



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 04:23 PM UTC

PDB ID : 6RQC / pdb_00006rqc
EMDB ID : EMD-4980
Title : Cryo-EM structure of an MCM loading intermediate
Authors : Miller, T.C.R.; Locke, J.; Costa, A.
Deposited on : 2019-05-15
Resolution : 4.40 Å(reported)
Based on initial models : 5ZR1, 5BK4, 6EYC, 6F0L

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

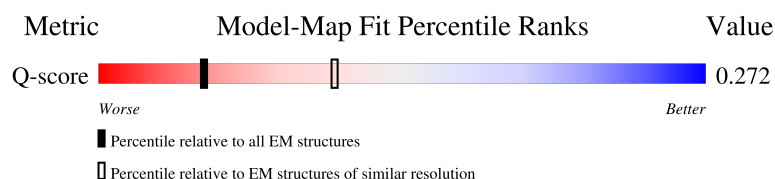
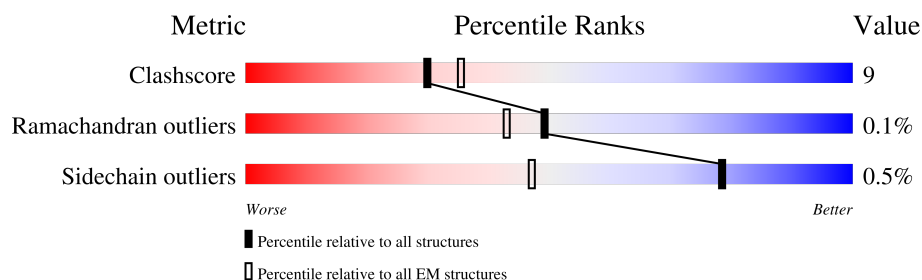
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	949	36% 39% 13% 48%
2	B	620	5% 31% 8% 60%
3	C	616	22% 75% 20% 6%
4	D	529	33% 62% 21% 17%

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Mol	Chain	Length	Quality of chain
5	E	479	
6	F	435	
7	2	868	
8	3	1006	
9	4	933	
10	5	775	
11	6	1017	
12	7	845	
13	X	88	
14	Y	88	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 105307 atoms, of which 52062 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 Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	494	Total	C	H	N	O	S	0	0
			8028	2527	4070	676	736	19		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP P54784
A	-33	LYS	-	expression tag	UNP P54784
A	-32	ARG	-	expression tag	UNP P54784
A	-31	ARG	-	expression tag	UNP P54784
A	-30	TRP	-	expression tag	UNP P54784
A	-29	LYS	-	expression tag	UNP P54784
A	-28	LYS	-	expression tag	UNP P54784
A	-27	ASN	-	expression tag	UNP P54784
A	-26	PHE	-	expression tag	UNP P54784
A	-25	ILE	-	expression tag	UNP P54784
A	-24	ALA	-	expression tag	UNP P54784
A	-23	VAL	-	expression tag	UNP P54784
A	-22	SER	-	expression tag	UNP P54784
A	-21	ALA	-	expression tag	UNP P54784
A	-20	ALA	-	expression tag	UNP P54784
A	-19	ASN	-	expression tag	UNP P54784
A	-18	ARG	-	expression tag	UNP P54784
A	-17	PHE	-	expression tag	UNP P54784
A	-16	LYS	-	expression tag	UNP P54784
A	-15	LYS	-	expression tag	UNP P54784
A	-14	ILE	-	expression tag	UNP P54784
A	-13	SER	-	expression tag	UNP P54784
A	-12	SER	-	expression tag	UNP P54784
A	-11	SER	-	expression tag	UNP P54784
A	-10	GLY	-	expression tag	UNP P54784
A	-9	ALA	-	expression tag	UNP P54784
A	-8	LEU	-	expression tag	UNP P54784
A	-7	GLU	-	expression tag	UNP P54784

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASN	-	expression tag	UNP P54784
A	-5	LEU	-	expression tag	UNP P54784
A	-4	TYR	-	expression tag	UNP P54784
A	-3	PHE	-	expression tag	UNP P54784
A	-2	GLN	-	expression tag	UNP P54784
A	-1	GLY	-	expression tag	UNP P54784
A	0	GLU	-	expression tag	UNP P54784

- Molecule 2 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	247	Total	C	H	N	O	S	0	0
			4067	1330	2018	339	372	8		

- Molecule 3 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	582	Total	C	H	N	O	S	0	0
			9579	3102	4766	794	901	16		

- Molecule 4 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	437	Total	C	H	N	O	S	0	0
			7193	2285	3627	605	663	13		

- Molecule 5 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	459	Total	C	H	N	O	S	0	0
			7529	2431	3780	609	695	14		

- Molecule 6 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	242	Total	C	H	N	O	S	0	0
			4046	1274	2051	343	358	20		

- Molecule 7 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	2	601	Total	C	H	N	O	S	0	0
			9573	2998	4820	845	891	19		

- Molecule 8 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	3	599	Total	C	H	N	O	S	0	0
			9448	2956	4752	840	887	13		

There are 35 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 9 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	4	641	Total	C	H	N	O	S	0	0
			10282	3210	5172	883	989	28		

- Molecule 10 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	5	602	Total	C	H	N	O	S	0	0
			9532	2976	4802	813	917	24		

- Molecule 11 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	6	616	Total	C	H	N	O	S	0	0
			9782	3072	4908	853	924	25		

- Molecule 12 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	7	654	Total	C	H	N	O	S	0	0
			10353	3244	5215	886	979	29		

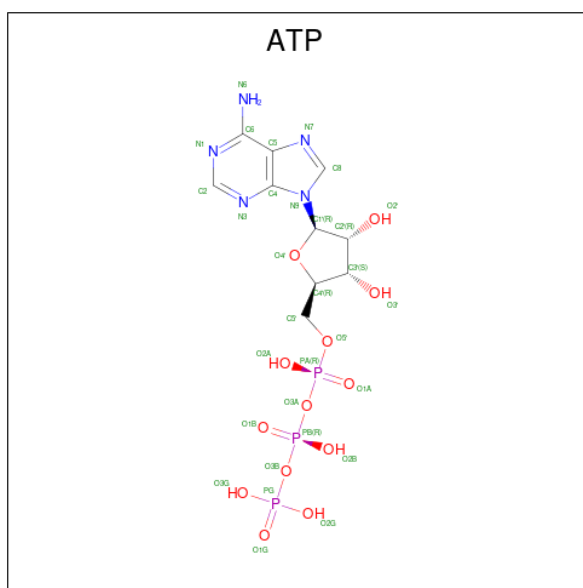
- Molecule 13 is a DNA chain called DNA (88-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
13	X	88	Total	C	H	N	O	P	0	0
			2806	867	1010	294	548	87		

- Molecule 14 is a DNA chain called DNA (88-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
14	Y	88	Total	C	H	N	O	P	0	0
			2796	863	987	352	506	88		

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

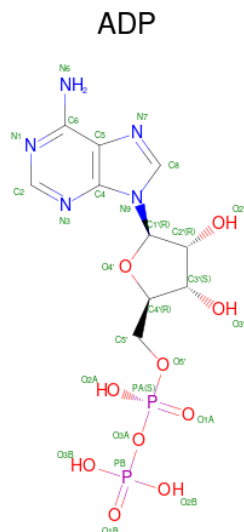


Mol	Chain	Residues	Atoms					AltConf	
15	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
15	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
15	E	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	Mg	0
			1	1	
16	D	1	Total	Mg	0
			1	1	
16	E	1	Total	Mg	0
			1	1	

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf	
17	2	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
17	3	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
17	5	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
17	7	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

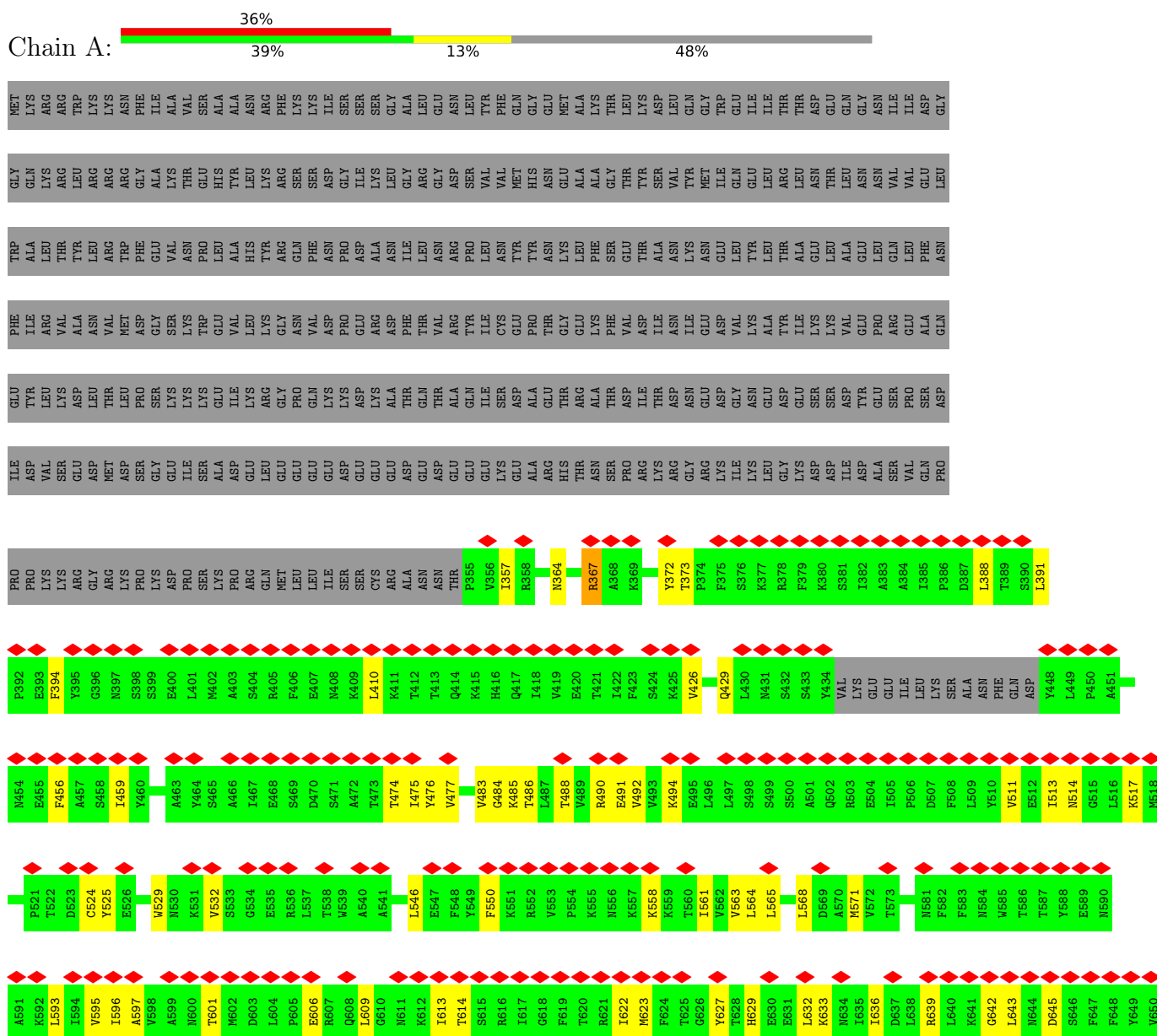
- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

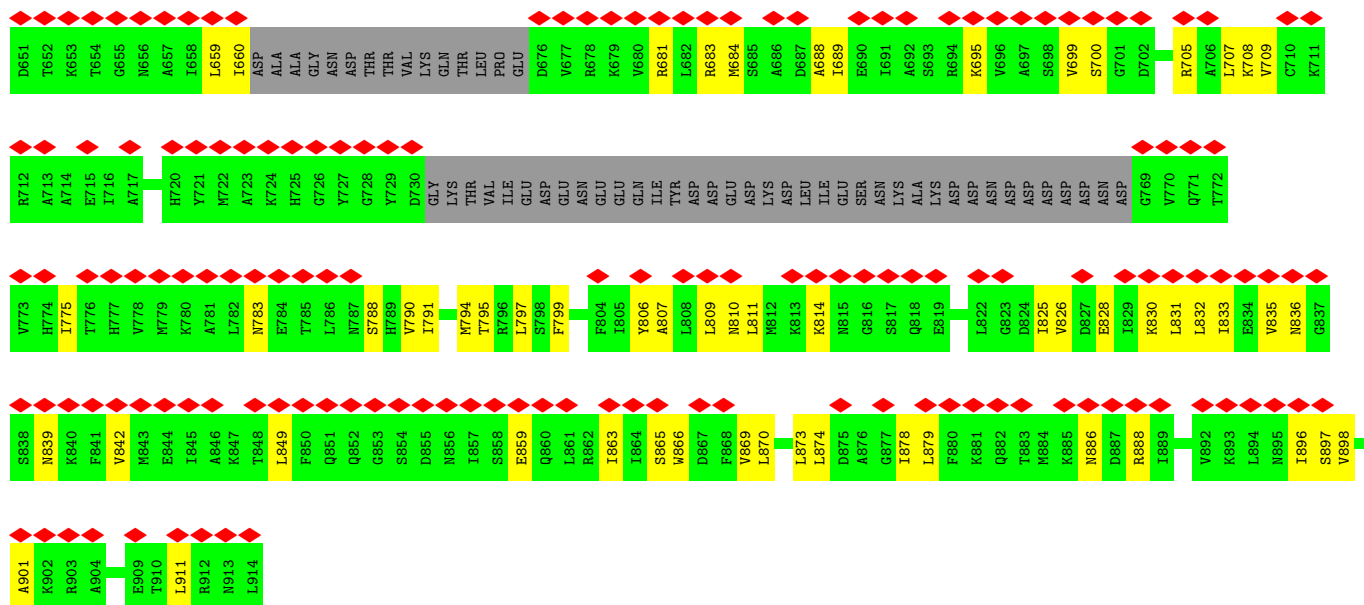
Mol	Chain	Residues	Atoms	AltConf
18	2	1	Total Zn 1 1	0
18	4	1	Total Zn 1 1	0
18	5	1	Total Zn 1 1	0
18	6	1	Total Zn 1 1	0
18	7	1	Total Zn 1 1	0

3 Residue-property plots

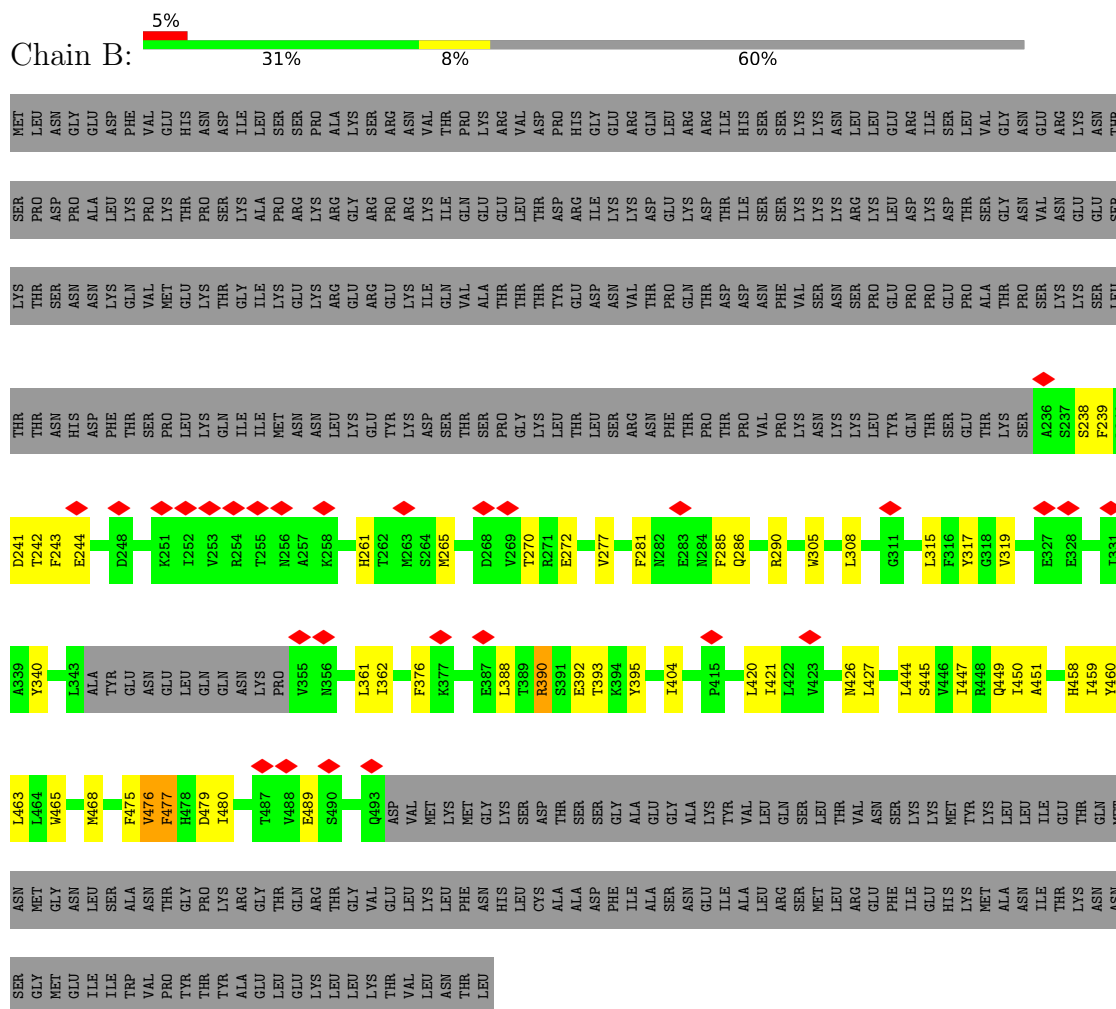
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Origin recognition complex subunit 1



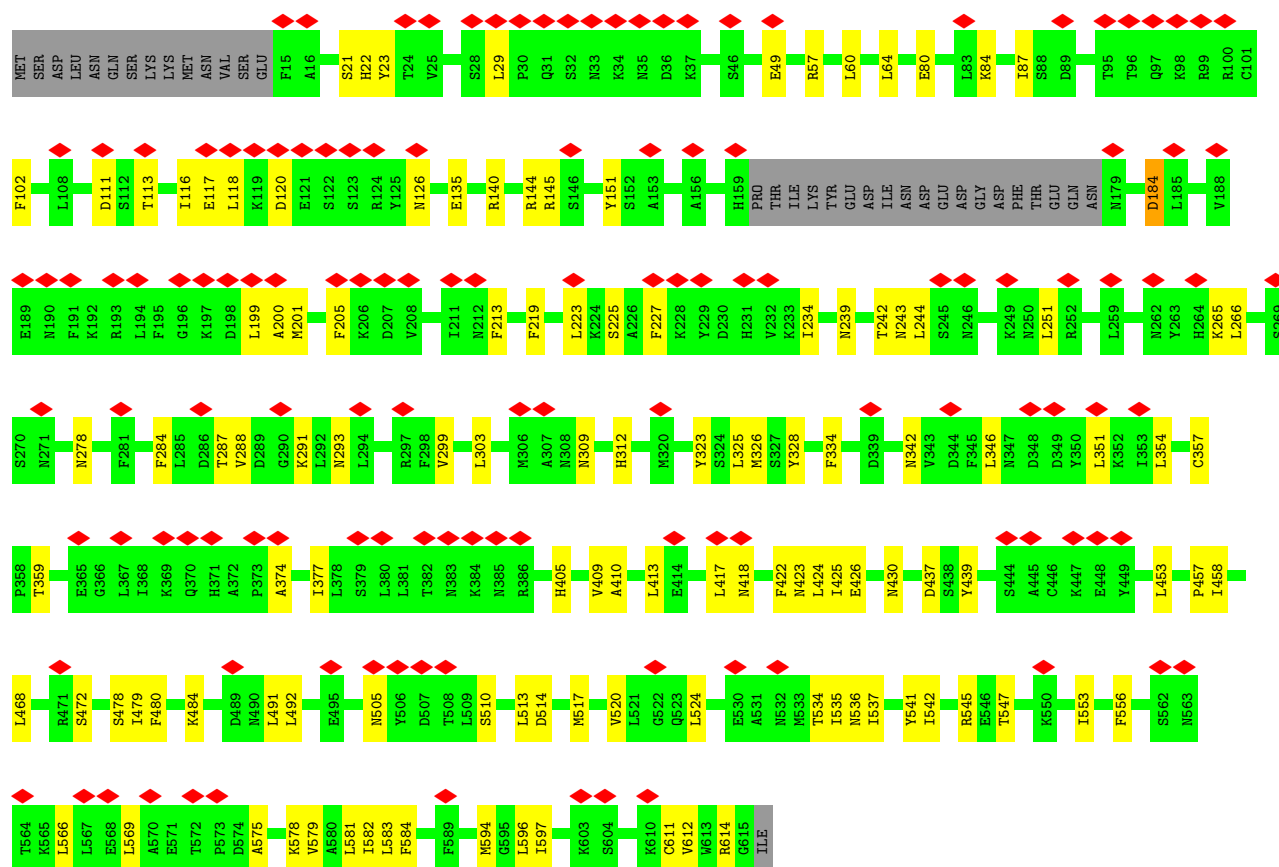


• Molecule 2: Origin recognition complex subunit 2



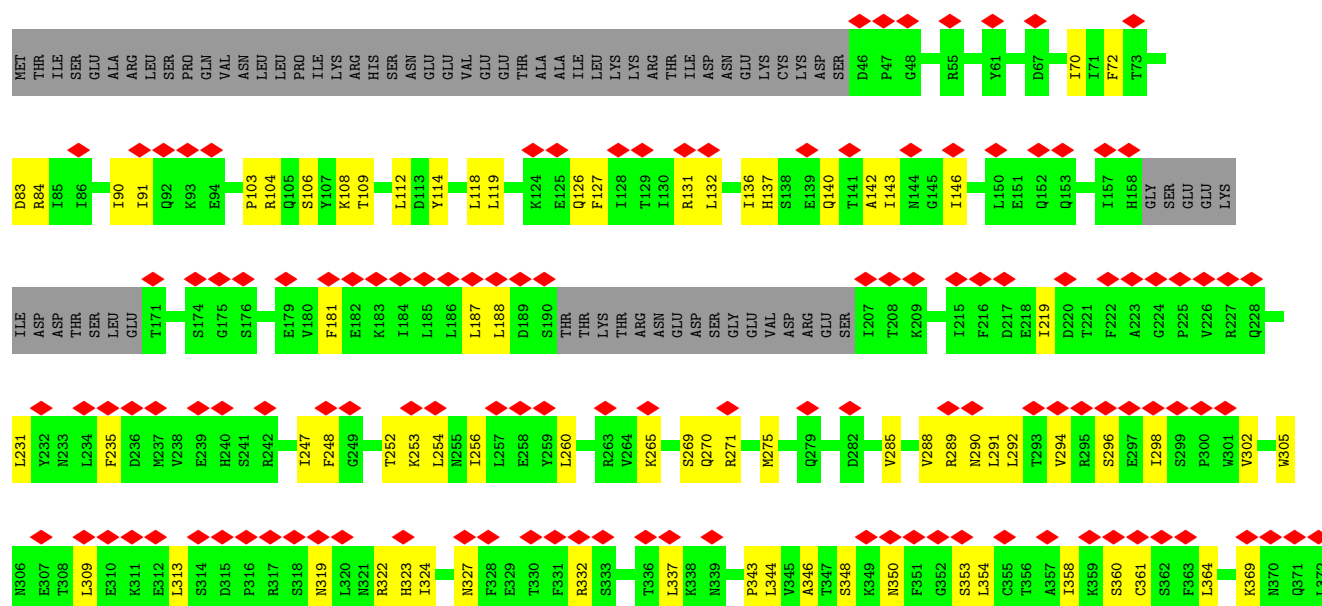
• Molecule 3: Origin recognition complex subunit 3

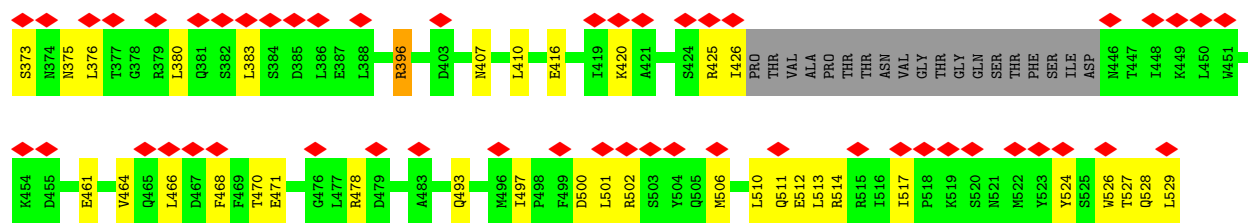
Chain C: 



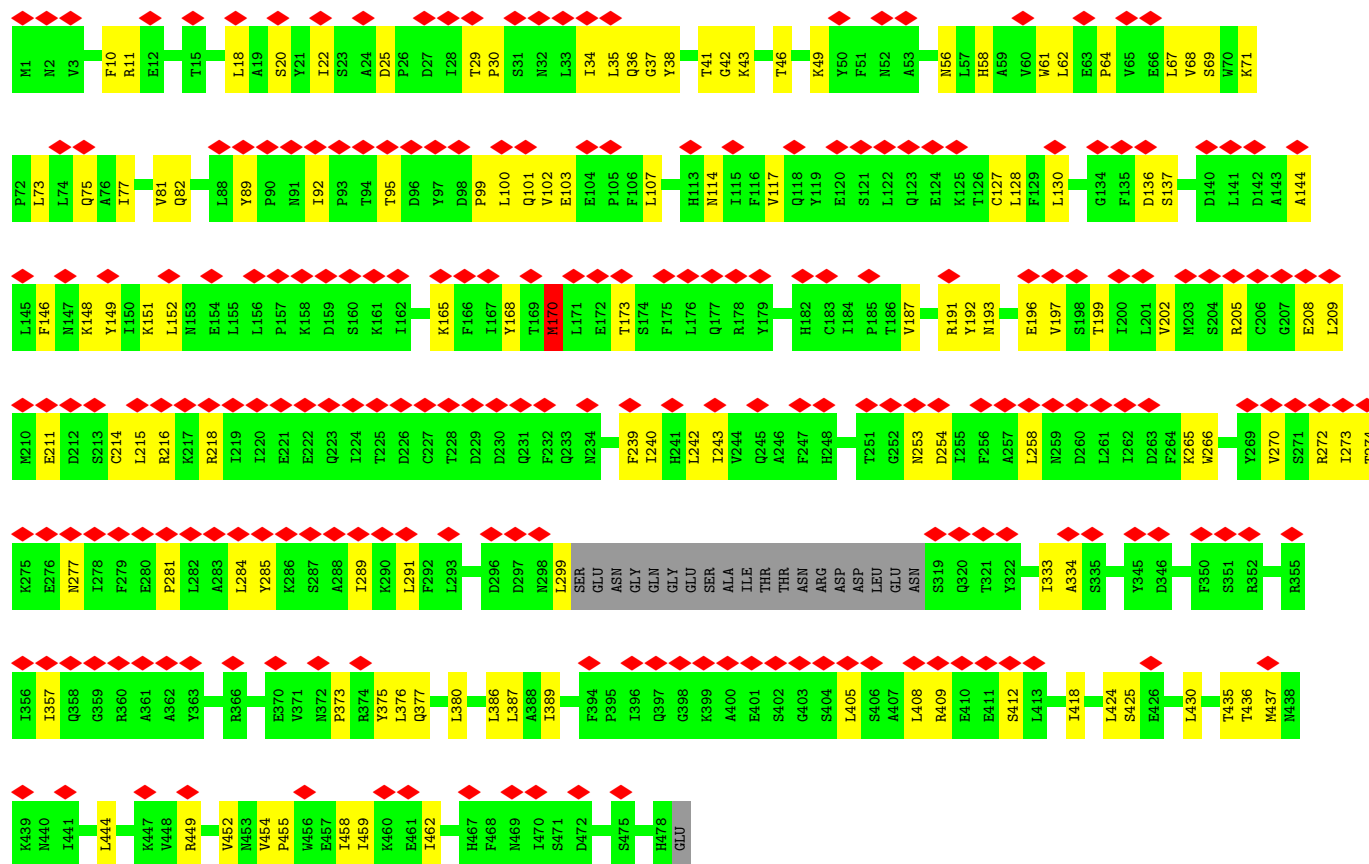
• Molecule 4: Origin recognition complex subunit 4

Chain D: 

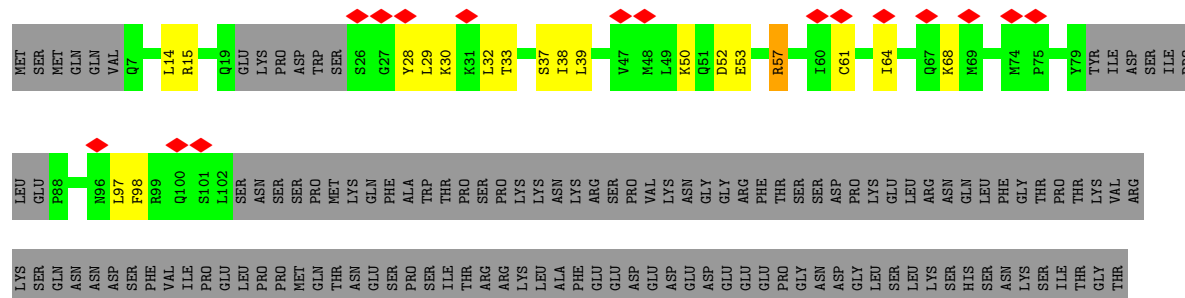
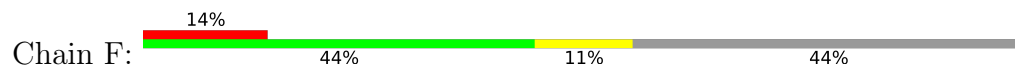


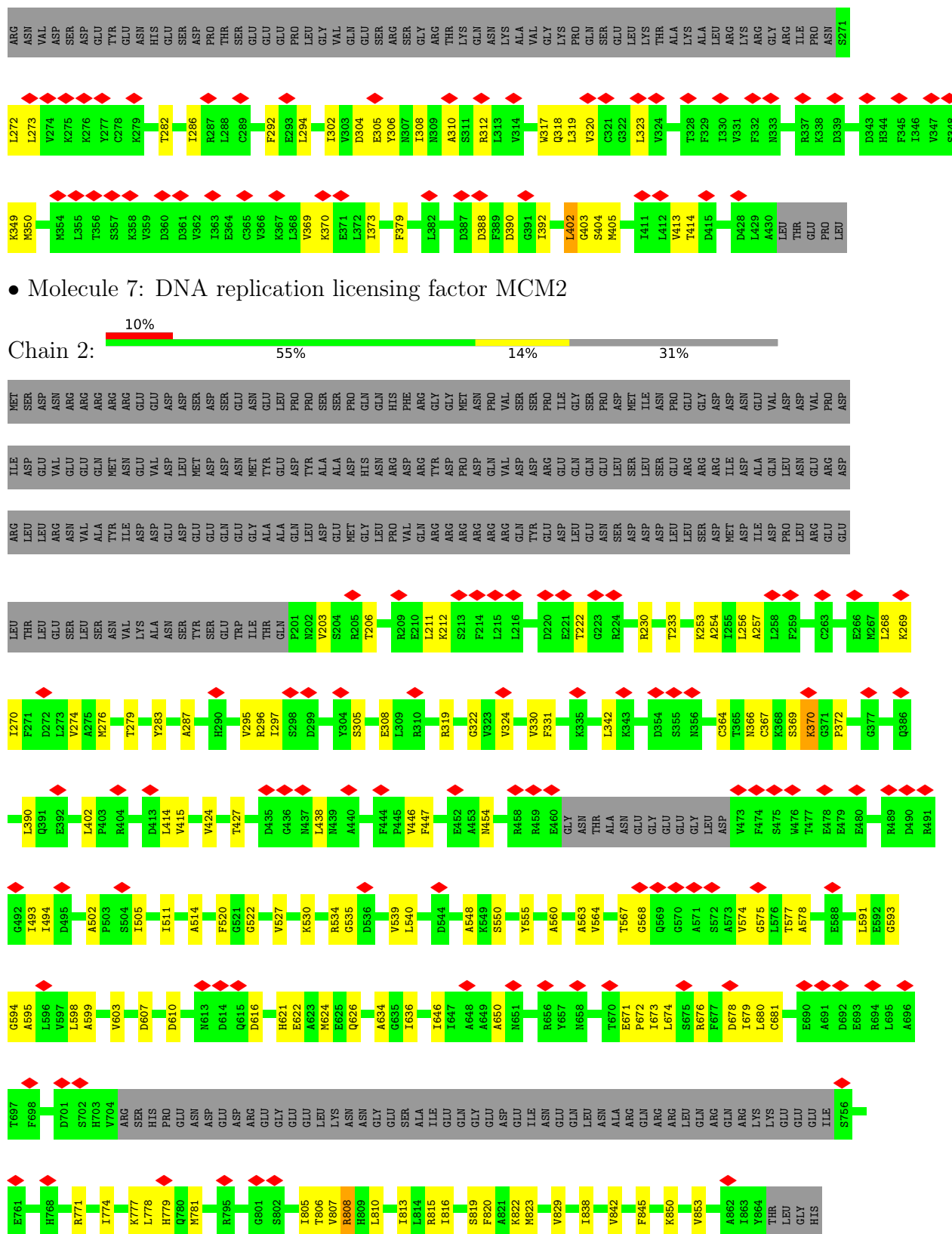


• Molecule 5: Origin recognition complex subunit 5



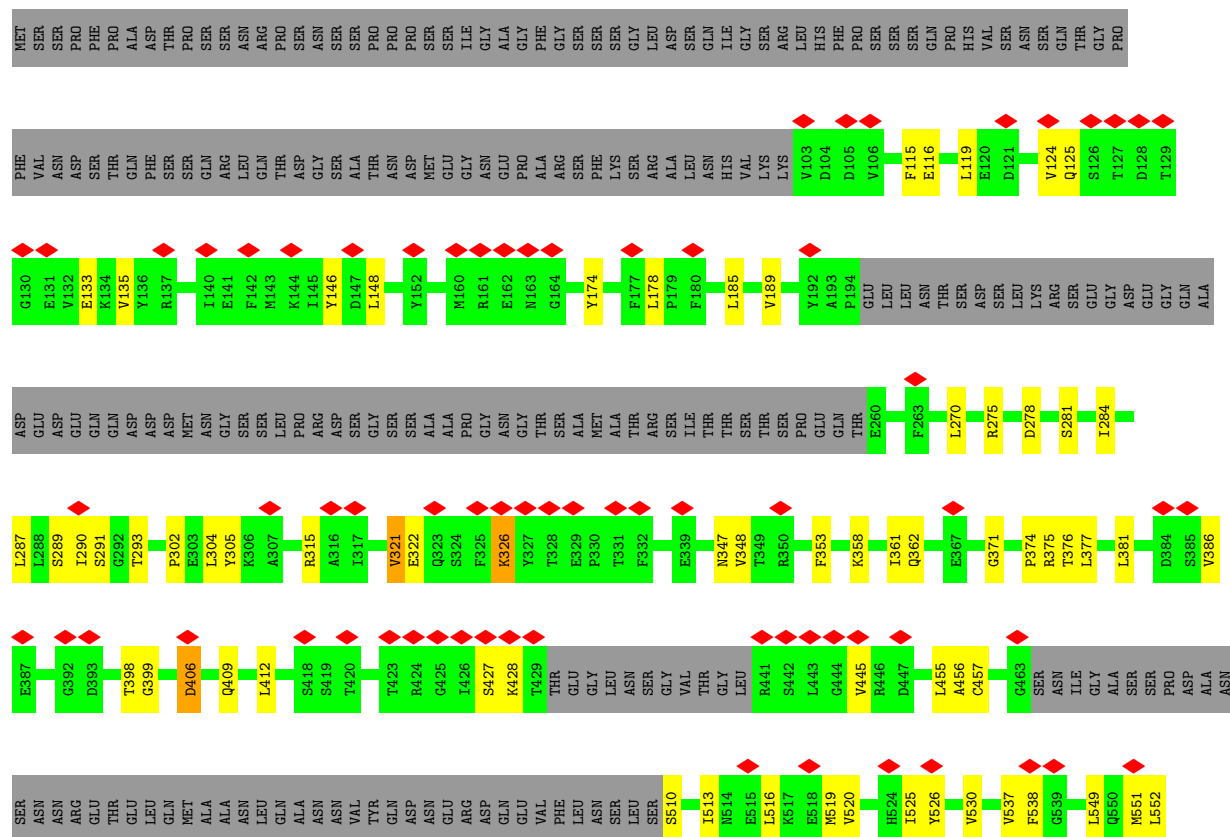
• Molecule 6: Origin recognition complex subunit 6

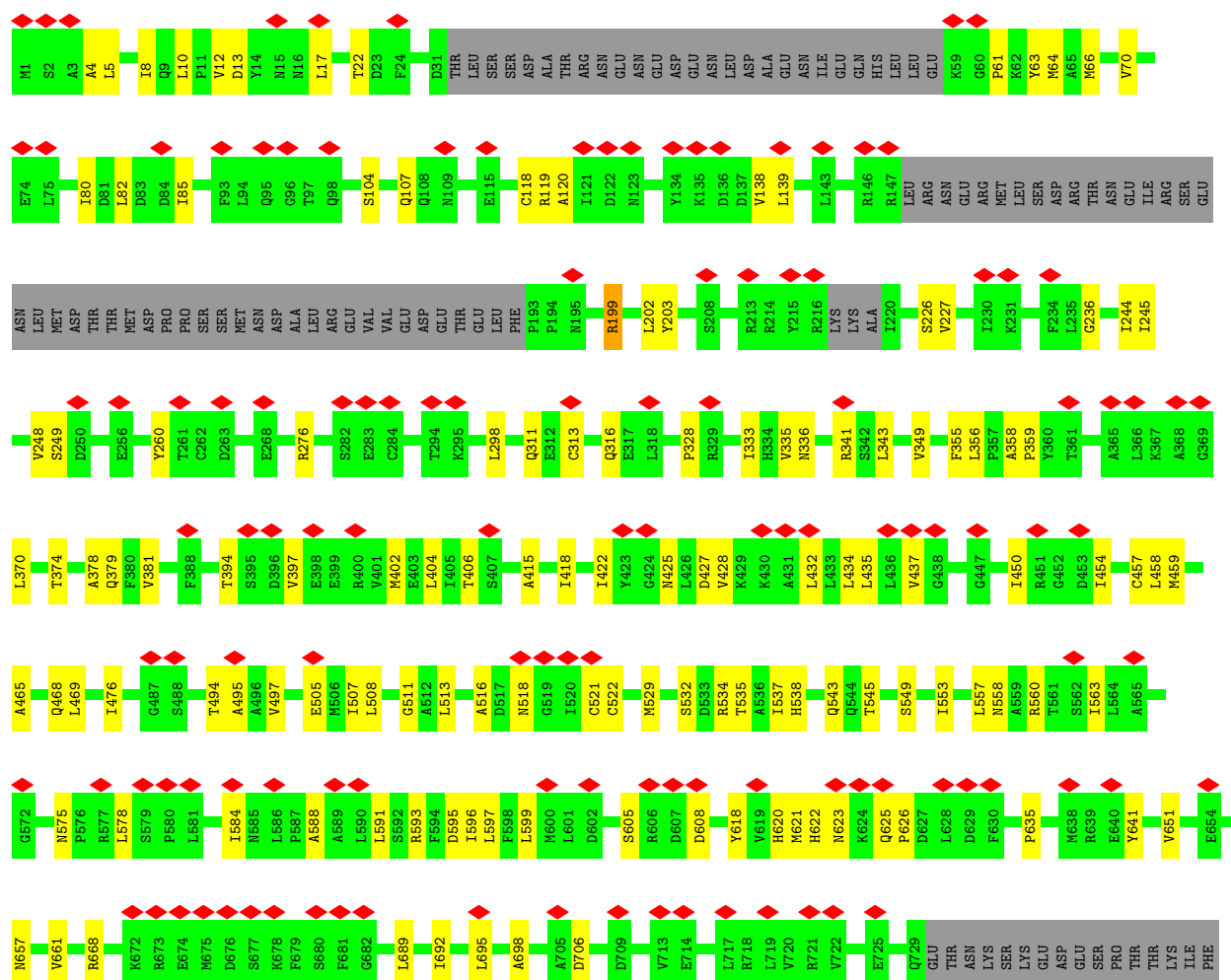




• Molecule 8: DNA replication licensing factor MCM3

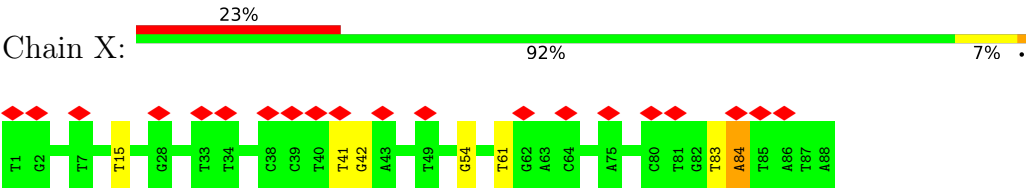




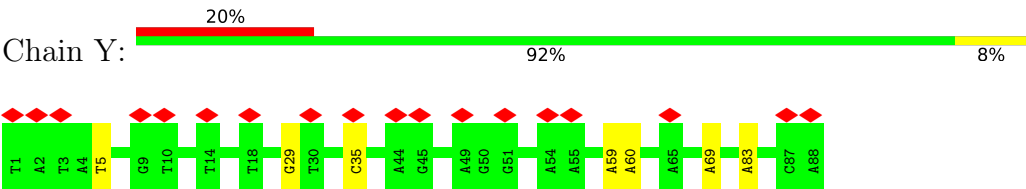


THR	ASP
ILE	GLY
ILE	THR
LYS	MET
LYS	ASP
MET	THR
LEU	ASP
GLN	GLN
THR	GLU
THR	ASP
GLY	SER
LYS	LEU
ASN	VAL
THR	SER
LEU	THR
SER	PRO
TYR	LYS
GLU	LEU
ASN	ALA
ILE	PRO
VAL	GLN
LYS	THR
THR	THR
VAL	ALA
ARG	SER
LEU	ALA
ARG	ASN
GLY	VAL
PHE	SER
THR	ALA
MET	GLN
LEU	ASP
GLN	SER
LEU	ILE
SER	ASP
ASN	ASP
CYS	LEU
ILE	GLN
GLN	ASP
GLU	ALA
TYR	
SER	
TYR	
LEU	
ASN	
VAL	
TRP	
HIS	
LEU	
ILE	
ASN	
GLY	
ASN	
THR	
LYS	
PHE	
VAL	
ASP	

● Molecule 13: DNA (88-MER)



● Molecule 14: DNA (88-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	177637	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 ($e^-/\text{\AA}^2$)	1.68	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	469.2, 469.2, 469.2	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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, ATP, ZN, MG

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	A	0.41	0/4020	0.63	1/5407 (0.0%)
2	B	0.53	0/2102	0.70	2/2844 (0.1%)
3	C	0.48	0/4918	0.69	0/6641
4	D	0.48	0/3628	0.67	0/4901
5	E	0.47	0/3835	0.67	1/5205 (0.0%)
6	F	0.55	0/2026	0.84	4/2722 (0.1%)
7	2	0.54	1/4835 (0.0%)	0.72	2/6529 (0.0%)
8	3	0.53	0/4775	0.75	2/6473 (0.0%)
9	4	0.50	0/5185	0.71	0/7009
10	5	0.59	1/4796 (0.0%)	0.81	9/6482 (0.1%)
11	6	0.54	0/4954	0.81	6/6683 (0.1%)
12	7	0.50	0/5219	0.71	0/7053
13	X	0.56	1/2006 (0.0%)	0.80	1/3097 (0.0%)
14	Y	0.54	0/2037	0.78	3/3139 (0.1%)
All	All	0.51	3/54336 (0.0%)	0.73	31/74185 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	84	DA	O3'-P	-10.07	1.46	1.61
7	2	370	LYS	N-CA	-5.55	1.39	1.46
10	5	486	ARG	CA-C	5.15	1.59	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	57	ARG	N-CA-C	9.41	126.00	113.20
11	6	321	VAL	N-CA-C	9.08	120.33	108.35
14	Y	60	DA	O3'-P-O5'	8.73	117.09	104.00
11	6	322	GLU	CB-CA-C	8.25	123.33	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	5	555	ILE	N-CA-C	-8.21	98.00	108.84
10	5	529	ARG	N-CA-C	7.99	123.14	113.23
11	6	322	GLU	N-CA-C	-7.99	96.19	109.46
2	B	477	PHE	N-CA-C	7.19	121.67	108.58
2	B	476	VAL	N-CA-C	-7.09	96.87	107.37
11	6	789	SER	N-CA-C	-6.83	96.18	108.48
11	6	790	ARG	N-CA-C	-6.79	102.01	111.52
6	F	68	LYS	N-CA-C	6.76	119.96	111.24
13	X	84	DA	O3'-P-O5'	6.71	114.07	104.00
7	2	370	LYS	N-CA-C	-6.69	102.22	110.65
10	5	567	SER	CA-C-N	6.59	131.11	120.30
10	5	567	SER	C-N-CA	6.59	131.11	120.30
10	5	528	GLY	N-CA-C	6.47	128.51	113.18
11	6	406	ASP	O-C-N	-6.42	116.75	123.56
10	5	523	ALA	N-CA-C	6.33	119.96	110.14
6	F	404	SER	N-CA-C	6.20	119.13	109.52
6	F	405	MET	CG-SD-CE	-5.92	87.89	100.90
10	5	486	ARG	N-CA-C	-5.68	101.03	110.17
8	3	703	GLU	N-CA-C	-5.66	105.11	111.28
10	5	437	VAL	N-CA-C	5.65	117.96	108.81
14	Y	59	DA	P-O3'-C3'	-5.55	111.87	120.20
10	5	169	THR	N-CA-C	-5.36	97.40	108.18
1	A	708	LYS	CG-CD-CE	5.29	123.46	111.30
5	E	170	MET	CB-CG-SD	-5.24	96.97	112.70
14	Y	5	DT	OP1-P-O3'	-5.23	92.32	108.00
8	3	432	THR	OG1-CB-CG2	5.09	119.48	109.30
7	2	808	ARG	N-CA-C	-5.03	105.07	111.11

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3958	4070	4070	92	0
2	B	2049	2018	2018	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4813	4766	4765	102	0
4	D	3566	3627	3627	80	0
5	E	3749	3780	3780	99	0
6	F	1995	2051	2051	36	0
7	2	4753	4820	4820	90	0
8	3	4696	4752	4752	104	0
9	4	5110	5172	5171	99	0
10	5	4730	4802	4803	96	0
11	6	4874	4908	4908	91	0
12	7	5138	5215	5214	109	0
13	X	1796	1010	1010	5	0
14	Y	1809	987	987	5	0
15	A	31	12	12	4	0
15	D	31	12	12	2	0
15	E	31	12	12	0	0
16	A	1	0	0	0	0
16	D	1	0	0	0	0
16	E	1	0	0	0	0
17	2	27	12	12	3	0
17	3	27	12	12	2	0
17	5	27	12	12	2	0
17	7	27	12	12	3	0
18	2	1	0	0	0	0
18	4	1	0	0	0	0
18	5	1	0	0	0	0
18	6	1	0	0	0	0
18	7	1	0	0	0	0
All	All	53245	52062	52060	960	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 9.

All (960) 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)
8:3:386:MET:HE3	8:3:715:VAL:HG22	1.39	0.98
1:A:550:PHE:O	1:A:558:LYS:NZ	2.09	0.86
6:F:302:ILE:HG23	6:F:323:LEU:HD13	1.60	0.83
3:C:80:GLU:OE2	3:C:84:LYS:HD2	1.79	0.81
8:3:488:GLU:O	8:3:493:GLN:N	2.15	0.79
9:4:775:VAL:HG21	11:6:725:THR:HG22	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3:554:ASN:O	10:5:630:ARG:NE	2.17	0.77
11:6:293:THR:N	11:6:362:GLN:O	2.18	0.76
3:C:410:ALA:HB2	3:C:424:LEU:HD21	1.66	0.76
12:7:236:GLY:N	12:7:355:PHE:O	2.19	0.75
3:C:346:LEU:HD21	3:C:351:LEU:HD21	1.68	0.74
1:A:874:LEU:HD22	1:A:879:LEU:HD23	1.69	0.74
5:E:36:GLN:NE2	5:E:37:GLY:O	2.22	0.73
10:5:422:LYS:HE3	17:5:801:ADP:O2B	1.89	0.73
12:7:80:ILE:HG13	12:7:202:LEU:HD21	1.71	0.73
4:D:396:ARG:NH2	4:D:528:GLN:O	2.22	0.73
1:A:564:LEU:O	1:A:564:LEU:HD12	1.89	0.73
1:A:645:ASP:OD1	1:A:681:ARG:NH2	2.22	0.72
9:4:594:LYS:O	9:4:594:LYS:HG2	1.90	0.72
6:F:50:LYS:O	11:6:315:ARG:NH1	2.22	0.72
6:F:402:LEU:HD23	6:F:402:LEU:C	2.15	0.71
8:3:367:LEU:HD12	8:3:378:LYS:HB3	1.71	0.71
12:7:434:LEU:HD23	12:7:695:LEU:HD22	1.72	0.71
10:5:425:LEU:O	10:5:429:VAL:HG23	1.90	0.71
4:D:108:LYS:N	15:D:2001:ATP:O1A	2.24	0.70
12:7:605:SER:HB2	12:7:608:ASP:OD2	1.91	0.70
8:3:167:SER:O	8:3:170:THR:OG1	2.09	0.70
4:D:396:ARG:NH1	4:D:526:TRP:O	2.24	0.70
1:A:849:LEU:HD21	1:A:863:ILE:HG22	1.72	0.70
11:6:362:GLN:HA	11:6:376:THR:HG22	1.74	0.70
11:6:695:LEU:N	11:6:792:SER:OG	2.24	0.70
12:7:199:ARG:O	12:7:199:ARG:HG3	1.90	0.70
12:7:203:TYR:OH	12:7:336:ASN:O	2.08	0.70
1:A:391:LEU:HD23	1:A:394:PHE:HB2	1.74	0.69
1:A:459:ILE:HD11	1:A:492:VAL:HG21	1.74	0.69
11:6:780:LEU:HD21	11:6:795:ILE:HD12	1.74	0.69
11:6:293:THR:O	11:6:362:GLN:N	2.25	0.69
1:A:476:TYR:OH	1:A:601:THR:O	2.11	0.68
3:C:111:ASP:OD2	3:C:312:HIS:NE2	2.27	0.68
3:C:541:TYR:OH	3:C:545:ARG:NH1	2.26	0.68
9:4:527:ALA:HB1	9:4:530:ILE:HD12	1.75	0.68
7:2:577:THR:O	7:2:594:GLY:N	2.28	0.67
3:C:140:ARG:HB3	5:E:68:VAL:HG21	1.75	0.67
4:D:478:ARG:NH1	14:Y:69:DA:OP1	2.27	0.67
12:7:343:LEU:HD21	12:7:381:VAL:HG21	1.75	0.67
9:4:392:ALA:O	11:6:281:SER:OG	2.08	0.66
5:E:64:PRO:HG3	5:E:73:LEU:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:357:CYS:SG	3:C:359:THR:OG1	2.53	0.66
1:A:636:ILE:HG22	1:A:707:LEU:HD21	1.77	0.66
11:6:807:SER:HB2	11:6:824:ILE:HD11	1.78	0.66
3:C:135:GLU:O	3:C:145:ARG:NH1	2.28	0.66
2:B:334:LEU:O	2:B:338:ILE:HG22	1.96	0.66
6:F:388:ASP:O	6:F:392:ILE:N	2.28	0.66
4:D:343:PRO:HA	4:D:346:ALA:HB3	1.78	0.66
11:6:361:ILE:HG22	11:6:377:LEU:O	1.96	0.66
11:6:572:CYS:SG	11:6:573:VAL:N	2.69	0.65
12:7:529:MET:O	12:7:534:ARG:NH1	2.28	0.65
5:E:144:ALA:O	5:E:148:LYS:NZ	2.28	0.65
10:5:600:LYS:O	10:5:604:THR:HG23	1.97	0.65
8:3:703:GLU:OE2	12:7:620:HIS:CD2	2.49	0.65
10:5:169:THR:O	10:5:169:THR:OG1	2.09	0.65
10:5:654:GLU:HA	10:5:657:ILE:HD12	1.78	0.65
12:7:402:MET:O	12:7:406:THR:HG23	1.97	0.65
7:2:268:LEU:HD12	7:2:269:LYS:HA	1.78	0.64
8:3:718:SER:OG	8:3:720:THR:O	2.14	0.64
4:D:126:GLN:N	4:D:126:GLN:OE1	2.30	0.64
5:E:273:ILE:HD12	5:E:284:LEU:HD21	1.80	0.64
9:4:437:GLY:HA2	9:4:464:VAL:HG22	1.78	0.64
7:2:560:ALA:HB3	7:2:563:ALA:HB2	1.80	0.64
3:C:457:PRO:O	3:C:458:ILE:HD13	1.98	0.64
5:E:240:ILE:HA	5:E:243:ILE:HD12	1.78	0.64
12:7:494:THR:O	12:7:511:GLY:N	2.31	0.64
1:A:426:VAL:HG22	1:A:643:LEU:HD23	1.79	0.63
1:A:849:LEU:HD21	1:A:863:ILE:CG2	2.28	0.63
6:F:52:ASP:O	6:F:57:ARG:HD2	1.98	0.63
4:D:361:CYS:HB3	4:D:364:LEU:HD12	1.79	0.63
7:2:514:ALA:HB1	7:2:679:ILE:HD13	1.80	0.63
11:6:566:ARG:NH1	11:6:656:MET:O	2.32	0.63
12:7:651:VAL:N	12:7:706:ASP:O	2.30	0.63
3:C:423:ASN:N	3:C:426:GLU:OE2	2.32	0.63
8:3:404:ASN:OD1	8:3:512:VAL:N	2.30	0.63
3:C:426:GLU:O	3:C:430:ASN:ND2	2.30	0.63
8:3:209:PHE:HB2	12:7:8:ILE:HG23	1.81	0.63
10:5:46:TYR:OH	10:5:67:HIS:ND1	2.29	0.63
12:7:313:CYS:SG	12:7:333:ILE:HD12	2.39	0.63
3:C:278:ASN:ND2	3:C:422:PHE:O	2.32	0.62
7:2:296:ARG:NH1	7:2:414:LEU:HD11	2.14	0.62
10:5:622:LEU:HD22	10:5:681:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:ILE:HD11	3:C:23:TYR:CZ	2.34	0.62
9:4:561:ASP:OD2	9:4:652:GLN:NE2	2.33	0.62
10:5:556:VAL:O	10:5:556:VAL:HG13	1.99	0.62
6:F:14:LEU:HD11	6:F:32:LEU:HB3	1.81	0.62
3:C:80:GLU:CD	3:C:84:LYS:HD2	2.23	0.62
7:2:342:LEU:HD12	7:2:372:PRO:HB2	1.80	0.62
3:C:278:ASN:OD1	3:C:424:LEU:N	2.31	0.62
3:C:323:TYR:HA	3:C:326:MET:HE3	1.80	0.62
10:5:482:PHE:O	10:5:485:MET:HE2	1.99	0.62
11:6:116:GLU:HA	11:6:119:LEU:HD12	1.82	0.62
2:B:241:ASP:O	2:B:242:THR:OG1	2.13	0.62
11:6:125:GLN:HB2	11:6:133:GLU:CB	2.29	0.62
12:7:591:LEU:HD21	12:7:597:LEU:HD13	1.82	0.62
1:A:490:ARG:O	1:A:490:ARG:NH1	2.30	0.62
10:5:301:TYR:O	10:5:325:THR:OG1	2.17	0.62
5:E:168:TYR:HB3	5:E:170:MET:HE2	1.82	0.61
8:3:421:PHE:O	8:3:425:THR:HG23	2.00	0.61
10:5:279:ASP:O	10:5:283:THR:HG23	1.99	0.61
8:3:212:ARG:NH1	8:3:230:ILE:O	2.33	0.61
9:4:245:ALA:HB1	9:4:258:TYR:HE1	1.65	0.61
1:A:797:LEU:O	4:D:332:ARG:NH1	2.34	0.61
6:F:15:ARG:HE	6:F:29:LEU:HD21	1.63	0.61
10:5:399:ILE:C	10:5:400:LEU:HD12	2.26	0.61
12:7:61:PRO:O	12:7:64:MET:N	2.33	0.61
2:B:286:GLN:O	2:B:290:ARG:NE	2.24	0.61
2:B:477:PHE:O	3:C:478:SER:HA	2.01	0.61
1:A:811:LEU:HD23	1:A:814:LYS:HE2	1.82	0.60
11:6:124:VAL:HG13	11:6:124:VAL:O	2.00	0.60
11:6:398:THR:O	11:6:457:CYS:N	2.33	0.60
8:3:386:MET:CE	8:3:715:VAL:HG22	2.25	0.60
4:D:470:THR:HG22	4:D:471:GLU:H	1.66	0.60
5:E:357:ILE:HD11	6:F:312:ARG:HE	1.66	0.60
7:2:805:ILE:HD11	7:2:845:PHE:CG	2.36	0.60
2:B:420:LEU:O	2:B:450:ILE:HG22	2.02	0.60
7:2:634:ALA:N	10:5:465:GLU:OE1	2.34	0.60
11:6:381:LEU:HB3	11:6:386:VAL:HG22	1.84	0.60
5:E:30:PRO:O	5:E:165:LYS:NZ	2.33	0.59
7:2:324:VAL:HG23	7:2:424:VAL:HG21	1.83	0.59
11:6:174:TYR:HE2	11:6:178:LEU:HD22	1.67	0.59
2:B:277:VAL:HG22	3:C:566:LEU:HD13	1.85	0.59
5:E:239:PHE:CZ	5:E:243:ILE:HD11	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:VAL:HG22	1:A:794:MET:HE2	1.84	0.59
9:4:339:ILE:HD11	11:6:412:LEU:HD13	1.84	0.59
8:3:400:ARG:NH1	8:3:402:ASP:O	2.36	0.59
10:5:206:SER:OG	10:5:207:LEU:N	2.36	0.59
12:7:591:LEU:HD21	12:7:597:LEU:CD1	2.33	0.59
8:3:656:LEU:O	8:3:660:VAL:HG23	2.02	0.59
9:4:712:VAL:HG12	12:7:668:ARG:NH2	2.17	0.59
9:4:428:ARG:NH2	9:4:481:ILE:HD11	2.18	0.59
9:4:558:TYR:OH	11:6:734:LEU:HD21	2.02	0.59
4:D:109:THR:N	15:D:2001:ATP:O1A	2.35	0.58
4:D:461:GLU:HA	4:D:464:VAL:HG22	1.84	0.58
5:E:199:THR:HA	5:E:202:VAL:HG22	1.85	0.58
7:2:505:ILE:HD13	7:2:548:ALA:HB3	1.85	0.58
3:C:374:ALA:HB1	3:C:377:ILE:HD11	1.84	0.58
11:6:519:MET:O	11:6:525:ILE:HD13	2.03	0.58
12:7:22:THR:HG22	12:7:120:ALA:HB1	1.84	0.58
5:E:193:ASN:N	5:E:196:GLU:OE2	2.36	0.58
8:3:410:ASP:OD2	8:3:551:ASP:N	2.36	0.58
2:B:277:VAL:CG2	3:C:566:LEU:HD13	2.33	0.58
5:E:386:LEU:HA	5:E:389:ILE:HG22	1.86	0.58
7:2:331:PHE:HB3	10:5:323:ILE:HD11	1.84	0.58
3:C:199:LEU:HD23	3:C:200:ALA:N	2.19	0.58
9:4:634:PHE:HE2	9:4:698:LEU:HD21	1.68	0.58
1:A:388:LEU:HD12	1:A:394:PHE:CD1	2.39	0.58
3:C:120:ASP:O	3:C:126:ASN:ND2	2.37	0.58
4:D:513:LEU:O	4:D:517:ILE:HG23	2.04	0.58
8:3:711:ALA:O	8:3:715:VAL:HG23	2.04	0.57
11:6:125:GLN:HB2	11:6:133:GLU:HB2	1.86	0.57
12:7:394:THR:HG22	12:7:397:VAL:HG22	1.86	0.57
7:2:296:ARG:O	7:2:297:ILE:HD13	2.04	0.57
7:2:331:PHE:CB	10:5:323:ILE:HD11	2.33	0.57
7:2:402:LEU:HD21	11:6:629:MET:HE2	1.86	0.57
10:5:426:LEU:CD2	10:5:520:LEU:HD13	2.34	0.57
11:6:574:VAL:HG22	11:6:682:ALA:CB	2.34	0.57
12:7:4:ALA:HB1	12:7:5:LEU:HD12	1.85	0.57
4:D:517:ILE:HD11	4:D:524:TYR:HD1	1.69	0.57
5:E:77:ILE:CD1	5:E:130:LEU:HD11	2.34	0.57
8:3:172:THR:OG1	10:5:252:ASP:OD2	2.20	0.57
9:4:224:LEU:HD22	9:4:227:ILE:HG13	1.86	0.57
10:5:25:THR:HA	10:5:28:ILE:HD12	1.86	0.57
5:E:18:LEU:CD2	5:E:187:VAL:HG21	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:564:VAL:HG11	7:2:595:ALA:CB	2.35	0.57
8:3:307:ASN:OD1	8:3:308:GLN:N	2.35	0.57
10:5:293:THR:C	10:5:294:ILE:HD12	2.29	0.57
1:A:874:LEU:CD2	1:A:879:LEU:HD23	2.33	0.57
12:7:557:LEU:HD23	12:7:558:ASN:N	2.19	0.57
2:B:390:ARG:O	2:B:390:ARG:HG2	2.02	0.57
8:3:43:ARG:O	8:3:47:VAL:HG23	2.05	0.56
8:3:712:HIS:ND1	8:3:725:ASP:OD1	2.37	0.56
12:7:404:LEU:HD22	12:7:641:TYR:CE1	2.40	0.56
1:A:807:ALA:HB1	1:A:828:GLU:HG3	1.86	0.56
5:E:11:ARG:NE	5:E:192:TYR:OH	2.38	0.56
8:3:416:SER:N	17:3:2001:ADP:O2B	2.34	0.56
3:C:184:ASP:N	3:C:184:ASP:OD1	2.35	0.56
8:3:307:ASN:HB3	10:5:207:LEU:HD12	1.86	0.56
8:3:420:ARG:NH2	10:5:501:THR:OG1	2.39	0.56
11:6:347:ASN:OD1	11:6:348:VAL:N	2.39	0.56
11:6:409:GLN:O	11:6:412:LEU:HD12	2.04	0.56
3:C:409:VAL:HG22	3:C:453:LEU:HD11	1.87	0.56
4:D:90:ILE:HG22	4:D:91:ILE:HG23	1.87	0.56
7:2:679:ILE:C	7:2:680:LEU:HD12	2.31	0.56
2:B:395:TYR:OH	13:X:15:DT:OP1	2.24	0.56
4:D:103:PRO:O	4:D:108:LYS:NZ	2.39	0.56
12:7:657:ASN:O	12:7:661:VAL:HG23	2.05	0.56
4:D:114:TYR:CZ	4:D:118:LEU:HD11	2.40	0.56
3:C:492:LEU:HD22	3:C:614:ARG:HE	1.71	0.56
12:7:66:MET:O	12:7:70:VAL:HG23	2.06	0.56
6:F:306:TYR:O	6:F:310:ALA:N	2.39	0.56
10:5:339:THR:HG22	10:5:340:SER:H	1.70	0.56
1:A:364:ASN:ND2	5:E:101:GLN:O	2.39	0.56
9:4:311:CYS:SG	9:4:326:ILE:HD11	2.46	0.56
10:5:496:ALA:O	10:5:500:GLN:N	2.39	0.56
12:7:605:SER:CB	12:7:608:ASP:OD2	2.53	0.55
4:D:346:ALA:HB1	5:E:20:SER:HB3	1.88	0.55
8:3:456:ARG:NH2	12:7:328:PRO:O	2.39	0.55
12:7:80:ILE:CG1	12:7:202:LEU:HD21	2.35	0.55
12:7:80:ILE:HD11	12:7:202:LEU:HD11	1.87	0.55
10:5:61:LEU:O	10:5:138:ILE:HD12	2.06	0.55
4:D:319:ASN:O	4:D:323:HIS:ND1	2.38	0.55
9:4:429:ALA:HB3	11:6:371:GLY:HA3	1.89	0.55
1:A:859:GLU:OE2	1:A:859:GLU:N	2.39	0.55
5:E:239:PHE:CE1	5:E:243:ILE:HD11	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:268:LEU:HD12	7:2:269:LYS:CA	2.37	0.55
10:5:279:ASP:OD1	10:5:279:ASP:N	2.39	0.55
8:3:559:ARG:O	8:3:562:SER:OG	2.24	0.55
12:7:335:VAL:HG13	12:7:378:ALA:HB3	1.89	0.55
1:A:486:THR:N	15:A:2001:ATP:O1A	2.39	0.55
1:A:790:VAL:HG23	4:D:254:LEU:CD2	2.36	0.55
5:E:69:SER:O	5:E:73:LEU:HD23	2.07	0.55
5:E:285:TYR:O	5:E:289:ILE:N	2.40	0.55
9:4:437:GLY:CA	9:4:464:VAL:HG22	2.37	0.55
9:4:585:THR:HG21	9:4:628:VAL:HB	1.89	0.55
12:7:497:VAL:HB	12:7:553:ILE:HD11	1.89	0.55
3:C:520:VAL:HG22	3:C:524:LEU:HD11	1.89	0.55
8:3:441:GLY:H	8:3:442:LEU:HD12	1.70	0.55
12:7:494:THR:HG22	12:7:495:ALA:H	1.71	0.55
3:C:242:THR:CG2	5:E:430:LEU:HD22	2.37	0.55
10:5:167:ILE:HD11	10:5:259:GLN:OE1	2.06	0.55
11:6:516:LEU:O	11:6:520:VAL:HG13	2.07	0.55
12:7:104:SER:O	12:7:107:GLN:NE2	2.38	0.55
1:A:475:ILE:HG23	1:A:596:ILE:HG23	1.89	0.54
2:B:444:LEU:HD23	2:B:445:SER:HA	1.88	0.54
7:2:813:ILE:HD13	7:2:838:ILE:CD1	2.37	0.54
1:A:629:HIS:HA	1:A:632:LEU:HD12	1.89	0.54
4:D:143:ILE:HD11	4:D:181:PHE:HA	1.88	0.54
5:E:214:CYS:SG	5:E:270:VAL:HG11	2.47	0.54
2:B:388:LEU:HD11	2:B:392:GLU:HB2	1.89	0.54
2:B:479:ASP:C	2:B:480:ILE:HD12	2.32	0.54
4:D:319:ASN:ND2	4:D:360:SER:O	2.40	0.54
8:3:195:LYS:N	8:3:251:ILE:O	2.40	0.54
8:3:363:LEU:O	8:3:366:SER:N	2.39	0.54
9:4:725:THR:HG21	12:7:657:ASN:CG	2.32	0.54
10:5:542:PHE:CE2	10:5:546:ILE:HD11	2.42	0.54
1:A:623:MET:SD	1:A:623:MET:N	2.80	0.54
5:E:75:GLN:HG2	5:E:100:LEU:HD12	1.88	0.54
7:2:212:LYS:HD3	7:2:274:VAL:HG13	1.90	0.54
8:3:100:LEU:HD11	8:3:161:PHE:CD1	2.42	0.54
8:3:320:LEU:HD12	8:3:321:ILE:N	2.23	0.54
10:5:387:ALA:HB1	10:5:552:MET:SD	2.47	0.54
12:7:437:VAL:HG11	12:7:698:ALA:HB1	1.89	0.54
12:7:465:ALA:N	17:7:901:ADP:N7	2.56	0.54
9:4:368:PRO:O	9:4:382:MET:HE2	2.08	0.54
9:4:637:MET:HE3	9:4:641:THR:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:7:260:TYR:HB3	12:7:298:LEU:HD13	1.88	0.54
5:E:10:PHE:O	5:E:11:ARG:NE	2.33	0.54
10:5:540:ILE:HG22	10:5:541:ASP:H	1.73	0.54
3:C:534:THR:C	3:C:535:ILE:HD12	2.33	0.54
5:E:333:ILE:HD11	5:E:462:ILE:HB	1.90	0.54
11:6:374:PRO:O	11:6:376:THR:HG23	2.07	0.54
1:A:488:THR:O	1:A:492:VAL:HG23	2.08	0.54
3:C:413:LEU:O	3:C:418:ASN:N	2.38	0.54
5:E:209:LEU:HD11	5:E:266:TRP:CE2	2.43	0.54
12:7:415:ALA:HA	12:7:418:ILE:HD12	1.90	0.54
4:D:327:ASN:O	4:D:332:ARG:N	2.39	0.53
1:A:790:VAL:HG23	4:D:254:LEU:HD22	1.91	0.53
3:C:64:LEU:HD21	3:C:288:VAL:CG2	2.37	0.53
9:4:491:ASP:OD2	9:4:493:ASN:ND2	2.42	0.53
6:F:97:LEU:HD22	11:6:315:ARG:HG2	1.91	0.53
11:6:573:VAL:HG12	11:6:713:PHE:HB2	1.90	0.53
8:3:42:VAL:HB	8:3:96:ILE:HD11	1.90	0.53
8:3:195:LYS:O	8:3:251:ILE:N	2.41	0.53
12:7:532:SER:O	12:7:535:THR:OG1	2.20	0.53
2:B:261:HIS:CG	2:B:265:MET:HE1	2.43	0.53
2:B:281:PHE:CZ	3:C:553:ILE:HD11	2.43	0.53
2:B:463:LEU:HD12	5:E:425:SER:HB2	1.90	0.53
5:E:205:ARG:HE	5:E:208:GLU:HB2	1.74	0.53
6:F:30:LYS:O	6:F:33:THR:HG22	2.09	0.53
9:4:248:LEU:O	9:4:254:THR:OG1	2.24	0.53
12:7:537:ILE:HG23	12:7:563:ILE:HD13	1.90	0.53
3:C:49:GLU:OE2	3:C:57:ARG:NH1	2.42	0.53
8:3:359:ILE:HA	8:3:362:ILE:HG22	1.90	0.53
11:6:549:LEU:HD23	11:6:552:LEU:HD12	1.90	0.53
7:2:567:THR:HG22	7:2:568:GLY:H	1.74	0.53
9:4:561:ASP:N	9:4:561:ASP:OD1	2.41	0.53
1:A:394:PHE:CZ	1:A:532:VAL:HG22	2.44	0.53
1:A:866:TRP:CE2	1:A:870:LEU:HD11	2.44	0.52
4:D:294:VAL:HG11	4:D:302:VAL:HG13	1.91	0.52
8:3:179:LEU:HD12	8:3:296:GLY:O	2.09	0.52
8:3:209:PHE:CE2	12:7:10:LEU:HD12	2.44	0.52
10:5:287:ILE:HG23	10:5:288:PRO:HD2	1.91	0.52
12:7:518:ASN:N	12:7:560:ARG:O	2.39	0.52
1:A:474:THR:HG22	1:A:595:VAL:CG1	2.40	0.52
5:E:192:TYR:O	5:E:253:ASN:ND2	2.42	0.52
5:E:333:ILE:HD13	5:E:459:ILE:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:4:417:LEU:HD12	9:4:418:CYS:N	2.24	0.52
11:6:636:CYS:SG	11:6:638:ILE:HD11	2.48	0.52
12:7:507:ILE:C	12:7:508:LEU:HD12	2.35	0.52
1:A:659:LEU:HD12	1:A:660:ILE:C	2.34	0.52
5:E:333:ILE:HD11	5:E:462:ILE:CG2	2.38	0.52
1:A:373:THR:HG23	14:Y:83:DA:O5'	2.09	0.52
2:B:319:VAL:HG21	3:C:491:LEU:HD21	1.91	0.52
3:C:579:VAL:HA	3:C:582:ILE:HD12	1.90	0.52
10:5:66:GLU:O	10:5:69:ILE:HG22	2.09	0.52
1:A:394:PHE:CE2	1:A:532:VAL:HG22	2.44	0.52
1:A:456:PHE:HD2	1:A:492:VAL:HG22	1.75	0.52
3:C:479:ILE:HG22	3:C:480:PHE:CD1	2.44	0.52
7:2:511:ILE:HD11	7:2:681:CYS:HB3	1.89	0.52
12:7:434:LEU:HD23	12:7:695:LEU:CD2	2.40	0.52
7:2:616:ASP:N	7:2:616:ASP:OD1	2.39	0.52
11:6:455:LEU:HD23	11:6:456:ALA:N	2.25	0.52
12:7:543:GLN:OE1	12:7:545:THR:OG1	2.13	0.52
6:F:273:LEU:HD13	6:F:318:GLN:CG	2.40	0.52
10:5:649:THR:HG1	10:5:652:GLN:H	1.57	0.52
11:6:305:TYR:O	11:6:321:VAL:HG11	2.10	0.52
1:A:565:LEU:HD21	1:A:568:LEU:HD13	1.92	0.52
5:E:103:GLU:H	5:E:107:LEU:HD12	1.75	0.52
7:2:850:LYS:O	7:2:853:VAL:HG12	2.10	0.52
11:6:721:GLU:O	11:6:725:THR:HG23	2.10	0.52
3:C:225:SER:O	3:C:225:SER:OG	2.28	0.52
5:E:67:LEU:HD23	5:E:73:LEU:HD22	1.92	0.52
5:E:452:VAL:CG2	5:E:454:VAL:HG22	2.40	0.52
1:A:809:LEU:HD22	1:A:898:VAL:HB	1.91	0.52
3:C:505:ASN:N	3:C:505:ASN:OD1	2.43	0.52
3:C:578:LYS:HA	3:C:581:LEU:HD12	1.91	0.51
8:3:683:TYR:HA	8:3:686:LEU:HD12	1.92	0.51
10:5:375:ALA:HB1	10:5:378:ILE:HB	1.92	0.51
1:A:388:LEU:HD12	1:A:394:PHE:CG	2.46	0.51
1:A:683:ARG:HE	1:A:684:MET:H	1.58	0.51
4:D:294:VAL:HG12	4:D:296:SER:H	1.76	0.51
4:D:104:ARG:NE	4:D:252:THR:OG1	2.43	0.51
4:D:119:LEU:HD23	4:D:127:PHE:CE1	2.46	0.51
8:3:368:ALA:HB3	8:3:378:LYS:CE	2.41	0.51
6:F:369:VAL:O	6:F:373:ILE:HG22	2.11	0.51
10:5:282:LEU:HD11	10:5:333:ILE:HG22	1.93	0.51
10:5:426:LEU:HD23	10:5:520:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:6:115:PHE:CZ	11:6:119:LEU:HD11	2.45	0.51
2:B:459:ILE:HD11	3:C:484:LYS:HD3	1.92	0.51
5:E:128:LEU:O	5:E:165:LYS:N	2.43	0.51
8:3:350:ILE:HA	8:3:353:LEU:HD12	1.92	0.51
3:C:328:TYR:HD1	3:C:468:LEU:HD21	1.76	0.51
3:C:334:PHE:HZ	3:C:354:LEU:HD23	1.75	0.51
5:E:218:ARG:NE	5:E:270:VAL:O	2.43	0.51
10:5:374:ILE:HD11	10:5:388:ILE:HG21	1.92	0.51
11:6:185:LEU:O	11:6:189:VAL:HG23	2.11	0.51
11:6:646:ILE:O	11:6:650:VAL:HG23	2.09	0.51
1:A:514:ASN:OD1	1:A:517:LYS:N	2.43	0.51
1:A:613:ILE:HD12	1:A:613:ILE:H	1.76	0.51
2:B:241:ASP:OD1	2:B:241:ASP:N	2.44	0.51
7:2:494:ILE:HD13	7:2:820:PHE:HD1	1.76	0.51
7:2:567:THR:HG23	7:2:607:ASP:OD1	2.10	0.51
7:2:598:LEU:O	7:2:598:LEU:HD12	2.11	0.51
1:A:791:ILE:O	1:A:795:THR:HG23	2.11	0.51
10:5:677:VAL:O	10:5:680:ALA:HB3	2.11	0.51
1:A:357:ILE:HD13	3:C:151:TYR:CD2	2.45	0.51
3:C:102:PHE:HD1	3:C:227:PHE:CE2	2.28	0.51
7:2:671:GLU:O	7:2:674:LEU:N	2.44	0.51
1:A:484:GLY:N	15:A:2001:ATP:O2A	2.43	0.50
6:F:28:TYR:O	6:F:32:LEU:HD23	2.11	0.50
10:5:655:ALA:O	10:5:659:ILE:HD12	2.11	0.50
12:7:80:ILE:HG22	12:7:82:LEU:HD21	1.93	0.50
12:7:521:CYS:SG	12:7:522:CYS:N	2.85	0.50
4:D:292:LEU:O	4:D:305:TRP:NE1	2.43	0.50
5:E:376:LEU:HD12	5:E:377:GLN:H	1.75	0.50
8:3:294:VAL:HG12	8:3:326:VAL:HG22	1.93	0.50
8:3:702:LEU:O	8:3:706:ILE:HD12	2.11	0.50
1:A:826:VAL:HG12	1:A:830:LYS:NZ	2.25	0.50
3:C:87:ILE:HG21	3:C:116:ILE:HD12	1.92	0.50
3:C:535:ILE:HG22	3:C:536:ASN:O	2.10	0.50
6:F:305:GLU:OE2	6:F:319:LEU:HD13	2.11	0.50
9:4:455:SER:N	12:7:276:ARG:O	2.44	0.50
12:7:202:LEU:HD23	12:7:203:TYR:N	2.25	0.50
1:A:799:PHE:CE1	1:A:911:LEU:HD21	2.47	0.50
1:A:429:GLN:HG3	1:A:643:LEU:HD13	1.93	0.50
3:C:117:GLU:O	3:C:118:LEU:HD12	2.12	0.50
6:F:53:GLU:O	6:F:57:ARG:HG3	2.12	0.50
8:3:262:PRO:CB	10:5:464:LEU:HD22	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3:356:LYS:O	8:3:359:ILE:HG23	2.12	0.50
9:4:279:CYS:O	9:4:283:LEU:HD23	2.11	0.50
7:2:774:ILE:HG23	7:2:822:LYS:HG2	1.94	0.50
9:4:326:ILE:HG22	9:4:437:GLY:C	2.36	0.50
7:2:574:VAL:HG12	7:2:575:GLY:H	1.77	0.50
9:4:727:LEU:CD2	9:4:736:ILE:HD12	2.42	0.50
6:F:272:LEU:HD12	6:F:317:TRP:CE2	2.47	0.50
7:2:296:ARG:C	7:2:297:ILE:HD13	2.37	0.50
9:4:331:LEU:HD12	9:4:332:VAL:N	2.27	0.50
12:7:82:LEU:HA	12:7:85:ILE:HD12	1.94	0.50
3:C:242:THR:HG22	5:E:430:LEU:HD22	1.94	0.50
4:D:70:ILE:HD11	4:D:290:ASN:HB3	1.93	0.50
7:2:564:VAL:HG11	7:2:595:ALA:HB1	1.93	0.50
1:A:811:LEU:HD11	1:A:825:ILE:HA	1.94	0.49
4:D:112:LEU:HD21	4:D:248:PHE:CD1	2.47	0.49
4:D:131:ARG:O	4:D:132:LEU:HD23	2.12	0.49
5:E:455:PRO:CD	5:E:458:ILE:HD12	2.41	0.49
7:2:838:ILE:O	7:2:842:VAL:HG23	2.12	0.49
9:4:744:VAL:O	9:4:748:THR:HG23	2.11	0.49
11:6:566:ARG:NH1	11:6:657:GLU:O	2.45	0.49
11:6:759:ARG:O	11:6:812:ARG:NH1	2.43	0.49
12:7:584:ILE:HD11	12:7:599:LEU:HD21	1.94	0.49
2:B:315:LEU:HD21	2:B:317:TYR:HD1	1.76	0.49
7:2:806:THR:HG22	7:2:807:VAL:HG12	1.94	0.49
8:3:223:THR:HG21	10:5:244:ILE:HA	1.94	0.49
3:C:242:THR:OG1	3:C:243:ASN:N	2.46	0.49
10:5:178:TYR:HB2	10:5:193:THR:HG22	1.95	0.49
10:5:572:VAL:HG21	17:5:801:ADP:H2	1.77	0.49
2:B:376:PHE:CE1	2:B:404:ILE:HD11	2.48	0.49
3:C:244:LEU:HD13	3:C:265:LYS:NZ	2.28	0.49
7:2:268:LEU:HD12	7:2:269:LYS:N	2.28	0.49
8:3:201:HIS:HB3	8:3:241:LEU:HD22	1.94	0.49
5:E:239:PHE:HA	5:E:242:LEU:HD12	1.94	0.49
10:5:50:LEU:O	10:5:54:ILE:HD12	2.12	0.49
10:5:176:ALA:O	10:5:194:ILE:HD11	2.13	0.49
7:2:621:HIS:HA	7:2:673:ILE:HD12	1.94	0.49
4:D:410:LEU:HD22	5:E:375:TYR:HB3	1.94	0.49
7:2:322:GLY:HA3	7:2:390:LEU:HD11	1.95	0.49
12:7:343:LEU:HD21	12:7:381:VAL:CG2	2.41	0.49
2:B:242:THR:HG22	2:B:243:PHE:N	2.28	0.49
2:B:305:TRP:HA	2:B:308:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:GLU:OE1	1:A:494:LYS:NZ	2.36	0.49
3:C:219:PHE:O	3:C:223:LEU:HD23	2.13	0.49
5:E:46:THR:HG22	5:E:49:LYS:CE	2.43	0.49
8:3:388:GLY:O	8:3:714:LYS:NZ	2.45	0.49
9:4:326:ILE:HG22	9:4:437:GLY:O	2.13	0.49
8:3:703:GLU:OE2	12:7:620:HIS:NE2	2.45	0.48
11:6:574:VAL:HG22	11:6:682:ALA:HB3	1.95	0.48
12:7:591:LEU:HD23	12:7:591:LEU:O	2.13	0.48
2:B:388:LEU:HD23	2:B:393:THR:OG1	2.14	0.48
3:C:287:THR:HG23	3:C:288:VAL:HG23	1.94	0.48
4:D:187:LEU:HD23	4:D:188:LEU:HD22	1.94	0.48
8:3:425:THR:HB	8:3:656:LEU:HD21	1.95	0.48
9:4:763:THR:HG21	9:4:817:VAL:O	2.12	0.48
12:7:335:VAL:HG22	12:7:378:ALA:HB2	1.95	0.48
12:7:513:LEU:O	12:7:516:ALA:N	2.40	0.48
12:7:595:ASP:OD1	12:7:596:ILE:N	2.46	0.48
12:7:689:LEU:HA	12:7:692:ILE:HD12	1.96	0.48
1:A:705:ARG:O	1:A:709:VAL:HG23	2.12	0.48
1:A:806:TYR:CD2	1:A:832:LEU:HD21	2.47	0.48
6:F:292:PHE:HB2	6:F:294:LEU:HD13	1.96	0.48
8:3:368:ALA:HB3	8:3:378:LYS:HE2	1.95	0.48
9:4:277:LYS:NZ	9:4:299:LYS:O	2.39	0.48
9:4:428:ARG:HH22	9:4:481:ILE:HD11	1.78	0.48
10:5:278:CYS:HB3	10:5:330:ILE:HD12	1.95	0.48
10:5:286:VAL:HG21	10:5:333:ILE:HD11	1.94	0.48
1:A:485:LYS:NZ	15:A:2001:ATP:O1B	2.31	0.48
4:D:285:VAL:O	4:D:313:LEU:HD21	2.13	0.48
8:3:422:VAL:O	8:3:425:THR:OG1	2.31	0.48
12:7:245:ILE:HD11	12:7:349:VAL:HG21	1.95	0.48
3:C:244:LEU:HD13	3:C:265:LYS:HZ1	1.78	0.48
3:C:542:ILE:HD13	3:C:545:ARG:NH2	2.29	0.48
3:C:594:MET:HB2	3:C:596:LEU:HD13	1.96	0.48
4:D:253:LYS:O	4:D:256:ILE:HD11	2.13	0.48
5:E:89:TYR:O	5:E:92:ILE:HG22	2.13	0.48
8:3:36:THR:HG23	8:3:39:ARG:NH2	2.27	0.48
11:6:358:LYS:NZ	11:6:617:GLU:OE1	2.46	0.48
12:7:608:ASP:OD2	12:7:608:ASP:N	2.46	0.48
2:B:458:HIS:CE1	5:E:444:LEU:HD11	2.48	0.48
8:3:676:ILE:O	8:3:680:VAL:HG23	2.14	0.48
8:3:424:ASN:O	8:3:657:ARG:NE	2.39	0.48
8:3:480:ASP:O	8:3:484:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:7:465:ALA:HB2	17:7:901:ADP:C5	2.49	0.48
1:A:791:ILE:HA	1:A:794:MET:HE3	1.96	0.48
5:E:270:VAL:O	5:E:273:ILE:HG22	2.13	0.48
9:4:728:TYR:OH	12:7:450:ILE:HD12	2.13	0.48
10:5:539:ASN:O	10:5:540:ILE:HD13	2.14	0.48
11:6:710:ASP:C	11:6:711:LEU:HD22	2.38	0.48
2:B:270:THR:HG22	2:B:272:GLU:H	1.79	0.48
3:C:293:ASN:N	3:C:293:ASN:OD1	2.45	0.48
5:E:22:ILE:HA	5:E:29:THR:HG22	1.96	0.48
8:3:350:ILE:HG23	8:3:659:TYR:HE1	1.79	0.48
3:C:244:LEU:HD11	5:E:299:LEU:C	2.38	0.48
4:D:253:LYS:C	4:D:256:ILE:HD11	2.39	0.48
8:3:262:PRO:HB3	10:5:464:LEU:HD22	1.96	0.48
3:C:102:PHE:HD1	3:C:227:PHE:HE2	1.62	0.47
3:C:288:VAL:HG13	3:C:291:LYS:NZ	2.28	0.47
5:E:99:PRO:O	5:E:102:VAL:HG12	2.14	0.47
9:4:199:MET:CE	9:4:283:LEU:HD21	2.44	0.47
9:4:526:ILE:HD12	9:4:541:LEU:CD2	2.43	0.47
11:6:782:LYS:O	11:6:785:ALA:HB3	2.14	0.47
5:E:455:PRO:HD2	5:E:458:ILE:HD12	1.95	0.47
9:4:436:THR:OG1	9:4:464:VAL:HG23	2.13	0.47
1:A:639:ARG:NH1	15:A:2001:ATP:N3	2.62	0.47
2:B:459:ILE:HG23	2:B:460:TYR:CG	2.49	0.47
3:C:520:VAL:HG22	3:C:524:LEU:CD1	2.44	0.47
5:E:18:LEU:HD11	5:E:35:LEU:HD21	1.94	0.47
7:2:279:THR:O	7:2:283:TYR:N	2.47	0.47
7:2:295:VAL:O	7:2:454:ASN:ND2	2.45	0.47
7:2:295:VAL:O	7:2:296:ARG:NE	2.47	0.47
6:F:292:PHE:CZ	6:F:350:MET:HE3	2.50	0.47
8:3:392:ASN:O	12:7:623:ASN:ND2	2.47	0.47
9:4:199:MET:HE2	9:4:227:ILE:HD11	1.95	0.47
11:6:146:TYR:HB3	11:6:148:LEU:HD21	1.96	0.47
12:7:459:MET:HE3	12:7:584:ILE:CG2	2.44	0.47
1:A:367:ARG:HG3	1:A:367:ARG:HH11	1.79	0.47
1:A:568:LEU:HD12	1:A:571:MET:HB2	1.95	0.47
1:A:633:LYS:HG2	1:A:689:ILE:HG22	1.97	0.47
4:D:106:SER:O	4:D:275:MET:HE1	2.15	0.47
4:D:323:HIS:NE2	4:D:364:LEU:HD13	2.30	0.47
9:4:609:VAL:HG11	12:7:505:GLU:HA	1.97	0.47
10:5:198:ASN:CG	10:5:251:ILE:HD11	2.40	0.47
1:A:799:PHE:HE1	1:A:911:LEU:HD21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:LEU:HD21	2:B:317:TYR:CD1	2.50	0.47
2:B:463:LEU:HD12	2:B:463:LEU:O	2.15	0.47
3:C:265:LYS:O	3:C:266:LEU:HD22	2.15	0.47
8:3:209:PHE:CZ	12:7:10:LEU:HD12	2.50	0.47
9:4:535:ASP:CB	9:4:828:LEU:HD11	2.44	0.47
1:A:372:TYR:N	14:Y:83:DA:OP1	2.48	0.47
1:A:695:LYS:NZ	1:A:783:ASN:OD1	2.47	0.47
5:E:265:LYS:HB3	5:E:291:LEU:HD22	1.96	0.47
6:F:370:LYS:HZ2	6:F:379:PHE:HZ	1.62	0.47
7:2:305:SER:OG	7:2:308:GLU:N	2.47	0.47
9:4:314:MET:SD	9:4:415:ILE:HD11	2.54	0.47
9:4:437:GLY:N	9:4:464:VAL:HG22	2.30	0.47
9:4:705:VAL:HG12	9:4:706:TYR:N	2.30	0.47
10:5:675:ARG:O	10:5:678:ASP:OD2	2.32	0.47
11:6:710:ASP:O	11:6:711:LEU:HD22	2.14	0.47
12:7:10:LEU:HB2	12:7:12:VAL:HG12	1.97	0.47
12:7:422:ILE:HG21	12:7:468:GLN:HB2	1.97	0.47
1:A:477:VAL:HG23	1:A:622:ILE:HG23	1.97	0.47
2:B:238:SER:OG	2:B:239:PHE:N	2.48	0.47
3:C:542:ILE:HD12	3:C:545:ARG:HB3	1.96	0.47
5:E:77:ILE:O	5:E:81:VAL:HG12	2.14	0.47
7:2:527:VAL:N	7:2:530:LYS:O	2.44	0.47
7:2:610:ASP:CG	7:2:650:ALA:HB1	2.39	0.47
10:5:178:TYR:O	10:5:249:LYS:N	2.44	0.47
10:5:415:LEU:HA	10:5:523:ALA:HB3	1.96	0.47
11:6:270:LEU:HD12	11:6:289:SER:HB2	1.96	0.47
3:C:517:MET:HE1	3:C:553:ILE:HD13	1.97	0.47
5:E:34:ILE:HD11	5:E:146:PHE:CZ	2.49	0.47
8:3:116:VAL:HG22	8:3:178:LYS:HD3	1.97	0.47
8:3:387:GLY:O	8:3:714:LYS:NZ	2.43	0.47
9:4:635:ASP:O	9:4:642:ARG:NH2	2.48	0.47
11:6:304:LEU:HD12	11:6:353:PHE:HE1	1.79	0.47
1:A:788:SER:OG	1:A:790:VAL:HG12	2.15	0.47
1:A:826:VAL:HG12	1:A:830:LYS:HZ1	1.80	0.47
9:4:191:THR:HG23	9:4:275:THR:HB	1.98	0.47
9:4:526:ILE:HD12	9:4:541:LEU:HD21	1.97	0.47
7:2:438:LEU:HD22	7:2:447:PHE:HE1	1.79	0.46
11:6:570:ASN:O	11:6:571:ILE:HD13	2.15	0.46
11:6:649:GLN:HA	11:6:652:ILE:HD12	1.97	0.46
2:B:281:PHE:HZ	3:C:553:ILE:HD11	1.81	0.46
2:B:447:ILE:HG22	2:B:449:GLN:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:136:ASP:OD2	5:E:137:SER:N	2.48	0.46
7:2:364:CYS:SG	7:2:366:ASN:ND2	2.83	0.46
8:3:398:HIS:NE2	8:3:492:GLN:O	2.46	0.46
10:5:622:LEU:HD21	10:5:677:VAL:CG1	2.45	0.46
11:6:554:GLY:HA2	11:6:808:GLU:HG2	1.98	0.46
4:D:187:LEU:CD2	4:D:188:LEU:HD22	2.46	0.46
6:F:282:THR:HG22	6:F:286:ILE:HD12	1.97	0.46
7:2:624:MET:HE2	7:2:646:ILE:HG21	1.97	0.46
9:4:335:SER:O	11:6:375:ARG:NH1	2.48	0.46
10:5:480:ASP:HA	10:5:522:ALA:HB3	1.98	0.46
4:D:140:GLN:O	4:D:143:ILE:HG22	2.15	0.46
5:E:376:LEU:HD12	5:E:377:GLN:N	2.31	0.46
7:2:534:ARG:HE	7:2:815:ARG:HH22	1.64	0.46
12:7:138:VAL:HG13	12:7:139:LEU:HD22	1.98	0.46
1:A:811:LEU:HD21	1:A:828:GLU:HB2	1.97	0.46
1:A:873:LEU:HD11	1:A:878:ILE:HD12	1.98	0.46
3:C:265:LYS:C	3:C:266:LEU:HD22	2.41	0.46
6:F:349:LYS:HD3	6:F:350:MET:HE3	1.98	0.46
7:2:319:ARG:HB2	7:2:427:THR:HG22	1.97	0.46
9:4:757:HIS:ND1	9:4:757:HIS:O	2.48	0.46
11:6:174:TYR:CE2	11:6:178:LEU:HD22	2.48	0.46
1:A:688:ALA:HB2	1:A:775:ILE:HA	1.97	0.46
3:C:484:LYS:NZ	5:E:387:LEU:HD13	2.31	0.46
4:D:425:ARG:O	4:D:426:ILE:HD13	2.16	0.46
7:2:778:LEU:HD23	10:5:577:THR:OG1	2.16	0.46
17:3:2001:ADP:O3B	10:5:651:ARG:NH1	2.49	0.46
9:4:451:ARG:HH21	11:6:445:VAL:HG21	1.81	0.46
12:7:13:ASP:O	12:7:17:LEU:HD13	2.16	0.46
2:B:421:ILE:HG23	2:B:451:ALA:O	2.16	0.46
9:4:259:HIS:O	9:4:263:ASN:ND2	2.47	0.46
9:4:528:PRO:O	9:4:736:ILE:HD11	2.15	0.46
9:4:581:VAL:O	9:4:585:THR:HG22	2.15	0.46
9:4:770:LEU:HD21	9:4:802:ILE:CG2	2.46	0.46
2:B:340:TYR:HE1	3:C:29:LEU:HD21	1.80	0.46
4:D:407:ASN:HB2	4:D:410:LEU:HD23	1.98	0.46
5:E:334:ALA:HB3	5:E:386:LEU:HD11	1.98	0.46
6:F:15:ARG:NE	6:F:29:LEU:HD21	2.30	0.46
9:4:451:ARG:NH2	11:6:445:VAL:HG21	2.30	0.46
7:2:678:ASP:OD1	7:2:678:ASP:N	2.49	0.46
9:4:707:LEU:HD12	9:4:708:VAL:N	2.30	0.46
12:7:249:SER:O	12:7:311:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:VAL:O	1:A:627:TYR:OH	2.29	0.46
3:C:288:VAL:HG12	3:C:288:VAL:O	2.15	0.46
3:C:303:LEU:HD21	3:C:425:ILE:HB	1.98	0.46
7:2:203:VAL:HG12	7:2:203:VAL:O	2.16	0.46
7:2:813:ILE:HA	7:2:816:ILE:HD12	1.98	0.46
9:4:234:ARG:NH1	9:4:289:LEU:HD22	2.32	0.46
10:5:487:ASP:O	10:5:491:VAL:HG23	2.16	0.46
11:6:526:TYR:O	11:6:530:VAL:HG23	2.16	0.46
1:A:833:ILE:O	1:A:836:ASN:N	2.49	0.45
1:A:888:ARG:NH2	4:D:512:GLU:OE1	2.48	0.45
3:C:21:SER:O	3:C:22:HIS:ND1	2.49	0.45
3:C:309:ASN:OD1	3:C:312:HIS:N	2.42	0.45
4:D:143:ILE:HA	4:D:146:ILE:HD12	1.97	0.45
5:E:333:ILE:HD11	5:E:462:ILE:HG21	1.97	0.45
6:F:402:LEU:HD23	6:F:402:LEU:O	2.16	0.45
7:2:222:THR:HG22	7:2:222:THR:O	2.15	0.45
8:3:442:LEU:HD12	8:3:442:LEU:N	2.31	0.45
8:3:472:ILE:HD12	8:3:512:VAL:CG1	2.46	0.45
10:5:35:ILE:HD13	10:5:97:VAL:HG21	1.98	0.45
6:F:273:LEU:HD13	6:F:318:GLN:HG3	1.98	0.45
6:F:319:LEU:HD12	6:F:320:VAL:N	2.31	0.45
7:2:254:ALA:O	7:2:257:ALA:N	2.49	0.45
7:2:548:ALA:HB2	17:2:901:ADP:C5	2.51	0.45
10:5:402:ASP:OD1	10:5:403:GLY:N	2.49	0.45
12:7:605:SER:HB2	12:7:608:ASP:CG	2.42	0.45
13:X:54:DG:N2	14:Y:35:DC:O2	2.32	0.45
2:B:390:ARG:NH2	2:B:390:ARG:HG3	2.30	0.45
5:E:38:TYR:O	5:E:41:THR:HG22	2.17	0.45
8:3:332:ARG:CZ	10:5:512:VAL:HG11	2.46	0.45
12:7:356:LEU:O	12:7:374:THR:OG1	2.27	0.45
4:D:72:PHE:HZ	4:D:291:LEU:HD21	1.81	0.45
4:D:319:ASN:OD1	4:D:322:ARG:NH2	2.43	0.45
4:D:514:ARG:HG2	4:D:514:ARG:HH11	1.82	0.45
7:2:591:LEU:HD21	7:2:636:ILE:CD1	2.47	0.45
8:3:176:LEU:HD11	10:5:250:PHE:HB2	1.98	0.45
8:3:196:LEU:HB3	12:7:370:LEU:HD23	1.98	0.45
8:3:569:HIS:NE2	10:5:657:ILE:HD13	2.30	0.45
8:3:695:SER:HB2	8:3:737:LEU:HD23	1.98	0.45
11:6:287:LEU:HD12	11:6:399:GLY:O	2.16	0.45
1:A:873:LEU:HD23	1:A:879:LEU:HB2	1.99	0.45
3:C:205:PHE:O	3:C:239:ASN:ND2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:235:PHE:CE1	4:D:247:ILE:HD13	2.52	0.45
7:2:330:VAL:HG12	7:2:415:VAL:CG2	2.46	0.45
8:3:460:GLY:O	8:3:464:LEU:N	2.49	0.45
9:4:234:ARG:HH11	9:4:289:LEU:HD22	1.82	0.45
10:5:139:LEU:HD12	10:5:140:ASN:N	2.31	0.45
10:5:360:LEU:HD13	10:5:594:ILE:HD11	1.99	0.45
7:2:813:ILE:HD13	7:2:838:ILE:HD12	1.99	0.45
12:7:341:ARG:HG3	12:7:341:ARG:HH11	1.82	0.45
12:7:553:ILE:HD12	12:7:553:ILE:H	1.81	0.45
2:B:447:ILE:HG22	2:B:449:GLN:N	2.31	0.45
3:C:201:MET:HB2	3:C:234:ILE:HG22	1.97	0.45
3:C:413:LEU:O	3:C:417:LEU:N	2.50	0.45
5:E:254:ASP:O	5:E:258:LEU:HD12	2.16	0.45
8:3:21:PHE:O	8:3:25:VAL:HG23	2.16	0.45
8:3:172:THR:HA	10:5:172:LEU:HD13	1.99	0.45
9:4:332:VAL:HG11	9:4:428:ARG:C	2.42	0.45
11:6:601:LYS:O	11:6:603:SER:N	2.50	0.45
1:A:456:PHE:CD2	1:A:492:VAL:HG22	2.51	0.45
3:C:346:LEU:HD23	3:C:346:LEU:O	2.17	0.45
3:C:513:LEU:HD22	3:C:556:PHE:CD1	2.52	0.45
4:D:288:VAL:HG21	4:D:324:ILE:HD11	1.97	0.45
4:D:344:LEU:O	4:D:348:SER:OG	2.29	0.45
5:E:209:LEU:O	5:E:215:LEU:HD11	2.17	0.45
10:5:347:THR:OG1	10:5:348:MET:HE2	2.17	0.45
12:7:335:VAL:HG22	12:7:378:ALA:CB	2.47	0.45
13:X:41:DT:H1'	13:X:42:DG:H5'	1.99	0.45
1:A:606:GLU:HB3	1:A:614:THR:HG21	1.99	0.45
4:D:294:VAL:HG11	4:D:302:VAL:CG1	2.47	0.45
4:D:375:ASN:C	4:D:376:LEU:HD22	2.42	0.45
9:4:770:LEU:HD21	9:4:802:ILE:HG22	1.98	0.45
11:6:694:SER:OG	11:6:792:SER:O	2.35	0.45
1:A:511:VAL:HB	1:A:563:VAL:HG12	1.99	0.45
4:D:70:ILE:HG21	4:D:291:LEU:CD2	2.47	0.45
5:E:61:TRP:C	5:E:62:LEU:HD12	2.42	0.45
5:E:409:ARG:NH1	6:F:392:ILE:HD11	2.32	0.45
8:3:653:ILE:O	8:3:656:LEU:N	2.41	0.45
9:4:637:MET:O	9:4:642:ARG:NH1	2.44	0.45
3:C:284:PHE:CE1	3:C:325:LEU:HD11	2.51	0.44
9:4:257:LEU:HD21	9:4:272:MET:HE1	1.99	0.44
9:4:552:PHE:HA	11:6:738:ARG:HE	1.81	0.44
9:4:707:LEU:HD12	9:4:708:VAL:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:327:ASN:HD22	4:D:337:LEU:HD13	1.82	0.44
7:2:610:ASP:OD2	7:2:650:ALA:HB1	2.17	0.44
10:5:276:MET:HE2	10:5:328:ILE:CD1	2.47	0.44
11:6:663:ILE:HB	11:6:670:ALA:HB3	1.97	0.44
12:7:22:THR:CG2	12:7:120:ALA:HB1	2.46	0.44
9:4:193:ASN:ND2	9:4:253:GLN:O	2.45	0.44
10:5:540:ILE:HG22	10:5:541:ASP:N	2.32	0.44
1:A:688:ALA:HA	1:A:775:ILE:HD13	1.98	0.44
7:2:276:MET:HE2	7:2:287:ALA:HB2	1.99	0.44
9:4:518:LEU:HD11	9:4:522:LEU:HD11	1.99	0.44
10:5:168:SER:OG	10:5:257:LYS:N	2.49	0.44
9:4:272:MET:O	9:4:276:ILE:HD12	2.18	0.44
9:4:609:VAL:HG13	9:4:610:ASP:OD1	2.16	0.44
11:6:557:LYS:C	11:6:564:LYS:HZ1	2.24	0.44
12:7:538:HIS:NE2	12:7:593:ARG:NH1	2.64	0.44
3:C:583:LEU:HD12	3:C:584:PHE:N	2.32	0.44
4:D:375:ASN:O	4:D:376:LEU:HD22	2.18	0.44
4:D:497:ILE:HD11	4:D:502:ARG:HB3	2.00	0.44
5:E:435:THR:HG22	5:E:436:THR:H	1.81	0.44
7:2:520:PHE:O	7:2:771:ARG:NH1	2.50	0.44
7:2:779:HIS:HB2	7:2:781:MET:HE2	1.99	0.44
8:3:488:GLU:O	8:3:492:GLN:C	2.60	0.44
9:4:323:ASP:N	9:4:439:PHE:O	2.45	0.44
10:5:529:ARG:HD3	10:5:529:ARG:N	2.33	0.44
12:7:118:CYS:SG	12:7:119:ARG:N	2.91	0.44
3:C:80:GLU:O	3:C:84:LYS:HG3	2.18	0.44
4:D:83:ASP:OD1	4:D:84:ARG:N	2.51	0.44
7:2:211:LEU:HD11	7:2:274:VAL:HG21	2.00	0.44
7:2:564:VAL:HG11	7:2:595:ALA:HB2	1.99	0.44
8:3:48:TYR:CD2	8:3:92:LEU:HD11	2.53	0.44
12:7:341:ARG:HG3	12:7:341:ARG:NH1	2.33	0.44
7:2:806:THR:HG21	10:5:419:GLY:N	2.32	0.44
8:3:468:GLY:O	8:3:511:SER:OG	2.36	0.44
11:6:552:LEU:CD1	11:6:813:ALA:HB2	2.48	0.44
3:C:405:HIS:O	3:C:409:VAL:HG23	2.18	0.44
4:D:219:ILE:HD11	4:D:231:LEU:HD22	2.00	0.44
4:D:466:LEU:HD21	5:E:191:ARG:NH1	2.32	0.44
7:2:548:ALA:N	17:2:901:ADP:N7	2.66	0.44
7:2:402:LEU:HD21	11:6:629:MET:CE	2.48	0.43
8:3:100:LEU:HD11	8:3:161:PHE:CE1	2.53	0.43
9:4:565:LEU:C	9:4:566:LEU:HD12	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:4:750:TYR:HE1	9:4:813:LEU:HD21	1.82	0.43
11:6:551:MET:HE1	11:6:755:ILE:HD13	1.98	0.43
5:E:41:THR:HG23	5:E:43:LYS:H	1.82	0.43
10:5:412:VAL:HG12	10:5:413:LEU:N	2.32	0.43
12:7:476:ILE:HG23	12:7:635:PRO:CB	2.48	0.43
4:D:510:LEU:HD23	4:D:511:GLN:N	2.32	0.43
5:E:56:ASN:O	5:E:58:HIS:NE2	2.51	0.43
5:E:333:ILE:HD11	5:E:462:ILE:CB	2.48	0.43
8:3:173:ALA:HB2	10:5:252:ASP:HB3	2.00	0.43
8:3:280:ASP:OD1	8:3:280:ASP:N	2.51	0.43
9:4:616:LEU:CD2	9:4:661:ILE:HD12	2.48	0.43
10:5:542:PHE:HE2	10:5:546:ILE:HD11	1.83	0.43
12:7:248:VAL:HG12	12:7:313:CYS:CB	2.48	0.43
2:B:468:MET:HE3	3:C:113:THR:HG21	2.00	0.43
3:C:409:VAL:O	3:C:413:LEU:HD13	2.18	0.43
4:D:493:GLN:N	5:E:437:MET:HE1	2.32	0.43
5:E:211:GLU:OE2	5:E:216:ARG:NH2	2.51	0.43
6:F:64:ILE:HD13	6:F:98:PHE:HE2	1.84	0.43
8:3:42:VAL:HG23	8:3:153:TRP:CZ3	2.53	0.43
6:F:402:LEU:C	6:F:402:LEU:CD2	2.85	0.43
7:2:230:ARG:O	7:2:233:THR:OG1	2.36	0.43
11:6:115:PHE:CE2	11:6:119:LEU:HD11	2.54	0.43
12:7:378:ALA:O	12:7:379:GLN:NE2	2.45	0.43
12:7:435:LEU:HD12	12:7:454:ILE:HB	2.00	0.43
1:A:886:ASN:ND2	4:D:506:MET:O	2.49	0.43
2:B:426:ASN:ND2	2:B:489:GLU:OE1	2.51	0.43
5:E:357:ILE:HD11	6:F:312:ARG:NE	2.31	0.43
8:3:419:LEU:HD11	8:3:473:ASP:HB3	2.00	0.43
8:3:687:ARG:CG	8:3:697:ILE:HG21	2.49	0.43
10:5:204:THR:HG22	10:5:205:VAL:HG13	1.99	0.43
12:7:459:MET:HE3	12:7:584:ILE:HG21	2.00	0.43
3:C:64:LEU:HD21	3:C:288:VAL:HG21	2.00	0.43
4:D:296:SER:O	4:D:298:ILE:HD12	2.18	0.43
5:E:149:TYR:HA	5:E:152:LEU:HD23	2.00	0.43
8:3:187:THR:HG21	10:5:461:GLU:CD	2.43	0.43
8:3:384:MET:HE1	8:3:513:ILE:HG13	2.01	0.43
9:4:311:CYS:N	9:4:327:ASN:OD1	2.52	0.43
12:7:437:VAL:HG11	12:7:698:ALA:CB	2.48	0.43
2:B:390:ARG:HG3	2:B:390:ARG:HH21	1.84	0.43
3:C:60:LEU:O	3:C:60:LEU:HD23	2.19	0.43
4:D:510:LEU:HD21	4:D:527:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:452:VAL:HG21	5:E:454:VAL:HG22	2.01	0.43
7:2:672:PRO:O	7:2:676:ARG:NH1	2.51	0.43
9:4:798:LEU:HD23	11:6:731:ILE:HG21	2.01	0.43
4:D:466:LEU:HD21	5:E:191:ARG:HH11	1.84	0.43
5:E:273:ILE:HD12	5:E:284:LEU:CD2	2.47	0.43
7:2:367:CYS:SG	7:2:369:SER:OG	2.75	0.43
12:7:80:ILE:HG22	12:7:82:LEU:CD2	2.49	0.43
2:B:285:PHE:CE1	3:C:513:LEU:HD23	2.54	0.43
4:D:416:GLU:C	4:D:420:LYS:HZ3	2.27	0.43
5:E:25:ASP:OD1	5:E:25:ASP:N	2.52	0.43
5:E:114:ASN:HA	5:E:117:VAL:HG22	2.01	0.43
8:3:666:ARG:HG3	8:3:666:ARG:O	2.18	0.43
9:4:435:VAL:HG23	9:4:466:VAL:HG23	2.01	0.43
10:5:660:THR:HG22	10:5:680:ALA:HB2	2.00	0.43
11:6:549:LEU:CD2	11:6:552:LEU:HD12	2.49	0.43
1:A:609:LEU:HD13	1:A:613:ILE:CG2	2.49	0.42
2:B:239:PHE:CD2	2:B:244:GLU:HB3	2.54	0.42
3:C:547:THR:HG22	3:C:547:THR:O	2.19	0.42
3:C:611:CYS:SG	3:C:612:VAL:HG13	2.59	0.42
4:D:235:PHE:HE1	4:D:247:ILE:HD13	1.84	0.42
4:D:380:LEU:HD11	4:D:468:PHE:CE1	2.53	0.42
5:E:34:ILE:HD11	5:E:146:PHE:CE2	2.54	0.42
6:F:304:ASP:OD2	6:F:308:ILE:HD12	2.19	0.42
7:2:276:MET:HE3	7:2:279:THR:HB	2.01	0.42
7:2:522:GLY:N	7:2:535:GLY:O	2.45	0.42
7:2:777:LYS:O	7:2:829:VAL:N	2.49	0.42
9:4:601:LEU:HD12	12:7:549:SER:HB3	2.01	0.42
9:4:678:ILE:HG22	9:4:691:ASN:O	2.19	0.42
10:5:476:VAL:HG22	10:5:477:VAL:N	2.34	0.42
1:A:839:ASN:HB3	1:A:842:VAL:HG22	2.01	0.42
4:D:269:SER:HB2	4:D:271:ARG:NE	2.33	0.42
9:4:393:ASP:OD1	11:6:281:SER:OG	2.36	0.42
9:4:518:LEU:CD1	9:4:522:LEU:HD11	2.49	0.42
11:6:427:SER:OG	11:6:428:LYS:N	2.51	0.42
12:7:428:VAL:O	12:7:432:LEU:HD23	2.19	0.42
13:X:61:DT:O2	14:Y:29:DG:N2	2.52	0.42
2:B:427:LEU:HD22	2:B:465:TRP:HZ2	1.83	0.42
4:D:396:ARG:HB2	4:D:529:LEU:HD12	2.01	0.42
5:E:281:PRO:HA	5:E:284:LEU:HB3	2.00	0.42
7:2:493:ILE:HD11	7:2:823:MET:O	2.19	0.42
7:2:622:GLU:OE1	10:5:440:SER:OG	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3:166:LEU:N	8:3:166:LEU:HD23	2.34	0.42
11:6:648:ASP:OD1	11:6:649:GLN:N	2.51	0.42
12:7:618:TYR:CD1	12:7:621:MET:HE2	2.54	0.42
1:A:809:LEU:HD11	1:A:901:ALA:HB3	2.01	0.42
2:B:444:LEU:HD23	2:B:445:SER:CA	2.48	0.42
5:E:380:LEU:HD13	5:E:449:ARG:CB	2.49	0.42
10:5:453:VAL:HG11	10:5:509:ILE:CD1	2.50	0.42
3:C:479:ILE:HG22	3:C:480:PHE:CE1	2.54	0.42
3:C:536:ASN:C	3:C:537:ILE:HD13	2.45	0.42
8:3:472:ILE:HD12	8:3:512:VAL:HG11	2.01	0.42
9:4:631:ILE:HG22	9:4:632:ASP:N	2.35	0.42
1:A:831:LEU:O	1:A:835:VAL:HG12	2.20	0.42
3:C:80:GLU:OE1	3:C:84:LYS:HD2	2.19	0.42
4:D:265:LYS:O	4:D:270:GLN:NE2	2.53	0.42
7:2:624:MET:HG3	7:2:646:ILE:HD13	2.02	0.42
8:3:169:ARG:HH21	10:5:287:ILE:HD11	1.84	0.42
8:3:368:ALA:HB2	8:3:421:PHE:CE1	2.55	0.42
8:3:687:ARG:HG3	8:3:697:ILE:HG21	2.01	0.42
9:4:712:VAL:HG12	12:7:668:ARG:CZ	2.49	0.42
11:6:275:ARG:HG2	11:6:278:ASP:HB2	2.02	0.42
11:6:510:SER:O	11:6:513:ILE:HG22	2.20	0.42
12:7:226:SER:OG	12:7:227:VAL:N	2.53	0.42
12:7:457:CYS:SG	12:7:458:LEU:N	2.93	0.42
11:6:537:VAL:HG13	11:6:583:GLN:OE1	2.20	0.42
12:7:244:ILE:O	12:7:316:GLN:N	2.48	0.42
1:A:513:ILE:HG21	1:A:565:LEU:HD12	2.01	0.42
1:A:529:TRP:HA	1:A:532:VAL:HG12	2.01	0.42
2:B:340:TYR:CE1	3:C:29:LEU:HD21	2.55	0.42
5:E:274:THR:H	5:E:277:ASN:HB2	1.85	0.42
7:2:370:LYS:O	7:2:370:LYS:HG2	2.20	0.42
8:3:221:LEU:HD12	8:3:221:LEU:H	1.84	0.42
10:5:673:GLN:O	10:5:677:VAL:HG23	2.19	0.42
11:6:574:VAL:HG13	11:6:684:PRO:HD3	2.01	0.42
2:B:277:VAL:HG22	3:C:566:LEU:HD22	2.02	0.42
2:B:421:ILE:HD12	2:B:451:ALA:O	2.20	0.42
3:C:437:ASP:N	3:C:437:ASP:OD1	2.52	0.42
6:F:37:SER:OG	6:F:38:ILE:N	2.52	0.42
7:2:819:SER:OG	7:2:820:PHE:N	2.52	0.42
8:3:364:SER:HA	8:3:367:LEU:HD11	2.02	0.42
12:7:469:LEU:HD12	12:7:469:LEU:H	1.84	0.42
4:D:260:LEU:HD22	4:D:265:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3:447:THR:OG1	8:3:456:ARG:O	2.31	0.42
11:6:455:LEU:HD23	11:6:456:ALA:C	2.45	0.42
1:A:524:CYS:SG	1:A:525:TYR:N	2.93	0.41
6:F:413:VAL:HG12	6:F:414:THR:N	2.35	0.41
7:2:599:ALA:HB1	7:2:603:VAL:N	2.35	0.41
8:3:413:THR:OG1	8:3:415:LYS:NZ	2.41	0.41
8:3:698:THR:O	8:3:701:THR:N	2.51	0.41
9:4:384:LEU:HD23	9:4:385:ILE:N	2.35	0.41
12:7:358:ALA:HB1	12:7:359:PRO:HD2	2.01	0.41
5:E:36:GLN:OE1	5:E:173:THR:HG22	2.20	0.41
5:E:380:LEU:HD13	5:E:449:ARG:HB3	2.03	0.41
8:3:100:LEU:HD12	8:3:160:SER:N	2.34	0.41
8:3:116:VAL:HG13	8:3:178:LYS:CE	2.49	0.41
9:4:421:ASP:OD2	9:4:422:GLU:N	2.50	0.41
11:6:836:ILE:HG22	11:6:837:ARG:O	2.20	0.41
12:7:422:ILE:HG21	12:7:468:GLN:CB	2.50	0.41
12:7:476:ILE:HG23	12:7:635:PRO:HB2	2.01	0.41
12:7:575:ASN:ND2	12:7:578:LEU:HD23	2.34	0.41
13:X:83:DT:H1'	13:X:84:DA:H5'	2.01	0.41
1:A:561:ILE:O	1:A:593:LEU:HD23	2.20	0.41
3:C:144:ARG:HG2	3:C:144:ARG:NH2	2.34	0.41
3:C:299:VAL:HG23	3:C:425:ILE:HG23	2.02	0.41
3:C:426:GLU:OE1	3:C:439:TYR:OH	2.24	0.41
4:D:136:ILE:HD11	5:E:151:LYS:HB2	2.02	0.41
5:E:193:ASN:O	5:E:197:VAL:HG12	2.21	0.41
8:3:197:ILE:HD11	8:3:251:ILE:HB	2.02	0.41
10:5:387:ALA:HB1	10:5:552:MET:CE	2.50	0.41
12:7:625:GLN:HB3	12:7:626:PRO:HD2	2.02	0.41
1:A:546:LEU:HD22	1:A:550:PHE:CZ	2.56	0.41
1:A:896:ILE:HG13	1:A:897:SER:H	1.86	0.41
3:C:213:PHE:HD1	3:C:251:LEU:HD13	1.85	0.41
8:3:403:ILE:HG13	8:3:707:ARG:HD2	2.02	0.41
9:4:522:LEU:HB3	9:4:541:LEU:HD13	2.01	0.41
9:4:609:VAL:HG21	12:7:505:GLU:N	2.35	0.41
9:4:708:VAL:HG12	9:4:708:VAL:O	2.20	0.41
10:5:65:MET:SD	10:5:139:LEU:HD13	2.61	0.41
1:A:410:LEU:HD23	1:A:410:LEU:H	1.85	0.41
1:A:642:GLY:C	1:A:643:LEU:HD12	2.46	0.41
3:C:596:LEU:HB2	3:C:597:ILE:HD12	2.03	0.41
5:E:272:ARG:O	5:E:277:ASN:ND2	2.53	0.41
7:2:211:LEU:HD21	7:2:270:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:621:HIS:CA	7:2:673:ILE:HD12	2.50	0.41
8:3:724:VAL:O	8:3:728:VAL:HG23	2.20	0.41
9:4:360:ILE:HD12	9:4:360:ILE:N	2.35	0.41
10:5:32:LYS:CG	10:5:93:ALA:HB1	2.51	0.41
10:5:375:ALA:CA	10:5:378:ILE:HD13	2.50	0.41
1:A:474:THR:HG22	1:A:595:VAL:HG12	2.01	0.41
6:F:302:ILE:HG23	6:F:323:LEU:CD1	2.42	0.41
7:2:502:ALA:HB2	7:2:555:TYR:CE2	2.54	0.41
8:3:706:ILE:HD12	8:3:706:ILE:H	1.86	0.41
10:5:472:ALA:O	10:5:517:THR:HG22	2.20	0.41
11:6:576:ASP:O	11:6:579:THR:OG1	2.33	0.41
11:6:663:ILE:HG22	11:6:664:ALA:N	2.34	0.41
11:6:811:ALA:HB2	11:6:819:ILE:HD13	2.02	0.41
4:D:289:ARG:HB2	4:D:313:LEU:HD23	2.03	0.41
7:2:810:LEU:HA	7:2:813:ILE:HD12	2.03	0.41
9:4:343:LYS:HA	9:4:360:ILE:HD13	2.02	0.41
9:4:616:LEU:HD12	9:4:616:LEU:N	2.36	0.41
2:B:361:LEU:H	2:B:361:LEU:HD23	1.86	0.41
3:C:80:GLU:OE1	3:C:84:LYS:CD	2.69	0.41
3:C:510:SER:OG	3:C:514:ASP:OD2	2.32	0.41
5:E:95:THR:O	5:E:95:THR:HG23	2.21	0.41
7:2:203:VAL:HG12	7:2:206:THR:OG1	2.21	0.41
7:2:591:LEU:HD21	7:2:636:ILE:HD11	2.02	0.41
8:3:545:LEU:HD11	8:3:708:LEU:CD1	2.51	0.41
9:4:331:LEU:HD12	9:4:331:LEU:C	2.46	0.41
10:5:255:PHE:C	10:5:256:LEU:HD12	2.46	0.41
3:C:457:PRO:C	3:C:458:ILE:HD13	2.45	0.41
4:D:305:TRP:O	4:D:309:LEU:HD23	2.21	0.41
4:D:354:LEU:O	4:D:358:ILE:HG22	2.20	0.41
4:D:369:LYS:O	4:D:373:SER:HB3	2.21	0.41
5:E:71:LYS:O	5:E:75:GLN:NE2	2.54	0.41
5:E:409:ARG:NE	6:F:390:ASP:OD1	2.54	0.41
8:3:341:MET:SD	8:3:341:MET:N	2.94	0.41
8:3:698:THR:O	8:3:701:THR:OG1	2.38	0.41
9:4:268:VAL:HA	9:4:271:ILE:HD12	2.03	0.41
9:4:345:ALA:HB2	9:4:365:ILE:CD1	2.50	0.41
10:5:529:ARG:HD3	10:5:529:ARG:H	1.86	0.41
11:6:281:SER:HA	11:6:284:ILE:HD11	2.03	0.41
1:A:865:SER:O	1:A:869:VAL:HG12	2.21	0.41
2:B:315:LEU:HD12	2:B:475:PHE:HD2	1.86	0.41
2:B:459:ILE:HD11	3:C:484:LYS:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:HIS:HB3	4:D:142:ALA:HB2	2.02	0.41
5:E:81:VAL:HG13	5:E:82:GLN:N	2.36	0.41
7:2:253:LYS:O	7:2:256:LEU:HD12	2.21	0.41
7:2:539:VAL:HG12	7:2:540:LEU:N	2.36	0.41
9:4:565:LEU:HD23	9:4:705:VAL:HG13	2.03	0.41
12:7:427:ASP:OD2	12:7:427:ASP:N	2.53	0.41
4:D:350:ASN:O	4:D:353:SER:OG	2.39	0.40
7:2:446:VAL:HG13	11:6:302:PRO:O	2.22	0.40
7:2:550:SER:N	17:2:901:ADP:O2A	2.54	0.40
9:4:311:CYS:SG	9:4:312:LYS:N	2.94	0.40
9:4:647:GLU:OE2	11:6:586:LYS:NZ	2.54	0.40
10:5:282:LEU:HD21	10:5:330:ILE:CG2	2.50	0.40
12:7:245:ILE:CD1	12:7:349:VAL:HG11	2.51	0.40
12:7:358:ALA:HB1	12:7:359:PRO:CD	2.51	0.40
1:A:429:GLN:HG3	1:A:643:LEU:HD22	2.03	0.40
1:A:596:ILE:HG22	1:A:597:ALA:H	1.87	0.40
2:B:462:PRO:HB3	5:E:418:ILE:HD11	2.03	0.40
2:B:463:LEU:HD13	5:E:424:LEU:HD23	2.02	0.40
5:E:18:LEU:HD21	5:E:187:VAL:HG21	2.03	0.40
8:3:667:VAL:HG11	8:3:714:LYS:HA	2.02	0.40
11:6:135:VAL:HG12	11:6:135:VAL:O	2.21	0.40
2:B:315:LEU:HD12	2:B:475:PHE:CD2	2.55	0.40
5:E:405:LEU:HA	5:E:408:LEU:HD13	2.04	0.40
6:F:39:LEU:HD22	6:F:61:CYS:HB3	2.03	0.40
7:2:578:ALA:HB2	7:2:593:GLY:HA2	2.04	0.40
8:3:717:LEU:HD12	8:3:717:LEU:N	2.37	0.40
9:4:308:VAL:HG11	9:4:325:LEU:HD21	2.04	0.40
11:6:574:VAL:HG12	11:6:575:GLY:N	2.36	0.40
1:A:699:VAL:HG13	1:A:700:SER:H	1.86	0.40
3:C:569:LEU:O	3:C:575:ALA:HB2	2.21	0.40
4:D:500:ASP:C	4:D:501:LEU:HD22	2.46	0.40
5:E:127:CYS:C	5:E:128:LEU:HD22	2.47	0.40
7:2:330:VAL:HG12	7:2:415:VAL:HG22	2.04	0.40
10:5:375:ALA:HB3	10:5:385:LYS:HD3	2.03	0.40
11:6:326:LYS:HG3	11:6:326:LYS:O	2.22	0.40
11:6:326:LYS:O	11:6:326:LYS:CG	2.70	0.40
11:6:381:LEU:CB	11:6:386:VAL:HG22	2.51	0.40
11:6:537:VAL:HG12	11:6:538:PHE:H	1.87	0.40
12:7:465:ALA:HB2	17:7:901:ADP:N7	2.36	0.40
1:A:426:VAL:HG22	1:A:643:LEU:CD2	2.50	0.40
5:E:42:GLY:O	5:E:46:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:81:VAL:HG13	5:E:82:GLN:H	1.86	0.40
5:E:205:ARG:NE	5:E:208:GLU:OE1	2.54	0.40
9:4:191:THR:HG23	9:4:275:THR:CB	2.51	0.40
9:4:435:VAL:HG22	9:4:436:THR:H	1.86	0.40
9:4:680:SER:HB3	12:7:588:ALA:HB3	2.02	0.40
10:5:181:ILE:HD11	10:5:192:ILE:HD12	2.03	0.40
10:5:261:ILE:HG22	10:5:263:GLU:H	1.87	0.40
10:5:375:ALA:HA	10:5:378:ILE:HD13	2.02	0.40
11:6:290:ILE:HG22	11:6:291:SER:N	2.37	0.40
12:7:620:HIS:O	12:7:620:HIS:ND1	2.53	0.40
12:7:621:MET:HE3	12:7:622:HIS:NE2	2.36	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	A	486/949 (51%)	447 (92%)	39 (8%)	0	100	100
2	B	243/620 (39%)	215 (88%)	28 (12%)	0	100	100
3	C	578/616 (94%)	514 (89%)	64 (11%)	0	100	100
4	D	429/529 (81%)	389 (91%)	40 (9%)	0	100	100
5	E	455/479 (95%)	409 (90%)	44 (10%)	2 (0%)	30	66
6	F	234/435 (54%)	208 (89%)	25 (11%)	1 (0%)	30	66
7	2	595/868 (68%)	528 (89%)	67 (11%)	0	100	100
8	3	589/1006 (58%)	521 (88%)	68 (12%)	0	100	100
9	4	635/933 (68%)	572 (90%)	61 (10%)	2 (0%)	36	71
10	5	590/775 (76%)	526 (89%)	63 (11%)	1 (0%)	43	77
11	6	608/1017 (60%)	541 (89%)	67 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	7	646/845 (76%)	579 (90%)	67 (10%)	0	100	100
All	All	6088/9072 (67%)	5449 (90%)	633 (10%)	6 (0%)	49	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	4	373	ARG
9	4	668	ARG
5	E	412	SER
10	5	434	PRO
6	F	403	GLY
5	E	373	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/842 (52%)	436 (100%)	2 (0%)	81	81
2	B	230/573 (40%)	228 (99%)	2 (1%)	70	76
3	C	543/576 (94%)	540 (99%)	3 (1%)	78	80
4	D	404/488 (83%)	402 (100%)	2 (0%)	81	81
5	E	423/440 (96%)	422 (100%)	1 (0%)	87	85
6	F	228/406 (56%)	227 (100%)	1 (0%)	84	82
7	2	526/770 (68%)	524 (100%)	2 (0%)	84	82
8	3	518/864 (60%)	517 (100%)	1 (0%)	87	85
9	4	582/848 (69%)	579 (100%)	3 (0%)	81	81
10	5	539/688 (78%)	535 (99%)	4 (1%)	76	79
11	6	537/886 (61%)	531 (99%)	6 (1%)	65	74
12	7	575/753 (76%)	572 (100%)	3 (0%)	81	81
All	All	5543/8134 (68%)	5513 (100%)	30 (0%)	78	81

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	ARG
1	A	810	ASN
2	B	390	ARG
2	B	476	VAL
3	C	184	ASP
3	C	342	ASN
3	C	472	SER
4	D	383	LEU
4	D	396	ARG
5	E	170	MET
6	F	402	LEU
7	2	626	GLN
7	2	808	ARG
8	3	432	THR
9	4	534	GLU
9	4	682	TYR
9	4	685	ASN
10	5	169	THR
10	5	171	VAL
10	5	437	VAL
10	5	685	GLN
11	6	326	LYS
11	6	406	ASP
11	6	596	VAL
11	6	612	VAL
11	6	781	ARG
11	6	805	ARG
12	7	63	TYR
12	7	199	ARG
12	7	425	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	720	HIS
2	B	286	GLN
2	B	297	GLN
2	B	310	GLN
2	B	405	GLN
2	B	426	ASN
3	C	214	ASN

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Mol	Chain	Res	Type
3	C	308	ASN
4	D	270	GLN
4	D	370	ASN
4	D	489	ASN
6	F	383	GLN
6	F	407	GLN
7	2	245	ASN
7	2	356	ASN
7	2	366	ASN
7	2	621	HIS
7	2	666	ASN
7	2	703	HIS
8	3	29	GLN
8	3	46	GLN
8	3	141	HIS
8	3	151	HIS
8	3	175	HIS
8	3	731	ASN
9	4	240	ASN
9	4	320	ASN
9	4	488	ASN
9	4	666	ASN
9	4	676	ASN
9	4	683	ASN
9	4	685	ASN
9	4	797	GLN
10	5	43	GLN
10	5	254	GLN
10	5	344	ASN
10	5	524	ASN
10	5	560	HIS
10	5	576	HIS
10	5	579	ASN
10	5	586	GLN
10	5	587	GLN
10	5	617	GLN
10	5	636	ASN
11	6	556	HIS
11	6	653	HIS
12	7	112	HIS
12	7	384	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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$
17	ADP	5	801	-	28,29,29	1.41	4 (14%)	43,45,45	1.90	11 (25%)
15	ATP	A	2001	16	32,33,33	1.32	4 (12%)	48,52,52	1.85	11 (22%)
15	ATP	D	2001	16	32,33,33	1.29	5 (15%)	48,52,52	1.90	10 (20%)
15	ATP	E	2001	16	32,33,33	1.37	5 (15%)	48,52,52	1.75	9 (18%)
17	ADP	2	901	-	28,29,29	1.36	4 (14%)	43,45,45	2.00	13 (30%)
17	ADP	3	2001	-	28,29,29	1.42	6 (21%)	43,45,45	1.88	10 (23%)
17	ADP	7	901	-	28,29,29	1.37	5 (17%)	43,45,45	1.86	10 (23%)

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
17	ADP	5	801	-	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	ATP	A	2001	16	-	3/22/38/38	0/3/3/3
15	ATP	D	2001	16	-	3/22/38/38	0/3/3/3
15	ATP	E	2001	16	-	4/22/38/38	0/3/3/3
17	ADP	2	901	-	-	3/16/32/32	0/3/3/3
17	ADP	3	2001	-	-	5/16/32/32	0/3/3/3
17	ADP	7	901	-	-	2/16/32/32	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	801	ADP	C5-C4	4.64	1.47	1.39
15	E	2001	ATP	C5-C4	4.50	1.47	1.39
15	D	2001	ATP	C5-C4	4.39	1.46	1.39
15	A	2001	ATP	C5-C4	4.33	1.46	1.39
17	2	901	ADP	C5-C4	3.99	1.46	1.39
17	7	901	ADP	C5-C4	3.89	1.46	1.39
17	3	2001	ADP	C5-C4	3.69	1.45	1.39
17	2	901	ADP	C5-N7	-3.10	1.33	1.39
17	3	2001	ADP	C4-N9	-2.87	1.31	1.37
17	5	801	ADP	C5-C6	2.75	1.48	1.41
17	7	901	ADP	C5-N7	-2.75	1.34	1.39
17	3	2001	ADP	C5-N7	-2.71	1.34	1.39
15	E	2001	ATP	C5-C6	2.69	1.48	1.41
15	A	2001	ATP	C5-C6	2.67	1.48	1.41
15	E	2001	ATP	C5-N7	-2.60	1.34	1.39
17	7	901	ADP	C8-N9	-2.59	1.33	1.37
17	7	901	ADP	C4-N9	-2.59	1.32	1.37
17	3	2001	ADP	C5-C6	2.45	1.47	1.41
17	2	901	ADP	C8-N9	-2.44	1.33	1.37
15	D	2001	ATP	C5-C6	2.43	1.47	1.41
17	5	801	ADP	C8-N7	2.41	1.36	1.31
15	A	2001	ATP	C5-N7	-2.41	1.34	1.39
17	3	2001	ADP	C8-N9	-2.36	1.33	1.37
15	D	2001	ATP	C5-N7	-2.36	1.34	1.39
17	2	901	ADP	C4-N9	-2.31	1.32	1.37
17	5	801	ADP	C5-N7	-2.28	1.34	1.39
15	A	2001	ATP	C8-N7	2.28	1.36	1.31
17	3	2001	ADP	C8-N7	2.24	1.36	1.31
15	E	2001	ATP	C8-N7	2.19	1.35	1.31
15	D	2001	ATP	C8-N7	2.17	1.35	1.31
15	D	2001	ATP	C4-N9	-2.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	E	2001	ATP	C8-N9	-2.04	1.34	1.37
17	7	901	ADP	C8-N7	2.03	1.35	1.31

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	2001	ATP	C5-C4-N3	-5.91	118.59	126.72
17	5	801	ADP	C5-C4-N3	-5.89	118.61	126.72
15	E	2001	ATP	C5-C4-N3	-5.70	118.87	126.72
15	D	2001	ATP	C5-C4-N3	-5.60	119.01	126.72
17	3	2001	ADP	C5-C4-N3	-5.42	119.25	126.72
17	2	901	ADP	C5-C4-N3	-5.22	119.53	126.72
15	D	2001	ATP	N3-C4-N9	5.07	135.79	127.17
17	7	901	ADP	C5-C4-N3	-5.02	119.81	126.72
17	2	901	ADP	N3-C4-N9	4.89	135.48	127.17
17	5	801	ADP	N3-C4-N9	4.65	135.08	127.17
17	7	901	ADP	N3-C4-N9	4.47	134.76	127.17
15	E	2001	ATP	N3-C4-N9	4.36	134.58	127.17
15	A	2001	ATP	N3-C4-N9	4.36	134.58	127.17
15	A	2001	ATP	C2-N3-C4	4.07	121.78	111.83
15	A	2001	ATP	N3-C2-N1	-4.04	122.46	128.58
15	D	2001	ATP	C4-N9-C8	3.99	109.93	105.74
17	3	2001	ADP	N3-C4-N9	3.96	133.91	127.17
17	5	801	ADP	C2-N3-C4	3.89	121.34	111.83
17	3	2001	ADP	C4-C5-N7	-3.85	106.18	110.58
17	3	2001	ADP	C2-N3-C4	3.78	121.07	111.83
17	2	901	ADP	C2'-C1'-N9	-3.78	103.91	113.30
15	E	2001	ATP	C2-N3-C4	3.77	121.04	111.83
17	5	801	ADP	N3-C2-N1	-3.71	122.96	128.58
15	E	2001	ATP	C4-C5-N7	-3.70	106.35	110.58
15	A	2001	ATP	C4-C5-N7	-3.63	106.43	110.58
17	5	801	ADP	C4-C5-N7	-3.59	106.47	110.58
17	2	901	ADP	C4-N9-C8	3.58	109.50	105.74
15	D	2001	ATP	C2-N3-C4	3.56	120.52	111.83
17	7	901	ADP	C4-N9-C8	3.55	109.46	105.74
15	E	2001	ATP	N3-C2-N1	-3.53	123.24	128.58
17	2	901	ADP	N3-C2-N1	-3.49	123.30	128.58
17	3	2001	ADP	N3-C2-N1	-3.49	123.30	128.58
17	7	901	ADP	C2-N3-C4	3.39	120.11	111.83
17	2	901	ADP	C2-N3-C4	3.34	119.99	111.83
17	7	901	ADP	N3-C2-N1	-3.32	123.55	128.58
15	D	2001	ATP	N3-C2-N1	-3.30	123.59	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	2001	ATP	C2'-C1'-N9	-3.22	105.30	113.30
17	3	2001	ADP	C4-N9-C8	3.15	109.05	105.74
15	D	2001	ATP	C4-C5-N7	-2.99	107.17	110.58
17	5	801	ADP	C4-N9-C8	2.86	108.74	105.74
17	5	801	ADP	C5-N7-C8	2.79	107.84	103.45
17	3	2001	ADP	C6-C5-N7	2.76	137.41	132.09
17	2	901	ADP	C3'-C2'-C1'	2.75	106.67	101.46
17	2	901	ADP	N6-C6-N1	2.75	124.50	118.38
17	7	901	ADP	C2'-C1'-N9	-2.72	106.55	113.30
15	D	2001	ATP	N9-C8-N7	-2.68	110.14	113.94
15	A	2001	ATP	C3'-C2'-C1'	2.67	106.51	101.46
15	A	2001	ATP	C5-N7-C8	2.66	107.64	103.45
17	7	901	ADP	C4-C5-N7	-2.65	107.55	110.58
15	D	2001	ATP	C5-N7-C8	2.62	107.57	103.45
17	3	2001	ADP	C5-N7-C8	2.61	107.55	103.45
15	E	2001	ATP	C5-N7-C8	2.57	107.49	103.45
17	3	2001	ADP	N9-C8-N7	-2.52	110.37	113.94
17	7	901	ADP	N6-C6-N1	2.50	123.94	118.38
17	2	901	ADP	C4-C5-N7	-2.48	107.75	110.58
15	A	2001	ATP	C4-N9-C8	2.48	108.34	105.74
15	A	2001	ATP	C6-C5-N7	2.42	136.76	132.09
15	E	2001	ATP	C4-N9-C8	2.41	108.26	105.74
17	5	801	ADP	N9-C8-N7	-2.33	110.63	113.94
17	5	801	ADP	C3'-C2'-C1'	2.19	105.61	101.46
15	E	2001	ATP	C6-C5-N7	2.19	136.32	132.09
17	5	801	ADP	C6-C5-N7	2.18	136.29	132.09
17	2	901	ADP	C5-N7-C8	2.17	106.86	103.45
15	A	2001	ATP	N9-C8-N7	-2.14	110.89	113.94
17	7	901	ADP	C2'-C3'-C4'	2.14	106.75	102.61
17	2	901	ADP	N9-C8-N7	-2.13	110.91	113.94
15	E	2001	ATP	C2-N1-C6	2.12	122.21	118.73
17	3	2001	ADP	C3'-C2'-C1'	2.10	105.44	101.46
17	2	901	ADP	C5-C6-N6	-2.09	118.11	123.29
17	5	801	ADP	C2-N1-C6	2.08	122.16	118.73
17	7	901	ADP	C5-C6-N6	-2.08	118.13	123.29
15	D	2001	ATP	O2B-PB-O1B	2.06	122.01	112.44
17	2	901	ADP	C2-N1-C6	2.05	122.11	118.73
15	A	2001	ATP	C2-N1-C6	2.02	122.05	118.73

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	2001	ATP	C5'-O5'-PA-O1A
15	A	2001	ATP	C5'-O5'-PA-O2A
15	A	2001	ATP	C5'-O5'-PA-O3A
15	E	2001	ATP	C5'-O5'-PA-O1A
15	E	2001	ATP	C5'-O5'-PA-O2A
15	E	2001	ATP	C5'-O5'-PA-O3A
17	2	901	ADP	C5'-O5'-PA-O2A
17	2	901	ADP	C5'-O5'-PA-O3A
17	3	2001	ADP	C5'-O5'-PA-O1A
17	3	2001	ADP	C5'-O5'-PA-O2A
17	3	2001	ADP	C5'-O5'-PA-O3A
17	7	901	ADP	C5'-O5'-PA-O3A
17	3	2001	ADP	O4'-C4'-C5'-O5'
17	3	2001	ADP	C3'-C4'-C5'-O5'
17	5	801	ADP	O4'-C4'-C5'-O5'
17	5	801	ADP	C3'-C4'-C5'-O5'
15	E	2001	ATP	O4'-C4'-C5'-O5'
17	7	901	ADP	C5'-O5'-PA-O1A
15	D	2001	ATP	C3'-C4'-C5'-O5'
15	D	2001	ATP	O4'-C4'-C5'-O5'
17	5	801	ADP	PB-O3A-PA-O1A
17	5	801	ADP	PB-O3A-PA-O2A
15	D	2001	ATP	PG-O3B-PB-O1B
17	2	901	ADP	O4'-C4'-C5'-O5'

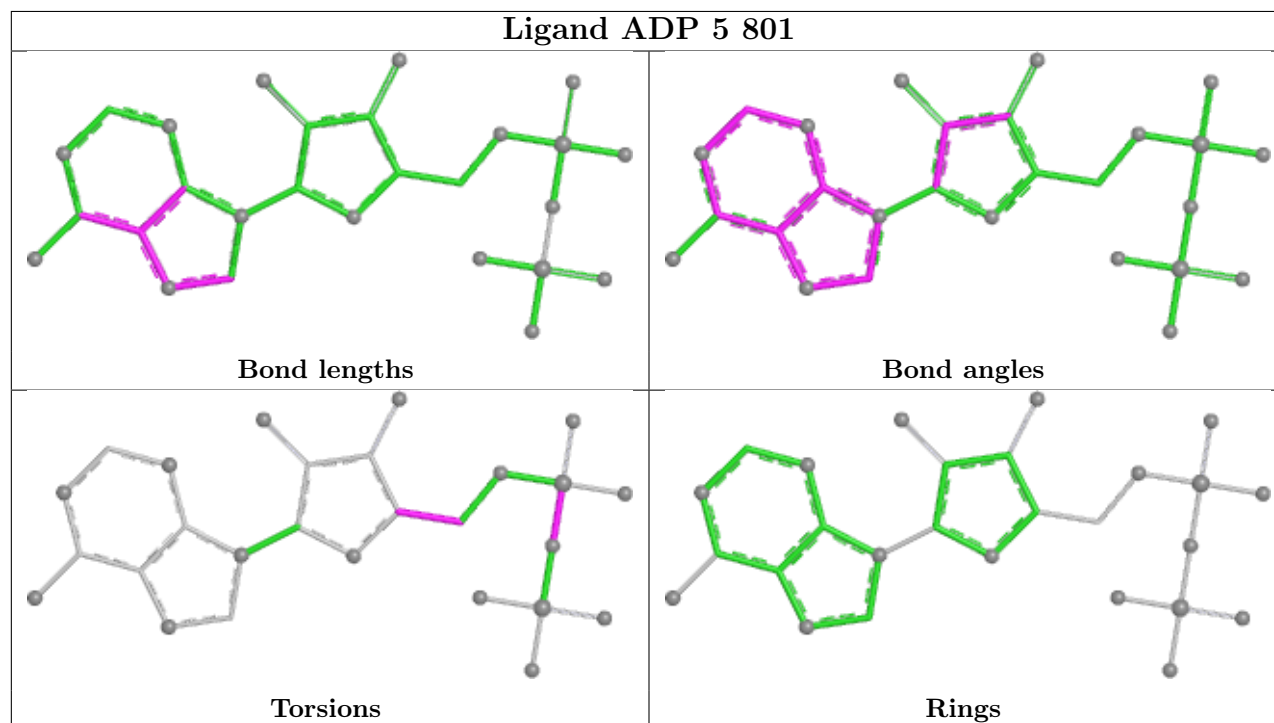
There are no ring outliers.

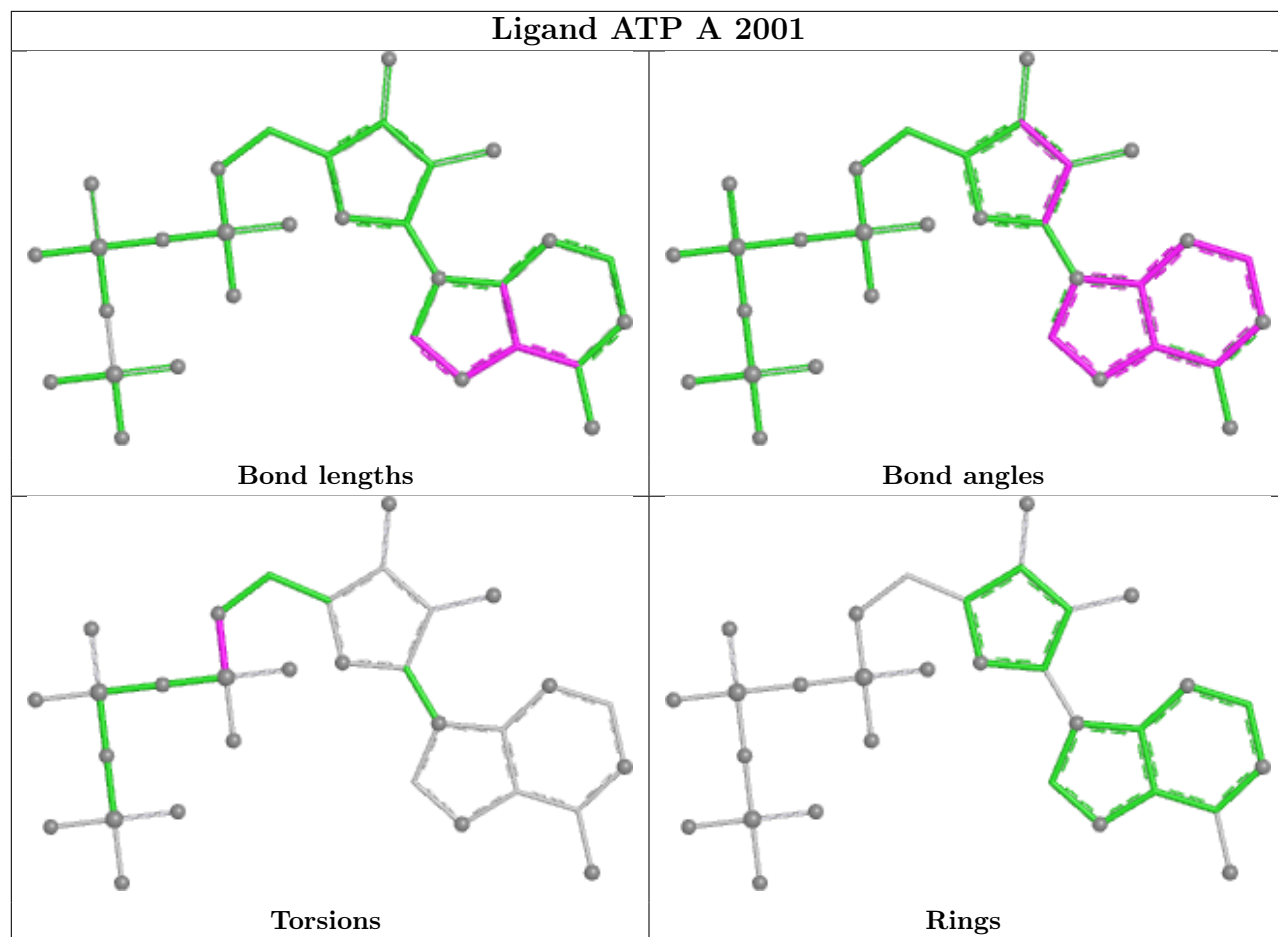
6 monomers are involved in 16 short contacts:

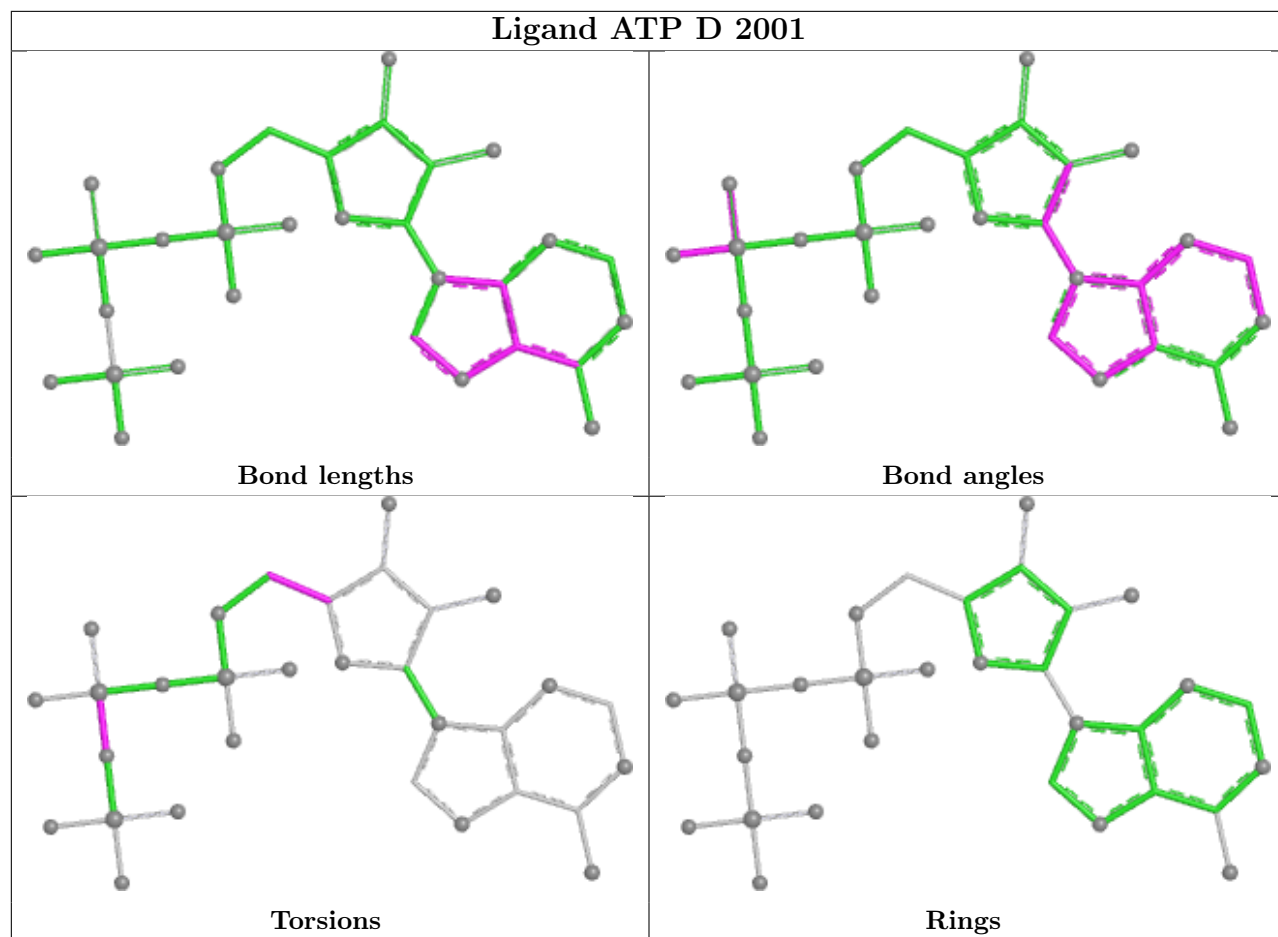
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	5	801	ADP	2	0
15	A	2001	ATP	4	0
15	D	2001	ATP	2	0
17	2	901	ADP	3	0
17	3	2001	ADP	2	0
17	7	901	ADP	3	0

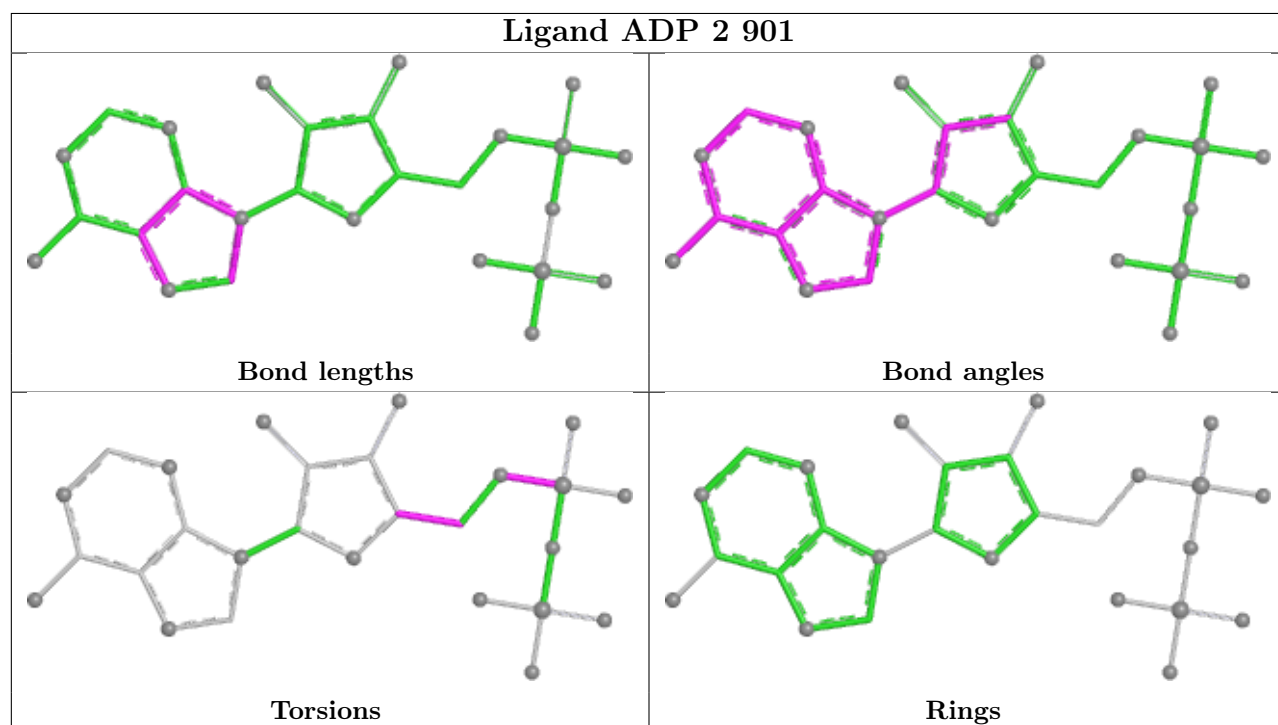
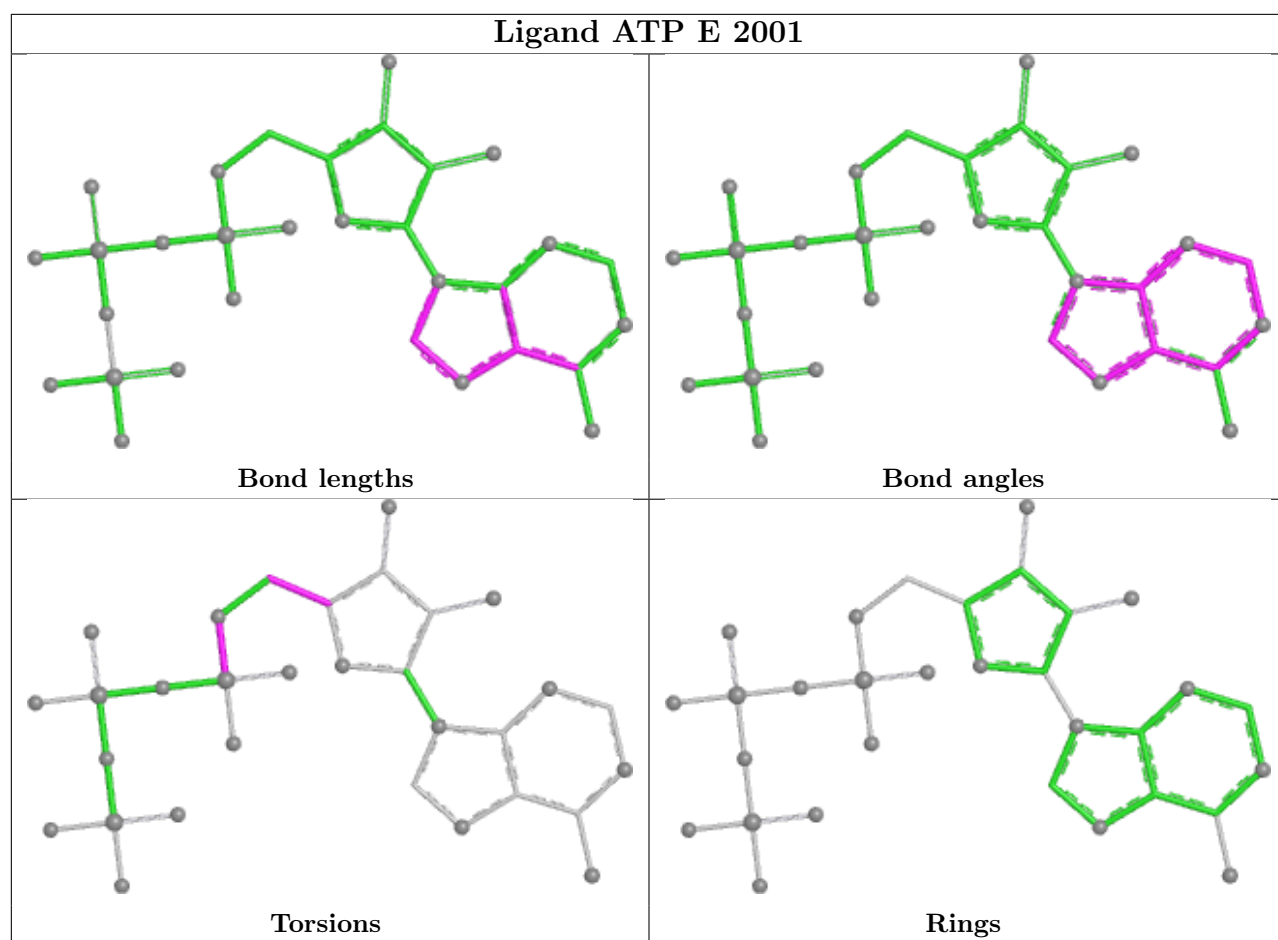
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

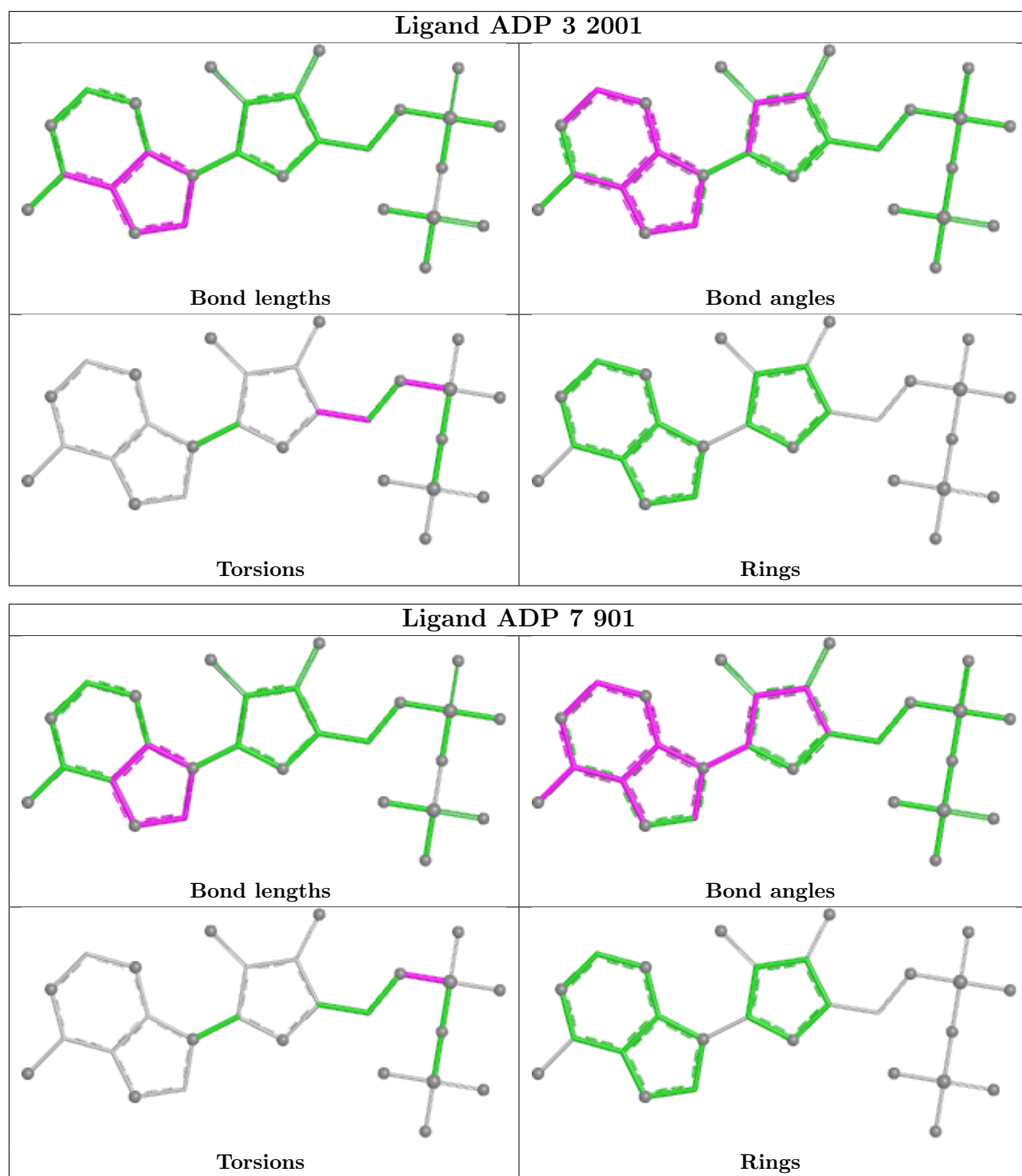
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

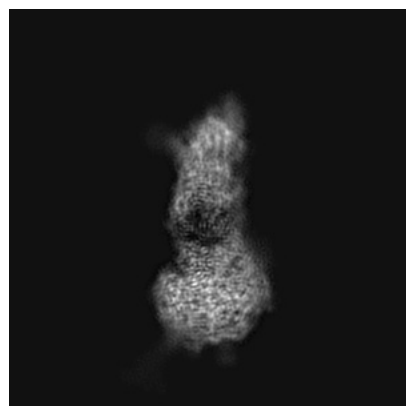
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4980. These allow visual inspection of the internal detail of the map and identification of artifacts.

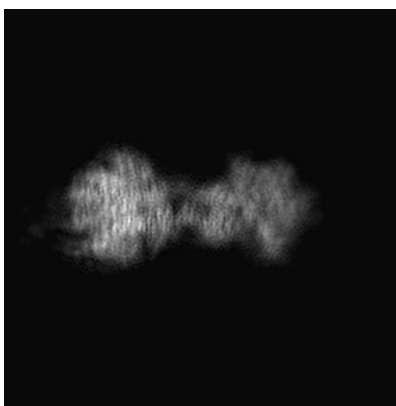
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

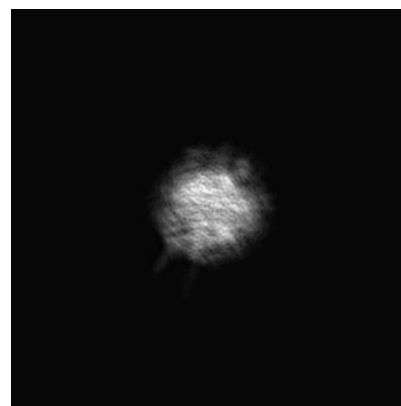
6.1.1 Primary map



X

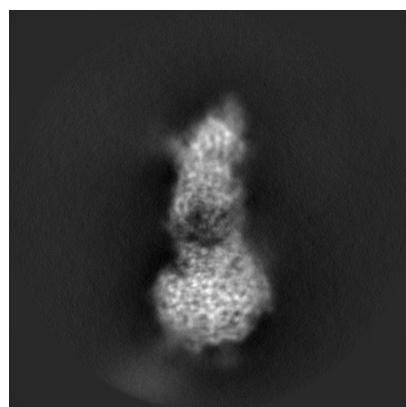


Y

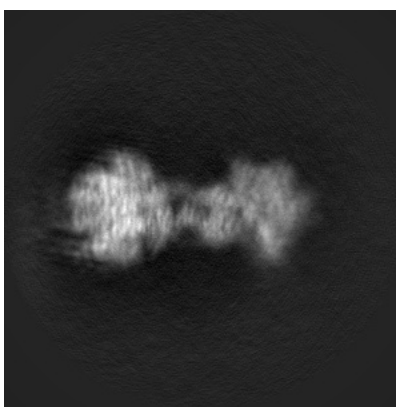


Z

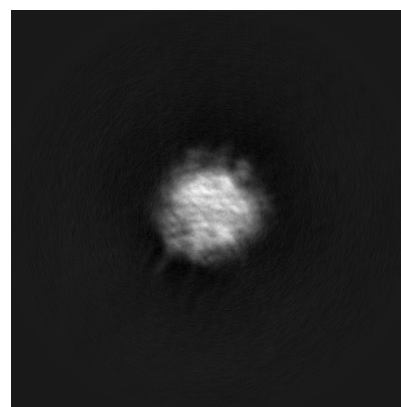
6.1.2 Raw map



X



Y

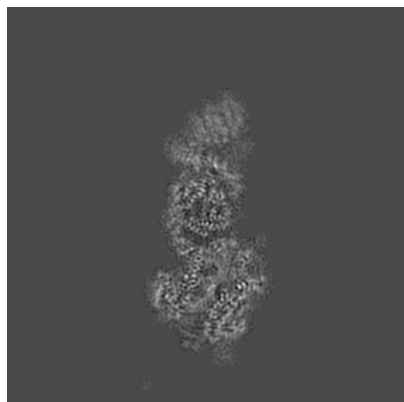


Z

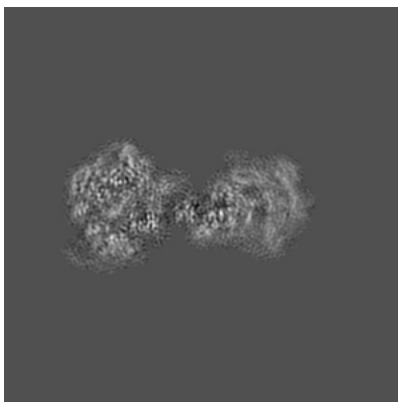
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

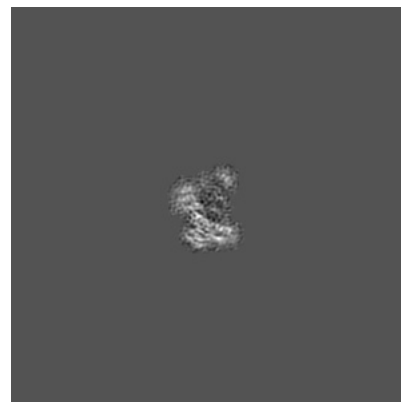
6.2.1 Primary map



X Index: 170

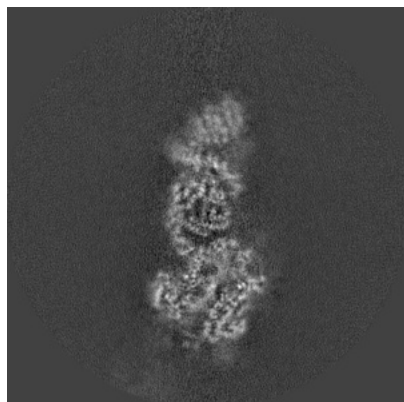


Y Index: 170

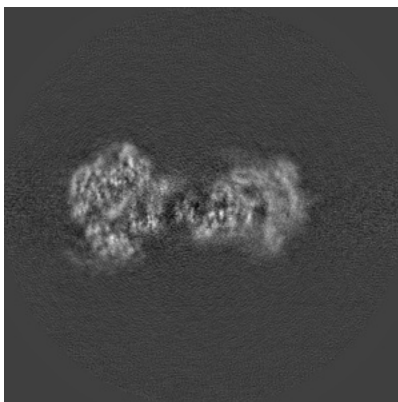


Z Index: 170

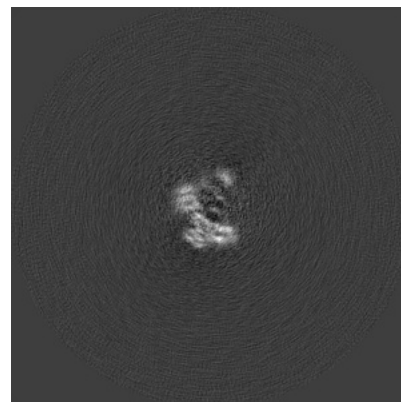
6.2.2 Raw map



X Index: 170



Y Index: 170

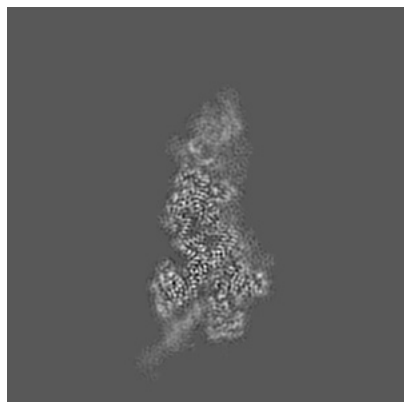


Z Index: 170

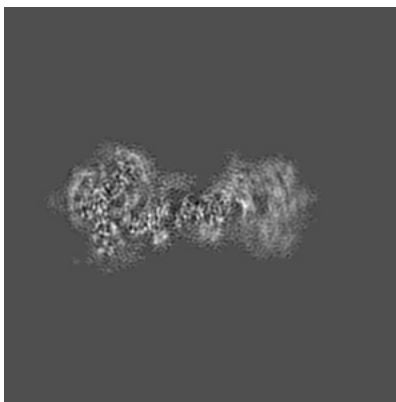
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

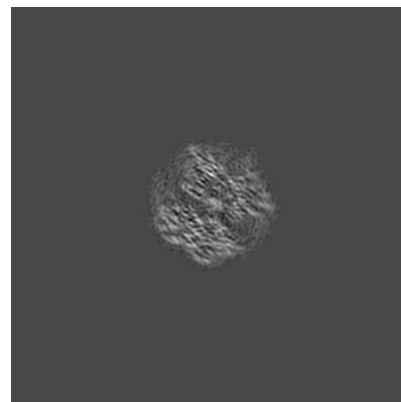
6.3.1 Primary map



X Index: 159

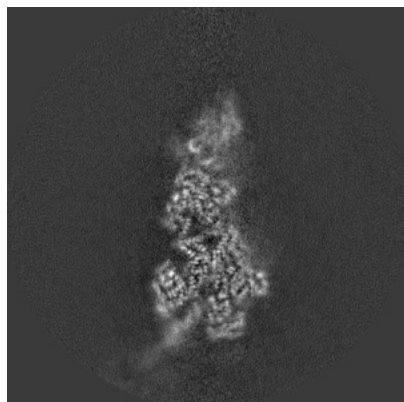


Y Index: 177

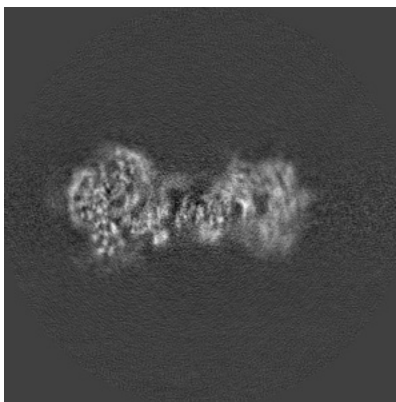


Z Index: 102

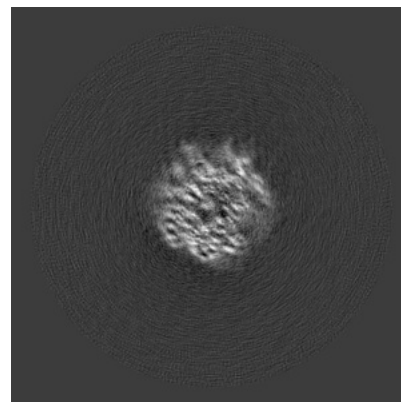
6.3.2 Raw map



X Index: 158



Y Index: 177

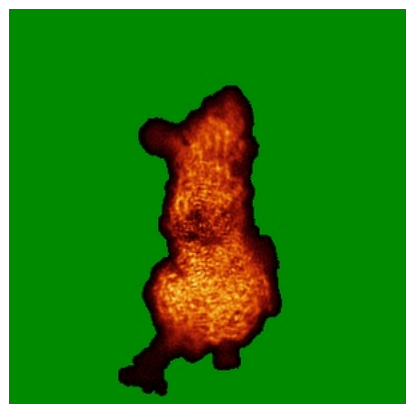


Z Index: 94

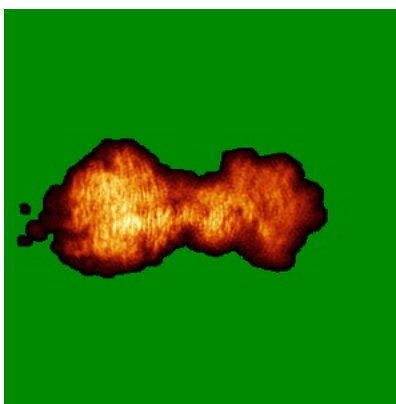
The images above show the largest variance slices of the map in three orthogonal directions.

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

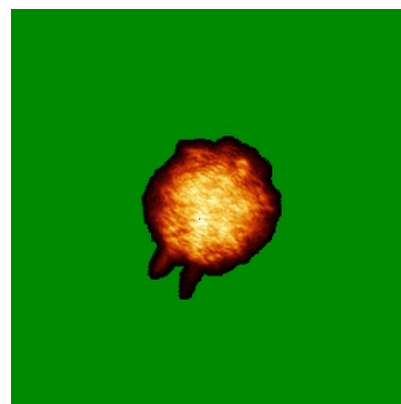
6.4.1 Primary map



X

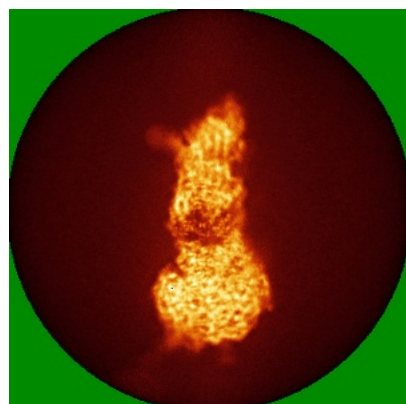


Y

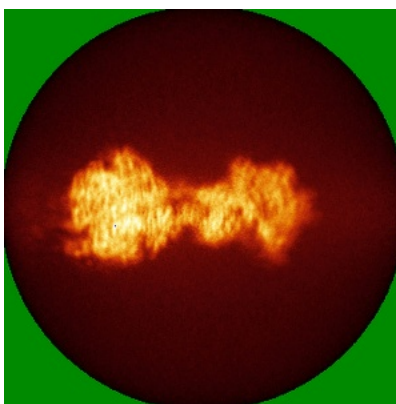


Z

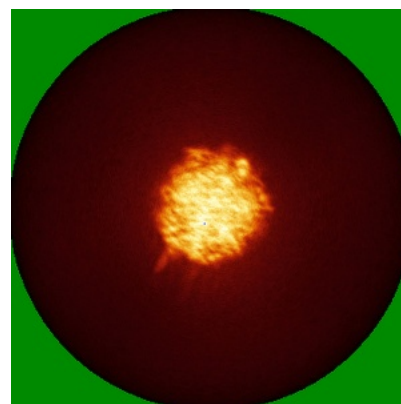
6.4.2 Raw map



X



Y

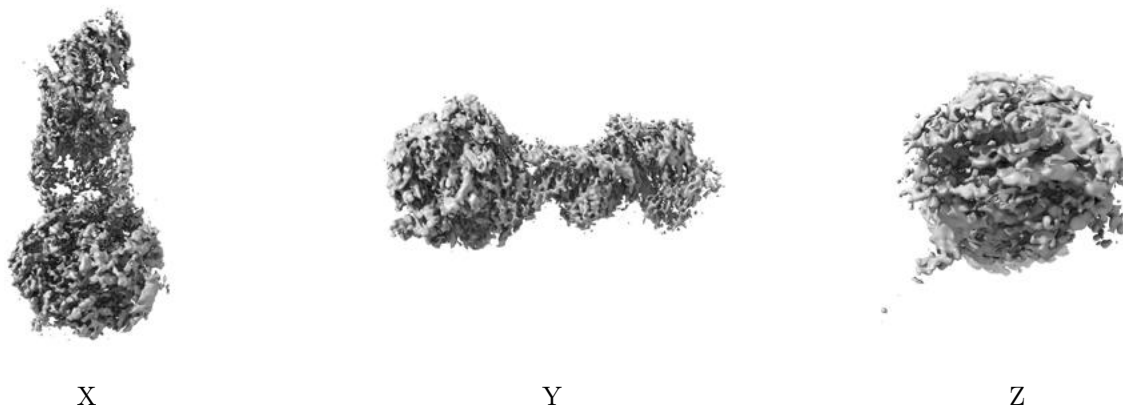


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

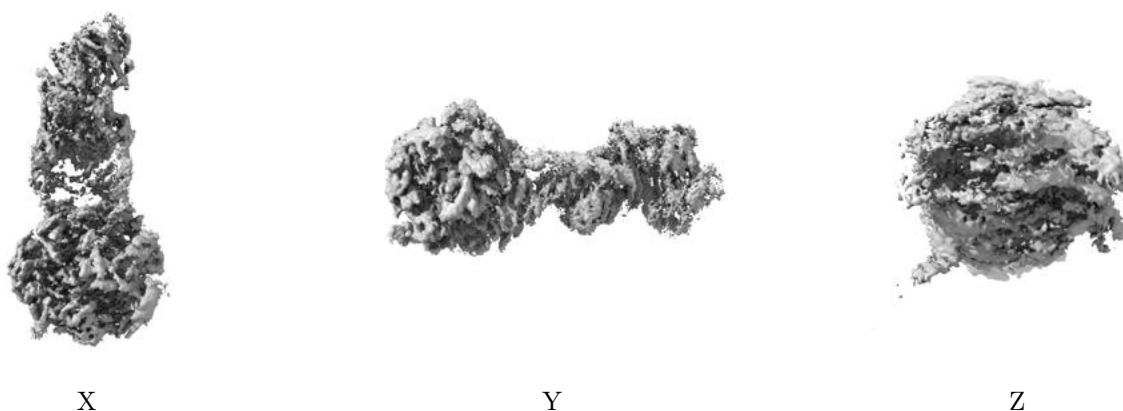
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

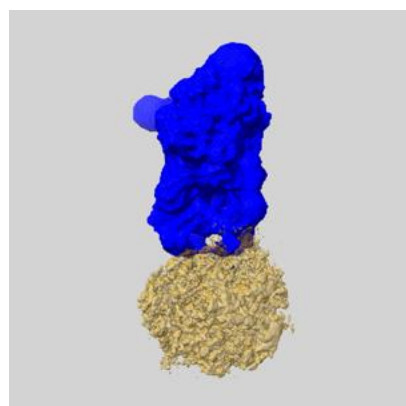
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

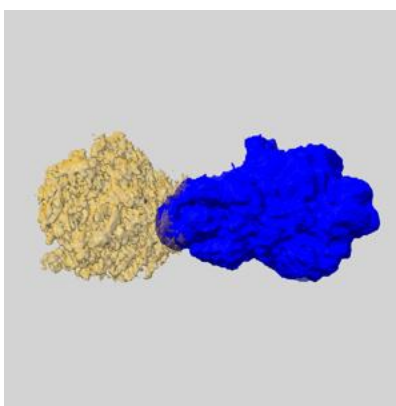
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

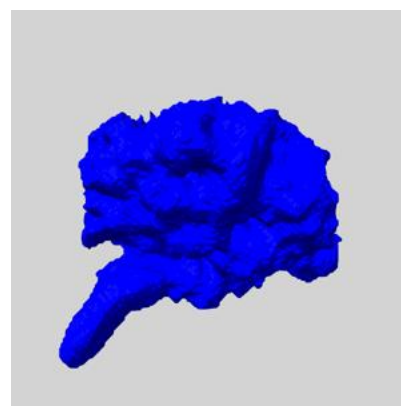
6.6.1 emd_4980_msk_2.map [i](#)



X

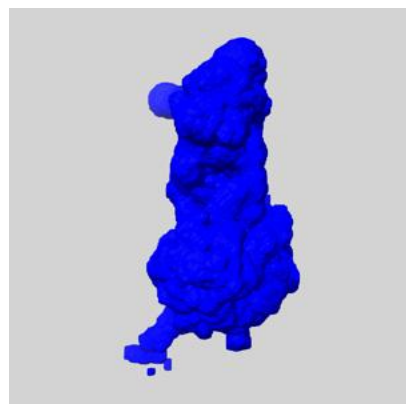


Y

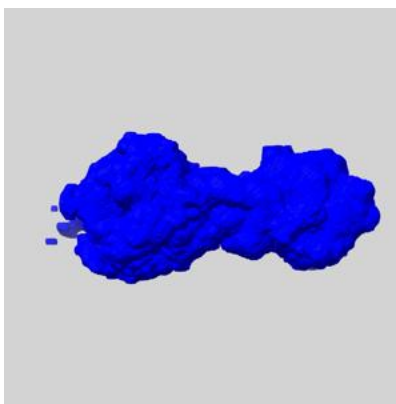


Z

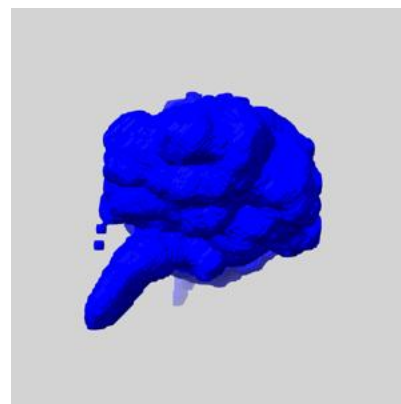
6.6.2 emd_4980_msk_3.map [i](#)



X

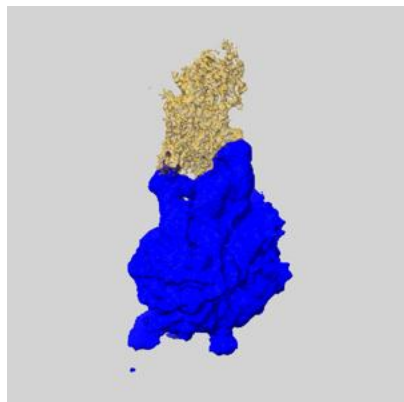


Y

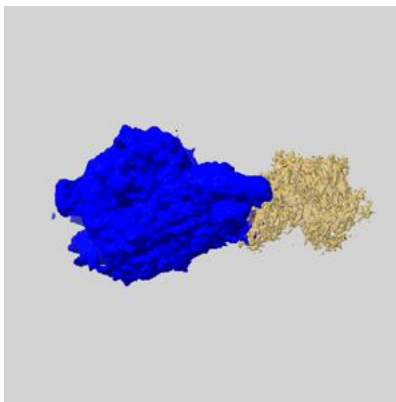


Z

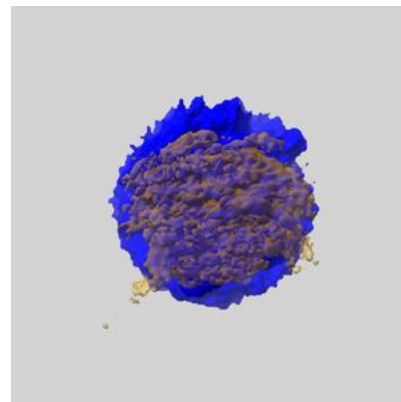
6.6.3 emd_4980_msk_1.map [i](#)



X



Y

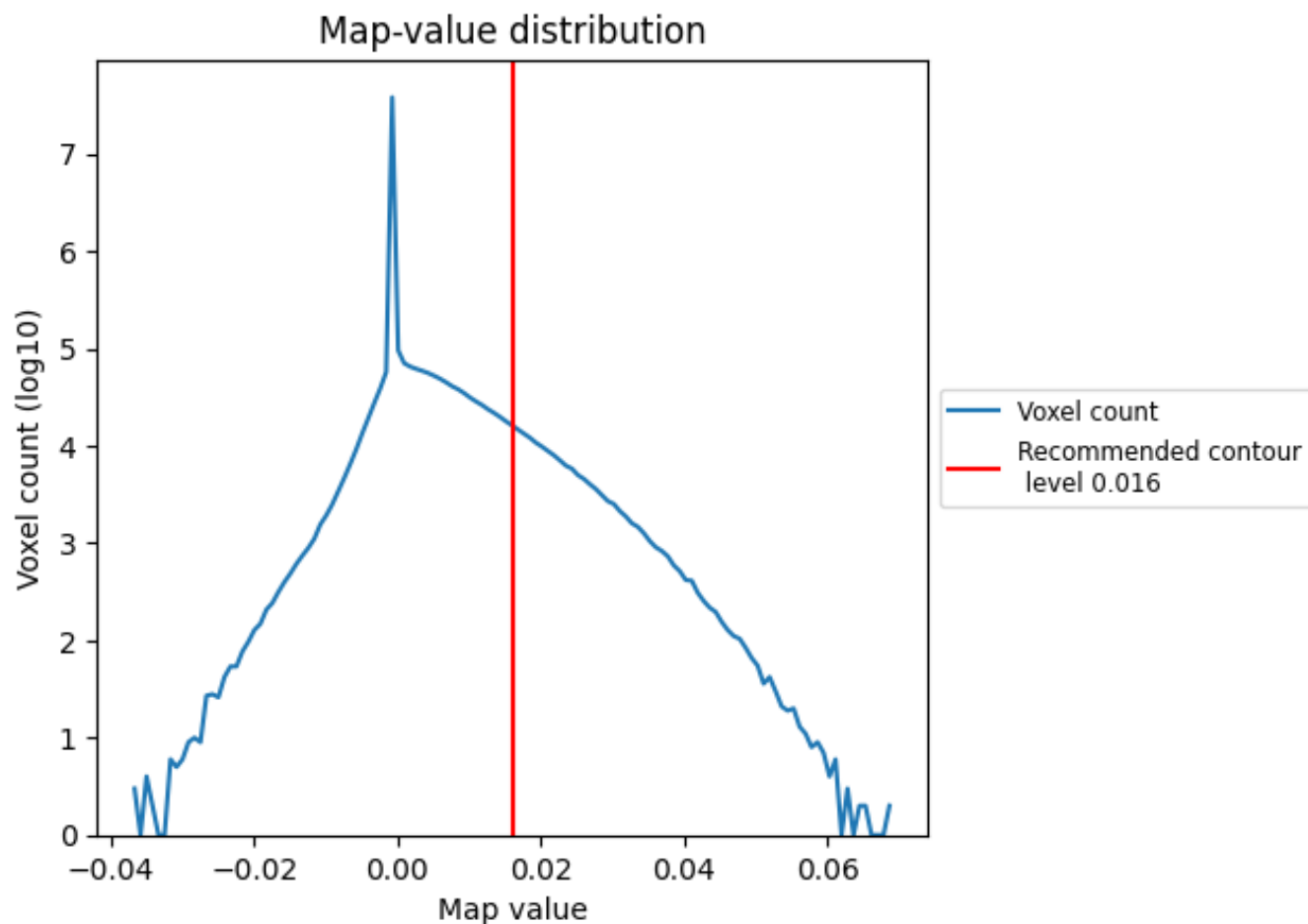


Z

7 Map analysis [i](#)

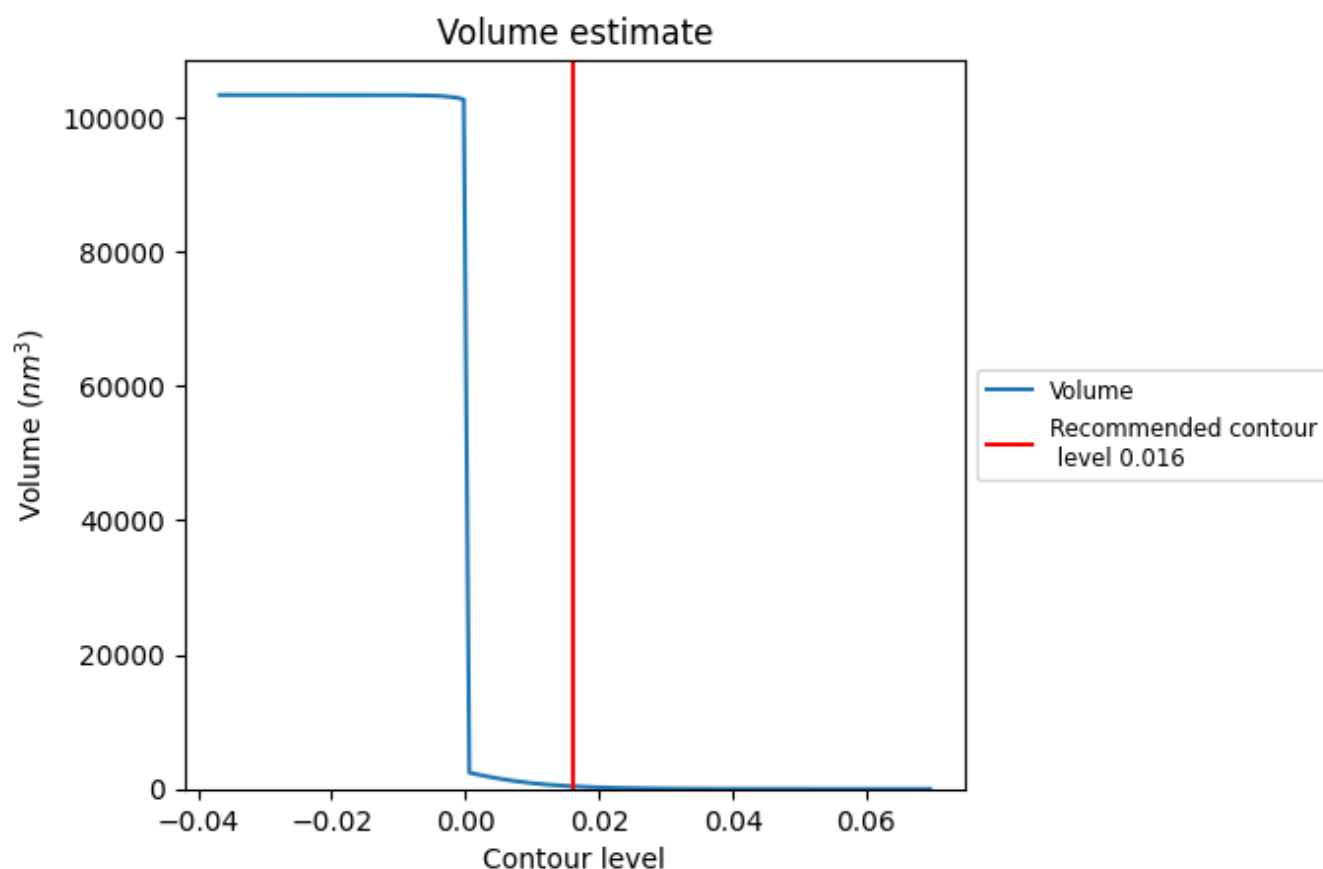
This section contains the results of statistical analysis of the map.

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.

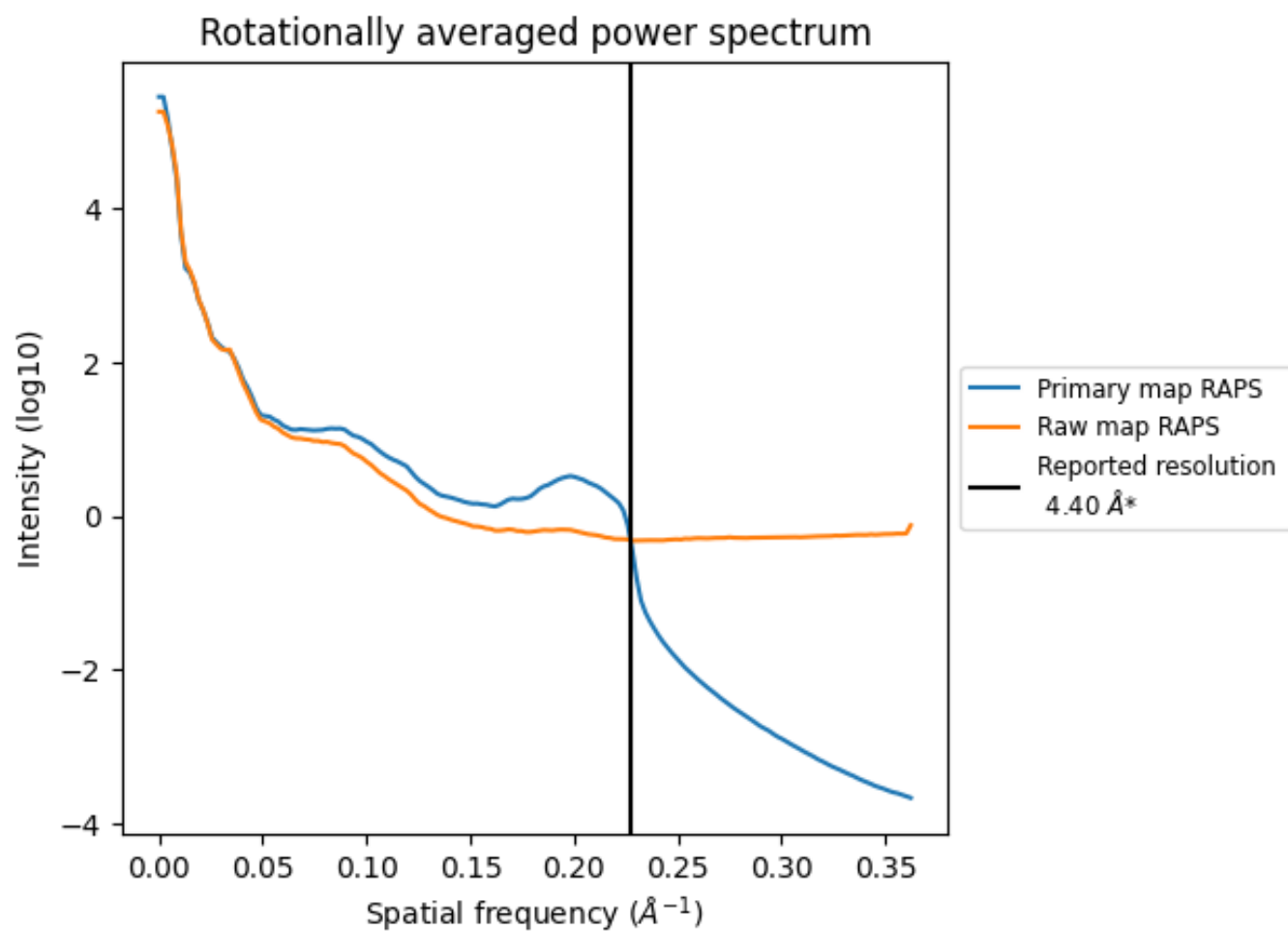
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 404 nm³; this corresponds to an approximate mass of 365 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

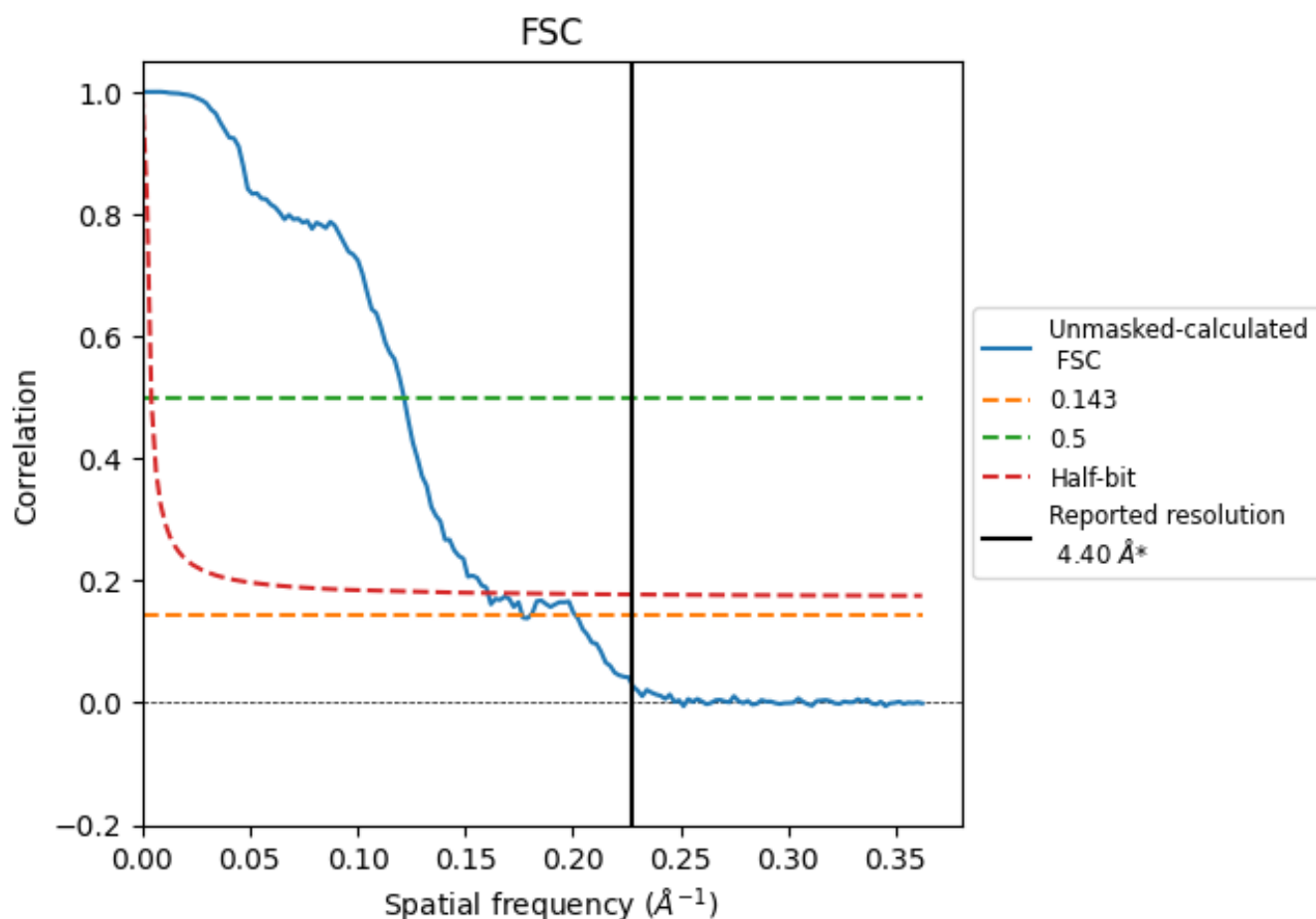


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

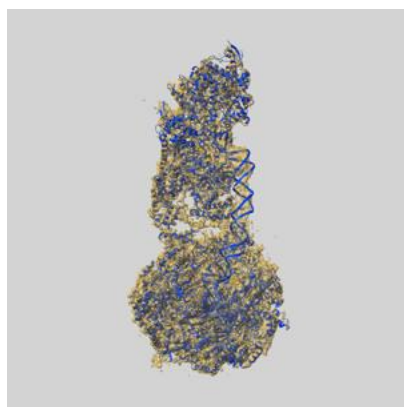
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.66	8.22	6.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.66 differs from the reported value 4.4 by more than 10 %

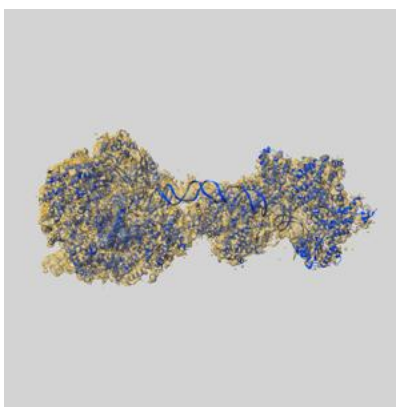
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4980 and PDB model 6RQC. Per-residue inclusion information can be found in section [3](#) on page [10](#).

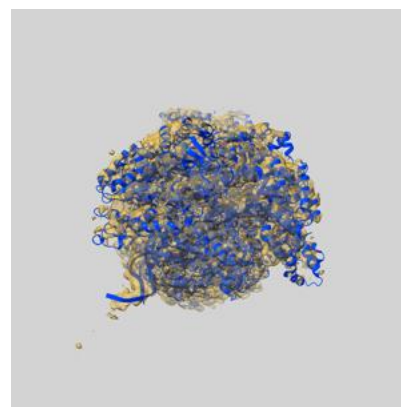
9.1 Map-model overlay [i](#)



X



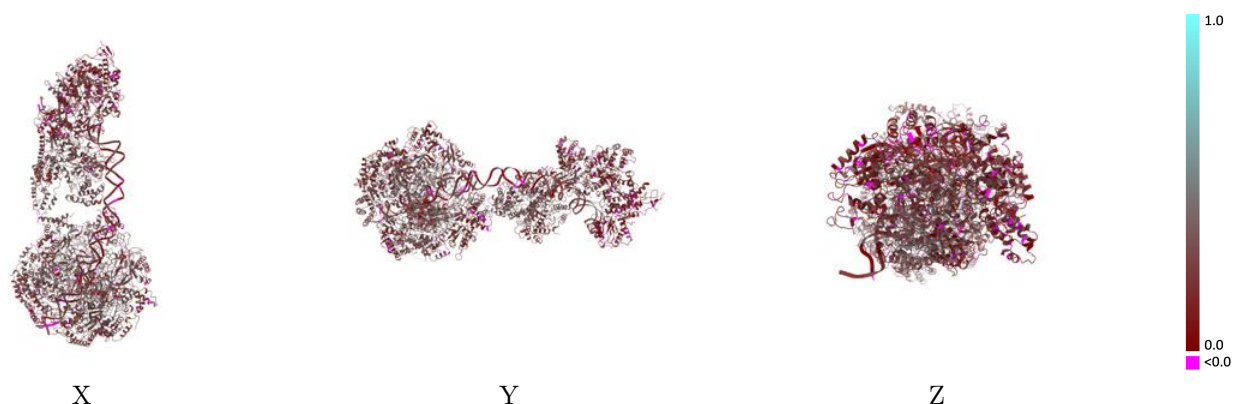
Y



Z

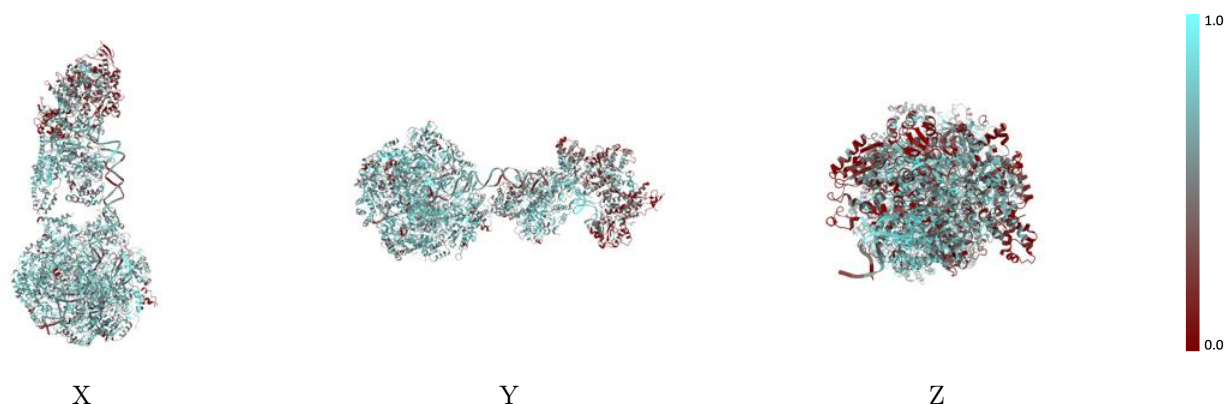
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



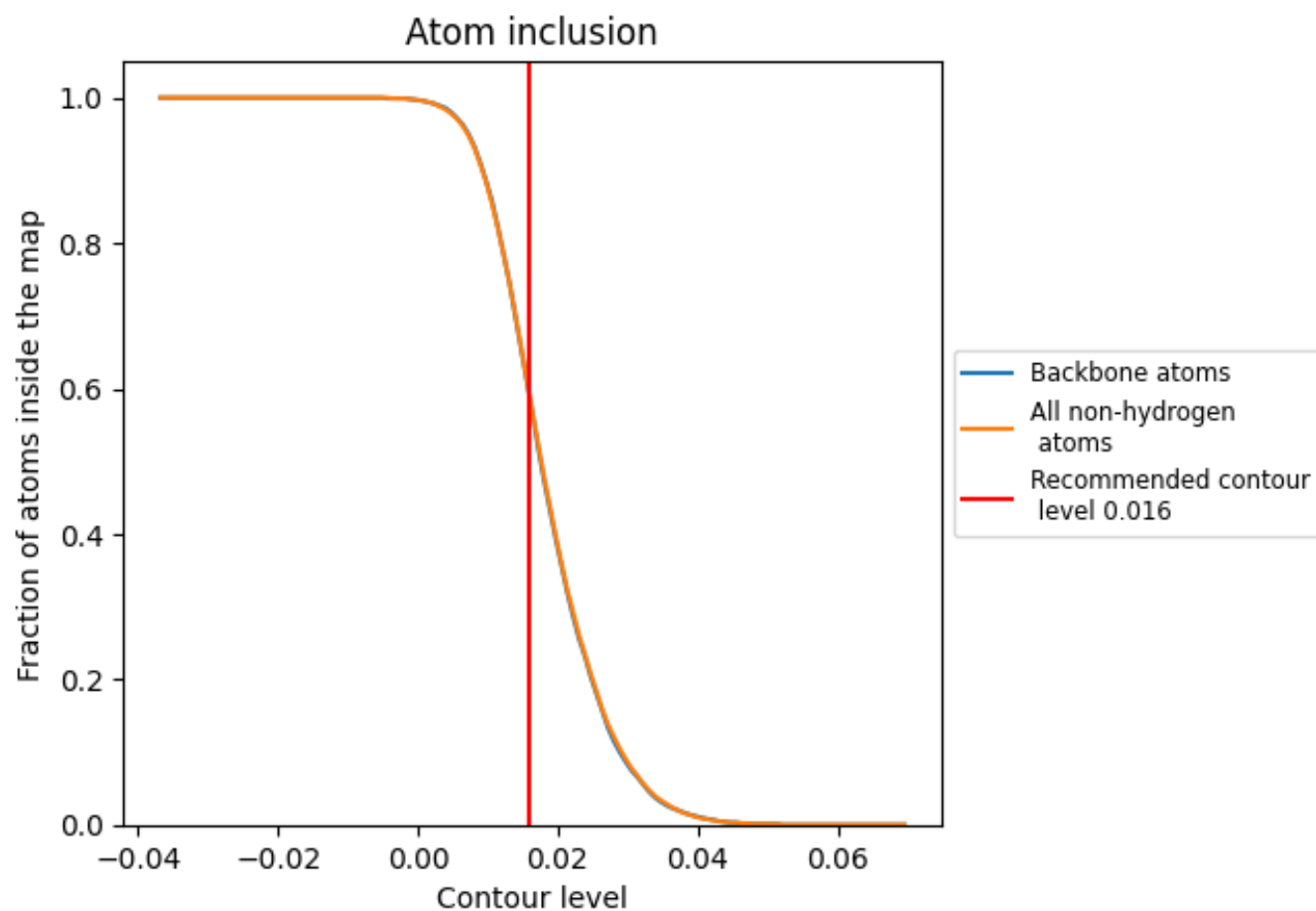
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5890	 0.2720
2	 0.6860	 0.3070
3	 0.6530	 0.3000
4	 0.6590	 0.3020
5	 0.7090	 0.3190
6	 0.6310	 0.2830
7	 0.6330	 0.2890
A	 0.2880	 0.1800
B	 0.7100	 0.3270
C	 0.6370	 0.2840
D	 0.4800	 0.2190
E	 0.4370	 0.2430
F	 0.5780	 0.2840
X	 0.5850	 0.1760
Y	 0.6030	 0.1800

