



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:43 AM UTC

PDB ID : 6WGG / pdb_00006wgg
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

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

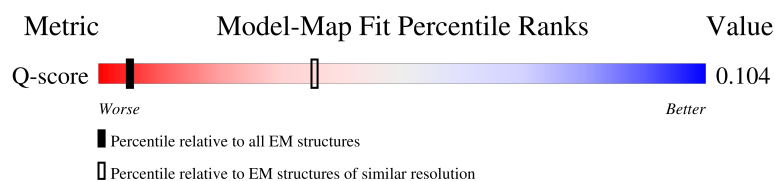
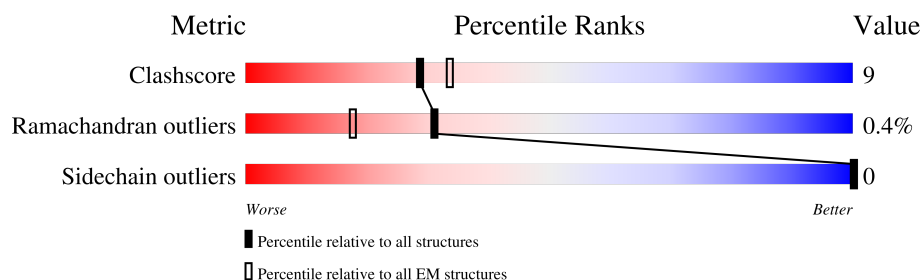
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



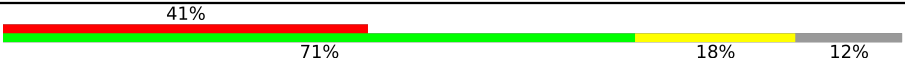
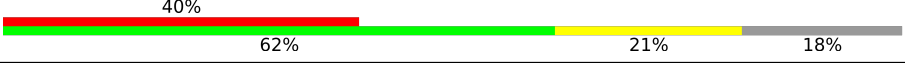
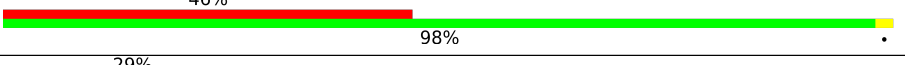
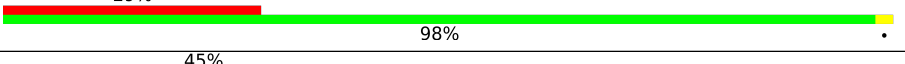
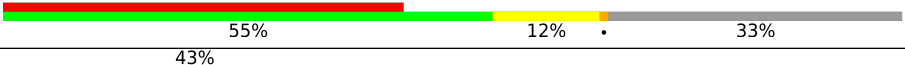
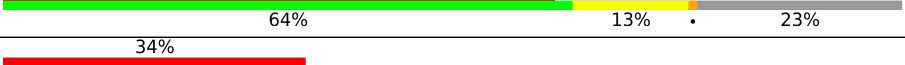
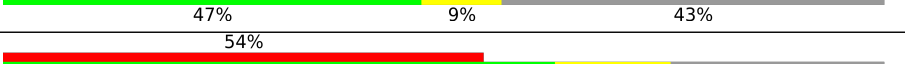
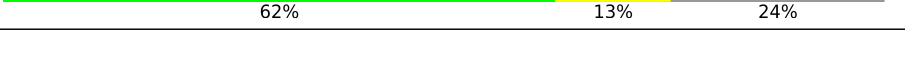
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	342 (7.60 - 8.60)

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	8	604	61% 41% 23% 36%
2	9	513	46% 49% 23% 27%
3	A	913	23% 37% 9% 54%
4	B	620	31% 40% 13% 47%

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Mol	Chain	Length	Quality of chain
5	C	616	
6	E	479	
7	D	529	
8	F	435	
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

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
1	8	388	Total	C	N	O	S	0	0
			3011	1916	518	566	11		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

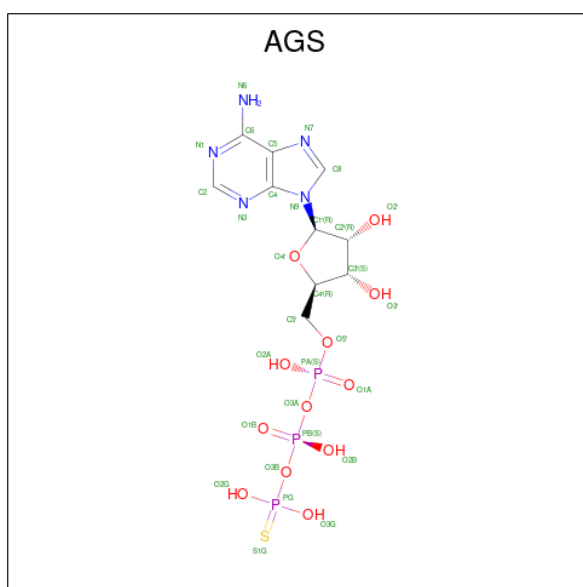
- Molecule 15 is a protein called DNA replication licensing factor MCM6.

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

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

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

- Molecule 17 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).

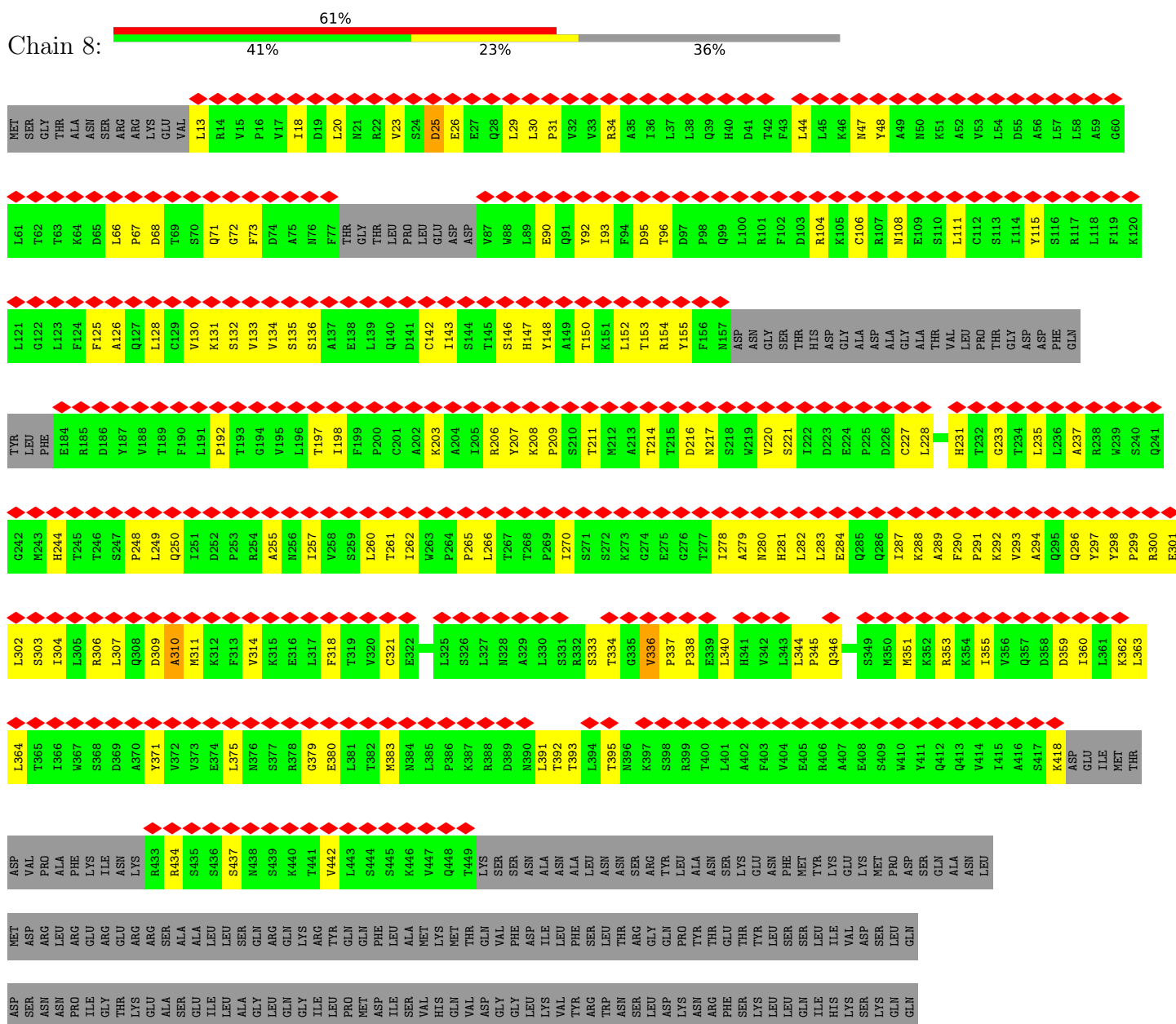


Mol	Chain	Residues	Atoms						AltConf
17	9	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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.

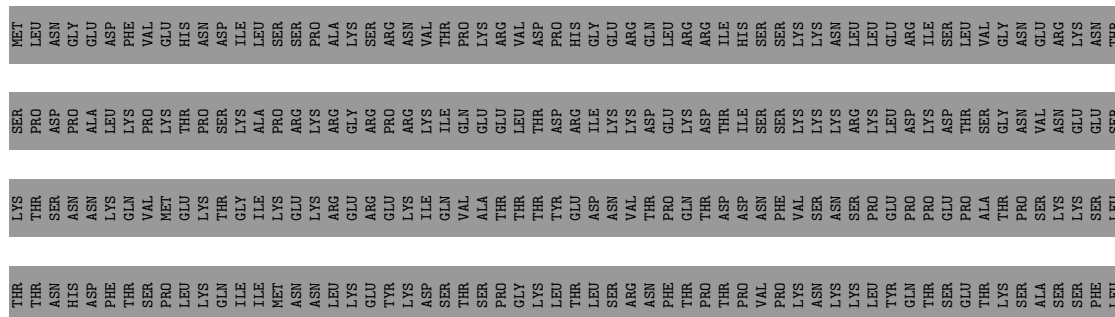
• Molecule 1: Cell division cycle protein CDT1

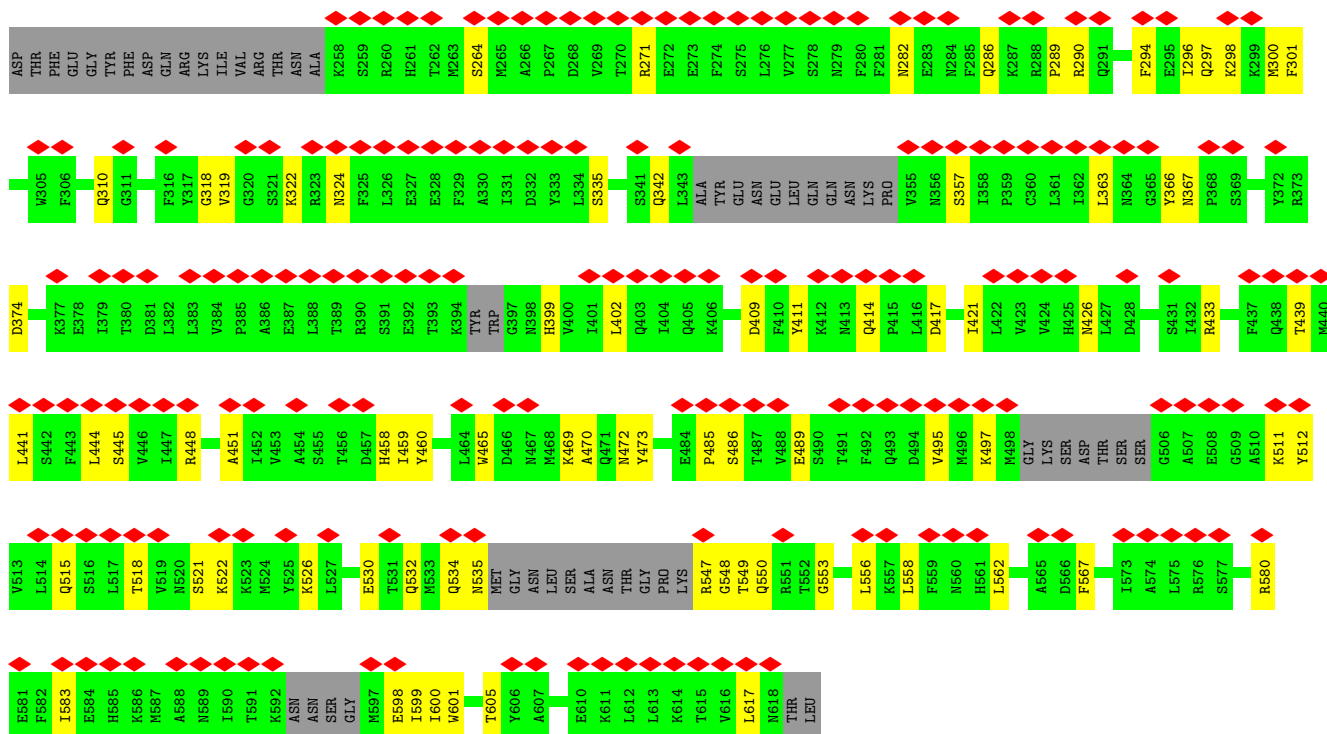


Chain 9:

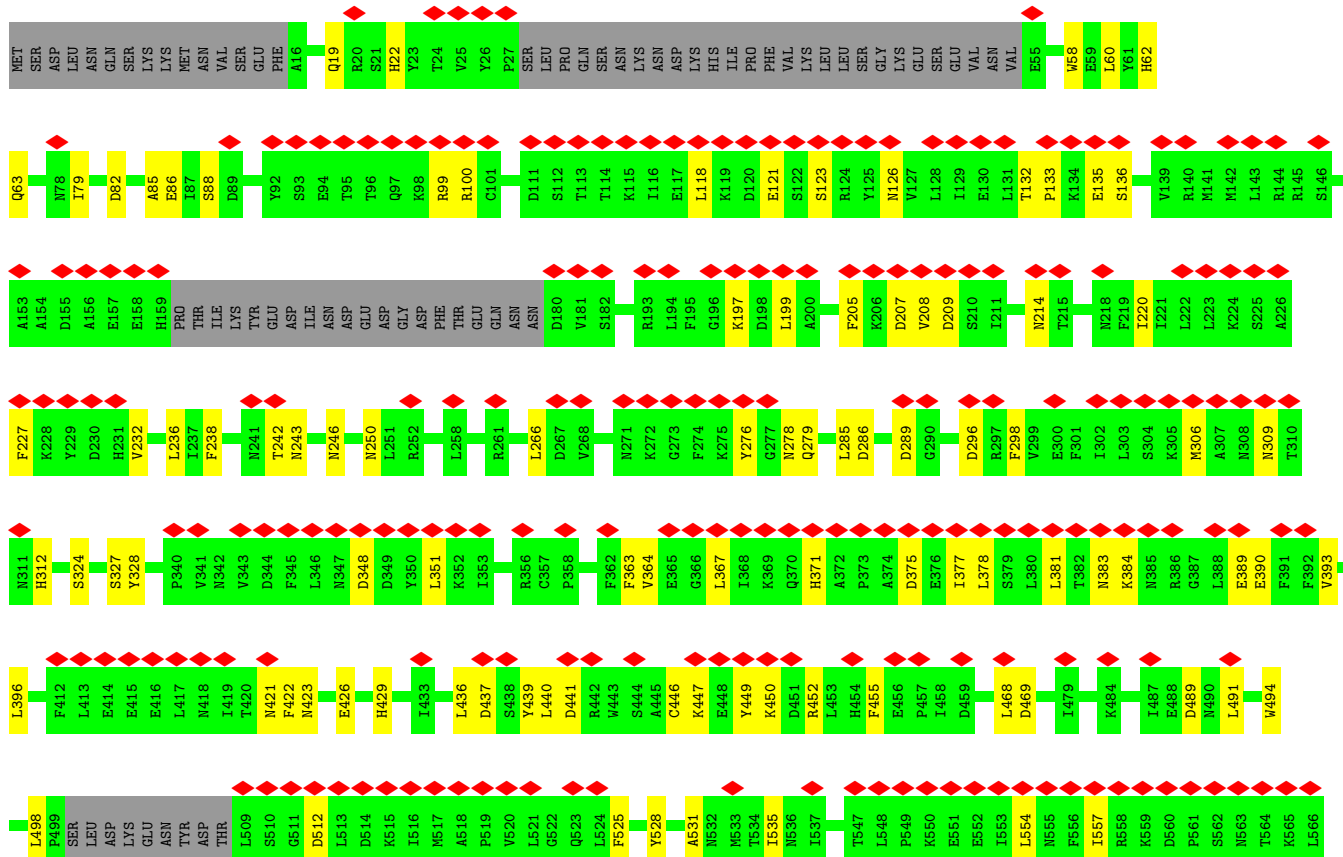
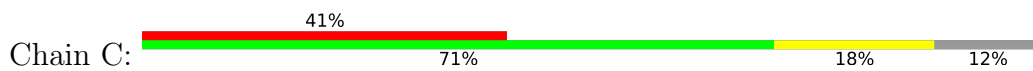
Chain A:





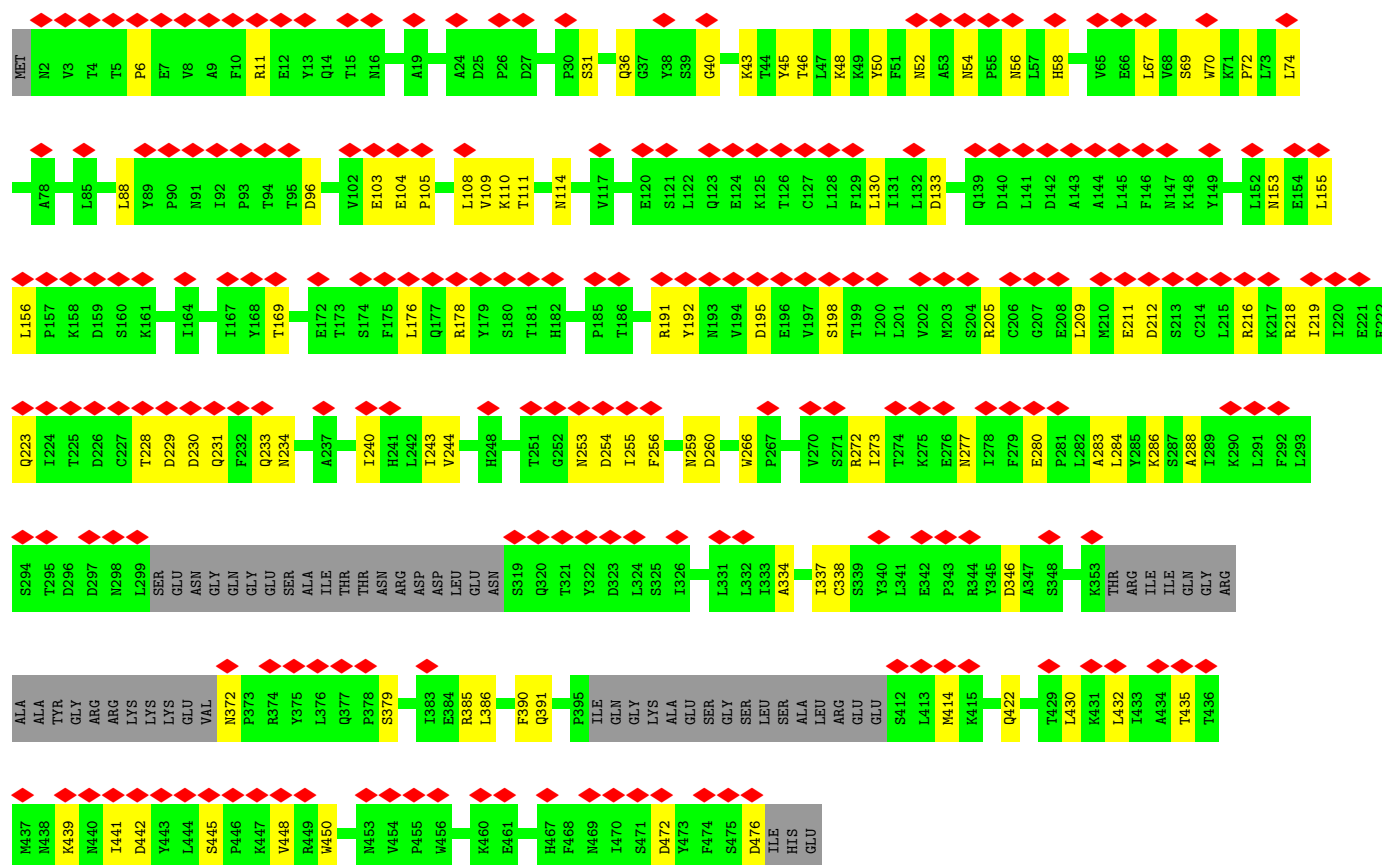


• Molecule 5: Origin recognition complex subunit 3

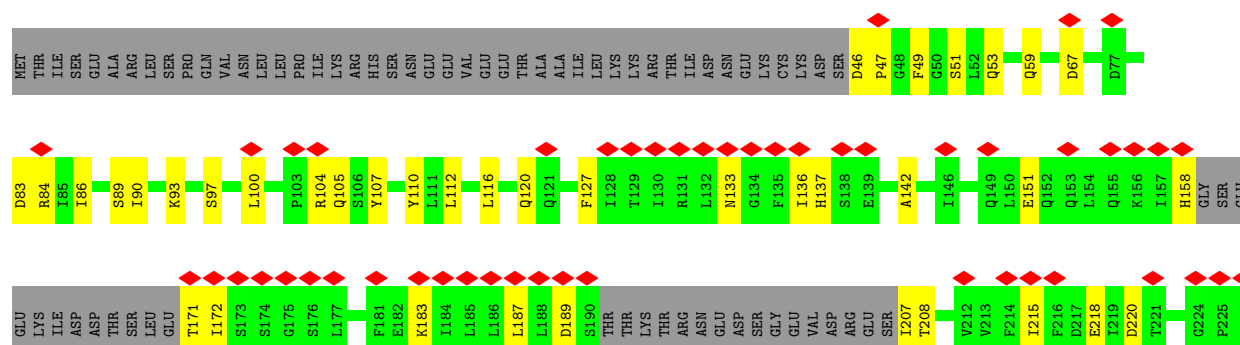
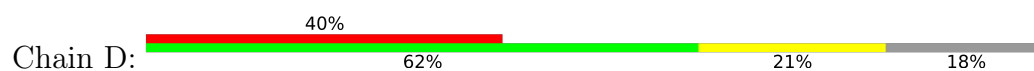


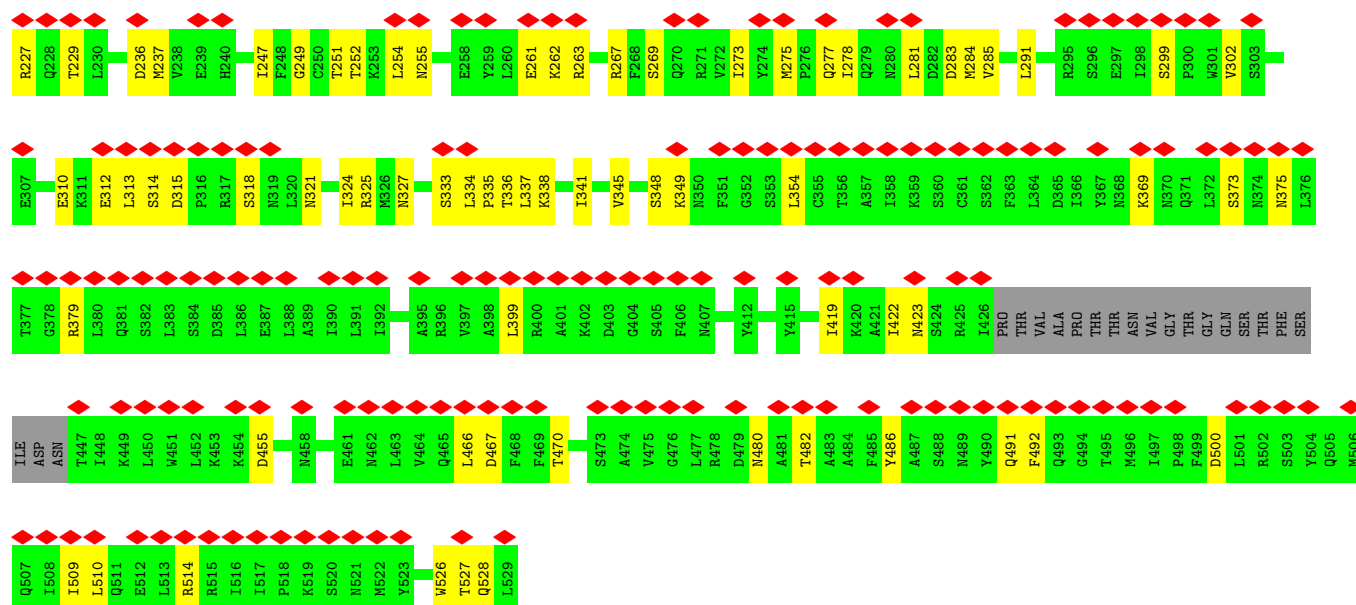


• Molecule 6: Origin recognition complex subunit 5

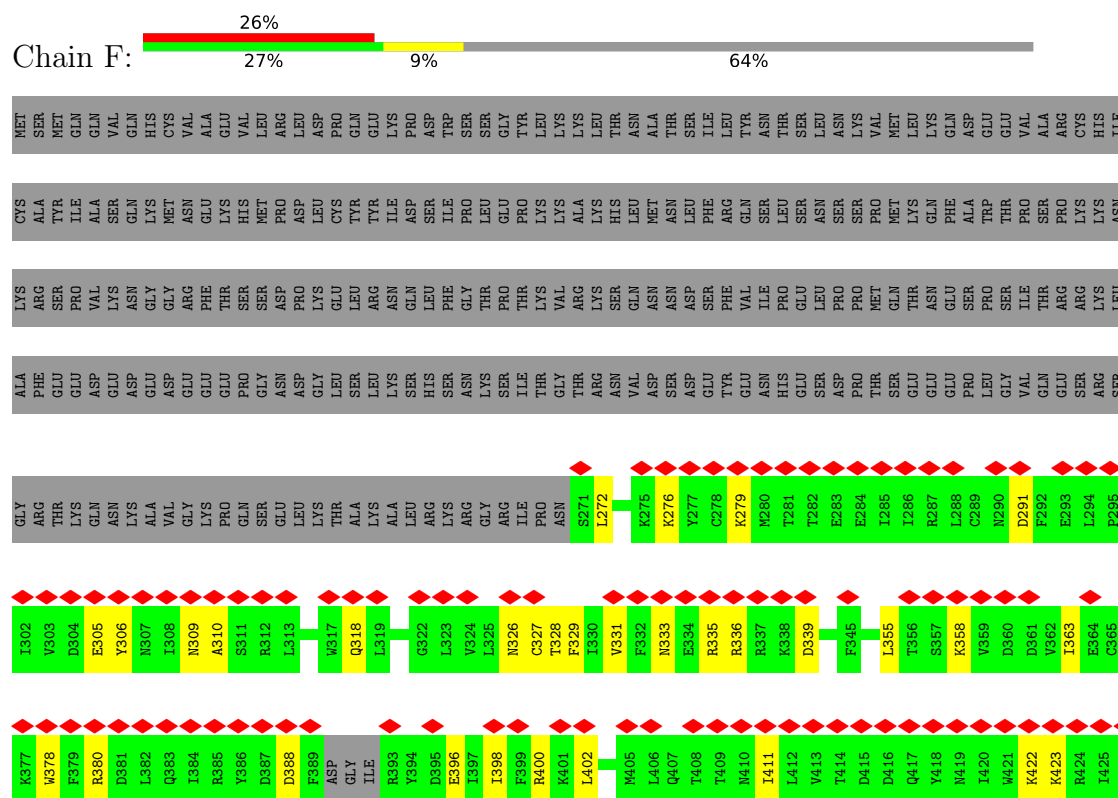


• Molecule 7: Origin recognition complex subunit 4

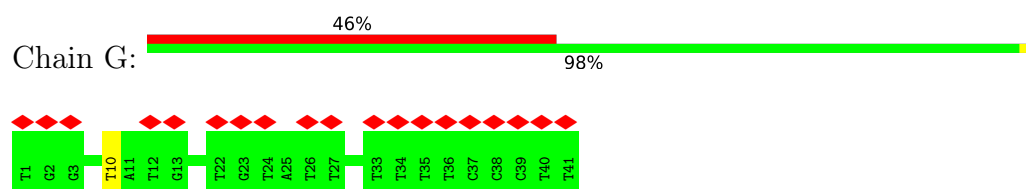




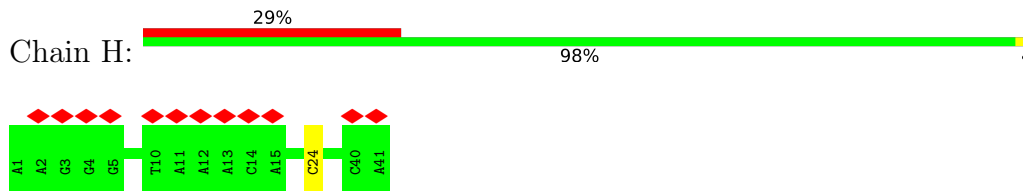
• Molecule 8: Origin recognition complex subunit 6



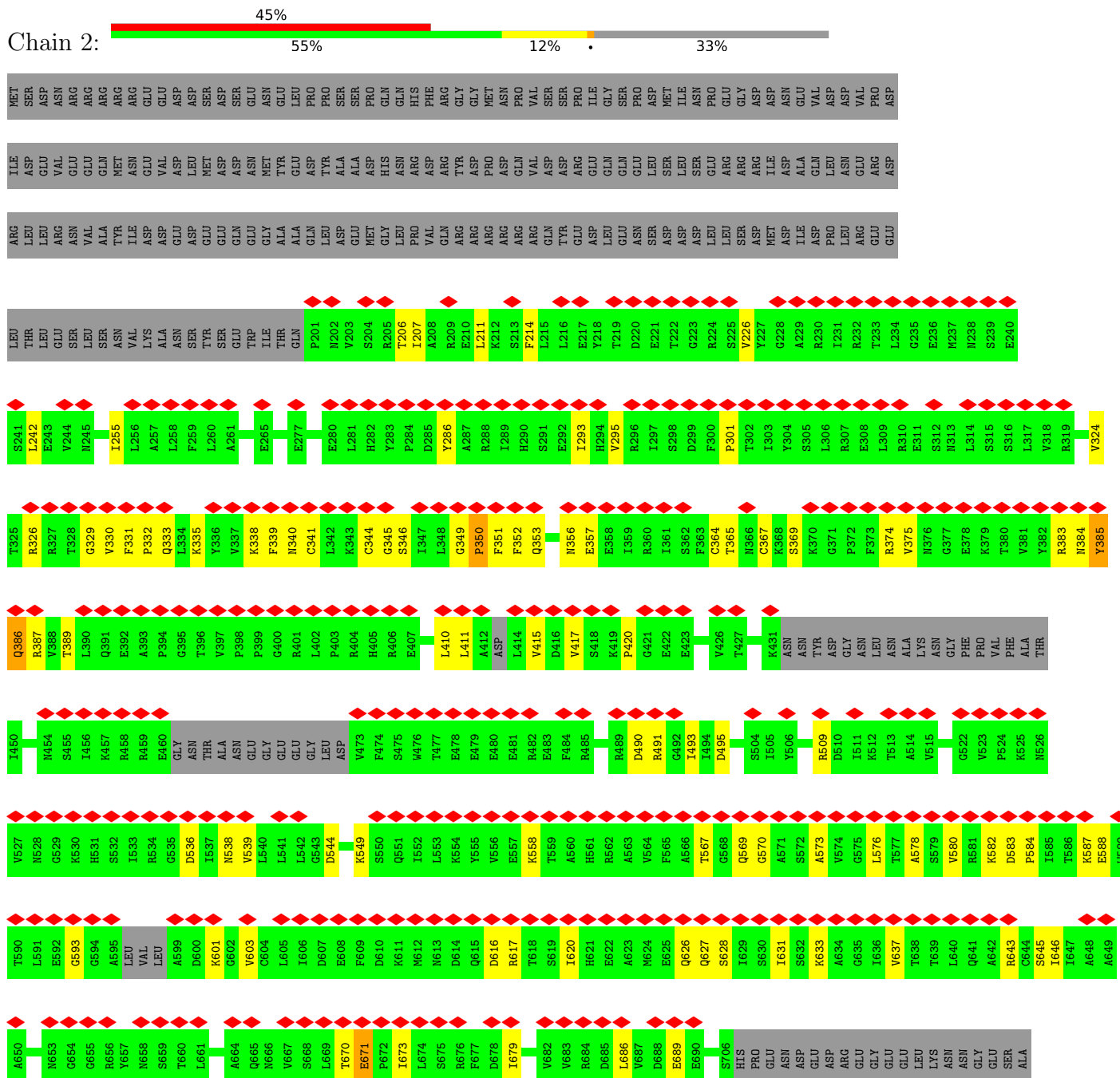
• Molecule 9: DNA (41-MER)

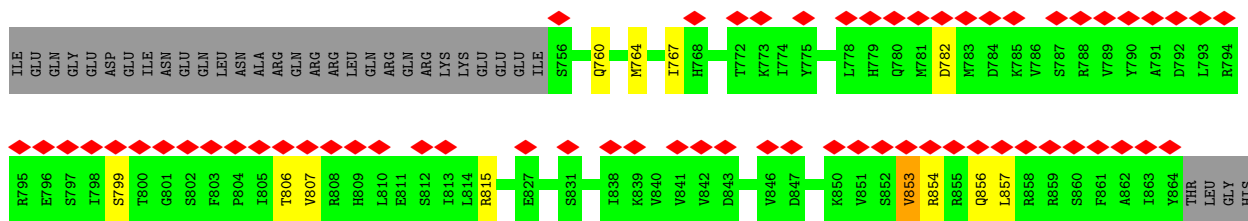


Chain H:

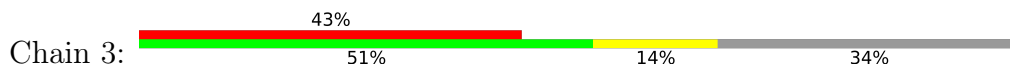


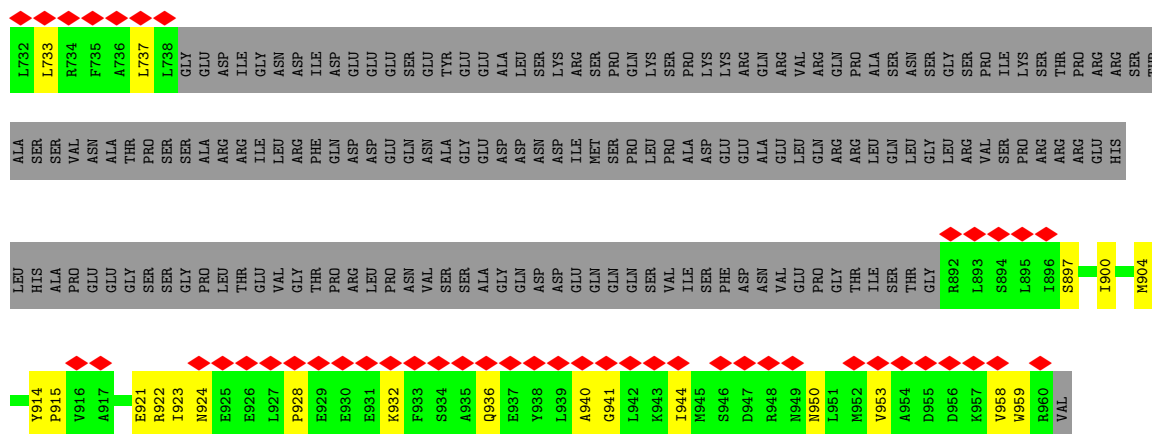
Chain 2:



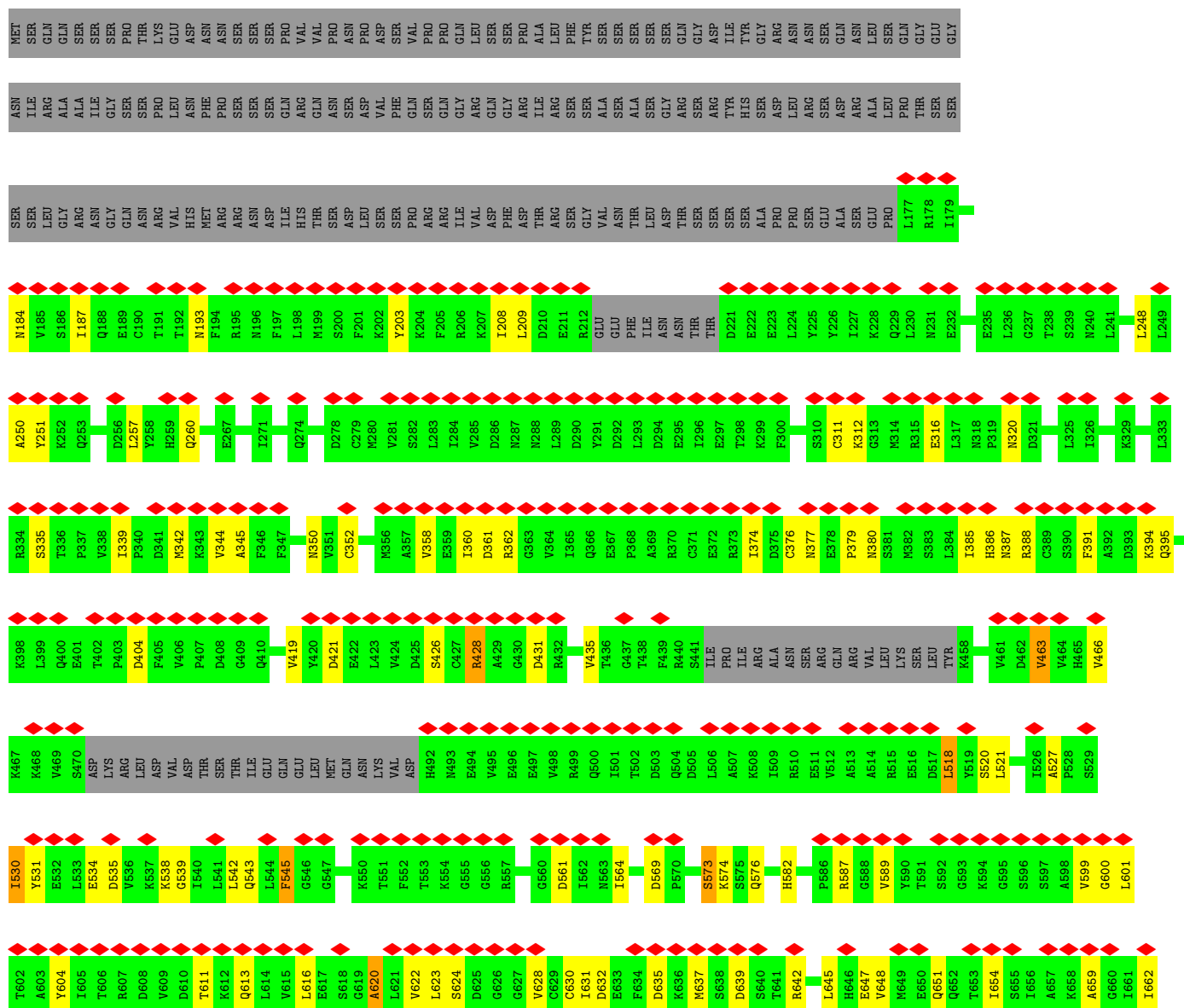


• Molecule 12: DNA replication licensing factor MCM3

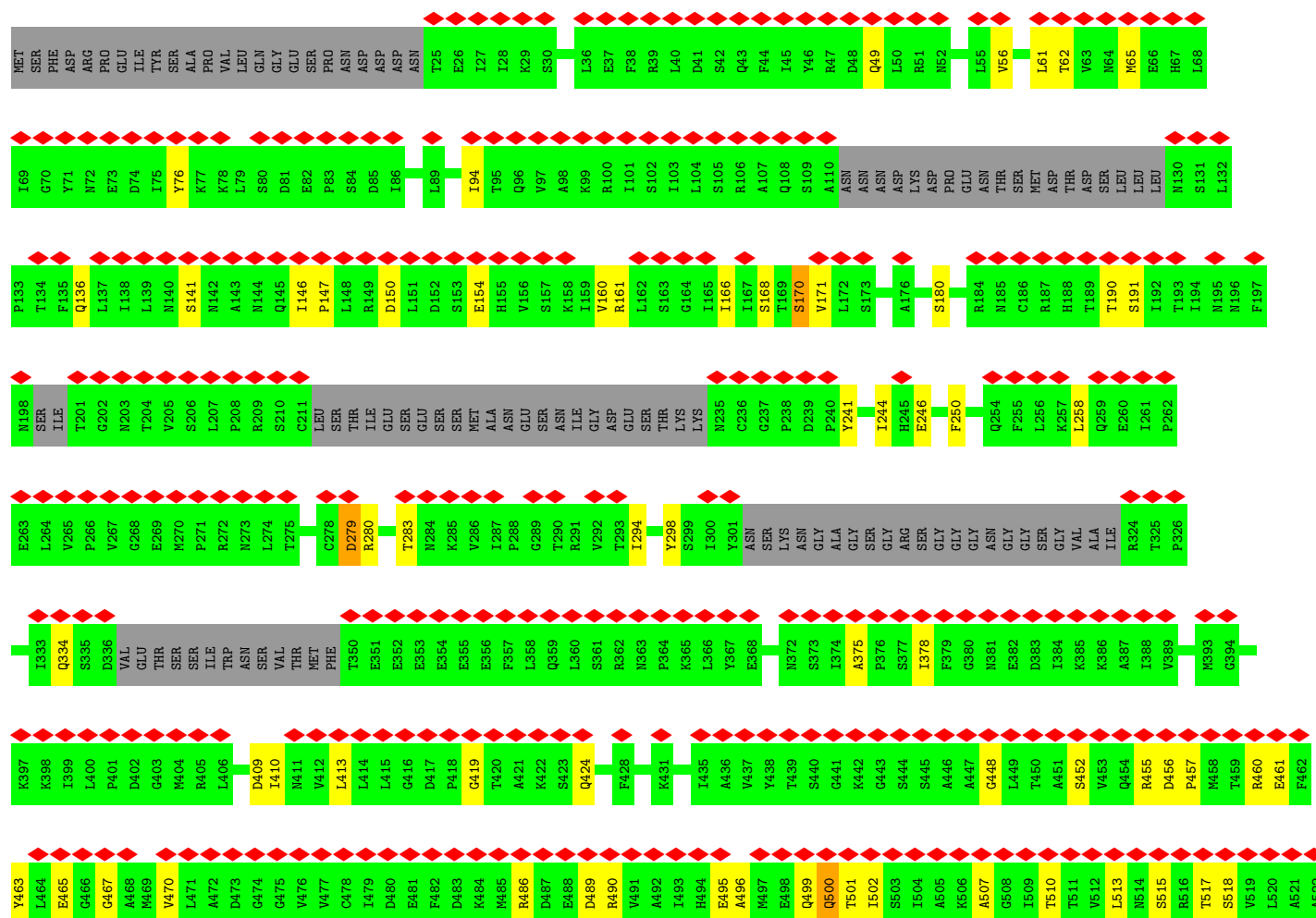


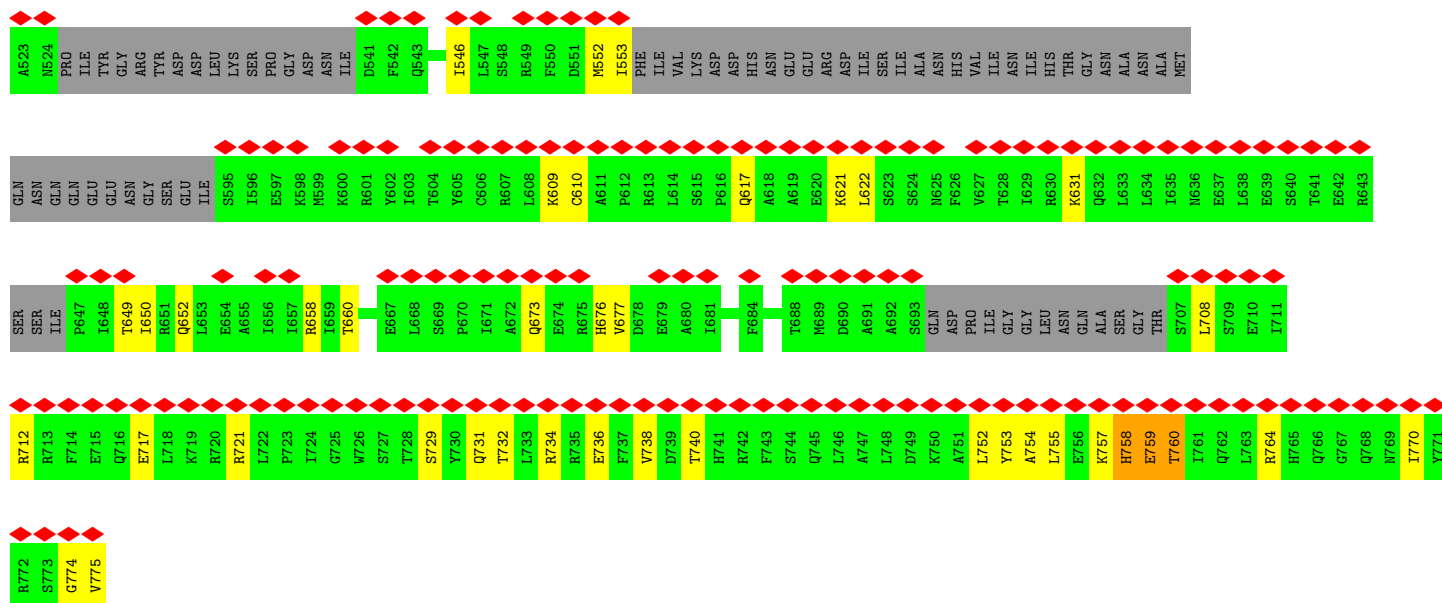


• Molecule 13: DNA replication licensing factor MCM4

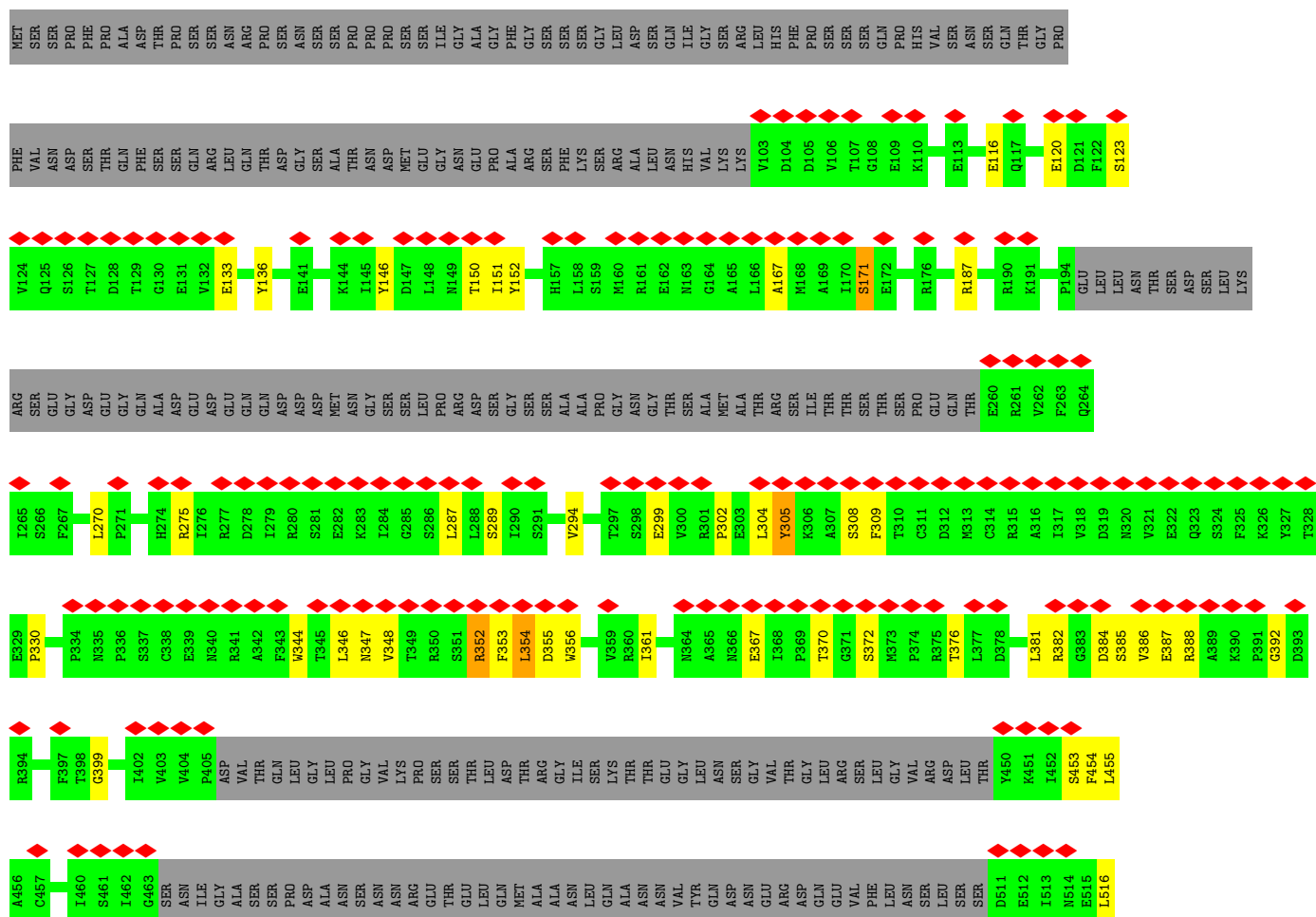


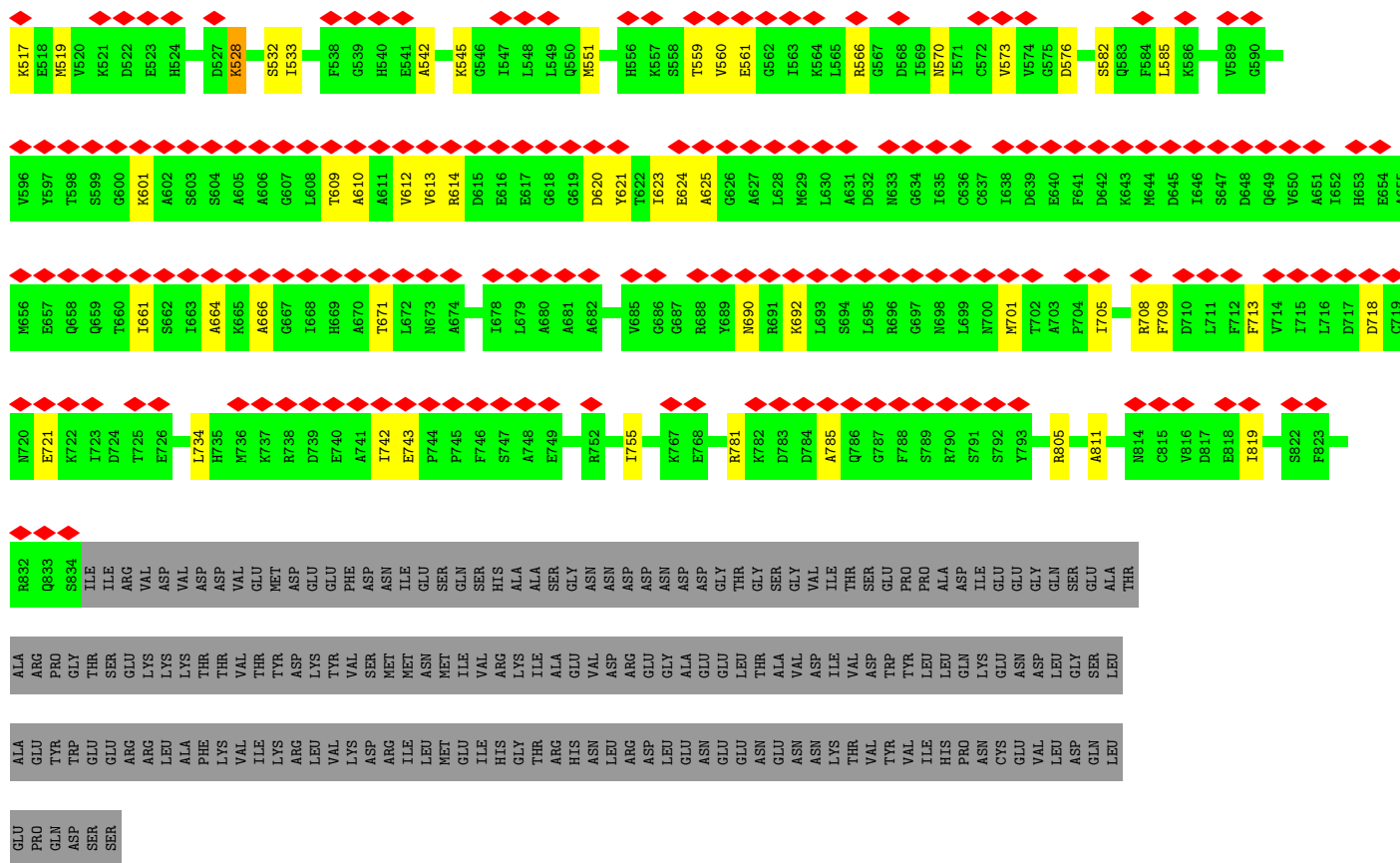
- Molecule 14: Minichromosome maintenance protein 5



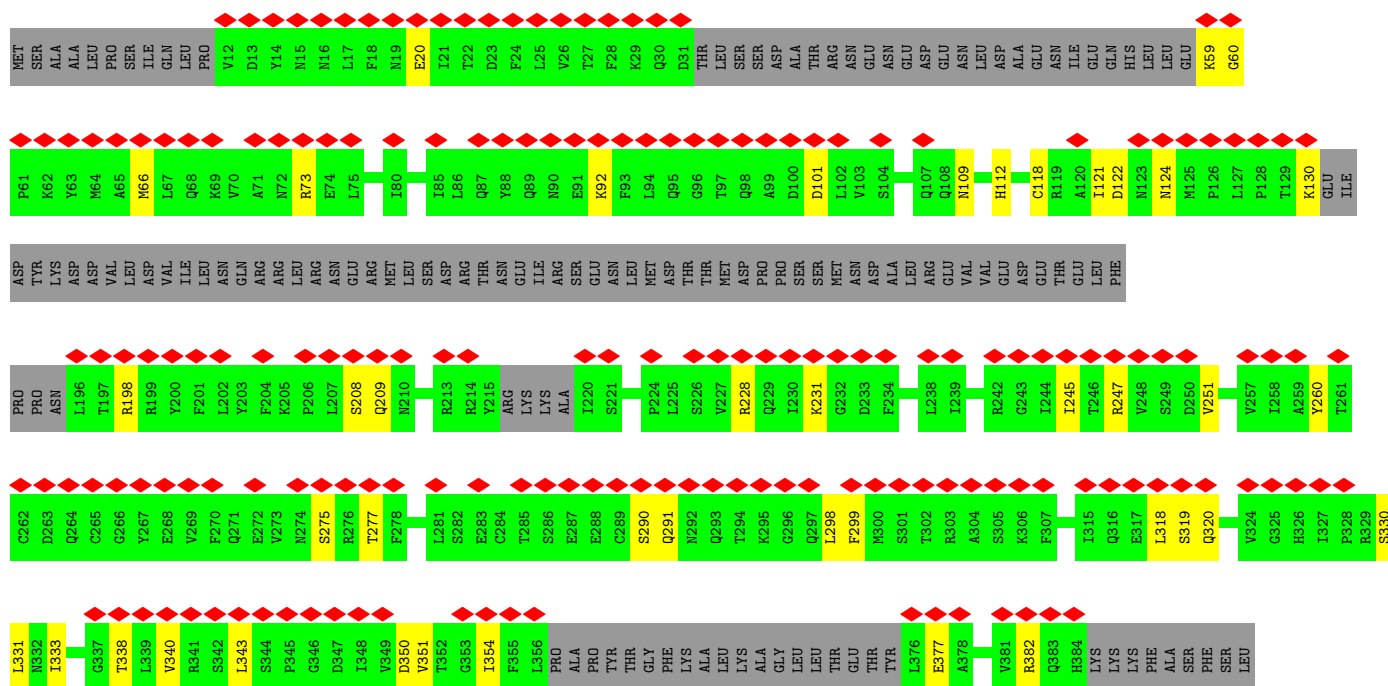


• Molecule 15: DNA replication licensing factor MCM6





● Molecule 16: DNA replication licensing factor MCM7



THR	SER	D396	E399	R400	V401	M402	E403	L404	I405	T406	S407	G408	D409	V410	Y411	M412	R413	L414	A415	K416	S417	I418	E421	G424	D427	V428	K429	K430	A431	L434	L435	L436	V437	G438	G439	V440	D441	K442	R443	V444	G445	D446	G447	M448	K449	I450	R451	G452	D453	I454	M455	V456	M459							
G460	D461	P462	G463	V464	Q468	L469	I473	C474	K475	I476	V481	Y482	T483	T484	G485	K486	G487	S488	S489	G490	V491	G492	L493	T494	A495	A496	V497	M498	K499	D500	P501	V502	T503	D504	E505	M506	I507	L508	Y509	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	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	L589	I590			
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	I642	A643	Y644	A645	K646	T647	K648	R649	P650	V651	M652	S653	E654	A655	V656	N657	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	G691	R694	L695	S696	Q697	A698	L699	A700	K701	L702	R703	L704	A705	D706	M707	V708	D709	I710	D711	D712	V713	E714	A715	L716	L717	R718	L719	V720	R721	V722	S723	K724	E725	S726			
L727	Y728	Q729	GLU	THR	ASN	GLY	ASN	LYS	SER	THR	LYS	GLU	ASP	PHE	VAL	GLU	SER	P740	T741	T742	K743	I744	I747	K750	M751	L752	Q753	E754	T755	G756	K757	N758	T759	L760	E763	N764	I765	V766	R770	L771	R772	G773	F774	T775	M776	L777	Q778	L779	S780	N781	C782	I783	Q784	E785	Y786	S787	Y788	L789	N790	V791
TRP	HIS	LEU	ILE	ASN	GLU	GLY	ASN	LYS	SER	THR	LEU	GLU	ASP	PHE	VAL	GLU	SER	ASP	ASP	GLY	THR	MET	ASP	THR	ASP	GLN	GLU	ASP	SER	LEU	VAL	VAL	VAL	ALA	GLN	ASP	ASP	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	0.22	0/3070	0.65	6/4175 (0.1%)
2	9	0.29	0/3014	0.70	4/4055 (0.1%)
3	A	0.31	0/3415	0.66	4/4596 (0.1%)
4	B	0.28	0/2717	0.60	0/3662
5	C	0.28	0/4602	0.58	0/6212
6	E	0.32	0/3505	0.59	1/4767 (0.0%)
7	D	0.31	0/3612	0.58	2/4879 (0.0%)
8	F	0.23	0/1336	0.59	1/1798 (0.1%)
9	G	0.34	0/923	0.63	0/1425
10	H	0.31	0/958	0.46	0/1474
11	2	0.38	0/4552	0.99	19/6152 (0.3%)
12	3	0.38	0/4944	0.97	20/6718 (0.3%)
13	4	0.42	0/5060	1.01	28/6863 (0.4%)
14	5	0.40	0/4362	0.98	18/5924 (0.3%)
15	6	0.39	0/4550	1.02	16/6148 (0.3%)
16	7	0.37	0/4918	0.96	19/6653 (0.3%)
All	All	0.35	0/55538	0.83	138/75501 (0.2%)

There are no bond length outliers.

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	6	743	GLU	CA-C-N	12.19	132.93	120.38
15	6	743	GLU	C-N-CA	12.19	132.93	120.38
1	8	310	ALA	N-CA-C	11.98	124.34	111.28
15	6	353	PHE	N-CA-C	9.82	123.80	110.55
15	6	136	TYR	N-CA-C	9.52	121.66	111.28
3	A	538	THR	CA-C-N	-9.20	105.88	120.60
3	A	538	THR	C-N-CA	-9.20	105.88	120.60
2	9	282	LEU	CA-C-N	9.19	131.32	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	282	LEU	C-N-CA	9.19	131.32	119.84
15	6	304	LEU	N-CA-C	9.17	122.11	111.11
12	3	223	THR	N-CA-C	9.09	123.72	108.90
1	8	334	THR	N-CA-C	8.90	123.64	111.54
11	2	853	VAL	N-CA-C	-8.13	103.31	111.77
11	2	491	ARG	N-CA-C	8.10	122.67	111.74
3	A	538	THR	N-CA-C	7.85	121.30	110.24
16	7	228	ARG	N-CA-C	-7.78	103.58	113.23
3	A	538	THR	CA-C-O	-7.75	112.63	121.15
16	7	406	THR	N-CA-C	7.74	122.16	112.87
14	5	170	SER	N-CA-C	7.59	119.56	111.28
14	5	171	VAL	N-CA-C	7.58	118.79	108.17
16	7	101	ASP	N-CA-C	7.50	121.37	110.42
11	2	493	ILE	N-CA-C	7.44	122.21	112.76
15	6	721	GLU	N-CA-C	7.39	120.27	111.33
12	3	460	GLY	N-CA-C	7.38	121.59	112.73
11	2	567	THR	N-CA-C	7.36	120.79	108.13
12	3	198	ARG	N-CA-C	7.31	121.75	111.52
12	3	281	ASP	N-CA-C	7.29	119.86	111.11
13	4	208	ILE	N-CA-C	7.05	119.94	113.10
15	6	352	ARG	N-CA-C	6.99	122.58	107.49
11	2	417	VAL	N-CA-C	-6.91	105.90	113.43
13	4	728	TYR	N-CA-C	-6.69	105.16	113.38
13	4	712	VAL	N-CA-C	6.66	118.03	109.30
12	3	667	VAL	N-CA-C	6.65	118.16	108.58
16	7	319	SER	N-CA-C	6.58	118.53	111.36
13	4	777	MET	N-CA-C	-6.57	105.26	113.28
12	3	440	VAL	N-CA-C	-6.55	105.17	113.22
14	5	609	LYS	N-CA-C	6.52	118.27	111.03
1	8	333	SER	N-CA-C	6.51	119.02	108.34
14	5	168	SER	N-CA-C	6.43	119.75	108.75
13	4	573	SER	N-CA-C	6.40	124.43	110.80
16	7	121	ILE	N-CA-C	-6.38	104.05	111.00
14	5	758	HIS	N-CA-C	-6.36	105.59	113.15
16	7	677	SER	CA-C-N	6.32	130.30	120.82
16	7	677	SER	C-N-CA	6.32	130.30	120.82
11	2	206	THR	N-CA-C	-6.30	105.63	113.38
16	7	515	LEU	N-CA-C	-6.27	105.45	113.23
13	4	187	ILE	N-CA-C	6.21	116.26	110.42
14	5	518	SER	N-CA-C	-6.19	101.36	110.52
12	3	715	VAL	N-CA-C	-6.16	103.19	111.44
12	3	487	HIS	N-CA-C	-6.15	104.13	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	411	ILE	N-CA-C	-6.12	104.05	113.16
12	3	360	PHE	N-CA-C	6.07	117.89	111.28
13	4	463	VAL	N-CA-C	6.03	117.50	109.37
11	2	799	SER	N-CA-C	5.95	117.76	111.28
1	8	25	ASP	N-CA-C	-5.94	104.38	111.69
12	3	94	HIS	N-CA-C	5.89	123.34	110.80
11	2	329	GLY	N-CA-C	5.88	119.68	111.10
14	5	76	TYR	N-CA-C	5.87	117.68	111.28
1	8	309	ASP	N-CA-C	5.83	123.22	110.80
13	4	193	ASN	CA-CB-CG	5.83	118.43	112.60
11	2	760	GLN	N-CA-C	5.81	117.62	111.28
16	7	338	THR	N-CA-C	5.79	119.82	112.87
15	6	171	SER	N-CA-C	5.79	119.44	112.38
14	5	760	THR	N-CA-C	-5.72	100.91	109.15
13	4	426	SER	N-CA-C	-5.72	106.64	113.97
12	3	706	ILE	N-CA-C	-5.70	106.75	113.42
13	4	668	ARG	N-CA-C	5.67	119.67	112.87
13	4	630	CYS	N-CA-C	5.65	117.94	108.73
12	3	694	LYS	N-CA-C	5.65	121.87	114.75
11	2	490	ASP	N-CA-C	5.65	119.27	110.17
12	3	280	ASP	CA-C-N	5.64	128.16	120.54
12	3	280	ASP	C-N-CA	5.64	128.16	120.54
11	2	673	ILE	N-CA-C	-5.64	104.76	113.16
15	6	151	ILE	N-CA-C	5.54	118.40	110.09
2	9	232	ASN	CA-C-N	5.54	129.56	121.31
2	9	232	ASN	C-N-CA	5.54	129.56	121.31
16	7	628	LEU	N-CA-C	-5.53	102.01	110.14
13	4	518	LEU	CA-C-N	5.53	128.24	120.28
13	4	518	LEU	C-N-CA	5.53	128.24	120.28
13	4	320	ASN	N-CA-C	-5.51	106.60	113.38
14	5	419	GLY	N-CA-C	-5.50	106.00	111.56
13	4	827	ARG	N-CA-C	-5.49	105.29	111.28
11	2	671	GLU	N-CA-C	5.48	121.92	109.81
13	4	545	PHE	N-CA-C	-5.47	105.33	112.23
15	6	146	TYR	N-CA-C	5.47	119.67	112.89
13	4	693	ASP	N-CA-C	5.44	118.75	111.24
12	3	540	LEU	N-CA-C	-5.44	105.38	112.23
14	5	546	ILE	N-CA-C	-5.42	106.41	111.45
15	6	354	LEU	N-CA-C	5.42	116.37	108.14
7	D	341	ILE	CA-C-N	5.40	124.65	120.33
7	D	341	ILE	C-N-CA	5.40	124.65	120.33
15	6	785	ALA	CA-C-N	5.39	129.78	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	6	785	ALA	C-N-CA	5.39	129.78	122.07
14	5	154	GLU	CA-C-N	5.38	129.76	122.07
14	5	154	GLU	C-N-CA	5.38	129.76	122.07
12	3	693	LYS	N-CA-C	5.38	119.54	111.96
6	E	223	GLN	N-CA-C	-5.35	101.44	109.15
16	7	592	SER	N-CA-C	-5.33	105.52	112.23
14	5	424	GLN	N-CA-C	-5.30	107.36	113.88
16	7	112	HIS	N-CA-C	-5.30	105.96	112.90
15	6	528	LYS	N-CA-C	-5.29	106.67	113.23
16	7	424	GLY	CA-C-N	5.26	129.88	122.46
16	7	424	GLY	C-N-CA	5.26	129.88	122.46
12	3	677	ASN	N-CA-C	5.26	117.01	111.28
14	5	610	CYS	N-CA-C	5.26	118.30	110.52
11	2	601	LYS	N-CA-C	-5.25	107.25	113.97
16	7	510	GLY	N-CA-C	5.25	119.26	111.18
14	5	241	TYR	N-CA-C	5.22	118.73	109.96
13	4	428	ARG	CA-C-N	5.22	128.51	121.05
13	4	428	ARG	C-N-CA	5.22	128.51	121.05
12	3	359	ILE	N-CA-C	5.21	115.43	110.53
13	4	203	TYR	N-CA-C	5.21	118.39	111.30
16	7	488	SER	CA-C-N	5.21	127.98	120.38
16	7	488	SER	C-N-CA	5.21	127.98	120.38
11	2	415	VAL	CA-C-N	5.21	129.73	122.08
11	2	415	VAL	C-N-CA	5.21	129.73	122.08
13	4	251	TYR	CA-C-N	5.21	127.78	120.28
13	4	251	TYR	C-N-CA	5.21	127.78	120.28
14	5	759	GLU	CA-C-N	-5.19	113.56	121.66
14	5	759	GLU	C-N-CA	-5.19	113.56	121.66
12	3	560	SER	N-CA-C	5.19	119.71	113.17
15	6	385	SER	N-CA-C	-5.18	106.96	113.28
13	4	620	ALA	N-CA-C	5.16	121.79	110.80
1	8	391	LEU	N-CA-C	5.15	116.65	108.67
16	7	456	VAL	N-CA-C	5.14	115.37	108.17
16	7	544	GLN	N-CA-C	5.14	121.75	110.80
13	4	700	SER	N-CA-C	-5.12	105.77	112.23
11	2	207	ILE	CA-C-N	5.11	127.44	120.54
11	2	207	ILE	C-N-CA	5.11	127.44	120.54
13	4	520	SER	N-CA-C	-5.08	107.63	113.88
13	4	582	HIS	N-CA-C	-5.07	106.35	112.54
14	5	56	VAL	N-CA-C	-5.07	108.03	112.90
15	6	356	TRP	CA-CB-CG	5.06	123.22	113.60
11	2	617	ARG	N-CA-C	-5.04	105.45	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	3	238	GLY	N-CA-C	5.03	125.09	113.18
11	2	385	TYR	N-CA-C	5.00	117.73	109.72
13	4	711	LYS	CA-C-N	5.00	128.00	120.69
13	4	711	LYS	C-N-CA	5.00	128.00	120.69

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	113	0
2	9	2972	0	3082	87	0
3	A	3368	0	3420	70	0
4	B	2663	0	2673	51	0
5	C	4505	0	4458	71	0
6	E	3425	0	3402	66	0
7	D	3551	0	3615	83	0
8	F	1315	0	1353	27	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	97	0
13	4	4995	0	4751	107	0
14	5	4317	0	4060	73	0
15	6	4475	0	4414	76	0
16	7	4858	0	4803	74	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	1012	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 (1012) 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
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
11:2:332:PRO:C	11:2:383:ARG:CB	2.55	0.80
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
11:2:335: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
11:2:569:GLN:H	11:2:569:GLN:CD	1.98	0.71
14:5:452:SER:HB2	14:5:465:GLU:HB2	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:8:321:CYS:HG	1:8:371:TYR:HH	1.38	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
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
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
13:4:812:LYS:O	13:4:812:LYS:HG2	1.95	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
15:6:354:LEU:C	15:6:354:LEU:HD12	2.23	0.64
13:4:379:PRO:O	13:4:380:ASN:ND2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:5:770:ILE:O	14:5:774:GLY:N	2.31	0.64
1:8:346:GLN:CB	11:2:301:PRO:C	2.71	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
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
12:3:386:MET:HE1	12:3:714:LYS:HB3	1.82	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
16:7:498:MET:HE2	16:7:509:GLU:OE1	2.01	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
1:8:142:CYS:O	1:8:265:PRO:HD3	2.00	0.61
15:6:551:MET:HE2	15:6:755:ILE:HD13	1.83	0.61
16:7:508:LEU:CD2	16:7:553:ILE:CD1	2.78	0.61
6:E:435:THR:HG21	6:E:442:ASP:CG	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:198:ARG:O	12:3:198:ARG:HG2	2.01	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
12:3:442:LEU:HB3	12:3:461:ALA:HB3	1.83	0.59
12:3:928:PRO:O	12:3:932:LYS:NZ	2.34	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
2:9:300:VAL:HG12	2:9:304:MET:HE2	1.83	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:8:302:LEU:C	1:8:304:ILE:H	2.13	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
11:2:411:LEU:C	11:2:411:LEU:HD12	2.30	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
16:7:260:TYR:HB3	16:7:298:LEU:HD12	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:5:757:LYS:C	14:5:759:GLU:H	2.14	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
8:F:326:ASN:HB2	8:F:370:LYS:HZ3	1.74	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
3:A:543:MET:HA	3:A:546:LEU:HB2	1.91	0.53
11:2:544:ASP:O	11:2:549:LYS:NZ	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:884:MET:HE3	3:A:886:ASN:H	1.74	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
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
1:8:375:LEU:HD12	1:8:380:GLU:C	2.35	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
14:5:729:SER:H	14:5:775:VAL:C	2.17	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
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:421:THR:OG1	3:A:422:ILE:N	2.39	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
16:7:747:ILE:HA	16:7:750:LYS:HZ2	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:9:491: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
13:4:622:VAL:CG2	13:4:665:LEU:HD13	2.39	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
6:E:439:LYS:NZ	7:D:491:GLN:OE1	2.41	0.51
2:9:495:MET:SD	2:9:495:MET:N	2.82	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
2:9:226:ASP:OD1	2:9:226:ASP:N	2.43	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
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
1:8:351:MET:C	1:8:353:ARG:H	2.18	0.50
1:8:360:ILE:HG21	1:8:383:MET:HE1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
16:7:751:MET:SD	16:7:751:MET:C	2.94	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:90:ILE:O	7:D:93:LYS:NZ	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
12:3:493:GLN:C	12:3:494:THR:HG23	2.38	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
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
5:C:569:LEU:O	5:C:572:THR:OG1	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:8:359:ASP:OD1	1:8:362:LYS:NZ	2.37	0.48
2:9:500:ASP:OD1	2:9:500:ASP:N	2.45	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
15:6:551:MET:HE1	15:6:755:ILE:CD1	2.42	0.48
16:7:776:MET:O	16:7:780:SER:OG	2.29	0.48
1:8:375:LEU:HD11	1:8:379:GLY:C	2.38	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
16:7:653:SER:OG	16:7:654:GLU:N	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:4:573:SER:O	13:4:576:GLN:HB2	2.14	0.48
15:6:354:LEU:C	15:6:354:LEU:CD1	2.86	0.48
1:8:302:LEU:C	1:8:304:ILE:N	2.71	0.47
2:9:495:MET:HA	2:9:498:PHE:HB2	1.96	0.47
5:C:423:ASN:O	5:C:439:TYR:OH	2.32	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
3:A:486:THR:OG1	17:A:2001:AGS:O3G	2.31	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
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
1:8:25:ASP:C	1:8:26:GLU:HG2	2.38	0.47
5:C:441:ASP:OD1	5:C:441:ASP:N	2.46	0.47
13:4:695:PRO:HA	13:4:696:PRO:HD3	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:2:670:THR:OG1	11:2:671:GLU:N	2.46	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
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
14:5:499:GLN:C	14:5:501:THR:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:620:THR:OG1	3:A:621:ARG:N	2.43	0.46
4:B:300:MET:HE2	8:F:402:LEU:HG	1.96	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
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
12:3:386:MET:HE2	12:3:386:MET:HB2	1.81	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
3:A:602:MET:HE2	3:A:602:MET:HB2	1.81	0.46
5:C:246:ASN:O	5:C:250:ASN:ND2	2.47	0.46
5:C:324:SER:O	5:C:327:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:45:TYR:HB2	17:E:2001:AGS:H3'	1.98	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
3:A:422:ILE:HG22	3:A:682:LEU:HD22	1.98	0.46
5:C:306:MET:HE3	5:C:306:MET:HB3	1.74	0.46
14:5:622:LEU:CD1	14:5:677:VAL:CG1	2.93	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
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
1:8:153:THR:OG1	1:8:257:ILE:O	2.30	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
13:4:386:HIS:C	13:4:388:ARG:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:B:495:VAL:HG13	4:B:497:LYS:H	1.82	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
7:D:284:MET:HE1	7:D:327:ASN:HD22	1.82	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
11:2:782:ASP:OD1	11:2:782:ASP:N	2.49	0.44
12:3:922:ARG:HD3	12:3:922:ARG:HA	1.85	0.44
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:85:ALA:O	5:C:88:SER:OG	2.32	0.44
5:C:363:PHE:O	5:C:367:LEU:N	2.51	0.44
2:9:409:LYS:O	2:9:415:LYS:NZ	2.39	0.43
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
2:9:432:THR:HG1	2:9:435:GLU:H	1.63	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
6:E:346:ASP:OD1	6:E:346:ASP:N	2.50	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
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
15:6:361:ILE:O	15:6:376:THR:OG1	2.33	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
3:A:855:ASP:OD1	3:A:855:ASP:N	2.50	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
12:3:220:THR:C	12:3:222:THR:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:567:LEU:HD23	5:C:567:LEU:HA	1.89	0.43
12:3:220:THR:C	12:3:222:THR:N	2.75	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
16:7:415:ALA:O	16:7:429:LYS:NZ	2.45	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
2:9:315:MET:HE3	2:9:315:MET:HB3	1.93	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
1:8:73:PHE:HA	1:8:92:TYR:HA	2.00	0.42
12:3:463:VAL:O	12:3:463:VAL:HG12	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
15:6:551:MET:HE1	15:6:755:ILE:HD13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:100:ARG:NH2	5:C:227:PHE:O	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
5:C:437:ASP:OD1	5:C:437:ASP:N	2.52	0.42
7:D:514:ARG:HH11	7:D:527:THR:HG1	1.66	0.42
8:F:301:LYS:HZ1	8:F:378:TRP:CD1	2.37	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
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
1:8:130: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
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
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
12:3:211:TYR:O	12:3:211:TYR:CG	2.72	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
7:D:189:ASP:HB2	7:D:237:MET:HE1	2.02	0.42
7:D:312:GLU:O	7:D:318:SER:OG	2.34	0.42
12:3:350:ILE:O	12:3:354:SER:OG	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:3:375:ASP:HA	12:3:378:LYS:HZ2	1.85	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
8:F:378:TRP:CD1	8:F:378:TRP:H	2.36	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
15:6:519:MET:HE3	15:6:519:MET:HB2	1.95	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
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
15:6:701:MET:HE3	15:6:705:ILE:HG13	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:8:298:TYR:O	1:8:300:ARG:N	2.53	0.41
2:9:63:GLN:O	2:9:66:SER:OG	2.33	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
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
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
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
16:7:330:SER:OG	16:7:331:LEU:N	2.52	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
8:F:422:LYS:HB3	8:F:423:LYS:HZ2	1.86	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
3:A:905:MET:HE3	3:A:905:MET:HB3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:ARG:O	5:C:100:ARG:NE	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
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
13:4:637:MET:HE1	13:4:645:LEU:HD21	2.02	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
3:A:780:LYS:HZ3	3:A:780:LYS:HG2	1.74	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
13:4:637:MET:HE2	13:4:637:MET:HB3	1.86	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
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
15:6:661:ILE:O	15:6:671:THR:HA	2.21	0.40
16:7:66:MET:HE3	16:7:66:MET:HB3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:6:354:LEU:HD12	15:6:354:LEU:O	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
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
12:3:914: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
14:5:410:ILE:HD12	14:5:552:MET:HE1	2.03	0.40
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%)	11	46
2	9	363/513 (71%)	319 (88%)	42 (12%)	2 (1%)	21	59
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%)	43	78
6	E	414/479 (86%)	385 (93%)	28 (7%)	1 (0%)	43	78
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%)	18	56
12	3	626/971 (64%)	582 (93%)	40 (6%)	4 (1%)	21	59
13	4	651/933 (70%)	603 (93%)	45 (7%)	3 (0%)	24	63
14	5	579/775 (75%)	552 (95%)	24 (4%)	3 (0%)	24	63
15	6	568/1017 (56%)	538 (95%)	28 (5%)	2 (0%)	30	67
16	7	623/845 (74%)	595 (96%)	25 (4%)	3 (0%)	24	63
All	All	6614/10118 (65%)	6183 (94%)	404 (6%)	27 (0%)	31	67

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	329 (100%)	0	100	100
2	9	338/470 (72%)	338 (100%)	0	100	100
3	A	370/812 (46%)	370 (100%)	0	100	100
4	B	298/573 (52%)	298 (100%)	0	100	100
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%)	402 (100%)	0	100	100
8	F	151/406 (37%)	151 (100%)	0	100	100
11	2	479/770 (62%)	479 (100%)	0	100	100
12	3	512/835 (61%)	512 (100%)	0	100	100
13	4	519/848 (61%)	519 (100%)	0	100	100
14	5	431/688 (63%)	431 (100%)	0	100	100
15	6	475/886 (54%)	475 (100%)	0	100	100
16	7	525/753 (70%)	525 (100%)	0	100	100
All	All	5721/9090 (63%)	5721 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123)

such sidechains are listed below:

Mol	Chain	Res	Type
1	8	108	ASN
1	8	147	HIS
1	8	217	ASN
1	8	250	GLN
1	8	256	ASN
1	8	281	HIS
1	8	285	GLN
1	8	412	GLN
2	9	90	ASN
2	9	206	GLN
2	9	295	GLN
2	9	388	ASN
2	9	400	ASN
3	A	454	ASN
3	A	530	ASN
3	A	882	GLN
4	B	279	ASN
4	B	282	ASN
4	B	297	GLN
4	B	310	GLN
4	B	364	ASN
4	B	405	GLN
4	B	414	GLN
4	B	425	HIS
4	B	426	ASN
4	B	458	HIS
4	B	472	ASN
4	B	532	GLN
4	B	535	ASN
4	B	585	HIS
5	C	19	GLN
5	C	63	GLN
5	C	65	HIS
5	C	69	HIS
5	C	78	ASN
5	C	159	HIS
5	C	231	HIS
5	C	243	ASN
5	C	253	GLN
5	C	309	ASN
5	C	400	ASN
5	C	477	GLN

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Mol	Chain	Res	Type
5	C	523	GLN
5	C	586	GLN
6	E	52	ASN
6	E	58	HIS
6	E	114	ASN
6	E	193	ASN
6	E	238	ASN
6	E	245	GLN
6	E	277	ASN
6	E	320	GLN
6	E	391	GLN
7	D	80	GLN
7	D	126	GLN
7	D	149	GLN
7	D	158	HIS
7	D	270	GLN
7	D	277	GLN
7	D	321	ASN
7	D	327	ASN
7	D	371	GLN
7	D	409	ASN
7	D	423	ASN
7	D	480	ASN
7	D	511	GLN
8	F	307	ASN
8	F	309	ASN
8	F	318	GLN
8	F	326	ASN
11	2	245	ASN
11	2	248	HIS
11	2	384	ASN
11	2	508	HIS
11	2	551	GLN
11	2	651	ASN
12	3	46	GLN
12	3	210	HIS
12	3	269	GLN
12	3	293	ASN
12	3	324	ASN
12	3	351	ASN
12	3	507	ASN
12	3	517	ASN

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Mol	Chain	Res	Type
12	3	691	ASN
12	3	924	ASN
12	3	950	ASN
13	4	193	ASN
13	4	247	ASN
13	4	253	GLN
13	4	380	ASN
13	4	395	GLN
13	4	543	GLN
13	4	579	GLN
13	4	646	HIS
13	4	652	GLN
13	4	691	ASN
13	4	738	GLN
13	4	808	HIS
13	4	815	ASN
14	5	43	GLN
14	5	49	GLN
14	5	67	HIS
14	5	145	GLN
14	5	203	ASN
14	5	254	GLN
14	5	411	ASN
14	5	625	ASN
14	5	676	HIS
15	6	524	HIS
15	6	556	HIS
15	6	570	ASN
15	6	720	ASN
15	6	750	GLN
16	7	68	GLN
16	7	108	GLN
16	7	210	ASN
16	7	271	GLN
16	7	336	ASN
16	7	379	GLN
16	7	425	ASN
16	7	568	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 ⓘ

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 ⓘ

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	-	32,33,33	1.05	3 (9%)	45,52,52	0.94	1 (2%)
17	AGS	9	2001	-	32,33,33	0.87	2 (6%)	45,52,52	0.89	1 (2%)
17	AGS	E	2001	-	32,33,33	0.93	2 (6%)	45,52,52	0.74	1 (2%)
17	AGS	D	2001	-	32,33,33	1.24	3 (9%)	45,52,52	1.08	1 (2%)

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	-	-	7/21/38/38	0/3/3/3
17	AGS	9	2001	-	-	7/21/38/38	0/3/3/3
17	AGS	E	2001	-	-	7/21/38/38	0/3/3/3
17	AGS	D	2001	-	-	2/21/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	2001	AGS	PB-O3B	-3.98	1.55	1.59
17	D	2001	AGS	PB-O3A	-3.88	1.55	1.59
17	A	2001	AGS	PB-O3B	-3.65	1.55	1.59
17	E	2001	AGS	PB-O3A	-3.64	1.55	1.59
17	D	2001	AGS	PA-O3A	-3.41	1.55	1.59
17	9	2001	AGS	PB-O3A	-3.16	1.56	1.59
17	A	2001	AGS	PB-O3A	-2.91	1.56	1.59
17	A	2001	AGS	PA-O3A	-2.87	1.56	1.59
17	E	2001	AGS	PA-O3A	-2.71	1.56	1.59
17	9	2001	AGS	PB-O3B	-2.36	1.57	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	2001	AGS	PB-O3B-PG	-6.59	109.04	133.17
17	A	2001	AGS	PB-O3B-PG	-5.36	113.56	133.17
17	9	2001	AGS	PB-O3B-PG	-4.85	115.42	133.17
17	E	2001	AGS	PB-O3B-PG	-3.39	120.77	133.17

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	C5'-O5'-PA-O3A
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	E	2001	AGS	O4'-C4'-C5'-O5'
17	9	2001	AGS	O4'-C4'-C5'-O5'
17	9	2001	AGS	C3'-C4'-C5'-O5'
17	E	2001	AGS	C3'-C4'-C5'-O5'
17	A	2001	AGS	O4'-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

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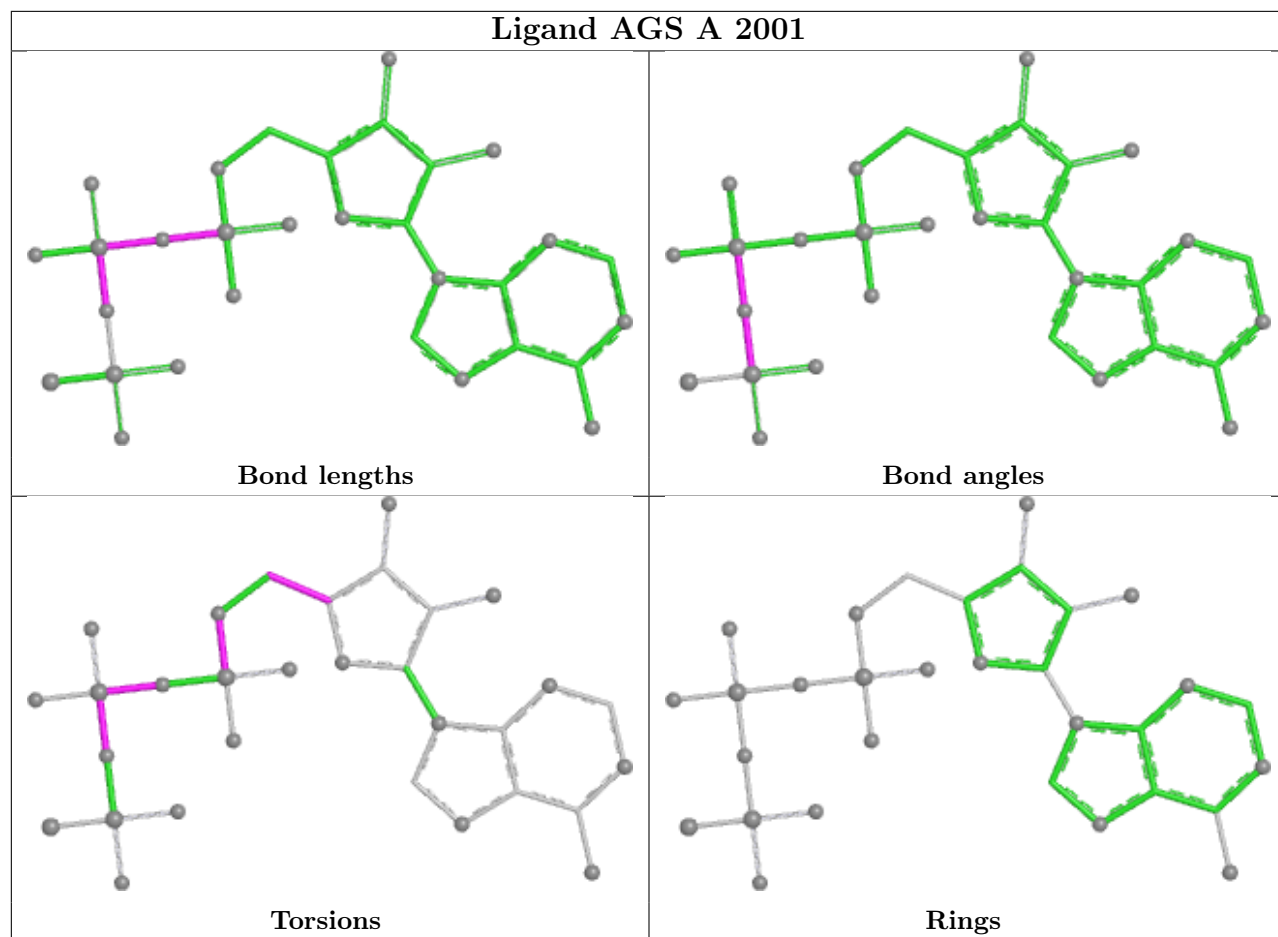
Mol	Chain	Res	Type	Atoms
17	D	2001	AGS	C3'-C4'-C5'-O5'
17	A	2001	AGS	PA-O3A-PB-O1B
17	9	2001	AGS	PB-O3A-PA-O2A
17	E	2001	AGS	PA-O3A-PB-O1B
17	A	2001	AGS	C3'-C4'-C5'-O5'

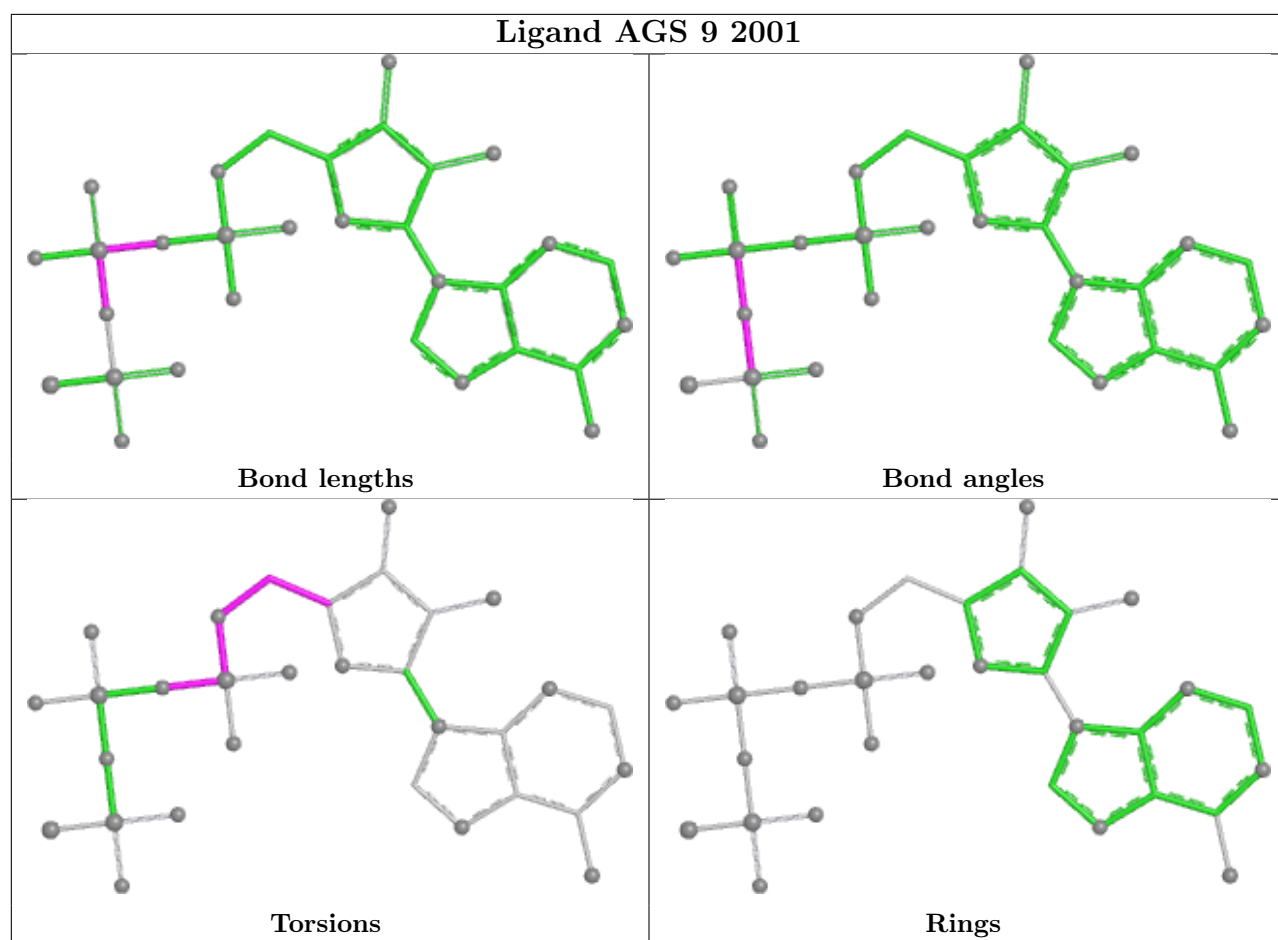
There are no ring outliers.

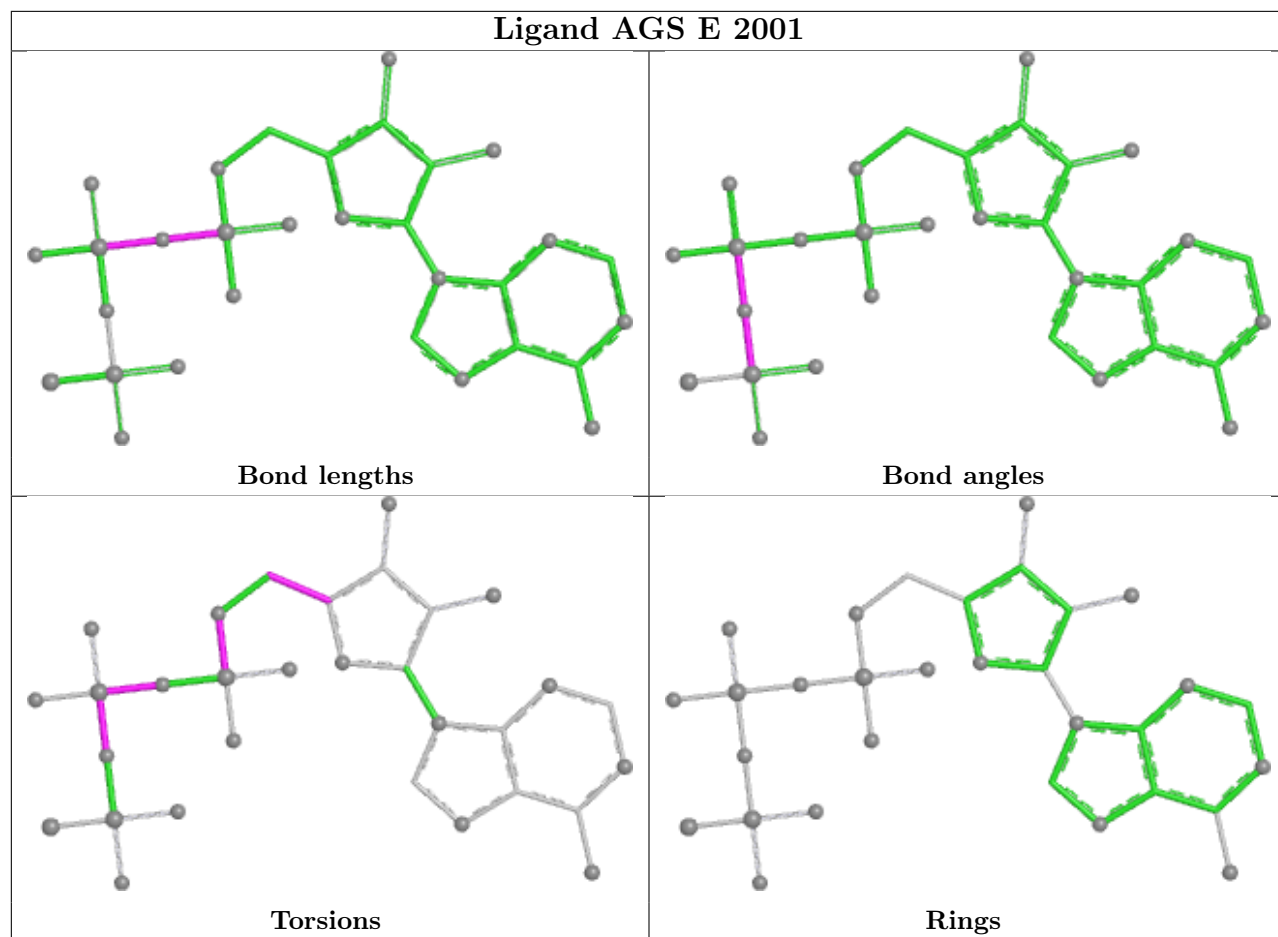
4 monomers are involved in 20 short contacts:

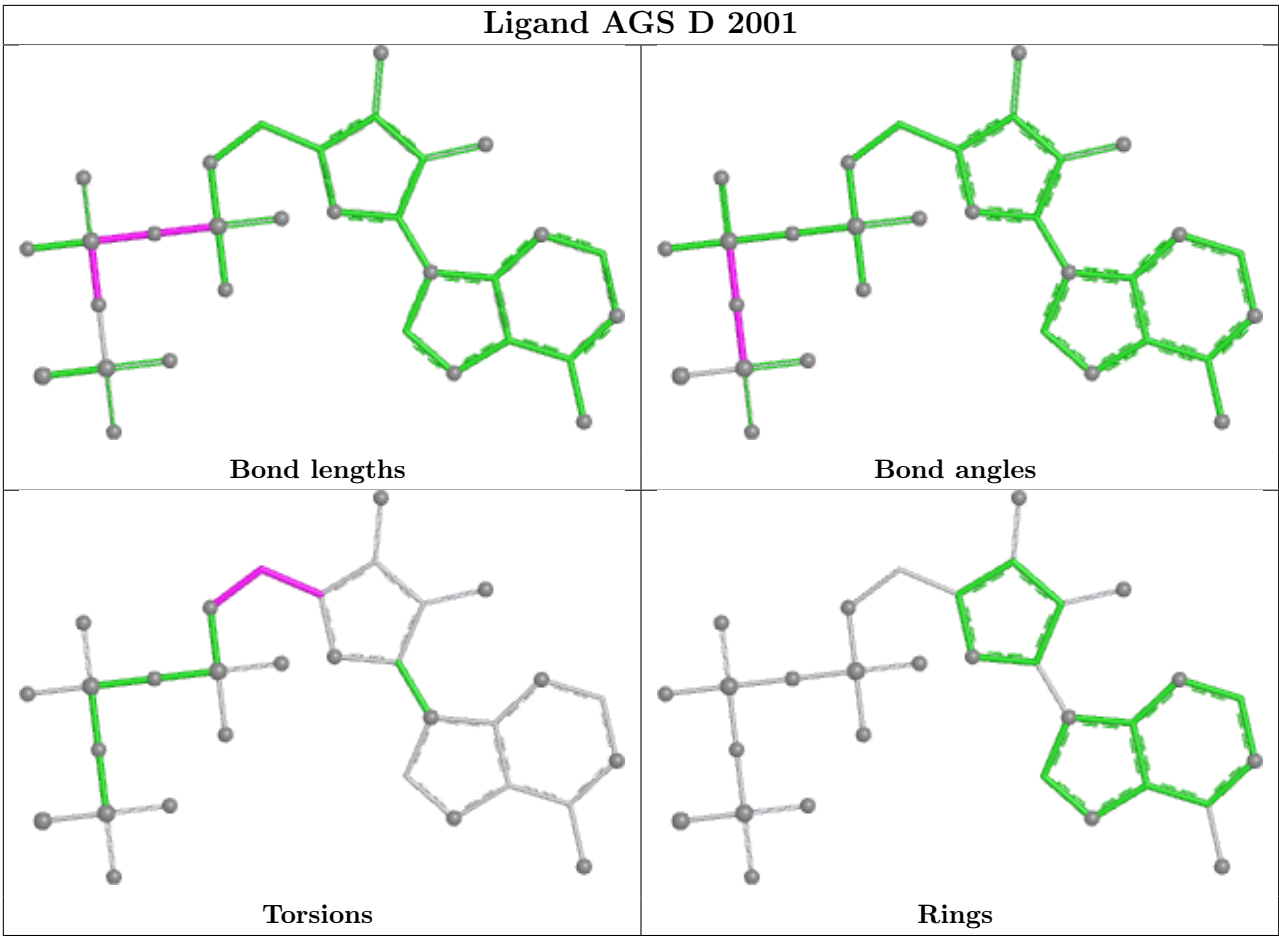
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	2001	AGS	7	0
17	9	2001	AGS	4	0
17	E	2001	AGS	5	0
17	D	2001	AGS	4	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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

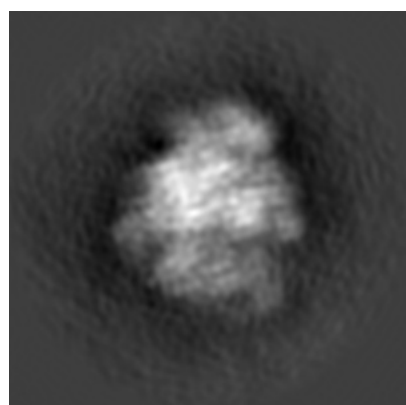
6 Map visualisation [i](#)

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.

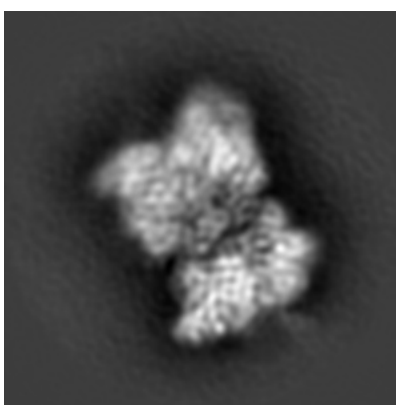
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

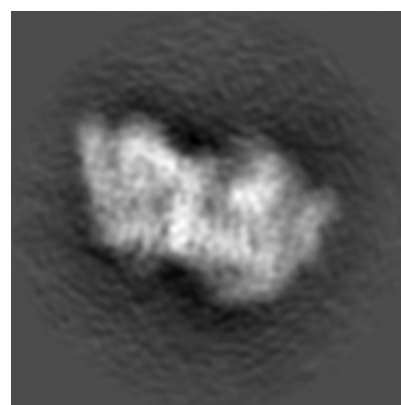
6.1.1 Primary map



X



Y

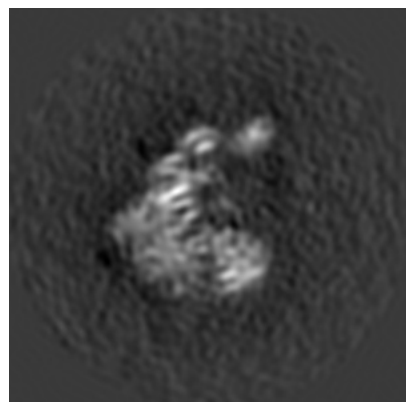


Z

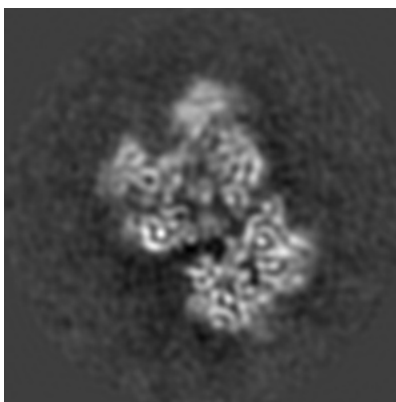
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

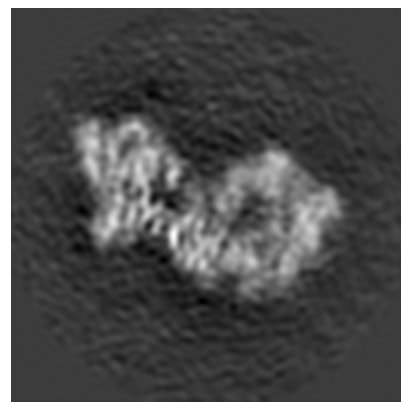
6.2.1 Primary map



X Index: 128



Y Index: 128

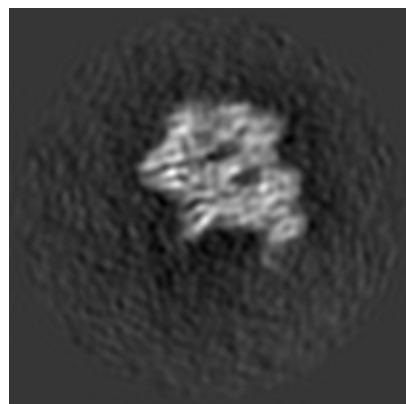


Z Index: 128

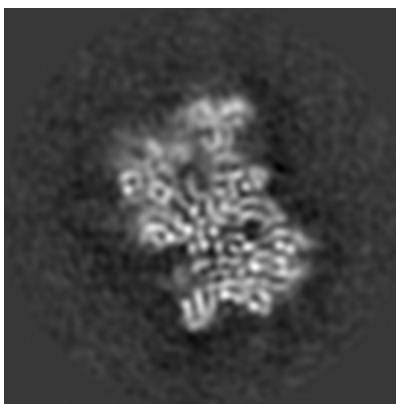
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

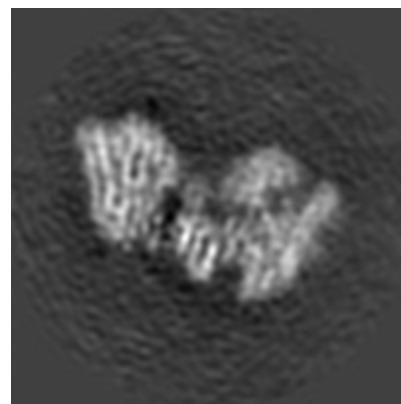
6.3.1 Primary map



X Index: 86



Y Index: 113

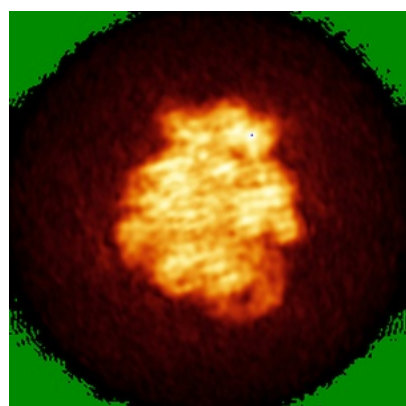


Z Index: 134

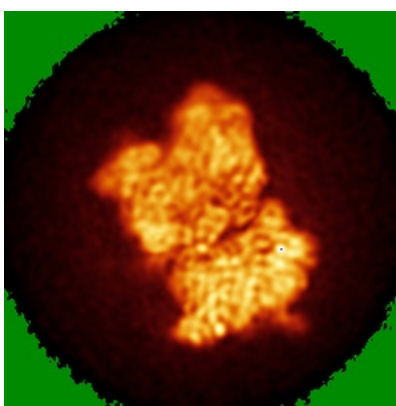
The images above show the largest variance slices of the map in three orthogonal directions.

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

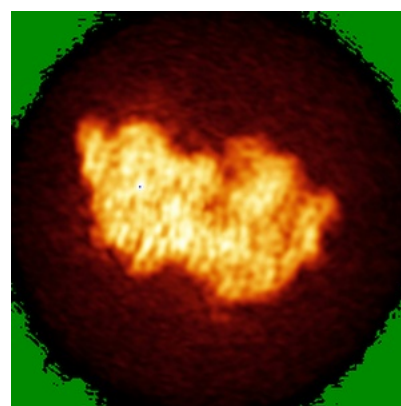
6.4.1 Primary map



X



Y

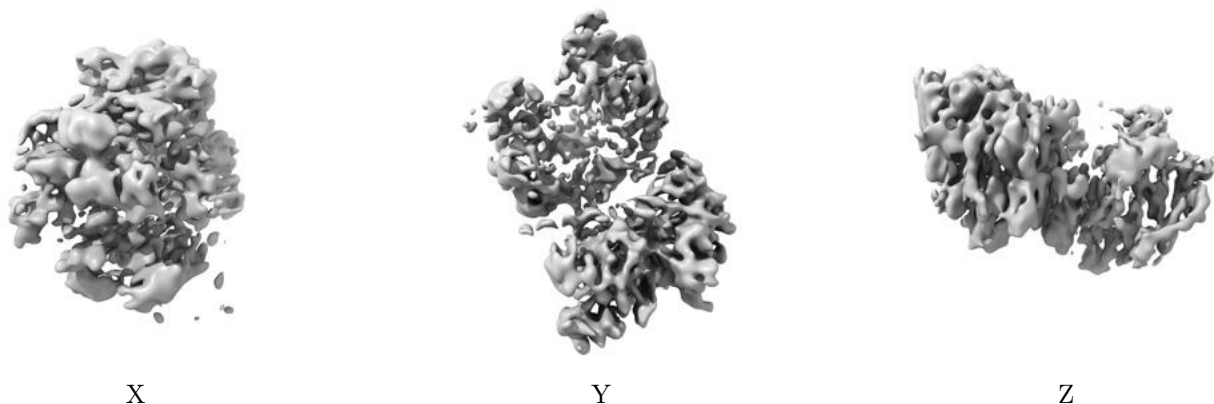


Z

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.

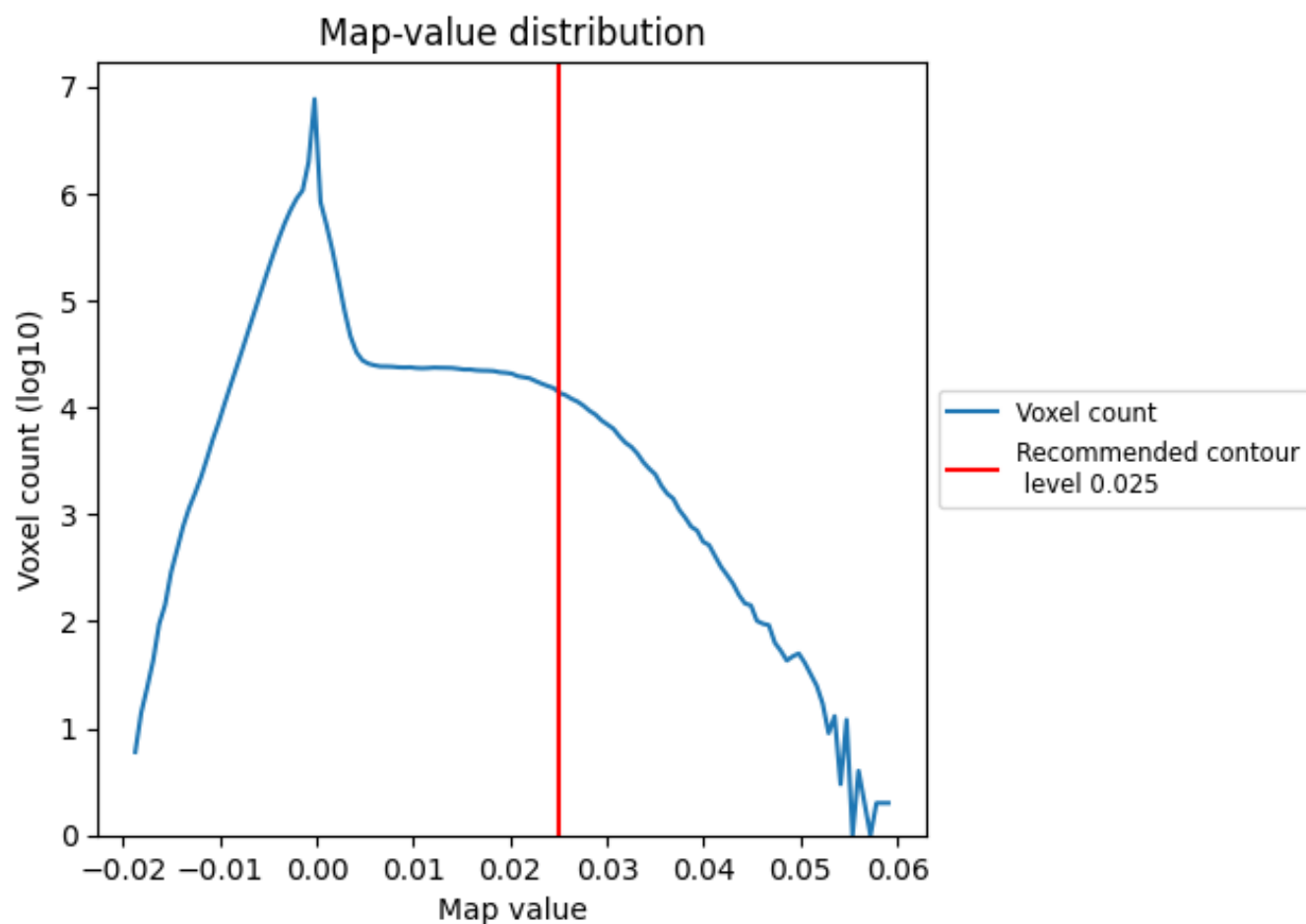
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

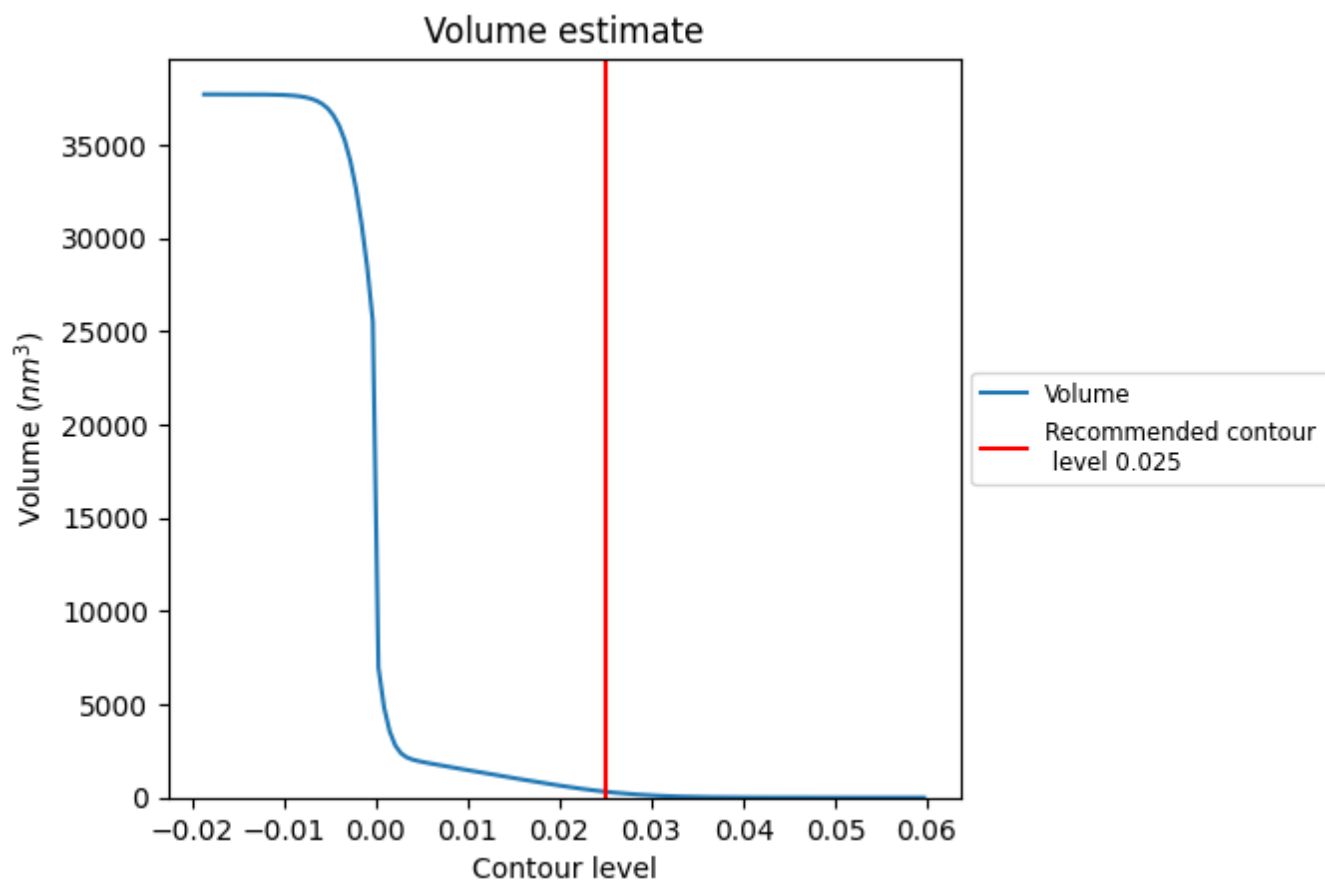
This section contains the results of statistical analysis of the map.

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.

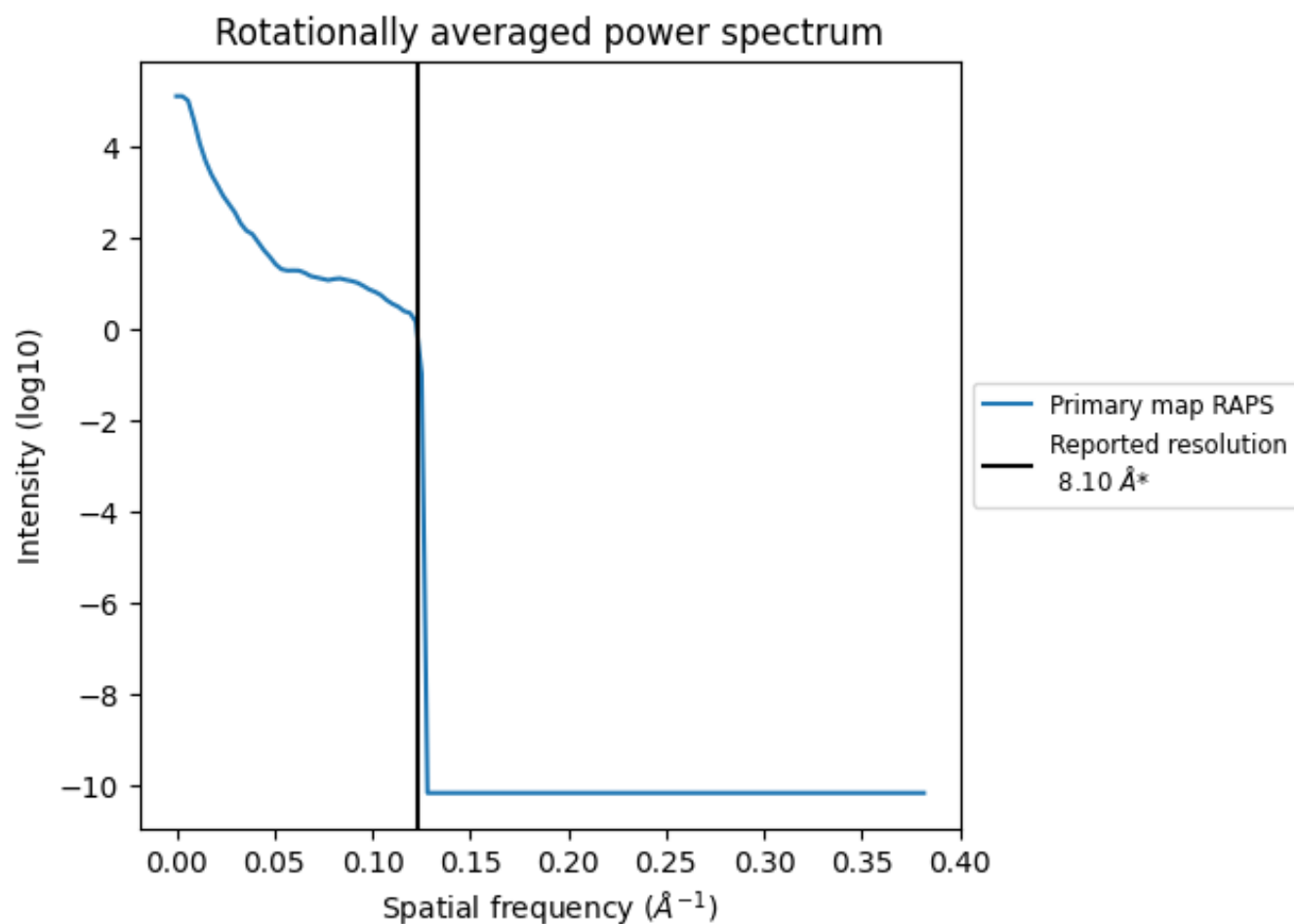
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.123 Å⁻¹

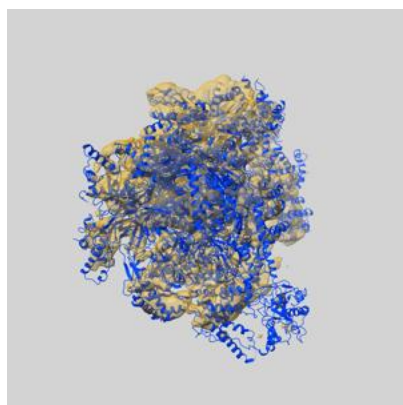
8 Fourier-Shell correlation

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

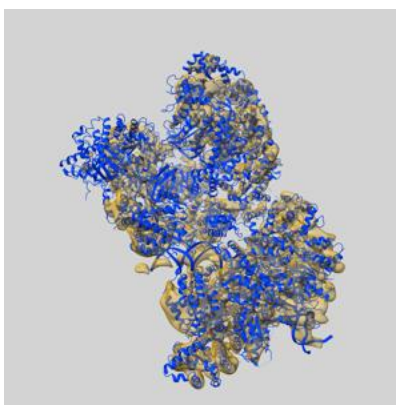
9 Map-model fit [i](#)

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

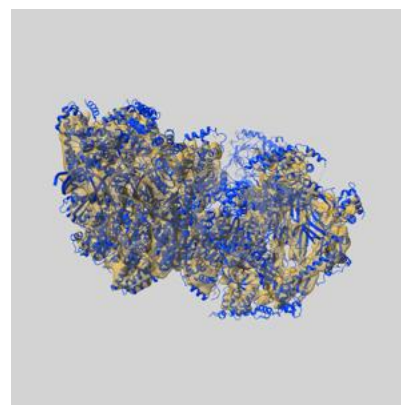
9.1 Map-model overlay [i](#)



X



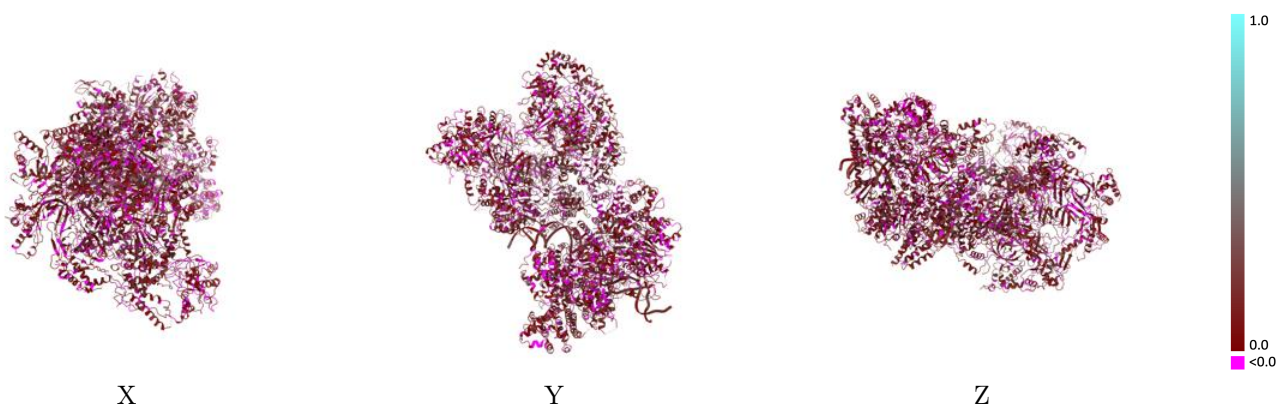
Y



Z

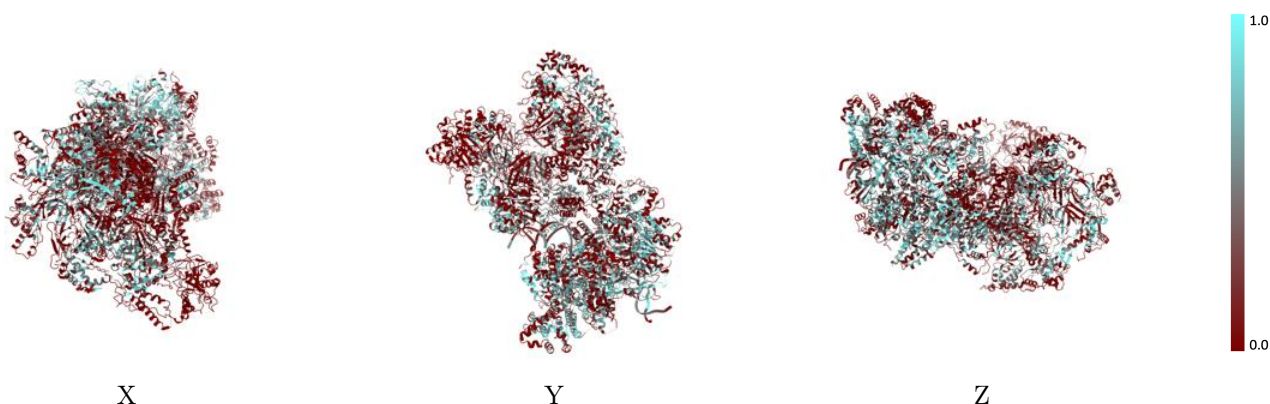
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



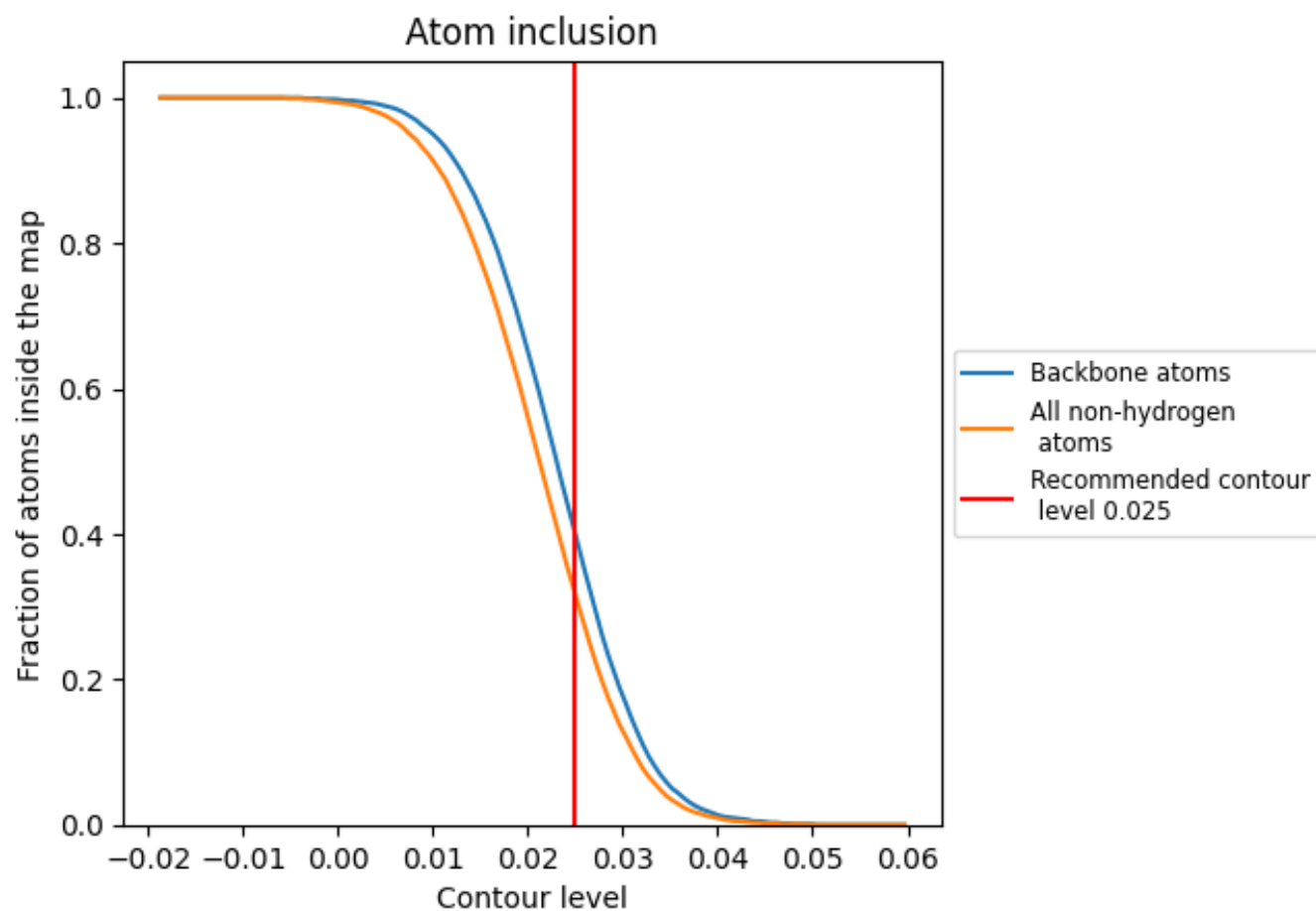
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

