



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Nov 29, 2017 – 07:38 PM 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 : unknown
Resolution : 3.90 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

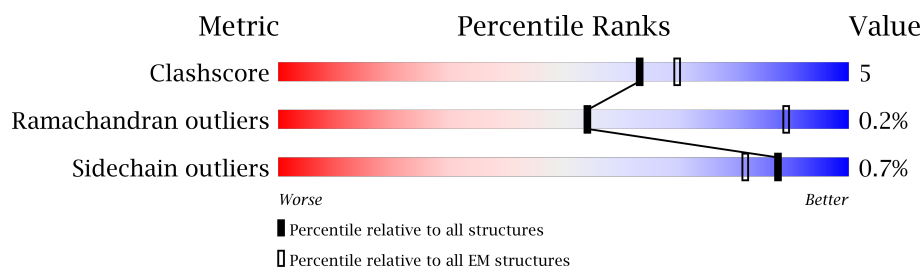
1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	2	868	59% 11% 31%
1	A	868	59% 11% 31%
2	3	971	54% 8% 38%
2	B	971	55% 7% 38%
3	4	933	59% 11% 31%
3	C	933	58% 11% 31%
4	5	775	74% 11% • 15%
4	D	775	74% 11% • 15%
5	6	1017	52% 9% 40%

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

2 Entry composition

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
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
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
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
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
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
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

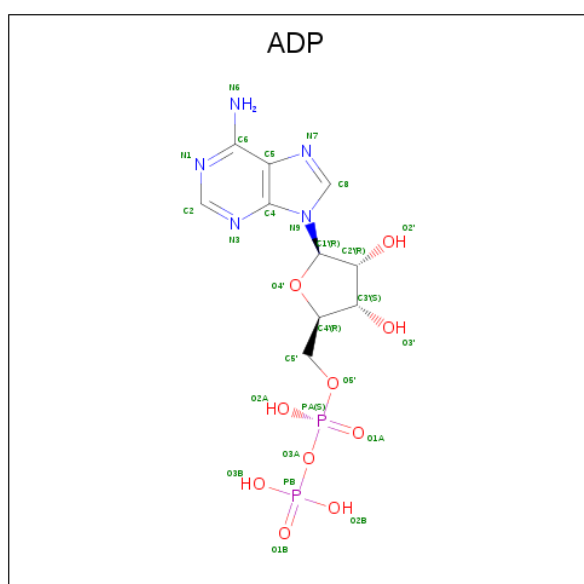
- Molecule 7 is a DNA chain called DNA (60-mer), strand 1.

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

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

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

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).

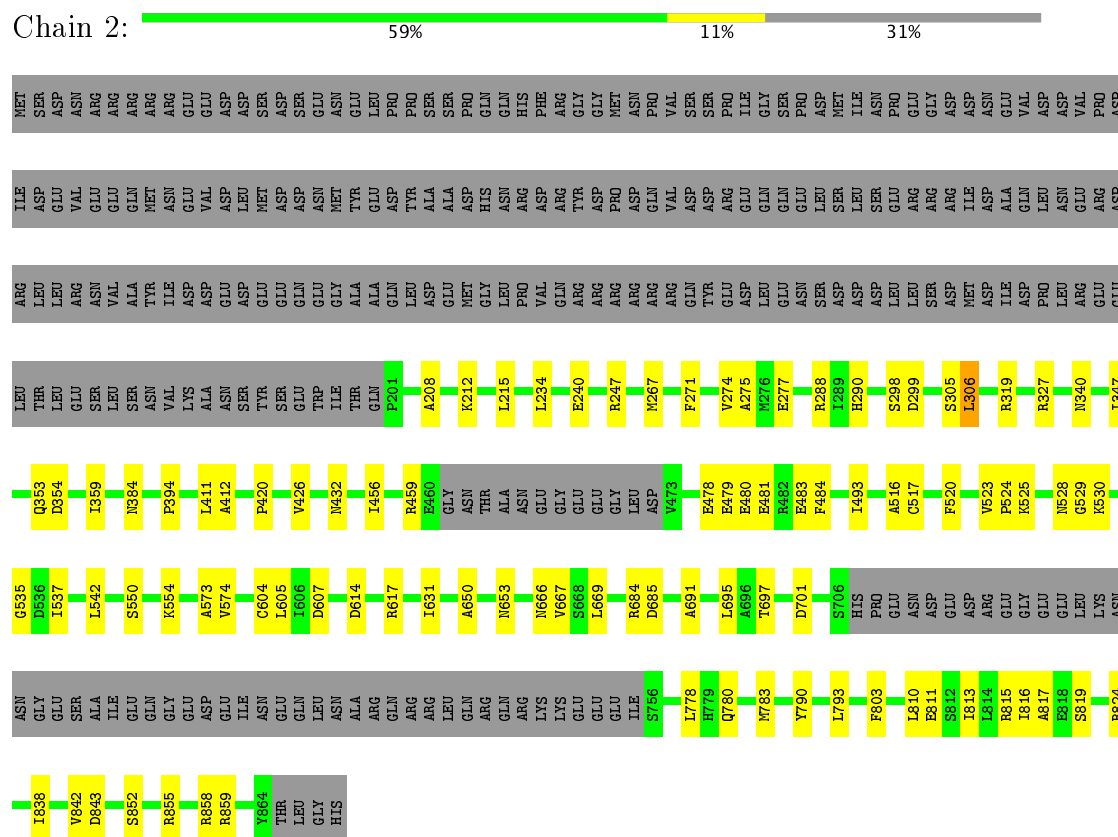


Mol	Chain	Residues	Atoms					AltConf
9	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	7	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	D	1	Total	C	N	O	P	0
			27	10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

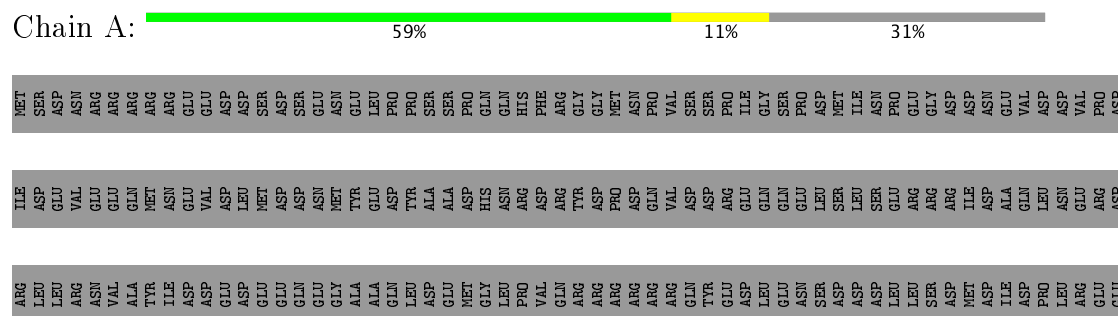
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

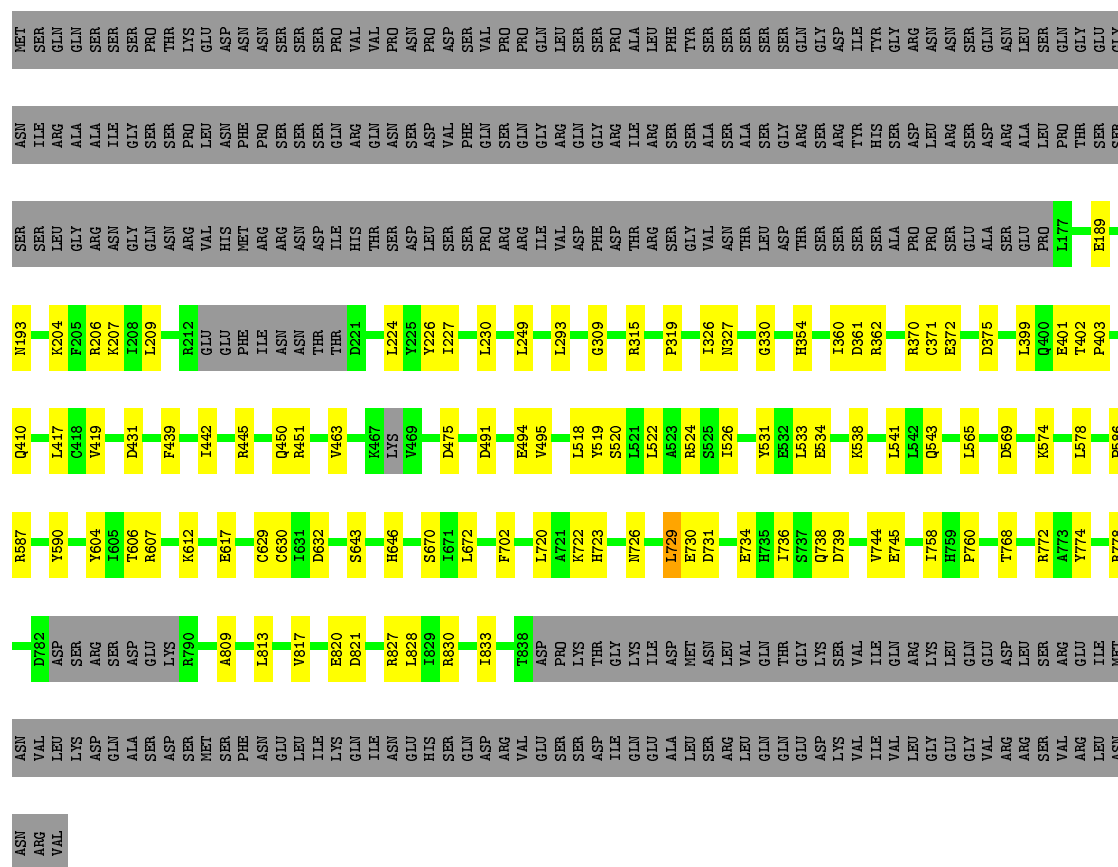
- Molecule 1: DNA replication licensing factor MCM2




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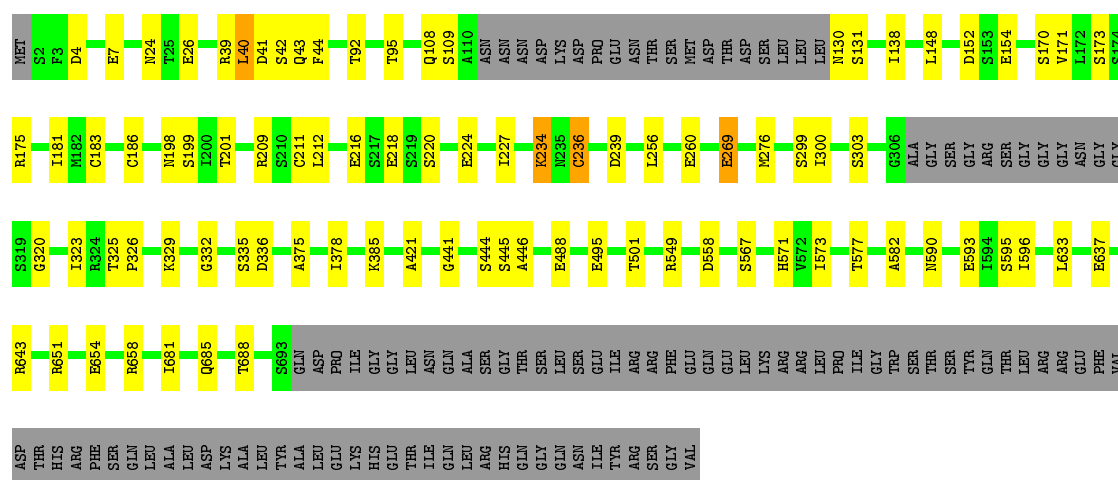


Chain C:  58% 11% 31%



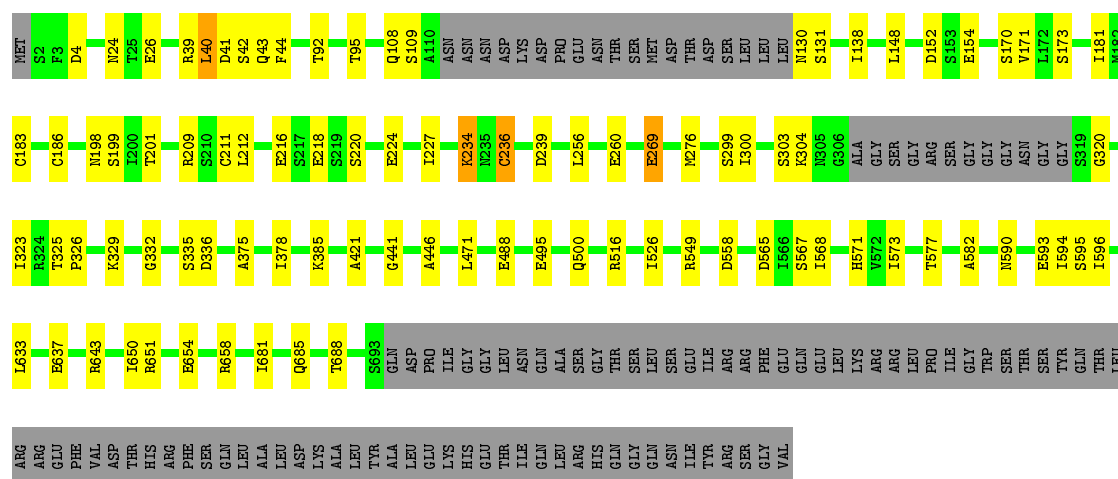
• Molecule 4: DNA replication licensing factor MCM5

Chain 5:  74% 11% 15%

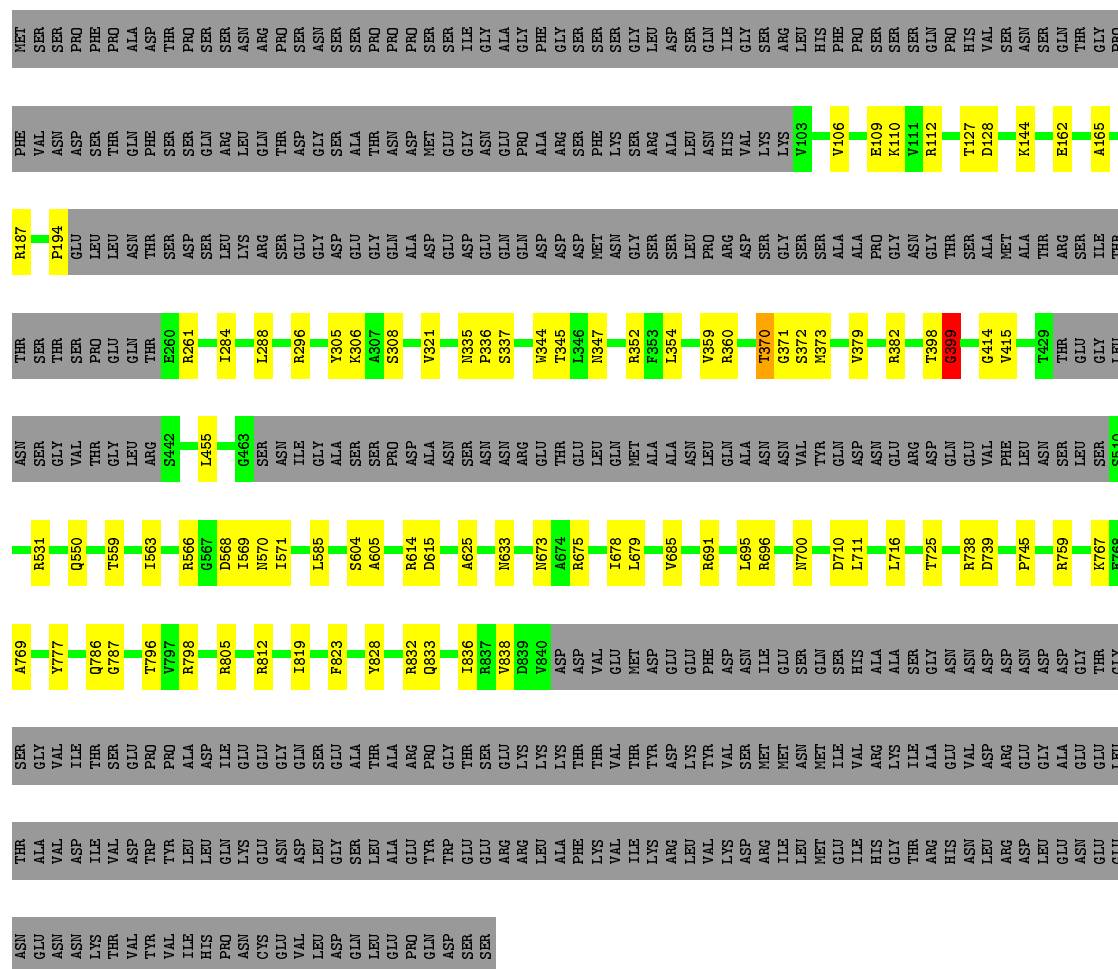


• Molecule 4: DNA replication licensing factor MCM5

Chain D:  74% 11% 15%

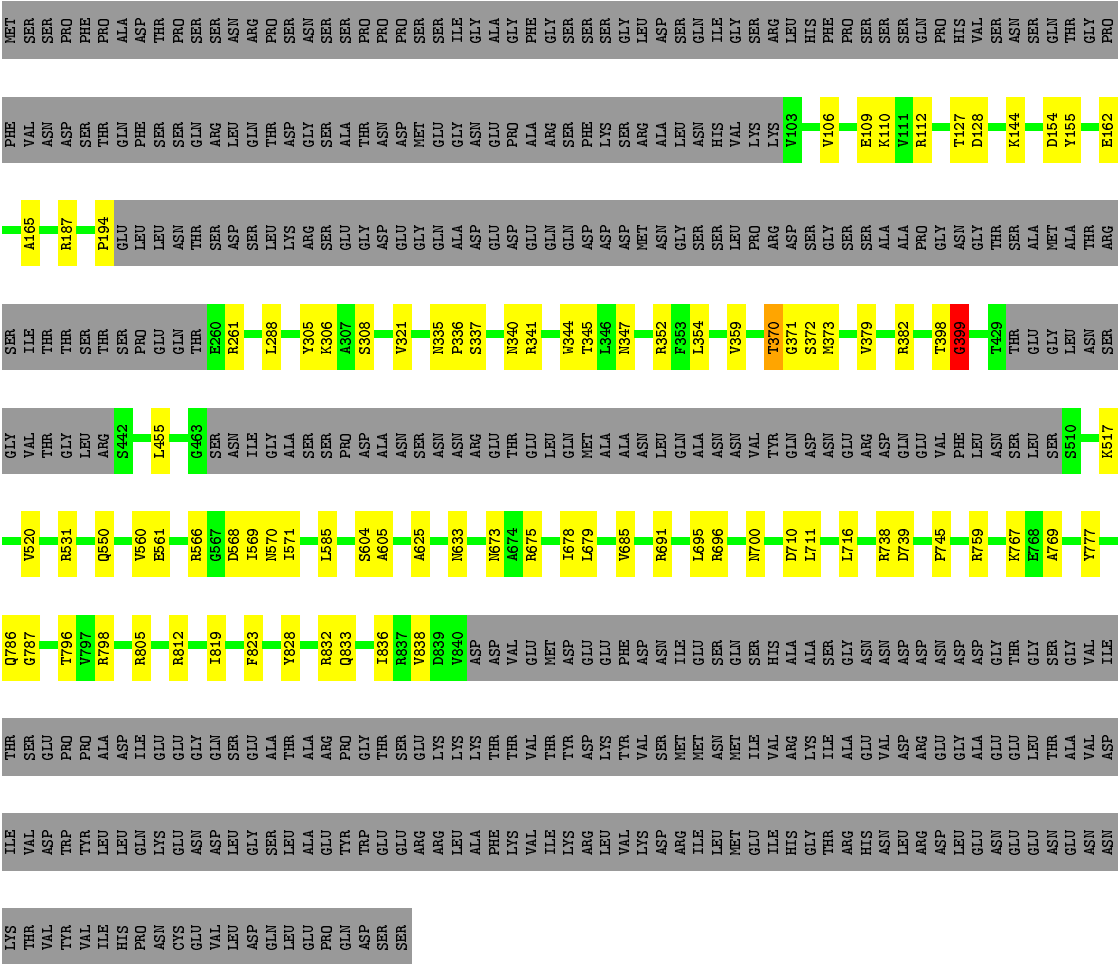


- Molecule 5: DNA replication licensing factor MCM6

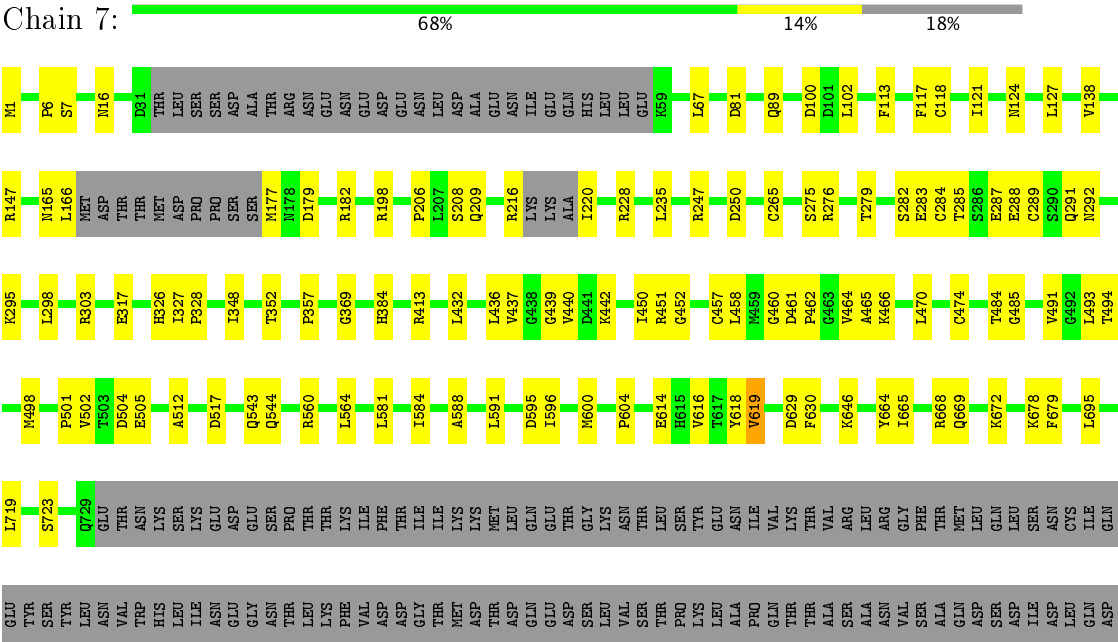


- Molecule 5: DNA replication licensing factor MCM6



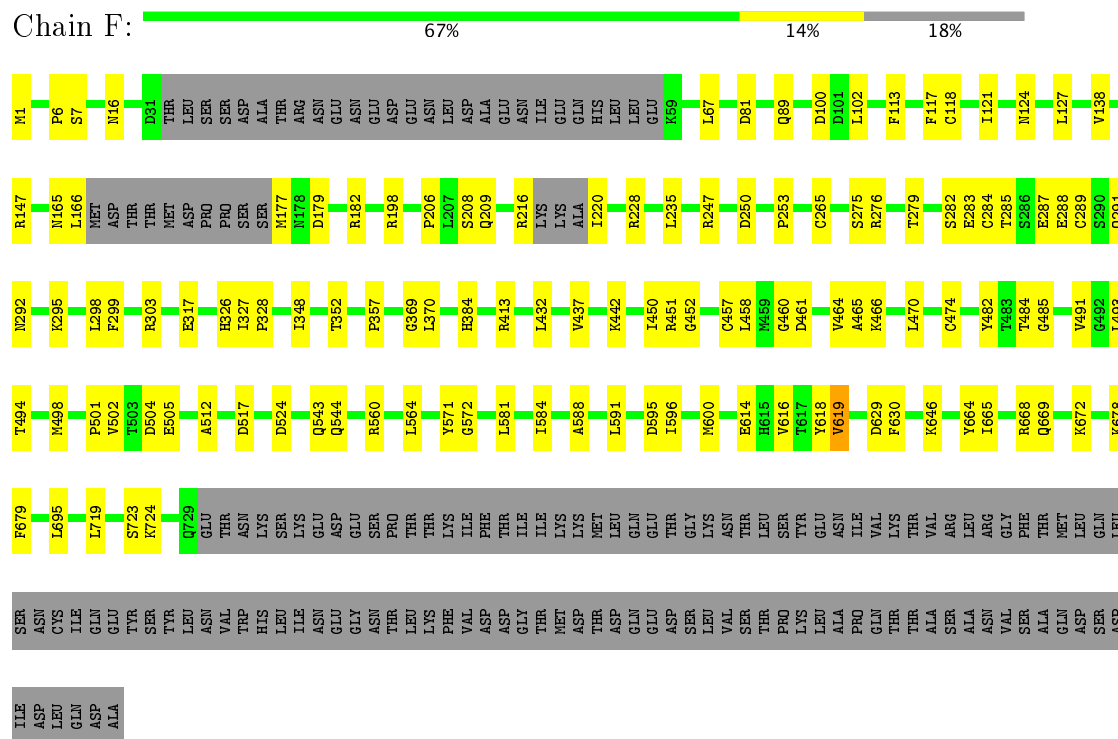


● Molecule 6: DNA replication licensing factor MCM7



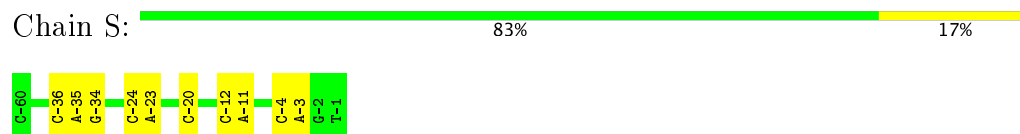
- Molecule 6: DNA replication licensing factor MCM7

Chain F:



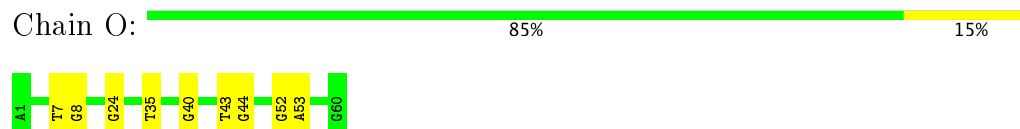
- Molecule 7: DNA (60-mer), strand 1

Chain S:



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

Chain O:



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
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	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 >2	RMSZ	# Z >2
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 ⓘ

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
3:4:578:LEU:HD21	3:4:672:LEU:HD22	1.84	0.60
1:2:780:GLN:NE2	4:5:577:THR:O	2.35	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
1:2:394:PRO:O	5:6:673:ASN:ND2	2.35	0.60
1:2:327:ARG:NH2	4:5:269:GLU:OE2	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
4:5:186:CYS:SG	4:5:234:LYS:NZ	2.76	0.58
2:3:420:ARG:NH1	4:5:495:GLU:OE2	2.37	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:N	4:5:4:ASP:OD1	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
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
2:B:195:LYS:NZ	6:F:369:GLY:O	2.38	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
4:5:421:ALA:HA	9:5:2001:ADP:H5'2	1.89	0.54
2:3:435:ARG:NH2	4:5:488:GLU:O	2.36	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
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
2:3:195:LYS:NZ	6:7:369:GLY:O	2.38	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
1:2:631:ILE:HG22	4:5:446:ALA:HB3	1.91	0.53
1:2:517:CYS:HG	1:2:819:SER:HG	1.56	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
3:C:531:TYR:HE2	3:C:720:LEU:HA	1.75	0.52
4:5:24:ASN:ND2	6:F:291:GLN:O	2.43	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:OD1	2:B:275:ASP:N	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:OD1	2:3:18:ASP:N	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:N	6:F:595:ASP:OD1	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:N	4:5:239:ASP:OD1	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:N	1:2:384:ASN:OD1	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:N	6:7:595:ASP:OD1	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
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
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
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:678:LYS:HG3	6:F:679:PHE:H	1.80	0.46
6:F:81:ASP:N	6:F:81:ASP:OD1	2.47	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:491:ASP:OD1	3:C:491:ASP:N	2.46	0.46
3:C:475:ASP:HB3	3:C:586:PRO:HD3	1.96	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:N	1:A:384:ASN:OD1	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:N	6:F:629:ASP:OD1	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
3:4:830:ARG:HD3	3:4:833:ILE:HD12	1.99	0.44
2:3:315:ILE:HG13	4:5:175:ARG:HE	1.83	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
4:D:549:ARG:HG2	4:D:651:ARG:HH22	1.83	0.44
2:B:236:THR:OG1	6:F:1:MET:SD	2.74	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:N	2:3:402:ASP:OD1	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:590:TYR:OH	3:C:632:ASP:OD2	2.29	0.43
3:C:531:TYR:CE2	3:C:720:LEU:HA	2.53	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:HD3	1:A:212:LYS:HA	1.77	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
2:B:267:ALA:HB1	4:D:471:LEU:HD23	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:HG13	2:3:553:ILE:H	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:HA	3:C:249:LEU:HD13	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:N	4:5:558:ASP:OD1	2.52	0.42
4:5:633:LEU:O	4:5:637:GLU:CB	2.62	0.42
1:A:432:ASN:N	1:A:432:ASN:OD1	2.52	0.42
3:C:729:LEU:HD22	3:C:730:GLU:H	1.84	0.42
4:D:558:ASP:N	4:D:558:ASP:OD1	2.52	0.42
4:D:92:THR:HA	4:D:95:THR:HG22	2.00	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:HA	3:4:578:LEU:HD23	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
4:5:40:LEU:O	4:5:43:GLN:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:3:211:TYR:HD2	6:7:6:PRO:HG2	1.84	0.42
2:B:216:ASP:N	2:B:216:ASP:OD1	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:N	6:F:124:ASN:OD1	2.53	0.41
6:F:432:LEU:HD23	6:F:432:LEU:HA	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:HD2	1:2:530:LYS:HA	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
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
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
5:6:559:THR:OG1	5:6:563:ILE:O	2.28	0.41
6:7:124:ASN:OD1	6:7:124:ASN:N	2.53	0.41
1:A:530:LYS:HD2	1:A:530:LYS:HA	1.88	0.41
3:C:370:ARG:HB2	3:C:371:CYS:HB2	2.03	0.41
6:F:461:ASP:OD1	6:F:461:ASP:N	2.54	0.41
6:F:571:TYR:HA	6:F:572:GLY:HA2	1.88	0.41
6:F:67:LEU:HD11	6:F:121:ILE:HG23	2.03	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:HD23	6:7:436:LEU:HA	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:S:-11:DA:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	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%)	51	84
2	B	596/971 (61%)	531 (89%)	64 (11%)	1 (0%)	51	84
3	4	638/933 (68%)	543 (85%)	93 (15%)	2 (0%)	44	80
3	C	638/933 (68%)	543 (85%)	93 (15%)	2 (0%)	44	80
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%)	44	80
5	E	607/1017 (60%)	527 (87%)	78 (13%)	2 (0%)	44	80
6	7	681/845 (81%)	606 (89%)	74 (11%)	1 (0%)	55	88
6	F	681/845 (81%)	605 (89%)	75 (11%)	1 (0%)	55	88
All	All	7548/10818 (70%)	6614 (88%)	922 (12%)	12 (0%)	54	84

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 ⓘ

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%)	93	96
1	A	509/770 (66%)	507 (100%)	2 (0%)	93	96
2	3	522/835 (62%)	517 (99%)	5 (1%)	80	90
2	B	522/835 (62%)	517 (99%)	5 (1%)	80	90
3	4	578/848 (68%)	576 (100%)	2 (0%)	94	97
3	C	578/848 (68%)	576 (100%)	2 (0%)	94	97
4	5	591/688 (86%)	582 (98%)	9 (2%)	70	87
4	D	591/688 (86%)	582 (98%)	9 (2%)	70	87
5	6	496/886 (56%)	494 (100%)	2 (0%)	93	96
5	E	496/886 (56%)	494 (100%)	2 (0%)	93	96
6	7	609/753 (81%)	607 (100%)	2 (0%)	94	97
6	F	609/753 (81%)	607 (100%)	2 (0%)	94	97
All	All	6610/9560 (69%)	6566 (99%)	44 (1%)	87	94

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

Some 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 carbohydrates 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	2	2001	-	25,29,29	0.96	1 (4%)	24,45,45	1.62	2 (8%)
9	ADP	3	2001	-	25,29,29	1.02	1 (4%)	24,45,45	1.72	4 (16%)
9	ADP	5	2001	-	25,29,29	1.00	1 (4%)	24,45,45	1.71	3 (12%)
9	ADP	7	2001	-	25,29,29	0.97	1 (4%)	24,45,45	1.78	3 (12%)
9	ADP	A	2001	-	25,29,29	0.96	1 (4%)	24,45,45	1.63	2 (8%)
9	ADP	B	2001	-	25,29,29	1.00	1 (4%)	24,45,45	1.69	2 (8%)
9	ADP	D	2001	-	25,29,29	0.99	1 (4%)	24,45,45	1.73	4 (16%)
9	ADP	F	2001	-	25,29,29	0.97	1 (4%)	24,45,45	1.79	3 (12%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2001	ADP	C5-C4	2.95	1.47	1.40
9	3	2001	ADP	C5-C4	2.96	1.47	1.40
9	7	2001	ADP	C5-C4	2.97	1.47	1.40
9	F	2001	ADP	C5-C4	2.98	1.47	1.40
9	D	2001	ADP	C5-C4	3.04	1.47	1.40
9	5	2001	ADP	C5-C4	3.04	1.47	1.40
9	2	2001	ADP	C5-C4	3.06	1.47	1.40
9	A	2001	ADP	C5-C4	3.10	1.47	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	2001	ADP	N3-C2-N1	-6.34	123.33	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	7	2001	ADP	N3-C2-N1	-6.23	123.43	128.86
9	B	2001	ADP	N3-C2-N1	-6.14	123.51	128.86
9	3	2001	ADP	N3-C2-N1	-6.10	123.55	128.86
9	A	2001	ADP	N3-C2-N1	-5.96	123.67	128.86
9	2	2001	ADP	N3-C2-N1	-5.92	123.70	128.86
9	5	2001	ADP	N3-C2-N1	-5.70	123.89	128.86
9	D	2001	ADP	N3-C2-N1	-5.64	123.95	128.86
9	A	2001	ADP	C4-C5-N7	-2.79	106.72	109.41
9	2	2001	ADP	C4-C5-N7	-2.79	106.72	109.41
9	3	2001	ADP	C4-C5-N7	-2.40	107.09	109.41
9	B	2001	ADP	C4-C5-N7	-2.38	107.11	109.41
9	D	2001	ADP	C4-C5-N7	-2.33	107.16	109.41
9	5	2001	ADP	C4-C5-N7	-2.28	107.21	109.41
9	F	2001	ADP	C4-C5-N7	-2.07	107.41	109.41
9	7	2001	ADP	C1'-N9-C4	2.00	130.09	126.64
9	3	2001	ADP	C2'-C3'-C4'	2.07	106.64	102.62
9	5	2001	ADP	C1'-N9-C4	2.08	130.23	126.64
9	3	2001	ADP	C4'-O4'-C1'	2.17	112.08	109.77
9	D	2001	ADP	C1'-N9-C4	2.22	130.46	126.64
9	D	2001	ADP	C4'-O4'-C1'	2.31	112.23	109.77
9	F	2001	ADP	C4'-O4'-C1'	2.54	112.47	109.77
9	7	2001	ADP	C4'-O4'-C1'	2.56	112.49	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.