



## Full wwPDB EM Validation Report ⓘ

Feb 26, 2024 – 07:36 AM EST

PDB ID : 6WGG  
EMDB ID : EMD-21665  
Title : Atomic model of pre-insertion mutant OCCM-DNA complex(ORC-Cdc6-Cdt1-Mcm2-7 with Mcm6 WHD truncation)  
Authors : Yuan, Z.; Schneider, S.; Dodd, T.; Riera, A.; Bai, L.; Yan, C.; Magdalou, I.; Ivanov, I.; Stillman, B.; Li, H.; Speck, C.  
Deposited on : 2020-04-05  
Resolution : 8.10 Å(reported)

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

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

---

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

EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

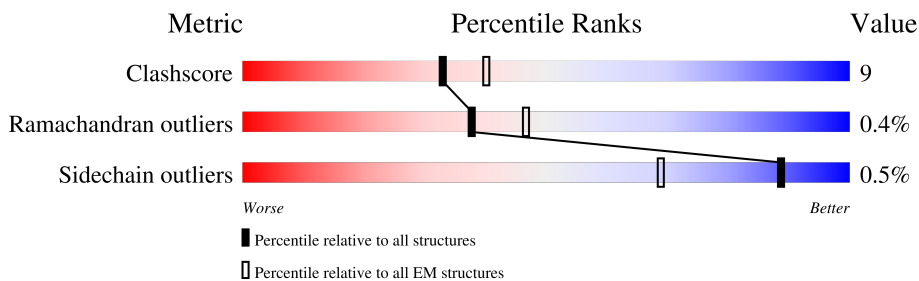
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.10 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	8	604	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">61%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">41%      23%      36%</div> </div>
2	9	513	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">46%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">50%      22%      27%</div> </div>
3	A	913	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">23%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">38%      9%      54%</div> </div>
4	B	620	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">31%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">40%      13%      47%</div> </div>
5	C	616	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">41%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">71%      17%      12%</div> </div>
6	E	479	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">45%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">68%      20%      12%</div> </div>
7	D	529	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">40%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">62%      20%      18%</div> </div>
8	F	435	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">26%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">28%      8%      64%</div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
9	G	41	
10	H	41	
11	2	868	
12	3	971	
13	4	933	
14	5	775	
15	6	1017	
16	7	845	

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 54601 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 Cell division cycle protein CDT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	8	388	3011	1916	518	566	11	0	0

- Molecule 2 is a protein called Cell division control protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	9	373	2972	1907	495	553	17	0	0

- Molecule 3 is a protein called Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	424	3368	2151	566	633	18	0	0

- Molecule 4 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	326	2663	1721	442	484	16	0	0

- Molecule 5 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	544	4505	2909	743	838	15	0	0

- Molecule 6 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	422	3425	2226	545	641	13	0	0

- Molecule 7 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	436	3551	2275	603	660	13	0	0

- Molecule 8 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	F	157	1315	846	222	235	12	0	0

- Molecule 9 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	G	41	831	407	118	266	40	0	0

- Molecule 10 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	H	41	847	404	178	224	41	0	0

- Molecule 11 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	2	581	4478	2824	786	849	19	0	0

- Molecule 12 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	3	642	4866	3073	837	942	14	0	0

- Molecule 13 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	4	665	4995	3126	864	981	24	0	0

- Molecule 14 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	5	599	4317	2699	750	849	19	0	0

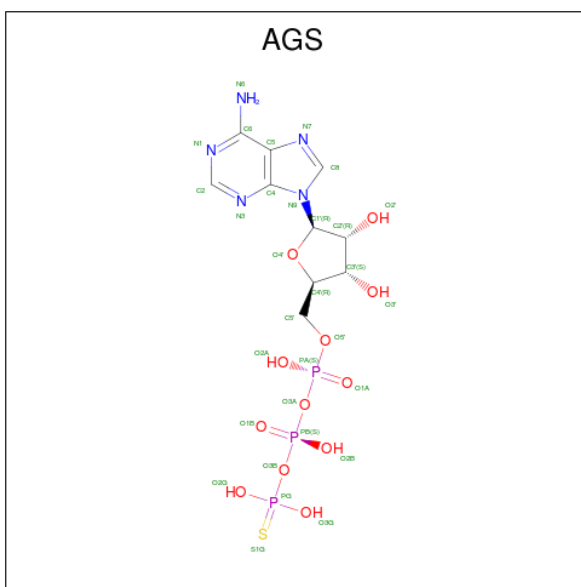
- Molecule 15 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	6	576	4475	2825	782	845	23	0	0

- Molecule 16 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	7	641	4858	3053	834	943	28	0	0

- Molecule 17 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).

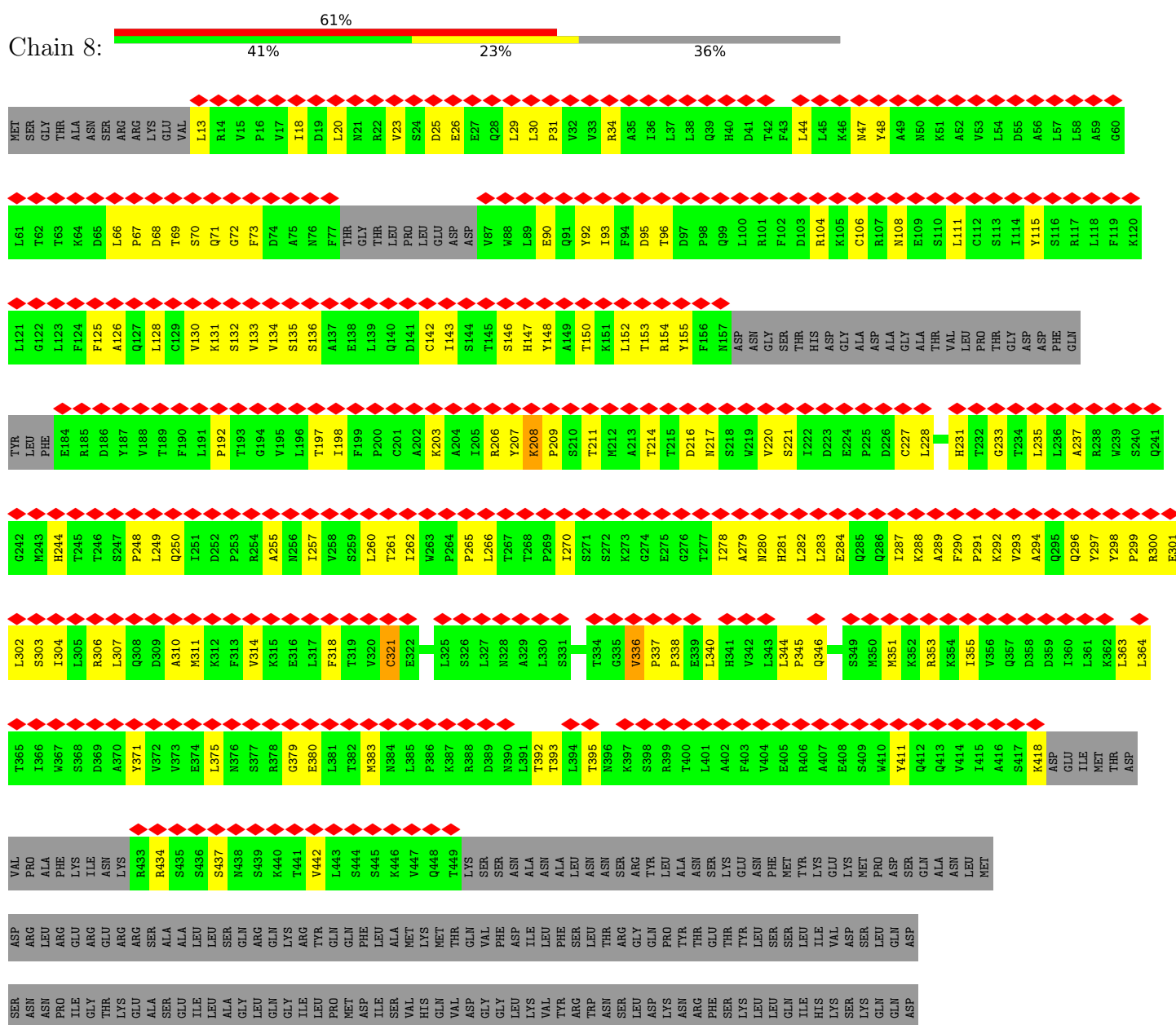


Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
17	9	1	31	10	5	12	3	1	0
17	A	1	31	10	5	12	3	1	0
17	E	1	31	10	5	12	3	1	0
17	D	1	31	10	5	12	3	1	0

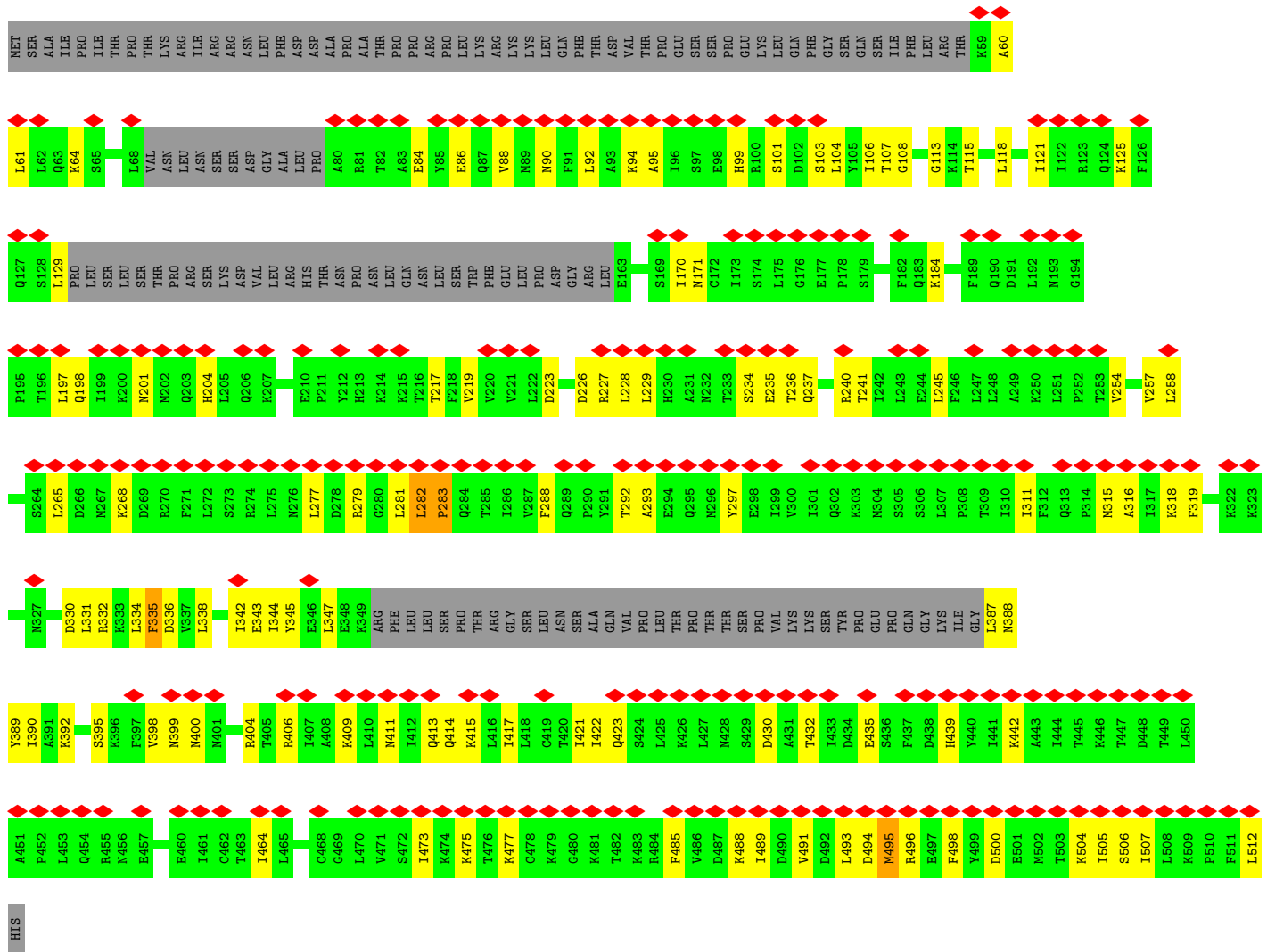
### 3 Residue-property plots

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.

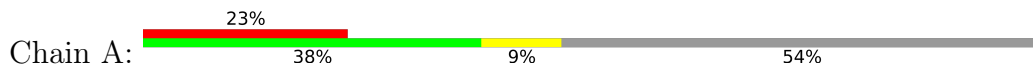
- Molecule 1: Cell division cycle protein CDT1



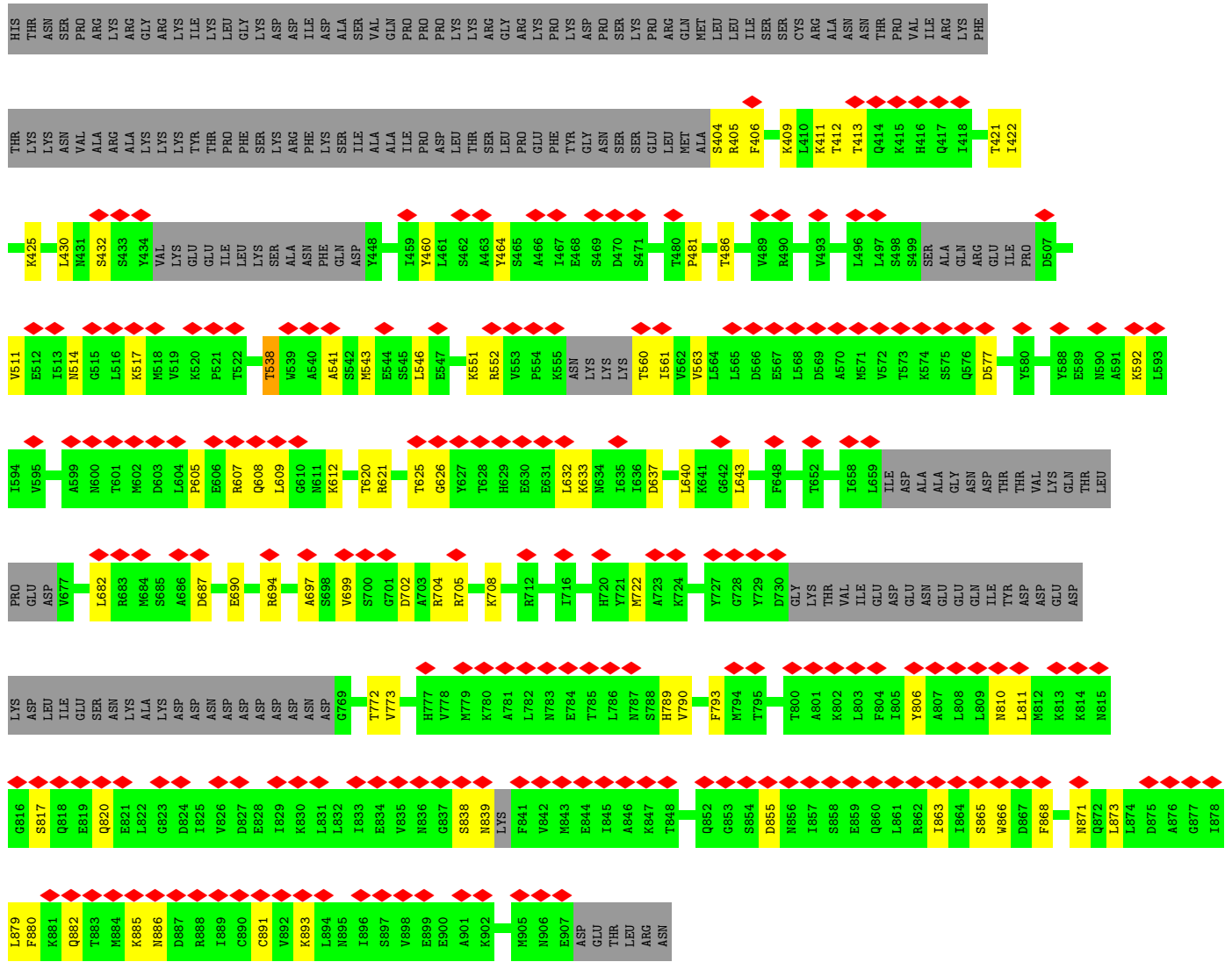
• Molecule 2: Cell division control protein 6



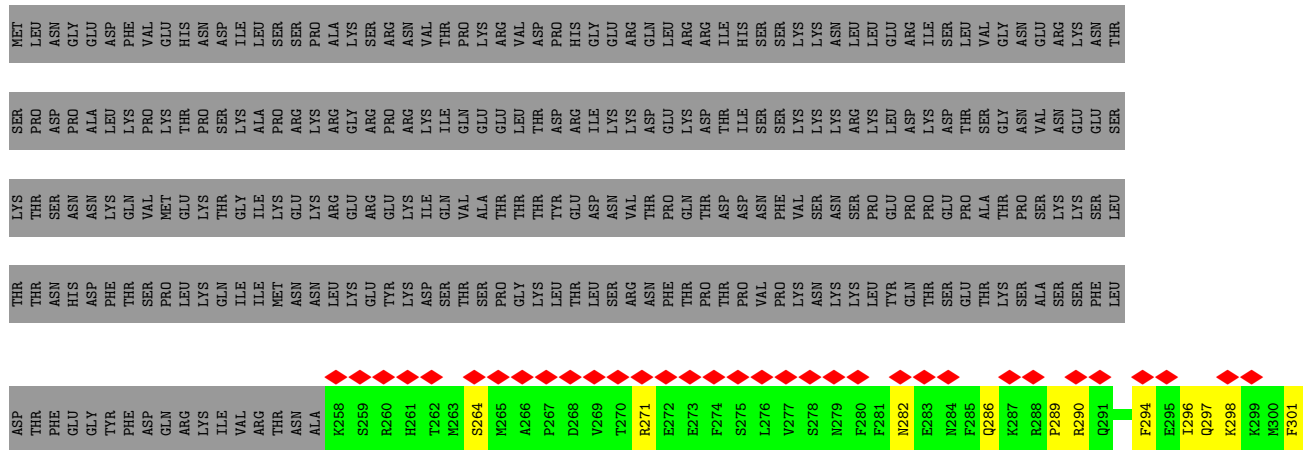
• Molecule 3: Origin recognition complex subunit 1

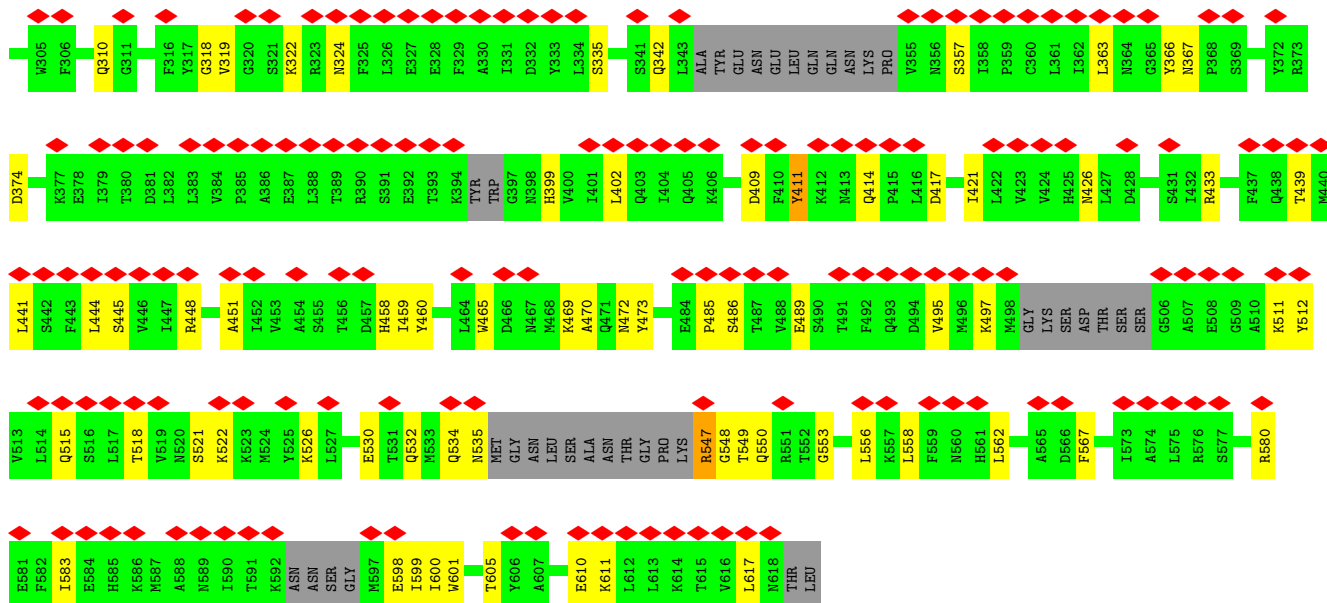




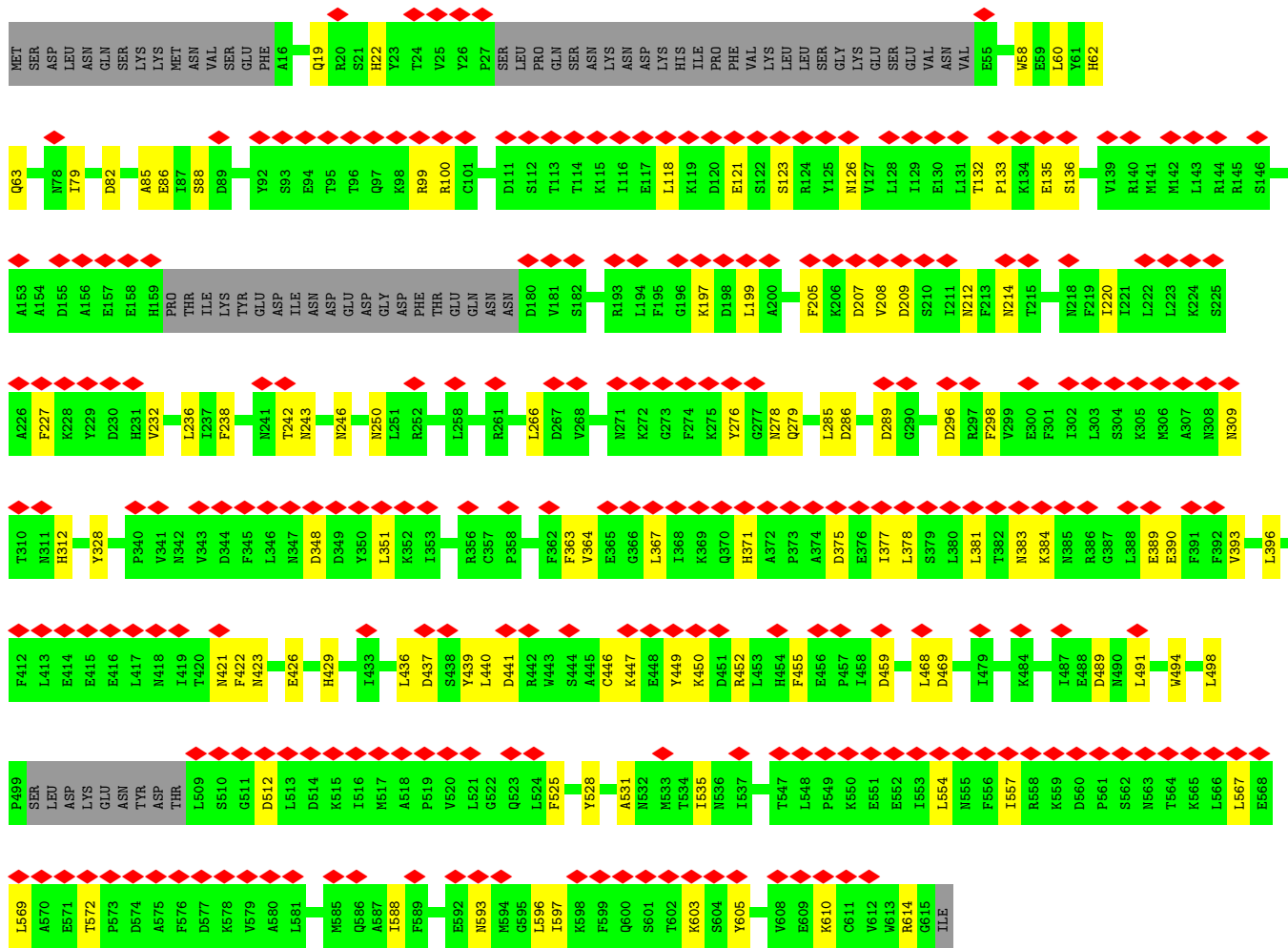
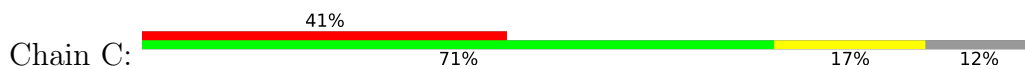


● Molecule 4: Origin recognition complex subunit 2

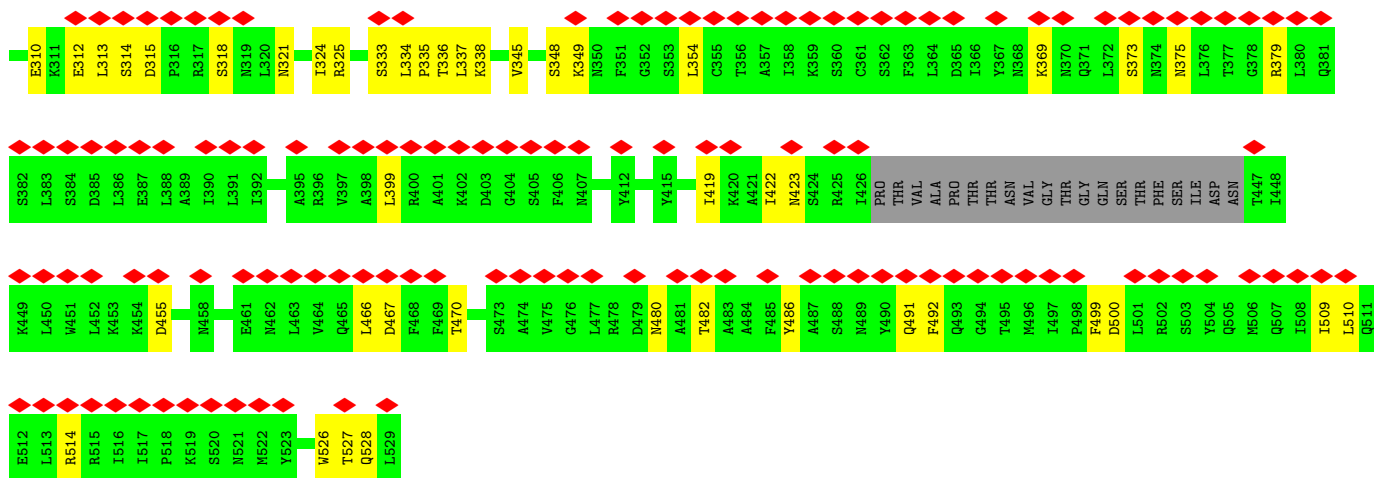




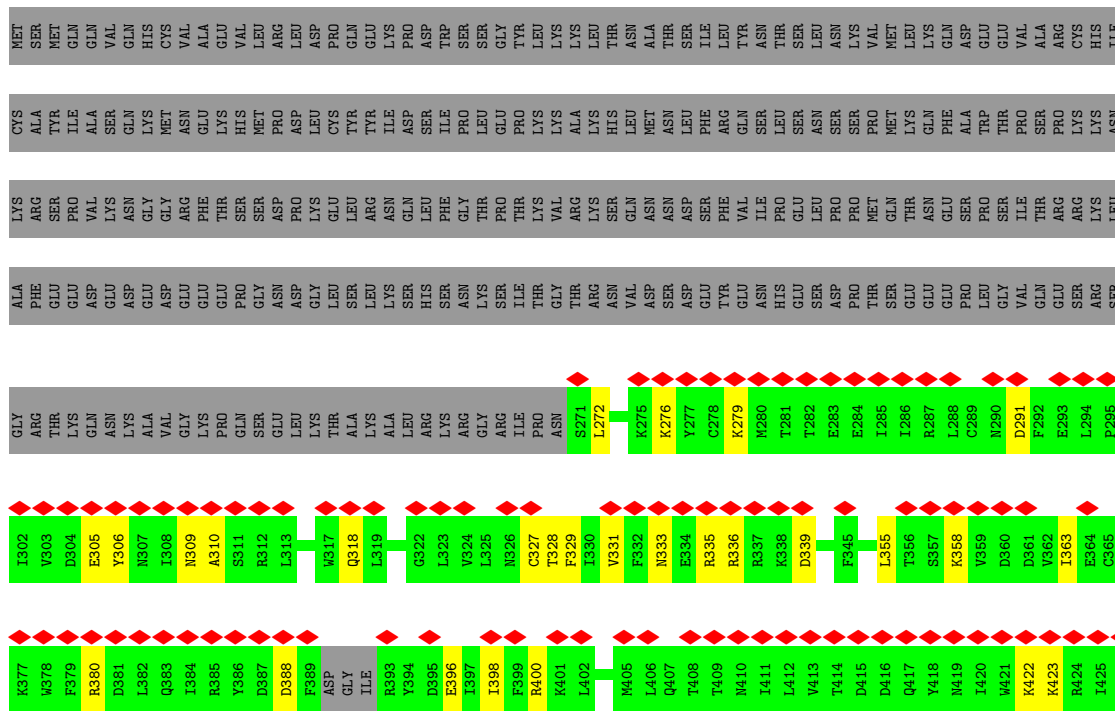
• Molecule 5: Origin recognition complex subunit 3



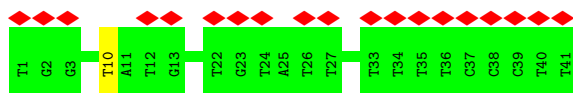




• Molecule 8: Origin recognition complex subunit 6

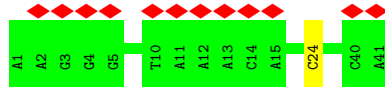


• Molecule 9: DNA (41-MER)



• Molecule 10: DNA (41-MER)



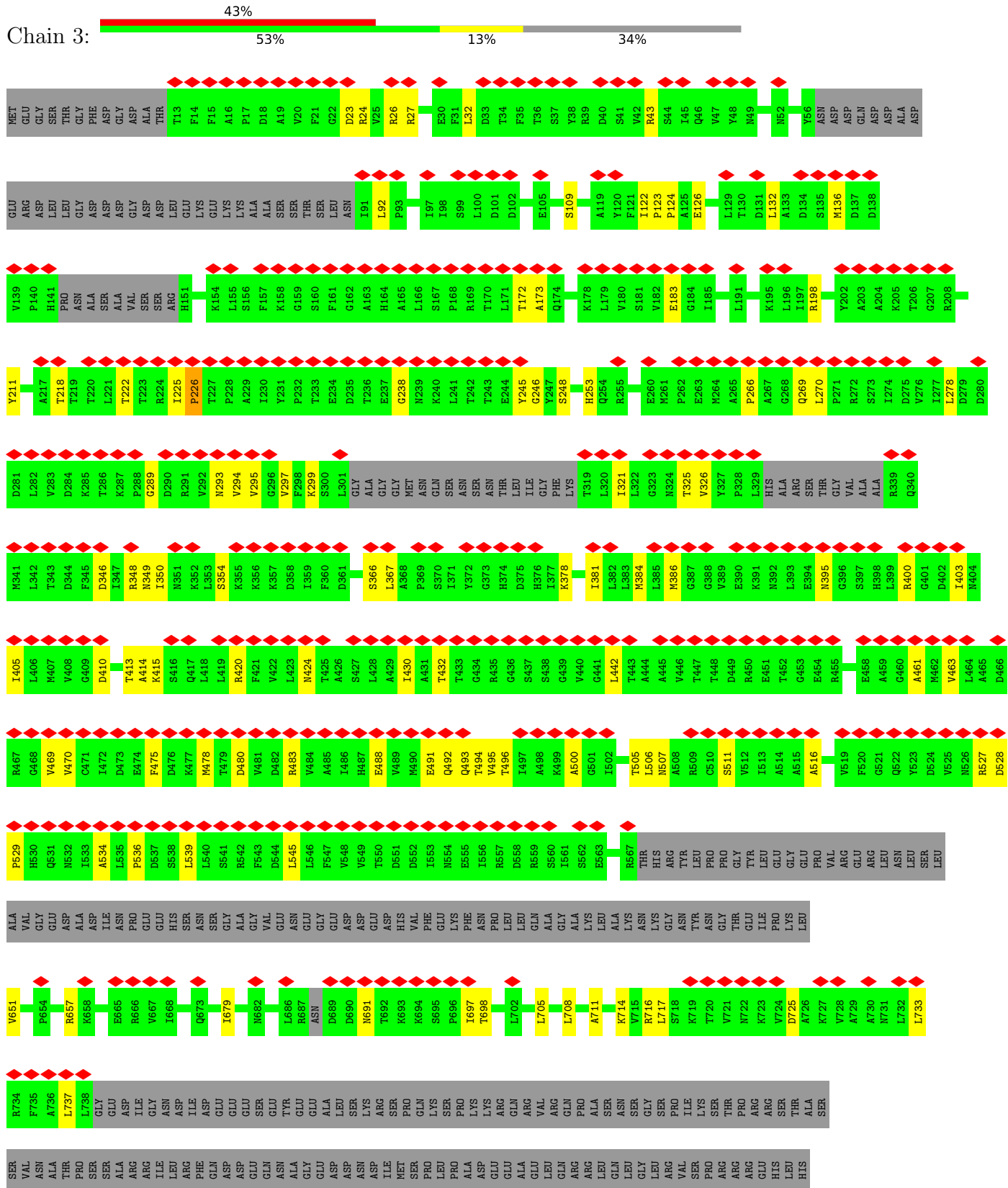


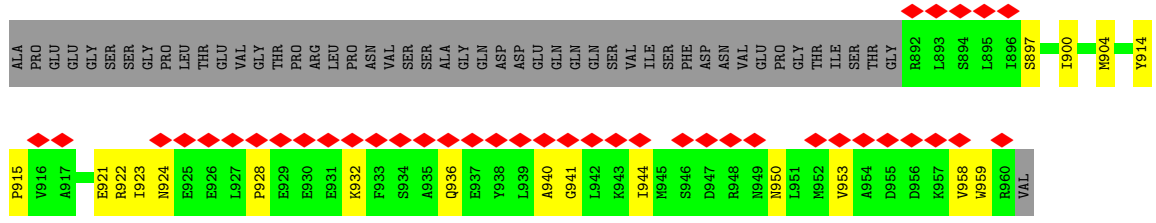
• Molecule 11: DNA replication licensing factor MCM2



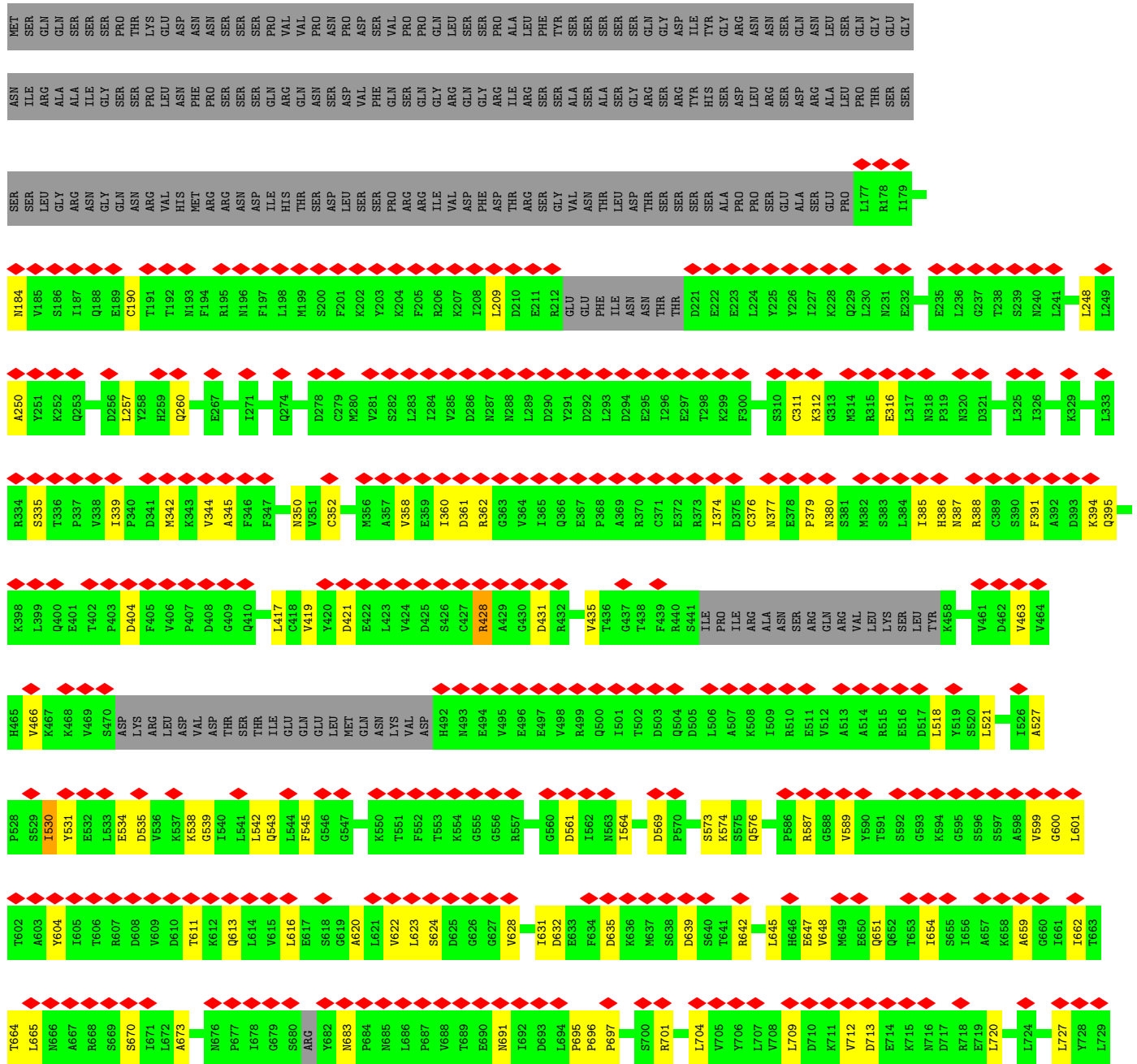
MET	ASP	LEU	THR	LEU	THR	E243	R327	V388	M454	N528	L591	M653	GLU	I798
SER	GLU	LEU	THR	LEU	THR	V244	T328	T389	S455	Q529	E592	G654	GLN	S799
ASN	VAL	ARG	GLU	LEU	LEU	N245	G329	L390	I456	K630	G593	G654	GLY	S799
ARG	GLU	ASN	SER	SER	SER	N245	V330	Q391	K457	H531	G594	R656	ASP	G801
ARG	GLN	VAL	LEU	LEU	LEU	I255	F331	E392	R468	S532	A595	R657	ILE	S802
ARG	MET	ALA	TYR	ASP	ASP	L256	P332	A393	R469	L533	LEU	M658	ASN	F803
ARG	ASN	ILE	ILE	ASP	VAL	A257	Q333	G395	E460	R534	VAL	S659	GLN	P804
GLU	VAL	ASP	LYS	ASP	ALA	F259	L334	T396	GLY	G535	A599	T660	LEU	T805
ASP	ASP	GLU	ASN	ASP	ASP	L260	K335	V397	THR	D536	D600	L661	ASN	T806
SER	MET	LEU	TYR	SER	TYR	A261	V336	P398	ALA	I537	R601	L664	ARG	V807
ASP	ASP	GLU	SER	GLU	SER	E265	K338	P399	ASN	N538	R602	Q665	ARG	R808
SER	ASP	GLU	GLU	GLU	GLU	E277	F339	G400	GLY	V539	V603	R666	ARG	H809
GLU	ASN	GLU	TRP	GLU	TRP	E280	N340	R401	GLU	L540	G604	R667	ARG	L810
ASN	GLY	GLY	ILE	ILE	ILE	E282	C341	R402	GLU	L542	L605	V667	ARG	E811
GLU	ALA	ALA	THR	THR	THR	Y283	L342	P403	LEU	L544	L606	L668	ARG	S812
LEU	ALA	ALA	GLN	GLN	GLN	P284	K343	R404	ASP	D544	D607	L669	ARG	T813
PRO	GLN	GLN	ASP	ASP	ASP	E285	L348	H405	V473	K549	E508	T670	ARG	L814
SER	VAL	LEU	LEU	LEU	LEU	Y286	G349	R406	F474	S550	D610	F672	ARG	R815
ARG	VAL	LEU	LEU	LEU	LEU	A287	A412	R407	S475	Q551	D611	P673	LYS	E827
HIS	GLM	ARG	ARG	ARG	ARG	R288	P350	E407	W476	I552	M612	S675	GLY	S831
GLY	GLY	ARG	ARG	ARG	ARG	I289	F351	ASP	E478	K554	M613	R676	ILE	I838
GLY	ASP	ARG	ARG	ARG	ARG	H290	F352	L414	E480	V555	D614	F677	ILE	K839
MET	PRO	ARG	ARG	ARG	ARG	S291	Q353	V415	E481	E556	D616	D678	ILE	V840
ASN	ASN	ARG	ARG	ARG	ARG	S291	N356	D416	R482	K558	T618	I679	ILE	V841
VAL	VAL	ARG	ARG	ARG	ARG	E292	E357	S418	F484	T559	T619	V682	ILE	V842
SER	ASP	VAL	TYR	ASP	ASP	E293	E358	R419	R485	A560	T620	R683	ILE	D843
PRO	ARG	GLN	GLU	ASP	ASP	H294	F359	K419	R486	S561	H621	R684	ILE	V844
ILE	ARG	LEU	LEU	ASP	ASP	V295	R360	P420	R489	A562	E522	D685	ILE	D847
GLY	ARG	LEU	LEU	LEU	LEU	R296	R361	G421	D490	A563	G623	L686	ILE	V846
GLY	GLN	LEU	LEU	LEU	LEU	S298	S362	E422	R491	V564	M624	D688	ILE	V847
PRO	ASN	PRO	ASN	PRO	PRO	D299	F363	E423	G492	F565	E625	L689	ILE	K850
ASP	ASP	SER	ASP	ASP	ASP	F300	C364	V426	D495	A566	Q626	E690	ILE	V851
MET	ILE	SER	ASP	ASP	ASP	P301	T365	T427	S504	T567	Q627	S706	ILE	V852
ASN	ASN	LEU	LEU	LEU	LEU	S225	N366	K431	I505	G566	S628	HIS	ILE	K853
PRO	PRO	LEU	LEU	LEU	LEU	V226	C367	ASN	Y506	G570	S630	PRO	ILE	R854
GLY	ARG	ARG	ARG	ARG	ARG	Y227	S369	ASN	T509	A571	I631	PRO	ILE	R855
ASP	ARG	ASP	ASP	ASP	ASP	G228	K370	TYR	B509	S572	S632	ASP	ILE	R856
ASP	ILE	ASP	ASP	ASP	ASP	A229	G371	ASP	D510	A573	R633	ASP	ILE	L857
ASN	ALA	ASP	ASP	ASP	ASP	R230	P372	GLY	K512	V574	A634	ASP	ILE	R858
VAL	ALA	ASP	ASP	ASP	ASP	I231	E307	LEU	T513	G575	G635	ASP	ILE	R859
ASP	ASP	ASP	ASP	ASP	ASP	R232	R307	LEU	T513	L576	L636	ASP	ILE	S860
ASP	ASP	ASP	ASP	ASP	ASP	T233	L309	ASN	A514	L577	L637	ASP	ILE	F861
VAL	ASP	ASP	ASP	ASP	ASP	L234	R310	ASN	A515	L578	L638	ASP	ILE	A862
ASP	ASP	ASP	ASP	ASP	ASP	G235	E311	LYS	V515	T577	T639	ASP	ILE	I863
VAL	ASP	ASP	ASP	ASP	ASP	E236	S312	ASN	A516	A578	L640	ASP	ILE	V864
ARG	ARG	ARG	ARG	ARG	ARG	M237	N313	GLY	C517	S579	L641	ASP	ILE	T864
PRO	ARG	ARG	ARG	ARG	ARG	N238	E378	PHE	G522	V580	M642	ASP	ILE	L864
ASP	ARG	ARG	ARG	ARG	ARG	S239	K379	VAL	V523	R581	R643	ASP	ILE	R794
ASP	ARG	ARG	ARG	ARG	ARG	E240	T380	PHE	F524	K582	R644	ASP	ILE	R795
ASP	ARG	ARG	ARG	ARG	ARG	S241	L317	ALA	F525	D583	R645	ASP	ILE	E796
ASP	ARG	ARG	ARG	ARG	ARG	V318	V382	THR	K525	F584	S645	ASP	ILE	S797
ASP	ARG	ARG	ARG	ARG	ARG	R319	R383	THR	N526	I585	T646	ASP	ILE	
ASP	ARG	ARG	ARG	ARG	ARG	Y324	N384	THR	V527	T586	I647	ASP	ILE	
ASP	ARG	ARG	ARG	ARG	ARG	I325	Q386	THR	V527	E588	L647	ASP	ILE	
ASP	ARG	ARG	ARG	ARG	ARG	R326	R387	THR	V527	W589	L647	ASP	ILE	

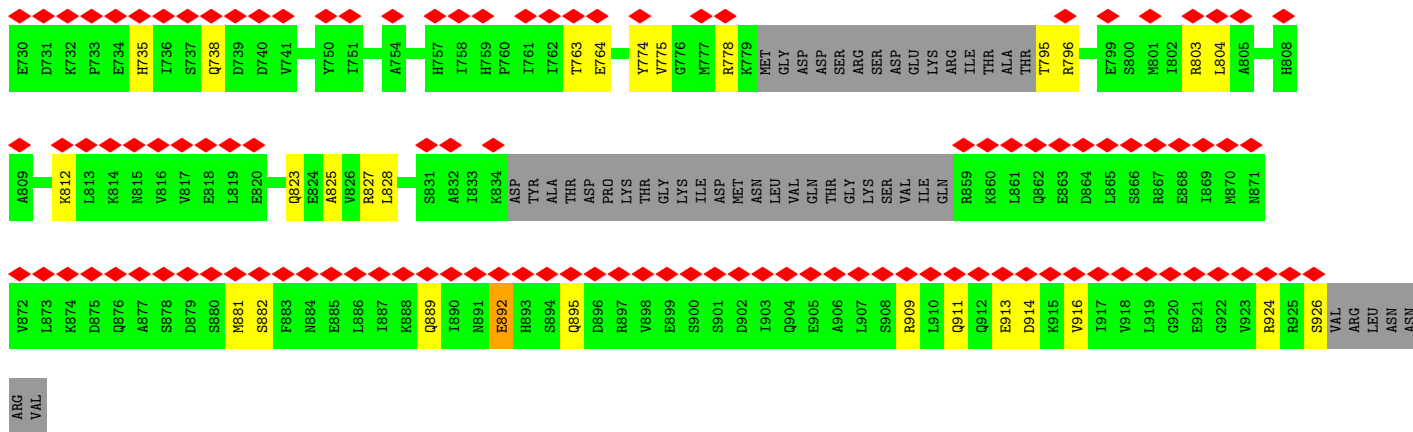
• Molecule 12: DNA replication licensing factor MCM3



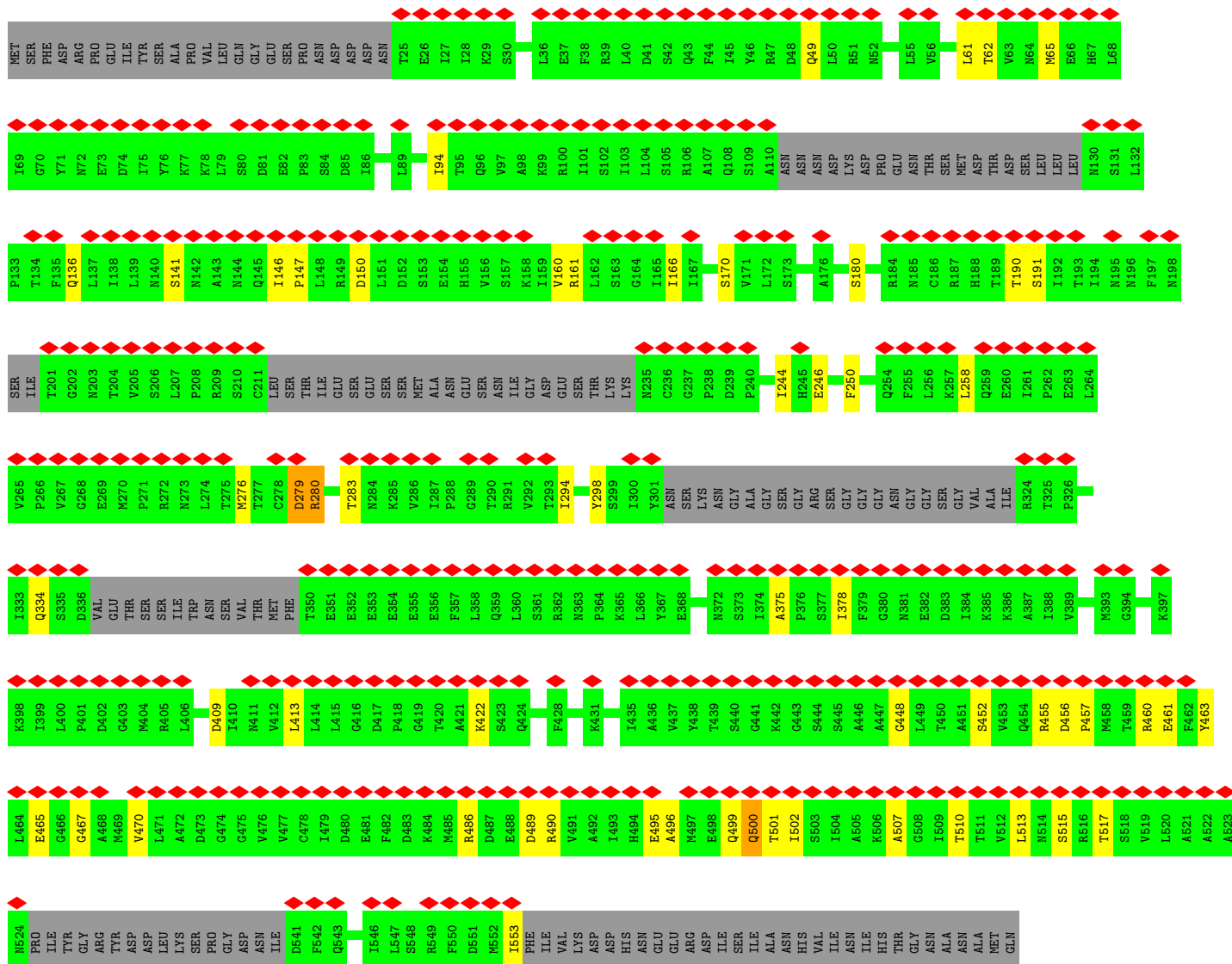


• Molecule 13: DNA replication licensing factor MCM4

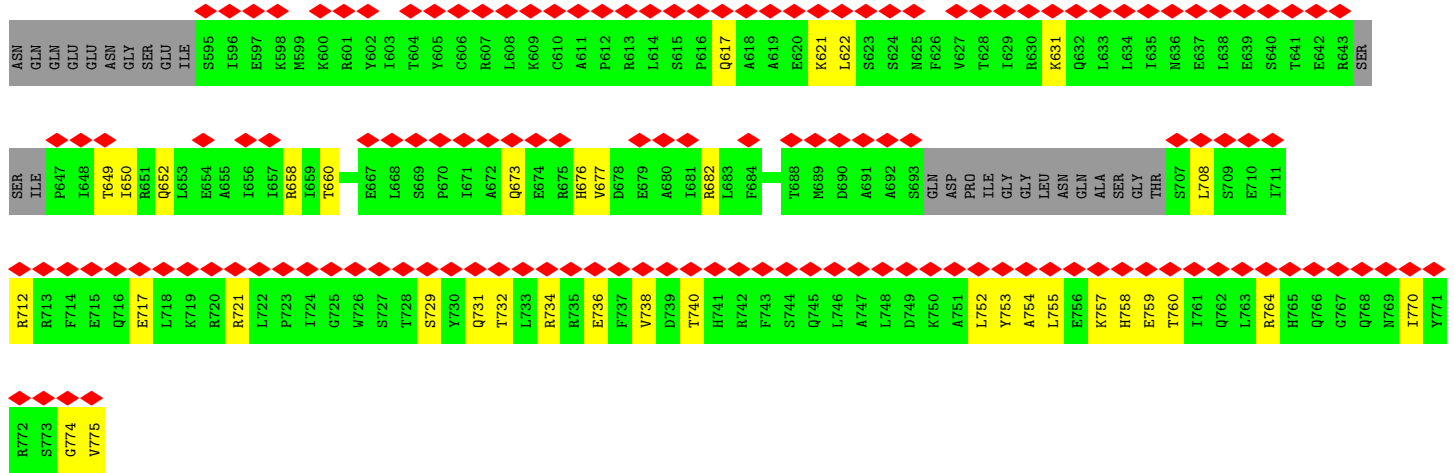




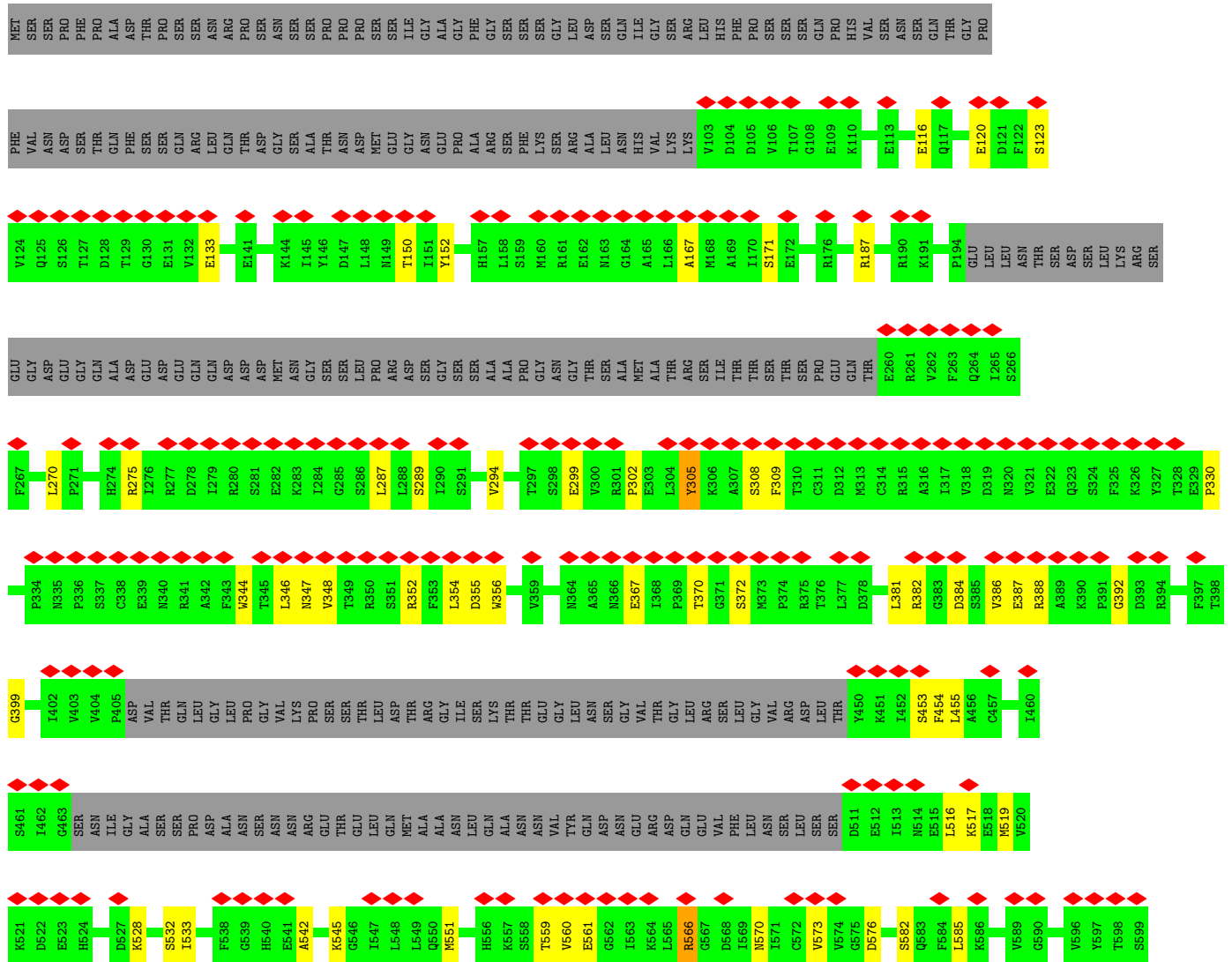
• Molecule 14: Minichromosome maintenance protein 5

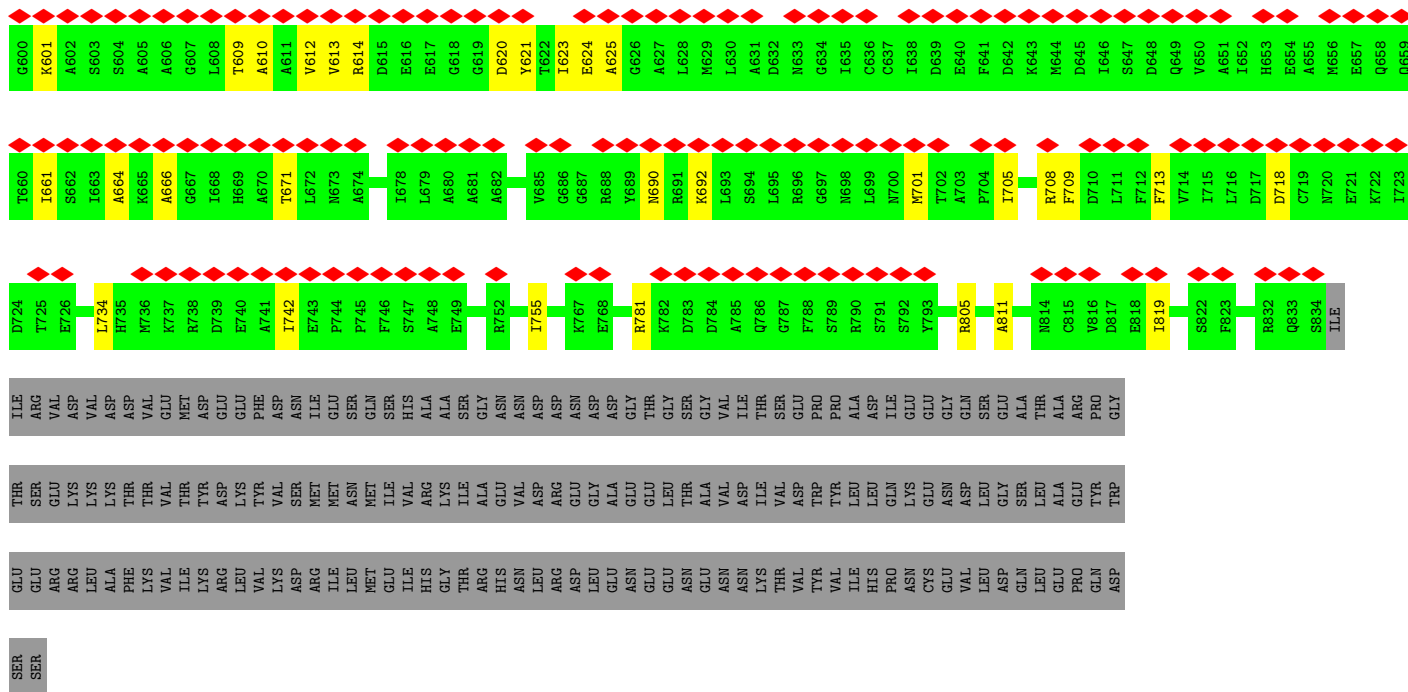




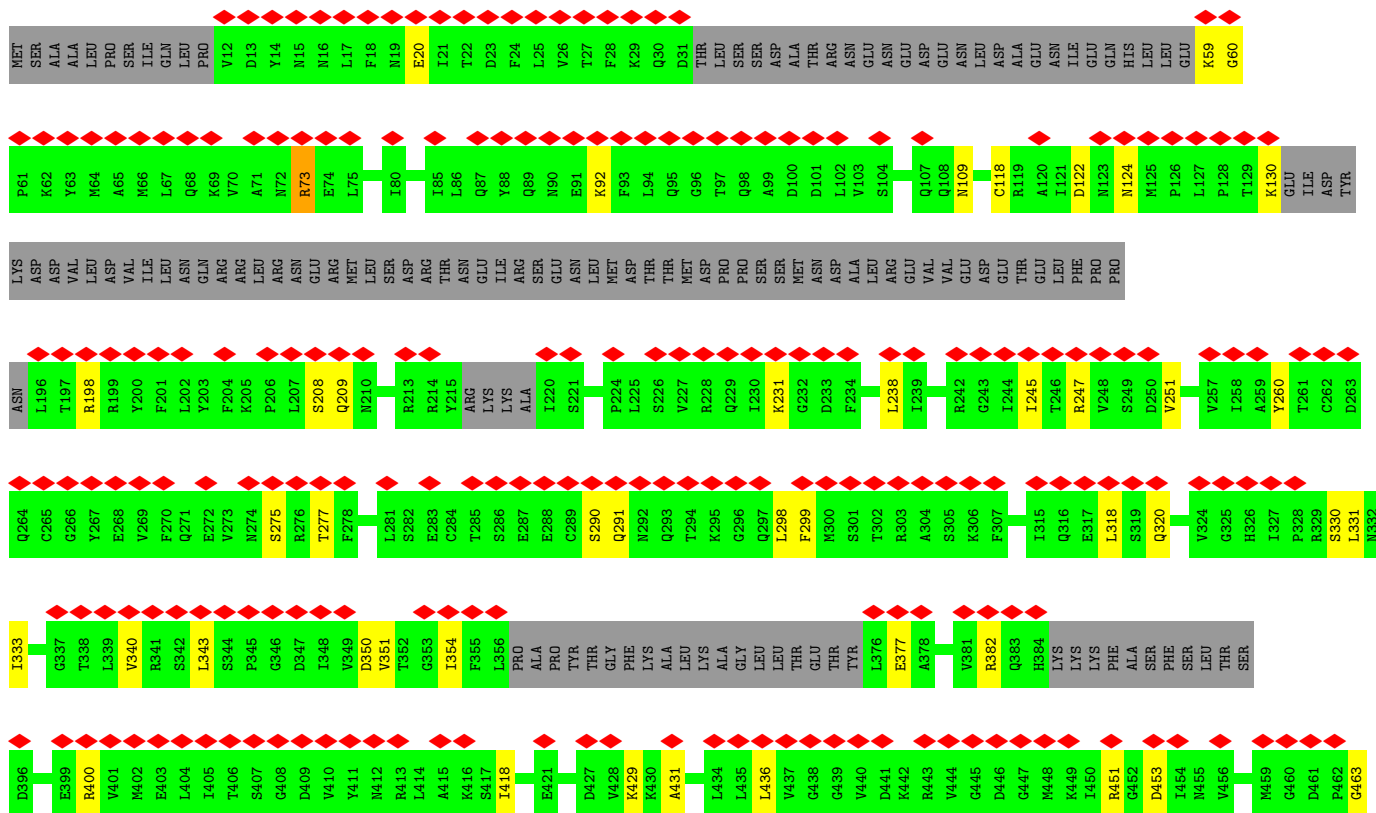


• Molecule 15: DNA replication licensing factor MCM6





• Molecule 16: DNA replication licensing factor MCM7



V464	Q468	L469	I473	C474	K475	I476	V481	Y482	T483	T484	C485	K486	G487	S488	S489	G490	V491	G492	L493	T494	A495	A496	V497	M498	K499	D500	P501	V502	I503	D504	E505	M506	I507	L508	E509	G510	V514	L515	A516	D517	N518	G519	I520	C521	C522	I523	D524	E525	F526	D527	K528	M529	D530	E531	S532			
D533	R534	T535	A536	I537	H538	E539	V540	M541	E542	Q543	Q544	T545	I546	S547	I548	S549	K550	A551	G552	I553	N554	T555	T556	L557	N558	A559	I563	L564	A565	A566	A567	N568	P569	L570	Y571	G572	R573	Y574	N575	P576	R577	L578	S579	P580	L581	D582	N583	I584	N585	L586	P587	A588	A589	L590	L591	S592	R593	F594
D595	I596	L597	F598	L599	M600	L601	D602	S605	R606	D607	D608	K611	V616	H620	K624	D627	L628	D629	F630	T631	E634	P635	S636	K637	M638	I642	A643	Y644	A645	K646	T647	K648	R649	P650	V651	M652	S653	E654	A655	V656	M657	D658	Y659	V660	V661	Q662	A663	Y664	I665	R666	L667							
R668	Q669	D670	S671	K672	ARG	GLU	MET	D676	S677	K678	F679	S680	F681	G682	Q683	A684	T685	P686	R687	T688	L689	L690	G691	R694	L695	S696	Q697	A698	L699	A700	K701	L702	R703	L704	A705	D706	M707	V708	D709	I710	D711	D712	V713	E714	E715	A716	L717	R718	L719	V720	R721	V722	S723	K724	E725	S726	L727	Y728
Q729	GLU	THR	ASN	LYS	SER	LYS	GLU	ASP	GLU	SER	P740	T741	T742	K743	I744	I747	K750	M751	L752	Q753	E754	T755	G756	K757	M758	I759	L760	E763	N764	I765	V766	R770	L771	R772	G773	F774	T775	M776	L777	Q778	L779	S780	M781	I783	Q784	E785	Y786	S787	Y788	L789	M790	V791	TRP	HIS				
LEU	ILE	ASN	GLU	GLY	ASN	THR	LEU	LYS	PHE	VAL	ASP	ASP	GLY	THR	MET	ASP	THR	ASP	GLN	GLU	ASP	SER	LEU	VAL	SER	THR	PRO	LYS	LEU	ALA	PRO	GLN	THR	THR	ALA	SER	ALA	ASN	VAL	SER	ALA	GLN	ASP	SER	ASP	ILE	ASP	LEU	GLN	ASP	ALA							

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25126	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 ( $e^-/\text{\AA}^2$ )	50	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	0.060	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	335.36, 335.36, 335.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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: AGS

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	8	0.25	0/3070	0.52	0/4175
2	9	0.32	0/3014	0.58	0/4055
3	A	0.35	0/3415	0.56	1/4596 (0.0%)
4	B	0.34	0/2717	0.53	0/3662
5	C	0.34	0/4602	0.55	0/6212
6	E	0.38	0/3505	0.55	0/4767
7	D	0.36	0/3612	0.52	0/4879
8	F	0.29	0/1336	0.50	0/1798
9	G	0.78	0/923	1.16	0/1425
10	H	0.76	0/958	0.94	0/1474
11	2	0.38	0/4552	0.66	1/6152 (0.0%)
12	3	0.39	0/4944	0.67	1/6718 (0.0%)
13	4	0.39	0/5060	0.68	2/6863 (0.0%)
14	5	0.38	0/4362	0.65	0/5924
15	6	0.39	0/4550	0.65	1/6148 (0.0%)
16	7	0.39	0/4918	0.64	1/6653 (0.0%)
All	All	0.39	0/55538	0.63	7/75501 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	3	717	LEU	CA-CB-CG	6.48	130.20	115.30
3	A	538	THR	C-N-CA	-6.33	105.88	121.70
13	4	804	LEU	CA-CB-CG	5.74	128.51	115.30
16	7	238	LEU	CA-CB-CG	5.49	127.93	115.30
11	2	211	LEU	CA-CB-CG	5.08	126.98	115.30
15	6	356	TRP	CA-CB-CG	5.01	123.22	113.70
13	4	417	LEU	CA-CB-CG	5.01	126.81	115.30

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	8	3011	0	2969	111	0
2	9	2972	0	3082	85	0
3	A	3368	0	3420	66	0
4	B	2663	0	2673	51	0
5	C	4505	0	4458	72	0
6	E	3425	0	3402	67	0
7	D	3551	0	3615	82	0
8	F	1315	0	1353	23	0
9	G	831	0	480	3	0
10	H	847	0	457	7	0
11	2	4478	0	4424	77	0
12	3	4866	0	4733	93	0
13	4	4995	0	4751	106	0
14	5	4317	0	4060	72	0
15	6	4475	0	4414	71	0
16	7	4858	0	4803	73	0
17	9	31	0	12	4	0
17	A	31	0	12	7	0
17	D	31	0	12	4	0
17	E	31	0	12	5	0
All	All	54601	0	53142	990	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 (990) 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)
12:3:534:ALA:HB1	14:5:757:LYS:O	1.52	1.08
13:4:601:LEU:HA	13:4:620:ALA:HB3	1.29	1.08
1:8:338:PRO:HG2	1:8:383:MET:O	1.55	1.07

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:541:ALA:HB2	9:G:10:DT:OP1	1.57	1.05
12:3:246:GLY:HA3	16:7:109:ASN:HA	1.05	1.04
12:3:246:GLY:HA3	16:7:109:ASN:CA	1.88	1.03
1:8:393:THR:CB	11:2:255:ILE:HB	1.90	1.00
2:9:282:LEU:CB	2:9:283:PRO:CD	2.43	0.96
13:4:601:LEU:HA	13:4:620:ALA:CB	1.97	0.94
11:2:332:PRO:CA	11:2:383:ARG:CB	2.47	0.91
11:2:332:PRO:HA	11:2:383:ARG:CB	2.03	0.88
12:3:246:GLY:CA	16:7:109:ASN:HA	1.99	0.86
14:5:170:SER:CB	14:5:463:TYR:HB2	2.05	0.86
13:4:696:PRO:HD2	13:4:697:PRO:HD2	1.57	0.86
1:8:25:ASP:O	1:8:26:GLU:HG2	1.76	0.85
13:4:696:PRO:CD	13:4:697:PRO:HD2	2.07	0.83
11:2:333:GLN:N	11:2:383:ARG:CB	2.42	0.83
14:5:448:GLY:O	14:5:467:GLY:HA3	1.79	0.81
11:2:386:GLN:CB	11:2:410:LEU:CB	2.59	0.81
14:5:734:ARG:O	14:5:738:VAL:CB	2.29	0.81
12:3:270:LEU:HA	14:5:510:THR:O	1.81	0.81
13:4:696:PRO:N	13:4:697:PRO:HD2	2.00	0.76
2:9:282:LEU:CB	2:9:283:PRO:HD3	2.15	0.75
13:4:881:MET:O	13:4:924:ARG:O	2.02	0.75
13:4:344:VAL:HG12	13:4:345:ALA:N	2.01	0.75
11:2:332:PRO:C	11:2:383:ARG:CB	2.55	0.75
11:2:335:LYS:HA	11:2:352:PHE:O	1.86	0.74
1:8:346:GLN:CB	11:2:301:PRO:O	2.36	0.73
13:4:911:GLN:HA	13:4:916:VAL:O	1.89	0.73
14:5:622:LEU:HD12	14:5:677:VAL:HG11	1.70	0.72
14:5:452:SER:HB2	14:5:465:GLU:HB2	1.73	0.71
15:6:551:MET:HE2	15:6:755:ILE:HD13	1.71	0.71
1:8:393:THR:CB	11:2:255:ILE:CB	2.68	0.71
2:9:282:LEU:CB	2:9:283:PRO:HD2	2.21	0.71
1:8:211:THR:HB	11:2:226:VAL:CB	2.21	0.70
3:A:538:THR:CB	3:A:541:ALA:H	2.04	0.70
1:8:375:LEU:HD11	1:8:379:GLY:O	1.91	0.70
12:3:123:PRO:HB2	12:3:124:PRO:CD	2.21	0.70
14:5:448:GLY:O	14:5:467:GLY:CA	2.38	0.70
16:7:251:VAL:HG23	16:7:340:VAL:HG21	1.73	0.70
13:4:647:GLU:O	13:4:651:GLN:HB2	1.90	0.70
16:7:588:ALA:O	16:7:592:SER:HB3	1.92	0.70
13:4:881:MET:H	13:4:926:SER:CB	2.06	0.69
6:E:435:THR:HG22	6:E:450:TRP:HE1	1.58	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:321:CYS:HG	1:8:371:TYR:HH	1.37	0.69
14:5:495:GLU:O	14:5:499:GLN:OE1	2.11	0.69
13:4:601:LEU:CA	13:4:620:ALA:HB3	2.16	0.69
14:5:280:ARG:HD3	14:5:280:ARG:N	2.08	0.69
13:4:622:VAL:HG21	13:4:665:LEU:CD1	2.23	0.68
14:5:486:ARG:O	14:5:489:ASP:OD1	2.11	0.68
14:5:729:SER:O	14:5:732:THR:N	2.24	0.68
12:3:534:ALA:CB	14:5:757:LYS:O	2.38	0.68
14:5:470:VAL:HG22	14:5:513:LEU:HD23	1.76	0.68
1:8:346:GLN:HA	11:2:301:PRO:O	1.94	0.68
14:5:500:GLN:O	14:5:515:SER:HB3	1.94	0.68
13:4:600:GLY:O	13:4:620:ALA:CB	2.41	0.67
1:8:71:GLN:NE2	1:8:104:ARG:O	2.27	0.67
12:3:494:THR:HG22	12:3:507:ASN:HA	1.74	0.67
2:9:118:LEU:HA	2:9:121:ILE:HD12	1.77	0.67
11:2:569:GLN:H	11:2:569:GLN:CD	1.98	0.67
12:3:222:THR:O	14:5:246:GLU:CB	2.42	0.66
13:4:344:VAL:HG12	13:4:345:ALA:H	1.60	0.66
1:8:249:LEU:HD13	1:8:257:ILE:HD13	1.78	0.66
1:8:126:ALA:O	1:8:130:VAL:HG12	1.95	0.66
1:8:266:LEU:HA	1:8:280:ASN:HB2	1.77	0.66
12:3:507:ASN:OD1	12:3:507:ASN:O	2.14	0.66
13:4:812:LYS:O	13:4:812:LYS:HG2	1.95	0.66
3:A:694:ARG:CZ	16:7:791:VAL:HG12	2.25	0.66
8:F:333:ASN:HA	8:F:336:ARG:HB2	1.77	0.66
16:7:500:ASP:O	16:7:504:ASP:HA	1.96	0.66
1:8:289:ALA:O	1:8:293:VAL:N	2.22	0.65
14:5:470:VAL:HG22	14:5:513:LEU:CD2	2.27	0.65
14:5:622:LEU:CD1	14:5:677:VAL:HG11	2.26	0.65
1:8:133:VAL:HG12	1:8:134:VAL:HG23	1.78	0.65
13:4:600:GLY:O	13:4:620:ALA:HB2	1.97	0.65
14:5:457:PRO:HA	14:5:460:ARG:HH21	1.61	0.65
1:8:20:LEU:HD11	1:8:48:TYR:HA	1.79	0.64
14:5:170:SER:CB	14:5:463:TYR:CB	2.74	0.64
4:B:421:ILE:HG22	4:B:451:ALA:HB3	1.78	0.64
7:D:324:ILE:HG12	7:D:337:LEU:HD11	1.79	0.64
13:4:622:VAL:CG2	13:4:665:LEU:CD1	2.75	0.64
13:4:379:PRO:O	13:4:380:ASN:ND2	2.31	0.64
14:5:770:ILE:O	14:5:774:GLY:N	2.31	0.64
7:D:486:TYR:CE2	10:H:24:DC:H6	2.16	0.64
1:8:307:LEU:HB2	1:8:434:ARG:HB2	1.79	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:298:PHE:HB2	5:C:469:ASP:HA	1.79	0.63
16:7:508:LEU:CD2	16:7:553:ILE:HD13	2.28	0.63
6:E:338:CYS:SG	6:E:385:ARG:NH1	2.71	0.63
15:6:299:GLU:OE2	15:6:620:ASP:OD2	2.16	0.63
15:6:302:PRO:HA	15:6:354:LEU:O	1.99	0.63
15:6:551:MET:CE	15:6:755:ILE:HD13	2.29	0.63
2:9:245:LEU:HB3	2:9:258:LEU:HD11	1.79	0.62
16:7:508:LEU:HD21	16:7:553:ILE:HD11	1.81	0.62
12:3:915:PRO:HA	12:3:958:VAL:HA	1.80	0.62
2:9:113:GLY:HA2	17:9:2001:AGS:H3'	1.80	0.62
12:3:218:THR:O	12:3:299:LYS:NZ	2.29	0.62
1:8:192:PRO:HG2	1:8:233:GLY:HA2	1.81	0.62
1:8:287:ILE:HG23	1:8:288:LYS:H	1.65	0.62
1:8:143:ILE:O	1:8:143:ILE:HG22	1.98	0.62
15:6:399:GLY:HA3	15:6:455:LEU:O	1.99	0.62
16:7:247:ARG:NH2	16:7:509:GLU:HG3	2.15	0.62
12:3:493:GLN:O	12:3:494:THR:HG23	2.00	0.62
15:6:305:TYR:CB	15:6:352:ARG:O	2.48	0.62
2:9:505:ILE:HG13	2:9:505:ILE:O	1.99	0.61
3:A:789:HIS:O	3:A:793:PHE:N	2.32	0.61
12:3:488:GLU:O	12:3:492:GLN:CB	2.48	0.61
2:9:315:MET:HA	2:9:318:LYS:HD2	1.82	0.61
2:9:171:ASN:HA	2:9:223:ASP:HB2	1.83	0.61
11:2:338:LYS:HD3	11:2:349:GLY:HA3	1.83	0.61
12:3:270:LEU:CA	14:5:510:THR:O	2.49	0.61
13:4:662:ILE:O	13:4:662:ILE:HG13	2.00	0.61
11:2:583:ASP:O	11:2:587:LYS:HA	2.00	0.61
12:3:198:ARG:O	12:3:198:ARG:HG2	2.01	0.61
1:8:142:CYS:O	1:8:265:PRO:HD3	2.00	0.61
16:7:508:LEU:CD2	16:7:553:ILE:CD1	2.78	0.61
4:B:294:PHE:HA	4:B:297:GLN:HE21	1.65	0.60
4:B:319:VAL:HG21	5:C:491:LEU:HD21	1.82	0.60
15:6:582:SER:O	15:6:585:LEU:HB3	2.01	0.60
5:C:132:THR:O	5:C:135:GLU:N	2.32	0.60
14:5:470:VAL:HG13	14:5:513:LEU:HD23	1.82	0.60
12:3:122:ILE:N	12:3:123:PRO:CD	2.64	0.60
13:4:622:VAL:HG21	13:4:665:LEU:HD11	1.82	0.60
1:8:318:PHE:HD1	1:8:363:LEU:HD21	1.65	0.60
13:4:882:SER:HA	13:4:924:ARG:O	2.01	0.60
2:9:240:ARG:NH2	2:9:241:THR:OG1	2.35	0.59
5:C:328:TYR:HB2	5:C:468:LEU:HD21	1.84	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:442:LEU:HB3	12:3:461:ALA:HB3	1.83	0.59
13:4:527:ALA:HB3	13:4:530:ILE:HD11	1.84	0.59
7:D:278:ILE:HG23	7:D:283:ASP:HB2	1.84	0.59
2:9:331:LEU:O	2:9:335:PHE:N	2.35	0.59
11:2:341:CYS:O	11:2:345:GLY:HA2	2.03	0.59
11:2:689:GLU:OE1	11:2:689:GLU:HA	2.00	0.59
14:5:455:ARG:HA	14:5:461:GLU:O	2.03	0.59
1:8:375:LEU:HD12	1:8:380:GLU:O	2.03	0.59
1:8:71:GLN:HG3	1:8:95:ASP:H	1.67	0.59
1:8:346:GLN:CB	11:2:301:PRO:C	2.71	0.59
4:B:470:ALA:HA	4:B:473:TYR:HB2	1.85	0.59
15:6:610:ALA:HA	15:6:624:GLU:O	2.02	0.59
3:A:790:VAL:HG12	7:D:254:LEU:HD13	1.85	0.59
1:8:214:THR:OG1	1:8:216:ASP:OD1	2.21	0.59
7:D:133:ASN:HB3	7:D:136:ILE:HG22	1.85	0.59
14:5:660:THR:HG21	14:5:677:VAL:HG22	1.84	0.59
15:6:354:LEU:C	15:6:354:LEU:HD12	2.23	0.59
1:8:13:LEU:HD11	1:8:220:VAL:HG11	1.83	0.58
1:8:300:ARG:O	1:8:300:ARG:HG3	2.03	0.58
1:8:221:SER:OG	1:8:250:GLN:NE2	2.36	0.58
3:A:722:MET:HB3	7:D:84:ARG:HH22	1.67	0.58
12:3:923:ILE:HG13	12:3:924:ASN:N	2.18	0.58
1:8:338:PRO:CG	1:8:383:MET:O	2.41	0.58
2:9:115:THR:OG1	17:9:2001:AGS:S1G	2.62	0.58
7:D:379:ARG:HH12	7:D:467:ASP:HB2	1.68	0.58
11:2:330:VAL:HG12	11:2:330:VAL:O	2.02	0.58
6:E:283:ALA:HA	6:E:286:LYS:HD2	1.86	0.58
13:4:342:MET:HG3	13:4:344:VAL:O	2.03	0.58
13:4:344:VAL:CG1	13:4:345:ALA:N	2.66	0.58
15:6:690:ASN:HB2	15:6:692:LYS:HG2	1.86	0.58
4:B:486:SER:HB2	4:B:489:GLU:HB2	1.85	0.58
17:E:2001:AGS:S1G	17:E:2001:AGS:O2B	2.62	0.58
7:D:486:TYR:CE2	10:H:24:DC:C6	2.91	0.58
13:4:344:VAL:CG1	13:4:345:ALA:H	2.17	0.58
15:6:609:THR:HG23	15:6:610:ALA:N	2.18	0.58
16:7:436:LEU:CD1	16:7:642:ILE:HD13	2.34	0.57
1:8:300:ARG:HG2	1:8:418:LYS:HB2	1.86	0.57
1:8:346:GLN:CA	11:2:301:PRO:O	2.51	0.57
7:D:486:TYR:CD1	10:H:24:DC:H5	2.22	0.57
7:D:486:TYR:CZ	10:H:24:DC:C6	2.92	0.57
14:5:279:ASP:O	14:5:283:THR:CG2	2.52	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:941:GLY:HA2	12:3:944:ILE:HD12	1.86	0.57
1:8:23:VAL:HG11	1:8:128:LEU:HD22	1.86	0.57
12:3:173:ALA:HB1	14:5:250:PHE:O	2.03	0.57
1:8:203:LYS:HD3	1:8:221:SER:HB3	1.86	0.57
3:A:625:THR:OG1	3:A:626:GLY:N	2.38	0.57
14:5:65:MET:SD	14:5:161:ARG:NH2	2.78	0.57
16:7:508:LEU:HD22	16:7:553:ILE:HD13	1.85	0.57
6:E:346:ASP:OD2	6:E:385:ARG:NH2	2.38	0.57
11:2:356:ASN:OD1	11:2:357:GLU:N	2.34	0.57
12:3:122:ILE:N	12:3:123:PRO:HD2	2.20	0.57
4:B:318:GLY:O	4:B:322:LYS:NZ	2.37	0.56
1:8:237:ALA:HB2	1:8:244:HIS:HB2	1.87	0.56
16:7:498:MET:CE	16:7:509:GLU:OE1	2.53	0.56
3:A:806:TYR:O	3:A:810:ASN:ND2	2.37	0.56
17:A:2001:AGS:O2G	7:D:267:ARG:NH1	2.37	0.56
13:4:622:VAL:HG21	13:4:665:LEU:HD13	1.87	0.56
3:A:694:ARG:NH1	16:7:791:VAL:HG12	2.21	0.56
5:C:309:ASN:ND2	5:C:312:HIS:O	2.38	0.56
6:E:103:GLU:HG2	6:E:104:GLU:HG2	1.87	0.56
7:D:261:GLU:OE2	7:D:263:ARG:NH1	2.38	0.56
6:E:435:THR:HG21	6:E:442:ASP:CG	2.26	0.56
16:7:260:TYR:HB3	16:7:298:LEU:HD12	1.88	0.56
3:A:421:THR:OG1	3:A:422:ILE:N	2.39	0.56
3:A:607:ARG:HE	3:A:608:GLN:HE22	1.51	0.56
8:F:291:ASP:OD1	8:F:291:ASP:N	2.38	0.56
1:8:111:LEU:HD21	1:8:150:THR:OG1	2.05	0.56
3:A:560:THR:HG23	3:A:592:LYS:HB3	1.88	0.56
1:8:44:LEU:HD11	1:8:227:CYS:HB2	1.88	0.56
2:9:104:LEU:H	2:9:281:LEU:HD12	1.70	0.56
5:C:378:LEU:O	5:C:383:ASN:ND2	2.38	0.56
6:E:50:TYR:O	6:E:54:ASN:ND2	2.35	0.56
5:C:199:LEU:HB3	5:C:232:VAL:HG12	1.88	0.56
5:C:528:TYR:O	5:C:610:LYS:NZ	2.39	0.56
3:A:704:ARG:HG3	17:A:2001:AGS:H5'2	1.88	0.55
13:4:534:GLU:O	13:4:538:LYS:HB2	2.06	0.55
1:8:304:ILE:HG22	1:8:306:ARG:H	1.72	0.55
7:D:486:TYR:CG	10:H:24:DC:H5	2.25	0.55
14:5:456:ASP:HB3	14:5:461:GLU:HB2	1.88	0.55
1:8:130:VAL:O	1:8:130:VAL:HG22	2.06	0.55
1:8:340:LEU:N	1:8:380:GLU:OE2	2.32	0.55
3:A:704:ARG:NH2	17:A:2001:AGS:O3A	2.39	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:328:THR:HA	8:F:331:VAL:HG12	1.88	0.55
11:2:584:PRO:O	15:6:614:ARG:NH2	2.40	0.55
6:E:31:SER:OG	6:E:153:ASN:ND2	2.39	0.55
11:2:764:MET:HA	11:2:767:ILE:HD12	1.89	0.55
12:3:405:ILE:HG12	12:3:545:LEU:HB2	1.89	0.55
12:3:410:ASP:O	12:3:415:LYS:NZ	2.40	0.55
16:7:722:VAL:HA	16:7:725:GLU:HB2	1.88	0.55
6:E:430:LEU:HB3	6:E:432:LEU:HG	1.89	0.55
2:9:94:LYS:HB3	2:9:99:HIS:HB3	1.89	0.54
2:9:268:LYS:NZ	4:B:512:TYR:OH	2.40	0.54
17:A:2001:AGS:O2A	17:A:2001:AGS:O1B	2.25	0.54
5:C:242:THR:OG1	5:C:243:ASN:N	2.39	0.54
1:8:304:ILE:HG21	1:8:437:SER:H	1.72	0.54
7:D:47:PRO:O	7:D:51:SER:N	2.40	0.54
11:2:544:ASP:O	11:2:549:LYS:NZ	2.38	0.54
12:3:123:PRO:HB2	12:3:124:PRO:HD3	1.89	0.54
13:4:600:GLY:O	13:4:620:ALA:HB3	2.06	0.54
13:4:654:ILE:O	13:4:664:THR:HA	2.07	0.54
14:5:729:SER:O	14:5:731:GLN:N	2.40	0.54
2:9:197:LEU:O	2:9:204:HIS:ND1	2.36	0.54
4:B:282:ASN:HB3	4:B:485:PRO:HG3	1.90	0.54
7:D:236:ASP:OD2	7:D:267:ARG:NE	2.39	0.54
12:3:432:THR:HG21	12:3:442:LEU:HD11	1.88	0.54
6:E:216:ARG:HA	6:E:219:ILE:HD12	1.88	0.54
13:4:645:LEU:HA	13:4:648:VAL:HG22	1.88	0.54
3:A:404:SER:OG	3:A:405:ARG:N	2.40	0.54
6:E:195:ASP:N	6:E:195:ASP:OD1	2.40	0.54
11:2:351:PHE:CE2	15:6:348:VAL:CG1	2.91	0.54
11:2:578:ALA:HA	11:2:593:GLY:HA2	1.89	0.54
3:A:538:THR:CB	9:G:10:DT:H3'	2.38	0.54
1:8:66:LEU:HD21	1:8:106:CYS:HB2	1.89	0.54
7:D:313:LEU:O	7:D:321:ASN:ND2	2.41	0.54
8:F:376:GLU:O	8:F:380:ARG:NH2	2.41	0.54
1:8:294:ALA:O	1:8:298:TYR:HB2	2.07	0.54
1:8:207:TYR:HA	1:8:248:PRO:HD2	1.90	0.54
2:9:103:SER:HB3	2:9:281:LEU:HA	1.90	0.54
2:9:494:ASP:OD1	2:9:494:ASP:N	2.41	0.54
6:E:56:ASN:OD1	6:E:56:ASN:N	2.41	0.54
7:D:375:ASN:O	7:D:379:ARG:NE	2.40	0.54
13:4:342:MET:HA	13:4:391:PHE:HD1	1.72	0.54
1:8:310:ALA:O	1:8:314:VAL:HG12	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:475:LYS:HB3	2:9:485:PHE:HB3	1.90	0.54
3:A:413:THR:HA	7:D:207:ILE:HD12	1.89	0.54
6:E:230:ASP:O	6:E:234:ASN:ND2	2.41	0.54
6:E:6:PRO:HG3	6:E:50:TYR:HA	1.89	0.53
11:2:332:PRO:CB	11:2:383:ARG:CB	2.86	0.53
6:E:111:THR:HA	6:E:114:ASN:HD22	1.74	0.53
7:D:455:ASP:OD1	7:D:455:ASP:N	2.38	0.53
12:3:733:LEU:O	12:3:737:LEU:HB2	2.08	0.53
4:B:526:LYS:NZ	4:B:530:GLU:OE2	2.40	0.53
6:E:218:ARG:NH2	6:E:273:ILE:O	2.40	0.53
13:4:622:VAL:CG2	13:4:665:LEU:HD11	2.38	0.53
14:5:136:GLN:HB2	14:5:280:ARG:HH21	1.73	0.53
6:E:153:ASN:OD1	6:E:153:ASN:N	2.40	0.53
11:2:286:TYR:HE2	11:2:293:ILE:HD11	1.74	0.53
2:9:464:ILE:HG12	3:A:699:VAL:HA	1.89	0.53
15:6:734:LEU:HD13	15:6:742:ILE:HG21	1.91	0.53
16:7:118:CYS:SG	16:7:198:ARG:NH2	2.82	0.53
2:9:60:ALA:O	2:9:64:LYS:N	2.40	0.53
5:C:375:ASP:N	5:C:375:ASP:OD1	2.40	0.53
11:2:331:PHE:O	11:2:385:TYR:HB2	2.08	0.53
12:3:495:VAL:HG22	12:3:496:THR:N	2.23	0.53
16:7:498:MET:HE2	16:7:509:GLU:OE1	2.09	0.53
3:A:543:MET:HA	3:A:546:LEU:HB2	1.91	0.53
2:9:330:ASP:OD1	2:9:330:ASP:N	2.41	0.53
5:C:603:LYS:O	5:C:603:LYS:HG2	2.09	0.53
7:D:53:GLN:NE2	7:D:345:VAL:O	2.42	0.53
12:3:698:THR:HA	16:7:463:GLY:HA2	1.91	0.53
12:3:897:SER:HA	12:3:900:ILE:HD12	1.91	0.53
12:3:923:ILE:HG13	12:3:924:ASN:H	1.74	0.53
13:4:561:ASP:H	13:4:803:ARG:HD2	1.73	0.53
2:9:227:ARG:NH2	3:A:577:ASP:OD1	2.41	0.53
12:3:32:LEU:HD13	12:3:132:LEU:HD22	1.90	0.53
14:5:489:ASP:OD1	14:5:490:ARG:N	2.42	0.53
12:3:493:GLN:O	12:3:494:THR:CG2	2.57	0.53
1:8:302:LEU:C	1:8:304:ILE:H	2.13	0.52
13:4:344:VAL:HG13	13:4:358:VAL:O	2.09	0.52
13:4:889:GLN:O	13:4:892:GLU:CB	2.57	0.52
2:9:345:TYR:OH	2:9:388:ASN:ND2	2.42	0.52
2:9:473:ILE:HG22	2:9:489:ILE:HG22	1.89	0.52
5:C:381:LEU:HD21	8:F:422:LYS:HE3	1.90	0.52
7:D:97:SER:HB2	7:D:247:ILE:HB	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:351:PHE:CE2	15:6:348:VAL:HG13	2.44	0.52
13:4:564:ILE:HG22	13:4:704:LEU:HB3	1.91	0.52
4:B:547:ARG:NH1	4:B:548:GLY:O	2.42	0.52
15:6:167:ALA:O	15:6:171:SER:HB3	2.09	0.52
2:9:234:SER:OG	2:9:235:GLU:N	2.40	0.52
6:E:11:ARG:NH2	6:E:192:TYR:OH	2.42	0.52
13:4:683:ASN:H	13:4:691:ASN:HD21	1.56	0.52
13:4:696:PRO:HD2	13:4:697:PRO:CD	2.36	0.52
2:9:409:LYS:O	2:9:415:LYS:NZ	2.39	0.52
6:E:442:ASP:HA	6:E:448:VAL:HG21	1.91	0.52
11:2:341:CYS:O	11:2:345:GLY:CA	2.58	0.52
12:3:469:VAL:HG12	12:3:511:SER:HB3	1.91	0.52
1:8:47:ASN:ND2	1:8:47:ASN:O	2.42	0.52
3:A:637:ASP:OD1	3:A:637:ASP:N	2.43	0.52
8:F:329:PHE:O	8:F:336:ARG:NH2	2.42	0.52
11:2:411:LEU:C	11:2:411:LEU:HD12	2.30	0.52
13:4:701:ARG:HG2	13:4:796:ARG:HE	1.74	0.52
16:7:648:LYS:HB2	16:7:701:LYS:HG2	1.92	0.52
2:9:226:ASP:HA	2:9:229:LEU:HB2	1.91	0.52
4:B:342:GLN:NE2	4:B:417:ASP:OD1	2.43	0.52
5:C:278:ASN:ND2	5:C:422:PHE:O	2.36	0.52
13:4:543:GLN:NE2	13:4:670:SER:OG	2.42	0.52
14:5:515:SER:OG	14:5:517:THR:OG1	2.17	0.52
13:4:342:MET:HA	13:4:391:PHE:CD1	2.44	0.52
3:A:541:ALA:CB	9:G:10:DT:OP1	2.46	0.52
11:2:335:LYS:CA	11:2:352:PHE:O	2.56	0.52
11:2:806:THR:OG1	11:2:807:VAL:N	2.43	0.52
14:5:190:THR:OG1	14:5:191:SER:N	2.43	0.52
11:2:286:TYR:CE2	11:2:293:ILE:HD11	2.45	0.51
13:4:611:THR:HG23	13:4:613:GLN:HB2	1.91	0.51
14:5:717:GLU:O	14:5:721:ARG:CB	2.58	0.51
2:9:61:LEU:HA	2:9:64:LYS:HB2	1.92	0.51
2:9:226:ASP:OD1	2:9:226:ASP:N	2.43	0.51
2:9:491:VAL:HG22	2:9:493:LEU:H	1.73	0.51
4:B:363:LEU:HD13	5:C:22:HIS:HB3	1.91	0.51
11:2:351:PHE:HE2	15:6:348:VAL:HG11	1.74	0.51
14:5:753:TYR:O	14:5:757:LYS:CB	2.58	0.51
17:9:2001:AGS:S1G	17:9:2001:AGS:O2B	2.68	0.51
4:B:433:ARG:HH21	6:E:441:ILE:HD11	1.76	0.51
8:F:305:GLU:O	8:F:309:ASN:ND2	2.43	0.51
11:2:854:ARG:HA	11:2:857:LEU:HD13	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:622:VAL:CG2	13:4:665:LEU:HD13	2.39	0.51
14:5:757:LYS:C	14:5:759:GLU:H	2.14	0.51
2:9:226:ASP:OD2	3:A:612:LYS:NZ	2.43	0.51
5:C:554:LEU:HA	5:C:557:ILE:HG22	1.93	0.51
2:9:495:MET:SD	2:9:495:MET:N	2.82	0.51
6:E:439:LYS:NZ	7:D:491:GLN:OE1	2.41	0.51
7:D:486:TYR:CD1	10:H:24:DC:C5	2.98	0.51
4:B:367:ASN:ND2	5:C:19:GLN:O	2.43	0.51
4:B:556:LEU:CD2	4:B:600:ILE:HG23	2.41	0.51
7:D:171:THR:HG23	7:D:172:ILE:HG13	1.92	0.51
7:D:500:ASP:OD1	7:D:500:ASP:N	2.36	0.51
12:3:27:ARG:NH2	12:3:109:SER:OG	2.43	0.51
1:8:111:LEU:HD11	1:8:150:THR:CB	2.41	0.51
6:E:96:ASP:OD1	6:E:96:ASP:N	2.43	0.51
11:2:576:LEU:HD13	11:2:620:ILE:HD13	1.93	0.51
15:6:382:ARG:HH11	15:6:455:LEU:HD21	1.74	0.51
3:A:481:PRO:O	7:D:262:LYS:NZ	2.43	0.51
3:A:620:THR:OG1	3:A:621:ARG:N	2.43	0.51
6:E:133:ASP:HA	6:E:169:THR:HB	1.93	0.51
6:E:338:CYS:O	6:E:379:SER:OG	2.29	0.51
11:2:333:GLN:H	11:2:383:ARG:CB	2.23	0.51
11:2:626:GLN:NE2	11:2:628:SER:O	2.43	0.51
12:3:921:GLU:O	12:3:922:ARG:NH2	2.38	0.51
4:B:534:GLN:OE1	4:B:535:ASN:ND2	2.44	0.51
6:E:192:TYR:O	6:E:253:ASN:ND2	2.43	0.51
7:D:83:ASP:HA	7:D:86:ILE:HG22	1.93	0.51
2:9:423:GLN:NE2	2:9:512:LEU:O	2.44	0.50
5:C:447:LYS:HA	5:C:450:LYS:HD3	1.92	0.50
7:D:251:THR:OG1	7:D:252:THR:N	2.43	0.50
13:4:428:ARG:NH2	15:6:370:THR:O	2.44	0.50
2:9:311:ILE:HG13	2:9:311:ILE:O	2.12	0.50
7:D:491:GLN:NE2	7:D:492:PHE:O	2.43	0.50
8:F:306:TYR:O	8:F:310:ALA:N	2.43	0.50
14:5:649:THR:HG23	14:5:652:GLN:H	1.76	0.50
2:9:88:VAL:HG22	2:9:92:LEU:HD23	1.93	0.50
2:9:234:SER:OG	2:9:235:GLU:OE1	2.28	0.50
3:A:873:LEU:HB3	3:A:879:LEU:HD23	1.94	0.50
7:D:112:LEU:HD13	7:D:215:ILE:HD12	1.93	0.50
7:D:171:THR:O	7:D:183:LYS:NZ	2.40	0.50
5:C:512:ASP:OD1	5:C:512:ASP:N	2.44	0.50
6:E:58:HIS:CD2	6:E:88:LEU:HD21	2.46	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:342:MET:CG	13:4:344:VAL:O	2.60	0.50
13:4:889:GLN:HA	13:4:892:GLU:CB	2.41	0.50
1:8:278:ILE:HG13	1:8:281:HIS:H	1.76	0.50
2:9:107:THR:OG1	2:9:108:GLY:N	2.45	0.50
5:C:426:GLU:HA	5:C:429:HIS:HB3	1.93	0.50
5:C:489:ASP:OD2	5:C:614:ARG:NH1	2.45	0.50
17:E:2001:AGS:O2B	17:E:2001:AGS:O1A	2.28	0.50
7:D:107:TYR:HB3	7:D:110:TYR:HD2	1.76	0.50
13:4:335:SER:OG	13:4:395:GLN:NE2	2.45	0.50
1:8:143:ILE:O	1:8:143:ILE:CG2	2.60	0.50
3:A:811:LEU:HB3	3:A:820:GLN:HG3	1.93	0.50
7:D:399:LEU:HD22	7:D:510:LEU:HD23	1.93	0.50
12:3:534:ALA:HA	14:5:758:HIS:HA	1.92	0.50
6:E:472:ASP:OD1	6:E:472:ASP:N	2.44	0.50
7:D:379:ARG:NH1	7:D:466:LEU:O	2.45	0.50
13:4:362:ARG:NH1	16:7:299:PHE:N	2.59	0.50
1:8:355:ILE:HG23	1:8:355:ILE:O	2.11	0.50
7:D:59:GLN:NE2	7:D:291:LEU:O	2.45	0.50
16:7:122:ASP:OD2	16:7:198:ARG:NH2	2.44	0.50
1:8:68:ASP:O	1:8:71:GLN:N	2.43	0.49
1:8:307:LEU:HD13	1:8:434:ARG:H	1.76	0.49
3:A:708:LYS:HD3	7:D:269:SER:HA	1.94	0.49
5:C:449:TYR:HD1	5:C:452:ARG:HD3	1.77	0.49
12:3:43:ARG:NH1	12:3:136:MET:O	2.45	0.49
1:8:71:GLN:OE1	1:8:104:ARG:N	2.45	0.49
2:9:292:THR:OG1	2:9:293:ALA:N	2.38	0.49
5:C:296:ASP:OD1	5:C:296:ASP:N	2.44	0.49
6:E:58:HIS:CE1	6:E:88:LEU:HD11	2.48	0.49
6:E:109:VAL:HG23	6:E:156:LEU:HD22	1.94	0.49
16:7:436:LEU:HD23	16:7:473:ILE:HD12	1.94	0.49
5:C:393:VAL:HA	5:C:396:LEU:HB2	1.93	0.49
11:2:558:LYS:NZ	15:6:561:GLU:OE2	2.46	0.49
14:5:736:GLU:O	14:5:740:THR:N	2.45	0.49
15:6:275:ARG:NH1	15:6:367:GLU:O	2.44	0.49
15:6:308:SER:O	15:6:347:ASN:HB3	2.13	0.49
2:9:88:VAL:O	2:9:92:LEU:N	2.44	0.49
3:A:486:THR:OG1	17:A:2001:AGS:O2B	2.30	0.49
11:2:364:CYS:HB3	11:2:367:CYS:HB2	1.94	0.49
12:3:928:PRO:O	12:3:932:LYS:NZ	2.34	0.49
13:4:911:GLN:O	13:4:914:ASP:HA	2.13	0.49
6:E:69:SER:OG	6:E:70:TRP:N	2.45	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:478:MET:O	12:3:483:ARG:NH2	2.45	0.49
2:9:331:LEU:HA	2:9:334:LEU:HB2	1.93	0.49
2:9:500:ASP:OD1	2:9:500:ASP:N	2.45	0.49
6:E:205:ARG:NH1	6:E:259:ASN:OD1	2.40	0.49
6:E:272:ARG:HH21	6:E:288:ALA:HA	1.77	0.49
7:D:299:SER:HB3	7:D:302:VAL:HG23	1.95	0.49
16:7:73:ARG:NH2	16:7:130:LYS:O	2.46	0.49
2:9:92:LEU:HD12	2:9:95:ALA:HB2	1.95	0.49
2:9:237:GLN:HA	2:9:240:ARG:HE	1.78	0.49
2:9:399:ASN:O	2:9:404:ARG:NH1	2.45	0.49
2:9:506:SER:O	2:9:506:SER:OG	2.31	0.49
12:3:494:THR:HB	12:3:506:LEU:O	2.13	0.49
12:3:679:ILE:HD11	12:3:705:LEU:HD12	1.94	0.49
14:5:258:LEU:HD22	14:5:294:ILE:HD12	1.93	0.49
7:D:486:TYR:CE1	10:H:24:DC:C5	3.00	0.49
17:D:2001:AGS:O1B	17:D:2001:AGS:O3G	2.31	0.49
12:3:172:THR:OG1	12:3:173:ALA:N	2.44	0.49
13:4:374:ILE:O	13:4:377:ASN:ND2	2.42	0.49
1:8:270:ILE:HD11	1:8:279:ALA:HB2	1.95	0.49
2:9:395:SER:HA	2:9:398:VAL:HG22	1.94	0.49
4:B:610:GLU:OE2	4:B:611:LYS:NZ	2.36	0.49
14:5:649:THR:OG1	14:5:650:ILE:N	2.44	0.49
4:B:310:GLN:O	4:B:448:ARG:NH1	2.43	0.49
5:C:371:HIS:HB2	5:C:377:ILE:HD11	1.94	0.49
11:2:603:VAL:HG22	11:2:645:SER:HB3	1.95	0.49
15:6:734:LEU:HD13	15:6:742:ILE:CG2	2.43	0.49
16:7:664:TYR:OH	16:7:668:ARG:NH1	2.45	0.49
3:A:880:PHE:HD2	3:A:893:LYS:HB3	1.78	0.48
6:E:67:LEU:HD23	6:E:72:PRO:HB2	1.95	0.48
16:7:436:LEU:CD1	16:7:642:ILE:CD1	2.91	0.48
1:8:130:VAL:HG22	1:8:135:SER:O	2.13	0.48
1:8:235:LEU:HD21	1:8:270:ILE:HG13	1.95	0.48
3:A:882:GLN:NE2	3:A:891:CYS:SG	2.86	0.48
4:B:296:ILE:HD13	8:F:398:ILE:HD12	1.95	0.48
4:B:599:ILE:HG22	4:B:601:TRP:HD1	1.77	0.48
7:D:104:ARG:NH2	7:D:218:GLU:OE2	2.46	0.48
15:6:123:SER:O	15:6:133:GLU:HG2	2.13	0.48
16:7:776:MET:O	16:7:780:SER:OG	2.29	0.48
3:A:817:SER:OG	3:A:820:GLN:OE1	2.31	0.48
11:2:351:PHE:HE2	15:6:348:VAL:CG1	2.25	0.48
13:4:631:ILE:O	13:4:673:ALA:HA	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:7:653:SER:OG	16:7:654:GLU:N	2.46	0.48
16:7:747:ILE:HA	16:7:750:LYS:HZ2	1.77	0.48
2:9:332:ARG:O	2:9:336:ASP:N	2.46	0.48
7:D:116:LEU:O	7:D:120:GLN:N	2.46	0.48
11:2:573:ALA:CB	15:6:664:ALA:HB3	2.43	0.48
13:4:350:ASN:N	13:4:350:ASN:OD1	2.47	0.48
15:6:570:ASN:ND2	15:6:708:ARG:O	2.46	0.48
1:8:235:LEU:HD12	1:8:282:LEU:HD23	1.94	0.48
3:A:412:THR:HG23	7:D:208:THR:HG23	1.95	0.48
3:A:871:ASN:ND2	6:E:178:ARG:O	2.46	0.48
6:E:260:ASP:OD1	6:E:260:ASP:N	2.42	0.48
7:D:151:GLU:HB3	7:D:172:ILE:HD12	1.94	0.48
7:D:333:SER:O	7:D:336:THR:OG1	2.31	0.48
12:3:253:HIS:HA	12:3:278:LEU:O	2.13	0.48
14:5:61:LEU:HD21	14:5:94:ILE:HD13	1.95	0.48
14:5:280:ARG:N	14:5:280:ARG:CD	2.73	0.48
15:6:811:ALA:HB2	15:6:819:ILE:HD13	1.95	0.48
16:7:509:GLU:HG2	16:7:510:GLY:N	2.29	0.48
3:A:865:SER:HB2	3:A:868:PHE:HB3	1.95	0.48
5:C:441:ASP:OD1	5:C:441:ASP:N	2.46	0.48
7:D:315:ASP:O	7:D:318:SER:OG	2.32	0.48
11:2:536:ASP:O	11:2:815:ARG:NH1	2.47	0.48
11:2:686:LEU:O	15:6:781:ARG:NH1	2.47	0.48
11:2:853:VAL:O	11:2:856:GLN:HB2	2.13	0.48
13:4:587:ARG:HG2	13:4:624:SER:HA	1.95	0.48
15:6:612:VAL:HG22	15:6:623:ILE:HD13	1.96	0.48
4:B:399:HIS:HB2	4:B:402:LEU:HD22	1.95	0.48
11:2:495:ASP:OD1	11:2:509:ARG:NH1	2.46	0.48
13:4:311:CYS:SG	13:4:312:LYS:N	2.87	0.48
4:B:289:PRO:HB2	5:C:498:LEU:HD12	1.96	0.48
16:7:436:LEU:HD13	16:7:642:ILE:HD13	1.94	0.48
11:2:411:LEU:HD12	11:2:411:LEU:O	2.13	0.48
12:3:348:ARG:NH2	12:3:349:ASN:OD1	2.47	0.48
14:5:470:VAL:CG2	14:5:513:LEU:HD23	2.44	0.48
16:7:208:SER:OG	16:7:209:GLN:N	2.45	0.48
16:7:656:VAL:HG23	16:7:710:ILE:HD12	1.95	0.48
16:7:677:SER:OG	16:7:678:LYS:N	2.46	0.48
1:8:198:ILE:HD11	1:8:228:LEU:HB3	1.95	0.48
3:A:486:THR:OG1	17:A:2001:AGS:O3G	2.31	0.48
13:4:573:SER:O	13:4:576:GLN:HB2	2.14	0.48
2:9:495:MET:HA	2:9:498:PHE:HB2	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:423:ASN:O	5:C:439:TYR:OH	2.32	0.47
11:2:670:THR:OG1	11:2:671:GLU:N	2.46	0.47
13:4:184:ASN:O	13:4:260:GLN:NE2	2.46	0.47
13:4:713:ASP:OD1	13:4:713:ASP:N	2.47	0.47
1:8:206:ARG:HG2	1:8:250:GLN:HB3	1.97	0.47
7:D:86:ILE:O	7:D:89:SER:OG	2.29	0.47
15:6:387:GLU:O	15:6:387:GLU:HG2	2.14	0.47
1:8:155:TYR:HB2	1:8:255:ALA:HB1	1.95	0.47
1:8:375:LEU:HD12	1:8:380:GLU:C	2.35	0.47
6:E:74:LEU:HD21	6:E:105:PRO:HA	1.96	0.47
6:E:74:LEU:HD23	6:E:108:LEU:HB2	1.96	0.47
7:D:281:LEU:HD21	7:D:325:ARG:HH21	1.79	0.47
7:D:419:ILE:O	7:D:423:ASN:ND2	2.47	0.47
12:3:123:PRO:O	12:3:126:GLU:HG2	2.13	0.47
12:3:266:PRO:O	12:3:269:GLN:NE2	2.47	0.47
14:5:470:VAL:CG2	14:5:513:LEU:CD2	2.92	0.47
13:4:695:PRO:HA	13:4:696:PRO:HD3	1.77	0.47
14:5:729:SER:H	14:5:775:VAL:C	2.17	0.47
2:9:439:HIS:HA	2:9:442:LYS:HG2	1.97	0.47
3:A:708:LYS:NZ	7:D:267:ARG:O	2.47	0.47
7:D:275:MET:O	7:D:277:GLN:NE2	2.47	0.47
12:3:367:LEU:HD21	12:3:378:LYS:HB2	1.95	0.47
13:4:339:ILE:HG13	13:4:394:LYS:HB3	1.97	0.47
13:4:543:GLN:HE22	13:4:628:VAL:HG12	1.78	0.47
16:7:436:LEU:HD11	16:7:642:ILE:HD11	1.95	0.47
1:8:235:LEU:HD13	1:8:283:LEU:HG	1.97	0.47
2:9:430:ASP:HA	2:9:488:LYS:HD3	1.97	0.47
17:9:2001:AGS:O2A	17:9:2001:AGS:O1B	2.31	0.47
5:C:123:SER:HA	5:C:197:LYS:HD3	1.97	0.47
7:D:100:LEU:N	7:D:249:GLY:O	2.42	0.47
13:4:435:VAL:HG23	13:4:466:VAL:HG12	1.97	0.47
15:6:453:SER:OG	15:6:454:PHE:N	2.48	0.47
16:7:715:GLU:OE2	16:7:718:ARG:NH1	2.46	0.47
1:8:197:THR:HB	1:8:231:HIS:HB3	1.97	0.47
1:8:393:THR:CB	11:2:255:ILE:CG2	2.92	0.47
2:9:170:ILE:HG12	2:9:184:LYS:HG3	1.97	0.47
2:9:219:VAL:HG13	2:9:257:VAL:HB	1.97	0.47
2:9:338:LEU:O	2:9:342:ILE:HG13	2.15	0.47
3:A:514:ASN:HB3	3:A:517:LYS:HB2	1.96	0.47
4:B:264:SER:HB2	4:B:605:THR:HG21	1.97	0.47
4:B:409:ASP:N	4:B:409:ASP:OD1	2.46	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:209:ASP:OD1	5:C:209:ASP:N	2.37	0.47
6:E:110:LYS:O	6:E:114:ASN:ND2	2.48	0.47
6:E:212:ASP:N	6:E:212:ASP:OD1	2.45	0.47
7:D:220:ASP:OD1	7:D:220:ASP:N	2.47	0.47
7:D:338:LYS:NZ	17:D:2001:AGS:O3'	2.48	0.47
8:F:333:ASN:HD21	8:F:388:ASP:HB3	1.80	0.47
8:F:369:VAL:HA	8:F:372:LEU:HD12	1.97	0.47
11:2:333:GLN:O	11:2:383:ARG:CB	2.63	0.47
11:2:350:PRO:HB2	11:2:351:PHE:H	1.58	0.47
12:3:936:GLN:O	12:3:940:ALA:N	2.48	0.47
13:4:421:ASP:N	13:4:421:ASP:OD1	2.46	0.47
6:E:212:ASP:OD2	6:E:266:TRP:NE1	2.47	0.47
12:3:384:MET:SD	12:3:511:SER:OG	2.71	0.47
12:3:708:LEU:O	12:3:711:ALA:HB3	2.15	0.47
13:4:735:HIS:O	13:4:738:GLN:NE2	2.48	0.47
14:5:409:ASP:O	14:5:658:ARG:NH1	2.48	0.47
15:6:576:ASP:OD1	15:6:576:ASP:N	2.48	0.47
3:A:633:LYS:HD3	3:A:690:GLU:HG2	1.97	0.47
3:A:886:ASN:HA	7:D:470:THR:HG21	1.97	0.47
2:9:217:THR:HA	2:9:254:VAL:HG12	1.97	0.47
2:9:316:ALA:HA	2:9:319:PHE:HB3	1.96	0.47
3:A:432:SER:O	17:A:2001:AGS:O2'	2.32	0.47
5:C:390:GLU:HA	5:C:393:VAL:HG22	1.97	0.47
17:E:2001:AGS:O2G	17:E:2001:AGS:O2A	2.32	0.47
15:6:566:ARG:O	15:6:805:ARG:NH1	2.48	0.47
2:9:504:LYS:HG3	2:9:505:ILE:HG23	1.97	0.46
4:B:286:GLN:H	4:B:290:ARG:HH21	1.61	0.46
4:B:549:THR:OG1	4:B:550:GLN:N	2.48	0.46
6:E:254:ASP:OD2	6:E:255:ILE:N	2.47	0.46
13:4:639:ASP:OD1	13:4:642:ARG:NH1	2.48	0.46
16:7:350:ASP:HB2	16:7:382:ARG:HG2	1.97	0.46
2:9:343:GLU:O	2:9:347:LEU:N	2.40	0.46
6:E:109:VAL:HG21	6:E:155:LEU:HB3	1.96	0.46
11:2:324:VAL:HG23	11:2:420:PRO:HA	1.96	0.46
12:3:294:VAL:HG12	12:3:326:VAL:HG22	1.96	0.46
12:3:716:ARG:NH2	12:3:725:ASP:OD1	2.49	0.46
13:4:542:LEU:HA	13:4:545:PHE:HB2	1.97	0.46
13:4:632:ASP:OD1	13:4:632:ASP:N	2.47	0.46
13:4:696:PRO:N	13:4:697:PRO:CD	2.73	0.46
13:4:825:ALA:O	13:4:828:LEU:HB3	2.15	0.46
7:D:269:SER:O	7:D:269:SER:OG	2.34	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2:242:LEU:HB3	11:2:295:VAL:HG12	1.97	0.46
14:5:500:GLN:HA	14:5:500:GLN:OE1	2.15	0.46
16:7:400:ARG:NH1	16:7:636:SER:OG	2.48	0.46
6:E:43:LYS:HA	6:E:46:THR:HG22	1.97	0.46
12:3:297:VAL:O	12:3:321:ILE:HA	2.16	0.46
13:4:531:TYR:HE1	13:4:720:LEU:HA	1.80	0.46
13:4:535:ASP:OD1	13:4:535:ASP:N	2.48	0.46
2:9:257:VAL:HG13	2:9:281:LEU:HD11	1.96	0.46
4:B:445:SER:OG	4:B:472:ASN:O	2.31	0.46
7:D:335:PRO:HA	7:D:338:LYS:HB3	1.98	0.46
13:4:696:PRO:CD	13:4:697:PRO:CD	2.89	0.46
15:6:150:THR:HG21	15:6:384:ASP:HB2	1.98	0.46
1:8:92:TYR:O	1:8:152:LEU:N	2.36	0.46
6:E:40:GLY:N	17:E:2001:AGS:O1B	2.43	0.46
7:D:310:GLU:O	7:D:314:SER:N	2.42	0.46
12:3:378:LYS:HA	12:3:381:ILE:HB	1.97	0.46
16:7:20:GLU:OE1	16:7:92:LYS:NZ	2.47	0.46
1:8:302:LEU:O	1:8:304:ILE:N	2.48	0.46
3:A:460:TYR:O	3:A:464:TYR:N	2.45	0.46
5:C:246:ASN:O	5:C:250:ASN:ND2	2.47	0.46
6:E:45:TYR:HB2	17:E:2001:AGS:H3'	1.98	0.46
11:2:782:ASP:OD1	11:2:782:ASP:N	2.49	0.46
13:4:763:THR:OG1	13:4:764:GLU:N	2.48	0.46
15:6:294:VAL:HG13	15:6:392:GLY:H	1.81	0.46
16:7:451:ARG:NH2	16:7:453:ASP:O	2.48	0.46
1:8:289:ALA:H	1:8:292:LYS:HB3	1.80	0.46
1:8:351:MET:C	1:8:353:ARG:H	2.18	0.46
3:A:422:ILE:HG22	3:A:682:LEU:HD22	1.98	0.46
14:5:622:LEU:CD1	14:5:677:VAL:CG1	2.93	0.46
16:7:751:MET:SD	16:7:751:MET:C	2.94	0.46
16:7:775:THR:HG23	16:7:777:LEU:H	1.80	0.46
2:9:198:GLN:HA	2:9:204:HIS:HB3	1.98	0.46
2:9:400:ASN:ND2	2:9:404:ARG:O	2.49	0.46
3:A:425:LYS:HD2	3:A:425:LYS:HA	1.82	0.46
7:D:105:GLN:N	17:D:2001:AGS:O1B	2.43	0.46
11:2:583:ASP:O	11:2:587:LYS:CA	2.64	0.46
13:4:419:VAL:HG12	13:4:463:VAL:HG11	1.97	0.46
1:8:34:ARG:HD3	1:8:132:SER:HB3	1.98	0.46
1:8:93:ILE:HA	1:8:150:THR:O	2.15	0.46
2:9:84:GLU:HB3	2:9:288:PHE:HE1	1.81	0.46
4:B:518:THR:HG23	4:B:521:SER:H	1.81	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:58:TRP:O	5:C:62:HIS:ND1	2.49	0.46
13:4:775:VAL:HA	13:4:778:ARG:HB2	1.97	0.46
4:B:511:LYS:O	4:B:515:GLN:NE2	2.46	0.45
7:D:369:LYS:O	7:D:373:SER:OG	2.33	0.45
13:4:209:LEU:HD12	13:4:250:ALA:HB2	1.97	0.45
13:4:909:ARG:O	13:4:913:GLU:N	2.40	0.45
6:E:277:ASN:HA	6:E:280:GLU:HB2	1.98	0.45
7:D:527:THR:OG1	7:D:528:GLN:N	2.48	0.45
16:7:591:LEU:HA	16:7:594:PHE:HB2	1.98	0.45
16:7:747:ILE:HA	16:7:750:LYS:NZ	2.31	0.45
11:2:339:PHE:CE2	11:2:375:VAL:HG22	2.52	0.45
12:3:246:GLY:HA3	16:7:109:ASN:CB	2.44	0.45
14:5:448:GLY:O	14:5:467:GLY:HA2	2.15	0.45
1:8:208:LYS:HB3	1:8:248:PRO:HG3	1.99	0.45
1:8:208:LYS:HD2	1:8:209:PRO:O	2.16	0.45
4:B:335:SER:O	4:B:357:SER:OG	2.34	0.45
14:5:160:VAL:HG11	14:5:298:TYR:HB2	1.98	0.45
16:7:418:ILE:HG13	16:7:429:LYS:HD3	1.97	0.45
1:8:73:PHE:HB2	1:8:90:GLU:HG3	1.98	0.45
2:9:277:LEU:O	2:9:279:ARG:NH1	2.43	0.45
5:C:348:ASP:HA	5:C:351:LEU:HB2	1.98	0.45
5:C:596:LEU:HB3	5:C:597:ILE:HD12	1.98	0.45
11:2:631:ILE:O	11:2:637:VAL:HA	2.16	0.45
13:4:248:LEU:HD11	13:4:257:LEU:HD23	1.99	0.45
1:8:108:ASN:ND2	1:8:108:ASN:O	2.50	0.45
2:9:399:ASN:HB3	2:9:404:ARG:HD3	1.97	0.45
3:A:605:PRO:HA	3:A:609:LEU:HB2	1.98	0.45
4:B:580:ARG:HA	4:B:583:ILE:HB	1.97	0.45
5:C:351:LEU:HD21	5:C:389:GLU:HB3	1.97	0.45
6:E:254:ASP:OD2	6:E:256:PHE:N	2.50	0.45
1:8:18:ILE:HD12	1:8:29:LEU:HD13	1.98	0.45
1:8:90:GLU:HB3	1:8:154:ARG:O	2.16	0.45
1:8:206:ARG:CG	1:8:250:GLN:HB3	2.47	0.45
3:A:855:ASP:OD1	3:A:855:ASP:N	2.50	0.45
4:B:495:VAL:HG13	4:B:497:LYS:H	1.82	0.45
7:D:514:ARG:HH11	7:D:527:THR:HG1	1.65	0.45
12:3:953:VAL:HA	12:3:959:TRP:HB3	1.99	0.45
2:9:388:ASN:O	2:9:392:LYS:NZ	2.41	0.45
4:B:600:ILE:O	4:B:600:ILE:HG13	2.16	0.45
5:C:60:LEU:HA	5:C:63:GLN:HE21	1.82	0.45
5:C:569:LEU:O	5:C:572:THR:OG1	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:5:166:ILE:HD11	14:5:294:ILE:HD11	1.98	0.45
16:7:597:LEU:O	16:7:723:SER:OG	2.34	0.45
2:9:201:ASN:HB3	2:9:204:HIS:CG	2.52	0.45
2:9:387:LEU:HD22	2:9:390:ILE:HG13	1.98	0.45
3:A:561:ILE:HG22	3:A:563:VAL:HG23	1.99	0.45
3:A:632:LEU:HD23	3:A:632:LEU:HA	1.88	0.45
3:A:772:THR:OG1	3:A:773:VAL:N	2.50	0.45
5:C:384:LYS:HA	5:C:384:LYS:HD3	1.85	0.45
7:D:46:ASP:OD2	7:D:49:PHE:N	2.45	0.45
8:F:363:ILE:HA	8:F:366:VAL:HG12	1.98	0.45
13:4:386:HIS:HD1	13:4:387:ASN:N	2.15	0.45
6:E:211:GLU:O	6:E:216:ARG:NH2	2.48	0.45
13:4:518:LEU:HA	13:4:521:LEU:HB3	1.99	0.45
15:6:287:LEU:HA	15:6:399:GLY:O	2.17	0.45
15:6:551:MET:CE	15:6:755:ILE:CD1	2.95	0.45
1:8:216:ASP:O	1:8:217:ASN:ND2	2.51	0.44
4:B:374:ASP:OD1	4:B:374:ASP:N	2.48	0.44
1:8:280:ASN:O	1:8:284:GLU:CB	2.65	0.44
1:8:292:LYS:HE2	1:8:296:GLN:HB2	2.00	0.44
4:B:556:LEU:HD21	4:B:600:ILE:HG23	1.99	0.44
12:3:245:TYR:HA	12:3:248:SER:OG	2.17	0.44
12:3:413:THR:HB	12:3:414:ALA:H	1.66	0.44
16:7:290:SER:OG	16:7:291:GLN:OE1	2.35	0.44
16:7:431:ALA:HB2	16:7:719:LEU:HD11	1.99	0.44
1:8:111:LEU:HD11	1:8:150:THR:HB	1.99	0.44
6:E:218:ARG:HA	6:E:218:ARG:HD2	1.72	0.44
11:2:344:CYS:SG	11:2:367:CYS:SG	3.16	0.44
11:2:582:LYS:HA	11:2:588:GLU:O	2.18	0.44
12:3:536:PRO:HD2	12:3:539:LEU:HD12	2.00	0.44
16:7:500:ASP:O	16:7:504:ASP:CA	2.65	0.44
16:7:549:SER:O	16:7:549:SER:OG	2.35	0.44
3:A:640:LEU:HD22	3:A:643:LEU:HD11	2.00	0.44
4:B:459:ILE:HD12	4:B:459:ILE:HA	1.82	0.44
12:3:493:GLN:C	12:3:494:THR:HG23	2.38	0.44
12:3:705:LEU:HD21	12:3:733:LEU:HD11	1.99	0.44
13:4:911:GLN:O	13:4:914:ASP:N	2.47	0.44
16:7:436:LEU:HD11	16:7:642:ILE:CD1	2.48	0.44
1:8:235:LEU:HD11	1:8:279:ALA:HA	1.99	0.44
3:A:885:LYS:HZ1	7:D:470:THR:HA	1.82	0.44
6:E:334:ALA:HA	6:E:337:ILE:HD12	1.99	0.44
12:3:922:ARG:HD3	12:3:922:ARG:HA	1.85	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:527:ALA:CB	13:4:530:ILE:HD11	2.48	0.44
13:4:812:LYS:O	13:4:812:LYS:CG	2.64	0.44
1:8:115:TYR:OH	1:8:146:SER:O	2.32	0.44
1:8:131:LYS:HB2	1:8:136:SER:HB3	2.00	0.44
1:8:296:GLN:O	1:8:299:PRO:HD3	2.17	0.44
1:8:302:LEU:C	1:8:304:ILE:N	2.71	0.44
3:A:838:SER:OG	13:4:823:GLN:O	2.36	0.44
12:3:496:THR:HG22	12:3:505:THR:CB	2.48	0.44
14:5:180:SER:OG	14:5:244:ILE:HB	2.17	0.44
1:8:364:LEU:HD22	1:8:442:VAL:HG11	2.00	0.44
5:C:276:TYR:HA	5:C:279:GLN:HB3	2.00	0.44
6:E:346:ASP:N	6:E:346:ASP:OD1	2.50	0.44
7:D:480:ASN:HD21	7:D:482:THR:HG22	1.82	0.44
12:3:225:ILE:HA	12:3:226:PRO:HD3	1.81	0.44
12:3:480:ASP:N	12:3:480:ASP:OD1	2.48	0.44
15:6:718:ASP:OD1	15:6:718:ASP:N	2.51	0.44
16:7:774:PHE:HB3	16:7:778:GLN:OE1	2.18	0.44
4:B:271:ARG:NH2	4:B:497:LYS:O	2.49	0.44
6:E:198:SER:HB3	6:E:244:VAL:HG21	2.00	0.44
6:E:386:LEU:O	6:E:390:PHE:N	2.48	0.44
7:D:255:ASN:N	7:D:255:ASN:OD1	2.50	0.44
8:F:422:LYS:HB3	8:F:423:LYS:HZ2	1.82	0.44
12:3:923:ILE:HB	12:3:932:LYS:HE2	1.99	0.44
14:5:141:SER:O	14:5:334:GLN:NE2	2.51	0.44
1:8:375:LEU:HD11	1:8:379:GLY:C	2.38	0.44
2:9:236:THR:OG1	2:9:237:GLN:N	2.51	0.44
4:B:522:LYS:HG2	4:B:617:LEU:HD23	1.99	0.44
5:C:363:PHE:O	5:C:367:LEU:N	2.51	0.44
11:2:854:ARG:O	11:2:857:LEU:HB2	2.17	0.43
14:5:49:GLN:NE2	14:5:62:THR:OG1	2.47	0.43
4:B:550:GLN:HA	4:B:601:TRP:CG	2.54	0.43
12:3:430:ILE:HB	12:3:470:VAL:HG12	1.99	0.43
13:4:616:LEU:H	13:4:616:LEU:HD23	1.82	0.43
15:6:609:THR:HG23	15:6:610:ALA:H	1.83	0.43
16:7:124:ASN:N	16:7:124:ASN:OD1	2.51	0.43
5:C:86:GLU:HG3	5:C:266:LEU:HD21	2.00	0.43
6:E:48:LYS:HD2	6:E:52:ASN:HD21	1.84	0.43
17:D:2001:AGS:O1A	17:D:2001:AGS:O2B	2.34	0.43
12:3:400:ARG:HD3	12:3:491:GLU:HA	1.99	0.43
1:8:304:ILE:HG21	1:8:437:SER:N	2.34	0.43
2:9:106:ILE:HD12	2:9:118:LEU:HD21	1.99	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:240:ILE:HA	6:E:243:ILE:HG22	1.99	0.43
7:D:509:ILE:HD12	7:D:509:ILE:HA	1.93	0.43
11:2:349:GLY:HA2	11:2:350:PRO:HD3	1.72	0.43
12:3:295:VAL:HB	12:3:325:THR:HB	2.00	0.43
13:4:385:ILE:HD13	13:4:385:ILE:HA	1.83	0.43
13:4:622:VAL:HG22	13:4:665:LEU:CD1	2.49	0.43
14:5:752:LEU:O	14:5:755:LEU:N	2.51	0.43
15:6:354:LEU:C	15:6:354:LEU:CD1	2.86	0.43
15:6:701:MET:HB2	15:6:705:ILE:HD11	2.00	0.43
1:8:148:TYR:CB	1:8:262:ILE:HA	2.48	0.43
11:2:539:VAL:HG12	11:2:679:ILE:HB	1.99	0.43
11:2:580:VAL:HG21	11:2:633:LYS:CB	2.49	0.43
12:3:366:SER:OG	12:3:651:VAL:O	2.37	0.43
12:3:475:PHE:HB3	12:3:516:ALA:HB2	1.99	0.43
1:8:336:VAL:HA	1:8:337:PRO:HD3	1.90	0.43
3:A:702:ASP:OD1	3:A:705:ARG:N	2.47	0.43
8:F:276:LYS:HD2	8:F:318:GLN:HE22	1.83	0.43
14:5:146:ILE:HD11	14:5:160:VAL:HG23	1.99	0.43
15:6:381:LEU:HG	15:6:386:VAL:HG12	2.01	0.43
3:A:481:PRO:HD2	7:D:262:LYS:HD2	2.00	0.43
4:B:298:LYS:HE2	4:B:301:PHE:HE2	1.83	0.43
4:B:324:ASN:N	4:B:324:ASN:OD1	2.51	0.43
5:C:236:LEU:HD23	5:C:238:PHE:HE2	1.84	0.43
5:C:437:ASP:OD1	5:C:437:ASP:N	2.52	0.43
5:C:567:LEU:HD23	5:C:567:LEU:HA	1.89	0.43
13:4:360:ILE:HG13	13:4:361:ASP:N	2.34	0.43
14:5:496:ALA:HB2	14:5:502:ILE:HG12	2.00	0.43
14:5:631:LYS:HD2	14:5:631:LYS:HA	1.90	0.43
14:5:708:LEU:O	14:5:712:ARG:CB	2.66	0.43
15:6:601:LYS:HD2	15:6:601:LYS:HA	1.88	0.43
3:A:839:ASN:OD1	13:4:827:ARG:CB	2.67	0.43
5:C:367:LEU:HB3	5:C:377:ILE:HD13	2.01	0.43
11:2:549:LYS:HE2	11:2:549:LYS:HB2	1.86	0.43
12:3:430:ILE:O	12:3:470:VAL:HA	2.19	0.43
16:7:542:GLU:HG3	16:7:593:ARG:HH21	1.83	0.43
1:8:297:TYR:O	1:8:297:TYR:CG	2.71	0.43
6:E:273:ILE:HA	6:E:284:LEU:HD11	2.01	0.43
7:D:349:LYS:HA	7:D:349:LYS:HD3	1.82	0.43
12:3:691:ASN:HD21	12:3:697:ILE:H	1.67	0.43
1:8:25:ASP:C	1:8:26:GLU:HG2	2.38	0.42
1:8:73:PHE:HA	1:8:92:TYR:HA	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:463:VAL:HG12	12:3:463:VAL:O	2.19	0.42
13:4:312:LYS:HB2	13:4:316:GLU:HB2	2.00	0.42
14:5:754:ALA:O	14:5:758:HIS:N	2.51	0.42
15:6:270:LEU:HD12	15:6:289:SER:HB3	2.01	0.42
16:7:685:THR:O	16:7:688:THR:OG1	2.35	0.42
5:C:79:ILE:HA	5:C:82:ASP:HB3	2.00	0.42
5:C:588:ILE:HD12	5:C:588:ILE:HA	1.91	0.42
11:2:211:LEU:HA	11:2:214:PHE:HB3	2.02	0.42
12:3:424:ASN:O	12:3:657:ARG:NH1	2.44	0.42
14:5:413:LEU:HD23	14:5:553:ILE:HG12	2.00	0.42
16:7:703:ARG:NH1	16:7:712:ASP:OD1	2.47	0.42
2:9:411:ASN:HB3	2:9:414:GLN:HB2	2.01	0.42
6:E:435:THR:HG22	6:E:450:TRP:NE1	2.30	0.42
11:2:616:ASP:OD1	11:2:616:ASP:N	2.53	0.42
13:4:428:ARG:NE	15:6:372:SER:OG	2.52	0.42
13:4:539:GLY:O	13:4:543:GLN:HB2	2.19	0.42
14:5:279:ASP:O	14:5:283:THR:HG23	2.18	0.42
16:7:333:ILE:HD13	16:7:351:VAL:HG11	2.02	0.42
1:8:197:THR:HG23	1:8:261:THR:HG22	2.00	0.42
5:C:100:ARG:NH2	5:C:227:PHE:O	2.47	0.42
6:E:476:ASP:N	6:E:476:ASP:OD1	2.47	0.42
12:3:289:GLY:HA2	12:3:463:VAL:HG12	2.01	0.42
16:7:484:THR:OG1	16:7:485:GLY:N	2.53	0.42
1:8:344:LEU:N	1:8:345:PRO:HD2	2.35	0.42
3:A:687:ASP:OD1	3:A:687:ASP:N	2.52	0.42
4:B:465:TRP:O	6:E:422:GLN:NE2	2.52	0.42
5:C:364:VAL:HA	5:C:367:LEU:HD12	2.01	0.42
8:F:429:LEU:HD12	8:F:429:LEU:HA	1.89	0.42
11:2:374:ARG:HA	11:2:374:ARG:HD3	1.77	0.42
12:3:211:TYR:O	12:3:211:TYR:CG	2.72	0.42
14:5:499:GLN:C	14:5:501:THR:H	2.22	0.42
15:6:152:TYR:OH	15:6:388:ARG:NH1	2.52	0.42
15:6:330:PRO:HG2	15:6:344:TRP:CD2	2.54	0.42
15:6:559:THR:OG1	15:6:560:VAL:N	2.52	0.42
15:6:570:ASN:HB2	15:6:709:PHE:HA	2.02	0.42
1:8:69:THR:O	1:8:70:SER:OG	2.35	0.42
1:8:130:VAL:HG13	1:8:136:SER:HA	2.01	0.42
1:8:392:THR:N	1:8:395:THR:OG1	2.52	0.42
3:A:430:LEU:HD12	3:A:430:LEU:HA	1.86	0.42
5:C:118:LEU:HD23	5:C:118:LEU:HA	1.88	0.42
7:D:67:ASP:OD1	7:D:67:ASP:N	2.48	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:396:GLU:O	8:F:400:ARG:N	2.47	0.42
12:3:346:ASP:HA	12:3:349:ASN:HD22	1.83	0.42
16:7:245:ILE:HD13	16:7:343:LEU:HD12	2.00	0.42
1:8:153:THR:OG1	1:8:257:ILE:HB	2.19	0.42
2:9:107:THR:HG21	2:9:265:LEU:HD11	2.01	0.42
2:9:432:THR:HG1	2:9:435:GLU:H	1.66	0.42
3:A:411:LYS:HA	3:A:411:LYS:HD2	1.81	0.42
3:A:863:ILE:HG12	3:A:866:TRP:HB2	2.01	0.42
5:C:593:ASN:N	5:C:593:ASN:OD1	2.50	0.42
7:D:137:HIS:HB3	7:D:142:ALA:HB2	2.01	0.42
16:7:275:SER:OG	16:7:277:THR:O	2.37	0.42
4:B:366:TYR:HB3	4:B:426:ASN:HD22	1.85	0.42
5:C:220:ILE:HD12	5:C:220:ILE:HA	1.90	0.42
5:C:531:ALA:HB1	5:C:535:ILE:HG21	2.01	0.42
5:C:557:ILE:HD12	5:C:557:ILE:HA	1.90	0.42
15:6:621:TYR:CE1	15:6:666:ALA:CB	3.03	0.42
1:8:30:LEU:HB2	1:8:31:PRO:HD3	2.02	0.42
1:8:96:THR:HG21	1:8:147:HIS:HA	2.02	0.42
1:8:283:LEU:O	1:8:287:ILE:HG22	2.20	0.42
3:A:409:LYS:HB3	7:D:158:HIS:HE1	1.84	0.42
3:A:511:VAL:CG2	3:A:563:VAL:HG22	2.50	0.42
7:D:227:ARG:HB3	7:D:229:THR:HG23	2.02	0.42
13:4:569:ASP:H	13:4:709:LEU:HA	1.84	0.42
13:4:735:HIS:HB3	13:4:738:GLN:HE22	1.85	0.42
16:7:354:ILE:HG22	16:7:377:GLU:HB3	2.00	0.42
2:9:421:ILE:HG22	2:9:422:ILE:HD13	2.02	0.42
4:B:556:LEU:HD23	4:B:598:GLU:HG2	2.02	0.42
5:C:447:LYS:O	5:C:450:LYS:NZ	2.39	0.42
7:D:284:MET:HB2	7:D:284:MET:HE3	1.77	0.42
12:3:679:ILE:HD12	12:3:679:ILE:HA	1.92	0.42
13:4:635:ASP:OD2	13:4:635:ASP:N	2.53	0.42
3:A:551:LYS:O	3:A:552:ARG:NH1	2.53	0.41
3:A:607:ARG:HE	3:A:608:GLN:NE2	2.17	0.41
4:B:567:PHE:HB3	12:3:950:ASN:HB3	2.01	0.41
5:C:136:SER:O	5:C:136:SER:OG	2.32	0.41
5:C:494:TRP:HZ2	8:F:380:ARG:HH11	1.68	0.41
5:C:525:PHE:HA	5:C:528:TYR:HB3	2.02	0.41
8:F:272:LEU:HG	8:F:355:LEU:HB2	2.00	0.41
11:2:627:GLN:HB3	11:2:643:ARG:HG2	2.01	0.41
12:3:528:ASP:HA	12:3:529:PRO:HD3	1.93	0.41
14:5:673:GLN:H	14:5:676:HIS:HD2	1.67	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:6:309:PHE:CD2	15:6:330:PRO:HD3	2.55	0.41
16:7:318:LEU:HD23	16:7:320:GLN:H	1.85	0.41
3:A:406:PHE:HB2	7:D:187:LEU:HD22	2.03	0.41
4:B:441:LEU:HD13	4:B:444:LEU:HD12	2.02	0.41
4:B:558:LEU:O	4:B:562:LEU:N	2.46	0.41
5:C:446:CYS:O	5:C:450:LYS:N	2.53	0.41
6:E:209:LEU:HD12	6:E:266:TRP:CE2	2.54	0.41
11:2:340:ASN:HA	11:2:346:SER:O	2.21	0.41
13:4:518:LEU:HD12	13:4:521:LEU:HD23	2.02	0.41
13:4:538:LYS:HE3	13:4:828:LEU:HD12	2.02	0.41
15:6:116:GLU:OE2	15:6:187:ARG:NH1	2.52	0.41
16:7:549:SER:HA	16:7:554:ASN:HA	2.02	0.41
2:9:125:LYS:HG2	2:9:129:LEU:HD13	2.01	0.41
5:C:121:GLU:HB3	5:C:126:ASN:HD21	1.86	0.41
5:C:285:LEU:HD12	5:C:285:LEU:HA	1.92	0.41
11:2:538:ASN:HA	11:2:646:ILE:O	2.20	0.41
12:3:183:GLU:HA	12:3:293:ASN:HA	2.02	0.41
14:5:375:ALA:HB1	14:5:378:ILE:HB	2.02	0.41
16:7:330:SER:OG	16:7:331:LEU:N	2.52	0.41
1:8:298:TYR:O	1:8:300:ARG:N	2.53	0.41
2:9:86:GLU:O	2:9:90:ASN:ND2	2.54	0.41
4:B:458:HIS:CE1	4:B:460:TYR:HB2	2.55	0.41
6:E:391:GLN:NE2	6:E:414:MET:SD	2.93	0.41
13:4:428:ARG:NH1	13:4:431:ASP:OD2	2.53	0.41
13:4:574:LYS:HE2	13:4:574:LYS:HB2	1.95	0.41
15:6:566:ARG:HH22	15:6:708:ARG:HE	1.68	0.41
15:6:610:ALA:HB1	15:6:623:ILE:HG22	2.02	0.41
2:9:94:LYS:HB2	2:9:101:SER:HA	2.02	0.41
2:9:228:LEU:HD11	2:9:241:THR:HG21	2.01	0.41
6:E:191:ARG:HH21	6:E:253:ASN:HB2	1.85	0.41
7:D:348:SER:HB3	7:D:354:LEU:HD12	2.03	0.41
7:D:422:ILE:HD11	7:D:526:TRP:HE1	1.86	0.41
12:3:386:MET:HE3	12:3:714:LYS:HB3	2.02	0.41
16:7:59:LYS:HB2	16:7:60:GLY:H	1.67	0.41
1:8:67:PRO:O	1:8:72:GLY:HA3	2.20	0.41
2:9:414:GLN:HA	2:9:417:ILE:HG22	2.03	0.41
5:C:133:PRO:HG3	5:C:207:ASP:HB3	2.03	0.41
5:C:459:ASP:N	5:C:459:ASP:OD1	2.49	0.41
7:D:285:VAL:HG13	7:D:313:LEU:HD11	2.02	0.41
8:F:279:LYS:HA	8:F:279:LYS:HD3	1.86	0.41
13:4:589:VAL:CG1	13:4:623:LEU:HD23	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:774:TYR:HH	13:4:795:THR:N	2.19	0.41
14:5:147:PRO:HG2	14:5:150:ASP:HB2	2.03	0.41
14:5:470:VAL:CG1	14:5:513:LEU:HD23	2.48	0.41
15:6:517:LYS:HD2	15:6:517:LYS:HA	1.86	0.41
2:9:389:TYR:HA	2:9:392:LYS:HG2	2.02	0.41
6:E:229:ASP:O	6:E:233:GLN:N	2.54	0.41
7:D:112:LEU:HD23	7:D:112:LEU:HA	1.83	0.41
8:F:327:CYS:O	8:F:331:VAL:N	2.52	0.41
8:F:335:ARG:O	8:F:339:ASP:N	2.52	0.41
11:2:384:ASN:HD22	11:2:384:ASN:HA	1.68	0.41
1:8:125:PHE:HA	1:8:128:LEU:HG	2.02	0.41
2:9:411:ASN:HD21	2:9:413:GLN:HB3	1.86	0.41
11:2:364:CYS:SG	11:2:365:THR:N	2.94	0.41
13:4:404:ASP:OD1	13:4:404:ASP:N	2.47	0.41
15:6:573:VAL:HG12	15:6:713:PHE:HB2	2.03	0.41
15:6:621:TYR:CE1	15:6:666:ALA:HB3	2.56	0.41
1:8:30:LEU:HD22	1:8:128:LEU:HA	2.03	0.41
1:8:150:THR:HG22	1:8:260:LEU:HD13	2.03	0.41
1:8:318:PHE:HA	1:8:363:LEU:HD11	2.02	0.41
2:9:170:ILE:HD12	2:9:170:ILE:HA	1.88	0.41
5:C:85:ALA:O	5:C:88:SER:OG	2.32	0.41
5:C:99:ARG:O	5:C:100:ARG:NE	2.53	0.41
5:C:212:ASN:N	5:C:212:ASN:OD1	2.53	0.41
5:C:214:ASN:OD1	5:C:214:ASN:N	2.53	0.41
6:E:228:THR:OG1	6:E:231:GLN:N	2.47	0.41
7:D:312:GLU:O	7:D:318:SER:OG	2.34	0.41
12:3:366:SER:OG	12:3:366:SER:O	2.38	0.41
12:3:415:LYS:HE2	12:3:415:LYS:HB2	1.95	0.41
13:4:599:VAL:O	13:4:604:TYR:HD2	2.04	0.41
13:4:712:VAL:HG11	16:7:668:ARG:HE	1.86	0.41
15:6:533:ILE:HD12	15:6:533:ILE:HA	1.97	0.41
16:7:354:ILE:HD12	16:7:354:ILE:HA	1.96	0.41
16:7:624:LYS:HE3	16:7:624:LYS:HB2	1.90	0.41
3:A:422:ILE:H	3:A:422:ILE:HG13	1.72	0.41
3:A:632:LEU:HD12	3:A:697:ALA:HB2	2.03	0.41
6:E:36:GLN:HG3	6:E:176:LEU:HD22	2.02	0.41
6:E:372:ASN:HD22	6:E:476:ASP:HB3	1.86	0.41
7:D:90:ILE:HD12	7:D:127:PHE:HB3	2.03	0.41
7:D:100:LEU:HD23	7:D:273:ILE:HG23	2.03	0.41
13:4:659:ALA:HB1	15:6:613:VAL:HG11	2.03	0.41
15:6:542:ALA:HA	15:6:545:LYS:HE3	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:7:652:MET:HA	16:7:708:VAL:HB	2.03	0.41
2:9:507:ILE:HD12	2:9:507:ILE:HA	1.90	0.40
11:2:326:ARG:HD3	11:2:389:THR:HG23	2.03	0.40
12:3:900:ILE:O	12:3:904:MET:N	2.54	0.40
13:4:386:HIS:C	13:4:388:ARG:H	2.25	0.40
15:6:661:ILE:O	15:6:671:THR:HA	2.21	0.40
1:8:290:PHE:HB3	1:8:291:PRO:HD3	2.02	0.40
2:9:344:ILE:HD13	2:9:344:ILE:HA	1.97	0.40
5:C:205:PHE:HB3	5:C:208:VAL:HG12	2.04	0.40
5:C:286:ASP:HA	5:C:289:ASP:HB2	2.03	0.40
5:C:440:LEU:HD13	5:C:446:CYS:HB3	2.03	0.40
6:E:130:LEU:HD12	6:E:130:LEU:HA	1.86	0.40
7:D:334:LEU:HD12	7:D:334:LEU:HA	1.89	0.40
12:3:403:ILE:O	12:3:511:SER:OG	2.39	0.40
15:6:116:GLU:O	15:6:120:GLU:HB2	2.21	0.40
15:6:354:LEU:O	15:6:354:LEU:HD12	2.21	0.40
15:6:528:LYS:O	15:6:532:SER:HB3	2.22	0.40
15:6:620:ASP:OD1	15:6:621:TYR:N	2.54	0.40
16:7:775:THR:OG1	16:7:776:MET:N	2.54	0.40
4:B:411:TYR:HA	4:B:414:GLN:HG2	2.01	0.40
5:C:421:ASN:N	5:C:421:ASN:OD1	2.52	0.40
7:D:90:ILE:O	7:D:93:LYS:NZ	2.43	0.40
12:3:23:ASP:HA	12:3:26:ARG:HE	1.85	0.40
12:3:92:LEU:HD23	12:3:92:LEU:HA	1.97	0.40
14:5:760:THR:O	14:5:764:ARG:N	2.43	0.40
15:6:516:LEU:HA	15:6:519:MET:HG2	2.04	0.40
8:F:298:VAL:HA	8:F:301:LYS:HB2	2.03	0.40
11:2:353:GLN:CG	15:6:348:VAL:HG11	2.51	0.40
11:2:367:CYS:HB3	11:2:369:SER:OG	2.22	0.40
12:3:350:ILE:O	12:3:354:SER:OG	2.35	0.40
12:3:914:TYR:O	12:3:959:TRP:N	2.49	0.40
14:5:617:GLN:OE1	14:5:621:LYS:NZ	2.55	0.40
16:7:495:ALA:HB1	16:7:508:LEU:HG	2.03	0.40
2:9:332:ARG:HA	2:9:335:PHE:HB3	2.02	0.40
2:9:496:ARG:O	2:9:496:ARG:NH1	2.53	0.40
4:B:439:THR:HG22	4:B:469:LYS:HE2	2.04	0.40
4:B:532:GLN:HG2	4:B:553:GLY:HA2	2.03	0.40
5:C:436:LEU:HD11	5:C:455:PHE:H	1.87	0.40
8:F:358:LYS:HD2	8:F:358:LYS:HA	1.98	0.40
12:3:420:ARG:HH11	14:5:499:GLN:HG2	1.86	0.40
13:4:352:CYS:CB	13:4:376:CYS:HB3	2.51	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:6:309:PHE:HD1	15:6:346:LEU:HA	1.86	0.40
15:6:355:ASP:OD1	15:6:355:ASP:N	2.55	0.40
15:6:610:ALA:HB1	15:6:623:ILE:CG2	2.52	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	8	380/604 (63%)	340 (90%)	36 (10%)	4 (1%)	14	52
2	9	363/513 (71%)	319 (88%)	42 (12%)	2 (1%)	25	66
3	A	410/913 (45%)	378 (92%)	32 (8%)	0	100	100
4	B	314/620 (51%)	292 (93%)	22 (7%)	0	100	100
5	C	536/616 (87%)	505 (94%)	30 (6%)	1 (0%)	47	81
6	E	414/479 (86%)	385 (93%)	28 (7%)	1 (0%)	47	81
7	D	428/529 (81%)	403 (94%)	25 (6%)	0	100	100
8	F	153/435 (35%)	146 (95%)	7 (5%)	0	100	100
11	2	569/868 (66%)	545 (96%)	20 (4%)	4 (1%)	22	63
12	3	626/971 (64%)	582 (93%)	40 (6%)	4 (1%)	25	66
13	4	651/933 (70%)	603 (93%)	45 (7%)	3 (0%)	29	69
14	5	579/775 (75%)	552 (95%)	24 (4%)	3 (0%)	29	69
15	6	568/1017 (56%)	538 (95%)	28 (5%)	2 (0%)	34	72
16	7	623/845 (74%)	595 (96%)	25 (4%)	3 (0%)	29	69
All	All	6614/10118 (65%)	6183 (94%)	404 (6%)	27 (0%)	38	72

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	605	TYR
6	E	445	SER
11	2	350	PRO
1	8	303	SER
2	9	282	LEU
12	3	395	ASN
12	3	500	ALA
13	4	892	GLU
14	5	507	ALA
16	7	544	GLN
1	8	301	GLU
1	8	311	MET
2	9	283	PRO
11	2	386	GLN
11	2	387	ARG
11	2	570	GLY
13	4	895	GLN
14	5	279	ASP
15	6	305	TYR
16	7	231	LYS
12	3	226	PRO
14	5	500	GLN
16	7	754	GLU
1	8	336	VAL
15	6	625	ALA
12	3	238	GLY
13	4	530	ILE

### 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	8	329/545 (60%)	326 (99%)	3 (1%)	78	87
2	9	338/470 (72%)	333 (98%)	5 (2%)	65	80
3	A	370/812 (46%)	370 (100%)	0	100	100
4	B	298/573 (52%)	296 (99%)	2 (1%)	84	90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C	505/576 (88%)	505 (100%)	0	100	100
6	E	387/440 (88%)	387 (100%)	0	100	100
7	D	402/488 (82%)	401 (100%)	1 (0%)	93	96
8	F	151/406 (37%)	151 (100%)	0	100	100
11	2	479/770 (62%)	475 (99%)	4 (1%)	81	89
12	3	512/835 (61%)	510 (100%)	2 (0%)	91	94
13	4	519/848 (61%)	516 (99%)	3 (1%)	86	92
14	5	431/688 (63%)	427 (99%)	4 (1%)	78	87
15	6	475/886 (54%)	474 (100%)	1 (0%)	93	96
16	7	525/753 (70%)	523 (100%)	2 (0%)	91	94
All	All	5721/9090 (63%)	5694 (100%)	27 (0%)	89	93

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	8	208	LYS
1	8	321	CYS
1	8	411	TYR
2	9	297	TYR
2	9	335	PHE
2	9	406	ARG
2	9	477	LYS
2	9	495	MET
4	B	411	TYR
4	B	547	ARG
7	D	499	PHE
11	2	341	CYS
11	2	385	TYR
11	2	517	CYS
11	2	794	ARG
12	3	24	ARG
12	3	527	ARG
13	4	190	CYS
13	4	428	ARG
13	4	727	LEU
14	5	276	MET
14	5	280	ARG
14	5	422	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	5	682	ARG
15	6	566	ARG
16	7	73	ARG
16	7	638	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	8	147	HIS
1	8	217	ASN
1	8	250	GLN
1	8	412	GLN
2	9	90	ASN
2	9	295	GLN
2	9	388	ASN
3	A	530	ASN
3	A	882	GLN
3	A	906	ASN
4	B	279	ASN
4	B	282	ASN
4	B	297	GLN
4	B	310	GLN
4	B	364	ASN
4	B	398	ASN
4	B	426	ASN
4	B	458	HIS
4	B	535	ASN
4	B	585	HIS
5	C	63	GLN
5	C	65	HIS
5	C	69	HIS
5	C	78	ASN
5	C	243	ASN
5	C	253	GLN
5	C	486	ASN
6	E	52	ASN
6	E	58	HIS
6	E	114	ASN
6	E	193	ASN
6	E	253	ASN
6	E	277	ASN
6	E	320	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	E	422	GLN
6	E	453	ASN
7	D	80	GLN
7	D	105	GLN
7	D	158	HIS
7	D	277	GLN
7	D	321	ASN
7	D	327	ASN
7	D	409	ASN
7	D	423	ASN
7	D	511	GLN
8	F	318	GLN
8	F	326	ASN
8	F	407	GLN
11	2	384	ASN
12	3	210	HIS
12	3	269	GLN
12	3	351	ASN
12	3	487	HIS
12	3	507	ASN
12	3	691	ASN
12	3	950	ASN
13	4	247	ASN
13	4	380	ASN
13	4	395	GLN
13	4	543	GLN
13	4	652	GLN
14	5	49	GLN
14	5	145	GLN
14	5	203	ASN
14	5	372	ASN
14	5	411	ASN
14	5	676	HIS
15	6	570	ASN
16	7	108	GLN
16	7	425	ASN
16	7	585	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	AGS	A	2001	-	26,33,33	0.72	1 (3%)	26,52,52	1.08	2 (7%)
17	AGS	9	2001	-	26,33,33	0.73	1 (3%)	26,52,52	1.30	2 (7%)
17	AGS	D	2001	-	26,33,33	0.76	0	26,52,52	1.41	2 (7%)
17	AGS	E	2001	-	26,33,33	0.68	0	26,52,52	1.33	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	AGS	A	2001	-	-	7/17/38/38	0/3/3/3
17	AGS	9	2001	-	-	7/17/38/38	0/3/3/3
17	AGS	D	2001	-	-	2/17/38/38	0/3/3/3
17	AGS	E	2001	-	-	7/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	2001	AGS	C8-N7	-2.02	1.31	1.34

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	2001	AGS	C8-N7	-2.01	1.31	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	2001	AGS	PA-O3A-PB	-5.96	112.37	132.83
17	9	2001	AGS	PA-O3A-PB	-5.46	114.08	132.83
17	E	2001	AGS	PA-O3A-PB	-5.21	114.94	132.83
17	A	2001	AGS	PA-O3A-PB	-3.84	119.66	132.83
17	D	2001	AGS	C5-C6-N6	2.31	123.87	120.35
17	A	2001	AGS	C5-C6-N6	2.25	123.76	120.35
17	E	2001	AGS	C5-C6-N6	2.20	123.70	120.35
17	9	2001	AGS	C5-C6-N6	2.15	123.62	120.35

There are no chirality outliers.

All (23) torsion outliers are listed below:

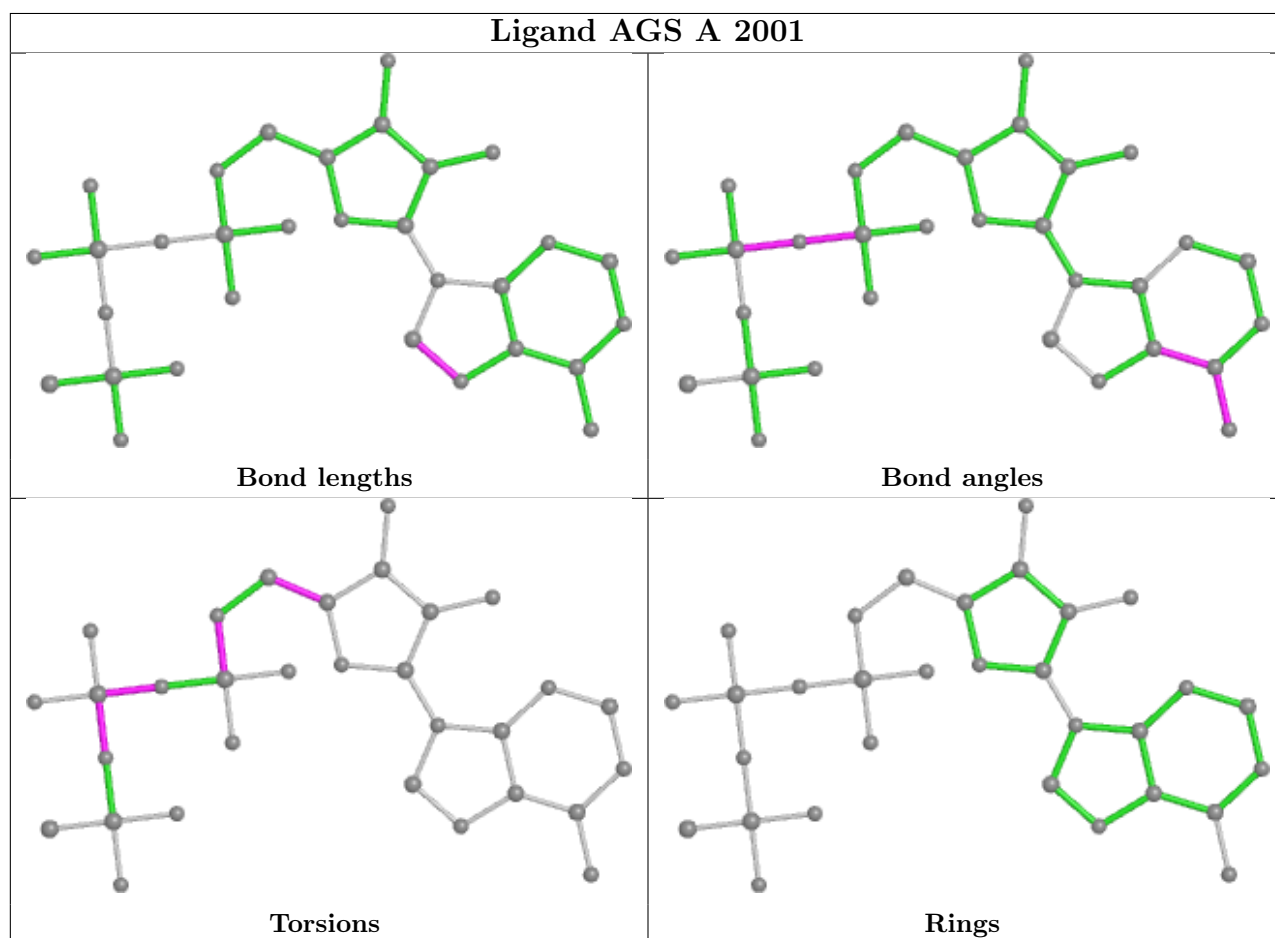
Mol	Chain	Res	Type	Atoms
17	9	2001	AGS	C5'-O5'-PA-O2A
17	9	2001	AGS	C5'-O5'-PA-O3A
17	A	2001	AGS	C5'-O5'-PA-O1A
17	A	2001	AGS	C5'-O5'-PA-O2A
17	A	2001	AGS	O4'-C4'-C5'-O5'
17	E	2001	AGS	C5'-O5'-PA-O1A
17	E	2001	AGS	C5'-O5'-PA-O2A
17	E	2001	AGS	C5'-O5'-PA-O3A
17	9	2001	AGS	O4'-C4'-C5'-O5'
17	E	2001	AGS	O4'-C4'-C5'-O5'
17	9	2001	AGS	C3'-C4'-C5'-O5'
17	E	2001	AGS	C3'-C4'-C5'-O5'
17	9	2001	AGS	PB-O3A-PA-O1A
17	A	2001	AGS	PG-O3B-PB-O1B
17	9	2001	AGS	C4'-C5'-O5'-PA
17	D	2001	AGS	C4'-C5'-O5'-PA
17	E	2001	AGS	PG-O3B-PB-O2B
17	D	2001	AGS	C3'-C4'-C5'-O5'
17	A	2001	AGS	PA-O3A-PB-O1B
17	A	2001	AGS	C5'-O5'-PA-O3A
17	9	2001	AGS	PB-O3A-PA-O2A
17	E	2001	AGS	PA-O3A-PB-O1B
17	A	2001	AGS	C3'-C4'-C5'-O5'

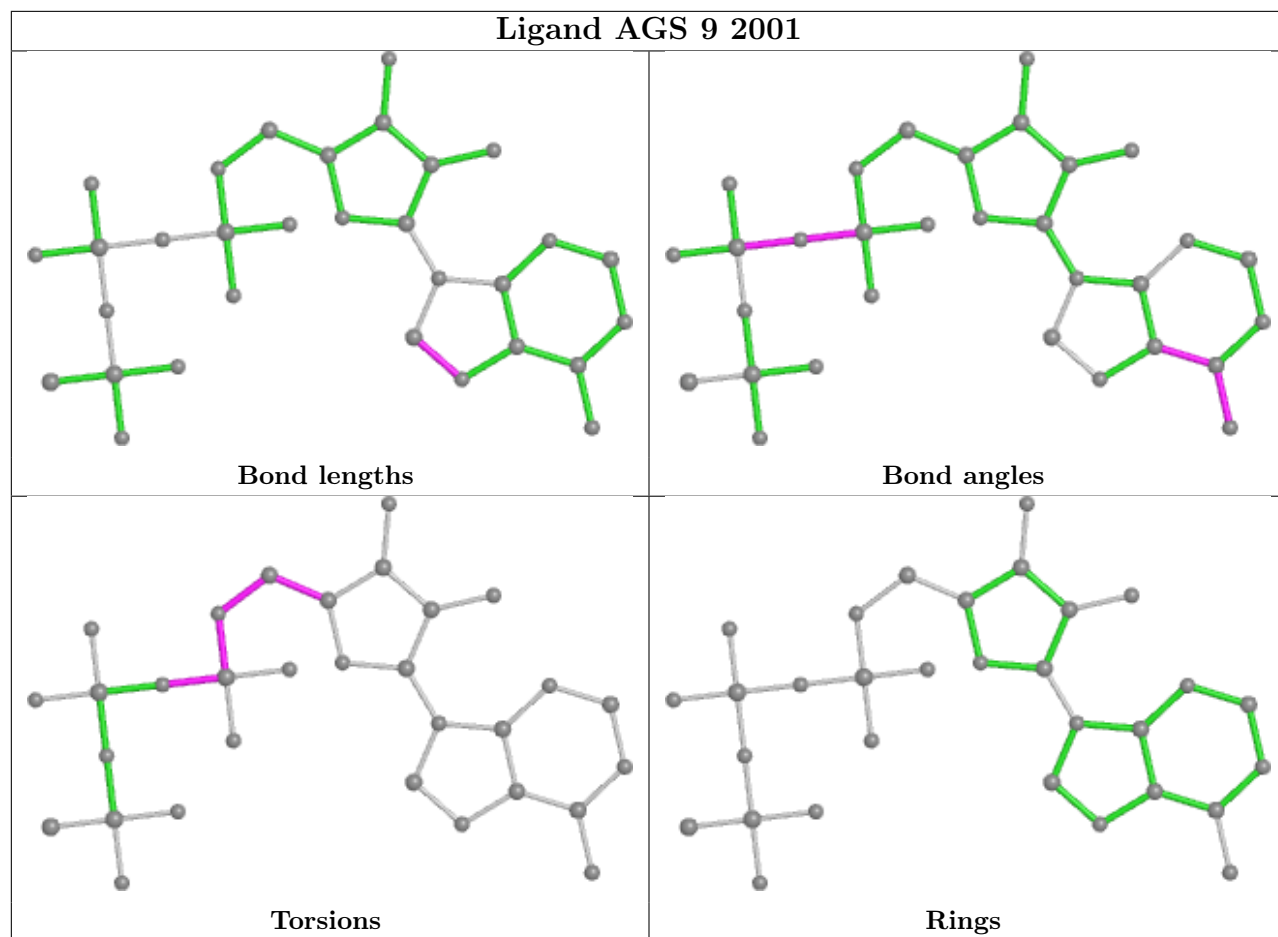
There are no ring outliers.

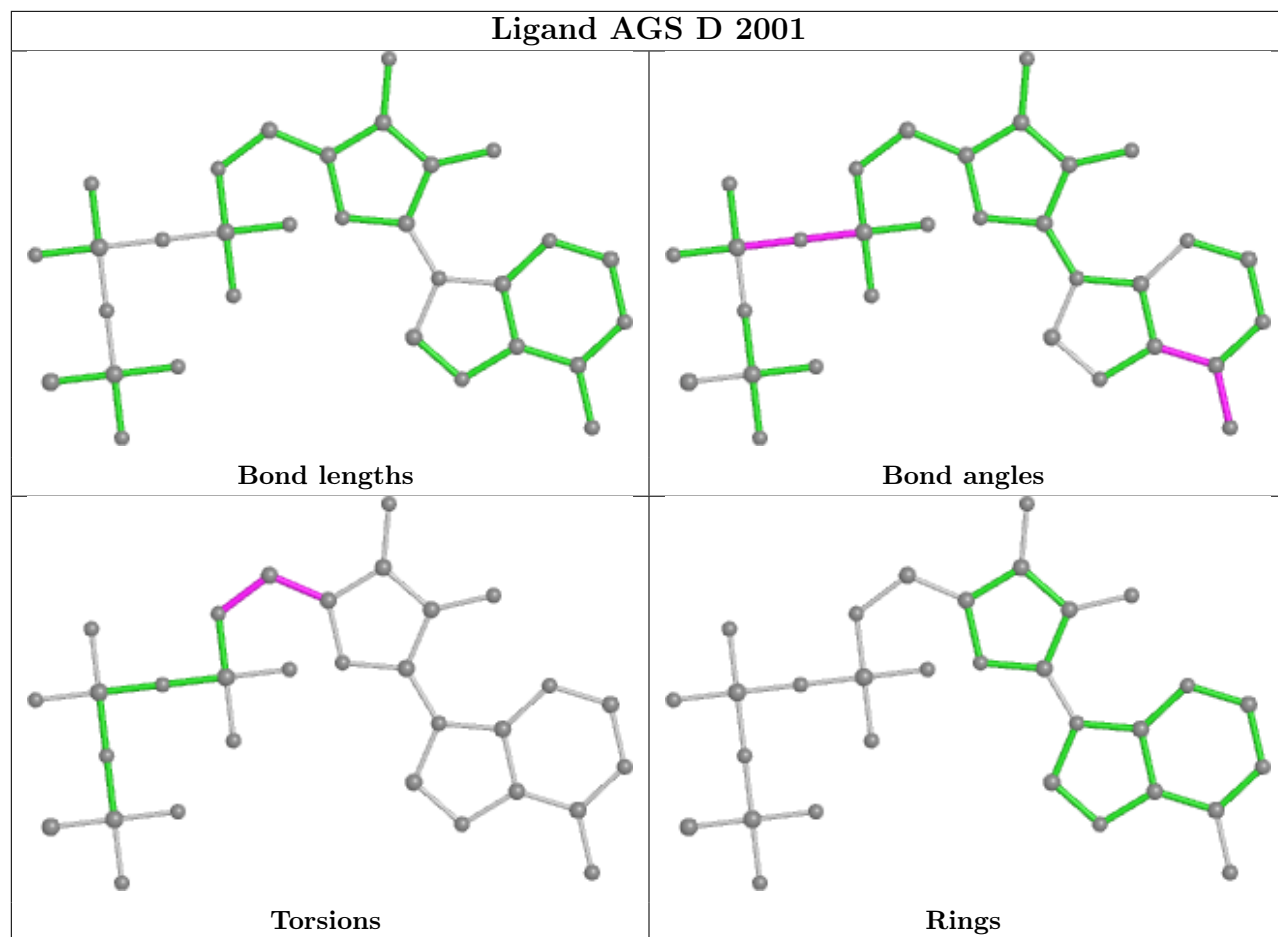
4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	2001	AGS	7	0
17	9	2001	AGS	4	0
17	D	2001	AGS	4	0
17	E	2001	AGS	5	0

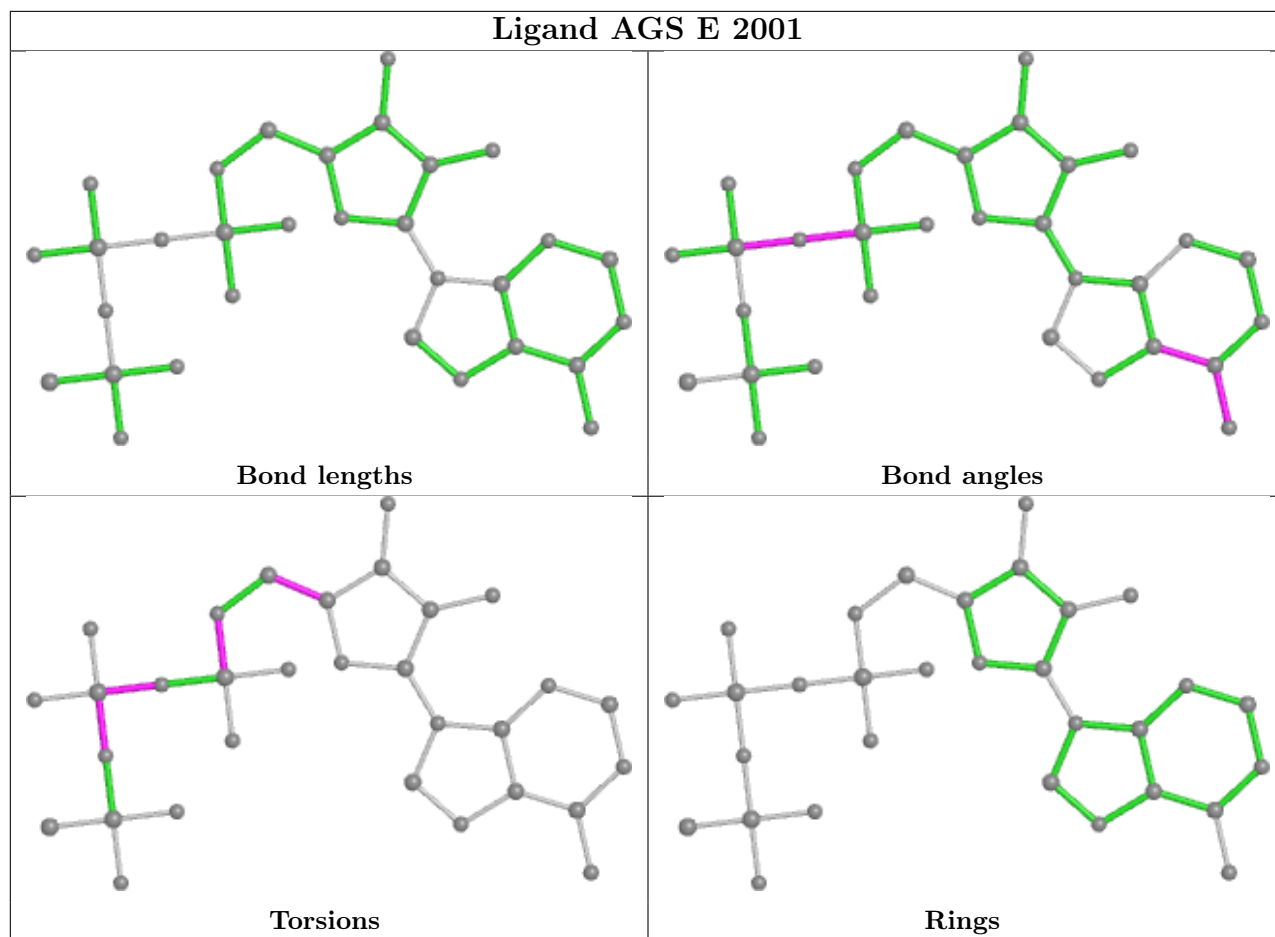
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	9	1
16	7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	399:ASN	C	400:ASN	N	3.97
1	7	785:GLU	C	786:TYR	N	3.65

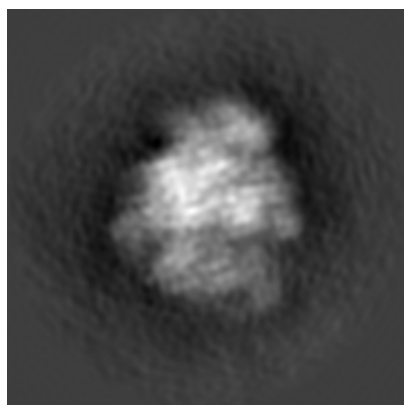
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21665. These allow visual inspection of the internal detail of the map and identification of artifacts.

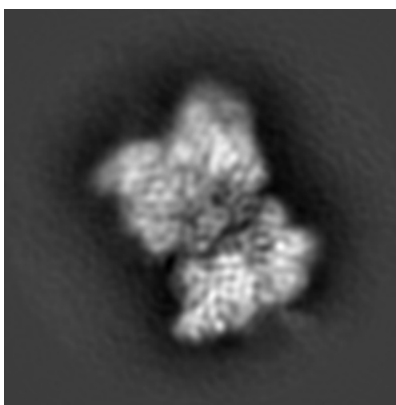
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

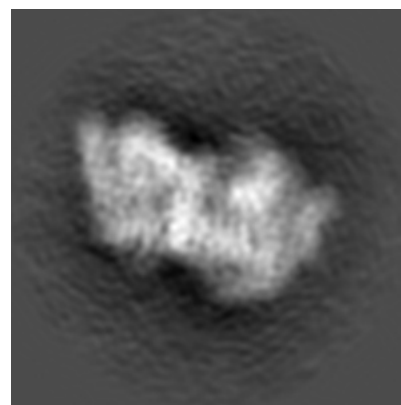
#### 6.1.1 Primary map



X



Y

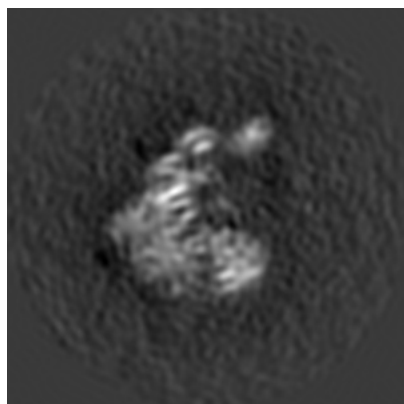


Z

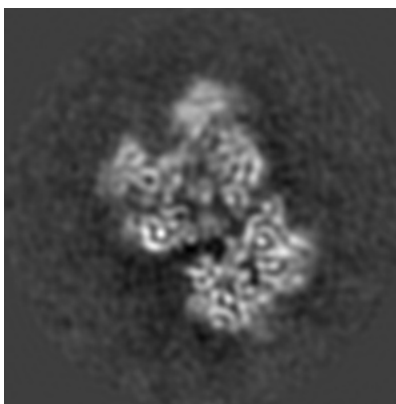
The images above show the map projected in three orthogonal directions.

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

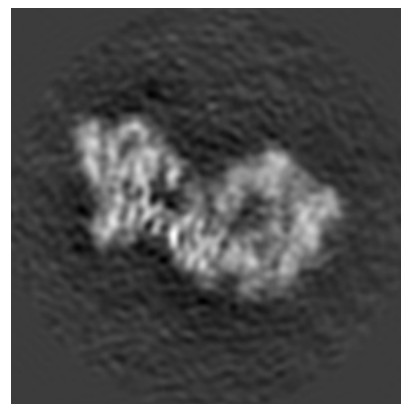
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

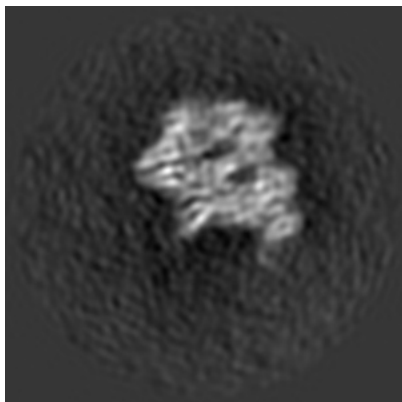


Z Index: 128

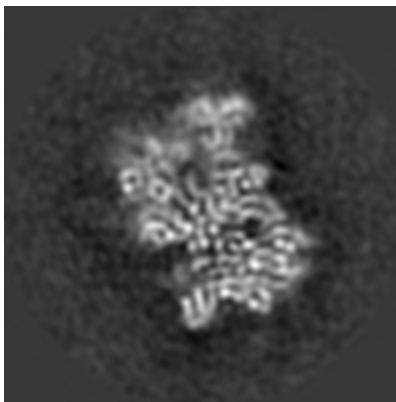
The images above show central slices of the map in three orthogonal directions.

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

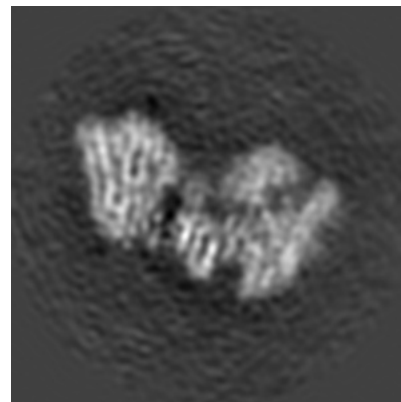
### 6.3.1 Primary map



X Index: 86



Y Index: 113

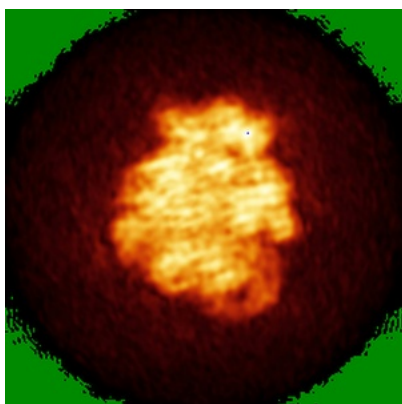


Z Index: 134

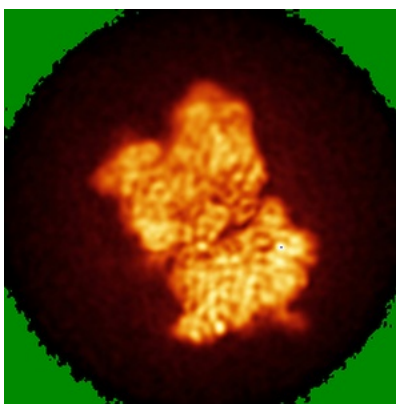
The images above show the largest variance slices of the map in three orthogonal directions.

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

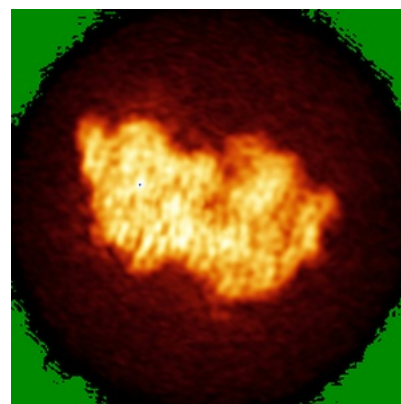
### 6.4.1 Primary map



X



Y

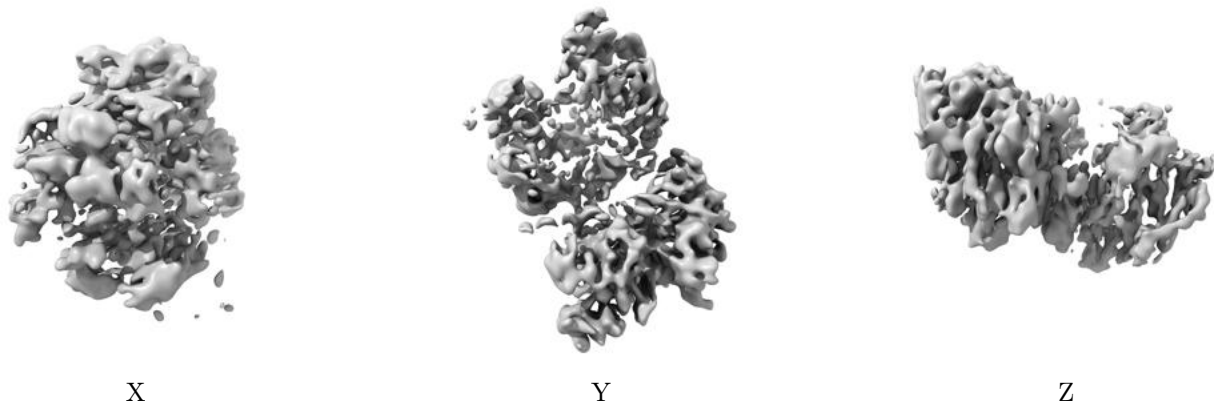


Z

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

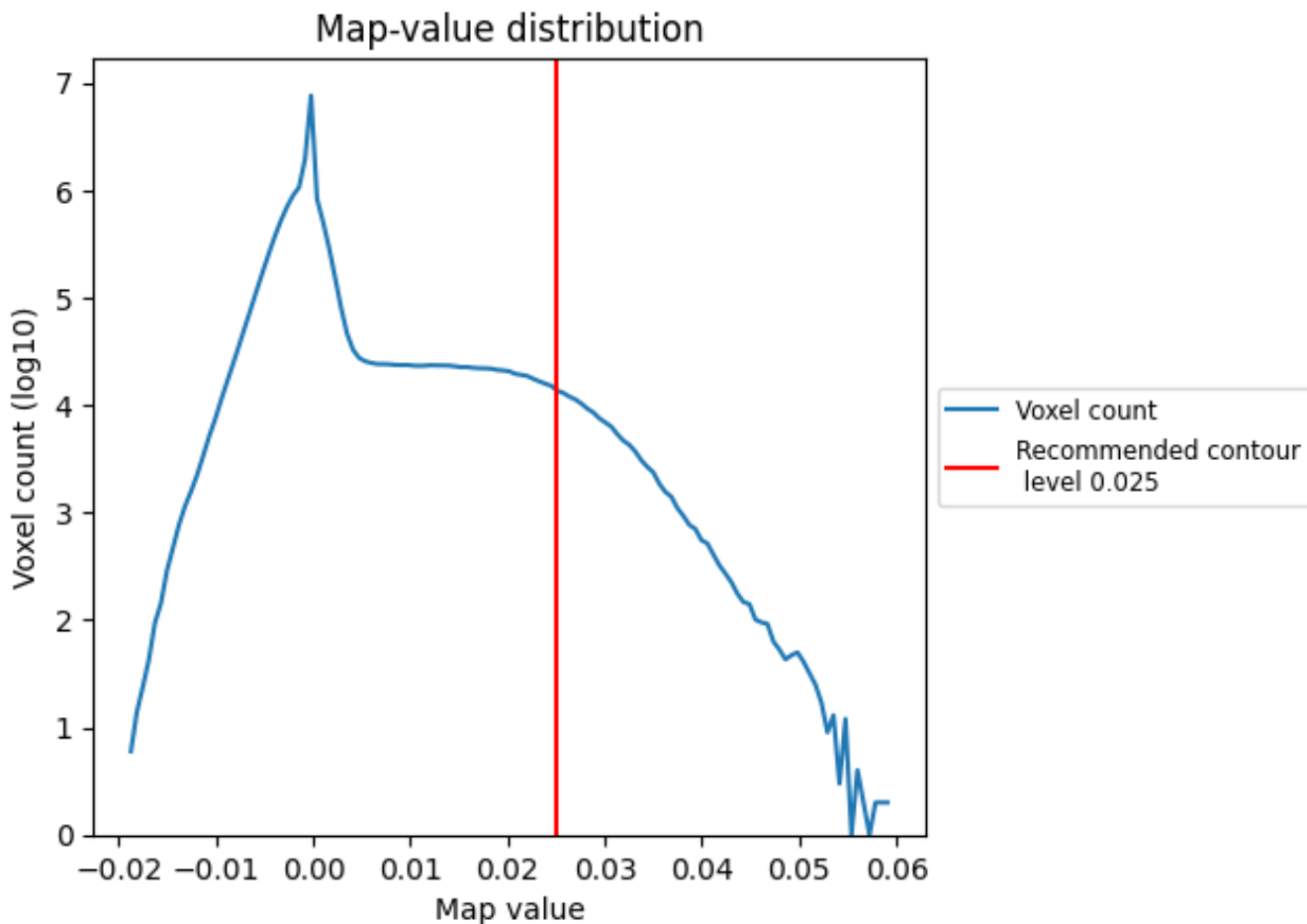
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

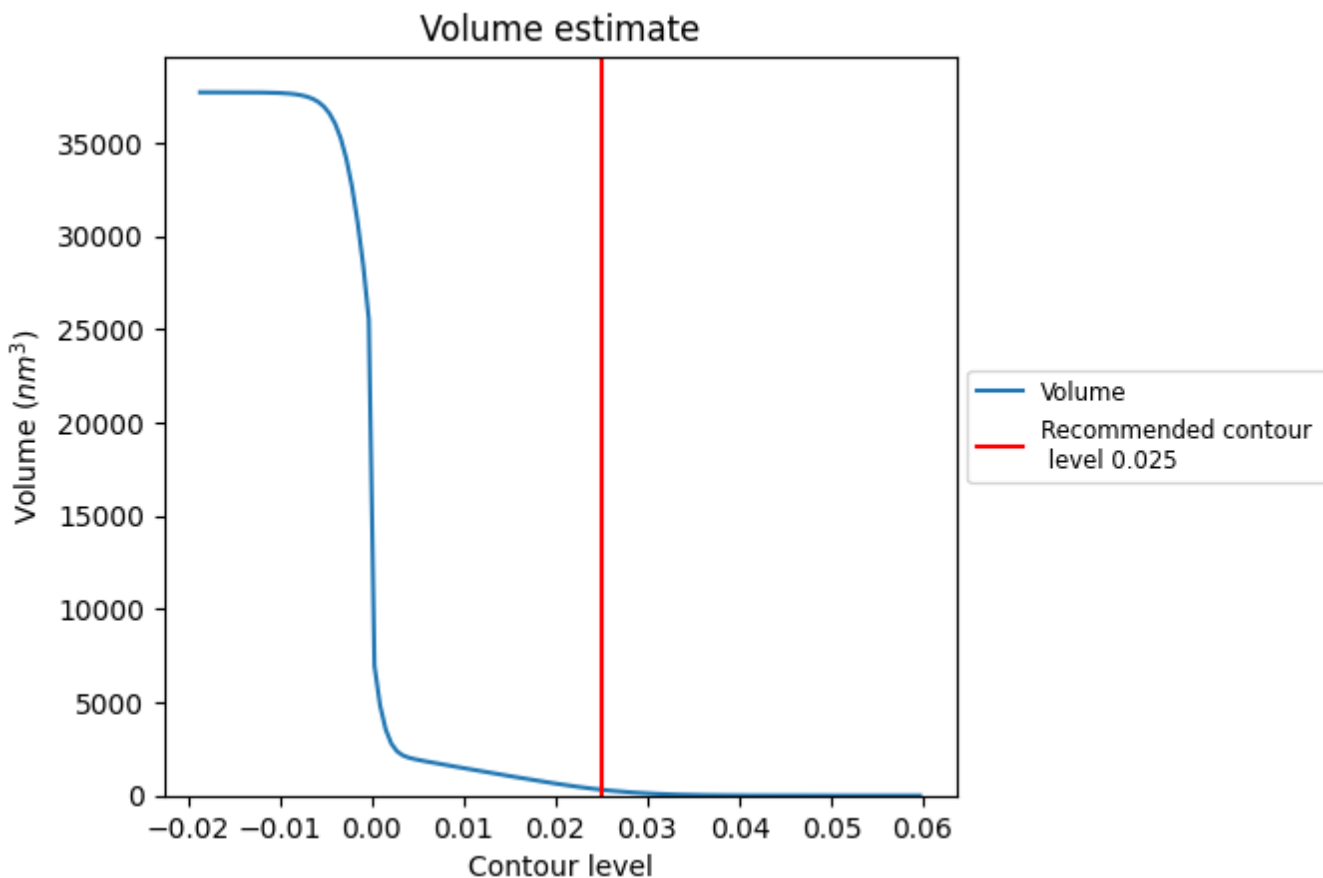
This section contains the results of statistical analysis of the map.

### 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.

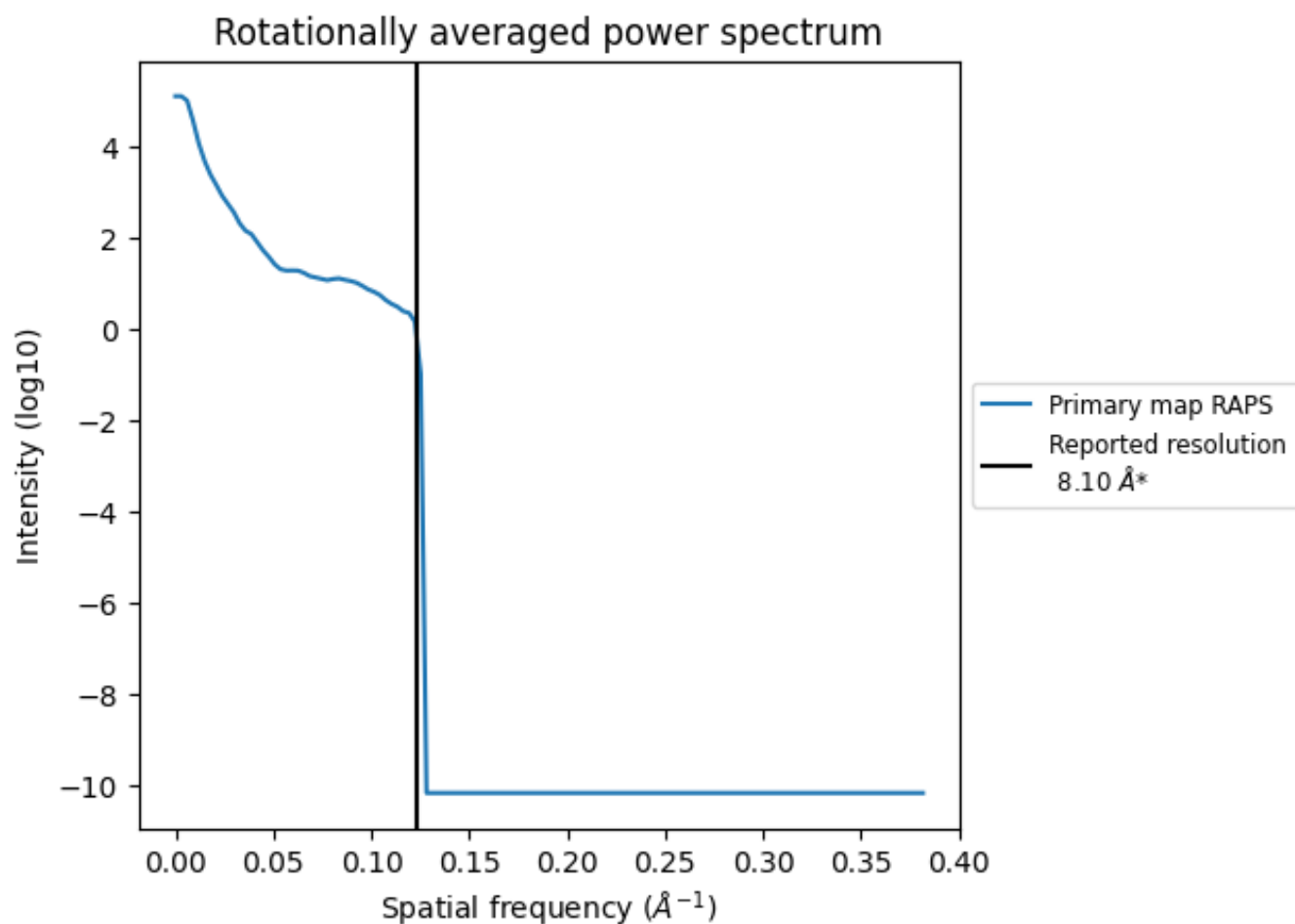
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm<sup>3</sup>; this corresponds to an approximate mass of 284 kDa.

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

### 7.3 Rotationally averaged power spectrum [\(i\)](#)



\*Reported resolution corresponds to spatial frequency of 0.123 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

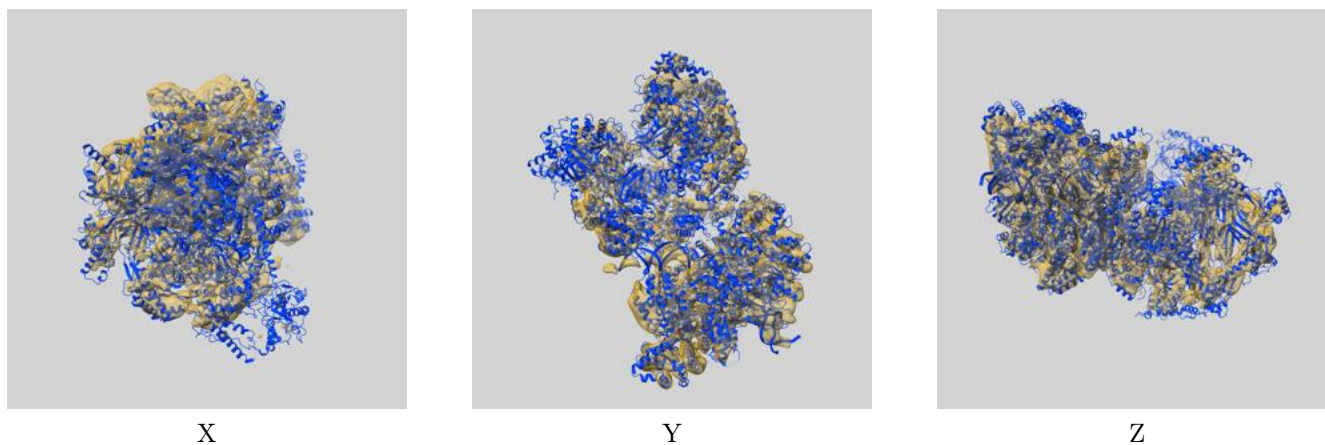
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit [i](#)

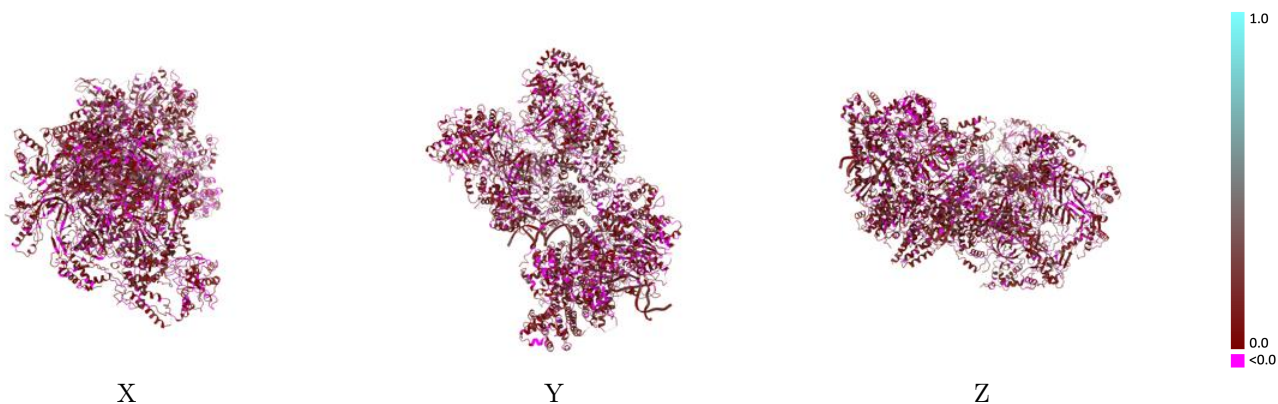
This section contains information regarding the fit between EMDB map EMD-21665 and PDB model 6WGG. Per-residue inclusion information can be found in section 3 on page 7.

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



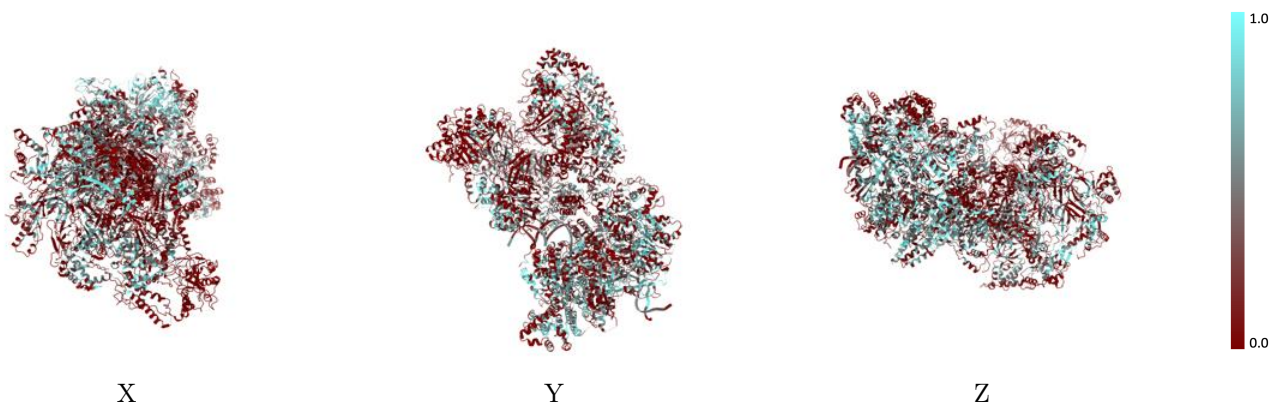
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



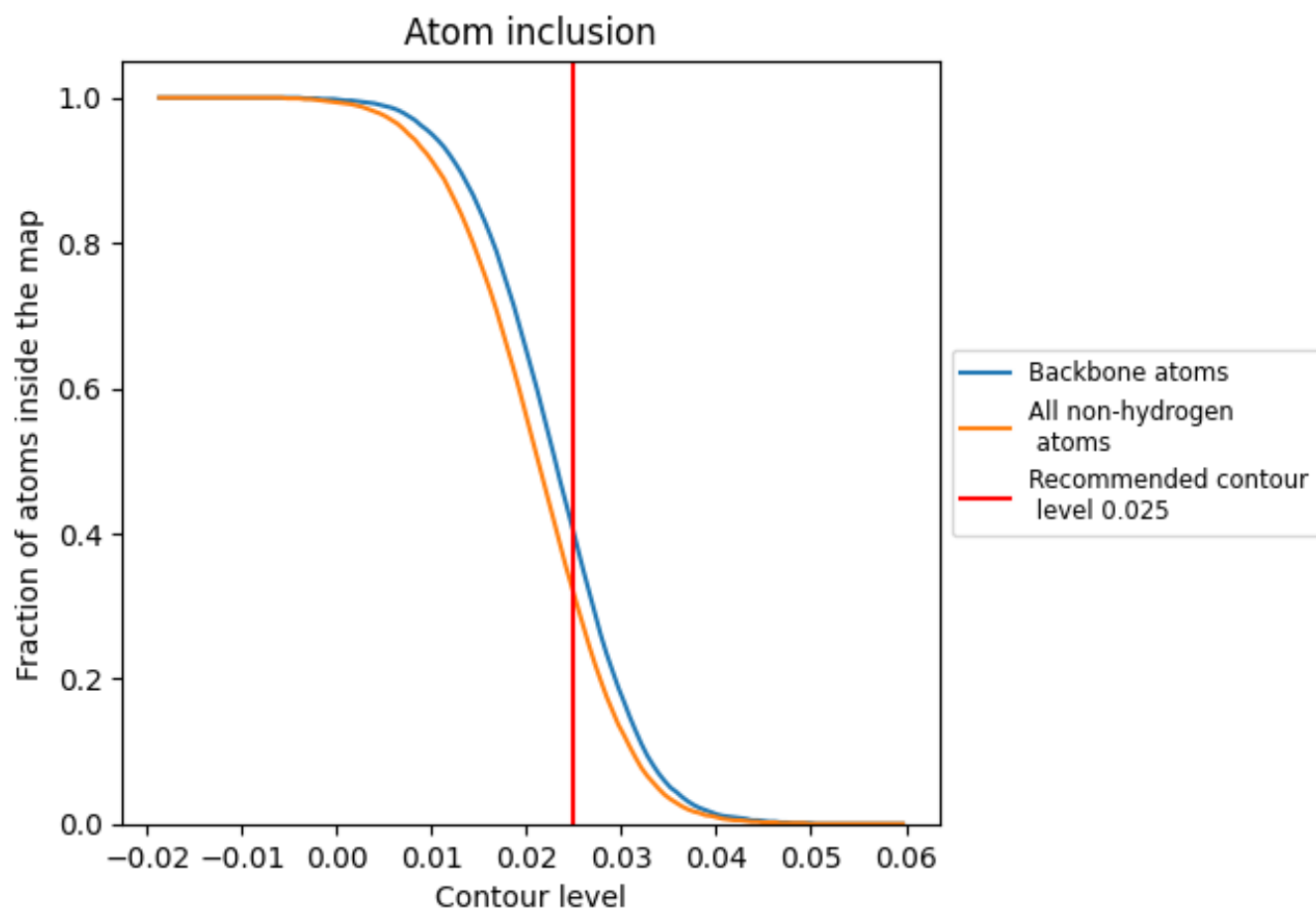
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 40% of all backbone atoms, 32% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3160	 0.1040
2	 0.2790	 0.1050
3	 0.3100	 0.1010
4	 0.2850	 0.1110
5	 0.1860	 0.0970
6	 0.3390	 0.1010
7	 0.2470	 0.1150
8	 0.0380	 0.0690
9	 0.3420	 0.0670
A	 0.4340	 0.1060
B	 0.3390	 0.0930
C	 0.4400	 0.1060
D	 0.4250	 0.1220
E	 0.4010	 0.1230
F	 0.2360	 0.0540
G	 0.4320	 0.1780
H	 0.5570	 0.2000

