



## Full wwPDB EM Validation Report ⓘ

Jun 30, 2022 – 06:30 pm BST

PDB ID : 7Z13  
EMDB ID : EMD-14439  
Title : S. cerevisiae CMGE dimer nucleating origin DNA melting  
Authors : Lewis, J.S.; Sousa, J.S.; Costa, A.  
Deposited on : 2022-02-24  
Resolution : 3.40 Å (reported)  
Based on initial models : 7QHS, ?

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev8  
Mogul : 1.8.4, 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)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

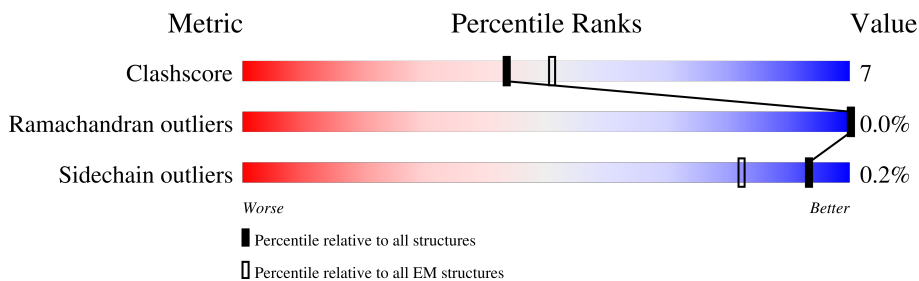
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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  $\geq 3$ , 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	1006	
2	b	1006	
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	51% 10% 38%
5	e	1017	61% 38%
6	7	845	60% 17% 22%
6	f	845	78% 22%
7	A	53	6% 74% 26%
8	B	53	6% 72% 28%
9	C	229	67% 9% 24%
9	J	229	68% 8% 24%
10	D	294	71% 12% 18%
10	K	294	70% 12% 18%
11	E	657	73% 13% 14%
11	L	657	73% 13% 14%
12	F	689	59% 21% 20%
12	M	689	59% 21% 20%
13	H	208	75% 25%
13	O	208	75% 25%
14	I	213	75% 14% 11%
14	P	213	74% 15% 11%
15	N	2222	27% 7% 66%
15	Q	2222	27% 7% 66%

## 2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 107381 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	660	5231	3284	937	991	19	0	0
1	a	660	5231	3284	937	991	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	633	4958	3119	882	944	13	0	0
2	b	633	4958	3119	882	944	13	0	0

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-34	MET	-	initiating methionine	UNP P24279
3	-33	LYS	-	expression tag	UNP P24279
3	-32	ARG	-	expression tag	UNP P24279
3	-31	ARG	-	expression tag	UNP P24279
3	-30	TRP	-	expression tag	UNP P24279
3	-29	LYS	-	expression tag	UNP P24279
3	-28	LYS	-	expression tag	UNP P24279
3	-27	ASN	-	expression tag	UNP P24279
3	-26	PHE	-	expression tag	UNP P24279
3	-25	ILE	-	expression tag	UNP P24279
3	-24	ALA	-	expression tag	UNP P24279
3	-23	VAL	-	expression tag	UNP P24279
3	-22	SER	-	expression tag	UNP P24279
3	-21	ALA	-	expression tag	UNP P24279
3	-20	ALA	-	expression tag	UNP P24279
3	-19	ASN	-	expression tag	UNP P24279
3	-18	ARG	-	expression tag	UNP P24279

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Chain	Residue	Modelled	Actual	Comment	Reference
3	-17	PHE	-	expression tag	UNP P24279
3	-16	LYS	-	expression tag	UNP P24279
3	-15	LYS	-	expression tag	UNP P24279
3	-14	ILE	-	expression tag	UNP P24279
3	-13	SER	-	expression tag	UNP P24279
3	-12	SER	-	expression tag	UNP P24279
3	-11	SER	-	expression tag	UNP P24279
3	-10	GLY	-	expression tag	UNP P24279
3	-9	ALA	-	expression tag	UNP P24279
3	-8	LEU	-	expression tag	UNP P24279
3	-7	GLU	-	expression tag	UNP P24279
3	-6	ASN	-	expression tag	UNP P24279
3	-5	LEU	-	expression tag	UNP P24279
3	-4	TYR	-	expression tag	UNP P24279
3	-3	PHE	-	expression tag	UNP P24279
3	-2	GLN	-	expression tag	UNP P24279
3	-1	GLY	-	expression tag	UNP P24279
3	0	GLU	-	expression tag	UNP P24279
b	-34	MET	-	initiating methionine	UNP P24279
b	-33	LYS	-	expression tag	UNP P24279
b	-32	ARG	-	expression tag	UNP P24279
b	-31	ARG	-	expression tag	UNP P24279
b	-30	TRP	-	expression tag	UNP P24279
b	-29	LYS	-	expression tag	UNP P24279
b	-28	LYS	-	expression tag	UNP P24279
b	-27	ASN	-	expression tag	UNP P24279
b	-26	PHE	-	expression tag	UNP P24279
b	-25	ILE	-	expression tag	UNP P24279
b	-24	ALA	-	expression tag	UNP P24279
b	-23	VAL	-	expression tag	UNP P24279
b	-22	SER	-	expression tag	UNP P24279
b	-21	ALA	-	expression tag	UNP P24279
b	-20	ALA	-	expression tag	UNP P24279
b	-19	ASN	-	expression tag	UNP P24279
b	-18	ARG	-	expression tag	UNP P24279
b	-17	PHE	-	expression tag	UNP P24279
b	-16	LYS	-	expression tag	UNP P24279
b	-15	LYS	-	expression tag	UNP P24279
b	-14	ILE	-	expression tag	UNP P24279
b	-13	SER	-	expression tag	UNP P24279
b	-12	SER	-	expression tag	UNP P24279
b	-11	SER	-	expression tag	UNP P24279

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Chain	Residue	Modelled	Actual	Comment	Reference
b	-10	GLY	-	expression tag	UNP P24279
b	-9	ALA	-	expression tag	UNP P24279
b	-8	LEU	-	expression tag	UNP P24279
b	-7	GLU	-	expression tag	UNP P24279
b	-6	ASN	-	expression tag	UNP P24279
b	-5	LEU	-	expression tag	UNP P24279
b	-4	TYR	-	expression tag	UNP P24279
b	-3	PHE	-	expression tag	UNP P24279
b	-2	GLN	-	expression tag	UNP P24279
b	-1	GLY	-	expression tag	UNP P24279
b	0	GLU	-	expression tag	UNP P24279

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	609	Total	C	N	O	S	0	0
			4850	3055	838	930	27		
3	c	609	Total	C	N	O	S	0	0
			4850	3055	838	930	27		

- Molecule 4 is a protein called DNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	690	Total	C	N	O	S	0	0
			5450	3423	948	1055	24		
4	d	690	Total	C	N	O	S	0	0
			5450	3423	948	1055	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	629	Total	C	N	O	S	0	0
			4972	3134	867	946	25		
5	e	629	Total	C	N	O	S	0	0
			4972	3134	867	946	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	658	Total	C	N	O	S	0	0
			5181	3268	897	987	29		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	658	5181	3268	897	987	29	0	0

- Molecule 7 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	A	53	1087	530	187	317	53	0	0

- Molecule 8 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	B	53	1086	530	184	319	53	0	0

- Molecule 9 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C	173	1398	911	224	256	7	0	0
9	J	173	1398	911	224	256	7	0	0

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-34	TRP	-	expression tag	UNP Q12146
C	-33	SER	-	expression tag	UNP Q12146
C	-32	HIS	-	expression tag	UNP Q12146
C	-31	PRO	-	expression tag	UNP Q12146
C	-30	GLN	-	expression tag	UNP Q12146
C	-29	PHE	-	expression tag	UNP Q12146
C	-28	GLU	-	expression tag	UNP Q12146
C	-27	LYS	-	expression tag	UNP Q12146
C	-26	GLY	-	expression tag	UNP Q12146
C	-25	GLY	-	expression tag	UNP Q12146
C	-24	GLY	-	expression tag	UNP Q12146
C	-23	SER	-	expression tag	UNP Q12146
C	-22	GLY	-	expression tag	UNP Q12146
C	-21	GLY	-	expression tag	UNP Q12146
C	-20	GLY	-	expression tag	UNP Q12146
C	-19	SER	-	expression tag	UNP Q12146

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	GLY	-	expression tag	UNP Q12146
C	-17	GLY	-	expression tag	UNP Q12146
C	-16	GLY	-	expression tag	UNP Q12146
C	-15	SER	-	expression tag	UNP Q12146
C	-14	TRP	-	expression tag	UNP Q12146
C	-13	SER	-	expression tag	UNP Q12146
C	-12	HIS	-	expression tag	UNP Q12146
C	-11	PRO	-	expression tag	UNP Q12146
C	-10	GLN	-	expression tag	UNP Q12146
C	-9	PHE	-	expression tag	UNP Q12146
C	-8	GLU	-	expression tag	UNP Q12146
C	-7	LYS	-	expression tag	UNP Q12146
C	-6	GLU	-	expression tag	UNP Q12146
C	-5	ASN	-	expression tag	UNP Q12146
C	-4	LEU	-	expression tag	UNP Q12146
C	-3	TYR	-	expression tag	UNP Q12146
C	-2	PHE	-	expression tag	UNP Q12146
C	-1	GLN	-	expression tag	UNP Q12146
C	0	SER	-	expression tag	UNP Q12146
J	-34	TRP	-	expression tag	UNP Q12146
J	-33	SER	-	expression tag	UNP Q12146
J	-32	HIS	-	expression tag	UNP Q12146
J	-31	PRO	-	expression tag	UNP Q12146
J	-30	GLN	-	expression tag	UNP Q12146
J	-29	PHE	-	expression tag	UNP Q12146
J	-28	GLU	-	expression tag	UNP Q12146
J	-27	LYS	-	expression tag	UNP Q12146
J	-26	GLY	-	expression tag	UNP Q12146
J	-25	GLY	-	expression tag	UNP Q12146
J	-24	GLY	-	expression tag	UNP Q12146
J	-23	SER	-	expression tag	UNP Q12146
J	-22	GLY	-	expression tag	UNP Q12146
J	-21	GLY	-	expression tag	UNP Q12146
J	-20	GLY	-	expression tag	UNP Q12146
J	-19	SER	-	expression tag	UNP Q12146
J	-18	GLY	-	expression tag	UNP Q12146
J	-17	GLY	-	expression tag	UNP Q12146
J	-16	GLY	-	expression tag	UNP Q12146
J	-15	SER	-	expression tag	UNP Q12146
J	-14	TRP	-	expression tag	UNP Q12146
J	-13	SER	-	expression tag	UNP Q12146
J	-12	HIS	-	expression tag	UNP Q12146

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-11	PRO	-	expression tag	UNP Q12146
J	-10	GLN	-	expression tag	UNP Q12146
J	-9	PHE	-	expression tag	UNP Q12146
J	-8	GLU	-	expression tag	UNP Q12146
J	-7	LYS	-	expression tag	UNP Q12146
J	-6	GLU	-	expression tag	UNP Q12146
J	-5	ASN	-	expression tag	UNP Q12146
J	-4	LEU	-	expression tag	UNP Q12146
J	-3	TYR	-	expression tag	UNP Q12146
J	-2	PHE	-	expression tag	UNP Q12146
J	-1	GLN	-	expression tag	UNP Q12146
J	0	SER	-	expression tag	UNP Q12146

- Molecule 10 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D	242	1990	1267	328	381	14	0	0
10	K	242	1990	1267	328	381	14	0	0

- Molecule 11 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	E	566	4599	2937	778	870	14	0	0
11	L	566	4599	2937	778	870	14	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	167G	TYR	-	linker	UNP Q08032
E	167H	LYS	-	linker	UNP Q08032
E	167I	ASP	-	linker	UNP Q08032
E	167J	ASP	-	linker	UNP Q08032
E	167K	ASP	-	linker	UNP Q08032
E	167L	GLY	-	linker	UNP Q08032
E	167M	ASP	-	linker	UNP Q08032
E	167N	TYR	-	linker	UNP Q08032
E	167O	LYS	-	linker	UNP Q08032
E	167P	ASP	-	linker	UNP Q08032

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Chain	Residue	Modelled	Actual	Comment	Reference
E	167Q	ASP	-	linker	UNP Q08032
L	167G	TYR	-	linker	UNP Q08032
L	167H	LYS	-	linker	UNP Q08032
L	167I	ASP	-	linker	UNP Q08032
L	167J	ASP	-	linker	UNP Q08032
L	167K	ASP	-	linker	UNP Q08032
L	167L	GLY	-	linker	UNP Q08032
L	167M	ASP	-	linker	UNP Q08032
L	167N	TYR	-	linker	UNP Q08032
L	167O	LYS	-	linker	UNP Q08032
L	167P	ASP	-	linker	UNP Q08032
L	167Q	ASP	-	linker	UNP Q08032

- Molecule 12 is a protein called DNA polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	F	551	4396	2819	755	804	18	0	0
12	M	551	4396	2819	755	804	18	0	0

- Molecule 13 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	H	208	1697	1065	290	332	10	0	0
13	O	208	1697	1065	290	332	10	0	0

- Molecule 14 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	I	189	1581	1018	277	282	4	0	0
14	P	189	1581	1018	277	282	4	0	0

- Molecule 15 is a protein called DNA polymerase epsilon catalytic subunit A.

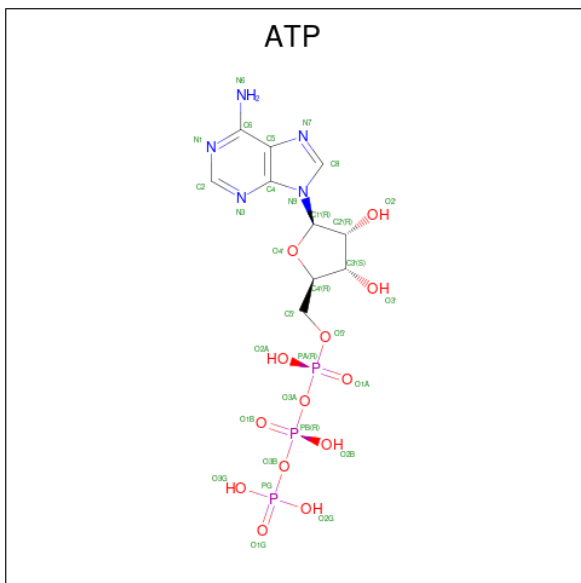
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	N	756	6113	3956	1006	1114	37	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Q	756	6113	3956	1006	1114	37	0	0

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
16	2	1	31	10	5	13	3	0
16	3	1	31	10	5	13	3	0
16	5	1	31	10	5	13	3	0
16	7	1	31	10	5	13	3	0
16	a	1	31	10	5	13	3	0
16	b	1	31	10	5	13	3	0
16	d	1	31	10	5	13	3	0
16	f	1	31	10	5	13	3	0

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	2	1	Total 1	Zn 1	0
17	4	1	Total 1	Zn 1	0
17	5	1	Total 1	Zn 1	0
17	6	1	Total 1	Zn 1	0
17	7	1	Total 1	Zn 1	0
17	N	2	Total 2	Zn 2	0
17	Q	2	Total 2	Zn 2	0
17	a	1	Total 1	Zn 1	0
17	c	1	Total 1	Zn 1	0
17	d	1	Total 1	Zn 1	0
17	e	1	Total 1	Zn 1	0
17	f	1	Total 1	Zn 1	0

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

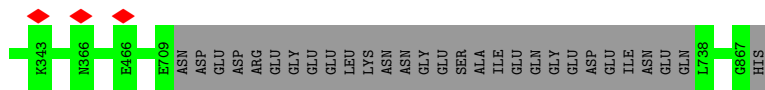
Mol	Chain	Residues	Atoms		AltConf
18	3	1	Total 1	Mg 1	0
18	5	1	Total 1	Mg 1	0
18	7	1	Total 1	Mg 1	0
18	b	1	Total 1	Mg 1	0
18	d	1	Total 1	Mg 1	0
18	f	1	Total 1	Mg 1	0

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

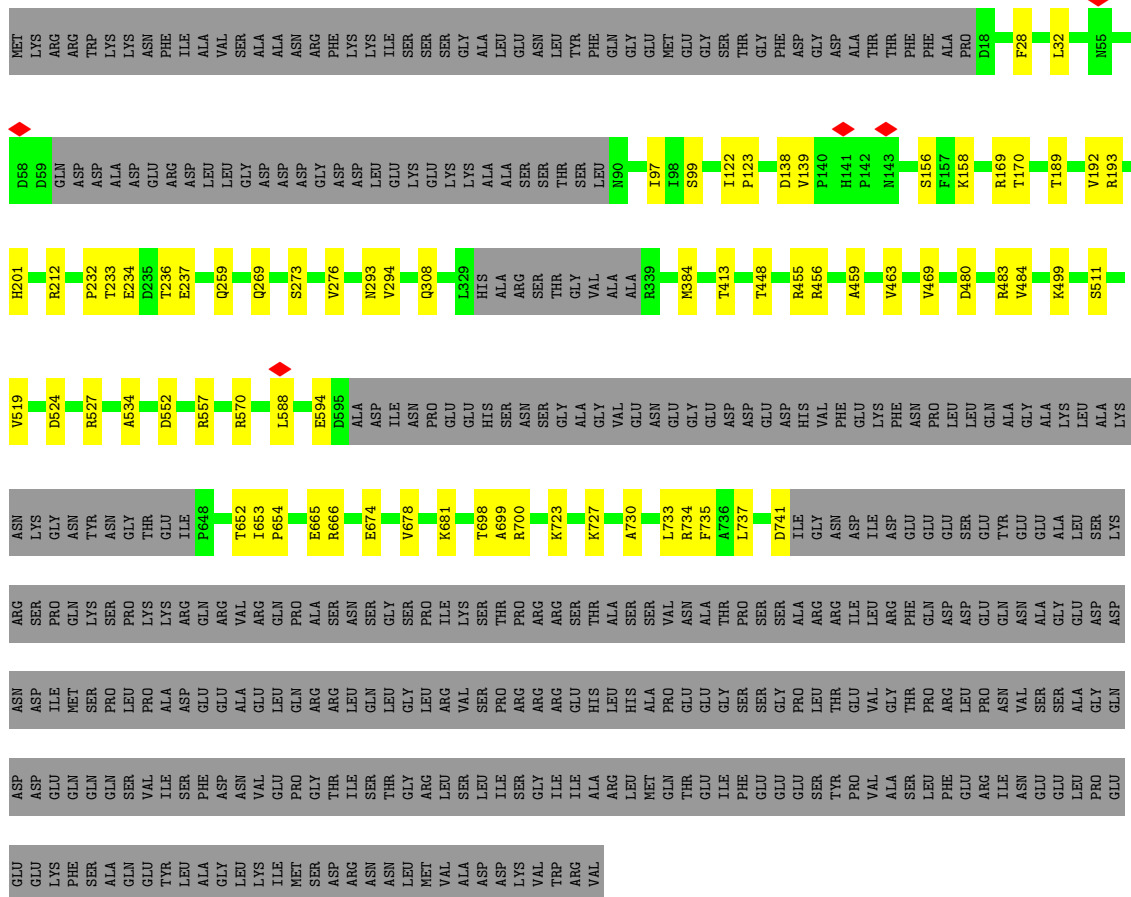


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
19	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	6	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

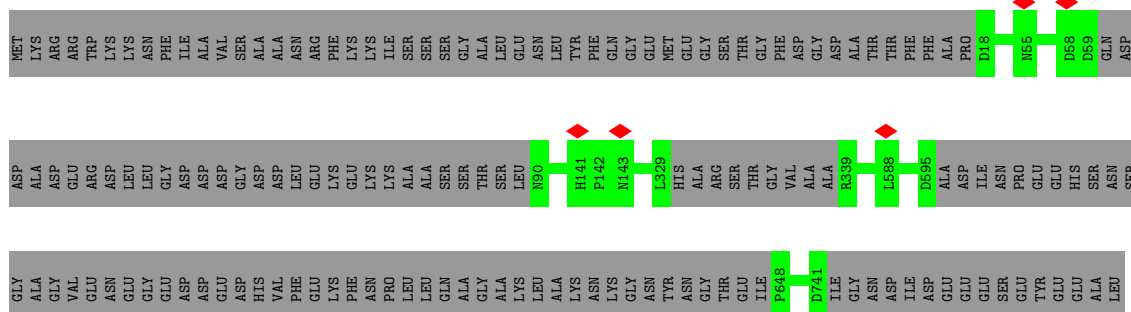




● Molecule 2: DNA replication licensing factor MCM3



● Molecule 2: DNA replication licensing factor MCM3





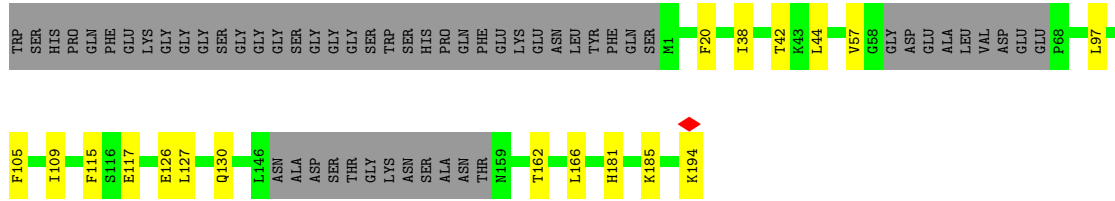




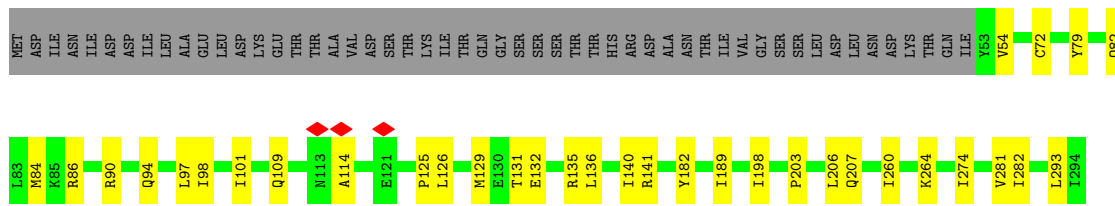




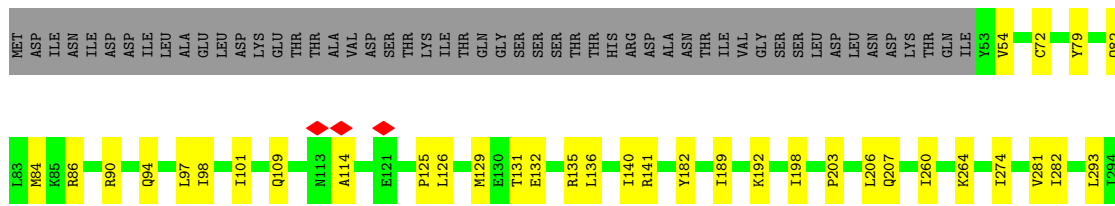




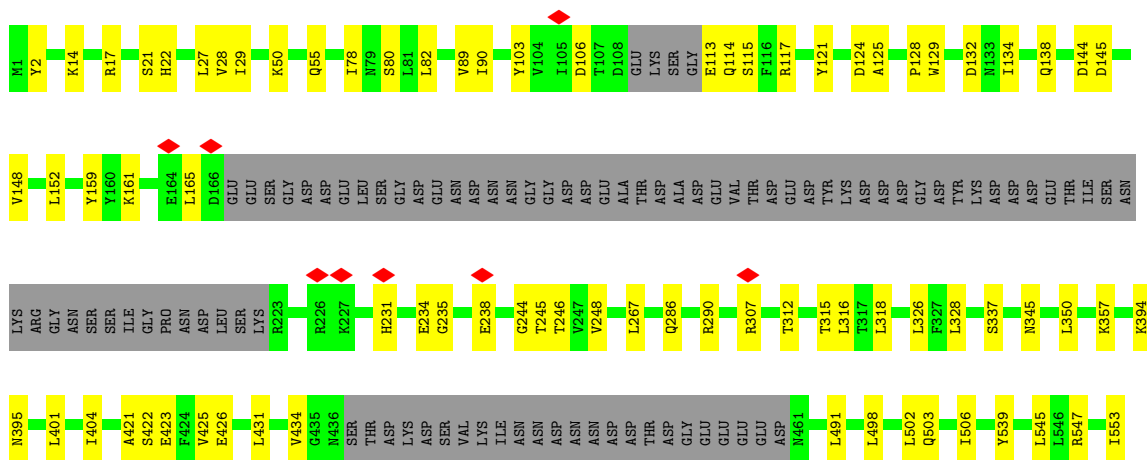
• Molecule 10: DNA replication complex GINS protein SLD5



• Molecule 10: DNA replication complex GINS protein SLD5



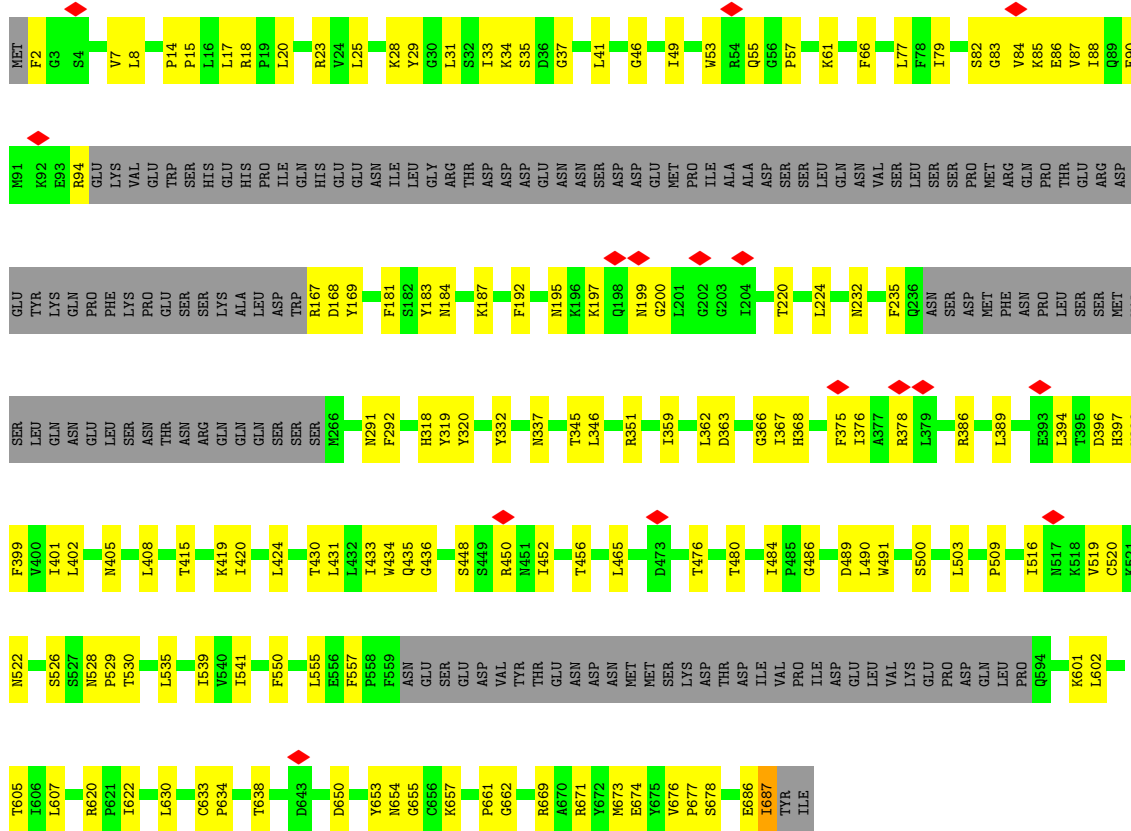
• Molecule 11: Cell division control protein 45



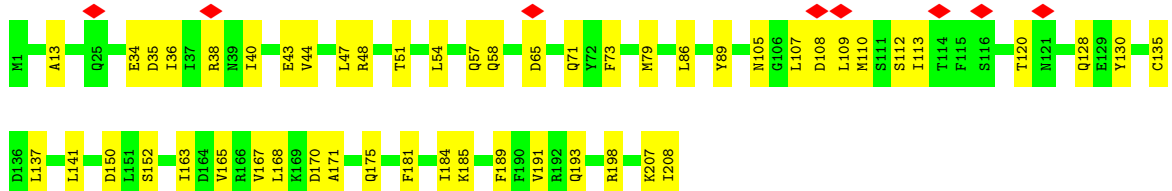




• Molecule 12: DNA polymerase epsilon subunit B



• Molecule 13: DNA replication complex GINS protein PSF1

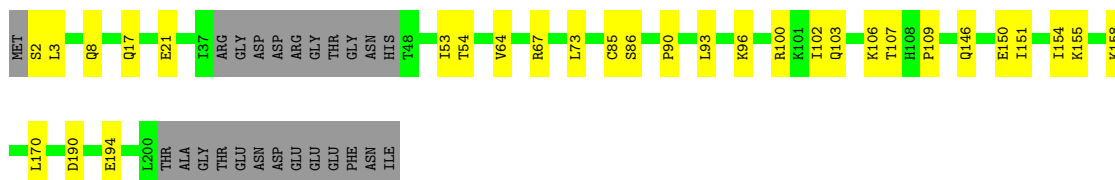


• Molecule 13: DNA replication complex GINS protein PSF1

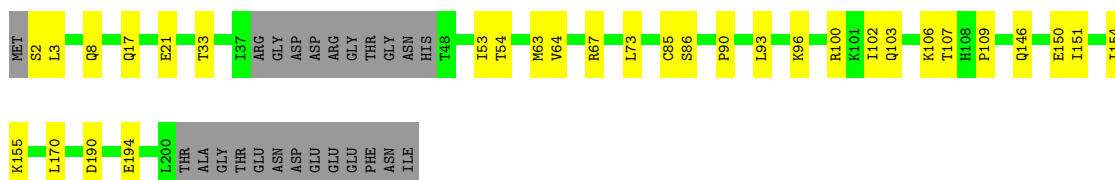




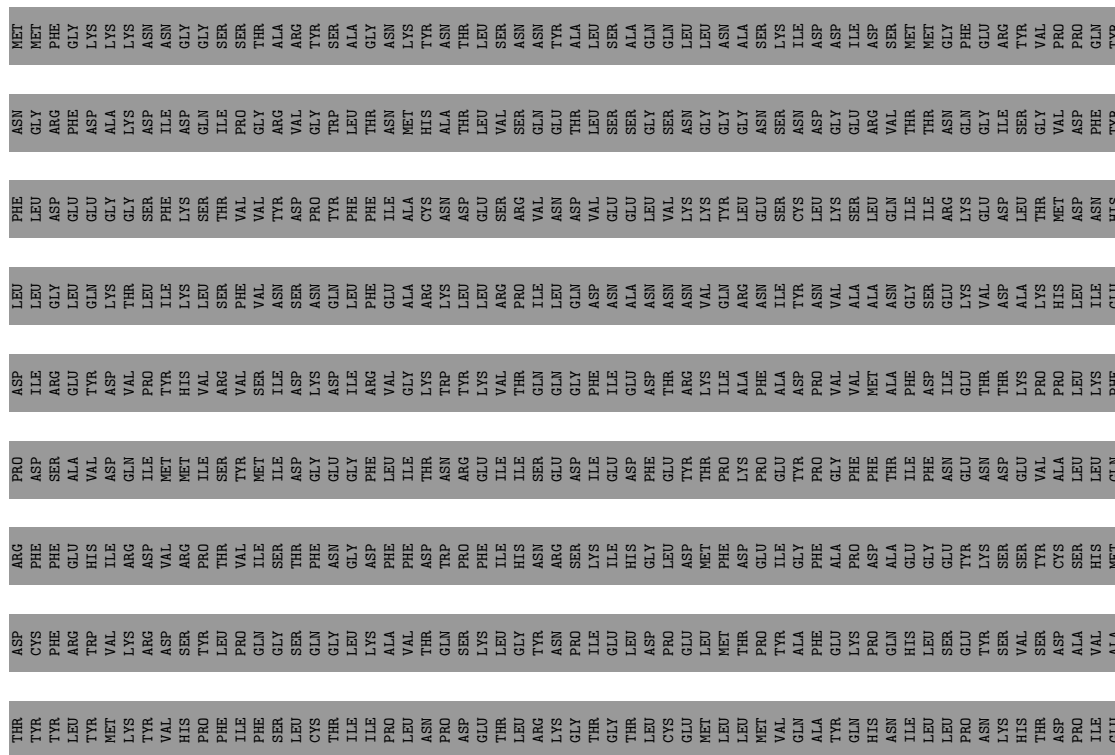
• Molecule 14: DNA replication complex GINS protein PSF2



• Molecule 14: DNA replication complex GINS protein PSF2



• Molecule 15: DNA polymerase epsilon catalytic subunit A











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	71348	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.913	Depositor
Minimum map value	-0.926	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	277.56, 387.72, 184.68001	wwPDB
Map dimensions	257, 359, 171	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	2	0.25	0/5319	0.52	0/7182
1	a	0.25	0/5319	0.52	0/7182
2	3	0.25	0/5044	0.50	0/6842
2	b	0.25	0/5044	0.50	0/6842
3	4	0.25	0/4921	0.52	0/6651
3	c	0.25	0/4921	0.52	0/6651
4	5	0.25	0/5530	0.50	0/7471
4	d	0.25	0/5530	0.50	0/7471
5	6	0.26	0/5051	0.52	0/6813
5	e	0.26	0/5051	0.51	0/6813
6	7	0.27	0/5261	0.51	0/7110
6	f	0.27	0/5261	0.51	0/7110
7	A	0.53	0/1219	0.98	0/1879
8	B	0.52	0/1217	1.00	0/1876
9	C	0.24	0/1431	0.41	0/1933
9	J	0.25	0/1431	0.41	0/1933
10	D	0.26	0/2032	0.48	0/2750
10	K	0.26	0/2032	0.48	0/2750
11	E	0.25	0/4685	0.48	0/6341
11	L	0.25	0/4685	0.48	0/6341
12	F	0.27	0/4492	0.51	0/6078
12	M	0.27	0/4492	0.51	0/6078
13	H	0.26	0/1719	0.52	0/2314
13	O	0.26	0/1719	0.52	0/2314
14	I	0.23	0/1613	0.49	0/2182
14	P	0.23	0/1613	0.49	0/2182
15	N	0.26	0/6250	0.47	0/8458
15	Q	0.26	0/6250	0.46	0/8458
All	All	0.26	0/109132	0.52	0/148005

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	5231	0	5280	58	0
1	a	5231	0	5280	0	0
2	3	4958	0	5005	43	0
2	b	4958	0	5005	0	0
3	4	4850	0	4926	114	0
3	c	4850	0	4926	0	0
4	5	5450	0	5510	59	0
4	d	5450	0	5510	0	0
5	6	4972	0	5007	80	0
5	e	4972	0	5007	0	0
6	7	5181	0	5258	103	0
6	f	5181	0	5258	0	0
7	A	1087	0	610	11	0
8	B	1086	0	611	12	0
9	C	1398	0	1418	12	0
9	J	1398	0	1418	11	0
10	D	1990	0	1985	27	0
10	K	1990	0	1985	27	0
11	E	4599	0	4603	50	0
11	L	4599	0	4603	49	0
12	F	4396	0	4442	103	0
12	M	4396	0	4442	100	0
13	H	1697	0	1698	38	0
13	O	1697	0	1698	39	0
14	I	1581	0	1635	21	0
14	P	1581	0	1635	19	0
15	N	6113	0	6177	89	0
15	Q	6113	0	6177	94	0
16	2	31	0	12	0	0
16	3	31	0	12	0	0
16	5	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	7	31	0	12	1	0
16	a	31	0	12	0	0
16	b	31	0	12	0	0
16	d	31	0	12	0	0
16	f	31	0	12	0	0
17	2	1	0	0	0	0
17	4	1	0	0	0	0
17	5	1	0	0	0	0
17	6	1	0	0	0	0
17	7	1	0	0	0	0
17	N	2	0	0	0	0
17	Q	2	0	0	0	0
17	a	1	0	0	0	0
17	c	1	0	0	0	0
17	d	1	0	0	0	0
17	e	1	0	0	0	0
17	f	1	0	0	0	0
18	3	1	0	0	0	0
18	5	1	0	0	0	0
18	7	1	0	0	0	0
18	b	1	0	0	0	0
18	d	1	0	0	0	0
18	f	1	0	0	0	0
19	4	27	0	12	0	0
19	6	27	0	12	4	0
19	c	27	0	12	0	0
19	e	27	0	12	0	0
All	All	107381	0	107253	1074	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 7.

All (1074) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:333:CYS:SG	5:6:334:PRO:HD2	1.73	1.28
5:6:333:CYS:SG	5:6:334:PRO:CD	2.30	1.17
12:M:526:SER:HB2	12:M:530:THR:HG21	1.48	0.92
12:F:526:SER:HB2	12:F:530:THR:HG21	1.48	0.91
5:6:333:CYS:SG	5:6:334:PRO:HD3	2.06	0.91
15:Q:1438:ILE:HD11	15:Q:1658:ILE:HG23	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:1438:ILE:HD11	15:N:1658:ILE:HG23	1.56	0.86
2:3:652:THR:HG22	2:3:654:PRO:HD2	1.60	0.84
15:Q:1649:LEU:HB3	15:Q:1660:ILE:HD11	1.65	0.79
15:N:1649:LEU:HB3	15:N:1660:ILE:HD11	1.65	0.78
12:F:169:TYR:OH	12:F:368:HIS:ND1	2.20	0.75
10:K:98:ILE:HG23	10:K:126:LEU:HD11	1.70	0.74
12:M:169:TYR:OH	12:M:368:HIS:ND1	2.20	0.74
5:6:335:ASN:N	5:6:336:PRO:HD3	2.03	0.74
11:L:615:GLU:HG3	11:L:616:THR:HG23	1.71	0.72
10:D:98:ILE:HG23	10:D:126:LEU:HD11	1.70	0.72
11:E:615:GLU:HG3	11:E:616:THR:HG23	1.71	0.71
1:2:339:PHE:HB2	1:2:348:LEU:HD12	1.72	0.71
13:H:35:ASP:HA	13:H:38:ARG:HE	1.56	0.70
13:O:35:ASP:HA	13:O:38:ARG:HE	1.56	0.70
3:4:621:LEU:HD13	3:4:648:VAL:HG21	1.74	0.70
12:M:351:ARG:HG2	12:M:654:ASN:HB3	1.74	0.70
12:F:662:GLY:O	12:F:671:ARG:NH2	2.24	0.70
6:7:368:ALA:HB1	6:7:371:LEU:HB2	1.73	0.70
12:M:662:GLY:O	12:M:671:ARG:NH2	2.24	0.70
15:N:2166:ARG:NH1	15:N:2182:ALA:O	2.25	0.70
15:Q:2166:ARG:NH1	15:Q:2182:ALA:O	2.25	0.70
12:F:351:ARG:HG2	12:F:654:ASN:HB3	1.74	0.69
1:2:211:LEU:HD13	1:2:271:PHE:HD1	1.58	0.69
1:2:577:THR:HG22	1:2:578:ALA:H	1.57	0.69
12:M:401:ILE:HG13	12:M:433:ILE:HD12	1.75	0.69
3:4:407:PRO:HG2	3:4:410:GLN:HG3	1.73	0.69
3:4:234:ARG:O	3:4:234:ARG:NH1	2.24	0.69
12:F:401:ILE:HG13	12:F:433:ILE:HD12	1.75	0.68
4:5:400:LEU:HD12	4:5:404:MET:HB3	1.73	0.68
4:5:685:GLN:NE2	15:Q:2180:PRO:O	2.27	0.68
12:F:528:ASN:HB3	12:F:529:PRO:HD3	1.74	0.68
5:6:151:ILE:HD11	5:6:265:ILE:HG12	1.75	0.68
12:M:528:ASN:HB3	12:M:529:PRO:HD3	1.74	0.67
5:6:318:VAL:HG21	5:6:330:PRO:HG3	1.75	0.67
6:7:494:THR:HG21	6:7:546:ILE:HG21	1.78	0.67
3:4:210:ASP:OD1	3:4:211:GLU:N	2.28	0.66
6:7:457:CYS:HB3	6:7:597:LEU:HD13	1.76	0.66
5:6:314:CYS:SG	5:6:338:CYS:HB3	2.34	0.66
5:6:270:LEU:HD12	5:6:289:SER:HB3	1.76	0.66
15:N:1385:ASN:ND2	15:N:1782:ALA:O	2.28	0.66
15:Q:1385:ASN:ND2	15:Q:1782:ALA:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:188:HIS:NE2	4:5:212:LEU:O	2.28	0.66
15:Q:1362:LYS:O	15:Q:1396:GLN:NE2	2.28	0.66
5:6:689:TYR:HA	5:6:698:ASN:HD21	1.61	0.66
15:N:1362:LYS:O	15:N:1396:GLN:NE2	2.28	0.66
4:5:493:ILE:HG22	4:5:497:MET:HG3	1.78	0.66
6:7:358:ALA:HB3	6:7:373:GLU:HB2	1.77	0.65
11:L:148:VAL:HG22	11:L:152:LEU:HD12	1.77	0.65
12:M:500:SER:OG	12:M:620:ARG:NH1	2.29	0.65
12:M:539:ILE:HG12	12:M:638:THR:HB	1.78	0.65
15:N:1679:LYS:HD3	15:N:1794:MET:HE2	1.77	0.65
12:M:345:THR:HG22	12:M:346:LEU:H	1.61	0.65
14:P:2:SER:OG	14:P:3:LEU:N	2.29	0.65
12:M:183:TYR:HD1	12:M:224:LEU:HD22	1.62	0.65
3:4:207:LYS:HE3	3:4:215:PHE:HB2	1.79	0.64
7:A:34:DA:N6	8:B:19:DT:O4	2.31	0.64
11:E:148:VAL:HG22	11:E:152:LEU:HD12	1.77	0.64
7:A:19:DT:O4	8:B:34:DA:N6	2.31	0.64
11:E:422:SER:O	11:E:426:GLU:HG2	1.97	0.64
12:F:183:TYR:HD1	12:F:224:LEU:HD22	1.61	0.64
14:I:2:SER:OG	14:I:3:LEU:N	2.29	0.64
2:3:698:THR:HG22	2:3:699:ALA:H	1.61	0.64
6:7:262:CYS:O	6:7:265:CYS:N	2.24	0.64
12:F:345:THR:HG22	12:F:346:LEU:H	1.61	0.64
2:3:169:ARG:NH1	2:3:269:GLN:OE1	2.30	0.64
11:L:422:SER:O	11:L:426:GLU:HG2	1.97	0.64
1:2:353:GLN:HA	1:2:359:ILE:HD11	1.80	0.64
12:M:480:THR:HG23	12:M:522:ASN:HB3	1.79	0.64
11:E:244:GLY:HA3	11:E:602:LEU:HB3	1.79	0.64
12:F:35:SER:HA	13:H:175:GLN:HE21	1.63	0.64
12:F:539:ILE:HG12	12:F:638:THR:HB	1.78	0.63
11:L:244:GLY:HA3	11:L:602:LEU:HB3	1.79	0.63
15:Q:2164:CYS:HB3	15:Q:2167:CYS:O	1.98	0.63
15:N:2164:CYS:HB3	15:N:2167:CYS:O	1.98	0.63
6:7:262:CYS:SG	6:7:284:CYS:HB3	2.37	0.63
12:F:386:ARG:HD3	12:F:389:LEU:HD12	1.81	0.63
12:F:480:THR:HG23	12:F:522:ASN:HB3	1.78	0.63
3:4:246:ARG:HH21	3:4:249:LEU:HD22	1.63	0.63
12:M:633:CYS:HB3	12:M:634:PRO:HD3	1.81	0.63
3:4:797:GLN:O	3:4:801:MET:HG3	1.99	0.63
6:7:212:ALA:O	6:7:216:ARG:N	2.32	0.63
14:I:190:ASP:O	14:I:194:GLU:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:583:LYS:HE3	3:4:583:LYS:HA	1.79	0.62
12:M:35:SER:HA	13:O:175:GLN:HE21	1.63	0.62
14:P:190:ASP:O	14:P:194:GLU:HG3	1.99	0.62
12:M:77:LEU:HD11	13:O:113:ILE:HG21	1.81	0.62
12:F:77:LEU:HD11	13:H:113:ILE:HG21	1.81	0.62
12:F:633:CYS:HB3	12:F:634:PRO:HD3	1.81	0.62
3:4:284:ILE:HG13	3:4:285:VAL:HG13	1.81	0.62
5:6:314:CYS:SG	5:6:338:CYS:CB	2.87	0.62
9:J:181:HIS:O	9:J:185:LYS:HG3	1.99	0.62
12:M:386:ARG:HD3	12:M:389:LEU:HD12	1.81	0.62
9:C:181:HIS:O	9:C:185:LYS:HG3	1.99	0.62
2:3:700:ARG:NH2	16:7:901:ATP:O3G	2.32	0.62
11:L:503:GLN:OE1	11:L:547:ARG:NH1	2.33	0.62
3:4:607:ARG:NH1	5:6:616:GLU:OE2	2.32	0.61
12:M:82:SER:O	12:M:85:LYS:N	2.33	0.61
6:7:284:CYS:SG	6:7:289:CYS:HB3	2.39	0.61
11:E:503:GLN:OE1	11:E:547:ARG:NH1	2.33	0.61
2:3:308:GLN:OE1	4:5:209:ARG:NH1	2.29	0.61
3:4:812:LYS:O	3:4:814:LYS:HG3	2.00	0.61
6:7:82:LEU:HD23	6:7:103:VAL:HG23	1.82	0.61
13:H:58:GLN:NE2	13:H:65:ASP:OD1	2.33	0.61
11:L:106:ASP:HB2	11:L:115:SER:HB3	1.83	0.61
15:Q:1679:LYS:HD3	15:Q:1794:MET:HE2	1.82	0.61
6:7:578:LEU:HD22	6:7:678:LYS:HB3	1.82	0.61
12:M:405:ASN:H	12:M:436:GLY:HA3	1.65	0.61
15:N:1333:PRO:HB2	15:N:1404:GLU:HB3	1.82	0.61
15:Q:1333:PRO:HB2	15:Q:1404:GLU:HB3	1.82	0.61
5:6:644:MET:HE1	5:6:652:ILE:HD12	1.83	0.61
3:4:454:LYS:HA	6:7:277:THR:HA	1.83	0.61
13:H:163:ILE:HD13	13:H:193:GLN:HG3	1.83	0.61
15:N:1345:LYS:HG2	15:N:1346:VAL:H	1.65	0.61
15:Q:1345:LYS:HG2	15:Q:1346:VAL:H	1.65	0.60
12:F:82:SER:O	12:F:85:LYS:N	2.33	0.60
12:M:676:VAL:HG12	12:M:678:SER:H	1.67	0.60
13:O:163:ILE:HD13	13:O:193:GLN:HG3	1.83	0.60
3:4:796:ARG:NH1	19:6:1201:ADP:O3'	2.34	0.60
6:7:670:ASP:OD1	6:7:673:ARG:NH1	2.34	0.60
1:2:319:ARG:NE	1:2:425:GLU:OE1	2.30	0.60
3:4:569:ASP:OD2	3:4:710:ASP:N	2.34	0.60
12:F:405:ASN:H	12:F:436:GLY:HA3	1.65	0.60
12:F:500:SER:OG	12:F:620:ARG:NH1	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:2205:ALA:HB2	15:N:2213:LEU:HD23	1.84	0.60
2:3:189:THR:O	2:3:456:ARG:NH1	2.35	0.60
12:F:431:LEU:HD23	12:F:480:THR:HB	1.84	0.60
15:N:1352:HIS:HB2	15:N:1464:GLU:HA	1.84	0.60
2:3:236:THR:OG1	2:3:237:GLU:OE2	2.19	0.59
3:4:711:LYS:HD3	3:4:712:VAL:H	1.66	0.59
12:M:431:LEU:HD23	12:M:480:THR:HB	1.84	0.59
12:M:486:GLY:N	12:M:489:ASP:OD2	2.34	0.59
13:O:58:GLN:NE2	13:O:65:ASP:OD1	2.33	0.59
15:Q:2205:ALA:HB2	15:Q:2213:LEU:HD23	1.84	0.59
1:2:587:LYS:NZ	8:B:12:DT:O3'	2.34	0.59
5:6:134:LYS:HG2	5:6:137:ARG:HD3	1.84	0.59
6:7:92:LYS:HD2	6:7:97:THR:HB	1.85	0.59
11:E:106:ASP:HB2	11:E:115:SER:HB3	1.83	0.59
12:F:168:ASP:OD1	12:F:169:TYR:N	2.34	0.59
3:4:370:ARG:HE	3:4:379:PRO:HG3	1.67	0.59
5:6:143:MET:HG2	5:6:148:LEU:HB2	1.84	0.59
9:C:38:ILE:HD11	9:C:42:THR:HG21	1.84	0.59
12:F:486:GLY:N	12:F:489:ASP:OD2	2.34	0.59
4:5:704:SER:HB2	4:5:707:SER:HB2	1.84	0.59
10:K:90:ARG:HD3	14:P:53:ILE:HB	1.84	0.59
9:C:57:VAL:HG11	13:H:73:PHE:HE2	1.68	0.59
5:6:608:LEU:HD23	5:6:652:ILE:HD11	1.85	0.58
6:7:584:ILE:HD11	6:7:591:LEU:HD11	1.85	0.58
11:L:124:ASP:OD1	11:L:125:ALA:N	2.36	0.58
10:D:90:ARG:HD3	14:I:53:ILE:HB	1.84	0.58
11:E:124:ASP:OD1	11:E:125:ALA:N	2.36	0.58
12:F:676:VAL:HG12	12:F:678:SER:H	1.66	0.58
12:M:291:ASN:OD1	12:M:292:PHE:N	2.35	0.58
2:3:480:ASP:OD1	2:3:483:ARG:NH2	2.36	0.58
3:4:510:ARG:NH2	3:4:753:TYR:OH	2.37	0.58
12:M:46:GLY:HA2	12:M:49:ILE:HB	1.84	0.58
2:3:678:VAL:HG21	2:3:723:LYS:HG3	1.86	0.58
12:F:291:ASN:OD1	12:F:292:PHE:N	2.35	0.58
12:F:359:ILE:HG12	12:F:362:LEU:HD12	1.86	0.58
15:Q:1352:HIS:HB2	15:Q:1464:GLU:HA	1.84	0.58
15:Q:1465:MET:O	15:Q:1469:SER:OG	2.22	0.58
3:4:281:VAL:HA	3:4:284:ILE:HG12	1.86	0.58
3:4:370:ARG:NH1	3:4:377:ASN:OD1	2.37	0.58
12:F:46:GLY:HA2	12:F:49:ILE:HB	1.84	0.58
12:M:168:ASP:OD1	12:M:169:TYR:N	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:325:THR:HG22	1:2:326:ARG:HG3	1.86	0.57
3:4:762:ILE:HA	3:4:817:VAL:HG22	1.86	0.57
5:6:335:ASN:H	5:6:336:PRO:HD3	1.69	0.57
6:7:451:ARG:HG2	6:7:453:ASP:H	1.67	0.57
11:L:89:VAL:HG23	11:L:90:ILE:HG23	1.86	0.57
9:J:38:ILE:HD11	9:J:42:THR:HG21	1.84	0.57
9:J:126:GLU:OE2	9:J:130:GLN:NE2	2.29	0.57
12:M:359:ILE:HG12	12:M:362:LEU:HD12	1.86	0.57
11:E:89:VAL:HG23	11:E:90:ILE:HG23	1.86	0.57
14:P:90:PRO:HD2	14:P:93:LEU:HD12	1.86	0.57
15:Q:1336:LEU:HD11	15:Q:1434:HIS:HA	1.86	0.57
5:6:134:LYS:HB3	5:6:137:ARG:HB2	1.87	0.57
15:N:1435:GLN:HA	15:N:1438:ILE:HG22	1.87	0.57
15:N:2117:ILE:HD11	15:N:2127:ILE:HA	1.86	0.57
5:6:581:LYS:NZ	5:6:682:ALA:O	2.37	0.57
6:7:77:SER:HG	6:7:338:THR:HG1	1.50	0.57
15:Q:2117:ILE:HD11	15:Q:2127:ILE:HA	1.86	0.57
6:7:68:GLN:O	6:7:72:ASN:ND2	2.38	0.57
6:7:597:LEU:O	6:7:723:SER:OG	2.23	0.57
15:Q:1376:ILE:HG22	15:Q:1400:ILE:HG23	1.87	0.57
9:J:57:VAL:HG11	13:O:73:PHE:HE2	1.68	0.57
15:N:1336:LEU:HD11	15:N:1434:HIS:HA	1.86	0.57
15:N:1376:ILE:HG22	15:N:1400:ILE:HG23	1.87	0.57
4:5:167:ILE:HD11	4:5:257:LYS:HE3	1.87	0.56
13:H:36:ILE:O	13:H:40:ILE:HD12	2.06	0.56
10:K:198:ILE:HD13	13:O:86:LEU:HB3	1.88	0.56
11:L:2:TYR:OH	11:L:138:GLN:OE1	2.24	0.56
12:M:399:PHE:HE1	12:M:677:PRO:HG3	1.70	0.56
15:Q:1374:CYS:HB3	15:Q:1402:LEU:HD12	1.87	0.56
2:3:665:GLU:HG3	2:3:666:ARG:HG2	1.87	0.56
9:C:126:GLU:OE2	9:C:130:GLN:NE2	2.29	0.56
10:D:198:ILE:HD13	13:H:86:LEU:HB3	1.88	0.56
12:F:31:LEU:HD11	12:F:77:LEU:HD23	1.87	0.56
12:F:601:LYS:O	12:F:605:THR:HG23	2.05	0.56
15:N:1465:MET:O	15:N:1469:SER:OG	2.22	0.56
13:O:36:ILE:O	13:O:40:ILE:HD12	2.06	0.56
4:5:104:LEU:HD21	14:I:151:ILE:HG23	1.86	0.56
12:F:319:TYR:HB2	12:F:605:THR:HG21	1.88	0.56
11:L:21:SER:O	11:L:55:GLN:NE2	2.39	0.56
12:F:398:LYS:O	12:F:430:THR:N	2.32	0.56
14:I:90:PRO:HD2	14:I:93:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:522:LEU:HD12	3:4:811:MET:HE1	1.87	0.56
11:E:2:TYR:OH	11:E:138:GLN:OE1	2.24	0.56
12:M:491:TRP:HZ3	15:N:2147:ILE:HG21	1.71	0.56
15:Q:1435:GLN:HA	15:Q:1438:ILE:HG22	1.86	0.56
3:4:767:LYS:HE2	5:6:732:VAL:HG13	1.88	0.55
2:3:570:ARG:NH1	4:5:614:LEU:O	2.39	0.55
11:E:21:SER:O	11:E:55:GLN:NE2	2.39	0.55
12:F:399:PHE:HE1	12:F:677:PRO:HG3	1.70	0.55
11:L:598:LYS:HG2	11:L:599:LYS:H	1.71	0.55
12:M:319:TYR:HB2	12:M:605:THR:HG21	1.88	0.55
4:5:718:LEU:HD21	4:5:761:ILE:HD11	1.88	0.55
11:E:267:LEU:HD13	11:E:316:LEU:HD22	1.88	0.55
12:M:601:LYS:O	12:M:605:THR:HG23	2.05	0.55
1:2:379:LYS:HD2	1:2:379:LYS:O	2.07	0.55
15:N:1365:THR:HG22	15:N:1366:MET:H	1.72	0.55
1:2:792:ASP:OD1	1:2:795:ARG:NH2	2.39	0.55
2:3:233:THR:HG23	2:3:234:GLU:HG2	1.89	0.55
6:7:101:ASP:OD2	6:7:104:SER:OG	2.24	0.55
10:K:125:PRO:O	10:K:129:MET:HG2	2.07	0.55
12:M:375:PHE:HA	13:O:120:THR:HG21	1.88	0.55
12:F:491:TRP:HZ3	15:Q:2147:ILE:HG21	1.71	0.55
14:P:150:GLU:O	14:P:154:ILE:HG13	2.07	0.55
15:N:1374:CYS:HB3	15:N:1402:LEU:HD12	1.87	0.55
15:Q:1637:ASN:OD1	15:Q:1638:HIS:N	2.40	0.55
15:Q:1797:GLU:O	15:Q:1801:GLU:HG3	2.07	0.55
12:M:398:LYS:O	12:M:430:THR:N	2.32	0.54
15:N:1850:GLU:HG3	15:N:1895:PHE:HE2	1.73	0.54
14:I:150:GLU:O	14:I:154:ILE:HG13	2.07	0.54
12:M:31:LEU:HD11	12:M:77:LEU:HD23	1.87	0.54
15:Q:1967:THR:HG21	15:Q:2003:PHE:HB3	1.89	0.54
1:2:222:THR:HG23	1:2:224:ARG:HG3	1.89	0.54
2:3:499:LYS:HE2	7:A:41:DA:H5'	1.89	0.54
11:L:267:LEU:HD13	11:L:316:LEU:HD22	1.88	0.54
1:2:743:ARG:HA	1:2:746:GLN:HG2	1.89	0.54
3:4:525:SER:HA	3:4:742:LEU:HD22	1.89	0.54
15:N:1797:GLU:O	15:N:1801:GLU:HG3	2.07	0.54
3:4:193:ASN:HB3	3:4:254:THR:HG22	1.89	0.54
13:H:40:ILE:HA	13:H:43:GLU:HG2	1.89	0.54
6:7:451:ARG:O	6:7:694:ARG:NH1	2.39	0.54
1:2:300:PHE:O	1:2:319:ARG:NH1	2.41	0.54
5:6:608:LEU:HD12	5:6:627:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:125:PRO:O	10:D:129:MET:HG2	2.07	0.54
14:I:21:GLU:HA	14:I:73:LEU:HD23	1.90	0.54
9:J:20:PHE:HE2	9:J:44:LEU:HD12	1.73	0.54
15:N:1637:ASN:OD1	15:N:1638:HIS:N	2.40	0.54
2:3:201:HIS:CE1	2:3:232:PRO:HD2	2.43	0.54
13:O:107:LEU:HD23	13:O:109:LEU:H	1.73	0.54
6:7:513:LEU:HD13	6:7:540:VAL:HG21	1.90	0.54
15:N:1709:THR:HA	15:N:1712:ILE:HG12	1.90	0.54
2:3:99:SER:HB3	2:3:158:LYS:HE2	1.89	0.54
4:5:734:ARG:HH12	12:F:293:LYS:HB3	1.72	0.54
11:E:598:LYS:HG2	11:E:599:LYS:H	1.71	0.54
10:K:182:TYR:CD1	13:O:141:LEU:HD11	2.43	0.54
12:M:195:ASN:HD21	12:M:197:LYS:HB3	1.73	0.54
12:F:375:PHE:HA	13:H:120:THR:HG21	1.88	0.53
15:N:1744:ILE:HD11	15:N:1836:VAL:HG22	1.91	0.53
15:Q:1365:THR:HG22	15:Q:1366:MET:H	1.72	0.53
13:O:40:ILE:HA	13:O:43:GLU:HG2	1.89	0.53
15:Q:1850:GLU:HG3	15:Q:1895:PHE:HE2	1.73	0.53
1:2:391:GLN:NE2	5:6:620:ASP:OD2	2.40	0.53
1:2:586:THR:HG22	1:2:588:GLU:HG3	1.91	0.53
3:4:265:PRO:HB3	3:4:325:LEU:HG	1.89	0.53
15:N:1967:THR:HG21	15:N:2003:PHE:HB3	1.89	0.53
3:4:587:ARG:NH1	3:4:623:LEU:O	2.42	0.53
11:L:161:LYS:O	11:L:165:LEU:HB2	2.09	0.53
3:4:319:PRO:HB3	6:7:253:PRO:HB3	1.91	0.53
12:F:195:ASN:HD21	12:F:197:LYS:HB3	1.74	0.53
12:M:516:ILE:HA	12:M:519:VAL:HG22	1.91	0.53
15:N:1361:PHE:HD2	15:N:1362:LYS:HG3	1.73	0.53
3:4:207:LYS:NZ	3:4:210:ASP:OD2	2.39	0.53
9:C:20:PHE:HE2	9:C:44:LEU:HD12	1.73	0.53
11:E:161:LYS:O	11:E:165:LEU:HB2	2.09	0.53
1:2:608:GLU:OE2	5:6:653:HIS:ND1	2.41	0.53
13:H:107:LEU:HD23	13:H:109:LEU:H	1.73	0.53
14:P:17:GLN:O	14:P:21:GLU:HG3	2.09	0.53
5:6:582:SER:OG	19:6:1201:ADP:O2B	2.23	0.53
6:7:18:PHE:HA	6:7:21:ILE:HD12	1.90	0.53
6:7:444:VAL:HB	6:7:448:MET:HB3	1.90	0.53
12:F:516:ILE:HA	12:F:519:VAL:HG22	1.91	0.53
1:2:321:THR:HG22	1:2:425:GLU:HG3	1.91	0.53
2:3:698:THR:HG22	2:3:699:ALA:N	2.24	0.53
5:6:140:ILE:HD11	5:6:189:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:7:441:ASP:OD1	6:7:452:GLY:N	2.43	0.53
10:D:182:TYR:CD1	13:H:141:LEU:HD11	2.43	0.53
3:4:525:SER:O	3:4:528:PRO:HD3	2.09	0.52
11:L:144:ASP:OD1	11:L:145:ASP:N	2.42	0.52
14:P:21:GLU:HA	14:P:73:LEU:HD23	1.90	0.52
15:Q:1361:PHE:HD2	15:Q:1362:LYS:HG3	1.73	0.52
4:5:31:PHE:CG	4:5:90:PHE:HD1	2.27	0.52
5:6:550:GLN:HB2	5:6:571:ILE:HD11	1.90	0.52
15:Q:1475:ARG:HG3	15:Q:1476:TYR:HD1	1.74	0.52
15:N:1664:ARG:HH12	15:N:1666:ASP:HB2	1.74	0.52
13:O:207:LYS:HG2	13:O:208:ILE:H	1.75	0.52
1:2:406:ARG:NH1	1:2:430:TYR:OH	2.42	0.52
5:6:262:VAL:HG21	5:6:354:LEU:HD21	1.91	0.52
5:6:777:TYR:HB2	5:6:800:LEU:HD13	1.91	0.52
11:E:82:LEU:HD23	11:E:121:TYR:HB2	1.92	0.52
1:2:478:GLU:OE1	11:E:357:LYS:NZ	2.29	0.52
11:E:248:VAL:O	11:E:290:ARG:NH2	2.43	0.52
11:L:82:LEU:HD23	11:L:121:TYR:HB2	1.92	0.52
15:Q:1744:ILE:HD11	15:Q:1836:VAL:HG22	1.91	0.52
6:7:435:LEU:HD13	6:7:564:LEU:HD13	1.92	0.52
6:7:548:ILE:HG13	6:7:549:SER:H	1.75	0.52
3:4:506:LEU:O	3:4:510:ARG:HG2	2.10	0.52
3:4:698:LEU:HD12	3:4:701:ARG:HD2	1.91	0.52
10:D:97:LEU:O	10:D:101:ILE:HD12	2.10	0.52
11:E:345:ASN:HA	11:E:350:LEU:HD13	1.92	0.52
11:E:401:LEU:HB3	11:E:404:ILE:HD12	1.92	0.52
14:I:17:GLN:O	14:I:21:GLU:HG3	2.09	0.52
15:Q:1709:THR:HA	15:Q:1712:ILE:HG12	1.90	0.52
6:7:458:LEU:HD23	6:7:598:PHE:HB2	1.91	0.52
8:B:25:DT:H2"	8:B:26:DT:OP2	2.10	0.52
11:E:144:ASP:OD1	11:E:145:ASP:N	2.42	0.52
5:6:816:VAL:HG12	5:6:818:GLU:H	1.75	0.52
6:7:400:ARG:HD2	6:7:637:LYS:HE2	1.91	0.52
11:L:345:ASN:HA	11:L:350:LEU:HD13	1.92	0.52
15:N:1593:GLN:OE1	15:N:1617:LEU:N	2.32	0.52
15:N:1670:TYR:O	15:N:1674:VAL:HG23	2.10	0.52
15:Q:1664:ARG:HH12	15:Q:1666:ASP:HB2	1.74	0.52
15:Q:1952:GLU:OE2	15:Q:2014:ARG:NH2	2.40	0.52
3:4:559:ARG:NH1	3:4:649:MET:O	2.43	0.52
6:7:596:ILE:HD11	6:7:695:LEU:HD11	1.91	0.52
9:J:105:PHE:O	9:J:109:ILE:HD12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:97:LEU:O	10:K:101:ILE:HD12	2.10	0.52
4:5:614:LEU:HD11	4:5:657:ILE:HG23	1.93	0.51
12:F:415:THR:O	12:F:419:LYS:HG3	2.10	0.51
15:Q:1670:TYR:O	15:Q:1674:VAL:HG23	2.10	0.51
1:2:196:GLU:HA	1:2:199:THR:HG22	1.92	0.51
1:2:341:CYS:O	1:2:345:GLY:HA2	2.11	0.51
9:C:105:PHE:O	9:C:109:ILE:HD12	2.09	0.51
12:M:415:THR:O	12:M:419:LYS:HG3	2.10	0.51
13:O:35:ASP:OD1	13:O:36:ILE:HD12	2.10	0.51
1:2:440:ALA:HB1	5:6:408:THR:HG22	1.93	0.51
12:F:84:VAL:O	12:F:88:ILE:HG13	2.10	0.51
12:F:550:PHE:HE2	12:F:602:LEU:HG	1.75	0.51
13:H:207:LYS:HG2	13:H:208:ILE:H	1.75	0.51
15:N:1475:ARG:HG3	15:N:1476:TYR:HD1	1.74	0.51
1:2:271:PHE:HA	1:2:274:VAL:HG12	1.92	0.51
6:7:142:ILE:O	6:7:146:ARG:HG2	2.09	0.51
12:F:394:LEU:HD22	12:F:397:HIS:HE1	1.76	0.51
12:F:669:ARG:NH1	12:F:687:ILE:HG12	2.26	0.51
11:L:328:LEU:HD23	11:L:423:GLU:HG2	1.91	0.51
12:M:669:ARG:NH1	12:M:687:ILE:HG12	2.26	0.51
12:M:378:ARG:NH1	13:O:128:GLN:OE1	2.44	0.51
15:N:1731:VAL:HB	15:N:1906:TRP:HB2	1.93	0.51
15:N:1895:PHE:HB3	15:N:1898:LEU:HD12	1.93	0.51
2:3:170:THR:HG21	2:3:588:LEU:HD11	1.92	0.51
2:3:293:ASN:ND2	2:3:594:GLU:OE2	2.33	0.51
3:4:316:GLU:HG2	3:4:316:GLU:O	2.11	0.51
5:6:152:TYR:HB3	5:6:268:PHE:HE1	1.76	0.51
10:D:94:GLN:O	10:D:98:ILE:HD12	2.11	0.51
13:H:107:LEU:HD21	13:H:112:SER:HB3	1.93	0.51
3:4:196:ASN:O	3:4:200:SER:HB2	2.11	0.51
12:F:378:ARG:NH1	13:H:128:GLN:OE1	2.44	0.51
2:3:519:VAL:HG22	2:3:534:ALA:HB2	1.93	0.51
3:4:209:LEU:HD13	3:4:250:ALA:HA	1.92	0.51
3:4:445:ARG:HA	3:4:453:LEU:HD23	1.92	0.51
3:4:728:TYR:HE1	6:7:450:ILE:HG21	1.76	0.51
3:4:826:VAL:HA	3:4:829:ILE:HG22	1.93	0.51
13:H:35:ASP:OD1	13:H:36:ILE:HD12	2.10	0.51
15:Q:1369:GLN:HG2	15:Q:1371:ILE:H	1.76	0.51
5:6:137:ARG:O	5:6:140:ILE:HG22	2.10	0.50
10:D:182:TYR:HD1	13:H:141:LEU:HD11	1.77	0.50
12:F:398:LYS:NZ	12:F:674:GLU:OE2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:394:LEU:HD22	12:M:397:HIS:HE1	1.76	0.50
12:M:550:PHE:HE2	12:M:602:LEU:HG	1.75	0.50
15:Q:1856:SER:HA	15:Q:1869:LYS:O	2.11	0.50
6:7:69:LYS:HD2	6:7:75:LEU:HB2	1.93	0.50
10:K:94:GLN:O	10:K:98:ILE:HD12	2.11	0.50
12:M:84:VAL:O	12:M:88:ILE:HG13	2.10	0.50
13:O:107:LEU:HD21	13:O:112:SER:HB3	1.93	0.50
6:7:216:ARG:HG2	6:7:217:LYS:H	1.76	0.50
6:7:432:LEU:HD13	6:7:473:ILE:HD11	1.93	0.50
6:7:575:ASN:OD1	6:7:576:PRO:HD2	2.11	0.50
11:E:328:LEU:HD23	11:E:423:GLU:HG2	1.91	0.50
9:J:97:LEU:HD11	9:J:127:LEU:HD21	1.93	0.50
15:Q:1731:VAL:HB	15:Q:1906:TRP:HB2	1.93	0.50
5:6:652:ILE:HG22	5:6:656:MET:HG3	1.93	0.50
12:M:18:ARG:NE	13:O:175:GLN:OE1	2.44	0.50
15:N:1369:GLN:HG2	15:N:1371:ILE:H	1.76	0.50
15:N:2155:GLU:O	15:N:2159:ILE:HG12	2.11	0.50
2:3:259:GLN:HG3	2:3:273:SER:HB3	1.94	0.50
15:N:1816:LEU:O	15:N:1820:VAL:HG23	2.12	0.50
15:N:1874:SER:OG	15:N:1876:GLU:OE1	2.30	0.50
1:2:589:TRP:HD1	4:5:454:GLN:HE22	1.60	0.50
14:I:109:PRO:HA	14:I:155:LYS:HE2	1.93	0.50
1:2:382:TYR:HB2	4:5:153:SER:HB2	1.92	0.50
5:6:690:ASN:HD22	5:6:693:LEU:HD23	1.77	0.50
11:L:401:LEU:HB3	11:L:404:ILE:HD12	1.92	0.50
15:N:1366:MET:HG2	15:N:1368:LEU:HG	1.94	0.50
12:M:20:LEU:HD22	12:M:23:ARG:HH21	1.77	0.50
1:2:341:CYS:O	1:2:345:GLY:CA	2.60	0.50
2:3:552:ASP:O	2:3:557:ARG:NH1	2.45	0.50
12:F:2:PHE:HE1	12:F:94:ARG:HG2	1.77	0.50
12:F:625:ASP:OD1	12:F:625:ASP:N	2.43	0.50
15:N:1952:GLU:OE2	15:N:2014:ARG:NH2	2.40	0.50
3:4:605:ILE:HD12	3:4:658:LYS:HB2	1.95	0.49
3:4:720:LEU:HD12	3:4:723:HIS:NE2	2.27	0.49
4:5:50:LEU:HG	4:5:61:LEU:HD13	1.94	0.49
6:7:260:TYR:HB3	6:7:298:LEU:HD12	1.94	0.49
6:7:322:VAL:HG21	6:7:328:PRO:HG3	1.93	0.49
9:C:97:LEU:HD11	9:C:127:LEU:HD21	1.93	0.49
12:F:529:PRO:HA	12:F:541:ILE:O	2.12	0.49
11:L:248:VAL:O	11:L:290:ARG:NH2	2.43	0.49
15:N:1856:SER:HA	15:N:1869:LYS:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:1816:LEU:O	15:Q:1820:VAL:HG23	2.12	0.49
15:Q:1895:PHE:HB3	15:Q:1898:LEU:HD12	1.93	0.49
3:4:520:SER:O	3:4:524:ARG:HG2	2.11	0.49
6:7:283:GLU:N	6:7:298:LEU:HD23	2.27	0.49
11:E:572:ILE:HD13	11:E:579:TYR:CE1	2.47	0.49
11:L:572:ILE:HD13	11:L:579:TYR:CE1	2.47	0.49
12:M:2:PHE:HE1	12:M:94:ARG:HG2	1.77	0.49
12:M:34:LYS:HB2	12:M:79:ILE:O	2.12	0.49
12:M:232:ASN:HB3	12:M:235:PHE:HD2	1.77	0.49
5:6:335:ASN:N	5:6:336:PRO:CD	2.73	0.49
5:6:538:PHE:HB2	5:6:730:HIS:ND1	2.27	0.49
6:7:291:GLN:NE2	6:7:292:ASN:OD1	2.45	0.49
10:D:126:LEU:HD23	11:E:22:HIS:NE2	2.27	0.49
15:Q:1366:MET:HG2	15:Q:1368:LEU:HG	1.93	0.49
15:Q:2155:GLU:O	15:Q:2159:ILE:HG12	2.12	0.49
4:5:196:ASN:ND2	4:5:279:ASP:OD2	2.46	0.49
4:5:414:LEU:HD23	4:5:554:PHE:HB2	1.93	0.49
4:5:433:SER:HB3	4:5:436:ALA:HB2	1.94	0.49
7:A:13:DT:H3'	7:A:14:DT:H5''	1.95	0.49
12:F:41:LEU:HD11	12:F:66:PHE:CE2	2.47	0.49
14:I:146:GLN:O	14:I:150:GLU:HG3	2.13	0.49
12:M:529:PRO:HA	12:M:541:ILE:O	2.12	0.49
15:Q:1360:LYS:HG3	15:Q:1424:LEU:HB2	1.94	0.49
6:7:226:SER:OG	6:7:229:GLN:HG3	2.13	0.49
2:3:723:LYS:HE2	2:3:727:LYS:HE2	1.94	0.49
4:5:584:GLN:O	4:5:587:GLN:HG2	2.12	0.49
11:L:638:SER:OG	11:L:639:PRO:HD3	2.13	0.49
15:Q:1403:PRO:HG2	15:Q:1406:VAL:HG22	1.94	0.49
1:2:656:ARG:NH2	5:6:793:TYR:OH	2.46	0.49
3:4:191:THR:O	3:4:195:ARG:HG2	2.12	0.49
3:4:251:TYR:CE2	3:4:253:GLN:HB3	2.47	0.49
6:7:643:ALA:O	6:7:647:THR:HG23	2.13	0.49
12:F:18:ARG:NE	13:H:175:GLN:OE1	2.44	0.49
13:H:168:LEU:O	13:H:185:LYS:NZ	2.45	0.49
15:N:1360:LYS:HG3	15:N:1424:LEU:HB2	1.94	0.49
8:B:13:DT:H3'	8:B:14:DT:H5''	1.95	0.49
11:E:638:SER:OG	11:E:639:PRO:HD3	2.13	0.49
12:F:53:TRP:N	12:F:55:GLN:OE1	2.46	0.49
12:F:232:ASN:HB3	12:F:235:PHE:HD2	1.77	0.49
10:K:126:LEU:HD23	11:L:22:HIS:NE2	2.27	0.49
15:Q:1874:SER:OG	15:Q:1876:GLU:OE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:110:MET:SD	13:H:120:THR:HG22	2.53	0.49
10:K:182:TYR:HD1	13:O:141:LEU:HD11	1.77	0.49
15:N:1998:ASN:HA	15:N:2001:ASN:OD1	2.13	0.49
13:O:105:ASN:HA	13:O:152:SER:HB2	1.95	0.49
14:P:146:GLN:O	14:P:150:GLU:HG3	2.13	0.49
1:2:271:PHE:CD2	1:2:295:VAL:HG21	2.48	0.49
5:6:690:ASN:ND2	5:6:693:LEU:HD23	2.28	0.49
6:7:235:LEU:HD22	6:7:357:PRO:HG3	1.95	0.49
7:A:7:DT:H2''	7:A:8:DT:H5'	1.95	0.49
12:F:31:LEU:HD22	13:H:198:ARG:HD3	1.95	0.49
12:F:34:LYS:HB2	12:F:79:ILE:O	2.12	0.49
10:K:136:LEU:O	10:K:140:ILE:HG13	2.13	0.49
13:O:34:GLU:OE1	13:O:38:ARG:NH2	2.46	0.49
13:O:54:LEU:HD21	13:O:71:GLN:HB2	1.95	0.49
15:Q:1486:TYR:OH	15:Q:1642:SER:HB2	2.13	0.49
1:2:334:LEU:HD13	4:5:322:ALA:HB1	1.94	0.48
3:4:443:PRO:HB3	3:4:457:TYR:CE1	2.48	0.48
5:6:596:VAL:HG22	5:6:631:ALA:HB2	1.95	0.48
6:7:455:ASN:HB2	6:7:595:ASP:H	1.78	0.48
12:F:386:ARG:CD	12:F:389:LEU:HD12	2.43	0.48
15:N:1486:TYR:OH	15:N:1642:SER:HB2	2.13	0.48
13:O:170:ASP:OD1	13:O:171:ALA:N	2.46	0.48
14:P:109:PRO:HA	14:P:155:LYS:HE2	1.93	0.48
3:4:403:PRO:HD2	3:4:432:ARG:HH22	1.78	0.48
4:5:26:GLU:N	4:5:26:GLU:OE1	2.46	0.48
5:6:644:MET:HE2	5:6:649:GLN:HG2	1.95	0.48
13:H:34:GLU:OE1	13:H:38:ARG:NH2	2.46	0.48
12:M:41:LEU:HD11	12:M:66:PHE:CE2	2.47	0.48
12:M:84:VAL:O	12:M:87:VAL:HG22	2.12	0.48
15:Q:1593:GLN:OE1	15:Q:1617:LEU:N	2.33	0.48
7:A:30:DA:H2'	7:A:31:DA:C8	2.48	0.48
6:7:262:CYS:HB2	6:7:298:LEU:HD11	1.95	0.48
8:B:7:DT:H2''	8:B:8:DT:H5'	1.95	0.48
11:L:28:VAL:HG23	11:L:78:ILE:HD12	1.95	0.48
15:N:1403:PRO:HG2	15:N:1406:VAL:HG22	1.94	0.48
1:2:364:CYS:CB	1:2:367:CYS:HB3	2.43	0.48
3:4:333:LEU:HD12	3:4:398:LYS:HZ2	1.78	0.48
3:4:728:TYR:CE1	6:7:450:ILE:HG21	2.48	0.48
3:4:768:THR:O	3:4:772:ARG:HG2	2.13	0.48
4:5:209:ARG:HG3	4:5:209:ARG:HH11	1.78	0.48
5:6:585:LEU:HD22	5:6:637:CYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:84:VAL:O	12:F:87:VAL:HG22	2.12	0.48
12:M:398:LYS:NZ	12:M:674:GLU:OE2	2.38	0.48
13:O:168:LEU:O	13:O:185:LYS:NZ	2.45	0.48
10:D:132:GLU:OE2	14:I:54:THR:OG1	2.27	0.48
12:F:20:LEU:HD22	12:F:23:ARG:HH21	1.77	0.48
12:F:362:LEU:HD21	12:F:376:ILE:HD12	1.96	0.48
12:F:408:LEU:HD21	12:F:465:LEU:HD11	1.96	0.48
12:M:169:TYR:HH	12:M:368:HIS:HD1	1.56	0.48
4:5:544:THR:HG23	4:5:647:PRO:HG3	1.95	0.48
4:5:571:HIS:O	4:5:575:ILE:HG12	2.13	0.48
11:E:28:VAL:HG23	11:E:78:ILE:HD12	1.95	0.48
10:K:203:PRO:O	10:K:207:GLN:HG3	2.14	0.48
12:M:31:LEU:HD22	13:O:198:ARG:HD3	1.95	0.48
6:7:282:SER:HA	6:7:298:LEU:H	1.78	0.48
10:D:203:PRO:O	10:D:207:GLN:HG3	2.14	0.48
12:F:490:LEU:HD23	12:F:509:PRO:HG3	1.96	0.48
11:L:246:THR:HG23	11:L:602:LEU:HD23	1.95	0.48
12:M:386:ARG:CD	12:M:389:LEU:HD12	2.43	0.48
12:F:686:GLU:O	12:F:687:ILE:C	2.52	0.48
12:M:53:TRP:N	12:M:55:GLN:OE1	2.46	0.48
12:M:362:LEU:HD21	12:M:376:ILE:HD12	1.96	0.48
1:2:463:THR:HG22	1:2:558:LYS:HG3	1.95	0.48
6:7:349:VAL:HG12	6:7:383:GLN:HG2	1.96	0.48
12:M:17:LEU:HD13	12:M:53:TRP:HZ2	1.78	0.48
12:M:408:LEU:HD21	12:M:465:LEU:HD11	1.96	0.48
12:M:490:LEU:HD23	12:M:509:PRO:HG3	1.96	0.48
12:M:555:LEU:HD23	12:M:557:PHE:CZ	2.49	0.48
3:4:203:TYR:O	3:4:207:LYS:HG2	2.14	0.47
3:4:527:ALA:HB3	3:4:537:LYS:HD3	1.95	0.47
12:F:555:LEU:HD23	12:F:557:PHE:CZ	2.49	0.47
13:H:170:ASP:OD1	13:H:171:ALA:N	2.46	0.47
15:Q:1998:ASN:HA	15:Q:2001:ASN:OD1	2.13	0.47
3:4:272:MET:O	3:4:276:ILE:HG12	2.14	0.47
4:5:730:TYR:HE2	12:F:293:LYS:HG2	1.79	0.47
6:7:86:LEU:HD21	6:7:103:VAL:HG11	1.95	0.47
6:7:396:ASP:O	6:7:400:ARG:HG2	2.13	0.47
10:D:206:LEU:HD12	10:D:206:LEU:O	2.15	0.47
12:F:17:LEU:HD13	12:F:53:TRP:HZ2	1.78	0.47
15:N:1339:PHE:HD1	15:N:1611:PRO:HB3	1.80	0.47
13:O:110:MET:SD	13:O:120:THR:HG22	2.53	0.47
15:Q:1597:ILE:HG21	15:Q:1614:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:329:LYS:HG2	3:4:434:GLU:HB3	1.96	0.47
4:5:738:VAL:HG22	4:5:743:PHE:HB2	1.96	0.47
13:H:54:LEU:HD21	13:H:71:GLN:HB2	1.95	0.47
13:H:105:ASN:HA	13:H:152:SER:HB2	1.95	0.47
11:L:502:LEU:O	11:L:506:ILE:HG12	2.14	0.47
2:3:484:VAL:HG11	6:7:486:LYS:HE2	1.96	0.47
3:4:367:GLU:OE1	5:6:441:ARG:N	2.48	0.47
4:5:236:CYS:HB3	4:5:240:PRO:HG2	1.95	0.47
4:5:467:GLY:H	4:5:470:VAL:HB	1.78	0.47
5:6:451:LYS:NZ	5:6:453:SER:OG	2.47	0.47
5:6:751:LEU:O	5:6:755:ILE:HG12	2.14	0.47
11:E:246:THR:HG23	11:E:602:LEU:HD23	1.95	0.47
15:N:1795:LEU:HD13	15:N:1816:LEU:HD22	1.97	0.47
4:5:90:PHE:CD2	4:5:137:LEU:HD22	2.49	0.47
6:7:275:SER:OG	6:7:276:ARG:N	2.46	0.47
11:E:502:LEU:O	11:E:506:ILE:HG12	2.14	0.47
12:M:332:TYR:OH	12:M:337:ASN:OD1	2.22	0.47
12:M:435:GLN:HA	12:M:484:ILE:HB	1.97	0.47
15:N:1664:ARG:NH1	15:N:1666:ASP:HB2	2.30	0.47
15:Q:1944:PHE:HE1	15:Q:2043:SER:HB3	1.80	0.47
4:5:681:ILE:O	4:5:685:GLN:HG3	2.14	0.47
5:6:430:THR:HA	5:6:433:LEU:HB2	1.96	0.47
6:7:404:LEU:HD23	6:7:641:TYR:CD1	2.50	0.47
6:7:707:MET:SD	6:7:707:MET:N	2.87	0.47
12:M:420:ILE:O	12:M:424:LEU:HD13	2.15	0.47
12:M:686:GLU:O	12:M:687:ILE:C	2.52	0.47
15:Q:1450:LYS:HG3	15:Q:1451:ALA:H	1.79	0.47
2:3:469:VAL:HG12	2:3:511:SER:HB2	1.96	0.47
10:D:72:CYS:HB3	10:D:293:LEU:HD23	1.97	0.47
10:D:281:VAL:HG23	10:D:282:ILE:HG23	1.96	0.47
12:F:669:ARG:NH1	12:F:687:ILE:HG23	2.30	0.47
11:L:14:LYS:HG2	11:L:17:ARG:HH12	1.80	0.47
1:2:696:ALA:HB3	5:6:774:VAL:HG23	1.97	0.47
3:4:714:GLU:OE1	3:4:715:LYS:HD3	2.14	0.47
6:7:67:LEU:HD21	6:7:121:ILE:HD12	1.97	0.47
11:E:14:LYS:HG2	11:E:17:ARG:HH12	1.80	0.47
12:F:49:ILE:HG13	12:F:53:TRP:CZ3	2.49	0.47
12:M:184:ASN:HD22	12:M:187:LYS:HE2	1.80	0.47
15:N:1920:LEU:HG	15:N:1933:TYR:HB3	1.97	0.47
15:Q:1365:THR:HG22	15:Q:1366:MET:N	2.30	0.47
10:D:136:LEU:O	10:D:140:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:206:LEU:O	10:K:206:LEU:HD12	2.15	0.47
15:N:1956:TRP:O	15:N:1960:ILE:HG13	2.15	0.47
15:Q:1920:LEU:HG	15:Q:1933:TYR:HB3	1.97	0.47
3:4:220:THR:HA	3:4:223:GLU:HG3	1.97	0.46
12:F:435:GLN:HA	12:F:484:ILE:HB	1.97	0.46
10:K:281:VAL:HG23	10:K:282:ILE:HG23	1.96	0.46
15:N:1595:PRO:HA	15:N:1618:ASN:OD1	2.15	0.46
15:N:1944:PHE:HE1	15:N:2043:SER:HB3	1.80	0.46
15:Q:1956:TRP:O	15:Q:1960:ILE:HG13	2.15	0.46
4:5:759:GLU:O	4:5:774:GLY:N	2.47	0.46
12:F:650:ASP:HB2	12:F:657:LYS:HZ1	1.81	0.46
10:D:109:GLN:NE2	10:D:114:ALA:O	2.48	0.46
12:M:49:ILE:HG13	12:M:53:TRP:CZ3	2.49	0.46
15:N:1597:ILE:HG21	15:N:1614:LYS:HD2	1.96	0.46
15:N:1616:SER:OG	15:N:1664:ARG:NH2	2.48	0.46
15:Q:1616:SER:OG	15:Q:1664:ARG:NH2	2.48	0.46
15:Q:1795:LEU:HD13	15:Q:1816:LEU:HD22	1.97	0.46
1:2:578:ALA:HB1	1:2:591:LEU:HD22	1.97	0.46
3:4:269:ILE:O	3:4:272:MET:HB2	2.14	0.46
4:5:266:PRO:HG2	4:5:269:GLU:HG3	1.97	0.46
12:F:28:LYS:HE3	12:F:29:TYR:CE1	2.51	0.46
15:Q:2039:VAL:O	15:Q:2040:LEU:HD23	2.16	0.46
8:B:24:DT:H2''	8:B:25:DT:O5'	2.16	0.46
8:B:30:DA:H2'	8:B:31:DA:C8	2.50	0.46
12:F:420:ILE:O	12:F:424:LEU:HD13	2.15	0.46
3:4:197:PHE:HB2	3:4:254:THR:HG21	1.96	0.46
3:4:545:PHE:O	3:4:810:LYS:NZ	2.42	0.46
15:N:1450:LYS:HG3	15:N:1451:ALA:H	1.79	0.46
15:Q:1339:PHE:HD1	15:Q:1611:PRO:HB3	1.80	0.46
15:Q:1595:PRO:HA	15:Q:1618:ASN:OD1	2.16	0.46
3:4:209:LEU:HD22	3:4:250:ALA:HB2	1.98	0.46
4:5:87:ILE:O	4:5:91:GLU:HG2	2.16	0.46
5:6:645:ASP:OD2	5:6:647:SER:OG	2.24	0.46
12:F:661:PRO:HG3	12:F:673:MET:SD	2.56	0.46
12:M:28:LYS:HE3	12:M:29:TYR:CE1	2.50	0.46
12:M:476:THR:HG23	12:M:520:CYS:HA	1.98	0.46
15:N:1365:THR:HG22	15:N:1366:MET:N	2.30	0.46
3:4:607:ARG:HH21	3:4:612:LYS:HB3	1.80	0.46
5:6:335:ASN:N	5:6:335:ASN:OD1	2.49	0.46
5:6:796:THR:H	5:6:799:GLN:HG2	1.80	0.46
15:N:1887:LYS:O	15:N:1891:THR:OG1	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:2039:VAL:O	15:N:2040:LEU:HD23	2.16	0.46
15:Q:1655:TYR:OH	15:Q:1801:GLU:OE2	2.28	0.46
15:Q:1941:LEU:HD21	15:Q:2057:SER:HB2	1.97	0.46
3:4:778:ARG:HD3	3:4:793:ALA:O	2.16	0.46
6:7:63:TYR:HA	6:7:66:MET:HG2	1.98	0.46
6:7:459:MET:HG2	6:7:567:ALA:HB3	1.96	0.46
12:F:669:ARG:HH11	12:F:687:ILE:HG12	1.81	0.46
10:K:72:CYS:HB3	10:K:293:LEU:HD23	1.97	0.46
12:M:669:ARG:NH1	12:M:687:ILE:HG23	2.30	0.46
15:N:1721:ILE:O	15:N:1860:TYR:HA	2.16	0.46
15:Q:1721:ILE:O	15:Q:1860:TYR:HA	2.16	0.46
2:3:97:ILE:HG12	2:3:156:SER:HB2	1.97	0.46
3:4:251:TYR:HE2	3:4:253:GLN:HB3	1.81	0.46
6:7:70:VAL:HG22	6:7:75:LEU:HB3	1.98	0.46
10:K:131:THR:O	10:K:135:ARG:HG3	2.16	0.46
13:O:109:LEU:HD23	13:O:135:CYS:SG	2.56	0.46
15:Q:1664:ARG:NH1	15:Q:1666:ASP:HB2	2.30	0.46
1:2:783:MET:HG2	4:5:573:ILE:HG21	1.99	0.45
2:3:730:ALA:O	2:3:734:ARG:HG3	2.16	0.45
3:4:336:THR:HG22	3:4:396:VAL:H	1.81	0.45
6:7:668:ARG:HD2	6:7:684:ALA:HB3	1.98	0.45
13:H:109:LEU:HD23	13:H:135:CYS:SG	2.56	0.45
4:5:416:GLY:HA3	4:5:556:VAL:HB	1.99	0.45
6:7:360:TYR:HD1	6:7:373:GLU:HG3	1.81	0.45
12:M:669:ARG:HH11	12:M:687:ILE:HG12	1.81	0.45
15:Q:2048:LYS:HG3	15:Q:2049:ASN:N	2.31	0.45
3:4:245:ALA:HB1	3:4:258:TYR:HE1	1.82	0.45
12:F:650:ASP:OD1	12:F:650:ASP:N	2.48	0.45
15:N:1634:LYS:HD2	15:N:1634:LYS:HA	1.76	0.45
14:P:102:ILE:O	14:P:106:LYS:HG2	2.17	0.45
15:Q:1691:GLU:OE2	15:Q:1692:LYS:HG2	2.17	0.45
7:A:24:DT:H2''	7:A:25:DT:O5'	2.16	0.45
10:D:131:THR:O	10:D:135:ARG:HG3	2.16	0.45
12:F:476:THR:HG23	12:F:520:CYS:HA	1.98	0.45
13:H:44:VAL:HG23	13:H:79:MET:HG2	1.99	0.45
13:H:167:VAL:HG21	13:H:184:ILE:O	2.17	0.45
14:I:102:ILE:O	14:I:106:LYS:HG2	2.17	0.45
11:L:231:HIS:HA	11:L:234:GLU:HG2	1.99	0.45
15:N:1941:LEU:HD21	15:N:2057:SER:HB2	1.97	0.45
15:Q:2213:LEU:O	15:Q:2217:ILE:HG12	2.16	0.45
5:6:516:LEU:HD21	5:6:757:TYR:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:728:ALA:O	5:6:732:VAL:HG12	2.16	0.45
11:L:50:LYS:HB2	11:L:50:LYS:HE3	1.78	0.45
11:L:539:TYR:HB3	11:L:545:LEU:HD13	1.98	0.45
13:O:167:VAL:HG21	13:O:184:ILE:O	2.17	0.45
3:4:508:LYS:HA	3:4:511:GLU:HG2	1.99	0.45
4:5:104:LEU:HD12	14:I:158:LYS:NZ	2.31	0.45
6:7:149:ARG:NH1	6:7:267:TYR:HB3	2.32	0.45
12:F:181:PHE:CD1	12:F:192:PHE:HA	2.52	0.45
11:L:553:ILE:HD11	11:L:584:LEU:HB3	1.99	0.45
1:2:253:LYS:HB3	1:2:256:LEU:HD12	1.98	0.45
3:4:522:LEU:HA	3:4:525:SER:OG	2.17	0.45
3:4:704:LEU:HD11	3:4:804:LEU:HD21	1.99	0.45
4:5:254:GLN:HB3	4:5:278:CYS:SG	2.56	0.45
6:7:503:THR:HG23	6:7:505:GLU:HG2	1.99	0.45
6:7:686:PRO:O	6:7:690:LEU:HG	2.17	0.45
9:C:162:THR:O	9:C:166:LEU:HG	2.17	0.45
11:E:553:ILE:HD11	11:E:584:LEU:HB3	1.99	0.45
12:M:503:LEU:HD12	12:M:622:ILE:HG12	1.99	0.45
12:M:650:ASP:OD1	12:M:650:ASP:N	2.48	0.45
12:M:661:PRO:HG3	12:M:673:MET:SD	2.56	0.45
3:4:632:ASP:OD2	3:4:633:GLU:N	2.50	0.45
4:5:92:THR:HA	4:5:95:THR:HG22	1.99	0.45
15:N:2213:LEU:O	15:N:2217:ILE:HG12	2.16	0.45
14:P:96:LYS:O	14:P:100:ARG:HG3	2.17	0.45
1:2:763:LEU:O	1:2:767:ILE:HG13	2.17	0.45
3:4:608:ASP:HB2	3:4:615:VAL:HG23	1.99	0.45
4:5:246:GLU:O	4:5:247:SER:OG	2.32	0.45
5:6:332:PHE:O	5:6:332:PHE:CD1	2.70	0.45
6:7:662:GLN:HA	6:7:665:ILE:HG12	1.98	0.45
12:F:184:ASN:HD22	12:F:187:LYS:HE2	1.80	0.45
12:F:452:ILE:HG13	12:F:456:THR:OG1	2.17	0.45
10:K:54:VAL:HG12	10:K:54:VAL:O	2.16	0.45
15:N:2048:LYS:HG3	15:N:2049:ASN:N	2.31	0.45
14:P:151:ILE:HA	14:P:154:ILE:HD12	1.99	0.45
15:Q:1887:LYS:O	15:Q:1891:THR:OG1	2.26	0.45
3:4:203:TYR:HB2	3:4:220:THR:O	2.17	0.45
11:E:539:TYR:HB3	11:E:545:LEU:HD13	1.98	0.45
12:F:435:GLN:HG2	12:F:436:GLY:N	2.32	0.45
12:M:435:GLN:HG2	12:M:436:GLY:N	2.32	0.45
15:N:1454:ALA:O	15:N:1458:GLY:N	2.44	0.45
4:5:407:ARG:HH21	4:5:658:ARG:NH1	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:54:VAL:HG12	10:D:54:VAL:O	2.16	0.44
14:I:151:ILE:HA	14:I:154:ILE:HD12	1.99	0.44
5:6:109:GLU:O	5:6:113:GLU:HG2	2.16	0.44
6:7:531:GLU:HA	6:7:534:ARG:HB2	1.99	0.44
14:I:96:LYS:O	14:I:100:ARG:HG3	2.17	0.44
9:J:162:THR:O	9:J:166:LEU:HG	2.17	0.44
10:K:141:ARG:HD3	13:O:150:ASP:O	2.17	0.44
10:K:192:LYS:HB2	10:K:192:LYS:HE3	1.83	0.44
12:M:363:ASP:HB3	12:M:366:GLY:HA2	1.98	0.44
1:2:656:ARG:NH2	5:6:793:TYR:CZ	2.85	0.44
2:3:413:THR:O	2:3:413:THR:HG22	2.16	0.44
3:4:417:LEU:HD23	3:4:463:VAL:HG11	1.98	0.44
3:4:505:ASP:HA	3:4:508:LYS:HG2	1.99	0.44
4:5:707:SER:HA	4:5:710:GLU:HB2	1.99	0.44
6:7:260:TYR:O	6:7:268:GLU:HA	2.17	0.44
6:7:635:PRO:O	6:7:638:MET:HB2	2.18	0.44
6:7:693:ILE:O	6:7:697:GLN:HG2	2.18	0.44
10:D:141:ARG:HD3	13:H:150:ASP:O	2.17	0.44
11:E:103:TYR:O	11:E:117:ARG:N	2.50	0.44
11:E:231:HIS:HA	11:E:234:GLU:HG2	1.99	0.44
12:F:503:LEU:HD12	12:F:622:ILE:HG12	1.99	0.44
15:N:1691:GLU:OE2	15:N:1692:LYS:HG2	2.17	0.44
13:O:44:VAL:HG23	13:O:79:MET:HG2	1.99	0.44
1:2:234:LEU:HG	1:2:239:SER:HB3	1.99	0.44
5:6:367:GLU:N	5:6:367:GLU:OE2	2.50	0.44
6:7:282:SER:HB3	6:7:297:GLN:HB2	2.00	0.44
12:F:363:ASP:HB3	12:F:366:GLY:HA2	1.99	0.44
12:M:396:ASP:OD1	12:M:397:HIS:N	2.51	0.44
2:3:459:ALA:HB1	2:3:463:VAL:HG23	2.00	0.44
3:4:776:GLY:HA2	3:4:779:LYS:HG2	1.98	0.44
6:7:217:LYS:HE2	6:7:217:LYS:HA	1.99	0.44
12:F:345:THR:HG22	12:F:346:LEU:N	2.32	0.44
12:F:503:LEU:HD13	12:F:630:LEU:HD13	1.99	0.44
10:K:126:LEU:HA	10:K:129:MET:HG2	2.00	0.44
11:L:27:LEU:HD12	11:L:80:SER:HB2	2.00	0.44
11:L:129:TRP:CD2	11:L:134:ILE:HD11	2.53	0.44
12:M:181:PHE:CD1	12:M:192:PHE:HA	2.52	0.44
1:2:437:ASN:OD1	5:6:416:LYS:HB3	2.18	0.44
5:6:112:ARG:NH1	5:6:187:ARG:HH12	2.16	0.44
5:6:332:PHE:O	5:6:332:PHE:CG	2.70	0.44
11:E:431:LEU:HD23	11:E:431:LEU:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:14:PRO:N	12:F:15:PRO:HD2	2.33	0.44
12:M:452:ILE:HG13	12:M:456:THR:OG1	2.17	0.44
15:N:1863:ARG:HE	15:N:1863:ARG:HB3	1.63	0.44
3:4:227:ILE:HD11	3:4:283:LEU:HD21	1.99	0.44
3:4:234:ARG:HH21	3:4:291:TYR:HB3	1.83	0.44
3:4:413:HIS:CE1	6:7:250:ASP:HB3	2.52	0.44
3:4:775:VAL:HG21	5:6:725:THR:HG22	2.00	0.44
11:E:326:LEU:HB3	11:E:337:SER:HB3	2.00	0.44
11:L:326:LEU:HB3	11:L:337:SER:HB3	2.00	0.44
15:N:1696:PRO:HG3	15:N:1828:PHE:O	2.18	0.44
15:Q:1656:SER:HB3	15:Q:1658:ILE:HD12	2.00	0.44
2:3:733:LEU:HD21	2:3:737:LEU:HD12	1.99	0.44
2:3:735:PHE:CD2	2:3:741:ASP:HB3	2.53	0.44
19:6:1201:ADP:H8	19:6:1201:ADP:H2'	1.76	0.44
11:E:50:LYS:HB2	11:E:50:LYS:HE3	1.78	0.44
10:K:109:GLN:NE2	10:K:114:ALA:O	2.48	0.44
11:L:431:LEU:HD11	11:L:491:LEU:HG	2.00	0.44
12:M:86:GLU:O	12:M:90:GLU:HG3	2.18	0.44
12:M:220:THR:O	12:M:224:LEU:HD23	2.18	0.44
3:4:264:TYR:HA	6:7:303:ARG:HH22	1.83	0.44
9:C:194:LYS:HD3	9:C:194:LYS:HA	1.80	0.44
2:3:276:VAL:HG11	2:3:294:VAL:HG11	1.99	0.43
3:4:451:ARG:HH22	6:7:282:SER:HB2	1.83	0.43
11:E:129:TRP:CD2	11:E:134:ILE:HD11	2.53	0.43
12:F:396:ASP:OD1	12:F:397:HIS:N	2.51	0.43
12:M:402:LEU:HD13	12:M:434:TRP:HD1	1.81	0.43
3:4:819:LEU:HD12	3:4:819:LEU:H	1.82	0.43
4:5:760:THR:HG22	4:5:761:ILE:HG12	2.00	0.43
5:6:821:PRO:HA	5:6:824:ILE:HD13	2.01	0.43
6:7:117:PHE:O	6:7:121:ILE:HG12	2.18	0.43
6:7:360:TYR:CD1	6:7:373:GLU:HG3	2.53	0.43
11:E:434:VAL:HG23	11:E:498:LEU:HD13	2.00	0.43
12:F:402:LEU:HD13	12:F:434:TRP:HD1	1.81	0.43
12:M:181:PHE:HD1	12:M:192:PHE:HA	1.83	0.43
15:Q:1371:ILE:HG13	15:Q:1372:LYS:HG3	2.00	0.43
1:2:458:ARG:HE	1:2:460:GLU:HB3	1.83	0.43
3:4:418:CYS:O	3:4:463:VAL:HG22	2.18	0.43
6:7:634:GLU:OE1	6:7:636:SER:HB2	2.19	0.43
10:D:82:GLN:O	10:D:86:ARG:HG3	2.18	0.43
11:E:27:LEU:HD12	11:E:80:SER:HB2	2.00	0.43
12:F:49:ILE:HG13	12:F:53:TRP:HZ3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:49:ILE:HG13	12:M:53:TRP:HZ3	1.83	0.43
13:O:107:LEU:HD23	13:O:108:ASP:N	2.33	0.43
4:5:207:LEU:HD23	4:5:241:TYR:HB3	2.01	0.43
4:5:650:ILE:HD12	4:5:650:ILE:H	1.83	0.43
5:6:122:PHE:O	5:6:124:VAL:HG23	2.18	0.43
5:6:538:PHE:H	19:6:1201:ADP:N6	2.16	0.43
6:7:363:PHE:CD1	7:A:36:DA:H1'	2.52	0.43
6:7:451:ARG:HD2	6:7:453:ASP:HB2	2.01	0.43
10:D:274:ILE:HB	14:I:170:LEU:O	2.18	0.43
12:F:181:PHE:HD1	12:F:192:PHE:HA	1.84	0.43
12:F:220:THR:O	12:F:224:LEU:HD23	2.18	0.43
15:N:1402:LEU:HD21	15:N:1406:VAL:HG23	2.00	0.43
14:P:64:VAL:HG21	14:P:67:ARG:HE	1.83	0.43
1:2:707:HIS:CE1	1:2:709:GLU:HB2	2.53	0.43
3:4:224:LEU:HB3	3:4:227:ILE:HG22	1.99	0.43
5:6:594:ARG:HG3	5:6:594:ARG:HH11	1.83	0.43
10:K:274:ILE:HB	14:P:170:LEU:O	2.18	0.43
11:L:434:VAL:HG23	11:L:498:LEU:HD13	2.01	0.43
15:N:1328:LYS:O	15:N:1337:GLU:N	2.51	0.43
15:N:1905:TYR:HB2	15:N:1922:CYS:SG	2.59	0.43
15:Q:1905:TYR:HB2	15:Q:1922:CYS:SG	2.59	0.43
15:Q:2009:LYS:HB3	15:Q:2010:PRO:HD3	2.00	0.43
4:5:99:LYS:HG2	4:5:132:LEU:HD12	2.01	0.43
10:D:126:LEU:HA	10:D:129:MET:HG2	2.00	0.43
15:N:1656:SER:HB3	15:N:1658:ILE:HD12	2.00	0.43
15:Q:1368:LEU:HB3	15:Q:1370:LYS:NZ	2.34	0.43
15:Q:1656:SER:HB3	15:Q:1658:ILE:CD1	2.49	0.43
1:2:534:ARG:NH2	1:2:625:GLU:OE1	2.51	0.43
4:5:726:TRP:HB3	15:Q:1779:VAL:HG13	2.00	0.43
5:6:333:CYS:CB	5:6:334:PRO:HD2	2.47	0.43
6:7:608:ASP:O	6:7:611:LYS:HG2	2.18	0.43
11:E:132:ASP:OD1	11:E:159:TYR:OH	2.24	0.43
10:K:189:ILE:HG22	13:O:130:TYR:CD2	2.54	0.43
12:M:503:LEU:HD13	12:M:630:LEU:HD13	1.99	0.43
13:O:47:LEU:O	13:O:51:THR:HG23	2.18	0.43
15:Q:1863:ARG:HE	15:Q:1863:ARG:HB3	1.62	0.43
1:2:577:THR:HG22	1:2:578:ALA:N	2.31	0.43
3:4:403:PRO:O	3:4:406:VAL:HG12	2.18	0.43
3:4:728:TYR:OH	6:7:690:LEU:HD22	2.19	0.43
5:6:333:CYS:CB	5:6:334:PRO:CD	2.89	0.43
7:A:11:DT:H3	8:B:43:DA:H61	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:318:HIS:NE2	12:F:320:TYR:OH	2.49	0.43
13:H:47:LEU:O	13:H:51:THR:HG23	2.18	0.43
14:I:103:GLN:O	14:I:107:THR:HG23	2.19	0.43
15:N:2081:LYS:HB2	15:N:2081:LYS:HE2	1.87	0.43
1:2:304:TYR:HD2	1:2:308:GLU:HG3	1.84	0.43
1:2:342:LEU:HD12	1:2:343:LYS:N	2.33	0.43
1:2:353:GLN:HG2	1:2:355:SER:H	1.84	0.43
2:3:674:GLU:OE1	2:3:723:LYS:HB2	2.18	0.43
3:4:444:ILE:HG13	3:4:454:LYS:HZ3	1.83	0.43
3:4:644:VAL:O	3:4:647:GLU:HG2	2.19	0.43
5:6:720:ASN:OD1	5:6:723:ILE:HB	2.19	0.43
6:7:440:VAL:HG12	6:7:697:GLN:HG3	2.01	0.43
10:K:132:GLU:OE2	14:P:54:THR:N	2.48	0.43
15:N:1656:SER:HB3	15:N:1658:ILE:CD1	2.49	0.43
15:N:2004:SER:HA	15:N:2007:PHE:CE1	2.54	0.43
15:Q:1696:PRO:HG3	15:Q:1828:PHE:O	2.18	0.43
3:4:280:MET:O	3:4:284:ILE:HG23	2.18	0.43
13:H:107:LEU:HD23	13:H:108:ASP:N	2.33	0.43
9:J:194:LYS:HA	9:J:194:LYS:HD3	1.80	0.43
12:M:14:PRO:N	12:M:15:PRO:HD2	2.33	0.43
14:P:3:LEU:HA	14:P:8:GLN:OE1	2.19	0.43
3:4:602:THR:HB	3:4:654:ILE:HG21	2.01	0.42
4:5:40:LEU:HD23	4:5:40:LEU:HA	1.89	0.42
4:5:415:LEU:O	4:5:555:ILE:HA	2.19	0.42
5:6:752:ARG:HG3	5:6:752:ARG:HH11	1.83	0.42
7:A:43:DA:H61	8:B:11:DT:H3	1.66	0.42
1:2:564:VAL:HG23	1:2:599:ALA:HB2	2.01	0.42
6:7:494:THR:HB	6:7:548:ILE:HD12	2.01	0.42
9:C:174:LYS:HE2	9:C:174:LYS:HB3	1.78	0.42
12:F:86:GLU:O	12:F:90:GLU:HG3	2.18	0.42
15:N:1371:ILE:HG13	15:N:1372:LYS:HG3	2.00	0.42
15:Q:1669:ASP:HB2	15:Q:1819:TRP:HD1	1.84	0.42
1:2:486:LYS:HA	1:2:489:ARG:NH1	2.34	0.42
1:2:803:PHE:HD1	1:2:804:PRO:HD2	1.84	0.42
4:5:276:MET:HA	4:5:328:ILE:O	2.19	0.42
11:E:29:ILE:HG12	11:E:82:LEU:HD12	2.01	0.42
12:F:28:LYS:HE3	12:F:29:TYR:HE1	1.84	0.42
10:K:82:GLN:O	10:K:86:ARG:HG3	2.18	0.42
12:M:318:HIS:NE2	12:M:320:TYR:OH	2.49	0.42
12:M:399:PHE:HB2	12:M:431:LEU:HB2	2.02	0.42
15:N:2009:LYS:HB3	15:N:2010:PRO:HD3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:2193:SER:O	15:N:2197:LYS:HG3	2.19	0.42
13:O:105:ASN:OD1	13:O:152:SER:OG	2.25	0.42
15:Q:1402:LEU:HD21	15:Q:1406:VAL:HG23	2.00	0.42
15:Q:1681:LYS:HE2	15:Q:1687:LEU:HD11	2.01	0.42
1:2:300:PHE:HB3	1:2:319:ARG:HD2	2.02	0.42
4:5:72:ASN:HB3	4:5:75:ILE:HD12	2.01	0.42
5:6:722:LYS:O	5:6:725:THR:OG1	2.29	0.42
6:7:422:ILE:HD13	6:7:469:LEU:HD22	2.01	0.42
14:I:3:LEU:HA	14:I:8:GLN:OE1	2.19	0.42
14:P:103:GLN:O	14:P:107:THR:HG23	2.19	0.42
3:4:779:LYS:HB3	3:4:779:LYS:HE3	1.75	0.42
6:7:130:LYS:NZ	6:7:131:GLU:OE1	2.34	0.42
6:7:414:LEU:HD23	6:7:638:MET:SD	2.59	0.42
6:7:469:LEU:HD13	6:7:469:LEU:HA	1.77	0.42
15:N:1368:LEU:HB3	15:N:1370:LYS:NZ	2.34	0.42
6:7:286:SER:HB2	6:7:289:CYS:SG	2.58	0.42
6:7:508:LEU:HD11	6:7:548:ILE:HG12	2.01	0.42
10:D:189:ILE:HG22	13:H:130:TYR:CD2	2.54	0.42
12:F:7:VAL:HG23	12:F:8:LEU:N	2.35	0.42
13:H:13:ALA:HB2	13:H:89:TYR:HD1	1.85	0.42
15:Q:1679:LYS:HD3	15:Q:1794:MET:CE	2.49	0.42
15:Q:2004:SER:HA	15:Q:2007:PHE:CE1	2.54	0.42
1:2:327:ARG:NH1	1:2:420:PRO:HD3	2.35	0.42
1:2:692:ASP:OD1	5:6:781:ARG:NH2	2.52	0.42
2:3:28:PHE:O	2:3:32:LEU:HD23	2.20	0.42
3:4:341:ASP:OD2	5:6:435:SER:OG	2.29	0.42
4:5:442:LYS:HD2	4:5:442:LYS:HA	1.80	0.42
6:7:64:MET:HA	6:7:67:LEU:HD12	2.01	0.42
6:7:542:GLU:OE2	6:7:593:ARG:NH2	2.52	0.42
11:E:431:LEU:HD11	11:E:491:LEU:HG	2.00	0.42
12:F:199:ASN:OD1	12:F:200:GLY:N	2.53	0.42
9:J:38:ILE:HD12	9:J:38:ILE:HA	1.88	0.42
11:L:161:LYS:HB3	11:L:161:LYS:HE3	1.68	0.42
15:N:1669:ASP:HB2	15:N:1819:TRP:HD1	1.84	0.42
15:Q:2193:SER:O	15:Q:2197:LYS:HG3	2.19	0.42
3:4:258:TYR:O	3:4:262:LEU:HD13	2.19	0.42
12:F:399:PHE:CE1	12:F:677:PRO:HG3	2.53	0.42
14:I:64:VAL:HG21	14:I:67:ARG:HE	1.83	0.42
15:N:1916:ASN:HB3	15:N:1939:TRP:CZ3	2.55	0.42
1:2:615:GLN:O	4:5:442:LYS:NZ	2.48	0.42
1:2:756:SER:OG	1:2:758:ILE:O	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:196:ASN:O	3:4:200:SER:CB	2.67	0.42
3:4:293:LEU:HA	3:4:296:ILE:HD12	2.02	0.42
7:A:14:DT:H5''	7:A:14:DT:O2	2.20	0.42
10:D:260:ILE:O	10:D:264:LYS:N	2.53	0.42
10:K:79:TYR:CZ	10:K:84:MET:HG3	2.55	0.42
11:L:156:LYS:HZ1	11:L:160:TYR:HE2	1.67	0.42
11:L:394:LYS:HG3	11:L:395:ASN:OD1	2.20	0.42
15:N:1681:LYS:HE2	15:N:1687:LEU:HD11	2.01	0.42
2:3:678:VAL:O	2:3:681:LYS:HG2	2.20	0.42
3:4:365:ILE:HD11	5:6:437:VAL:HB	2.02	0.42
3:4:824:GLU:OE1	3:4:827:ARG:NH2	2.53	0.42
4:5:149:ARG:NH2	4:5:260:GLU:OE2	2.52	0.42
6:7:282:SER:HA	6:7:298:LEU:HB2	2.02	0.42
11:E:394:LYS:HG3	11:E:395:ASN:OD1	2.20	0.42
12:F:399:PHE:HB2	12:F:431:LEU:HB2	2.02	0.42
12:M:199:ASN:OD1	12:M:200:GLY:N	2.53	0.42
3:4:581:VAL:HG11	3:4:672:LEU:HD23	2.01	0.41
4:5:639:GLU:HG2	4:5:746:LEU:HD11	2.01	0.41
11:E:128:PRO:HD2	11:E:245:THR:HG22	2.02	0.41
13:H:105:ASN:OD1	13:H:152:SER:OG	2.26	0.41
10:K:203:PRO:HG3	13:O:48:ARG:HG2	2.01	0.41
10:K:260:ILE:O	10:K:264:LYS:N	2.53	0.41
11:L:103:TYR:O	11:L:117:ARG:N	2.50	0.41
15:Q:1330:SER:OG	15:Q:1331:GLY:N	2.53	0.41
1:2:761:GLU:HG2	1:2:762:LEU:N	2.35	0.41
2:3:138:ASP:OD1	2:3:139:VAL:N	2.53	0.41
3:4:435:VAL:HG12	3:4:466:VAL:HG13	2.01	0.41
5:6:350:ARG:HE	5:6:350:ARG:HB2	1.67	0.41
10:D:203:PRO:HG3	13:H:48:ARG:HG2	2.01	0.41
12:F:169:TYR:CE1	12:F:367:ILE:HG22	2.55	0.41
11:L:235:GLY:O	11:L:238:GLU:HG2	2.20	0.41
15:N:2141:LEU:HD23	15:N:2141:LEU:HA	1.80	0.41
15:Q:1616:SER:H	15:Q:1664:ARG:HH21	1.68	0.41
3:4:767:LYS:O	3:4:771:VAL:HG23	2.19	0.41
15:Q:1916:ASN:HB3	15:Q:1939:TRP:CZ3	2.54	0.41
2:3:448:THR:HG22	2:3:455:ARG:HG2	2.02	0.41
4:5:385:LYS:O	4:5:389:VAL:HG23	2.21	0.41
5:6:438:THR:HB	5:6:447:ASP:OD1	2.20	0.41
6:7:146:ARG:CZ	6:7:149:ARG:HD3	2.50	0.41
8:B:23:DT:H2''	8:B:24:DT:O5'	2.20	0.41
12:F:386:ARG:HE	12:F:535:LEU:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:28:LYS:HE3	12:M:29:TYR:HE1	1.84	0.41
12:M:85:LYS:HA	12:M:88:ILE:HD12	2.03	0.41
1:2:180:GLU:N	1:2:180:GLU:OE2	2.54	0.41
6:7:20:GLU:OE1	6:7:100:ASP:HB2	2.20	0.41
11:E:286:GLN:H	11:E:286:GLN:CD	2.24	0.41
11:L:29:ILE:HG12	11:L:82:LEU:HD12	2.01	0.41
12:M:7:VAL:HG23	12:M:8:LEU:N	2.35	0.41
12:M:653:TYR:O	12:M:655:GLY:N	2.54	0.41
15:Q:1328:LYS:O	15:Q:1337:GLU:N	2.51	0.41
15:Q:1391:ASN:HA	15:Q:1392:PRO:HD3	1.96	0.41
15:Q:1794:MET:O	15:Q:1797:GLU:HG2	2.21	0.41
5:6:586:LYS:HA	5:6:589:VAL:HG12	2.02	0.41
6:7:607:ASP:O	6:7:611:LYS:HE3	2.20	0.41
10:D:79:TYR:CZ	10:D:84:MET:HG3	2.55	0.41
11:E:421:ALA:O	11:E:425:VAL:HG13	2.21	0.41
11:E:598:LYS:HG2	11:E:599:LYS:N	2.35	0.41
12:F:83:GLY:O	12:F:87:VAL:HG13	2.21	0.41
12:M:650:ASP:HB2	12:M:657:LYS:HZ1	1.86	0.41
13:O:137:LEU:O	13:O:141:LEU:HG	2.21	0.41
15:Q:1358:TYR:CD2	15:Q:1397:LEU:HD21	2.56	0.41
15:Q:2130:CYS:SG	15:Q:2131:VAL:N	2.94	0.41
3:4:572:THR:OG1	3:4:573:SER:N	2.54	0.41
6:7:366:LEU:HD23	6:7:366:LEU:HA	1.92	0.41
6:7:600:MET:HE2	6:7:600:MET:HB2	1.92	0.41
6:7:669:GLN:O	6:7:672:LYS:HG2	2.21	0.41
9:C:133:GLN:H	9:C:133:GLN:HG2	1.71	0.41
12:M:83:GLY:O	12:M:87:VAL:HG13	2.21	0.41
15:N:1358:TYR:CD2	15:N:1397:LEU:HD21	2.56	0.41
15:N:1730:VAL:HG23	15:N:1870:THR:HB	2.03	0.41
1:2:364:CYS:HB3	1:2:367:CYS:H	1.86	0.41
2:3:192:VAL:O	2:3:193:ARG:HD2	2.20	0.41
2:3:698:THR:CG2	2:3:699:ALA:H	2.33	0.41
3:4:565:LEU:HB2	3:4:702:PHE:CD2	2.56	0.41
4:5:464:LEU:HD21	4:5:504:ILE:HG21	2.02	0.41
11:E:161:LYS:HE3	11:E:161:LYS:HB3	1.68	0.41
11:L:128:PRO:HD2	11:L:245:THR:HG22	2.02	0.41
11:L:255:ILE:O	11:L:259:LEU:HG	2.21	0.41
12:M:7:VAL:HG23	12:M:8:LEU:H	1.86	0.41
13:O:107:LEU:HD23	13:O:109:LEU:N	2.36	0.41
13:O:181:PHE:CZ	13:O:191:VAL:HG21	2.56	0.41
2:3:122:ILE:HB	2:3:123:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:601:LEU:HA	3:4:620:ALA:H	1.86	0.41
3:4:711:LYS:HD3	3:4:712:VAL:N	2.33	0.41
5:6:440:LEU:HD12	5:6:440:LEU:HA	1.88	0.41
6:7:531:GLU:HG3	6:7:534:ARG:HD2	2.03	0.41
11:E:318:LEU:HD23	11:E:318:LEU:HA	1.91	0.41
12:F:37:GLY:O	12:F:41:LEU:HD23	2.21	0.41
12:F:57:PRO:O	12:F:61:LYS:HG2	2.21	0.41
12:F:185:PRO:HG3	12:F:223:TYR:CE2	2.56	0.41
13:H:137:LEU:O	13:H:141:LEU:HG	2.21	0.41
13:H:165:VAL:HG23	13:H:189:PHE:HB2	2.03	0.41
9:J:115:PHE:O	9:J:117:GLU:HG3	2.21	0.41
11:L:431:LEU:HD23	11:L:431:LEU:HA	1.86	0.41
12:M:169:TYR:CE1	12:M:367:ILE:HG22	2.55	0.41
12:M:607:LEU:HD23	12:M:607:LEU:HA	1.80	0.41
15:N:1482:MET:HE1	15:N:1588:PHE:HA	2.03	0.41
15:N:1691:GLU:HA	15:N:1826:LYS:HE3	2.03	0.41
15:N:1957:MET:SD	15:N:2061:VAL:HG11	2.61	0.41
13:O:165:VAL:HG23	13:O:189:PHE:HB2	2.03	0.41
15:Q:1336:LEU:HD23	15:Q:1336:LEU:HA	1.92	0.41
15:Q:1634:LYS:HD2	15:Q:1634:LYS:HA	1.77	0.41
15:Q:1691:GLU:HA	15:Q:1826:LYS:HE3	2.03	0.41
15:Q:1730:VAL:HG23	15:Q:1870:THR:HB	2.03	0.41
1:2:601:LYS:HE3	1:2:643:ARG:HH21	1.86	0.41
3:4:623:LEU:HD23	3:4:623:LEU:HA	1.91	0.41
4:5:263:GLU:HG3	4:5:264:LEU:HD12	2.02	0.41
4:5:730:TYR:CE2	12:F:293:LYS:HG2	2.56	0.41
5:6:629:MET:SD	5:6:672:LEU:HD13	2.62	0.41
6:7:578:LEU:HD13	6:7:677:SER:HB2	2.03	0.41
8:B:14:DT:H5"	8:B:14:DT:O2	2.20	0.41
13:H:181:PHE:CZ	13:H:191:VAL:HG21	2.56	0.41
11:L:421:ALA:O	11:L:425:VAL:HG13	2.21	0.41
12:M:653:TYR:CG	12:M:654:ASN:N	2.88	0.41
2:3:212:ARG:NH1	2:3:232:PRO:HG3	2.36	0.40
3:4:333:LEU:HD11	3:4:400:GLN:OE1	2.21	0.40
3:4:337:PRO:HA	5:6:375:ARG:HH12	1.86	0.40
3:4:761:ILE:HG13	3:4:816:VAL:HG23	2.03	0.40
9:C:115:PHE:O	9:C:117:GLU:HG3	2.21	0.40
11:L:286:GLN:CD	11:L:286:GLN:H	2.24	0.40
12:M:57:PRO:O	12:M:61:LYS:HG2	2.21	0.40
12:M:386:ARG:HE	12:M:535:LEU:HD22	1.85	0.40
13:O:13:ALA:HB2	13:O:89:TYR:HD1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:2081:LYS:HB2	15:Q:2081:LYS:HE2	1.87	0.40
1:2:703:HIS:CE1	5:6:565:LEU:HD13	2.56	0.40
2:3:524:ASP:OD2	2:3:527:ARG:NH2	2.34	0.40
2:3:653:ILE:HD12	2:3:653:ILE:H	1.86	0.40
3:4:206:ARG:HH12	3:4:246:ARG:HG2	1.86	0.40
3:4:430:GLY:HA3	6:7:553:ILE:O	2.20	0.40
3:4:545:PHE:HE1	3:4:751:ILE:HG12	1.85	0.40
3:4:558:TYR:HD2	5:6:735:HIS:CE1	2.39	0.40
6:7:226:SER:HB3	6:7:321:GLN:NE2	2.36	0.40
10:D:132:GLU:OE2	14:I:54:THR:N	2.48	0.40
11:E:235:GLY:O	11:E:238:GLU:HG2	2.20	0.40
12:F:20:LEU:HD22	12:F:23:ARG:NH2	2.36	0.40
12:F:653:TYR:CG	12:F:654:ASN:N	2.88	0.40
12:F:653:TYR:O	12:F:655:GLY:N	2.54	0.40
11:L:598:LYS:HG2	11:L:599:LYS:N	2.35	0.40
15:N:1690:ASN:ND2	15:N:1695:LEU:O	2.51	0.40
14:P:85:CYS:SG	14:P:86:SER:N	2.95	0.40
2:3:384:MET:HB2	2:3:384:MET:HE2	1.95	0.40
6:7:570:LEU:HG	6:7:584:ILE:HA	2.03	0.40
11:E:312:THR:OG1	11:E:315:THR:HG23	2.22	0.40
15:N:1655:TYR:OH	15:N:1801:GLU:OE2	2.28	0.40
15:N:1794:MET:O	15:N:1797:GLU:HG2	2.21	0.40
14:P:33:THR:OG1	14:P:63:MET:HB2	2.22	0.40
3:4:257:LEU:HD23	3:4:257:LEU:HA	1.93	0.40
3:4:566:LEU:HD23	3:4:706:TYR:HB2	2.04	0.40
3:4:687:PRO:HG2	3:4:690:GLU:OE1	2.21	0.40
5:6:178:LEU:HB3	5:6:179:PRO:HD3	2.03	0.40
11:E:113:GLU:HB3	11:E:114:GLN:H	1.73	0.40
12:F:7:VAL:HG23	12:F:8:LEU:H	1.85	0.40
12:F:85:LYS:HA	12:F:88:ILE:HD12	2.02	0.40
11:L:26:GLN:HE21	11:L:26:GLN:HB2	1.63	0.40
15:N:2130:CYS:SG	15:N:2131:VAL:N	2.94	0.40
15:Q:1665:LEU:HD23	15:Q:1665:LEU:HA	1.83	0.40
3:4:296:ILE:HA	3:4:299:LYS:HG2	2.03	0.40
5:6:368:ILE:HG23	5:6:372:SER:HB3	2.04	0.40
6:7:634:GLU:HA	6:7:635:PRO:HD3	2.00	0.40
14:I:85:CYS:SG	14:I:86:SER:N	2.95	0.40
11:L:161:LYS:HA	11:L:164:GLU:HG3	2.03	0.40
12:M:25:LEU:HB2	12:M:33:ILE:HD11	2.04	0.40
12:M:37:GLY:O	12:M:41:LEU:HD23	2.21	0.40
12:M:448:SER:HB2	12:M:450:ARG:HH21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Q:1622:LEU:HA	15:Q:1622:LEU:HD23	1.82	0.40
15:Q:1718:PHE:HE2	15:Q:1844:LEU:HD23	1.87	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	656/868 (76%)	642 (98%)	14 (2%)	0	100	100
1	a	656/868 (76%)	641 (98%)	15 (2%)	0	100	100
2	3	625/1006 (62%)	609 (97%)	16 (3%)	0	100	100
2	b	625/1006 (62%)	609 (97%)	16 (3%)	0	100	100
3	4	601/933 (64%)	579 (96%)	22 (4%)	0	100	100
3	c	601/933 (64%)	579 (96%)	22 (4%)	0	100	100
4	5	680/775 (88%)	653 (96%)	27 (4%)	0	100	100
4	d	680/775 (88%)	653 (96%)	27 (4%)	0	100	100
5	6	619/1017 (61%)	594 (96%)	22 (4%)	3 (0%)	29	61
5	e	619/1017 (61%)	596 (96%)	22 (4%)	1 (0%)	47	78
6	7	650/845 (77%)	614 (94%)	36 (6%)	0	100	100
6	f	650/845 (77%)	614 (94%)	36 (6%)	0	100	100
9	C	167/229 (73%)	164 (98%)	3 (2%)	0	100	100
9	J	167/229 (73%)	164 (98%)	3 (2%)	0	100	100
10	D	240/294 (82%)	231 (96%)	9 (4%)	0	100	100
10	K	240/294 (82%)	231 (96%)	9 (4%)	0	100	100
11	E	558/657 (85%)	546 (98%)	12 (2%)	0	100	100
11	L	558/657 (85%)	546 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	F	543/689 (79%)	510 (94%)	33 (6%)	0	100	100
12	M	543/689 (79%)	510 (94%)	33 (6%)	0	100	100
13	H	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
13	O	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
14	I	185/213 (87%)	174 (94%)	11 (6%)	0	100	100
14	P	185/213 (87%)	174 (94%)	11 (6%)	0	100	100
15	N	748/2222 (34%)	716 (96%)	32 (4%)	0	100	100
15	Q	748/2222 (34%)	715 (96%)	33 (4%)	0	100	100
All	All	12956/19912 (65%)	12454 (96%)	498 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	6	334	PRO
5	6	336	PRO
5	e	337	SER
5	6	335	ASN

### 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	578/770 (75%)	578 (100%)	0	100	100
1	a	578/770 (75%)	578 (100%)	0	100	100
2	3	549/864 (64%)	549 (100%)	0	100	100
2	b	549/864 (64%)	549 (100%)	0	100	100
3	4	551/848 (65%)	551 (100%)	0	100	100
3	c	551/848 (65%)	551 (100%)	0	100	100
4	5	618/688 (90%)	618 (100%)	0	100	100
4	d	618/688 (90%)	618 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	6	549/886 (62%)	544 (99%)	5 (1%)	78	90
5	e	549/886 (62%)	545 (99%)	4 (1%)	84	92
6	7	580/753 (77%)	577 (100%)	3 (0%)	88	94
6	f	580/753 (77%)	577 (100%)	3 (0%)	88	94
9	C	157/199 (79%)	157 (100%)	0	100	100
9	J	157/199 (79%)	157 (100%)	0	100	100
10	D	232/279 (83%)	232 (100%)	0	100	100
10	K	232/279 (83%)	232 (100%)	0	100	100
11	E	512/592 (86%)	511 (100%)	1 (0%)	93	98
11	L	512/592 (86%)	511 (100%)	1 (0%)	93	98
12	F	494/629 (78%)	492 (100%)	2 (0%)	91	95
12	M	494/629 (78%)	492 (100%)	2 (0%)	91	95
13	H	193/193 (100%)	192 (100%)	1 (0%)	88	94
13	O	193/193 (100%)	192 (100%)	1 (0%)	88	94
14	I	179/198 (90%)	179 (100%)	0	100	100
14	P	179/198 (90%)	179 (100%)	0	100	100
15	N	694/2014 (34%)	694 (100%)	0	100	100
15	Q	694/2014 (34%)	694 (100%)	0	100	100
All	All	11772/17826 (66%)	11749 (100%)	23 (0%)	93	98

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	6	269	ASN
5	6	335	ASN
5	6	337	SER
5	6	338	CYS
5	6	339	GLU
6	7	469	LEU
6	7	470	LEU
6	7	639	ARG
11	E	307	ARG
12	F	167	ARG
12	F	687	ILE
13	H	57	GLN
11	L	307	ARG

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Mol	Chain	Res	Type
12	M	167	ARG
12	M	687	ILE
13	O	57	GLN
5	e	269	ASN
5	e	333	CYS
5	e	338	CYS
5	e	339	GLU
6	f	469	LEU
6	f	470	LEU
6	f	639	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	3	201	HIS
2	3	417	GLN
4	5	196	ASN
4	5	499	GLN
5	6	690	ASN
5	6	698	ASN
15	N	1391	ASN
1	a	238	ASN
2	b	201	HIS
2	b	417	GLN
4	d	284	ASN
4	d	499	GLN
5	e	690	ASN
5	e	698	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 32 ligands modelled in this entry, 20 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	ATP	7	901	18	26,33,33	0.62	0	31,52,52	0.79	1 (3%)
19	ADP	e	1201	-	24,29,29	0.93	1 (4%)	29,45,45	1.44	4 (13%)
16	ATP	5	1701	18	26,33,33	0.60	0	31,52,52	0.76	1 (3%)
16	ATP	d	1701	18	26,33,33	0.62	0	31,52,52	0.75	1 (3%)
16	ATP	f	901	18	26,33,33	0.62	0	31,52,52	0.78	1 (3%)
19	ADP	4	1001	-	24,29,29	0.95	1 (4%)	29,45,45	1.44	4 (13%)
19	ADP	6	1201	-	24,29,29	0.93	1 (4%)	29,45,45	1.45	4 (13%)
16	ATP	2	901	-	26,33,33	0.60	0	31,52,52	0.77	2 (6%)
19	ADP	c	1001	-	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
16	ATP	3	1101	18	26,33,33	0.62	0	31,52,52	0.76	1 (3%)
16	ATP	a	901	-	26,33,33	0.61	0	31,52,52	0.78	2 (6%)
16	ATP	b	1101	18	26,33,33	0.62	0	31,52,52	0.76	2 (6%)

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
16	ATP	7	901	18	-	6/18/38/38	0/3/3/3
19	ADP	e	1201	-	-	3/12/32/32	0/3/3/3
16	ATP	5	1701	18	-	1/18/38/38	0/3/3/3
16	ATP	d	1701	18	-	1/18/38/38	0/3/3/3
16	ATP	f	901	18	-	6/18/38/38	0/3/3/3
19	ADP	4	1001	-	-	5/12/32/32	0/3/3/3
19	ADP	6	1201	-	-	3/12/32/32	0/3/3/3
16	ATP	2	901	-	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ADP	c	1001	-	-	5/12/32/32	0/3/3/3
16	ATP	3	1101	18	-	2/18/38/38	0/3/3/3
16	ATP	a	901	-	-	3/18/38/38	0/3/3/3
16	ATP	b	1101	18	-	2/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	c	1001	ADP	C5-C4	2.50	1.47	1.40
19	4	1001	ADP	C5-C4	2.49	1.47	1.40
19	6	1201	ADP	C5-C4	2.44	1.47	1.40
19	e	1201	ADP	C5-C4	2.43	1.47	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	c	1001	ADP	C3'-C2'-C1'	3.64	106.46	100.98
19	4	1001	ADP	C3'-C2'-C1'	3.63	106.45	100.98
19	e	1201	ADP	PA-O3A-PB	-3.61	120.43	132.83
19	6	1201	ADP	PA-O3A-PB	-3.61	120.44	132.83
19	6	1201	ADP	N3-C2-N1	-3.25	123.59	128.68
19	e	1201	ADP	N3-C2-N1	-3.23	123.64	128.68
19	c	1001	ADP	N3-C2-N1	-3.20	123.68	128.68
19	6	1201	ADP	C3'-C2'-C1'	3.11	105.66	100.98
19	4	1001	ADP	N3-C2-N1	-3.09	123.84	128.68
19	e	1201	ADP	C3'-C2'-C1'	3.08	105.62	100.98
19	c	1001	ADP	PA-O3A-PB	-2.98	122.58	132.83
19	4	1001	ADP	PA-O3A-PB	-2.98	122.60	132.83
19	c	1001	ADP	C4-C5-N7	-2.58	106.71	109.40
19	4	1001	ADP	C4-C5-N7	-2.56	106.73	109.40
19	e	1201	ADP	C4-C5-N7	-2.54	106.75	109.40
19	6	1201	ADP	C4-C5-N7	-2.53	106.76	109.40
16	7	901	ATP	C5-C6-N6	2.31	123.86	120.35
16	3	1101	ATP	C5-C6-N6	2.29	123.84	120.35
16	b	1101	ATP	C5-C6-N6	2.27	123.80	120.35
16	5	1701	ATP	C5-C6-N6	2.26	123.79	120.35
16	f	901	ATP	C5-C6-N6	2.26	123.78	120.35
16	a	901	ATP	C5-C6-N6	2.25	123.77	120.35
16	2	901	ATP	C5-C6-N6	2.24	123.76	120.35
16	d	1701	ATP	C5-C6-N6	2.24	123.75	120.35
16	a	901	ATP	PB-O3B-PG	2.05	139.86	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	901	ATP	PB-O3B-PG	2.04	139.84	132.83
16	b	1101	ATP	PB-O3B-PG	2.00	139.71	132.83

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	7	901	ATP	PB-O3B-PG-O2G
16	7	901	ATP	C5'-O5'-PA-O3A
16	7	901	ATP	C4'-C5'-O5'-PA
16	f	901	ATP	PB-O3B-PG-O2G
16	f	901	ATP	C5'-O5'-PA-O3A
16	f	901	ATP	C4'-C5'-O5'-PA
19	4	1001	ADP	C5'-O5'-PA-O1A
19	4	1001	ADP	C5'-O5'-PA-O2A
19	6	1201	ADP	O4'-C4'-C5'-O5'
19	6	1201	ADP	C3'-C4'-C5'-O5'
19	c	1001	ADP	C5'-O5'-PA-O1A
19	c	1001	ADP	C5'-O5'-PA-O2A
19	e	1201	ADP	O4'-C4'-C5'-O5'
19	e	1201	ADP	C3'-C4'-C5'-O5'
16	2	901	ATP	O4'-C4'-C5'-O5'
16	a	901	ATP	O4'-C4'-C5'-O5'
16	2	901	ATP	C3'-C4'-C5'-O5'
16	a	901	ATP	C3'-C4'-C5'-O5'
19	6	1201	ADP	C4'-C5'-O5'-PA
19	e	1201	ADP	C4'-C5'-O5'-PA
16	7	901	ATP	PB-O3B-PG-O3G
16	f	901	ATP	PB-O3B-PG-O3G
19	4	1001	ADP	O4'-C4'-C5'-O5'
19	c	1001	ADP	O4'-C4'-C5'-O5'
16	7	901	ATP	C5'-O5'-PA-O1A
16	f	901	ATP	C5'-O5'-PA-O1A
16	3	1101	ATP	PA-O3A-PB-O2B
16	b	1101	ATP	PA-O3A-PB-O2B
16	2	901	ATP	PA-O3A-PB-O1B
16	a	901	ATP	PA-O3A-PB-O1B
16	7	901	ATP	PB-O3B-PG-O1G
16	f	901	ATP	PB-O3B-PG-O1G
16	3	1101	ATP	C5'-O5'-PA-O3A
16	5	1701	ATP	C5'-O5'-PA-O3A
16	b	1101	ATP	C5'-O5'-PA-O3A

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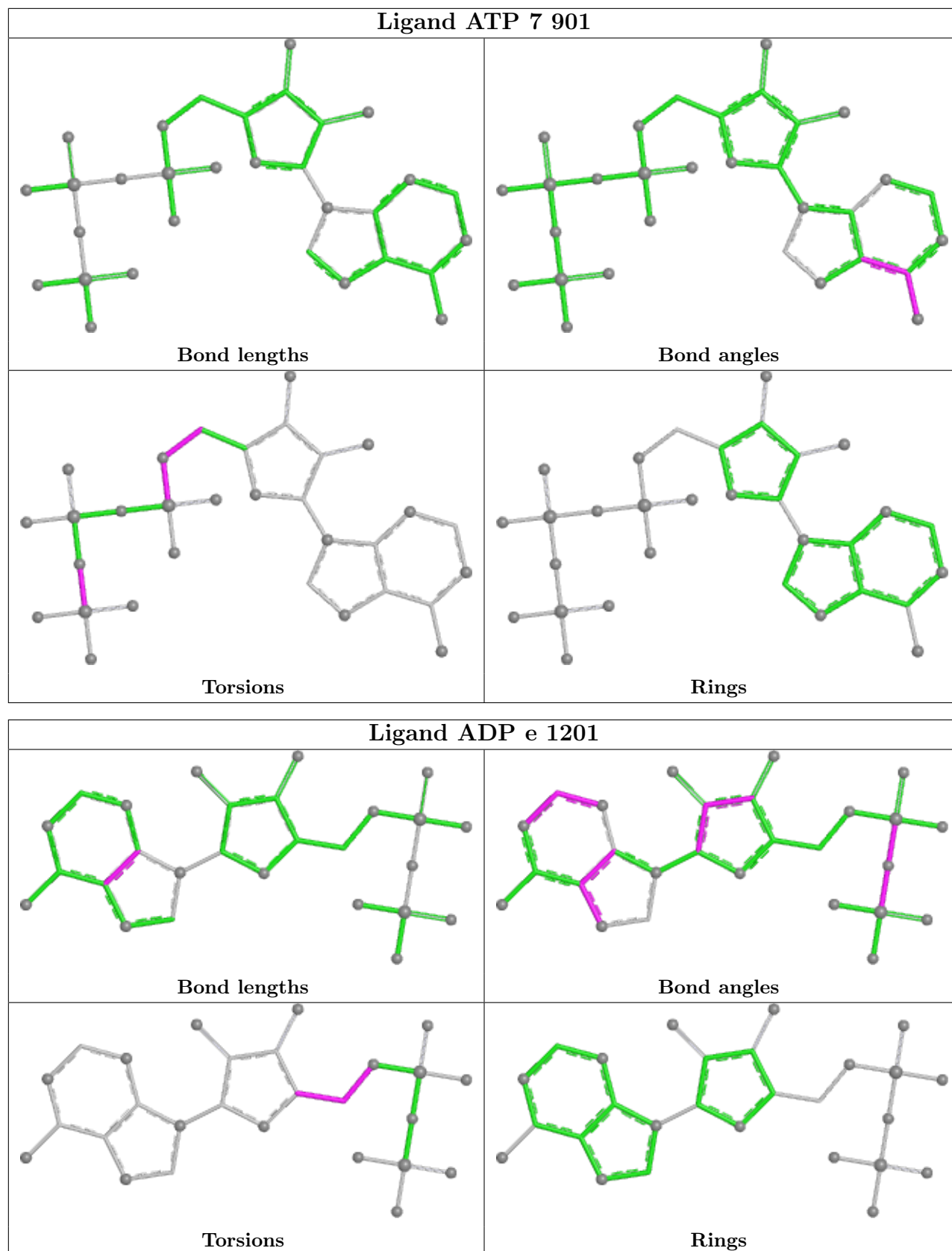
Mol	Chain	Res	Type	Atoms
16	d	1701	ATP	C5'-O5'-PA-O3A
19	4	1001	ADP	C5'-O5'-PA-O3A
19	c	1001	ADP	C5'-O5'-PA-O3A
19	4	1001	ADP	C3'-C4'-C5'-O5'
19	c	1001	ADP	C3'-C4'-C5'-O5'

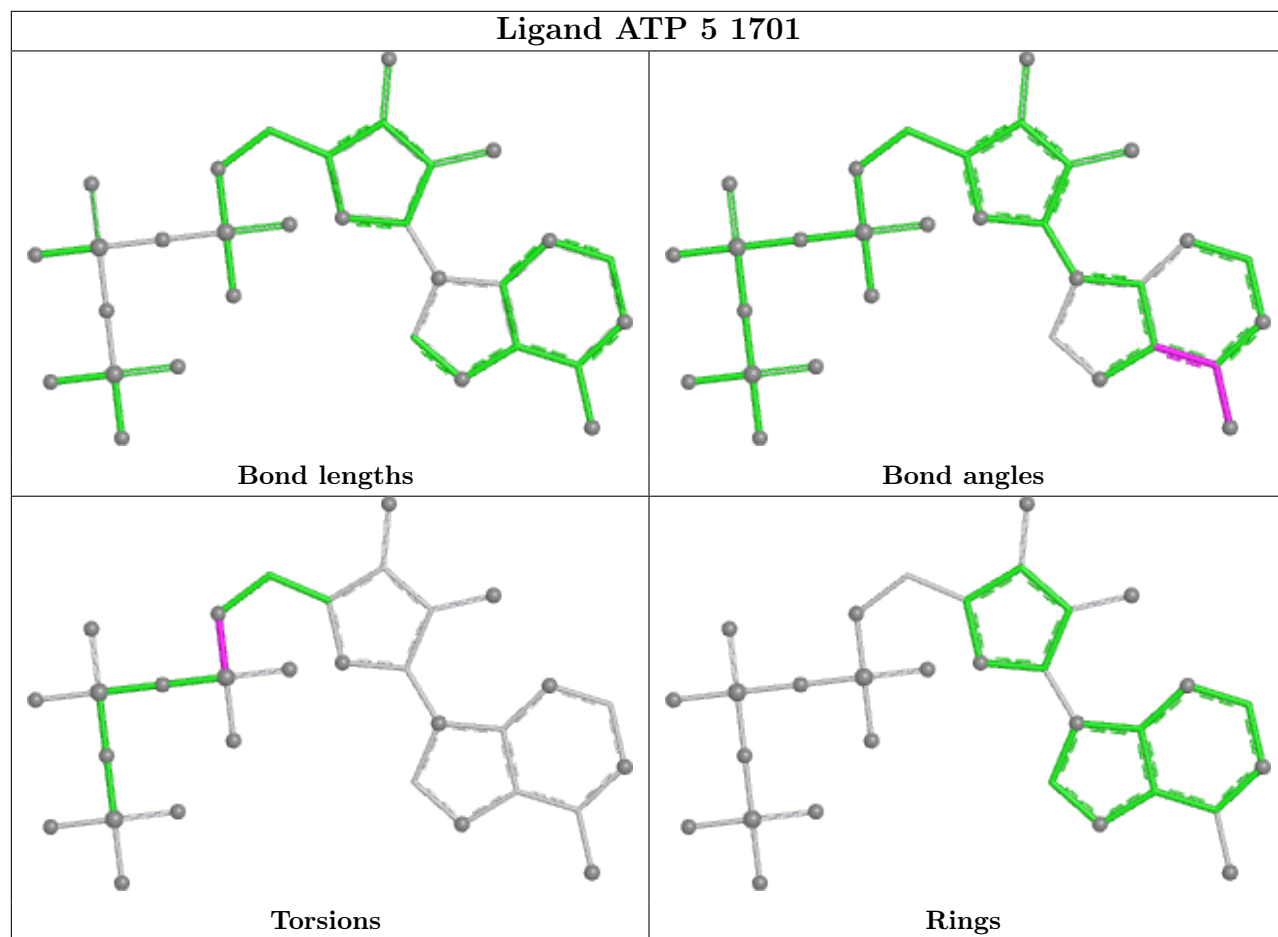
There are no ring outliers.

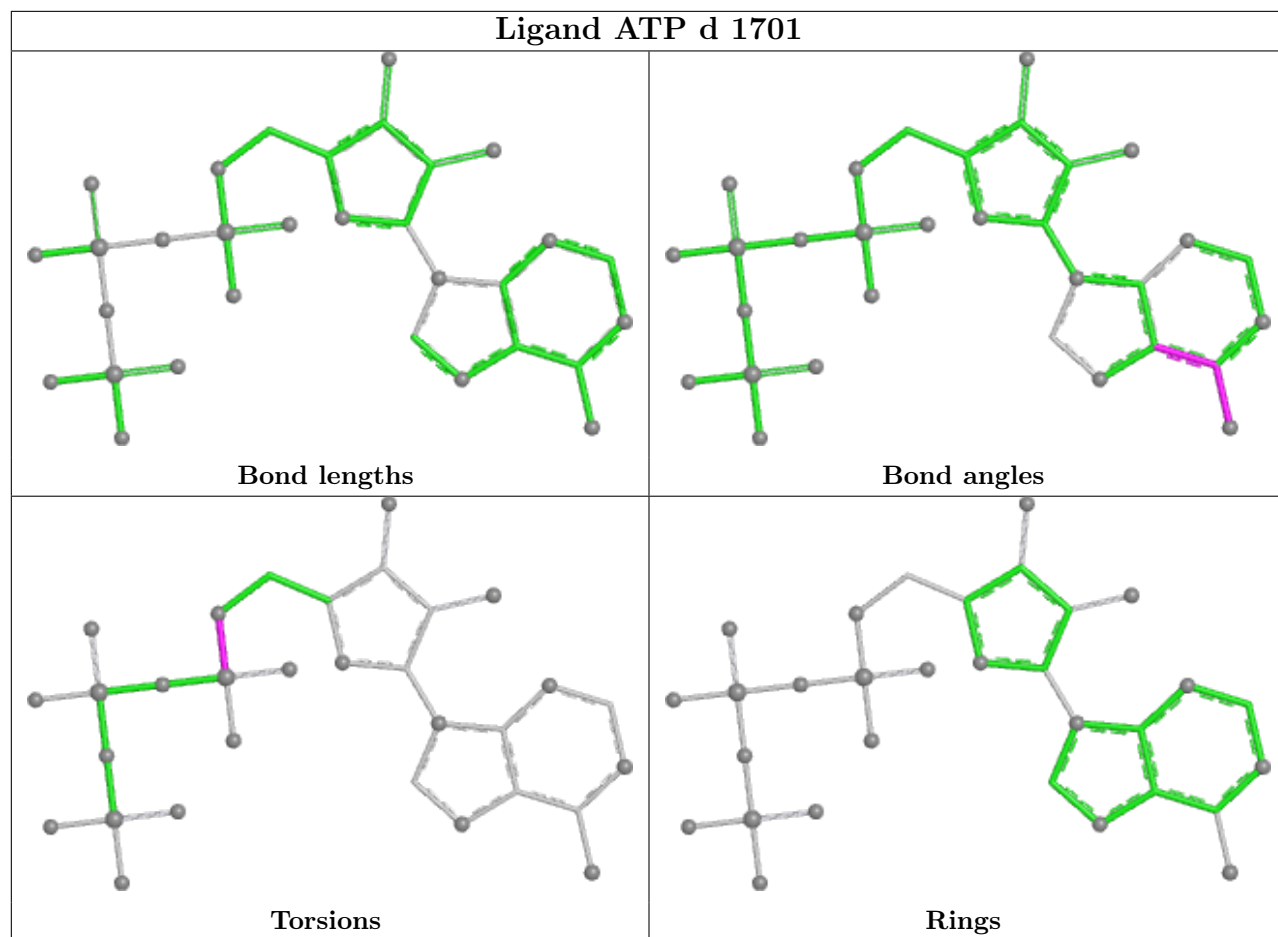
2 monomers are involved in 5 short contacts:

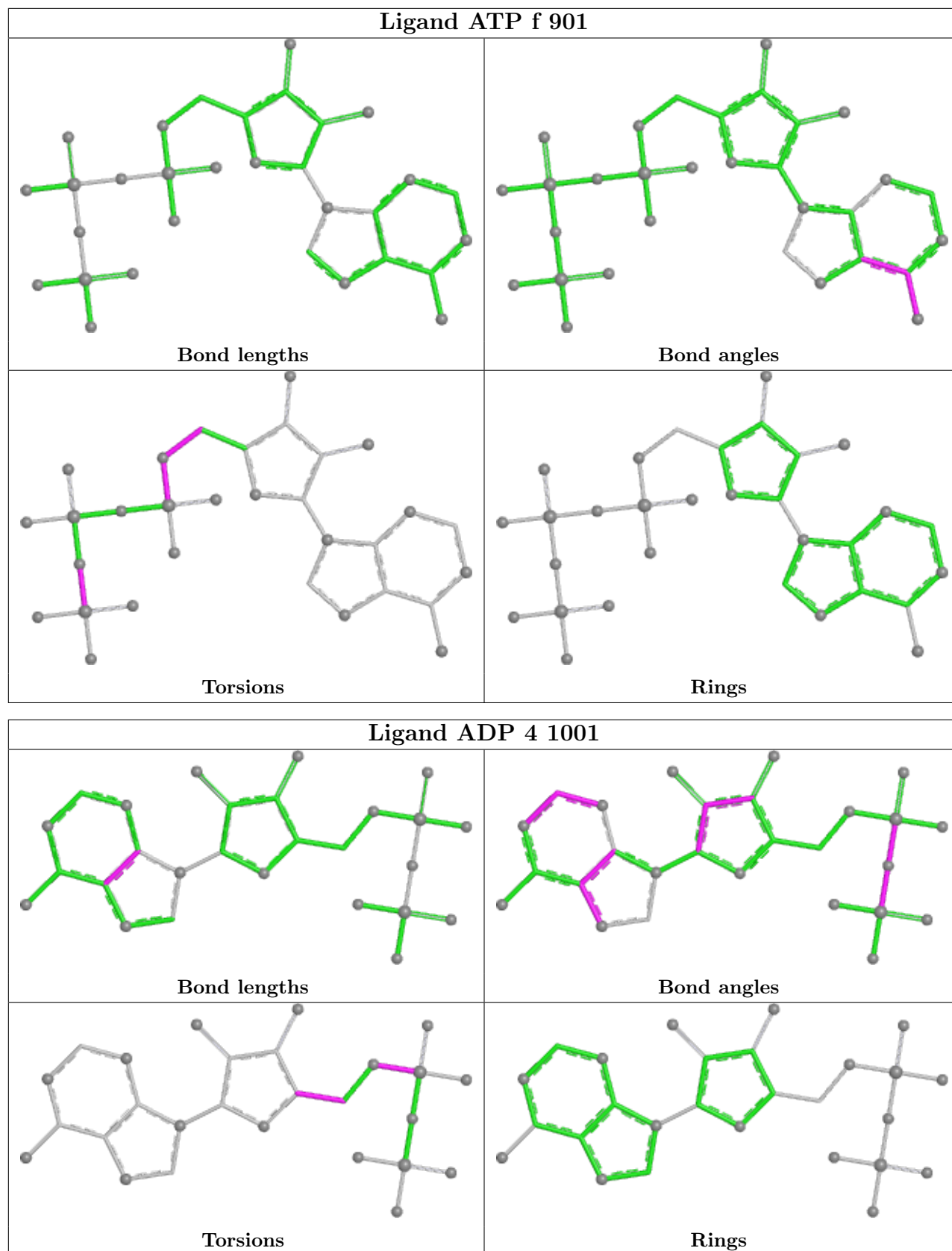
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	7	901	ATP	1	0
19	6	1201	ADP	4	0

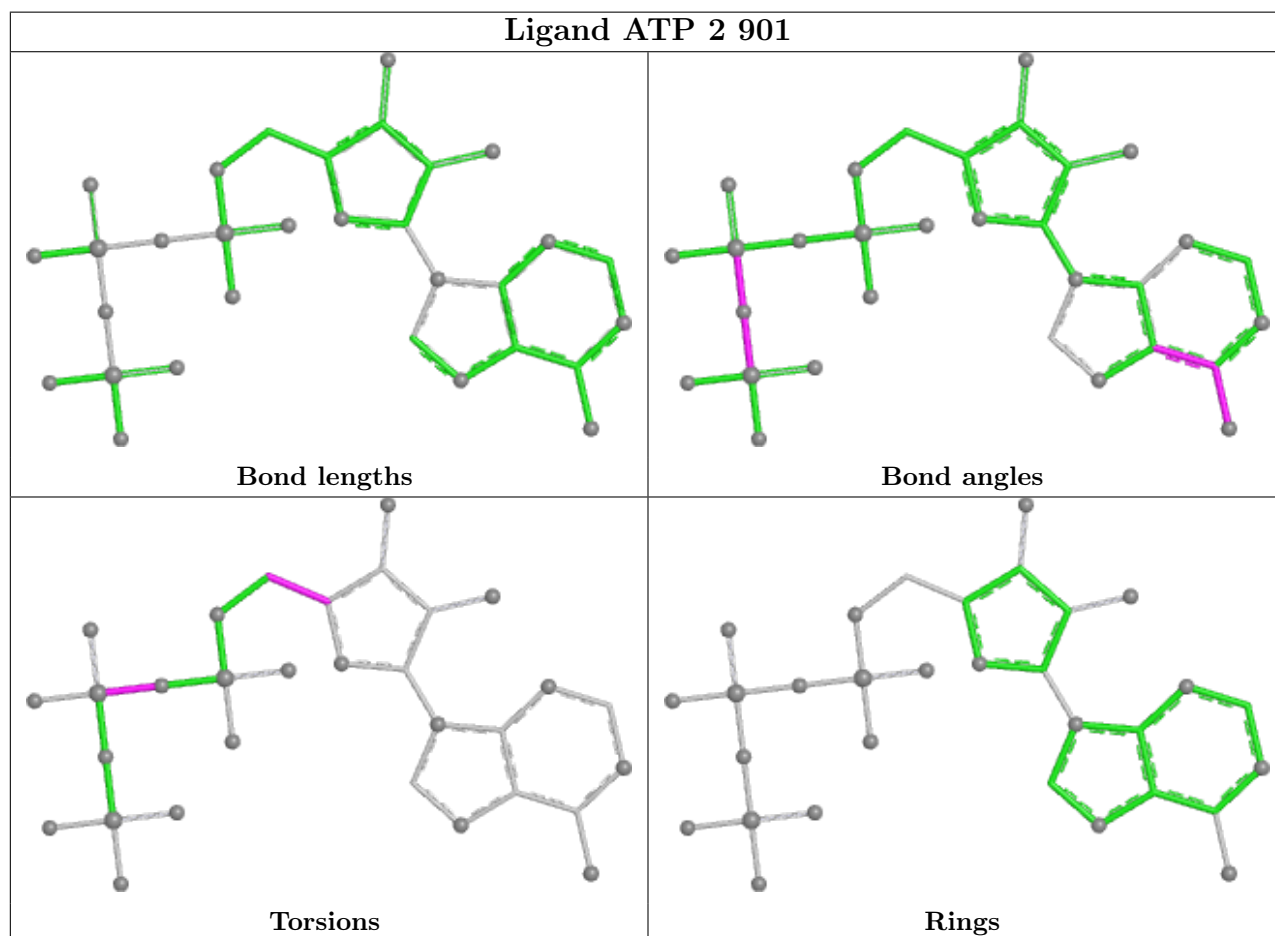
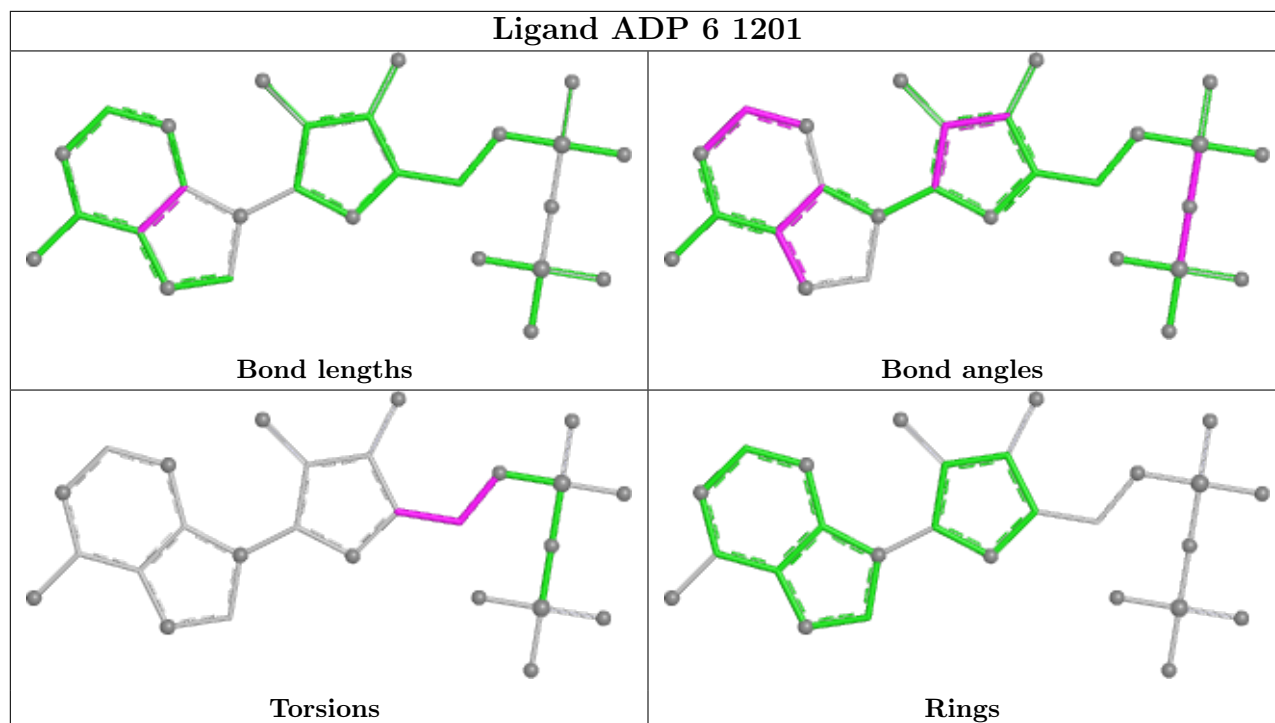
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

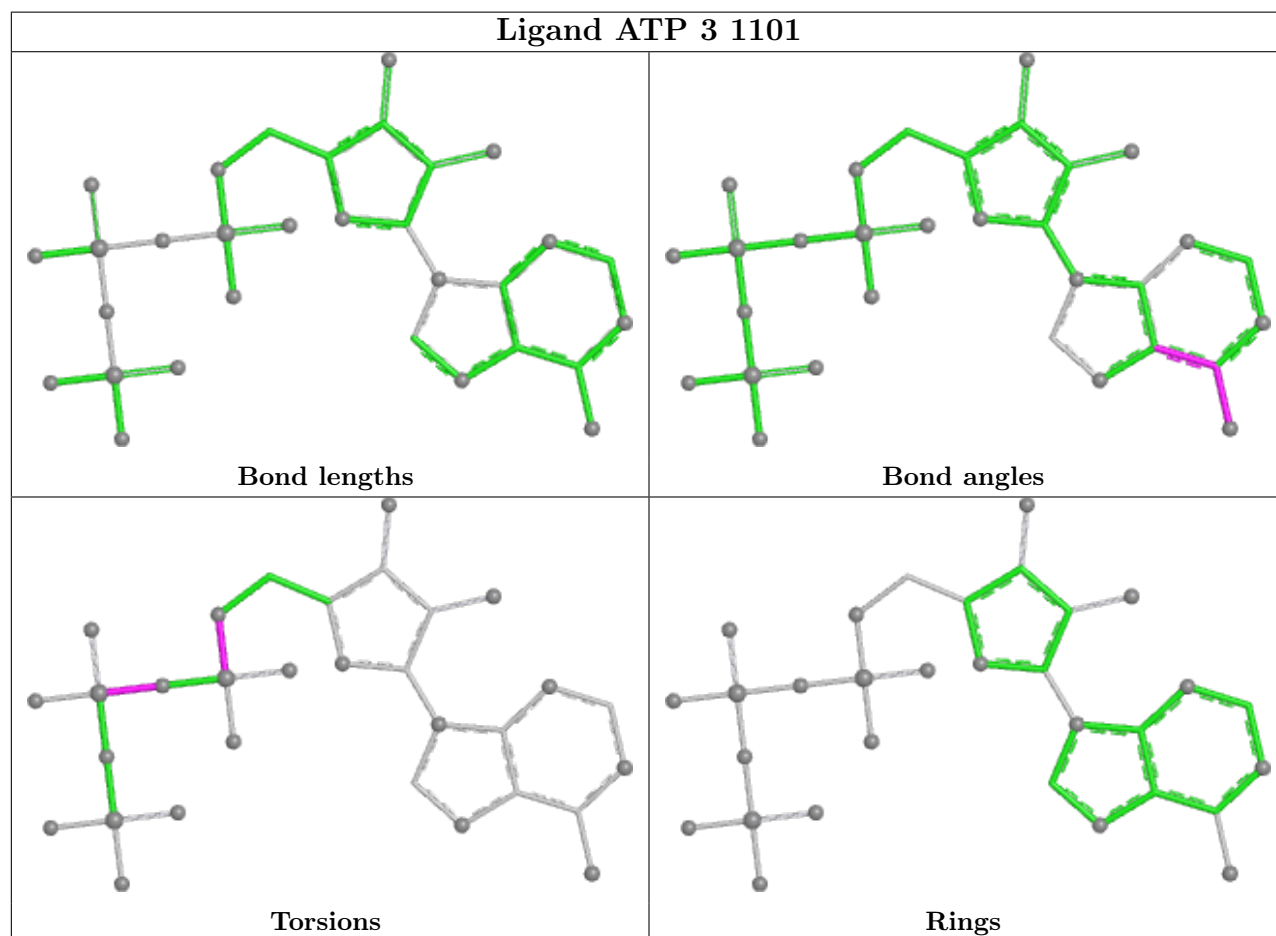
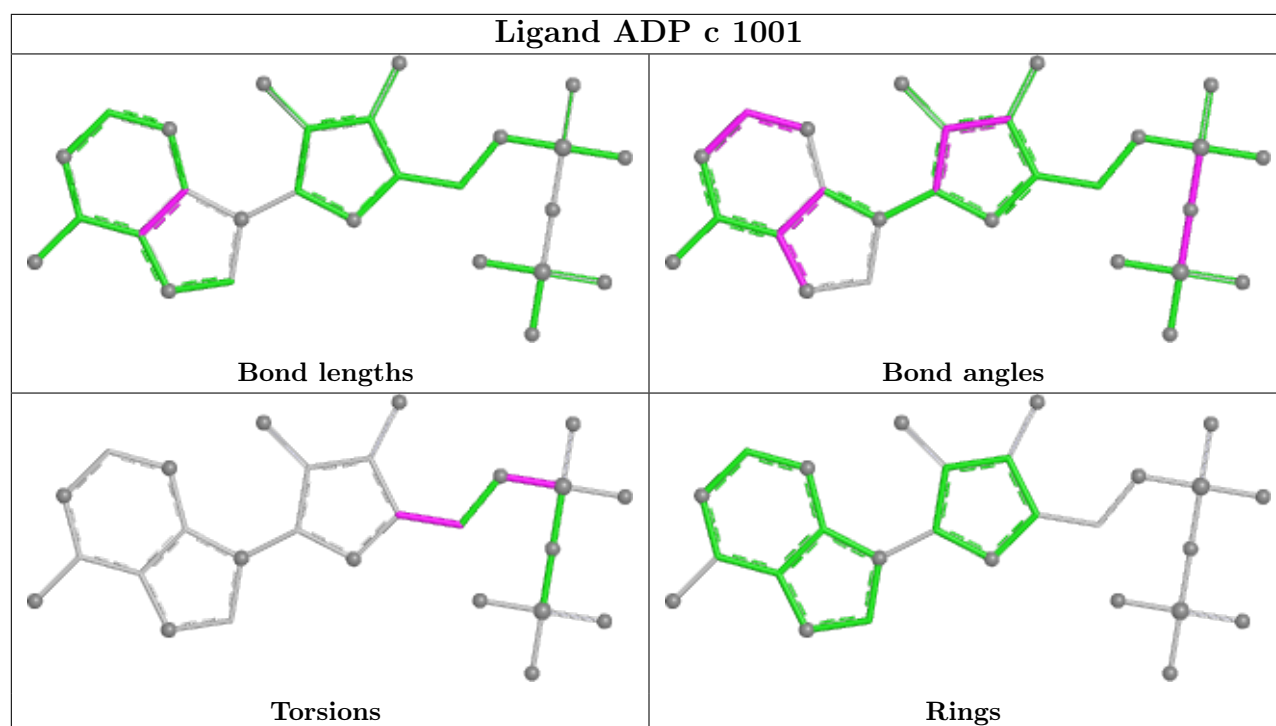


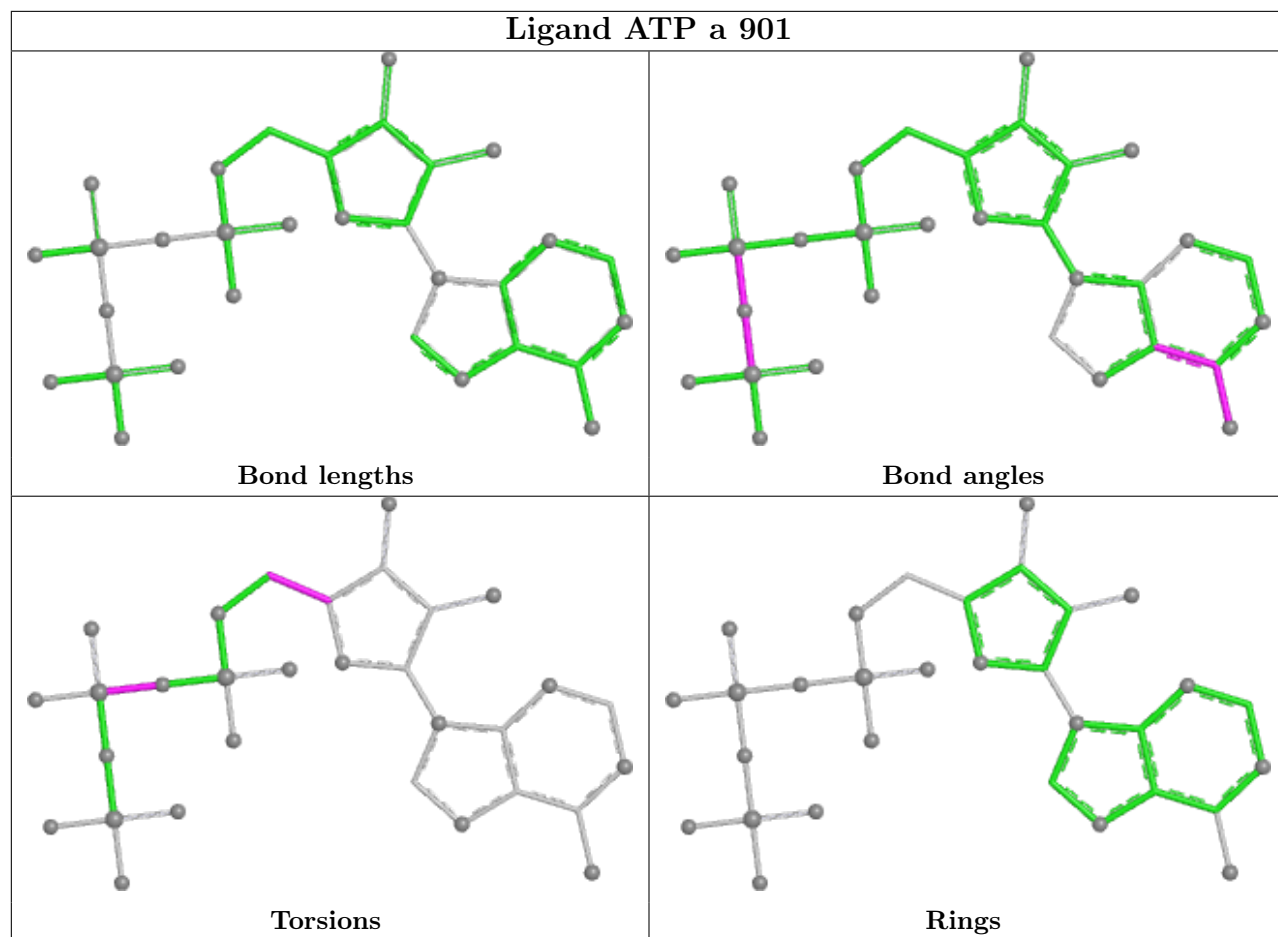




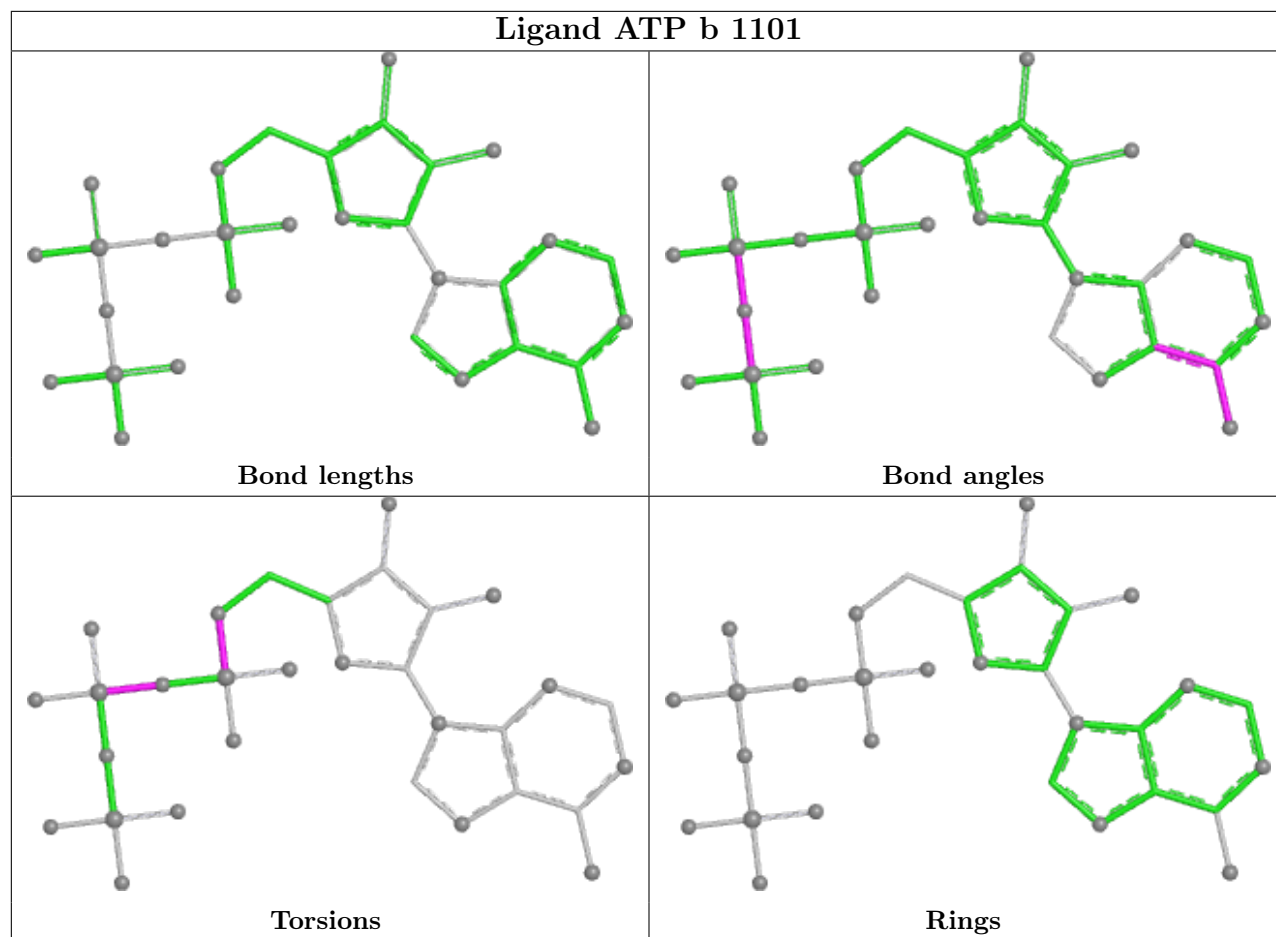












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

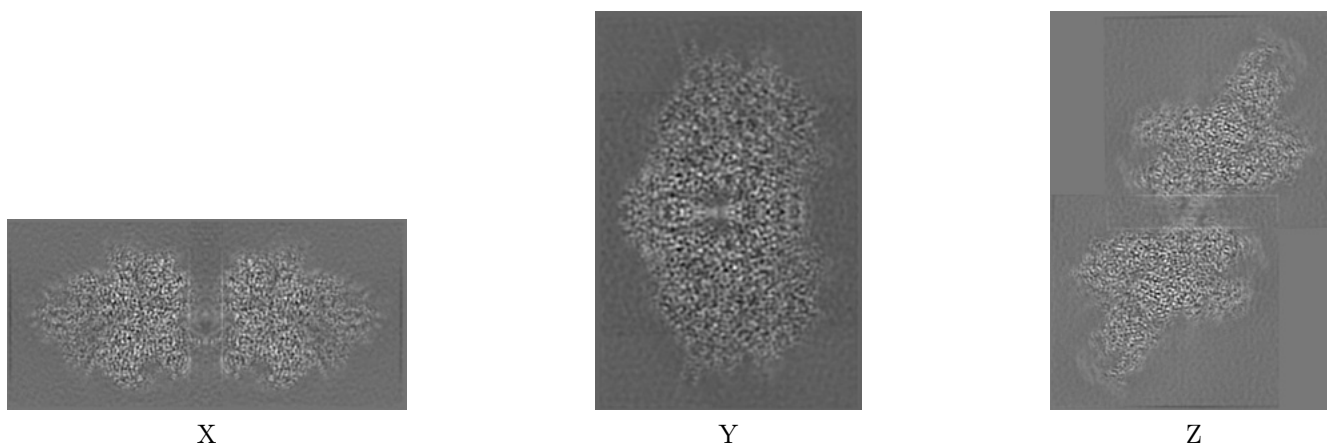
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14439. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

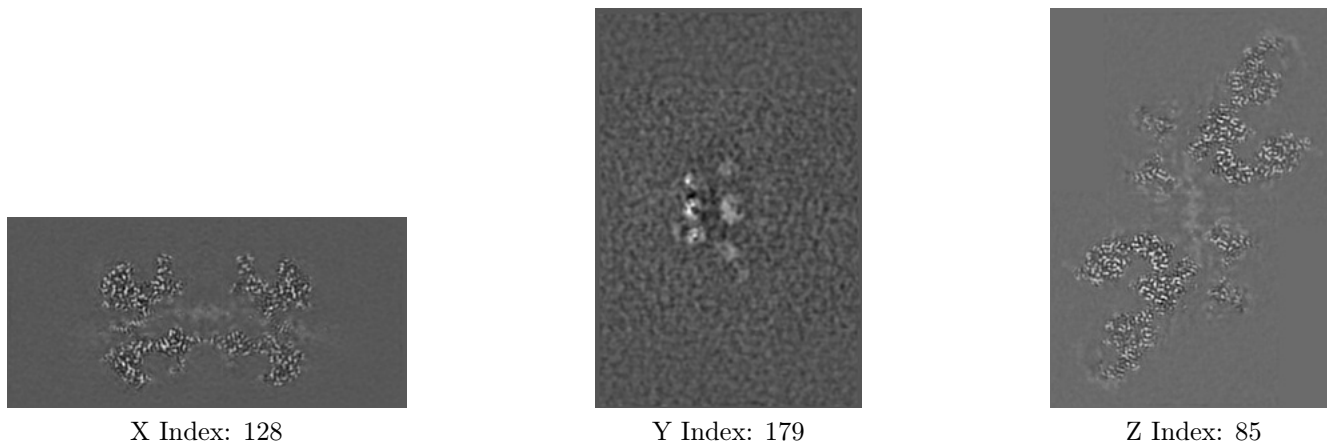
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

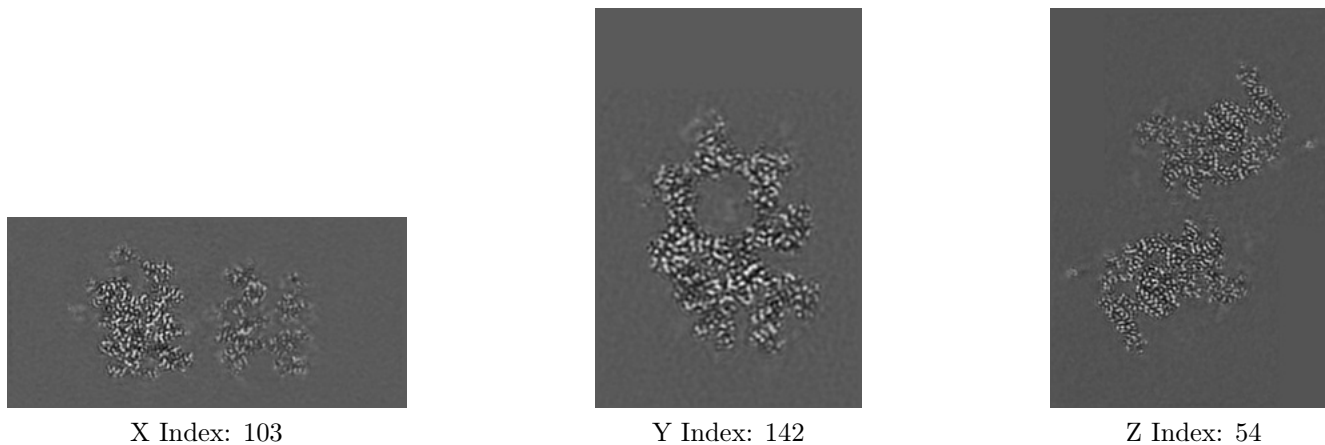
#### 6.2.1 Primary map



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

## 6.3 Largest variance slices [i](#)

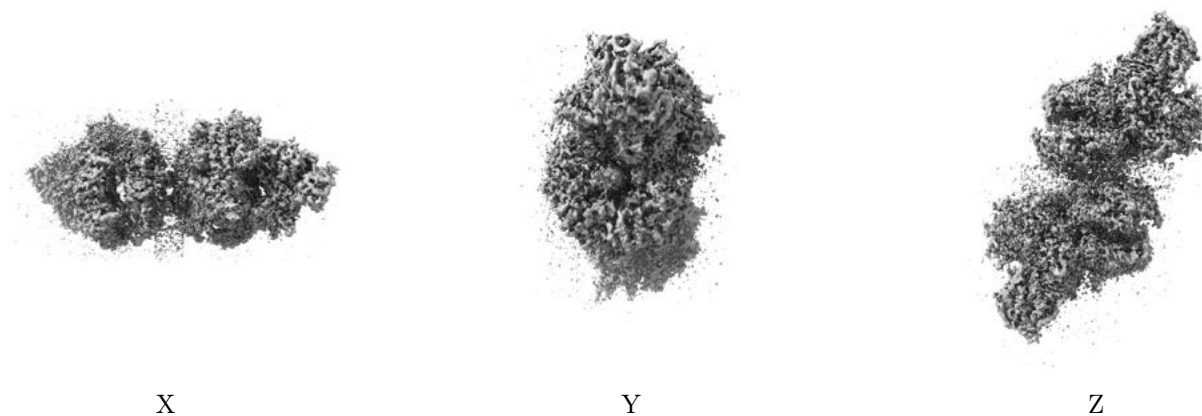
### 6.3.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

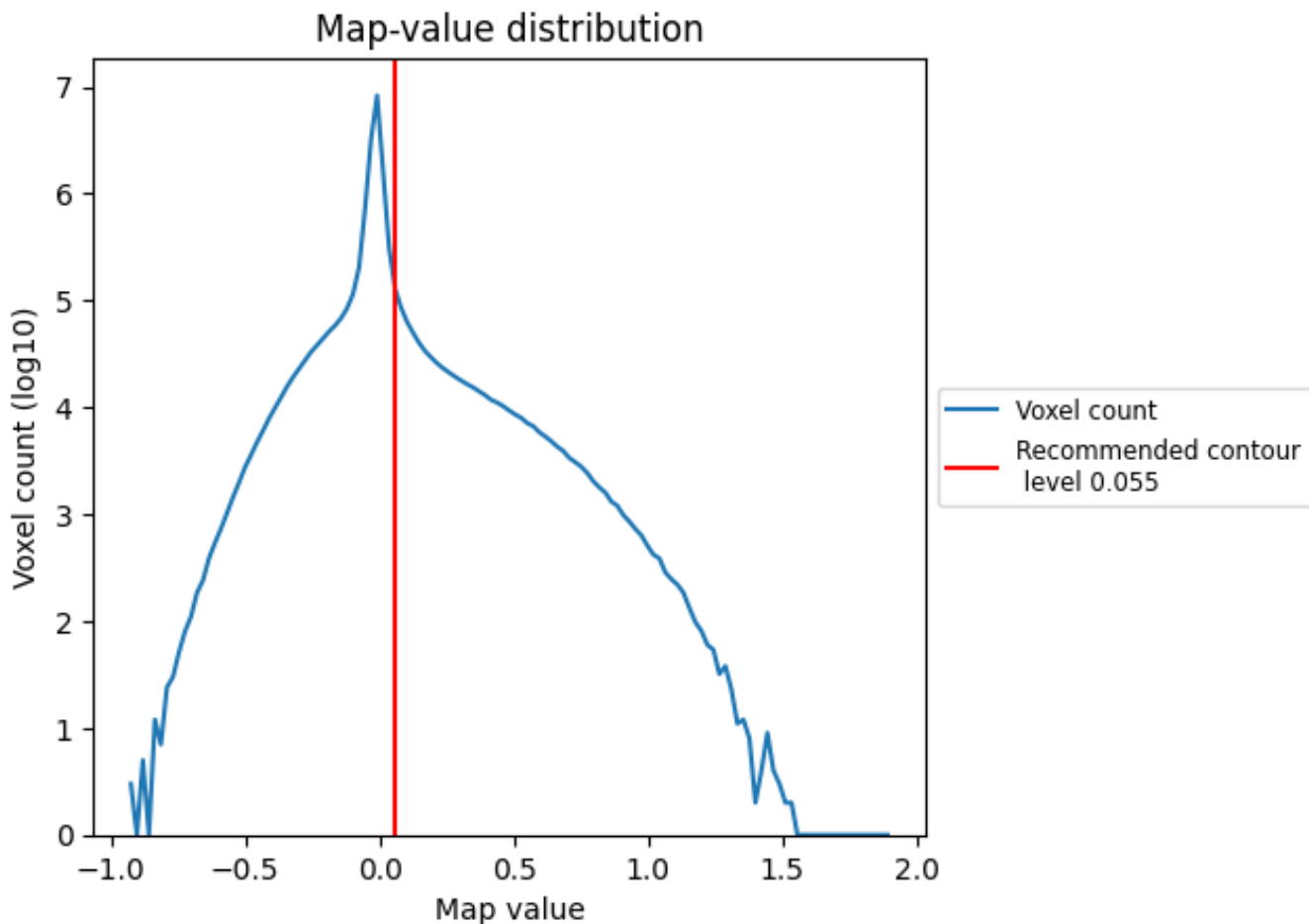
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

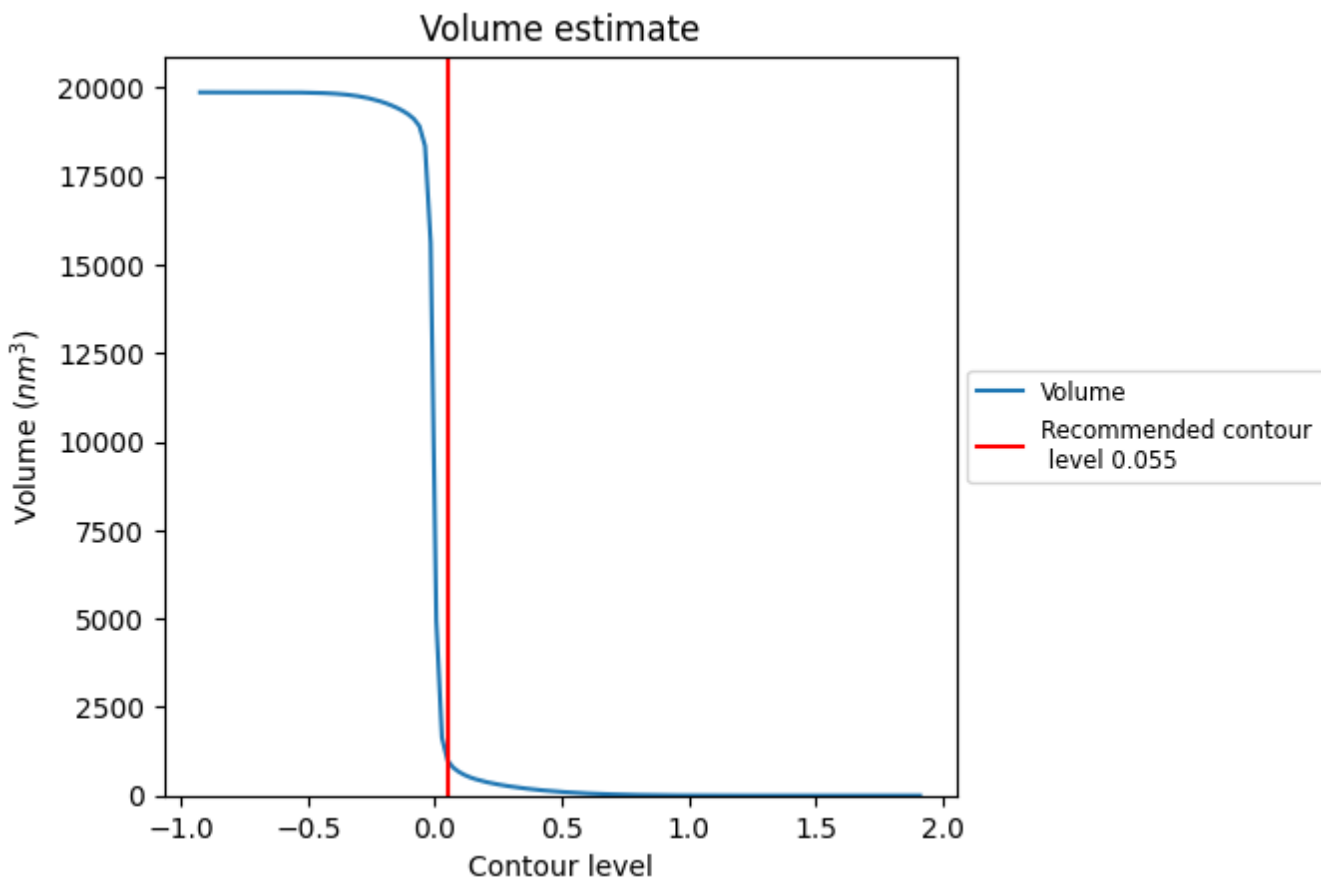
This section contains the results of statistical analysis of the map.

### 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 945 nm<sup>3</sup>; this corresponds to an approximate mass of 853 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

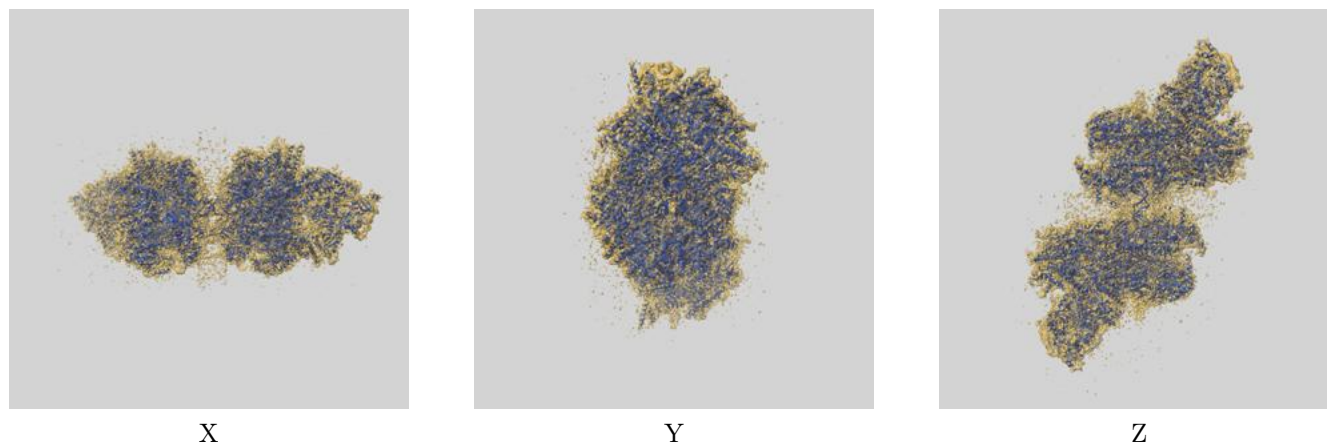
## 8 Fourier-Shell correlation

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-14439 and PDB model 7Z13. Per-residue inclusion information can be found in section 3 on page 14.

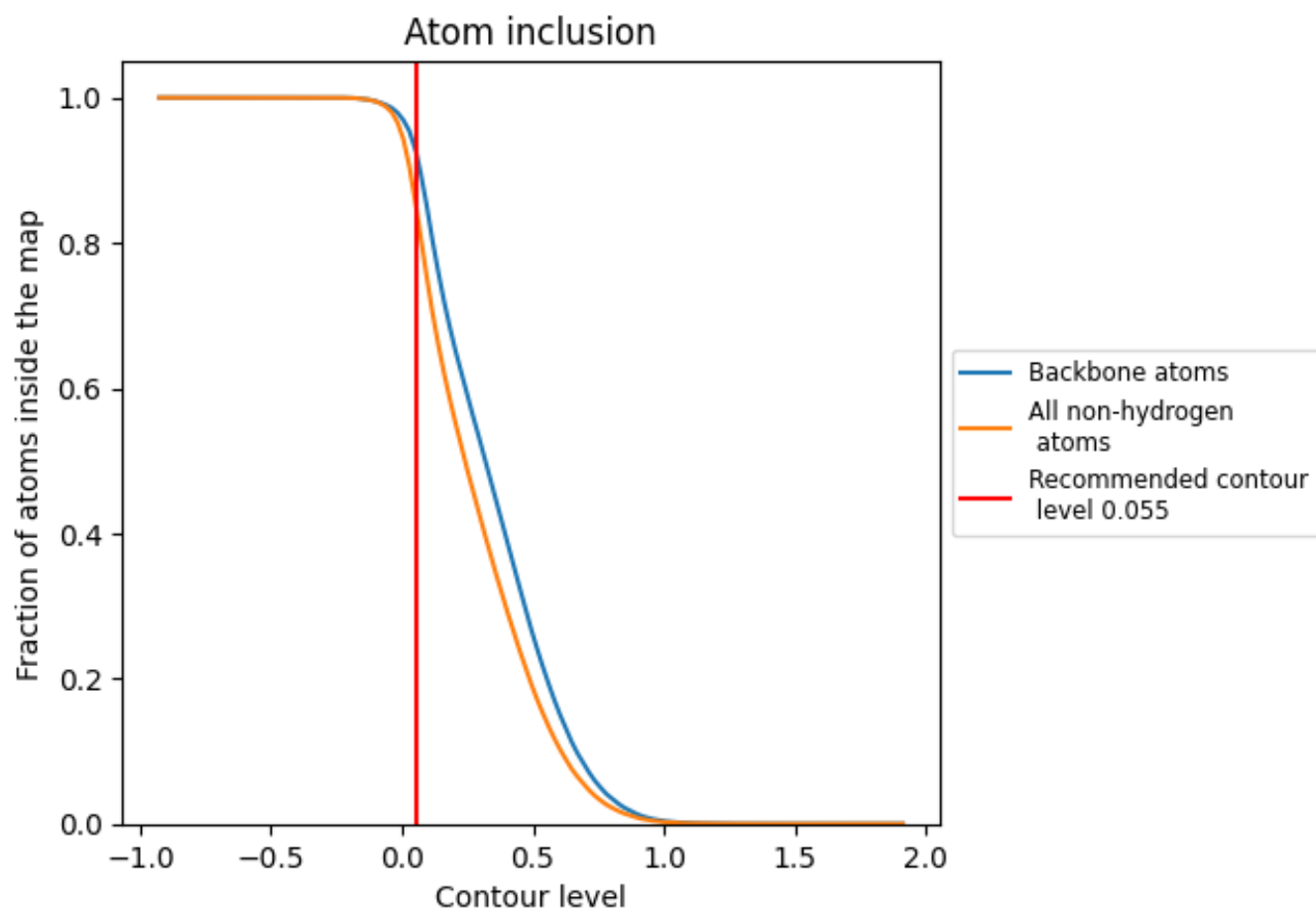
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.055 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 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.