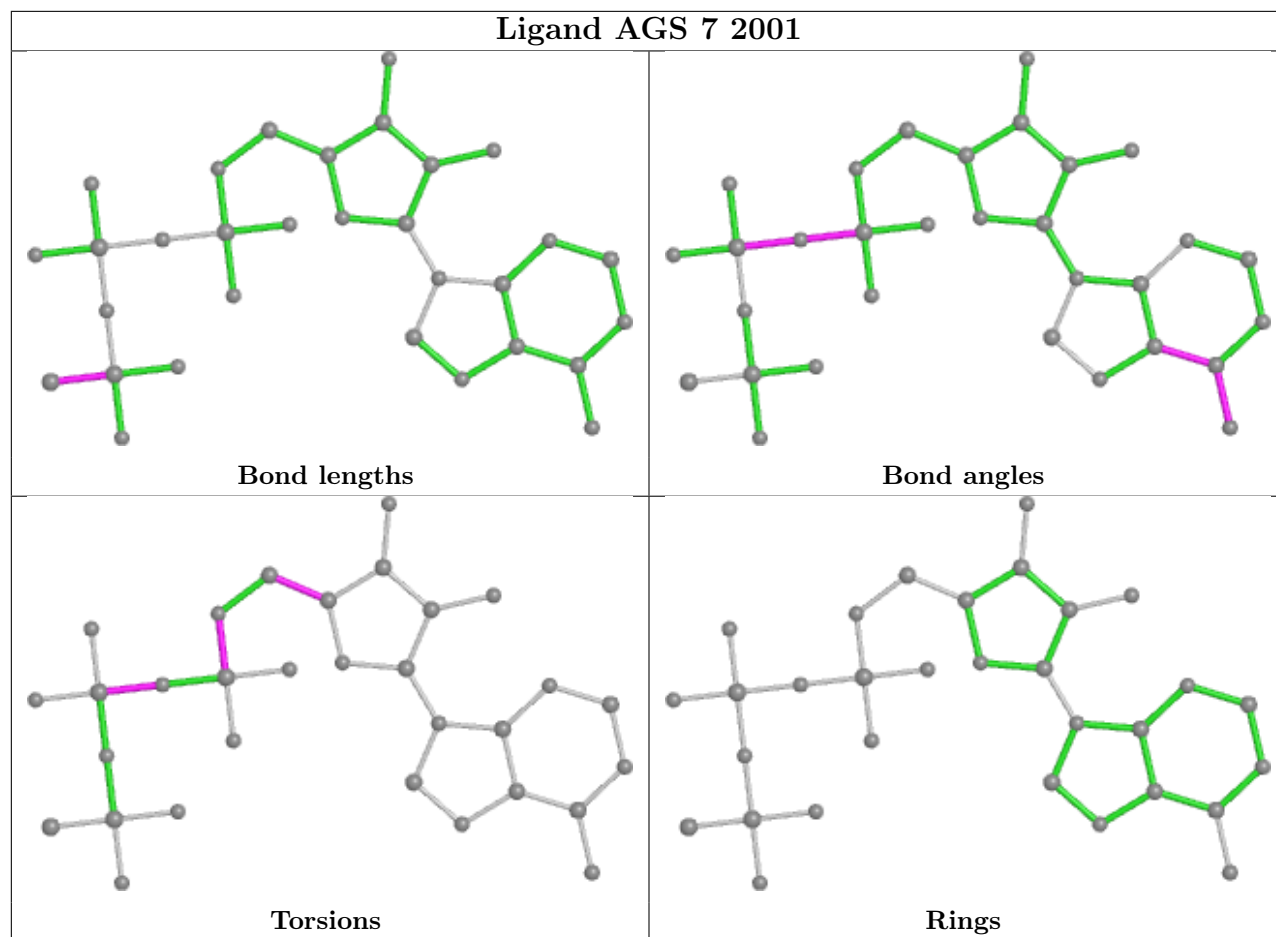












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

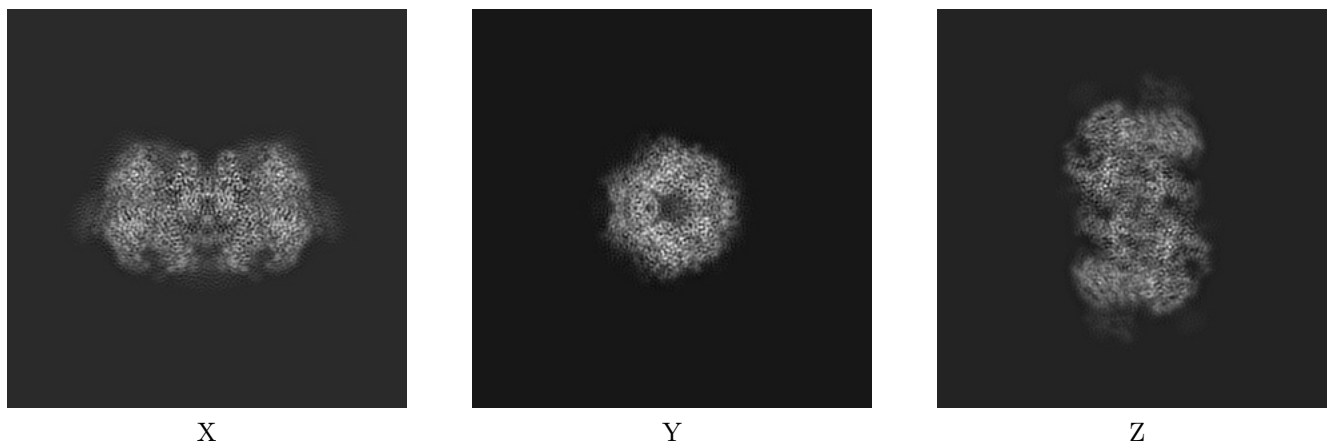
6 Map visualisation [i](#)

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

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

6.1 Orthogonal projections [i](#)

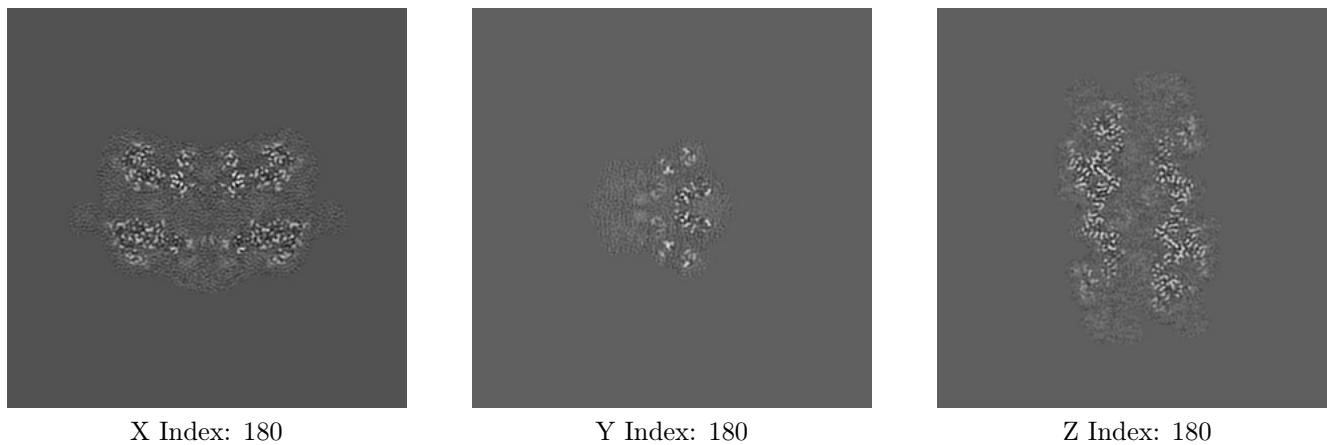
6.1.1 Primary map



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

6.2 Central slices [i](#)

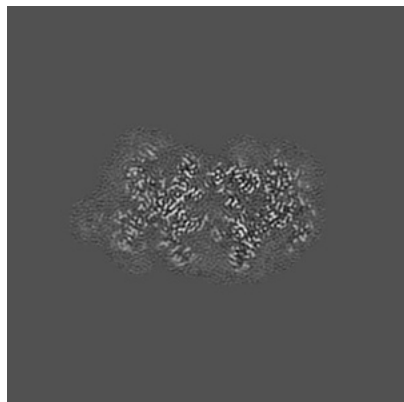
6.2.1 Primary map



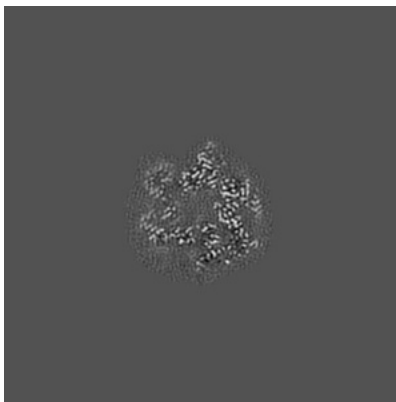
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

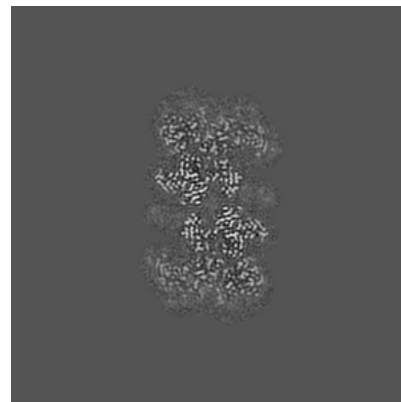
6.3.1 Primary map



X Index: 159



Y Index: 203

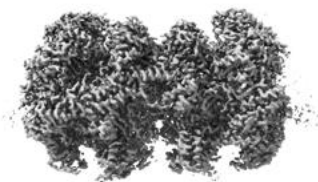


Z Index: 206

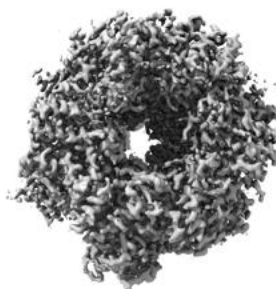
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

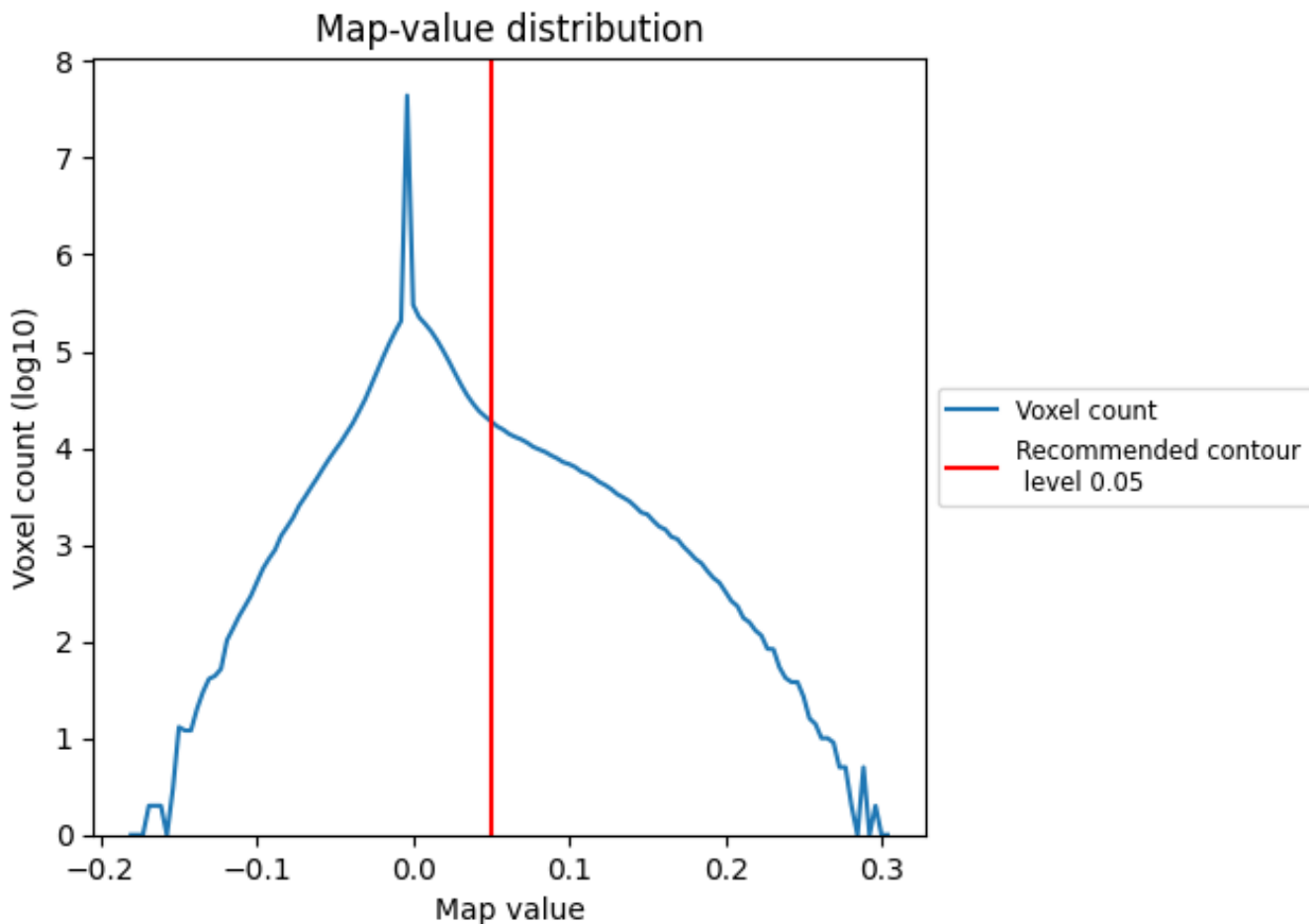
6.5 Mask visualisation

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

7 Map analysis [i](#)

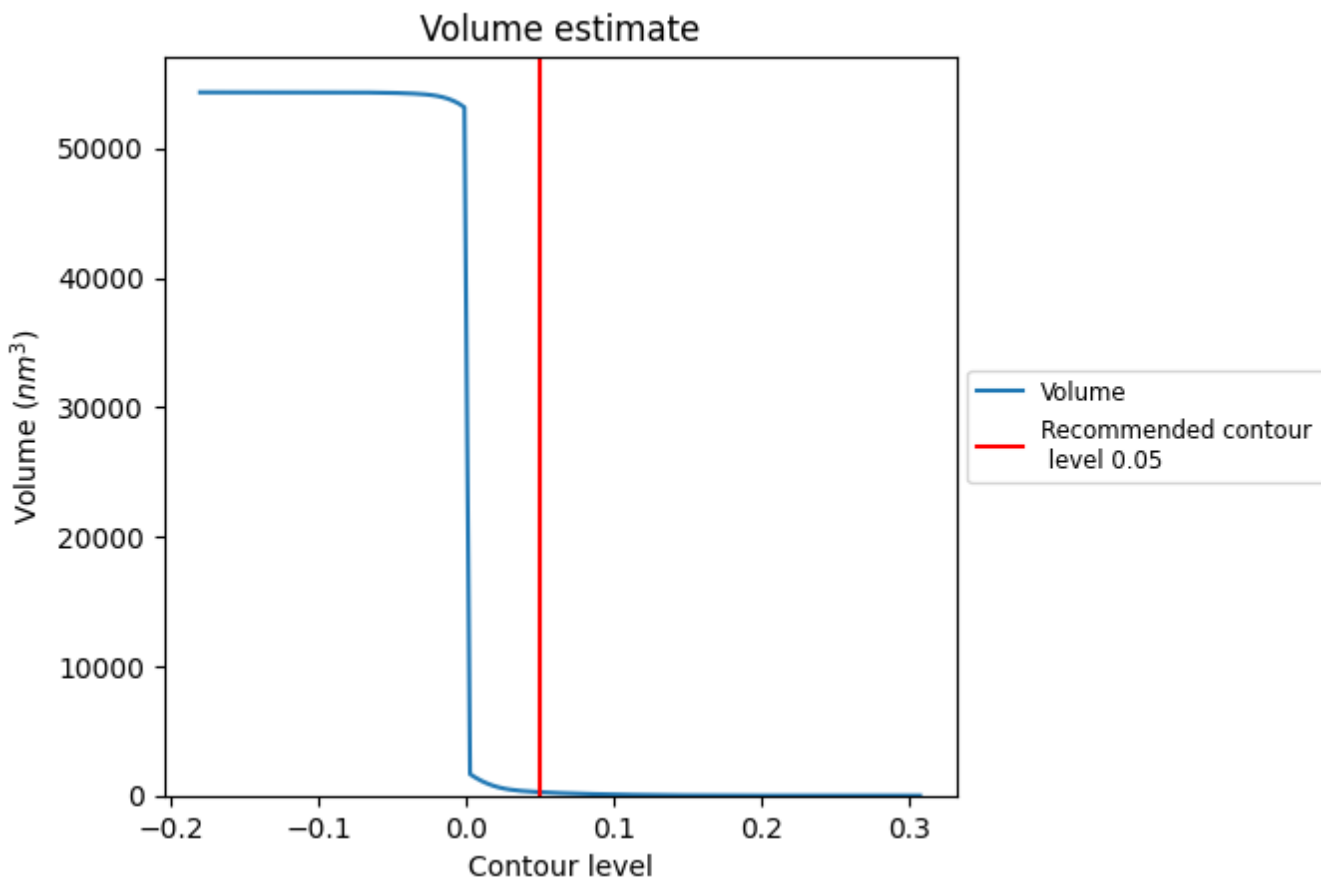
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

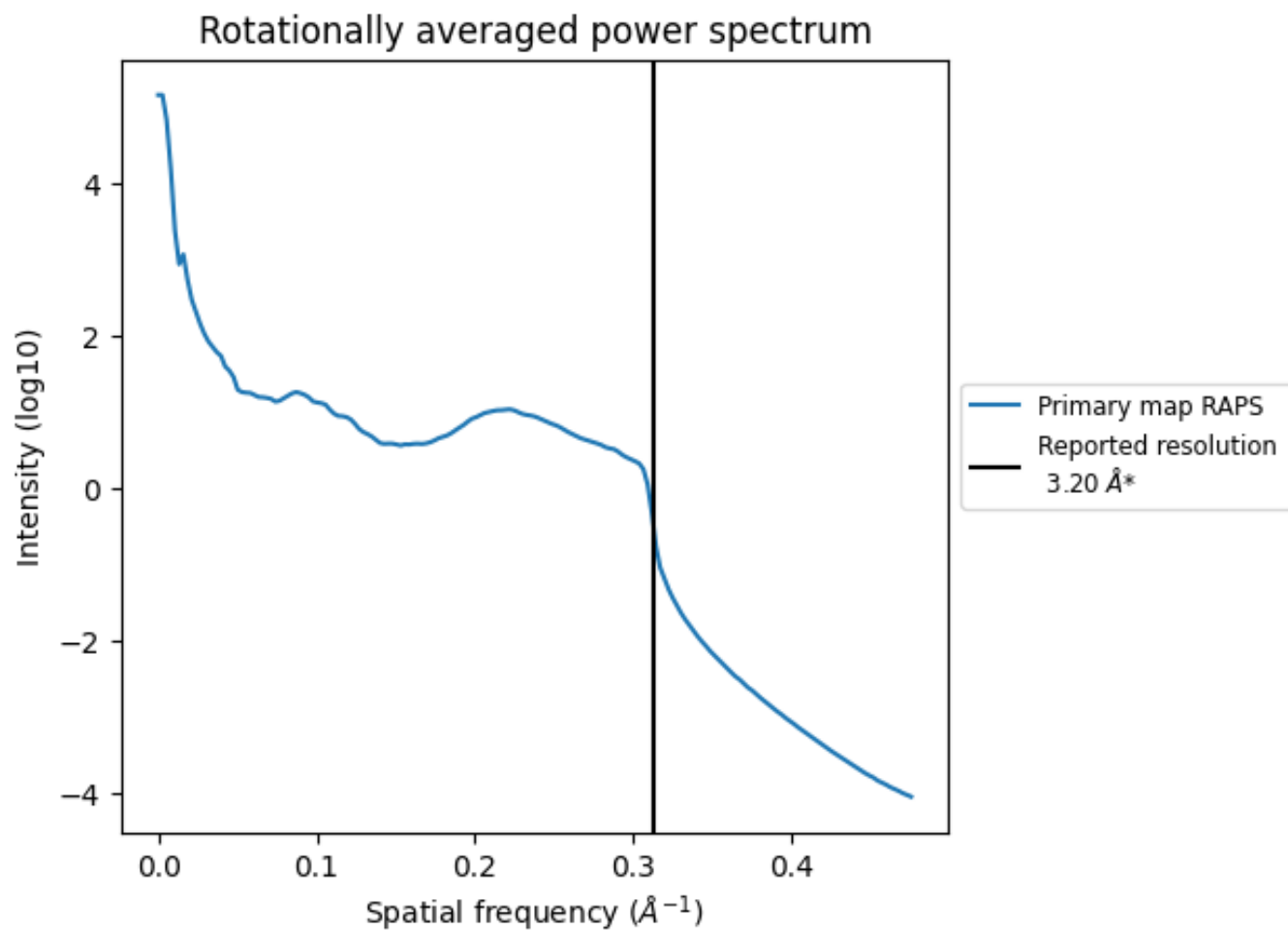
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 262 nm³; this corresponds to an approximate mass of 237 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.312\AA^{-1}

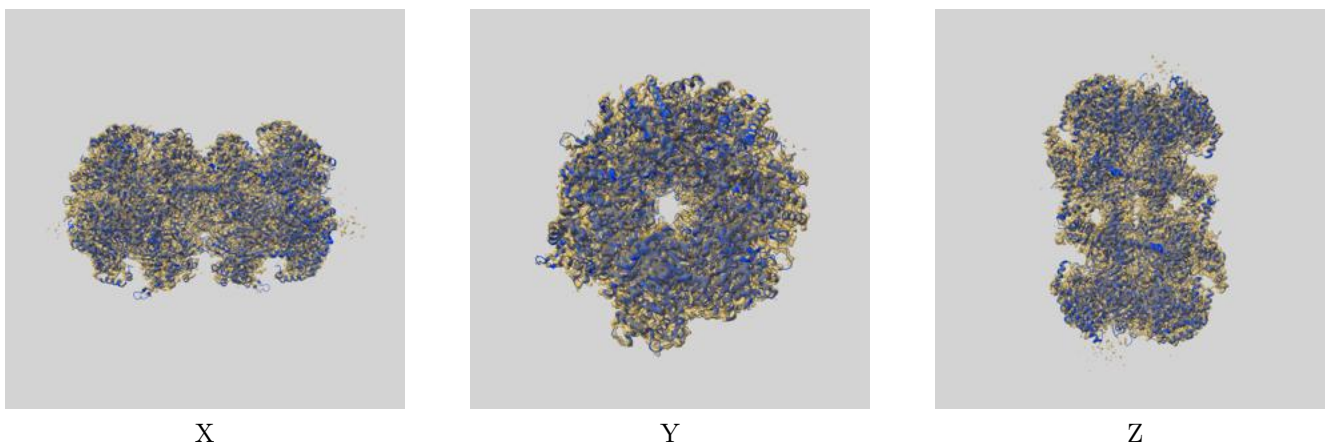
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

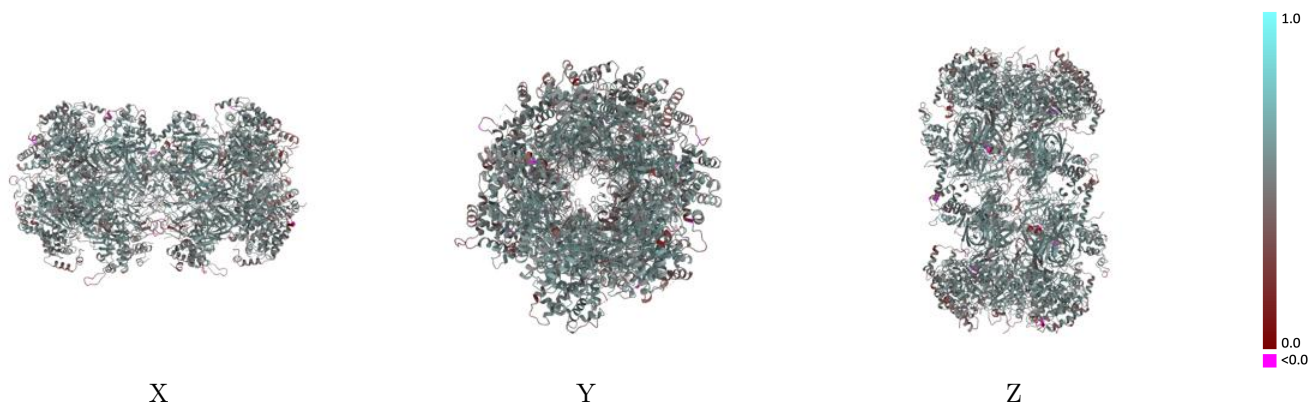
This section contains information regarding the fit between EMDB map EMD-31684 and PDB model 7V3U. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



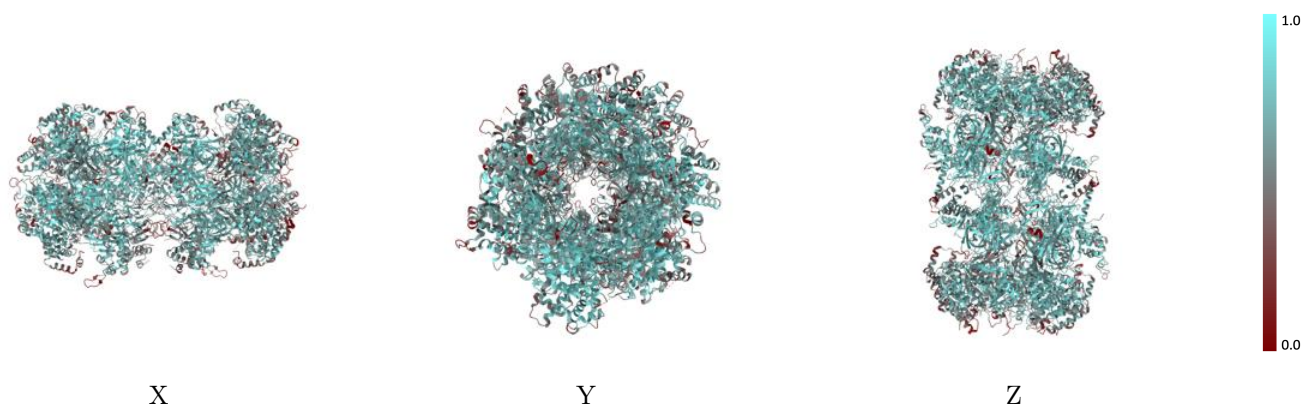
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



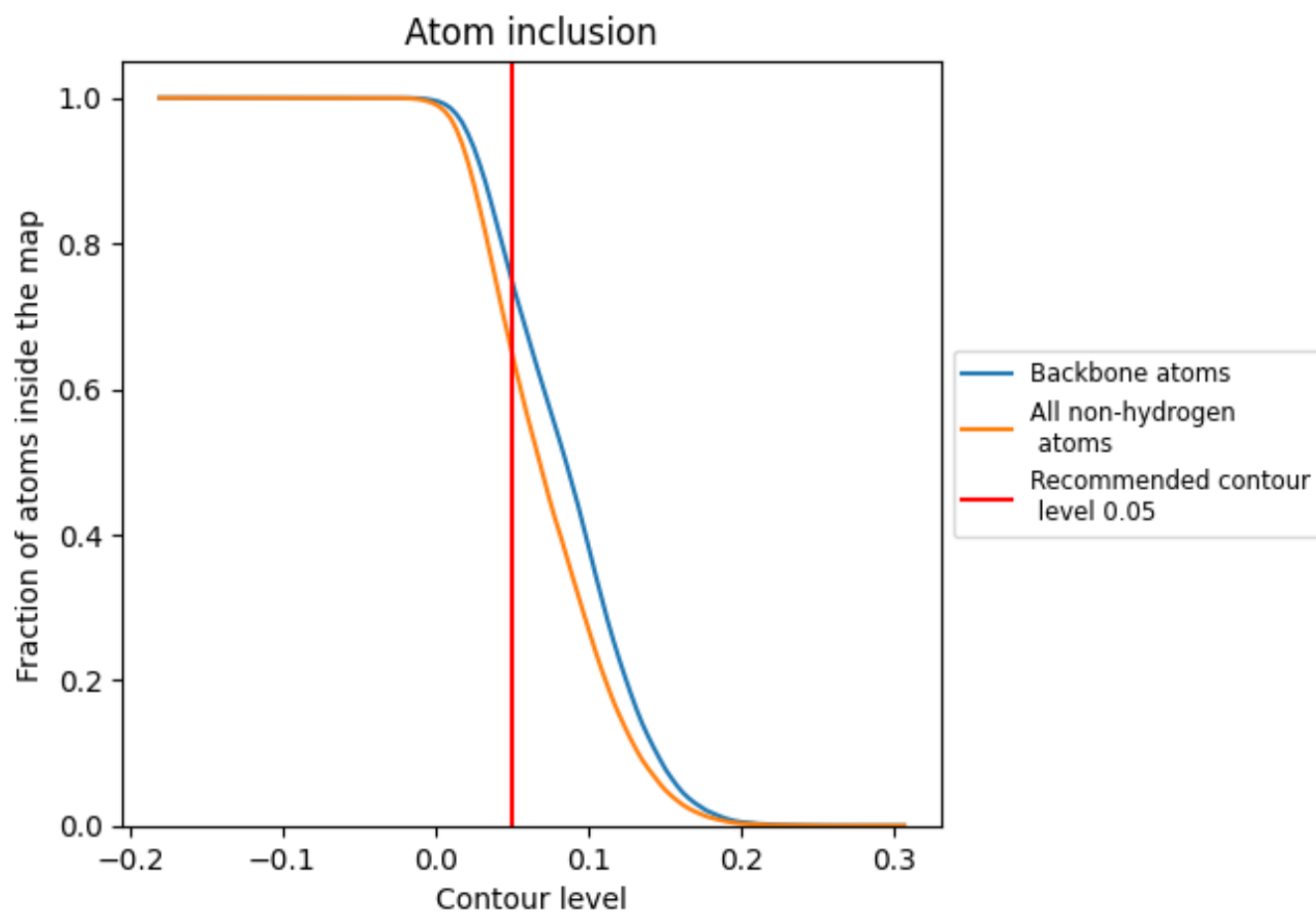
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6534	 0.5140
2	 0.6142	 0.5000
3	 0.6770	 0.5260
4	 0.7021	 0.5320
5	 0.6352	 0.5030
6	 0.6271	 0.5030
7	 0.6993	 0.5290
B	 0.6060	 0.5000
C	 0.6680	 0.5190
D	 0.6890	 0.5290
E	 0.6281	 0.5040
F	 0.6016	 0.4970
G	 0.6808	 0.5250

