



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:13 AM EST

PDB ID : 5BK4
EMDB ID : EMD-9400
Title : Cryo-EM structure of Mcm2-7 double hexamer on dsDNA
Authors : Li, H.; Yuan, Z.; Bai, L.
Deposited on : 2017-09-12
Resolution : 3.90 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.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

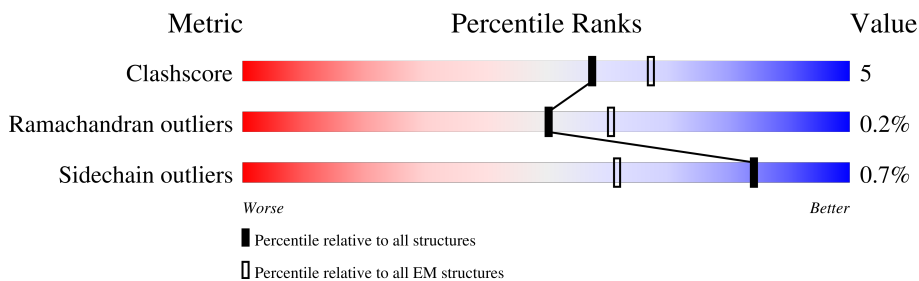
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.





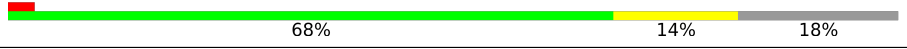



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
1	A	868	
2	3	971	
2	B	971	
3	4	933	
3	C	933	
4	5	775	
4	D	775	

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Mol	Chain	Length	Quality of chain
5	6	1017	 52% 9% 40%
5	E	1017	 52% 8% 40%
6	7	845	 68% 14% 18%
6	F	845	 67% 14% 18%
7	S	60	 7% 83% 17%
8	O	60	 8% 85% 15%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 62482 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	603	Total	C	N	O	S	0	0
			4714	2974	842	881	17		
1	A	603	Total	C	N	O	S	0	0
			4714	2974	842	881	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	604	Total	C	N	O	S	0	0
			4734	2981	844	896	13		
2	B	604	Total	C	N	O	S	0	0
			4734	2981	844	896	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	646	Total	C	N	O	S	0	0
			5127	3221	888	990	28		
3	C	646	Total	C	N	O	S	0	0
			5127	3221	888	990	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	661	Total	C	N	O	S	0	0
			5165	3231	887	1022	25		
4	D	661	Total	C	N	O	S	0	0
			5165	3231	887	1022	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	615	Total 4731	C 2979	N 837	O 895	S 20	0	0
5	E	615	Total 4731	C 2979	N 837	O 895	S 20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	689	Total 5432	C 3419	N 940	O 1042	S 31	0	0
6	F	689	Total 5432	C 3419	N 940	O 1042	S 31	0	0

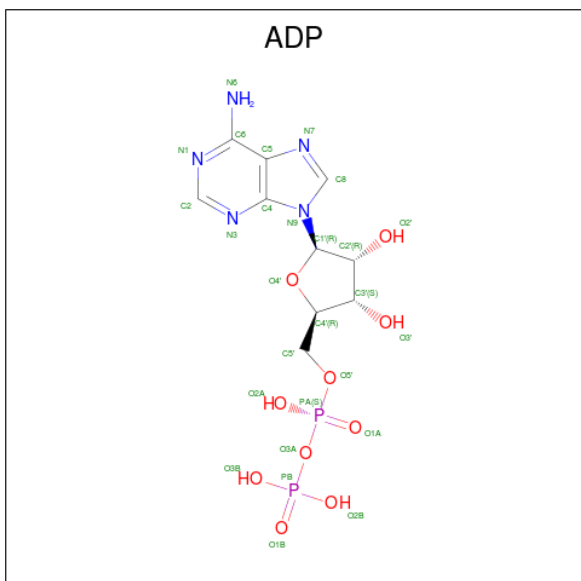
- Molecule 7 is a DNA chain called DNA (60-mer), strand 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	S	60	Total 1230	C 585	N 225	O 360	P 60	0	0

- Molecule 8 is a DNA chain called DNA (60-mer), strand 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	O	60	Total 1230	C 585	N 225	O 360	P 60	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

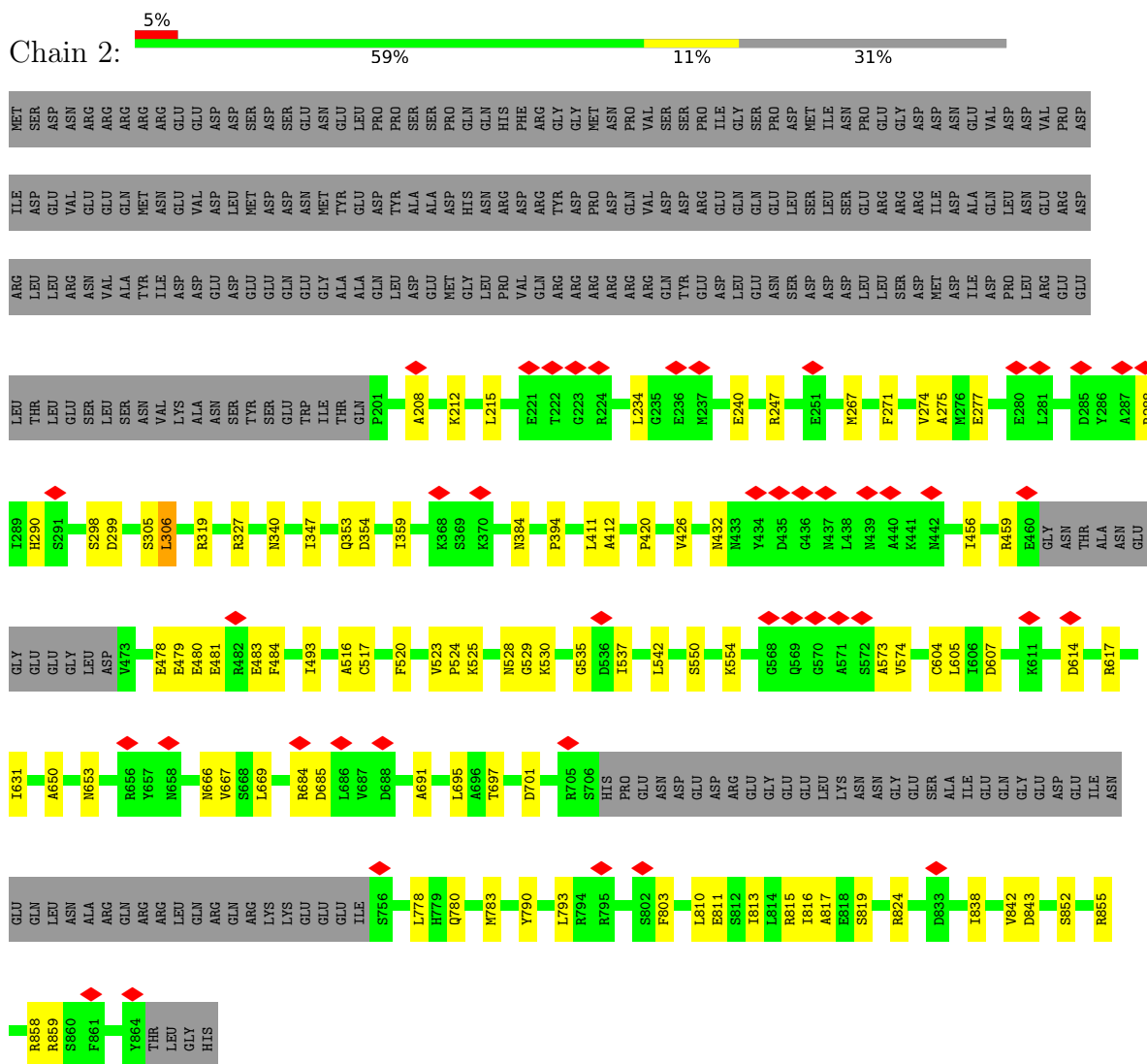


Mol	Chain	Residues	Atoms					AltConf
9	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	7	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots i

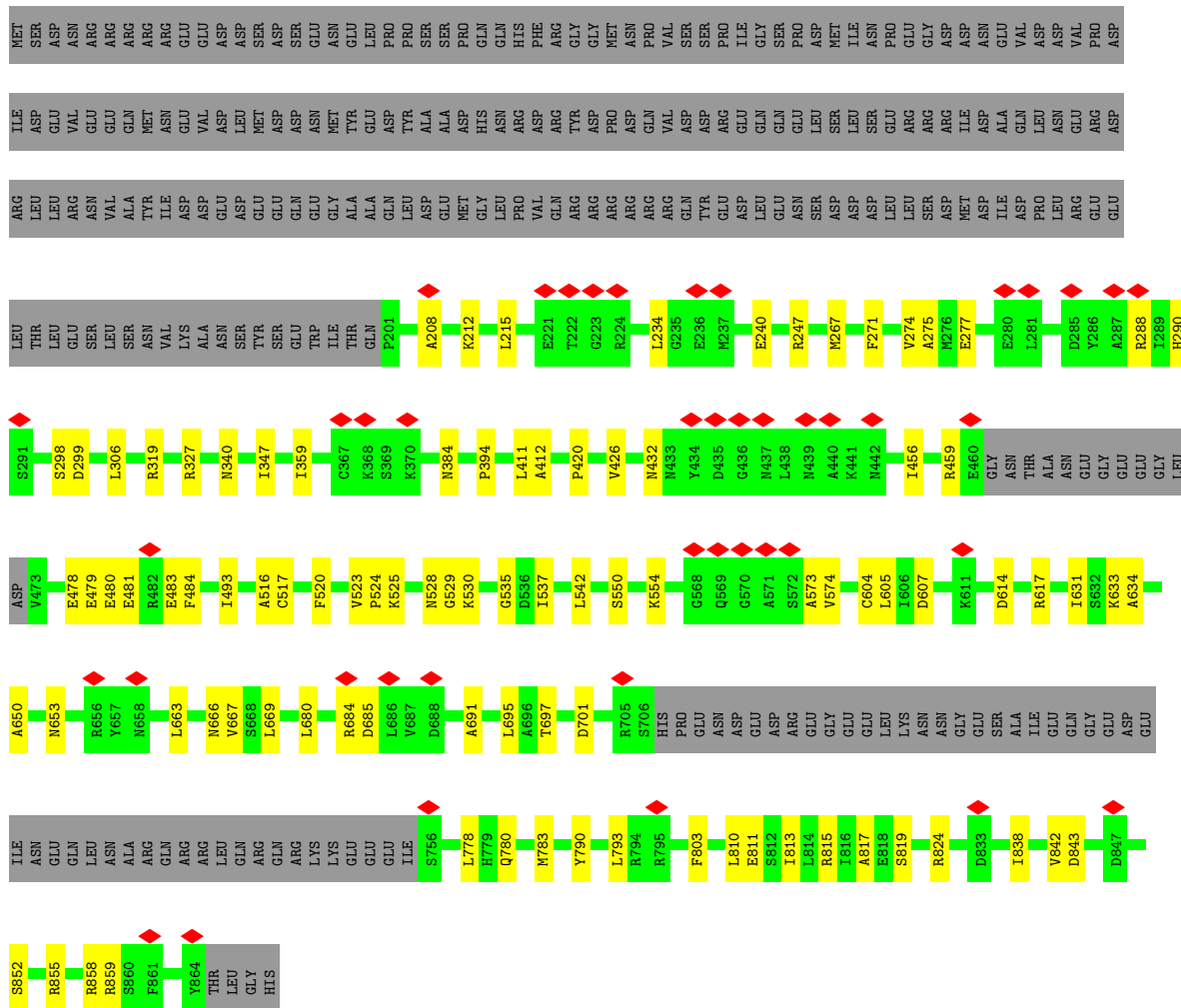
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

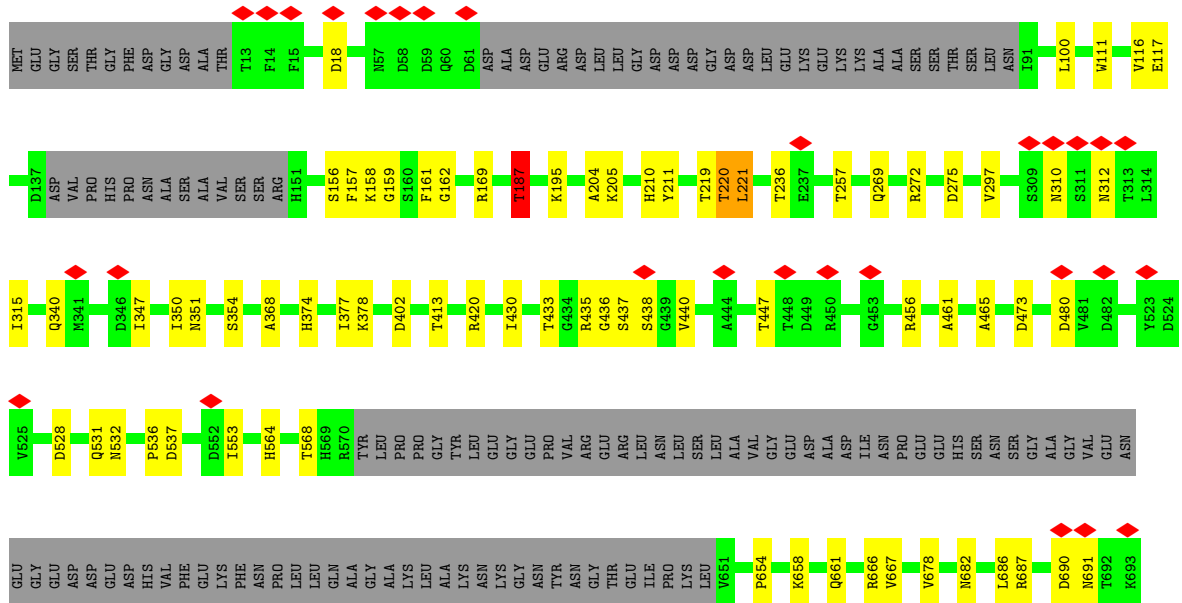


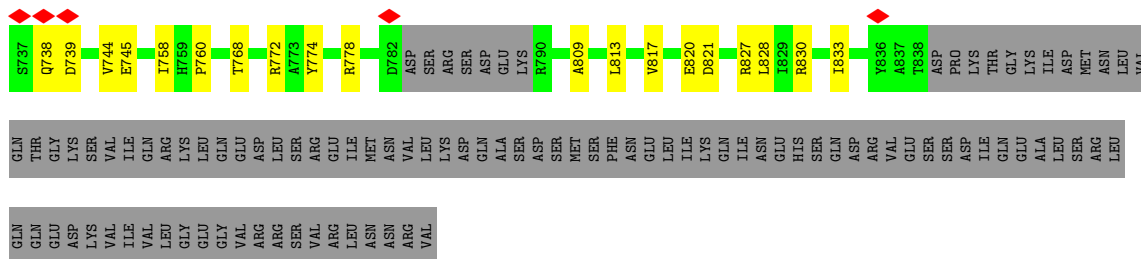
- Molecule 1: DNA replication licensing factor MCM2



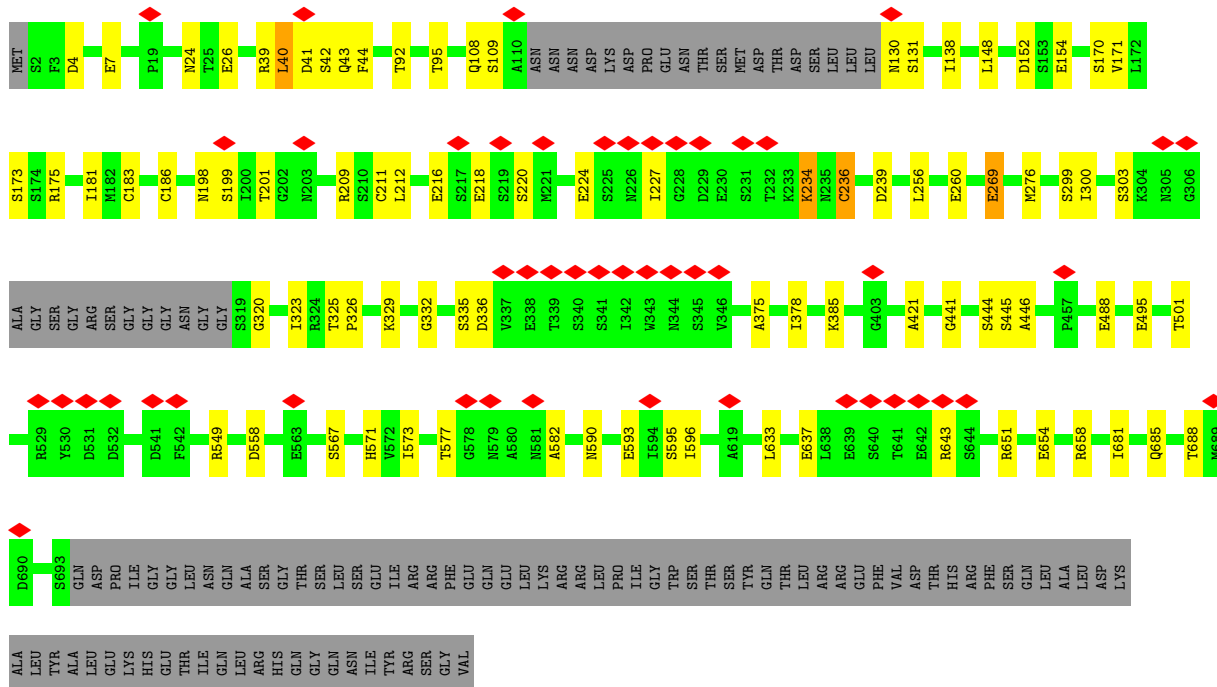


● Molecule 2: DNA replication licensing factor MCM3

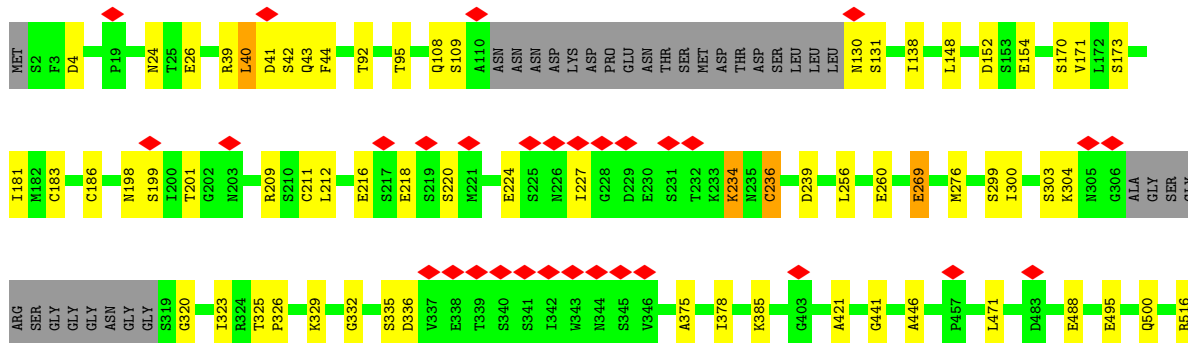


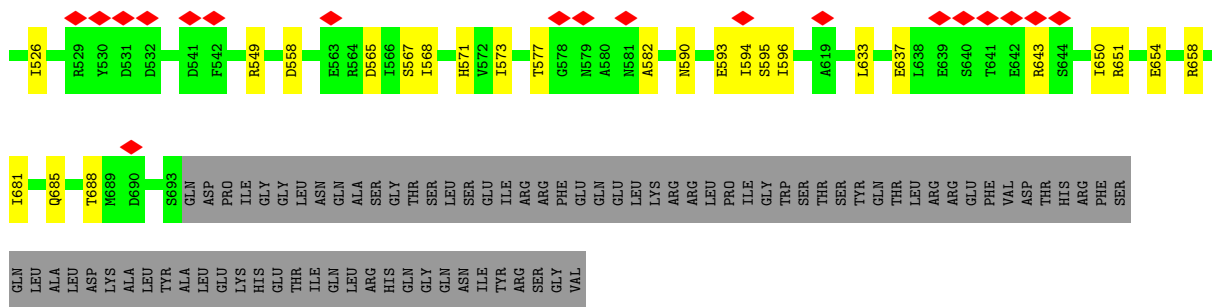


● Molecule 4: DNA replication licensing factor MCM5

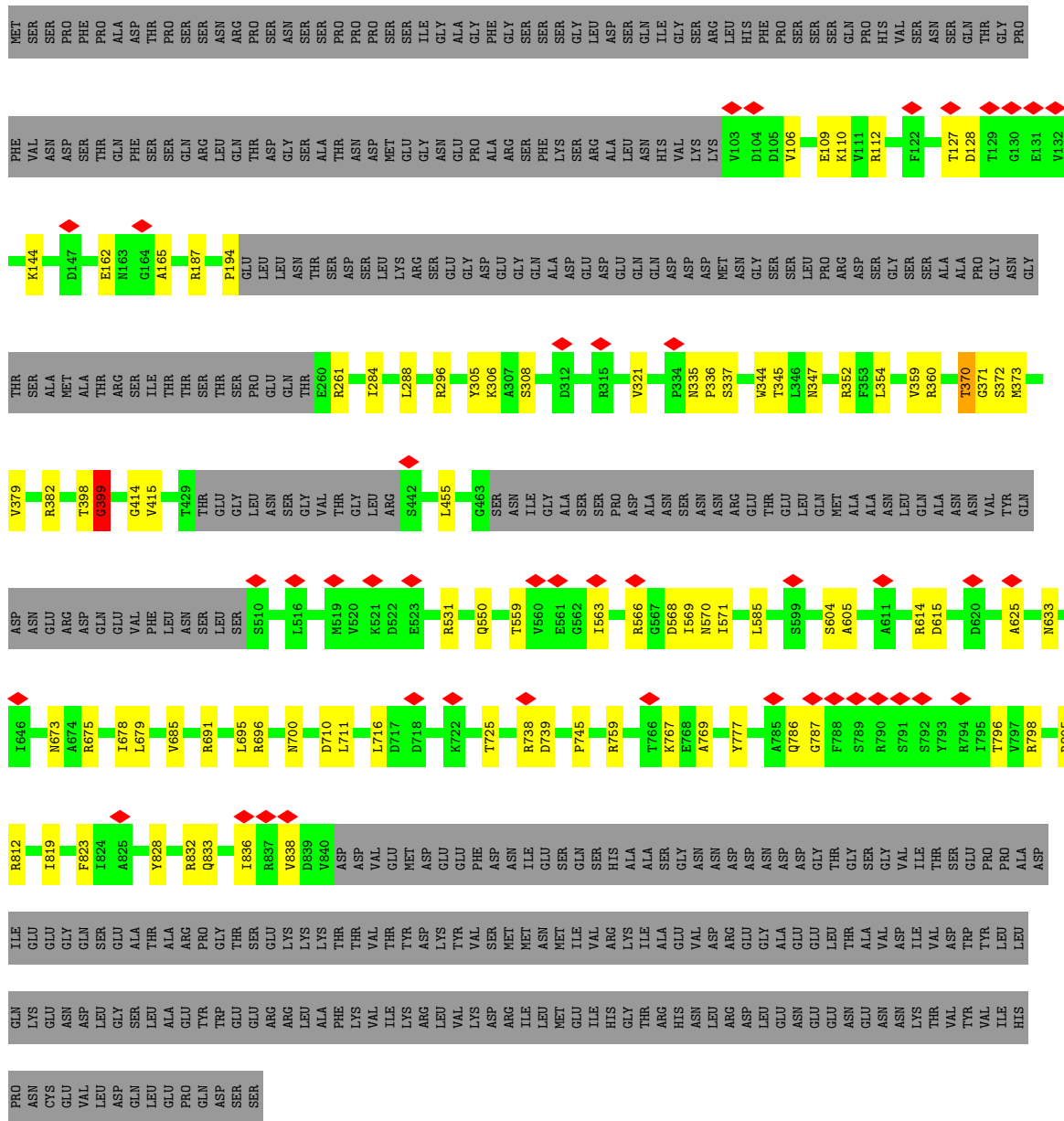


● Molecule 4: DNA replication licensing factor MCM5

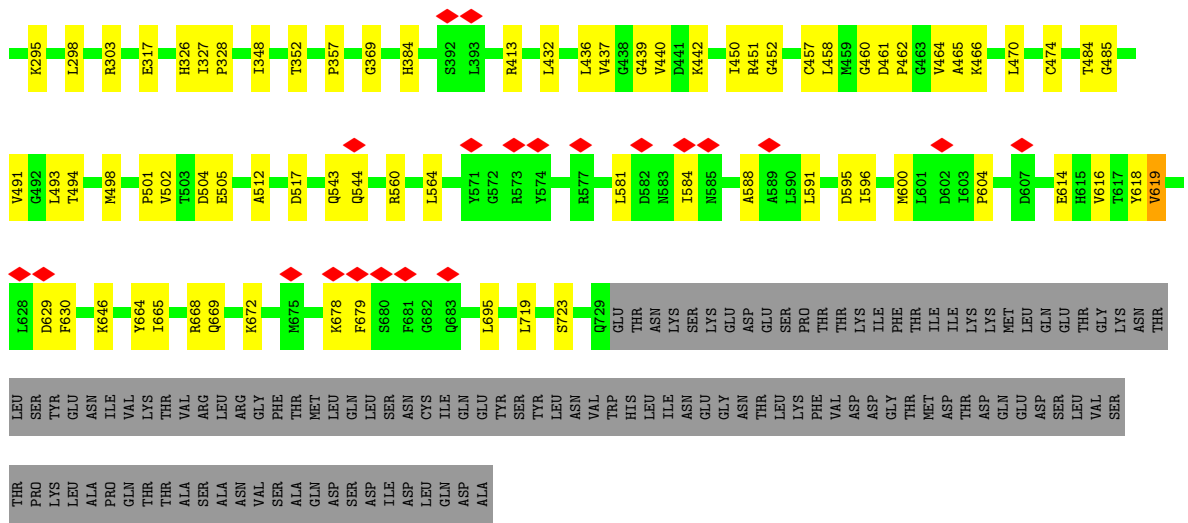




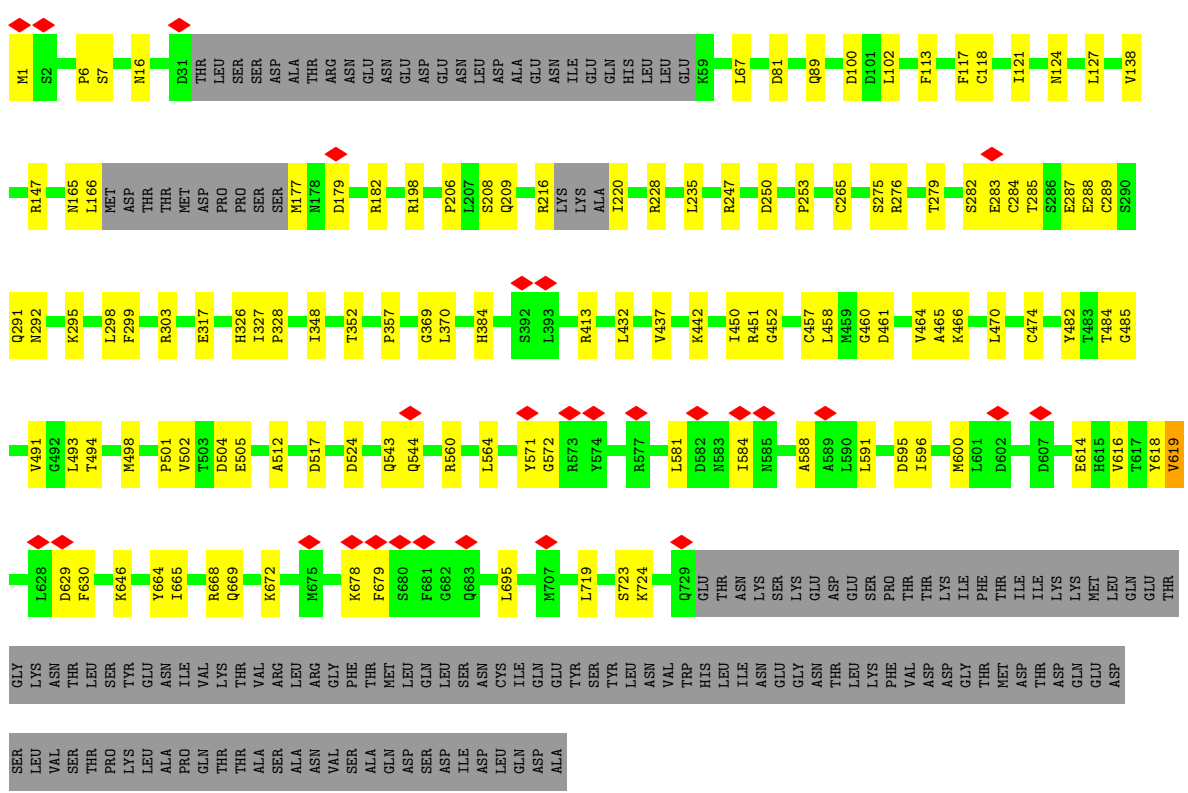
• Molecule 5: DNA replication licensing factor MCM6



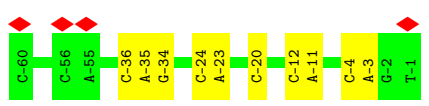
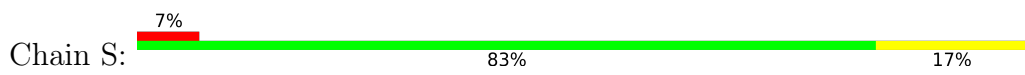
• Molecule 5: DNA replication licensing factor MCM6



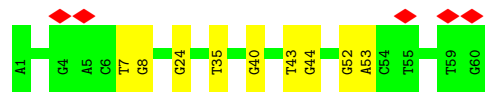
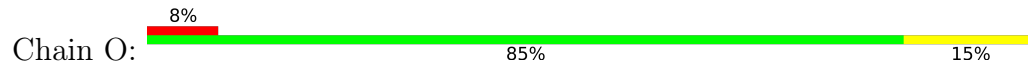
● Molecule 6: DNA replication licensing factor MCM7



● Molecule 7: DNA (60-mer), strand 1



- Molecule 8: DNA (60-mer), strand 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58772	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.254	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.026	Depositor
Map size (\AA)	278.528, 278.528, 278.528	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.088, 1.088, 1.088	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: ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	2	0.37	0/4794	0.65	4/6479 (0.1%)
1	A	0.37	0/4794	0.65	4/6479 (0.1%)
2	3	0.46	0/4815	0.64	1/6529 (0.0%)
2	B	0.46	0/4815	0.64	1/6529 (0.0%)
3	4	0.41	0/5200	0.71	6/7028 (0.1%)
3	C	0.41	0/5200	0.71	6/7028 (0.1%)
4	5	0.42	0/5238	0.67	5/7081 (0.1%)
4	D	0.42	0/5238	0.67	5/7081 (0.1%)
5	6	0.38	0/4801	0.69	4/6483 (0.1%)
5	E	0.38	0/4801	0.69	4/6483 (0.1%)
6	7	0.44	0/5514	0.65	0/7450
6	F	0.44	0/5514	0.65	0/7450
7	S	0.74	0/1379	1.04	0/2126
8	O	0.73	0/1379	1.02	0/2126
All	All	0.44	0/63482	0.69	40/86352 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	1
1	A	0	1
2	3	0	5
2	B	0	5
3	4	0	3
3	C	0	3
4	5	0	3
4	D	0	3
5	6	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	4
6	7	0	3
6	F	0	3
All	All	0	38

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	533	LEU	CA-CB-CG	9.39	136.89	115.30
3	C	533	LEU	CA-CB-CG	9.37	136.86	115.30
4	5	269	GLU	C-N-CA	8.60	143.19	121.70
4	D	269	GLU	C-N-CA	8.57	143.13	121.70
3	4	821	ASP	CB-CG-OD1	8.52	125.97	118.30
3	C	821	ASP	CB-CG-OD1	8.42	125.88	118.30
3	C	410	GLN	C-N-CA	8.40	142.69	121.70
3	4	410	GLN	C-N-CA	8.39	142.66	121.70
5	6	399	GLY	N-CA-C	7.46	131.75	113.10
5	E	399	GLY	N-CA-C	7.46	131.74	113.10
4	5	236	CYS	CA-CB-SG	7.22	126.99	114.00
4	D	236	CYS	CA-CB-SG	7.20	126.95	114.00
1	A	803	PHE	C-N-CD	-7.00	105.19	120.60
1	2	803	PHE	C-N-CD	-7.00	105.20	120.60
4	5	212	LEU	CA-CB-CG	6.32	129.82	115.30
4	D	212	LEU	CA-CB-CG	6.27	129.73	115.30
3	C	731	ASP	CB-CG-OD1	5.77	123.50	118.30
3	4	731	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	234	LEU	CA-CB-CG	5.65	128.30	115.30
1	2	234	LEU	CA-CB-CG	5.65	128.30	115.30
5	E	335	ASN	C-N-CA	5.58	145.44	122.00
5	6	335	ASN	C-N-CA	5.58	145.42	122.00
5	6	345	THR	N-CA-C	5.49	125.81	111.00
5	E	345	THR	N-CA-C	5.48	125.80	111.00
3	C	820	GLU	C-N-CA	5.45	135.32	121.70
3	4	820	GLU	C-N-CA	5.43	135.28	121.70
2	B	159	GLY	C-N-CA	5.42	135.24	121.70
2	3	159	GLY	C-N-CA	5.40	135.21	121.70
4	5	441	GLY	C-N-CA	5.40	135.20	121.70
4	D	441	GLY	C-N-CA	5.39	135.17	121.70
5	6	354	LEU	CA-CB-CG	5.30	127.48	115.30
5	E	354	LEU	CA-CB-CG	5.29	127.46	115.30
4	D	40	LEU	CA-CB-CG	5.26	127.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	40	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	459	ARG	C-N-CA	5.14	134.54	121.70
1	2	459	ARG	C-N-CA	5.13	134.53	121.70
1	2	843	ASP	CB-CG-OD1	5.07	122.86	118.30
3	C	729	LEU	CA-CB-CG	5.07	126.95	115.30
3	4	729	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	843	ASP	CB-CG-OD1	5.05	122.85	118.30

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	359	ILE	Peptide
2	3	161	PHE	Peptide
2	3	187	THR	Peptide
2	3	210	HIS	Peptide
2	3	220	THR	Peptide
2	3	531	GLN	Peptide
3	4	360	ILE	Peptide
3	4	375	ASP	Peptide
3	4	734	GLU	Peptide
4	5	199	SER	Peptide
4	5	26	GLU	Peptide
4	5	593	GLU	Peptide
5	6	344	TRP	Peptide
5	6	398	THR	Peptide
5	6	399	GLY	Peptide
5	6	625	ALA	Peptide
6	7	282	SER	Peptide
6	7	501	PRO	Peptide
6	7	619	VAL	Peptide
1	A	359	ILE	Peptide
2	B	161	PHE	Peptide
2	B	187	THR	Peptide
2	B	210	HIS	Peptide
2	B	220	THR	Peptide
2	B	531	GLN	Peptide
3	C	360	ILE	Peptide
3	C	375	ASP	Peptide
3	C	734	GLU	Peptide
4	D	199	SER	Peptide
4	D	26	GLU	Peptide

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Mol	Chain	Res	Type	Group
4	D	593	GLU	Peptide
5	E	344	TRP	Peptide
5	E	398	THR	Peptide
5	E	399	GLY	Peptide
5	E	625	ALA	Peptide
6	F	282	SER	Peptide
6	F	501	PRO	Peptide
6	F	619	VAL	Peptide

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	4714	0	4730	57	0
1	A	4714	0	4730	56	0
2	3	4734	0	4785	45	0
2	B	4734	0	4785	41	0
3	4	5127	0	5172	54	0
3	C	5127	0	5172	58	0
4	5	5165	0	5193	50	0
4	D	5165	0	5193	52	0
5	6	4731	0	4679	48	0
5	E	4731	0	4679	45	0
6	7	5432	0	5495	70	0
6	F	5432	0	5495	74	0
7	S	1230	0	676	8	0
8	O	1230	0	676	6	0
9	2	27	0	12	0	0
9	3	27	0	12	0	0
9	5	27	0	12	2	0
9	7	27	0	12	1	0
9	A	27	0	12	0	0
9	B	27	0	12	1	0
9	D	27	0	12	1	0
9	F	27	0	12	1	0
All	All	62482	0	61556	620	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 (620) 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)
6:F:719:LEU:O	6:F:723:SER:HB3	1.68	0.92
6:7:719:LEU:O	6:7:723:SER:HB3	1.68	0.92
1:2:480:GLU:O	1:2:484:PHE:HB2	1.77	0.84
1:A:480:GLU:O	1:A:484:PHE:HB2	1.77	0.84
4:D:633:LEU:O	4:D:637:GLU:HB2	1.89	0.72
4:5:633:LEU:O	4:5:637:GLU:HB2	1.89	0.71
5:6:566:ARG:HG3	5:6:805:ARG:HH22	1.57	0.70
5:E:566:ARG:HG3	5:E:805:ARG:HH22	1.57	0.69
6:F:113:PHE:O	6:F:117:PHE:HB2	1.93	0.69
3:C:226:TYR:O	3:C:230:LEU:HB2	1.93	0.68
6:7:113:PHE:O	6:7:117:PHE:HB2	1.93	0.68
3:4:226:TYR:O	3:4:230:LEU:HB2	1.93	0.67
1:2:550:SER:O	1:2:554:LYS:HB2	1.95	0.66
6:7:7:SER:H	2:B:18:ASP:HB3	1.60	0.65
2:3:350:ILE:O	2:3:354:SER:HB3	1.96	0.65
1:A:550:SER:O	1:A:554:LYS:HB2	1.95	0.65
2:B:315:ILE:HG21	4:D:173:SER:HB2	1.77	0.65
2:B:435:ARG:NH2	4:D:488:GLU:O	2.29	0.64
2:B:368:ALA:HB2	2:B:378:LYS:HE2	1.79	0.64
2:B:350:ILE:O	2:B:354:SER:HB3	1.96	0.64
2:3:368:ALA:HB2	2:3:378:LYS:HE2	1.79	0.64
2:3:430:ILE:HD12	2:3:465:ALA:HB2	1.80	0.64
6:7:177:MET:O	4:D:108:GLN:NE2	2.31	0.64
5:6:767:LYS:HG3	5:6:769:ALA:H	1.63	0.63
5:E:585:LEU:HD21	5:E:679:LEU:HD22	1.80	0.63
5:6:585:LEU:HD21	5:6:679:LEU:HD22	1.80	0.63
6:7:464:VAL:HG11	6:7:600:MET:HB3	1.81	0.63
1:A:479:GLU:O	1:A:483:GLU:HB2	1.99	0.63
5:E:194:PRO:O	5:E:261:ARG:NH2	2.32	0.63
5:6:194:PRO:O	5:6:261:ARG:NH2	2.32	0.63
5:E:767:LYS:HG3	5:E:769:ALA:H	1.63	0.62
6:F:235:LEU:HD23	6:F:357:PRO:HG3	1.81	0.62
2:B:430:ILE:HD12	2:B:465:ALA:HB2	1.80	0.62
1:2:523:VAL:HG12	1:2:525:LYS:HB3	1.81	0.62
1:2:479:GLU:O	1:2:483:GLU:HB2	1.99	0.62
6:F:464:VAL:HG11	6:F:600:MET:HB3	1.81	0.61
6:7:247:ARG:NH2	6:7:498:MET:SD	2.74	0.61
6:7:235:LEU:HD23	6:7:357:PRO:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:247:ARG:NH2	6:F:498:MET:SD	2.74	0.61
4:D:375:ALA:H	4:D:385:LYS:HE3	1.66	0.61
1:A:523:VAL:HG12	1:A:525:LYS:HB3	1.81	0.60
3:4:604:TYR:HB2	3:4:617:GLU:HB2	1.83	0.60
2:3:687:ARG:O	2:3:691:ASN:HB2	2.02	0.60
2:3:18:ASP:HB3	6:F:7:SER:H	1.66	0.60
3:C:604:TYR:HB2	3:C:617:GLU:HB2	1.83	0.60
1:2:780:GLN:NE2	4:5:577:THR:O	2.35	0.60
3:4:578:LEU:HD21	3:4:672:LEU:HD22	1.84	0.60
4:D:148:LEU:HD23	4:D:260:GLU:HB3	1.84	0.60
5:E:288:LEU:H	5:E:399:GLY:HA3	1.66	0.60
1:2:327:ARG:NH2	4:5:269:GLU:OE2	2.35	0.60
1:2:394:PRO:O	5:6:673:ASN:ND2	2.35	0.60
5:6:288:LEU:H	5:6:399:GLY:HA3	1.66	0.60
1:2:327:ARG:HH12	1:2:420:PRO:HD3	1.67	0.59
4:5:108:GLN:NE2	6:F:177:MET:O	2.34	0.59
4:5:148:LEU:HD23	4:5:260:GLU:HB3	1.84	0.59
2:B:687:ARG:O	2:B:691:ASN:HB2	2.02	0.59
4:5:595:SER:OG	4:5:596:ILE:N	2.36	0.59
6:7:437:VAL:O	6:7:646:LYS:NZ	2.36	0.59
1:A:327:ARG:HH12	1:A:420:PRO:HD3	1.67	0.59
4:5:375:ALA:H	4:5:385:LYS:HE3	1.66	0.59
5:6:308:SER:O	5:6:347:ASN:ND2	2.36	0.58
6:F:543:GLN:HG3	6:F:544:GLN:HG2	1.85	0.58
2:3:420:ARG:NH1	4:5:495:GLU:OE2	2.37	0.58
4:5:186:CYS:SG	4:5:234:LYS:NZ	2.76	0.58
5:6:550:GLN:HE21	5:6:571:ILE:H	1.51	0.58
3:C:330:GLY:HA3	3:C:401:GLU:HA	1.83	0.58
3:4:330:GLY:HA3	3:4:401:GLU:HA	1.83	0.58
4:D:595:SER:OG	4:D:596:ILE:N	2.36	0.58
6:F:437:VAL:O	6:F:646:LYS:NZ	2.36	0.58
4:5:198:ASN:HD22	4:5:329:LYS:HE2	1.69	0.58
5:E:550:GLN:HE21	5:E:571:ILE:H	1.51	0.58
2:B:420:ARG:NH1	4:D:495:GLU:OE2	2.36	0.58
3:4:224:LEU:HD11	3:4:227:ILE:HG12	1.86	0.58
3:C:578:LEU:HD21	3:C:672:LEU:HD22	1.84	0.58
5:E:308:SER:O	5:E:347:ASN:ND2	2.36	0.58
4:D:186:CYS:SG	4:D:234:LYS:NZ	2.76	0.58
4:D:198:ASN:HD22	4:D:329:LYS:HE2	1.68	0.58
6:7:543:GLN:HG3	6:7:544:GLN:HG2	1.85	0.57
3:4:774:TYR:OH	3:4:778:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:315:ARG:HH22	6:F:250:ASP:HA	1.68	0.57
3:C:309:GLY:O	3:C:327:ASN:ND2	2.37	0.57
4:5:39:ARG:HE	4:5:44:PHE:HD1	1.53	0.57
4:5:4:ASP:OD1	4:5:4:ASP:N	2.37	0.57
1:A:793:LEU:HA	1:A:859:ARG:HH12	1.70	0.57
4:D:39:ARG:HE	4:D:44:PHE:HD1	1.52	0.57
5:6:112:ARG:HH12	5:6:187:ARG:HH22	1.53	0.57
2:B:169:ARG:NH2	2:B:269:GLN:OE1	2.38	0.57
3:C:371:CYS:SG	3:C:372:GLU:N	2.78	0.56
1:2:793:LEU:HA	1:2:859:ARG:HH12	1.70	0.56
3:4:371:CYS:SG	3:4:372:GLU:N	2.78	0.56
3:C:534:GLU:O	3:C:538:LYS:HB2	2.05	0.56
3:4:534:GLU:O	3:4:538:LYS:HB2	2.06	0.56
1:A:394:PRO:O	5:E:673:ASN:ND2	2.38	0.56
2:3:169:ARG:NH2	2:3:269:GLN:OE1	2.38	0.56
3:4:744:VAL:HG12	3:4:745:GLU:HG2	1.87	0.56
3:4:569:ASP:O	3:4:574:LYS:NZ	2.39	0.56
3:C:569:ASP:O	3:C:574:LYS:NZ	2.39	0.56
3:C:224:LEU:HD11	3:C:227:ILE:HG12	1.86	0.56
6:F:288:GLU:O	6:F:292:ASN:ND2	2.39	0.56
6:7:138:VAL:HG21	6:7:303:ARG:HH21	1.71	0.56
1:A:212:LYS:HZ3	1:A:215:LEU:HD22	1.71	0.56
5:6:691:ARG:HH11	5:6:716:LEU:HD22	1.71	0.55
6:7:616:VAL:O	6:7:619:VAL:O	2.25	0.55
2:B:195:LYS:NZ	6:F:369:GLY:O	2.38	0.55
3:C:774:TYR:OH	3:C:778:ARG:NH2	2.37	0.55
4:D:201:THR:HG21	4:D:303:SER:HB3	1.87	0.55
6:F:138:VAL:HG21	6:F:303:ARG:HH21	1.71	0.55
1:2:855:ARG:HG3	1:2:858:ARG:HH21	1.72	0.55
6:7:288:GLU:O	6:7:292:ASN:ND2	2.39	0.55
6:7:228:ARG:NH2	6:7:327:ILE:O	2.39	0.55
1:A:667:VAL:HG13	1:A:669:LEU:H	1.72	0.55
5:E:695:LEU:HD13	5:E:838:VAL:HG13	1.88	0.55
6:F:228:ARG:NH2	6:F:327:ILE:O	2.39	0.55
6:7:89:GLN:HE22	6:7:102:LEU:H	1.55	0.55
3:4:315:ARG:HH22	6:7:250:ASP:HA	1.72	0.55
1:A:327:ARG:NH2	4:D:269:GLU:OE2	2.39	0.55
5:E:382:ARG:HH11	5:E:455:LEU:HD21	1.72	0.55
7:S:-36:DC:H2"	7:S:-35:DA:C8	2.41	0.55
1:A:855:ARG:HG3	1:A:858:ARG:HH21	1.72	0.55
6:F:616:VAL:O	6:F:619:VAL:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:309:GLY:O	3:4:327:ASN:ND2	2.37	0.55
5:6:382:ARG:HH11	5:6:455:LEU:HD21	1.72	0.55
6:F:118:CYS:SG	6:F:198:ARG:NH2	2.80	0.55
6:F:664:TYR:OH	6:F:668:ARG:NH2	2.31	0.55
4:5:201:THR:HG21	4:5:303:SER:HB3	1.88	0.55
4:D:681:ILE:O	4:D:685:GLN:HB2	2.07	0.55
5:E:566:ARG:O	5:E:805:ARG:NH2	2.40	0.55
7:S:-34:DG:N2	8:O:35:DT:O2	2.39	0.55
2:3:435:ARG:NH2	4:5:488:GLU:O	2.36	0.54
4:5:421:ALA:HA	9:5:2001:ADP:H5'2	1.89	0.54
3:C:744:VAL:HG12	3:C:745:GLU:HG2	1.87	0.54
5:E:112:ARG:HH12	5:E:187:ARG:HH22	1.53	0.54
6:F:465:ALA:HA	9:F:2001:ADP:H5'1	1.89	0.54
3:4:758:ILE:HD11	3:4:813:LEU:HD23	1.89	0.54
6:7:317:GLU:HB3	6:7:328:PRO:HB3	1.90	0.54
6:7:616:VAL:O	6:7:619:VAL:C	2.45	0.54
1:A:528:ASN:HB3	4:D:582:ALA:HB1	1.89	0.54
6:F:616:VAL:O	6:F:619:VAL:O	2.24	0.54
2:3:195:LYS:NZ	6:7:369:GLY:O	2.38	0.54
5:6:566:ARG:O	5:6:805:ARG:NH2	2.40	0.54
6:7:465:ALA:HA	9:7:2001:ADP:H5'1	1.89	0.54
5:6:695:LEU:HD13	5:6:838:VAL:HG13	1.88	0.54
1:A:298:SER:O	1:A:319:ARG:NH1	2.40	0.54
6:7:118:CYS:SG	6:7:198:ARG:NH2	2.80	0.54
1:A:780:GLN:NE2	4:D:577:THR:O	2.40	0.54
5:E:691:ARG:HH11	5:E:716:LEU:HD22	1.71	0.54
3:C:758:ILE:HD11	3:C:813:LEU:HD23	1.89	0.54
1:2:667:VAL:HG13	1:2:669:LEU:H	1.72	0.54
6:F:89:GLN:HE22	6:F:102:LEU:H	1.55	0.54
2:3:275:ASP:OD1	2:3:275:ASP:N	2.41	0.54
2:B:18:ASP:N	2:B:18:ASP:OD1	2.39	0.54
4:5:7:GLU:OE2	2:B:240:LYS:NZ	2.40	0.53
4:5:681:ILE:O	4:5:685:GLN:HB2	2.08	0.53
1:2:298:SER:O	1:2:319:ARG:NH1	2.40	0.53
3:4:450:GLN:NE2	7:S:-36:DC:OP1	2.42	0.53
6:7:470:LEU:O	6:7:474:CYS:HB2	2.09	0.53
6:7:460:GLY:O	6:7:466:LYS:NZ	2.29	0.53
6:7:664:TYR:OH	6:7:668:ARG:NH2	2.31	0.53
6:F:460:GLY:O	6:F:466:LYS:NZ	2.29	0.53
1:2:517:CYS:HG	1:2:819:SER:HG	1.56	0.53
1:2:631:ILE:HG22	4:5:446:ALA:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:722:LYS:O	3:4:726:ASN:HB2	2.09	0.53
6:F:317:GLU:HB3	6:F:328:PRO:HB3	1.90	0.53
6:F:413:ARG:HG3	6:F:630:PHE:HE1	1.74	0.53
1:2:542:LEU:HA	1:2:650:ALA:HB3	1.91	0.53
2:B:187:THR:O	2:B:257:THR:OG1	2.27	0.53
6:F:284:CYS:SG	6:F:285:THR:N	2.82	0.53
6:F:470:LEU:O	6:F:474:CYS:HB2	2.09	0.53
2:3:315:ILE:HG21	4:5:173:SER:HB2	1.91	0.53
6:7:284:CYS:SG	6:7:285:THR:N	2.82	0.53
5:E:106:VAL:O	5:E:110:LYS:HB2	2.09	0.53
3:4:543:GLN:HE21	3:4:670:SER:HB3	1.74	0.52
6:F:517:ASP:OD1	6:F:517:ASP:N	2.42	0.52
6:7:413:ARG:HG3	6:7:630:PHE:HE1	1.74	0.52
6:7:291:GLN:O	4:D:24:ASN:ND2	2.42	0.52
4:5:24:ASN:ND2	6:F:291:GLN:O	2.43	0.52
3:C:531:TYR:HE2	3:C:720:LEU:HA	1.75	0.52
3:4:612:LYS:NZ	8:O:40:DG:OP2	2.43	0.52
1:A:542:LEU:HA	1:A:650:ALA:HB3	1.91	0.52
3:C:722:LYS:O	3:C:726:ASN:HB2	2.09	0.52
5:E:306:LYS:HG3	5:E:352:ARG:HB2	1.92	0.52
5:6:306:LYS:HG3	5:6:352:ARG:HB2	1.91	0.52
1:A:614:ASP:OD1	1:A:617:ARG:NH1	2.43	0.52
4:D:170:SER:OG	4:D:171:VAL:N	2.43	0.52
6:7:265:CYS:SG	6:7:289:CYS:N	2.83	0.52
4:D:138:ILE:HG23	4:D:332:GLY:HA3	1.91	0.52
4:5:567:SER:O	4:5:571:HIS:HB2	2.10	0.51
3:4:401:GLU:HG2	3:4:403:PRO:HD3	1.92	0.51
5:6:796:THR:HG22	5:6:798:ARG:H	1.74	0.51
1:2:614:ASP:OD1	1:2:617:ARG:NH1	2.43	0.51
4:D:299:SER:OG	4:D:300:ILE:N	2.42	0.51
5:E:796:THR:HG22	5:E:798:ARG:H	1.74	0.51
5:6:106:VAL:O	5:6:110:LYS:HB2	2.09	0.51
1:A:684:ARG:HB3	1:A:685:ASP:HB3	1.92	0.51
2:B:275:ASP:N	2:B:275:ASP:OD1	2.41	0.51
3:C:543:GLN:HE21	3:C:670:SER:HB3	1.74	0.51
1:2:340:ASN:HB3	1:2:347:ILE:HG22	1.93	0.51
2:3:18:ASP:N	2:3:18:ASP:OD1	2.40	0.51
1:A:340:ASN:HB3	1:A:347:ILE:HG22	1.93	0.51
4:D:567:SER:O	4:D:571:HIS:HB2	2.10	0.51
4:5:681:ILE:O	4:5:685:GLN:CB	2.59	0.51
6:7:275:SER:OG	6:7:276:ARG:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:265:CYS:SG	6:F:289:CYS:N	2.84	0.51
2:3:187:THR:O	2:3:257:THR:OG1	2.27	0.51
3:4:531:TYR:HE2	3:4:720:LEU:HA	1.75	0.51
1:A:607:ASP:N	1:A:607:ASP:OD1	2.44	0.51
5:E:777:TYR:OH	5:E:796:THR:O	2.29	0.51
1:2:528:ASN:HB3	4:5:582:ALA:HB1	1.92	0.50
2:3:100:LEU:HB3	2:3:111:TRP:HZ3	1.76	0.50
3:4:189:GLU:O	3:4:193:ASN:HB2	2.11	0.50
6:7:581:LEU:HA	6:7:584:ILE:HB	1.93	0.50
1:2:212:LYS:HZ3	1:2:215:LEU:HD22	1.76	0.50
1:2:537:ILE:HG13	1:2:815:ARG:HE	1.76	0.50
6:7:588:ALA:HA	6:7:591:LEU:HB2	1.93	0.50
4:5:170:SER:OG	4:5:171:VAL:N	2.43	0.50
5:E:550:GLN:NE2	5:E:571:ILE:H	2.09	0.50
6:F:16:ASN:ND2	6:F:100:ASP:OD2	2.45	0.50
6:F:275:SER:OG	6:F:276:ARG:N	2.44	0.50
4:5:138:ILE:HG23	4:5:332:GLY:HA3	1.91	0.50
3:C:401:GLU:HG2	3:C:403:PRO:HD3	1.92	0.50
6:F:493:LEU:HA	6:F:512:ALA:H	1.77	0.50
6:7:16:ASN:ND2	6:7:100:ASP:OD2	2.45	0.50
6:F:595:ASP:OD1	6:F:595:ASP:N	2.45	0.50
3:4:226:TYR:O	3:4:230:LEU:CB	2.60	0.50
5:E:531:ARG:HD2	5:E:745:PRO:HG3	1.93	0.50
6:F:581:LEU:HA	6:F:584:ILE:HB	1.93	0.50
1:2:607:ASP:N	1:2:607:ASP:OD1	2.44	0.50
3:4:629:CYS:SG	3:4:630:CYS:N	2.85	0.50
6:7:493:LEU:HA	6:7:512:ALA:H	1.77	0.50
1:A:537:ILE:HG13	1:A:815:ARG:HE	1.76	0.50
2:B:100:LEU:HB3	2:B:111:TRP:HZ3	1.76	0.50
4:D:681:ILE:O	4:D:685:GLN:CB	2.59	0.50
3:C:629:CYS:SG	3:C:630:CYS:N	2.85	0.50
5:E:568:ASP:O	5:E:805:ARG:NH1	2.45	0.50
1:2:684:ARG:HB3	1:2:685:ASP:HB3	1.92	0.49
4:5:239:ASP:OD1	4:5:239:ASP:N	2.45	0.49
6:F:588:ALA:HA	6:F:591:LEU:HB2	1.93	0.49
5:6:531:ARG:HD2	5:6:745:PRO:HG3	1.93	0.49
6:7:517:ASP:OD1	6:7:517:ASP:N	2.42	0.49
3:C:189:GLU:O	3:C:193:ASN:HB2	2.11	0.49
3:C:827:ARG:HA	3:C:830:ARG:HB2	1.95	0.49
1:2:274:VAL:HA	1:2:277:GLU:HG2	1.95	0.49
5:6:568:ASP:O	5:6:805:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:374:HIS:HB3	2:B:377:ILE:HD12	1.94	0.49
4:D:218:GLU:OE1	4:D:220:SER:N	2.45	0.49
2:3:374:HIS:HB3	2:3:377:ILE:HD12	1.94	0.49
2:3:420:ARG:NH2	4:5:501:THR:OG1	2.43	0.49
1:A:550:SER:O	1:A:554:LYS:CB	2.60	0.49
1:A:631:ILE:HG22	4:D:446:ALA:HB3	1.94	0.49
2:B:447:THR:HG21	2:B:456:ARG:HB2	1.94	0.49
4:5:335:SER:OG	4:5:336:ASP:N	2.44	0.49
1:A:274:VAL:HA	1:A:277:GLU:HG2	1.95	0.49
4:D:335:SER:OG	4:D:336:ASP:N	2.44	0.49
1:2:426:VAL:HG12	1:2:456:ILE:HG13	1.95	0.49
2:3:654:PRO:O	2:3:658:LYS:NZ	2.39	0.49
3:4:809:ALA:HB2	3:4:817:VAL:HG23	1.94	0.49
3:C:612:LYS:NZ	7:S:-20:DC:OP2	2.45	0.49
5:E:685:VAL:HG22	5:E:700:ASN:HB2	1.95	0.49
3:4:326:ILE:HD12	3:4:439:PHE:HB2	1.95	0.49
5:6:685:VAL:HG22	5:6:700:ASN:HB2	1.95	0.49
6:7:665:ILE:O	6:7:669:GLN:HB2	2.13	0.49
3:C:606:THR:OG1	3:C:607:ARG:N	2.46	0.49
4:D:239:ASP:OD1	4:D:239:ASP:N	2.45	0.49
3:4:827:ARG:HA	3:4:830:ARG:HB2	1.94	0.49
1:2:573:ALA:HA	1:2:574:VAL:HA	1.61	0.48
5:6:550:GLN:NE2	5:6:571:ILE:H	2.09	0.48
5:6:777:TYR:OH	5:6:796:THR:O	2.29	0.48
3:C:326:ILE:HD12	3:C:439:PHE:HB2	1.95	0.48
6:F:596:ILE:HD11	6:F:695:LEU:HD11	1.94	0.48
1:2:524:PRO:HA	1:2:535:GLY:HA3	1.95	0.48
1:2:691:ALA:O	1:2:695:LEU:CB	2.61	0.48
3:4:606:THR:OG1	3:4:607:ARG:N	2.46	0.48
2:B:211:TYR:HD2	6:F:6:PRO:HG2	1.78	0.48
4:5:130:ASN:HA	4:5:131:SER:HA	1.66	0.48
4:5:218:GLU:OE1	4:5:220:SER:N	2.45	0.48
1:A:426:VAL:HG12	1:A:456:ILE:HG13	1.95	0.48
2:3:447:THR:HG21	2:3:456:ARG:HB2	1.94	0.48
2:B:528:ASP:O	2:B:532:ASN:ND2	2.47	0.48
3:C:226:TYR:O	3:C:230:LEU:CB	2.60	0.48
4:D:256:LEU:HB2	4:D:276:MET:HB2	1.96	0.48
1:2:493:ILE:HD11	1:2:824:ARG:HG2	1.95	0.48
1:A:478:GLU:HA	1:A:481:GLU:HG2	1.95	0.48
2:B:347:ILE:O	2:B:351:ASN:ND2	2.47	0.48
4:D:41:ASP:HA	4:D:42:SER:HA	1.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:347:ILE:O	2:3:351:ASN:ND2	2.47	0.48
5:6:370:THR:HA	5:6:371:GLY:HA2	1.56	0.48
1:A:691:ALA:O	1:A:695:LEU:CB	2.61	0.48
3:C:431:ASP:OD1	3:C:587:ARG:NH2	2.46	0.48
5:E:372:SER:OG	5:E:373:MET:N	2.46	0.48
6:F:665:ILE:O	6:F:669:GLN:HB2	2.13	0.48
6:7:228:ARG:HH22	6:7:326:HIS:HB3	1.79	0.48
6:7:596:ILE:HD11	6:7:695:LEU:HD11	1.94	0.48
3:C:450:GLN:NE2	8:O:24:DG:OP2	2.46	0.48
1:2:212:LYS:HZ1	1:2:275:ALA:HA	1.77	0.48
2:3:219:THR:OG1	2:3:220:THR:N	2.47	0.48
4:5:299:SER:OG	4:5:300:ILE:N	2.42	0.48
6:F:457:CYS:SG	6:F:458:LEU:N	2.87	0.48
1:2:384:ASN:OD1	1:2:384:ASN:N	2.46	0.48
1:2:478:GLU:HA	1:2:481:GLU:HG2	1.95	0.48
1:A:240:GLU:OE1	1:A:290:HIS:ND1	2.47	0.48
3:C:758:ILE:HG22	3:C:760:PRO:HD3	1.96	0.48
4:D:320:GLY:H	4:D:323:ILE:HD12	1.79	0.48
2:3:528:ASP:O	2:3:532:ASN:ND2	2.47	0.47
3:4:431:ASP:OD1	3:4:587:ARG:NH2	2.46	0.47
1:A:247:ARG:NH1	1:A:299:ASP:O	2.47	0.47
3:4:491:ASP:OD1	3:4:491:ASP:N	2.46	0.47
6:7:179:ASP:OD1	6:7:182:ARG:NH2	2.47	0.47
6:7:442:LYS:HB3	6:7:450:ILE:HD11	1.96	0.47
1:A:524:PRO:HA	1:A:535:GLY:HA3	1.95	0.47
5:6:372:SER:OG	5:6:373:MET:N	2.46	0.47
6:7:165:ASN:HA	6:7:166:LEU:HA	1.70	0.47
6:7:457:CYS:SG	6:7:458:LEU:N	2.87	0.47
4:D:304:LYS:NZ	7:S:-24:DC:OP2	2.36	0.47
4:5:320:GLY:H	4:5:323:ILE:HD12	1.79	0.47
6:7:595:ASP:OD1	6:7:595:ASP:N	2.45	0.47
3:C:809:ALA:HB2	3:C:817:VAL:HG23	1.94	0.47
4:D:4:ASP:OD1	4:D:4:ASP:N	2.37	0.47
1:2:208:ALA:HB1	1:2:274:VAL:HG21	1.96	0.47
3:4:758:ILE:HG22	3:4:760:PRO:HD3	1.96	0.47
2:B:156:SER:OG	2:B:157:PHE:N	2.48	0.47
2:B:480:ASP:N	2:B:480:ASP:OD1	2.47	0.47
4:5:256:LEU:HB2	4:5:276:MET:HB2	1.96	0.47
6:F:442:LYS:HB3	6:F:450:ILE:HD11	1.96	0.47
1:2:240:GLU:OE1	1:2:290:HIS:ND1	2.47	0.47
1:2:550:SER:O	1:2:554:LYS:CB	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:691:ALA:O	1:2:695:LEU:HB2	2.14	0.47
3:C:643:SER:HA	3:C:646:HIS:HD2	1.80	0.47
5:E:738:ARG:HA	5:E:739:ASP:HA	1.65	0.47
6:F:206:PRO:HG3	6:F:352:THR:HG21	1.97	0.47
6:F:228:ARG:HH22	6:F:326:HIS:HB3	1.79	0.47
1:A:493:ILE:HD11	1:A:824:ARG:HG2	1.95	0.47
3:4:643:SER:HA	3:4:646:HIS:HD2	1.80	0.47
6:7:216:ARG:HH11	6:7:220:ILE:HD13	1.80	0.47
2:B:654:PRO:O	2:B:658:LYS:NZ	2.39	0.47
2:3:156:SER:OG	2:3:157:PHE:N	2.48	0.47
4:D:40:LEU:O	4:D:43:GLN:N	2.46	0.47
1:2:247:ARG:NH1	1:2:299:ASP:O	2.47	0.46
1:2:479:GLU:O	1:2:483:GLU:CB	2.62	0.46
2:3:718:SER:OG	2:3:719:LYS:N	2.49	0.46
5:6:127:THR:OG1	5:6:128:ASP:N	2.47	0.46
1:A:691:ALA:O	1:A:695:LEU:HB2	2.14	0.46
3:C:445:ARG:HH12	3:C:451:ARG:HD3	1.79	0.46
5:E:759:ARG:HA	5:E:812:ARG:HH21	1.80	0.46
6:F:81:ASP:N	6:F:81:ASP:OD1	2.47	0.46
6:F:678:LYS:HG3	6:F:679:PHE:H	1.80	0.46
2:3:236:THR:OG1	6:7:1:MET:SD	2.73	0.46
3:4:445:ARG:HH12	3:4:451:ARG:HD3	1.79	0.46
6:7:206:PRO:HG3	6:7:352:THR:HG21	1.97	0.46
2:B:536:PRO:HA	2:B:537:ASP:HA	1.74	0.46
3:C:475:ASP:HB3	3:C:586:PRO:HD3	1.96	0.46
3:C:491:ASP:OD1	3:C:491:ASP:N	2.46	0.46
3:4:475:ASP:HB3	3:4:586:PRO:HD3	1.96	0.46
5:6:759:ARG:HA	5:6:812:ARG:HH21	1.80	0.46
1:A:653:ASN:ND2	1:A:666:ASN:O	2.48	0.46
2:B:169:ARG:HG3	2:B:272:ARG:HH21	1.80	0.46
4:D:685:GLN:OE1	4:D:688:THR:OG1	2.33	0.46
6:F:216:ARG:HH11	6:F:220:ILE:HD13	1.80	0.46
1:2:816:ILE:O	1:2:819:SER:OG	2.33	0.46
1:A:208:ALA:HB1	1:A:274:VAL:HG21	1.96	0.46
1:2:697:THR:O	1:2:701:ASP:HB2	2.16	0.46
4:5:685:GLN:OE1	4:5:688:THR:OG1	2.33	0.46
1:A:697:THR:O	1:A:701:ASP:HB2	2.16	0.46
2:B:440:VAL:HG13	2:B:461:ALA:HB3	1.98	0.46
2:3:480:ASP:N	2:3:480:ASP:OD1	2.47	0.46
4:D:421:ALA:HA	9:D:2001:ADP:H5'2	1.97	0.46
4:D:633:LEU:O	4:D:637:GLU:CB	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:144:LYS:HE2	5:E:194:PRO:HD2	1.98	0.46
6:F:614:GLU:O	6:F:618:TYR:HB2	2.16	0.46
1:2:653:ASN:ND2	1:2:666:ASN:O	2.48	0.46
3:4:738:GLN:HA	3:4:739:ASP:HA	1.67	0.46
3:C:768:THR:O	3:C:772:ARG:HB2	2.16	0.46
2:3:440:VAL:HG13	2:3:461:ALA:HB3	1.97	0.46
4:5:152:ASP:HB2	4:5:154:GLU:HG2	1.98	0.46
4:5:216:GLU:HG3	4:5:218:GLU:H	1.81	0.46
1:A:528:ASN:HA	1:A:529:GLY:HA2	1.58	0.46
2:B:219:THR:OG1	2:B:220:THR:N	2.47	0.46
2:B:666:ARG:HA	2:B:667:VAL:HA	1.74	0.46
1:2:267:MET:O	1:2:271:PHE:HB2	2.16	0.45
2:3:169:ARG:HG3	2:3:272:ARG:HH21	1.80	0.45
2:3:564:HIS:O	2:3:568:THR:OG1	2.24	0.45
3:C:362:ARG:HD3	6:F:299:PHE:CZ	2.51	0.45
3:C:526:ILE:HD11	3:C:541:LEU:HD12	1.98	0.45
4:D:216:GLU:HG3	4:D:218:GLU:H	1.81	0.45
6:7:678:LYS:HG3	6:7:679:PHE:H	1.80	0.45
4:D:152:ASP:HB2	4:D:154:GLU:HG2	1.98	0.45
5:E:828:TYR:OH	5:E:832:ARG:NH2	2.50	0.45
3:4:526:ILE:HD11	3:4:541:LEU:HD12	1.98	0.45
1:A:573:ALA:HA	1:A:574:VAL:HA	1.61	0.45
5:E:127:THR:OG1	5:E:128:ASP:N	2.47	0.45
5:E:560:VAL:HA	5:E:561:GLU:HA	1.67	0.45
6:7:614:GLU:O	6:7:618:TYR:HB2	2.16	0.45
1:A:267:MET:O	1:A:271:PHE:HB2	2.16	0.45
1:A:384:ASN:OD1	1:A:384:ASN:N	2.46	0.45
5:E:633:ASN:OD1	5:E:675:ARG:NH1	2.49	0.45
5:6:144:LYS:HE2	5:6:194:PRO:HD2	1.98	0.45
6:7:208:SER:OG	6:7:209:GLN:N	2.49	0.45
6:F:629:ASP:OD1	6:F:629:ASP:N	2.50	0.45
1:A:479:GLU:O	1:A:483:GLU:CB	2.62	0.45
2:B:678:VAL:O	2:B:682:ASN:HB2	2.17	0.45
2:3:666:ARG:HA	2:3:667:VAL:HA	1.74	0.45
2:B:718:SER:OG	2:B:719:LYS:N	2.49	0.45
4:D:224:GLU:HA	4:D:227:ILE:HG22	1.99	0.45
1:2:813:ILE:O	1:2:817:ALA:HB2	2.17	0.45
3:4:526:ILE:HD11	3:4:541:LEU:HB2	1.99	0.45
4:5:549:ARG:HG2	4:5:651:ARG:HH22	1.82	0.45
6:7:127:LEU:HD11	6:7:147:ARG:HH12	1.82	0.45
6:7:668:ARG:HH11	6:7:672:LYS:HE3	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:340:ASN:HA	5:E:341:ARG:HA	1.63	0.45
7:S:-4:DC:H2"	7:S:-3:DA:C8	2.52	0.45
3:4:768:THR:O	3:4:772:ARG:HB2	2.16	0.44
6:7:629:ASP:OD1	6:7:629:ASP:N	2.50	0.44
1:A:517:CYS:SG	1:A:819:SER:OG	2.74	0.44
2:3:158:LYS:HE2	2:3:158:LYS:HB3	1.85	0.44
6:7:451:ARG:HA	6:7:452:GLY:HA3	1.69	0.44
2:B:686:LEU:O	2:B:690:ASP:HB3	2.17	0.44
3:C:206:ARG:HA	3:C:209:LEU:HB3	1.99	0.44
2:3:315:ILE:HG13	4:5:175:ARG:HE	1.83	0.44
3:4:830:ARG:HD3	3:4:833:ILE:HD12	1.99	0.44
5:6:828:TYR:OH	5:6:832:ARG:NH2	2.50	0.44
6:F:208:SER:OG	6:F:209:GLN:N	2.49	0.44
2:3:686:LEU:O	2:3:690:ASP:HB3	2.17	0.44
5:6:633:ASN:OD1	5:6:675:ARG:NH1	2.50	0.44
2:B:564:HIS:O	2:B:568:THR:OG1	2.24	0.44
3:C:526:ILE:HD11	3:C:541:LEU:HB2	1.99	0.44
8:O:43:DT:H2"	8:O:44:DG:C8	2.52	0.44
2:3:435:ARG:HA	2:3:436:GLY:HA3	1.67	0.44
3:4:373:ARG:HA	3:4:374:ILE:HA	1.79	0.44
2:B:236:THR:OG1	6:F:1:MET:SD	2.74	0.44
4:D:549:ARG:HG2	4:D:651:ARG:HH22	1.83	0.44
6:F:543:GLN:HE22	6:F:560:ARG:HA	1.82	0.44
2:3:678:VAL:O	2:3:682:ASN:HB2	2.17	0.44
3:4:520:SER:O	3:4:524:ARG:HB2	2.18	0.44
4:5:224:GLU:HA	4:5:227:ILE:HG22	1.99	0.44
1:A:813:ILE:O	1:A:817:ALA:HB2	2.17	0.44
4:D:130:ASN:HA	4:D:131:SER:HA	1.66	0.44
6:F:179:ASP:OD1	6:F:182:ARG:NH2	2.47	0.44
1:2:604:CYS:SG	1:2:605:LEU:N	2.91	0.44
5:6:833:GLN:HA	5:6:836:ILE:HB	2.00	0.44
6:F:127:LEU:HD11	6:F:147:ARG:HH12	1.82	0.44
2:3:536:PRO:HA	2:3:537:ASP:HA	1.74	0.44
3:4:518:LEU:HG	3:4:522:LEU:HD23	2.00	0.44
4:5:375:ALA:HB1	4:5:378:ILE:HB	2.00	0.44
6:7:504:ASP:HB3	6:7:505:GLU:HB3	2.00	0.43
3:4:206:ARG:HA	3:4:209:LEU:HB3	1.99	0.43
4:5:108:GLN:HA	4:5:109:SER:HA	1.75	0.43
1:A:604:CYS:SG	1:A:605:LEU:N	2.91	0.43
5:E:336:PRO:HA	5:E:337:SER:HA	1.58	0.43
1:2:528:ASN:HA	1:2:529:GLY:HA2	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:402:ASP:OD1	2:3:402:ASP:N	2.51	0.43
3:4:204:LYS:HA	3:4:207:LYS:HD3	2.00	0.43
3:4:531:TYR:CE2	3:4:720:LEU:HA	2.53	0.43
6:7:543:GLN:HE22	6:7:560:ARG:HA	1.81	0.43
1:A:516:ALA:O	1:A:520:PHE:HB2	2.18	0.43
3:C:518:LEU:HG	3:C:522:LEU:HD23	1.99	0.43
6:F:668:ARG:HH11	6:F:672:LYS:HE3	1.83	0.43
1:2:212:LYS:HD3	1:2:212:LYS:HA	1.77	0.43
6:7:348:ILE:HG22	6:7:384:HIS:HD2	1.84	0.43
4:D:375:ALA:HB1	4:D:378:ILE:HB	2.00	0.43
6:F:348:ILE:HG22	6:F:384:HIS:HD2	1.84	0.43
5:6:336:PRO:HA	5:6:337:SER:HA	1.58	0.43
6:7:113:PHE:O	6:7:117:PHE:CB	2.63	0.43
3:C:531:TYR:CE2	3:C:720:LEU:HA	2.53	0.43
3:C:590:TYR:OH	3:C:632:ASP:OD2	2.29	0.43
5:E:109:GLU:HG2	5:E:112:ARG:HH21	1.84	0.43
6:F:451:ARG:HA	6:F:452:GLY:HA3	1.69	0.43
3:4:830:ARG:HA	3:4:833:ILE:HB	2.01	0.43
3:C:830:ARG:HD3	3:C:833:ILE:HD12	1.99	0.43
6:F:614:GLU:O	6:F:618:TYR:CB	2.66	0.43
6:7:614:GLU:O	6:7:618:TYR:CB	2.66	0.43
3:C:204:LYS:HA	3:C:207:LYS:HD3	2.00	0.43
5:E:604:SER:OG	5:E:605:ALA:N	2.52	0.43
1:2:432:ASN:OD1	1:2:432:ASN:N	2.52	0.43
4:5:421:ALA:HB2	9:5:2001:ADP:C8	2.54	0.43
5:6:570:ASN:HD22	5:6:678:ILE:H	1.67	0.43
3:C:520:SER:O	3:C:524:ARG:HB2	2.18	0.43
3:C:565:LEU:HB2	3:C:702:PHE:CD2	2.53	0.43
5:E:370:THR:HA	5:E:371:GLY:HA2	1.56	0.43
3:4:723:HIS:HE1	3:4:736:ILE:HD11	1.84	0.43
1:A:212:LYS:HA	1:A:212:LYS:HD3	1.77	0.43
2:B:267:ALA:HB1	4:D:471:LEU:HD23	2.01	0.43
2:B:435:ARG:HA	2:B:436:GLY:HA3	1.67	0.43
3:C:830:ARG:HA	3:C:833:ILE:HB	2.01	0.43
3:4:565:LEU:HB2	3:4:702:PHE:CD2	2.53	0.43
5:6:819:ILE:HG23	5:6:823:PHE:HD2	1.84	0.43
6:F:287:GLU:O	6:F:291:GLN:NE2	2.52	0.43
6:F:504:ASP:HB3	6:F:505:GLU:HB3	1.99	0.43
3:4:519:TYR:CZ	3:4:538:LYS:HD3	2.55	0.42
1:A:790:TYR:CG	1:A:810:LEU:HD12	2.53	0.42
5:E:833:GLN:HA	5:E:836:ILE:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:775:VAL:HG21	5:6:725:THR:HG22	2.00	0.42
4:5:41:ASP:HA	4:5:42:SER:HA	1.54	0.42
6:7:81:ASP:OD1	6:7:81:ASP:N	2.48	0.42
1:A:299:ASP:HA	1:A:319:ARG:HH12	1.85	0.42
1:2:790:TYR:CG	1:2:810:LEU:HD12	2.53	0.42
2:3:553:ILE:H	2:3:553:ILE:HG13	1.75	0.42
4:5:92:THR:HA	4:5:95:THR:HG22	2.00	0.42
5:6:109:GLU:HG2	5:6:112:ARG:HH21	1.84	0.42
5:6:162:GLU:HG3	5:6:165:ALA:HB3	2.01	0.42
1:A:838:ILE:O	1:A:842:VAL:HB	2.20	0.42
3:C:249:LEU:HD13	3:C:249:LEU:HA	1.90	0.42
3:C:723:HIS:HE1	3:C:736:ILE:HD11	1.84	0.42
6:F:113:PHE:O	6:F:117:PHE:CB	2.63	0.42
1:2:516:ALA:O	1:2:520:PHE:HB2	2.18	0.42
4:5:558:ASP:OD1	4:5:558:ASP:N	2.52	0.42
4:5:633:LEU:O	4:5:637:GLU:CB	2.62	0.42
1:A:432:ASN:OD1	1:A:432:ASN:N	2.52	0.42
3:C:729:LEU:HD22	3:C:730:GLU:H	1.84	0.42
4:D:92:THR:HA	4:D:95:THR:HG22	2.00	0.42
4:D:558:ASP:N	4:D:558:ASP:OD1	2.52	0.42
5:E:570:ASN:HD22	5:E:678:ILE:H	1.67	0.42
2:3:437:SER:HA	2:3:438:SER:HA	1.75	0.42
4:5:654:GLU:OE1	4:5:658:ARG:NH2	2.52	0.42
3:C:370:ARG:HA	3:C:371:CYS:HA	1.87	0.42
3:C:419:VAL:HG12	3:C:463:VAL:HG21	2.02	0.42
4:D:108:GLN:HA	4:D:109:SER:HA	1.75	0.42
5:E:550:GLN:HG2	5:E:569:ILE:HG23	2.02	0.42
6:F:470:LEU:HD21	6:F:564:LEU:HD22	2.01	0.42
3:4:578:LEU:HD23	3:4:578:LEU:HA	1.79	0.42
3:4:729:LEU:HD22	3:4:730:GLU:H	1.85	0.42
5:6:738:ARG:HA	5:6:739:ASP:HA	1.65	0.42
1:A:212:LYS:HZ1	1:A:275:ALA:HA	1.83	0.42
1:A:633:LYS:HA	1:A:634:ALA:HA	1.78	0.42
4:D:654:GLU:OE1	4:D:658:ARG:NH2	2.52	0.42
6:F:482:TYR:OH	6:F:524:ASP:OD2	2.23	0.42
2:3:116:VAL:HG12	2:3:117:GLU:HG3	2.01	0.42
2:3:221:LEU:HD21	2:3:297:VAL:HG11	2.02	0.42
5:6:414:GLY:HA3	5:6:415:VAL:HA	1.84	0.42
3:C:519:TYR:CZ	3:C:538:LYS:HD3	2.54	0.42
2:3:204:ALA:HA	2:3:205:LYS:HA	1.71	0.42
2:3:211:TYR:HD2	6:7:6:PRO:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:40:LEU:O	4:5:43:GLN:N	2.46	0.42
5:6:106:VAL:O	5:6:110:LYS:CB	2.68	0.42
5:6:284:ILE:HD12	5:6:284:ILE:HA	1.92	0.42
5:6:550:GLN:HG2	5:6:569:ILE:HG23	2.02	0.42
5:6:604:SER:OG	5:6:605:ALA:N	2.52	0.42
2:B:216:ASP:OD1	2:B:216:ASP:N	2.52	0.42
6:F:283:GLU:HG3	6:F:295:LYS:HG2	2.02	0.42
1:2:353:GLN:HA	1:2:354:ASP:HA	1.88	0.42
3:4:419:VAL:HG12	3:4:463:VAL:HG21	2.02	0.42
2:B:116:VAL:HG12	2:B:117:GLU:HG3	2.01	0.42
2:3:433:THR:HG22	2:3:473:ASP:HB2	2.02	0.42
6:7:287:GLU:O	6:7:291:GLN:NE2	2.52	0.42
2:B:221:LEU:HD21	2:B:297:VAL:HG11	2.02	0.42
6:7:432:LEU:HD23	6:7:432:LEU:HA	1.85	0.41
6:7:491:VAL:HA	6:7:494:THR:HG22	2.02	0.41
3:C:399:LEU:HD13	3:C:417:LEU:HD21	2.02	0.41
5:E:819:ILE:HG23	5:E:823:PHE:HD2	1.84	0.41
1:2:852:SER:OG	1:2:855:ARG:NH1	2.53	0.41
6:7:283:GLU:HG3	6:7:295:LYS:HG2	2.02	0.41
5:E:162:GLU:HG3	5:E:165:ALA:HB3	2.01	0.41
6:F:369:GLY:HA2	6:F:370:LEU:HA	1.69	0.41
7:S:-24:DC:H2"	7:S:-23:DA:C8	2.55	0.41
2:3:340:GLN:HB3	2:3:661:GLN:HE22	1.85	0.41
2:3:687:ARG:HH21	6:7:604:PRO:HA	1.85	0.41
1:A:411:LEU:HB3	1:A:412:ALA:H	1.73	0.41
5:E:154:ASP:OD1	5:E:155:TYR:N	2.53	0.41
1:2:778:LEU:HD13	1:2:783:MET:HG3	2.03	0.41
6:7:470:LEU:HD21	6:7:564:LEU:HD22	2.01	0.41
8:O:7:DT:H2"	8:O:8:DG:C8	2.55	0.41
1:2:838:ILE:O	1:2:842:VAL:HB	2.20	0.41
3:C:319:PRO:HB3	6:F:253:PRO:HB3	2.02	0.41
5:E:359:VAL:HG23	5:E:379:VAL:HG13	2.02	0.41
6:F:124:ASN:OD1	6:F:124:ASN:N	2.53	0.41
6:F:432:LEU:HA	6:F:432:LEU:HD23	1.85	0.41
5:6:288:LEU:HD12	5:6:288:LEU:HA	1.87	0.41
1:A:852:SER:OG	1:A:855:ARG:NH1	2.53	0.41
2:B:340:GLN:HB3	2:B:661:GLN:HE22	1.85	0.41
2:B:433:THR:HG22	2:B:473:ASP:HB2	2.02	0.41
3:C:738:GLN:HA	3:C:739:ASP:HA	1.67	0.41
8:O:52:DG:H2"	8:O:53:DA:C8	2.55	0.41
1:2:411:LEU:HB3	1:2:412:ALA:H	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:786:GLN:HA	5:E:787:GLY:HA2	1.62	0.41
6:F:484:THR:OG1	6:F:485:GLY:N	2.54	0.41
6:F:719:LEU:O	6:F:723:SER:CB	2.54	0.41
1:2:299:ASP:HA	1:2:319:ARG:HH12	1.85	0.41
1:2:530:LYS:HA	1:2:530:LYS:HD2	1.89	0.41
5:6:296:ARG:NH1	5:6:360:ARG:HH12	2.19	0.41
5:6:786:GLN:HA	5:6:787:GLY:HA2	1.62	0.41
9:B:2001:ADP:C8	4:D:650:ILE:HD11	2.55	0.41
1:2:811:GLU:OE1	1:2:815:ARG:NH1	2.54	0.41
3:4:399:LEU:HD13	3:4:417:LEU:HD21	2.02	0.41
5:6:614:ARG:HA	5:6:615:ASP:HA	1.67	0.41
5:6:710:ASP:HA	5:6:711:LEU:HA	1.72	0.41
1:A:811:GLU:OE1	1:A:815:ARG:NH1	2.54	0.41
4:D:211:CYS:HB2	4:D:236:CYS:HB2	1.30	0.41
4:D:565:ASP:HA	4:D:568:ILE:HG22	2.03	0.41
5:E:106:VAL:O	5:E:110:LYS:CB	2.68	0.41
5:E:710:ASP:HA	5:E:711:LEU:HA	1.72	0.41
6:F:491:VAL:HA	6:F:494:THR:HG22	2.02	0.41
5:6:559:THR:OG1	5:6:563:ILE:O	2.28	0.41
6:7:124:ASN:N	6:7:124:ASN:OD1	2.53	0.41
1:A:530:LYS:HA	1:A:530:LYS:HD2	1.88	0.41
3:C:370:ARG:HB2	3:C:371:CYS:HB2	2.03	0.41
6:F:67:LEU:HD11	6:F:121:ILE:HG23	2.03	0.41
6:F:461:ASP:N	6:F:461:ASP:OD1	2.54	0.41
6:F:571:TYR:HA	6:F:572:GLY:HA2	1.88	0.41
4:5:444:SER:HA	4:5:445:SER:HA	1.75	0.40
5:6:359:VAL:HG23	5:6:379:VAL:HG13	2.02	0.40
6:7:484:THR:OG1	6:7:485:GLY:N	2.54	0.40
4:D:526:ILE:H	4:D:526:ILE:HG13	1.73	0.40
4:D:594:ILE:HD12	4:D:595:SER:H	1.86	0.40
1:2:305:SER:OG	1:2:306:LEU:N	2.52	0.40
6:7:436:LEU:HA	6:7:436:LEU:HD23	1.91	0.40
6:7:461:ASP:HA	6:7:462:PRO:HA	1.90	0.40
3:C:494:GLU:HB3	3:C:495:VAL:H	1.76	0.40
3:C:828:LEU:HD23	3:C:828:LEU:HA	1.95	0.40
4:D:500:GLN:HE21	4:D:516:ARG:HA	1.86	0.40
6:F:165:ASN:HA	6:F:166:LEU:HA	1.70	0.40
6:7:439:GLY:HA2	6:7:440:VAL:HA	1.90	0.40
3:4:370:ARG:HA	3:4:371:CYS:HA	1.87	0.40
6:7:67:LEU:HD11	6:7:121:ILE:HG23	2.03	0.40
1:A:663:LEU:HD13	1:A:680:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:354:HIS:HB3	3:C:372:GLU:HB2	2.03	0.40
3:4:184:ASN:N	3:4:184:ASN:OD1	2.55	0.40
4:5:211:CYS:HB2	4:5:236:CYS:HB2	1.30	0.40
1:A:778:LEU:HD13	1:A:783:MET:HG3	2.03	0.40
2:B:172:THR:HA	2:B:173:ALA:HA	1.96	0.40
5:E:517:LYS:HA	5:E:520:VAL:HG22	2.03	0.40
6:F:723:SER:OG	6:F:724:LYS:N	2.55	0.40
7:S:-12:DC:H2 ⁷	7:S:-11:DA:C8	2.56	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	597/868 (69%)	522 (87%)	75 (13%)	0	100	100
1	A	597/868 (69%)	522 (87%)	75 (13%)	0	100	100
2	3	596/971 (61%)	531 (89%)	64 (11%)	1 (0%)	47	79
2	B	596/971 (61%)	531 (89%)	64 (11%)	1 (0%)	47	79
3	4	638/933 (68%)	543 (85%)	93 (15%)	2 (0%)	41	75
3	C	638/933 (68%)	543 (85%)	93 (15%)	2 (0%)	41	75
4	5	655/775 (84%)	578 (88%)	77 (12%)	0	100	100
4	D	655/775 (84%)	579 (88%)	76 (12%)	0	100	100
5	6	607/1017 (60%)	527 (87%)	78 (13%)	2 (0%)	41	75
5	E	607/1017 (60%)	527 (87%)	78 (13%)	2 (0%)	41	75
6	7	681/845 (81%)	606 (89%)	74 (11%)	1 (0%)	51	84
6	F	681/845 (81%)	605 (89%)	75 (11%)	1 (0%)	51	84
All	All	7548/10818 (70%)	6614 (88%)	922 (12%)	12 (0%)	50	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	293	LEU
3	4	361	ASP
6	7	502	VAL
3	C	293	LEU
3	C	361	ASP
6	F	502	VAL
5	6	305	TYR
5	E	305	TYR
5	6	321	VAL
5	E	321	VAL
2	3	162	GLY
2	B	162	GLY

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	509/770 (66%)	507 (100%)	2 (0%)	91	94
1	A	509/770 (66%)	507 (100%)	2 (0%)	91	94
2	3	522/835 (62%)	517 (99%)	5 (1%)	76	86
2	B	522/835 (62%)	517 (99%)	5 (1%)	76	86
3	4	578/848 (68%)	576 (100%)	2 (0%)	92	95
3	C	578/848 (68%)	576 (100%)	2 (0%)	92	95
4	5	591/688 (86%)	582 (98%)	9 (2%)	65	80
4	D	591/688 (86%)	582 (98%)	9 (2%)	65	80
5	6	496/886 (56%)	494 (100%)	2 (0%)	91	94
5	E	496/886 (56%)	494 (100%)	2 (0%)	91	94
6	7	609/753 (81%)	607 (100%)	2 (0%)	92	95
6	F	609/753 (81%)	607 (100%)	2 (0%)	92	95
All	All	6610/9560 (69%)	6566 (99%)	44 (1%)	84	90

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	288	ARG
1	2	306	LEU
2	3	187	THR
2	3	221	LEU
2	3	310	ASN
2	3	312	ASN
2	3	413	THR
3	4	402	THR
3	4	442	ILE
4	5	181	ILE
4	5	183	CYS
4	5	209	ARG
4	5	234	LYS
4	5	325	THR
4	5	326	PRO
4	5	573	ILE
4	5	590	ASN
4	5	643	ARG
5	6	370	THR
5	6	696	ARG
6	7	279	THR
6	7	298	LEU
1	A	288	ARG
1	A	306	LEU
2	B	187	THR
2	B	221	LEU
2	B	310	ASN
2	B	312	ASN
2	B	413	THR
3	C	402	THR
3	C	442	ILE
4	D	181	ILE
4	D	183	CYS
4	D	209	ARG
4	D	234	LYS
4	D	325	THR
4	D	326	PRO
4	D	573	ILE
4	D	590	ASN
4	D	643	ARG
5	E	370	THR
5	E	696	ARG

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Mol	Chain	Res	Type
6	F	279	THR
6	F	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	238	ASN
1	2	653	ASN
1	2	768	HIS
1	2	856	GLN
2	3	310	ASN
2	3	312	ASN
2	3	351	ASN
2	3	424	ASN
2	3	532	ASN
3	4	723	HIS
4	5	198	ASN
4	5	203	ASN
4	5	253	GLN
4	5	500	GLN
4	5	586	GLN
4	5	590	ASN
4	5	636	ASN
5	6	550	GLN
5	6	750	GLN
6	7	89	GLN
6	7	334	HIS
6	7	379	GLN
6	7	384	HIS
6	7	543	GLN
1	A	238	ASN
1	A	561	HIS
1	A	653	ASN
1	A	768	HIS
1	A	780	GLN
1	A	856	GLN
2	B	310	ASN
2	B	312	ASN
2	B	351	ASN
2	B	424	ASN
2	B	532	ASN
3	C	318	ASN

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Mol	Chain	Res	Type
3	C	723	HIS
4	D	198	ASN
4	D	203	ASN
4	D	500	GLN
4	D	586	GLN
4	D	590	ASN
4	D	636	ASN
5	E	550	GLN
5	E	750	GLN
6	F	89	GLN
6	F	334	HIS
6	F	379	GLN
6	F	384	HIS
6	F	543	GLN

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 [i](#)

8 ligands are modelled in this entry.

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	ADP	3	2001	-	24,29,29	0.97	1 (4%)	29,45,45	1.40	4 (13%)
9	ADP	D	2001	-	24,29,29	0.98	1 (4%)	29,45,45	1.59	5 (17%)
9	ADP	2	2001	-	24,29,29	0.94	1 (4%)	29,45,45	1.53	4 (13%)
9	ADP	A	2001	-	24,29,29	0.95	1 (4%)	29,45,45	1.53	4 (13%)
9	ADP	B	2001	-	24,29,29	0.96	1 (4%)	29,45,45	1.39	3 (10%)
9	ADP	7	2001	-	24,29,29	0.96	1 (4%)	29,45,45	1.57	3 (10%)
9	ADP	F	2001	-	24,29,29	0.96	1 (4%)	29,45,45	1.58	3 (10%)
9	ADP	5	2001	-	24,29,29	0.98	1 (4%)	29,45,45	1.59	5 (17%)

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	ADP	3	2001	-	-	3/12/32/32	0/3/3/3
9	ADP	D	2001	-	-	6/12/32/32	0/3/3/3
9	ADP	2	2001	-	-	3/12/32/32	0/3/3/3
9	ADP	A	2001	-	-	3/12/32/32	0/3/3/3
9	ADP	B	2001	-	-	3/12/32/32	0/3/3/3
9	ADP	7	2001	-	-	5/12/32/32	0/3/3/3
9	ADP	F	2001	-	-	5/12/32/32	0/3/3/3
9	ADP	5	2001	-	-	5/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2001	ADP	C5-C4	2.48	1.47	1.40
9	2	2001	ADP	C5-C4	2.45	1.47	1.40
9	5	2001	ADP	C5-C4	2.43	1.47	1.40
9	D	2001	ADP	C5-C4	2.43	1.47	1.40
9	F	2001	ADP	C5-C4	2.37	1.47	1.40
9	7	2001	ADP	C5-C4	2.37	1.47	1.40
9	3	2001	ADP	C5-C4	2.36	1.47	1.40
9	B	2001	ADP	C5-C4	2.36	1.47	1.40

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	2001	ADP	C3'-C2'-C1'	4.46	107.69	100.98
9	7	2001	ADP	C3'-C2'-C1'	4.32	107.48	100.98
9	D	2001	ADP	PA-O3A-PB	-3.98	119.15	132.83
9	5	2001	ADP	PA-O3A-PB	-3.95	119.28	132.83
9	2	2001	ADP	C3'-C2'-C1'	3.94	106.91	100.98
9	A	2001	ADP	C3'-C2'-C1'	3.93	106.90	100.98
9	2	2001	ADP	PA-O3A-PB	-3.75	119.96	132.83
9	A	2001	ADP	PA-O3A-PB	-3.72	120.07	132.83
9	3	2001	ADP	C3'-C2'-C1'	3.44	106.15	100.98
9	F	2001	ADP	N3-C2-N1	-3.42	123.33	128.68
9	D	2001	ADP	C3'-C2'-C1'	3.38	106.06	100.98
9	B	2001	ADP	C3'-C2'-C1'	3.37	106.05	100.98
9	7	2001	ADP	N3-C2-N1	-3.36	123.43	128.68
9	B	2001	ADP	N3-C2-N1	-3.31	123.51	128.68
9	5	2001	ADP	C3'-C2'-C1'	3.30	105.95	100.98
9	3	2001	ADP	N3-C2-N1	-3.28	123.55	128.68
9	A	2001	ADP	N3-C2-N1	-3.21	123.67	128.68
9	2	2001	ADP	N3-C2-N1	-3.18	123.70	128.68
9	7	2001	ADP	PA-O3A-PB	-3.12	122.14	132.83
9	5	2001	ADP	N3-C2-N1	-3.06	123.89	128.68
9	F	2001	ADP	PA-O3A-PB	-3.04	122.39	132.83
9	D	2001	ADP	N3-C2-N1	-3.03	123.95	128.68
9	A	2001	ADP	C4-C5-N7	-2.58	106.72	109.40
9	2	2001	ADP	C4-C5-N7	-2.57	106.72	109.40
9	3	2001	ADP	C4-C5-N7	-2.22	107.09	109.40
9	B	2001	ADP	C4-C5-N7	-2.19	107.11	109.40
9	D	2001	ADP	C1'-N9-C4	2.18	130.46	126.64
9	D	2001	ADP	C4-C5-N7	-2.15	107.16	109.40
9	5	2001	ADP	C4-C5-N7	-2.10	107.21	109.40
9	3	2001	ADP	C2'-C3'-C4'	2.06	106.64	102.64
9	5	2001	ADP	C1'-N9-C4	2.04	130.23	126.64

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	2	2001	ADP	PA-O3A-PB-O3B
9	3	2001	ADP	C5'-O5'-PA-O1A
9	3	2001	ADP	C5'-O5'-PA-O2A
9	5	2001	ADP	PA-O3A-PB-O3B
9	5	2001	ADP	C5'-O5'-PA-O1A
9	7	2001	ADP	PB-O3A-PA-O5'
9	7	2001	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
9	7	2001	ADP	C5'-O5'-PA-O2A
9	A	2001	ADP	PA-O3A-PB-O3B
9	B	2001	ADP	C5'-O5'-PA-O1A
9	B	2001	ADP	C5'-O5'-PA-O2A
9	D	2001	ADP	PA-O3A-PB-O3B
9	D	2001	ADP	C5'-O5'-PA-O3A
9	F	2001	ADP	PB-O3A-PA-O5'
9	F	2001	ADP	C5'-O5'-PA-O1A
9	F	2001	ADP	C5'-O5'-PA-O2A
9	D	2001	ADP	C3'-C4'-C5'-O5'
9	5	2001	ADP	C5'-O5'-PA-O3A
9	7	2001	ADP	C5'-O5'-PA-O3A
9	B	2001	ADP	C5'-O5'-PA-O3A
9	F	2001	ADP	C5'-O5'-PA-O3A
9	D	2001	ADP	C5'-O5'-PA-O1A
9	5	2001	ADP	C3'-C4'-C5'-O5'
9	2	2001	ADP	PA-O3A-PB-O2B
9	5	2001	ADP	PA-O3A-PB-O2B
9	A	2001	ADP	PA-O3A-PB-O2B
9	D	2001	ADP	PA-O3A-PB-O2B
9	3	2001	ADP	C5'-O5'-PA-O3A
9	2	2001	ADP	O4'-C4'-C5'-O5'
9	7	2001	ADP	O4'-C4'-C5'-O5'
9	A	2001	ADP	O4'-C4'-C5'-O5'
9	F	2001	ADP	O4'-C4'-C5'-O5'
9	D	2001	ADP	O4'-C4'-C5'-O5'

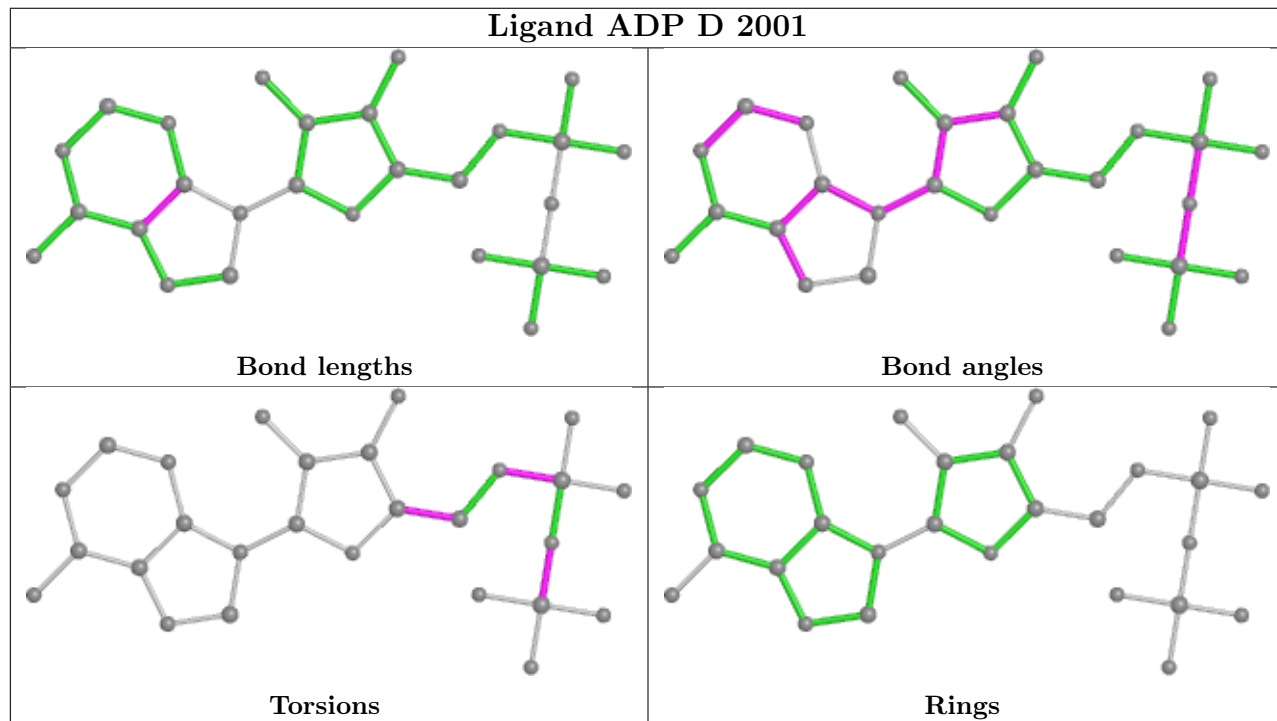
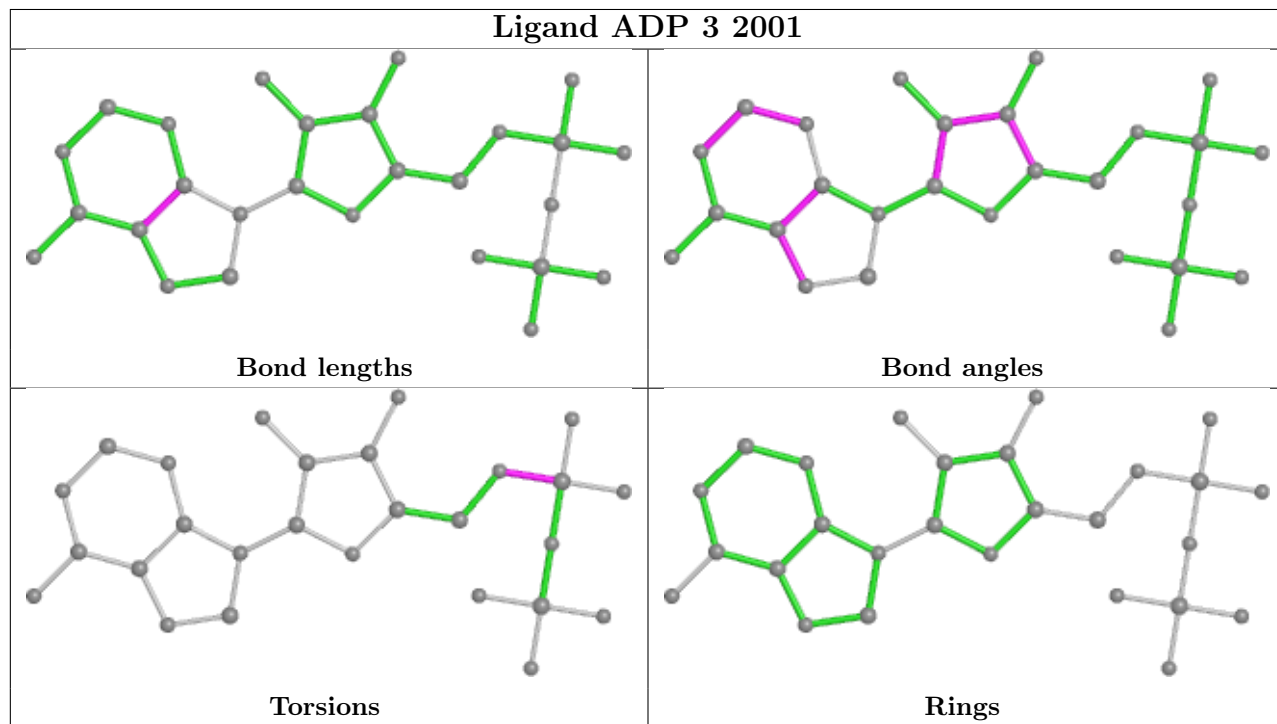
There are no ring outliers.

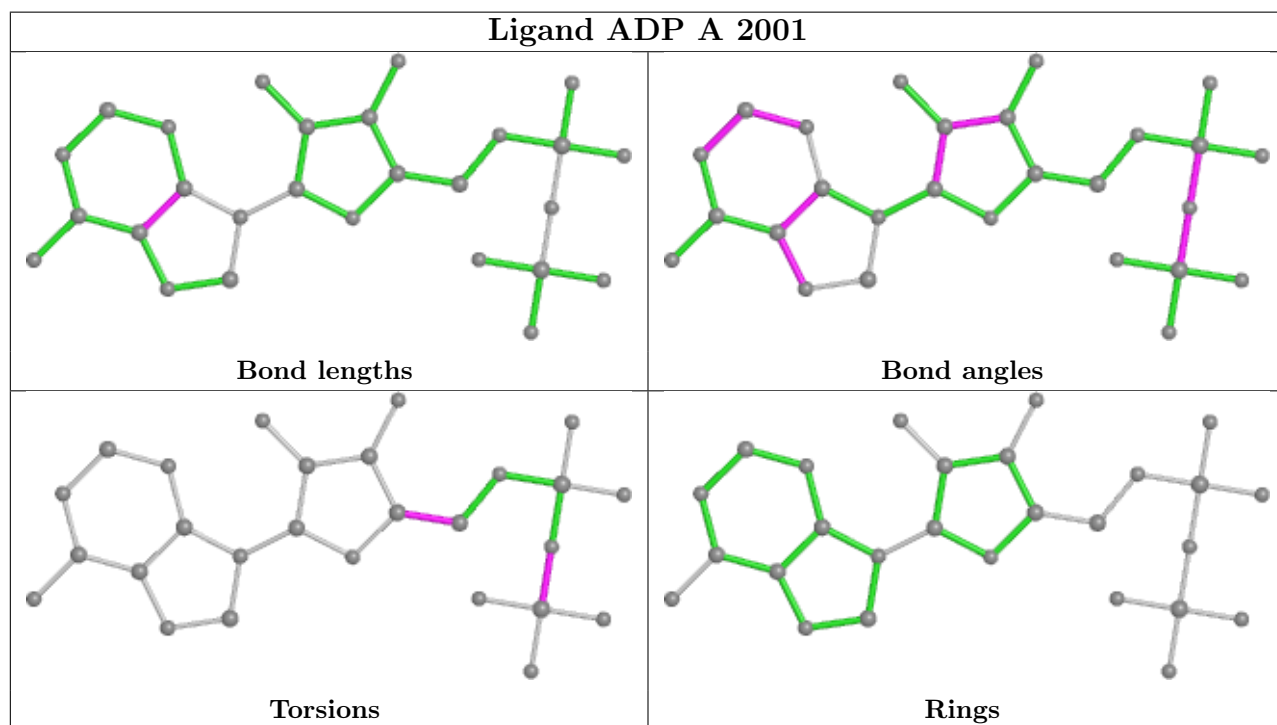
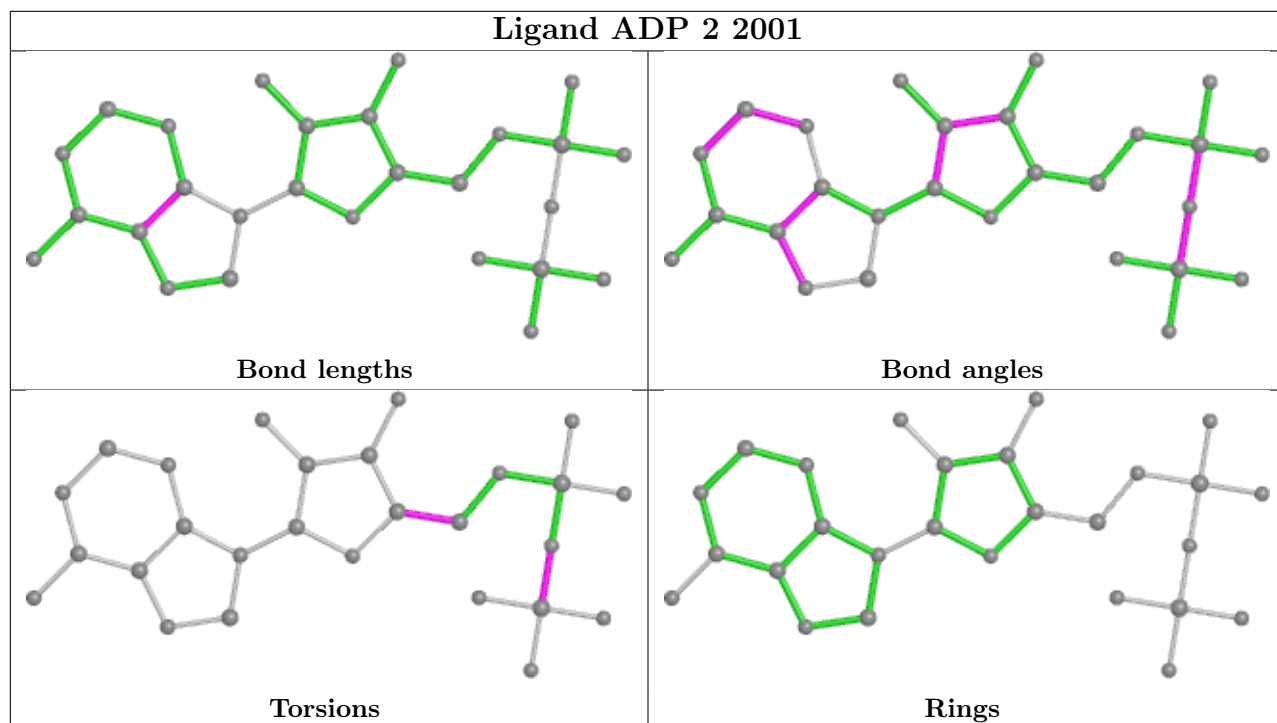
5 monomers are involved in 6 short contacts:

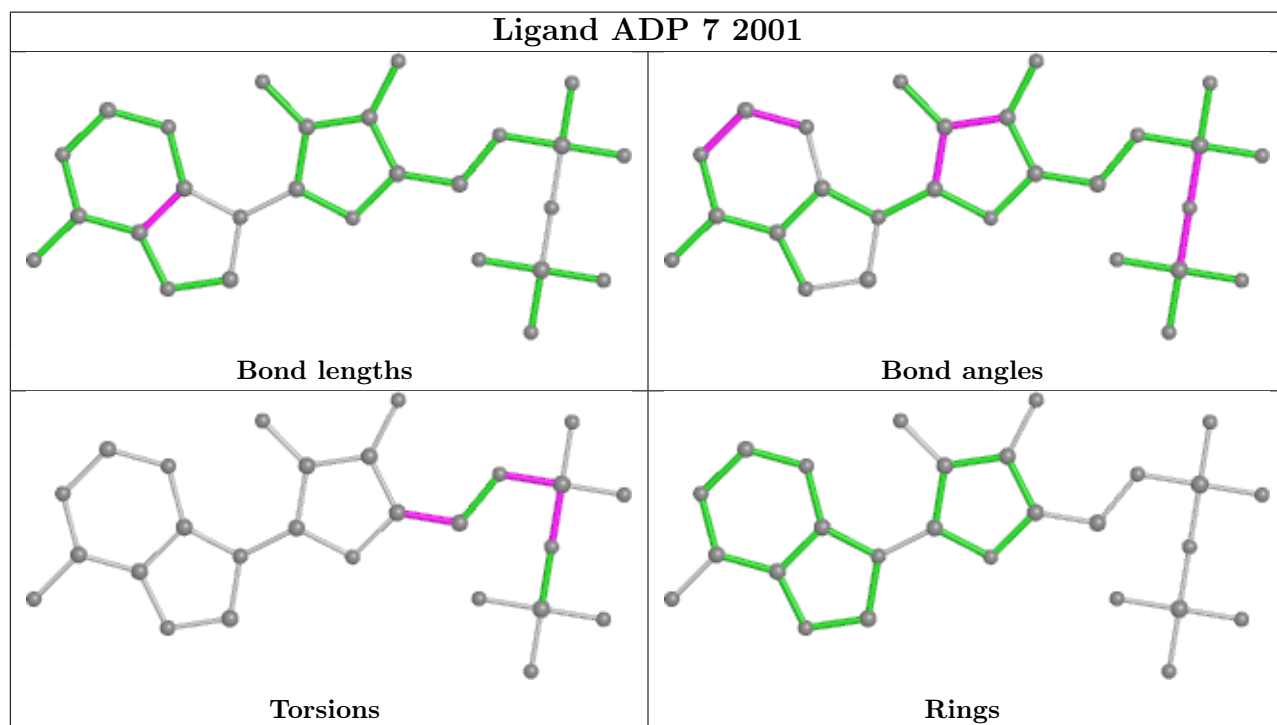
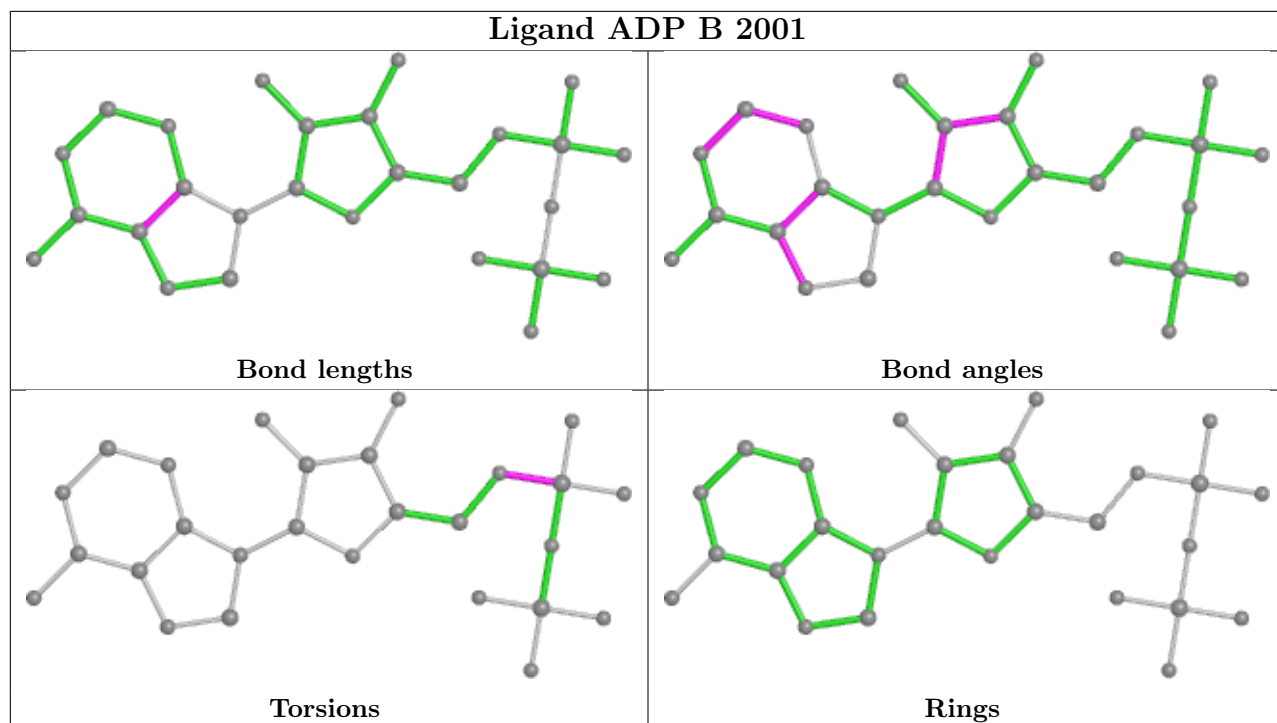
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	2001	ADP	1	0
9	B	2001	ADP	1	0
9	7	2001	ADP	1	0
9	F	2001	ADP	1	0
9	5	2001	ADP	2	0

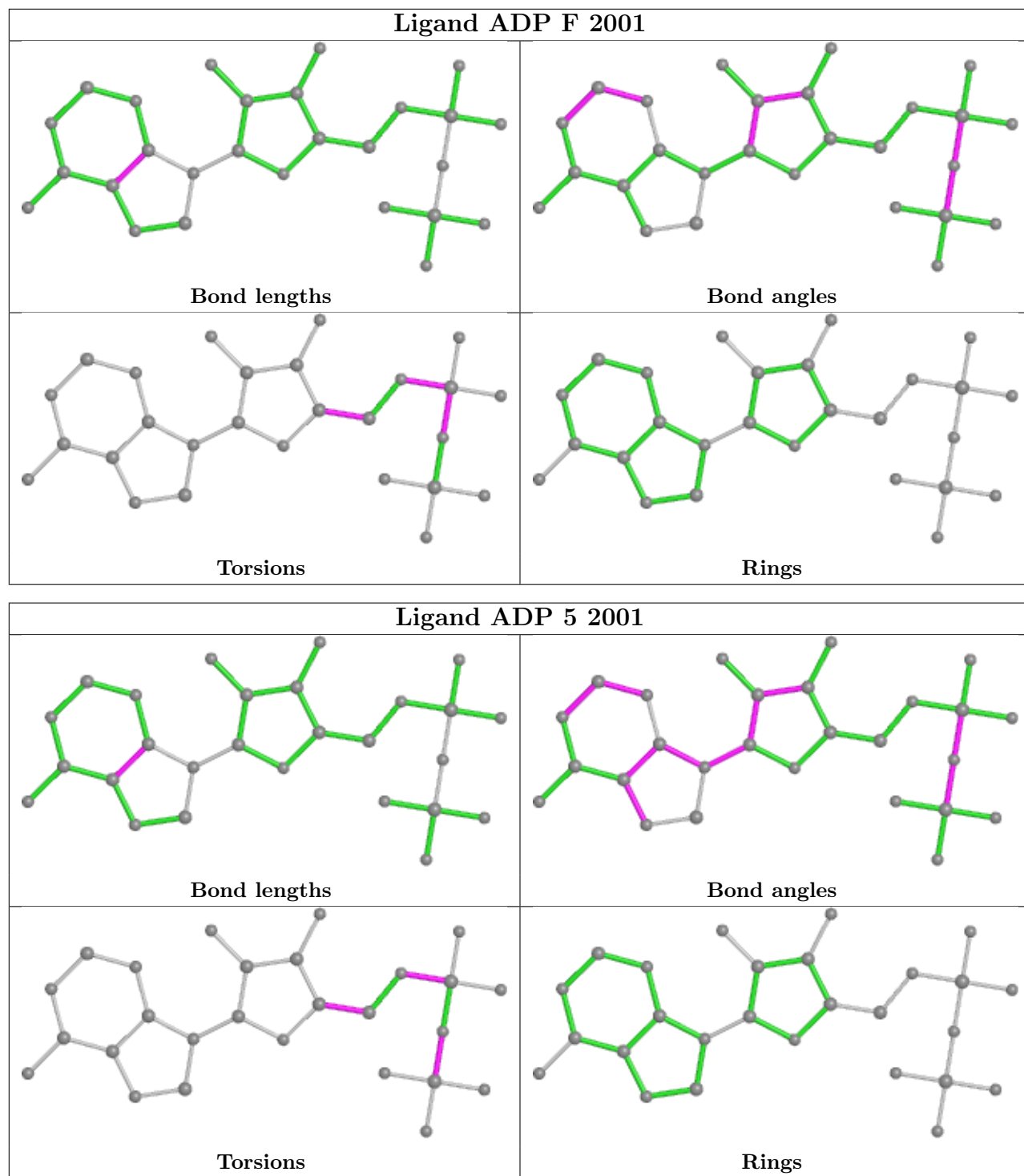
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

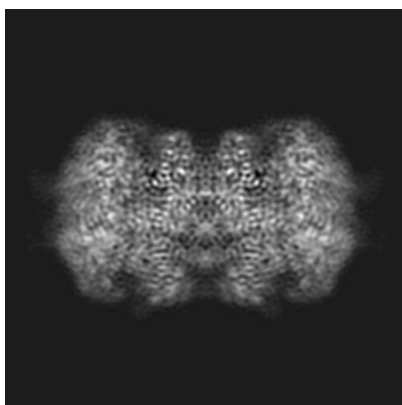
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9400. These allow visual inspection of the internal detail of the map and identification of artifacts.

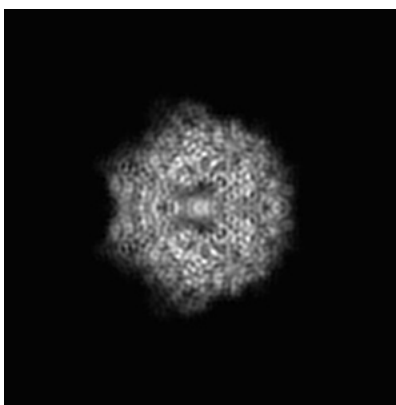
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

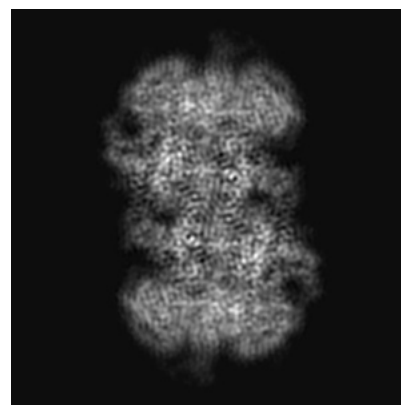
6.1.1 Primary map



X



Y

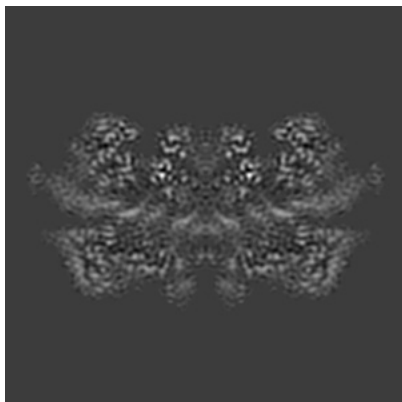


Z

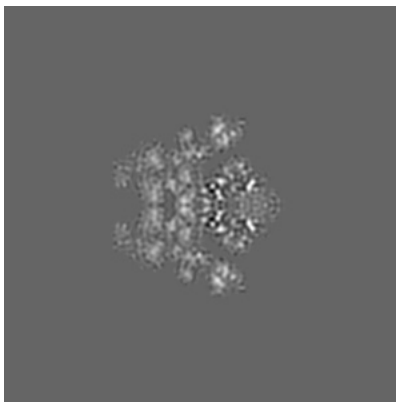
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

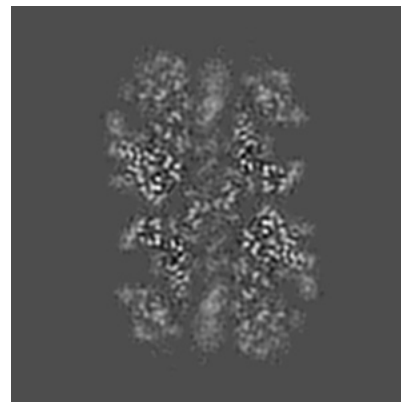
6.2.1 Primary map



X Index: 128



Y Index: 128

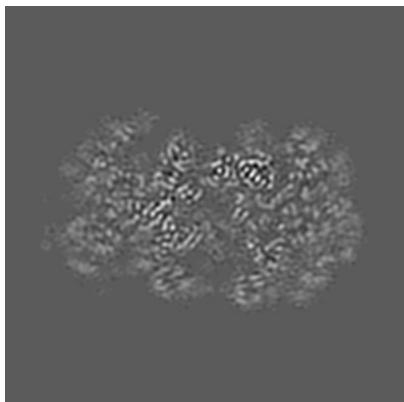


Z Index: 128

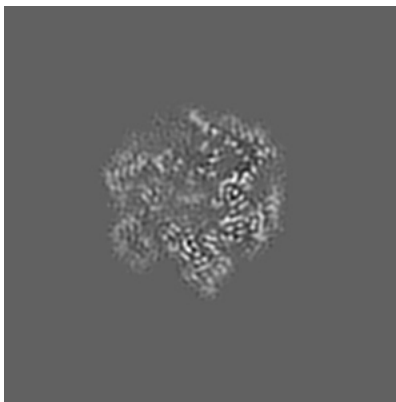
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

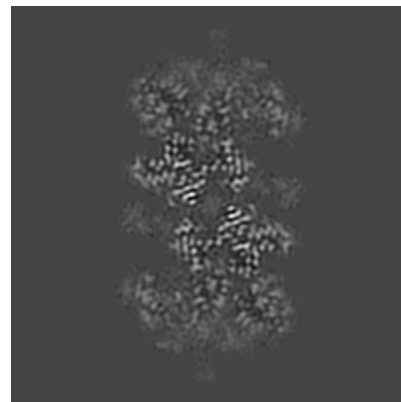
6.3.1 Primary map



X Index: 108



Y Index: 105

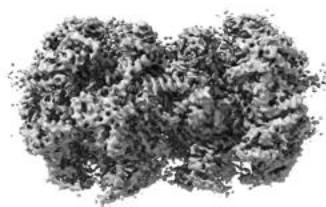


Z Index: 151

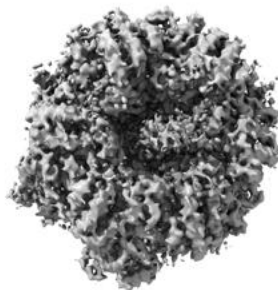
The images above show the largest variance slices of the map in three orthogonal directions.

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

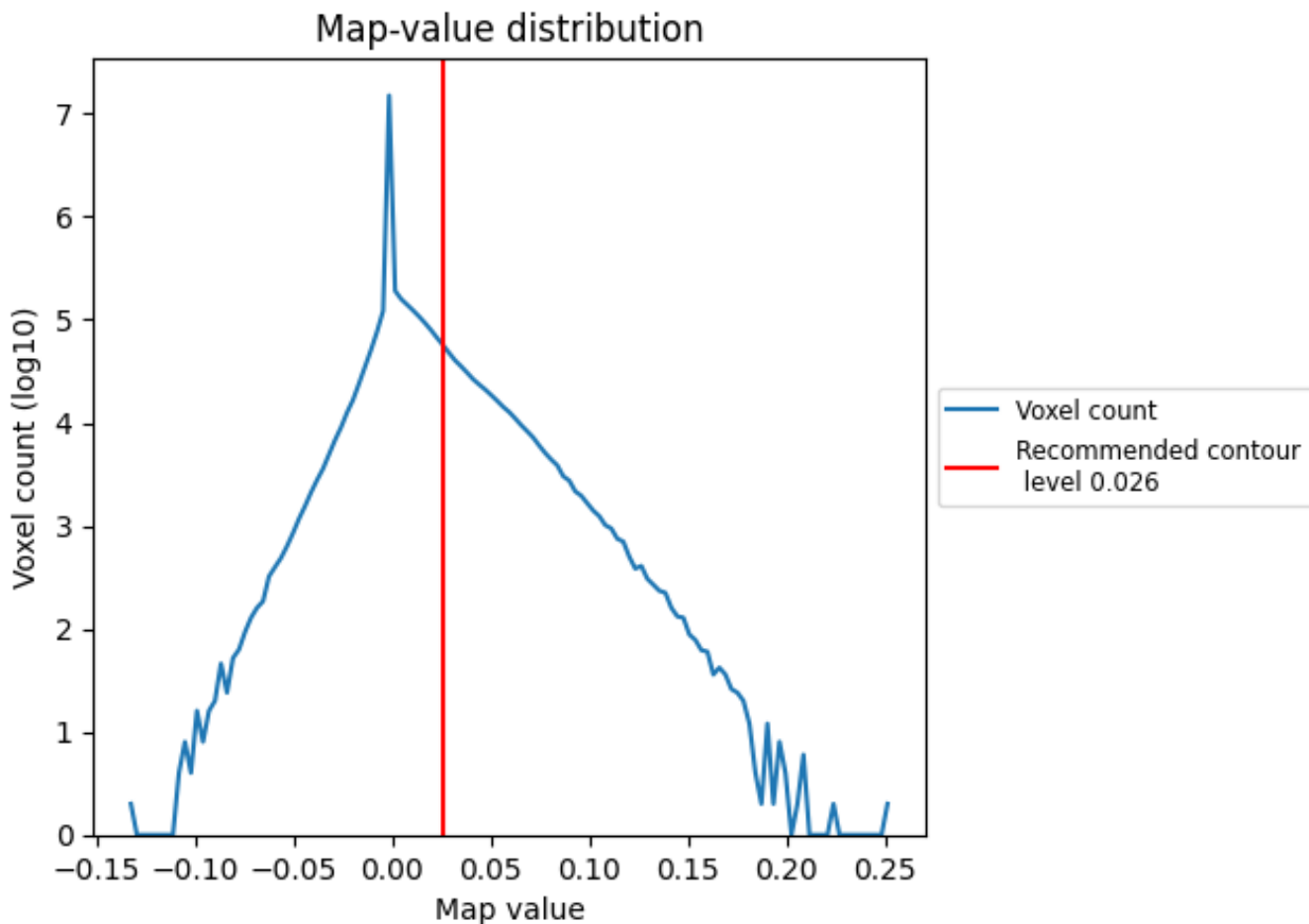
6.5 Mask visualisation

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

7 Map analysis [i](#)

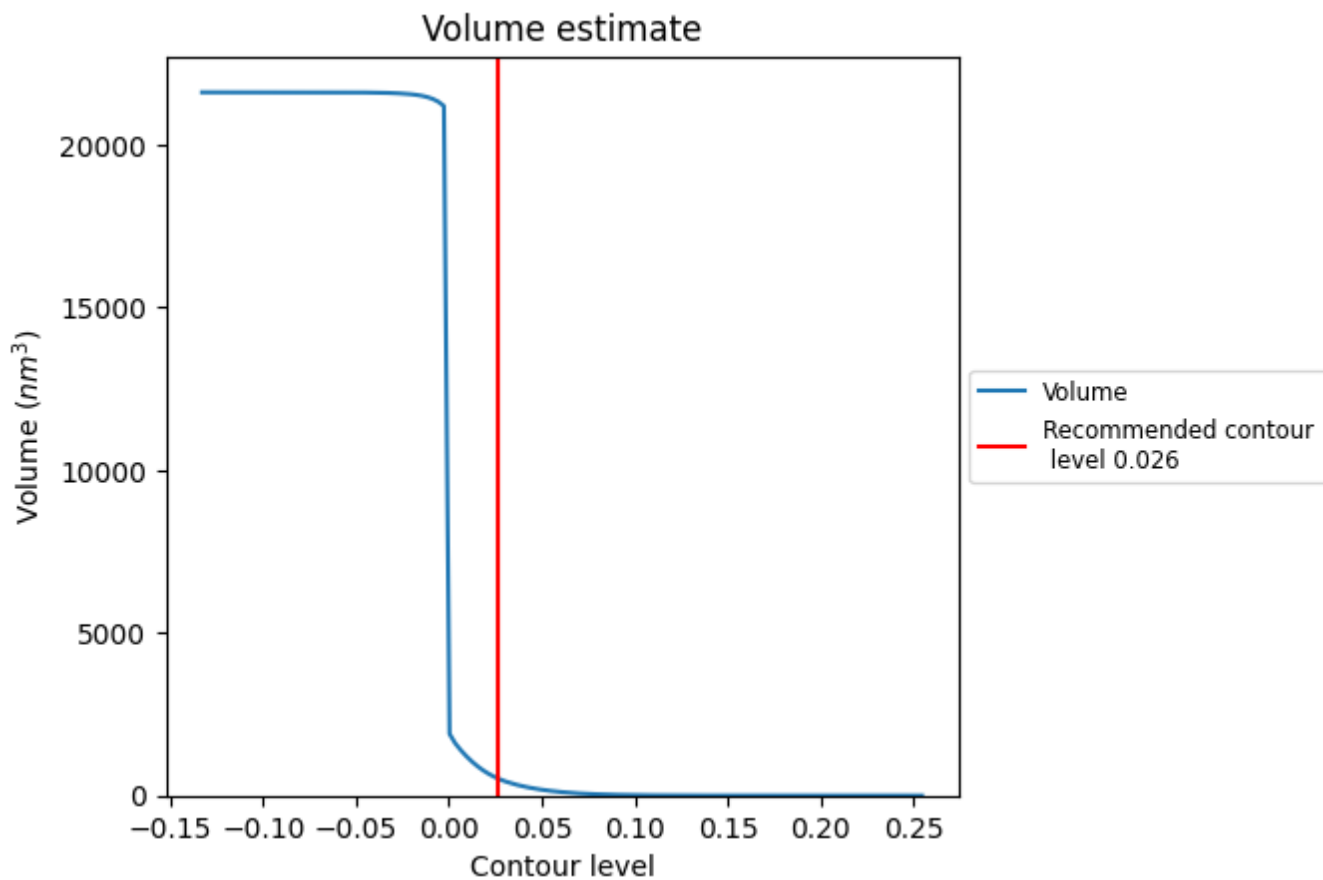
This section contains the results of statistical analysis of the map.

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.

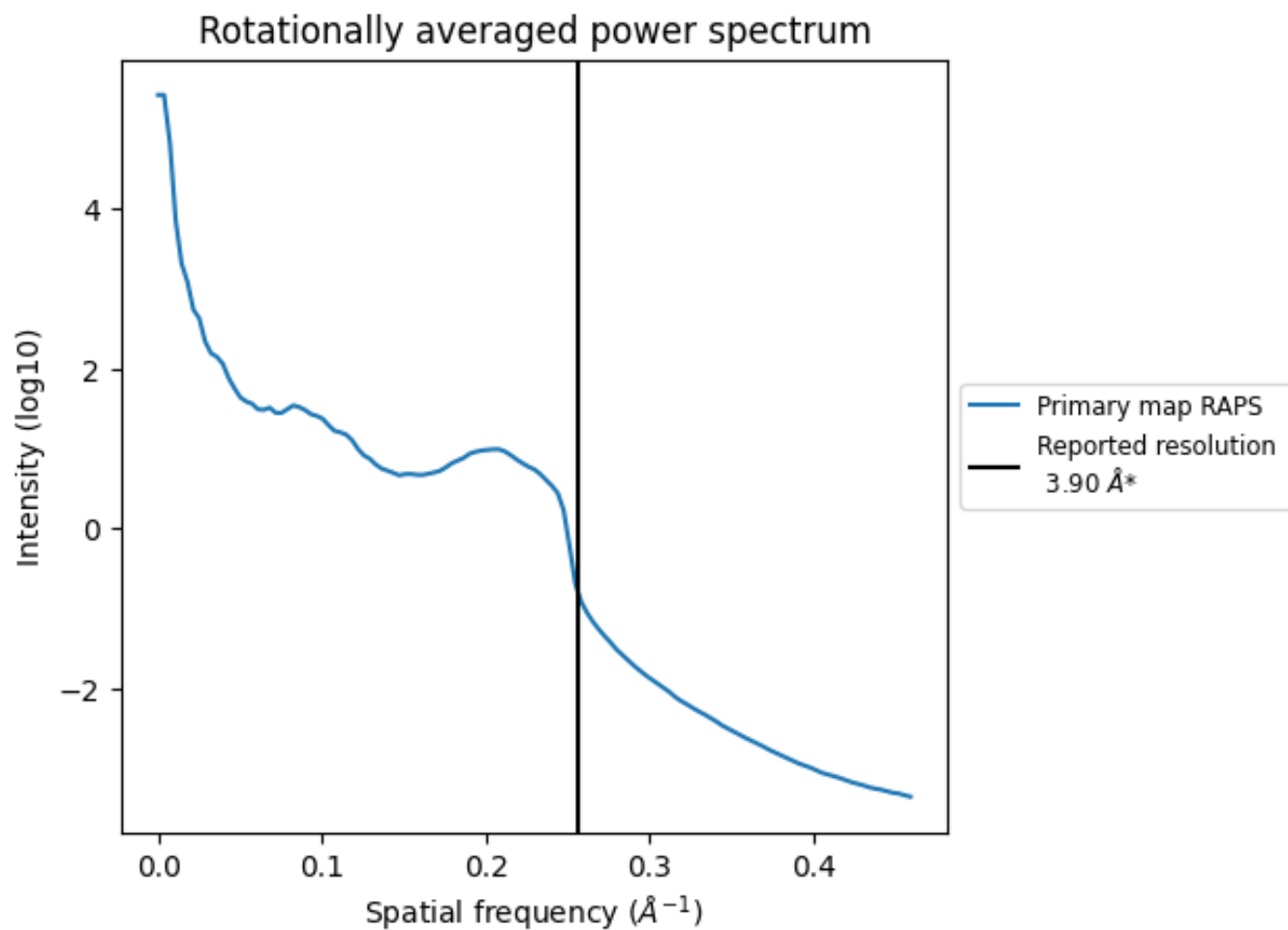
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 537 nm³; this corresponds to an approximate mass of 485 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 0.256\AA^{-1}

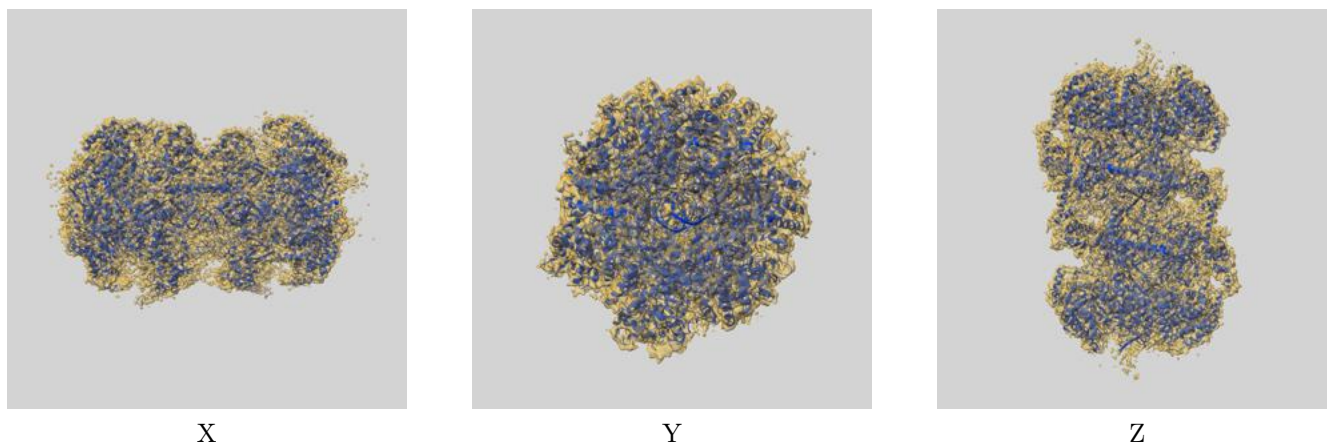
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

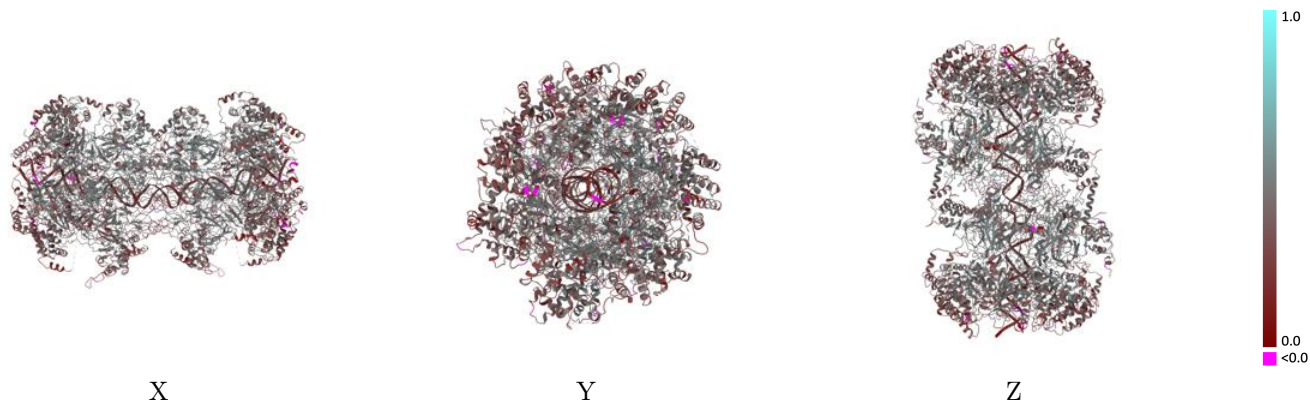
This section contains information regarding the fit between EMDB map EMD-9400 and PDB model 5BK4. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



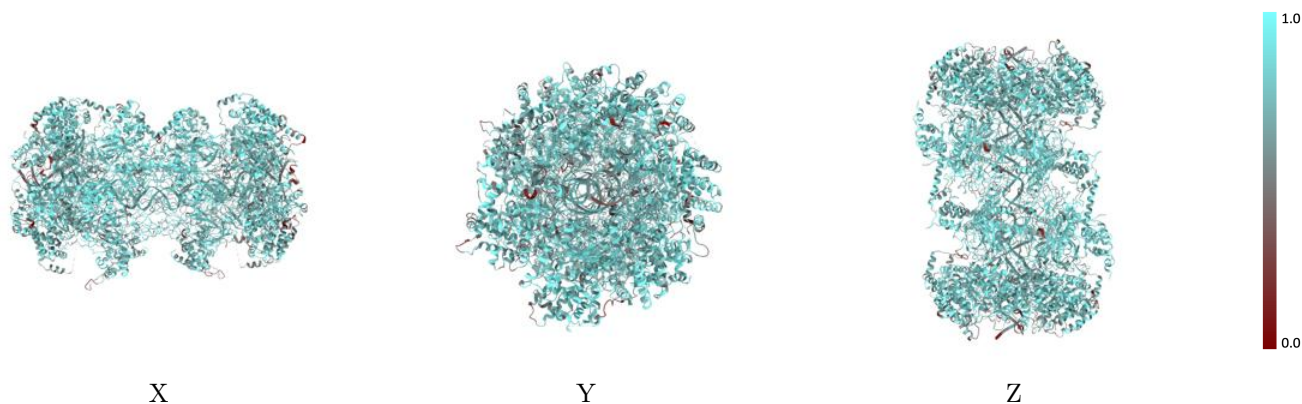
The images above show the 3D surface view of the map at the recommended contour level 0.026 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



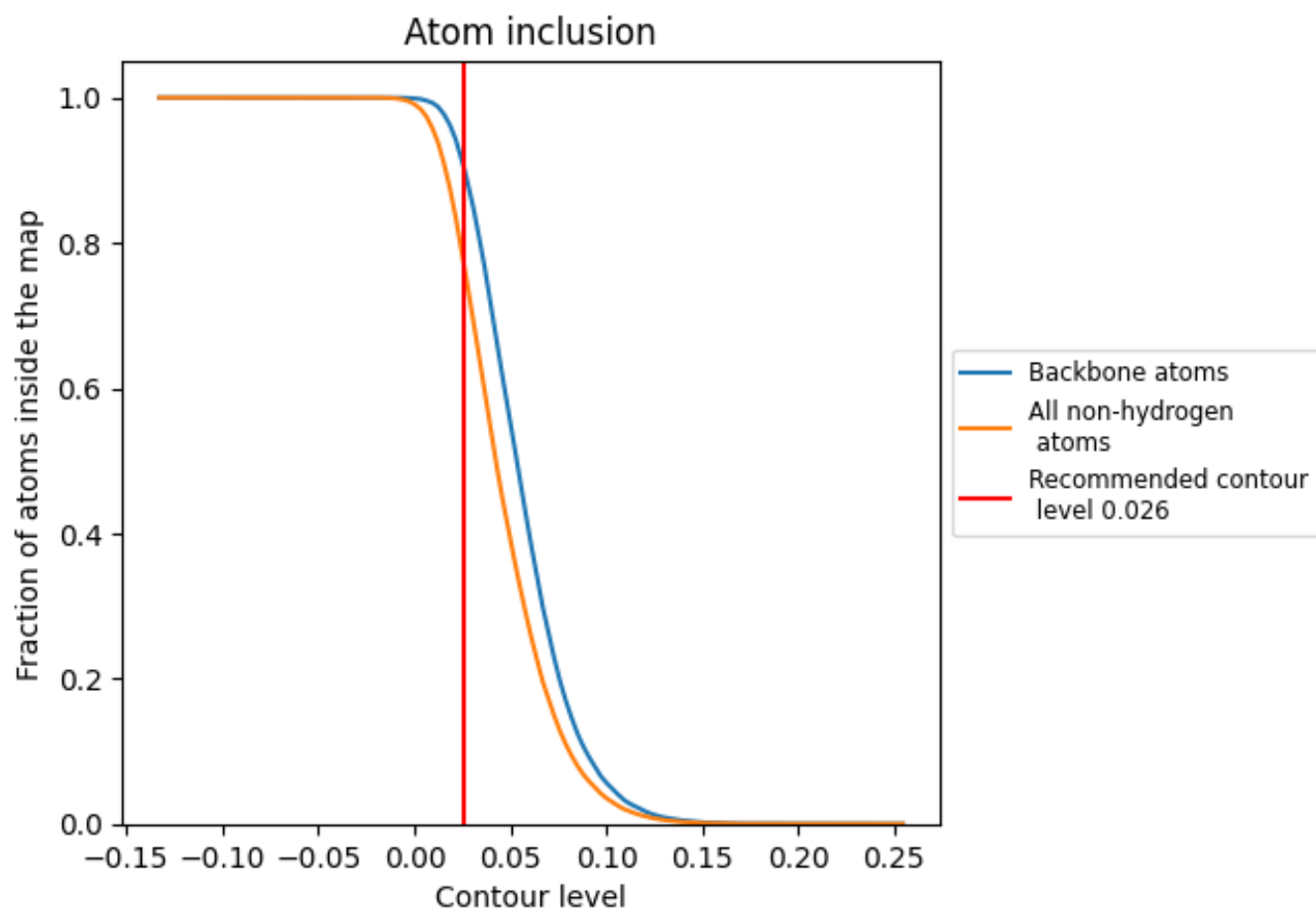
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.026).































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 77% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7692	 0.3930
2	 0.7391	 0.3760
3	 0.7901	 0.4240
4	 0.7889	 0.3980
5	 0.7653	 0.3990
6	 0.7456	 0.3700
7	 0.8006	 0.4220
A	 0.7398	 0.3730
B	 0.7918	 0.4250
C	 0.7891	 0.4000
D	 0.7622	 0.3990
E	 0.7423	 0.3670
F	 0.8006	 0.4220
O	 0.6911	 0.2470
S	 0.7065	 0.2470

