



Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 03:09 PM 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

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.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

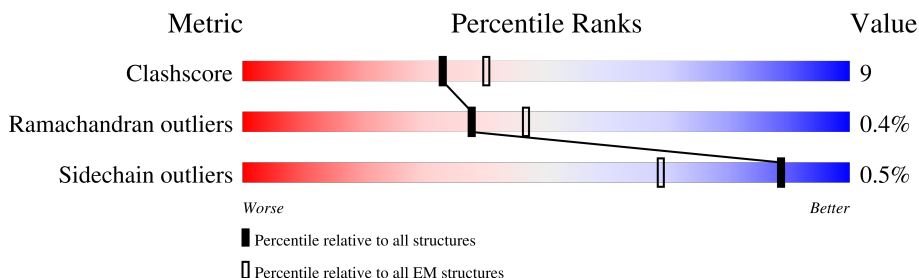
1 Overall quality at a glance

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)
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 ≥ 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> <div>61%</div> <div> <div>41%</div> <div>23%</div> <div>36%</div> </div> </div>
2	9	513	<div> <div>46%</div> <div> <div>50%</div> <div>22%</div> <div>27%</div> </div> </div>
3	A	913	<div> <div>23%</div> <div> <div>38%</div> <div>9%</div> <div>54%</div> </div> </div>
4	B	620	<div> <div>31%</div> <div> <div>40%</div> <div>13%</div> <div>47%</div> </div> </div>
5	C	616	<div> <div>41%</div> <div> <div>71%</div> <div>17%</div> <div>12%</div> </div> </div>
6	E	479	<div> <div>45%</div> <div> <div>68%</div> <div>20%</div> <div>12%</div> </div> </div>
7	D	529	<div> <div>40%</div> <div> <div>62%</div> <div>20%</div> <div>18%</div> </div> </div>
8	F	435	<div> <div>26%</div> <div> <div>28%</div> <div>8%</div> <div>64%</div> </div> </div>

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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

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		

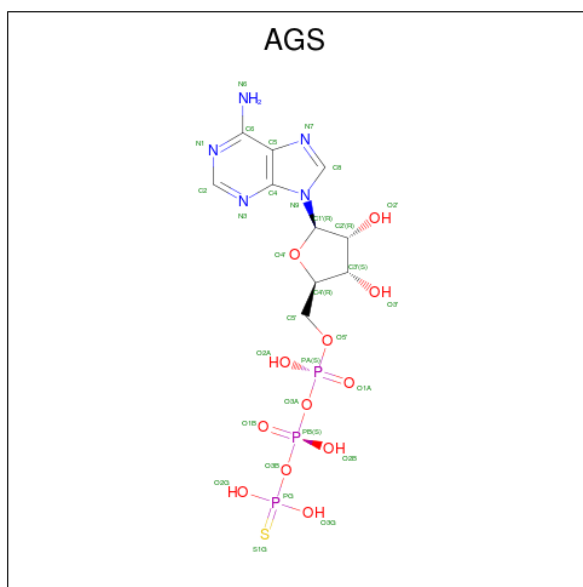
- Molecule 15 is a protein called DNA replication licensing factor MCM6.

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.

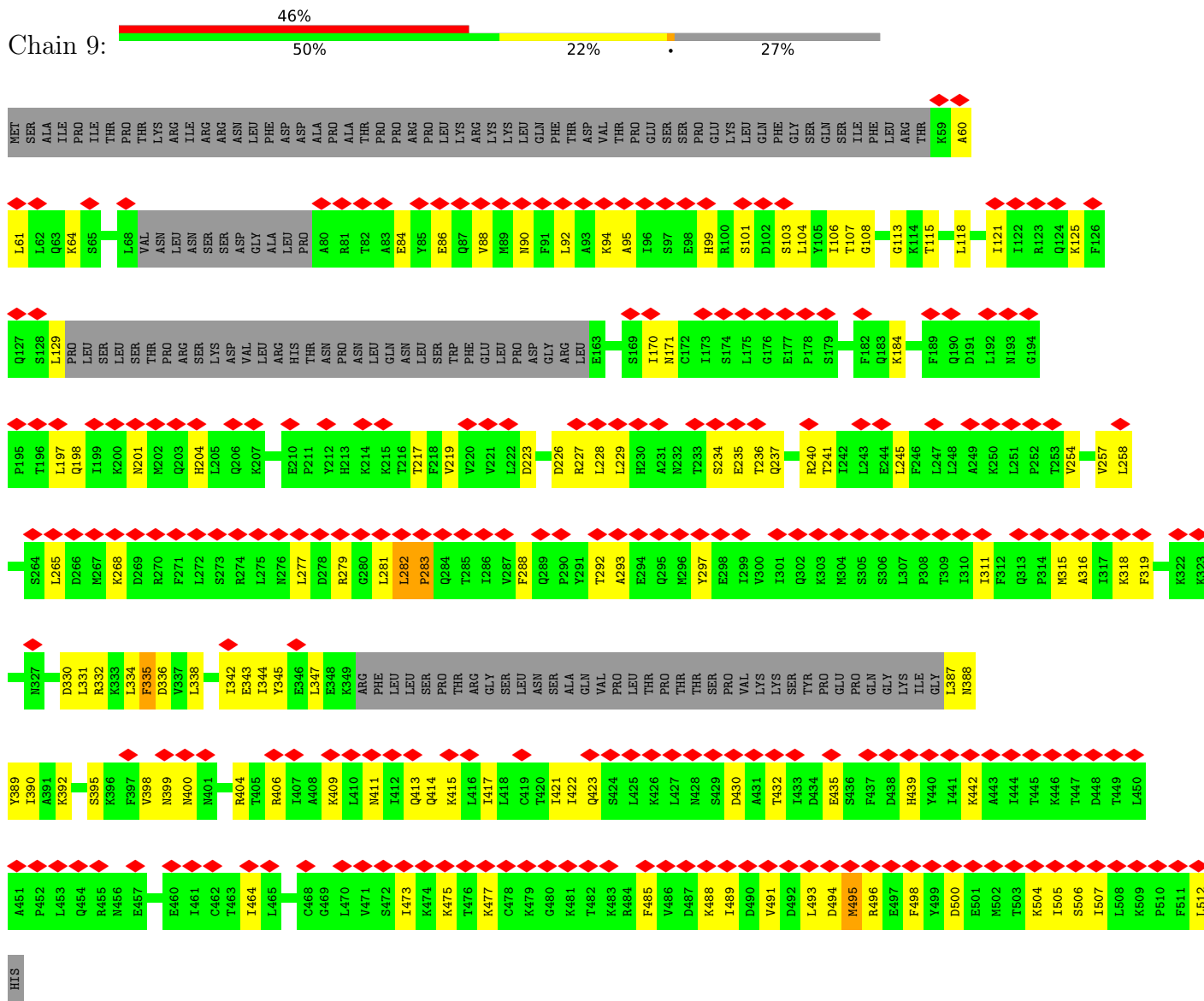
Mol	Chain	Residues	Atoms					AltConf	Trace
16	7	641	Total	C	N	O	S	0	0
			4858	3053	834	943	28		

- Molecule 17 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).

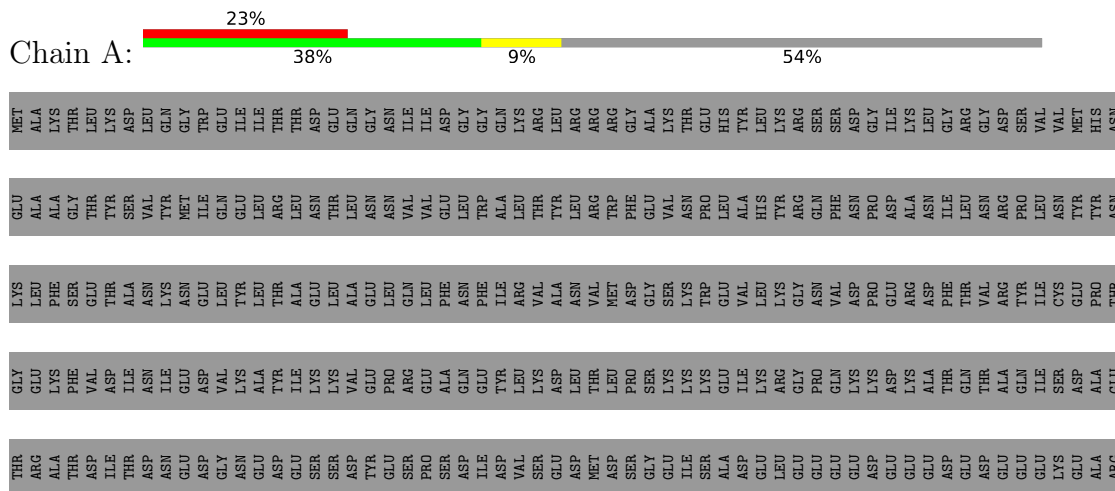


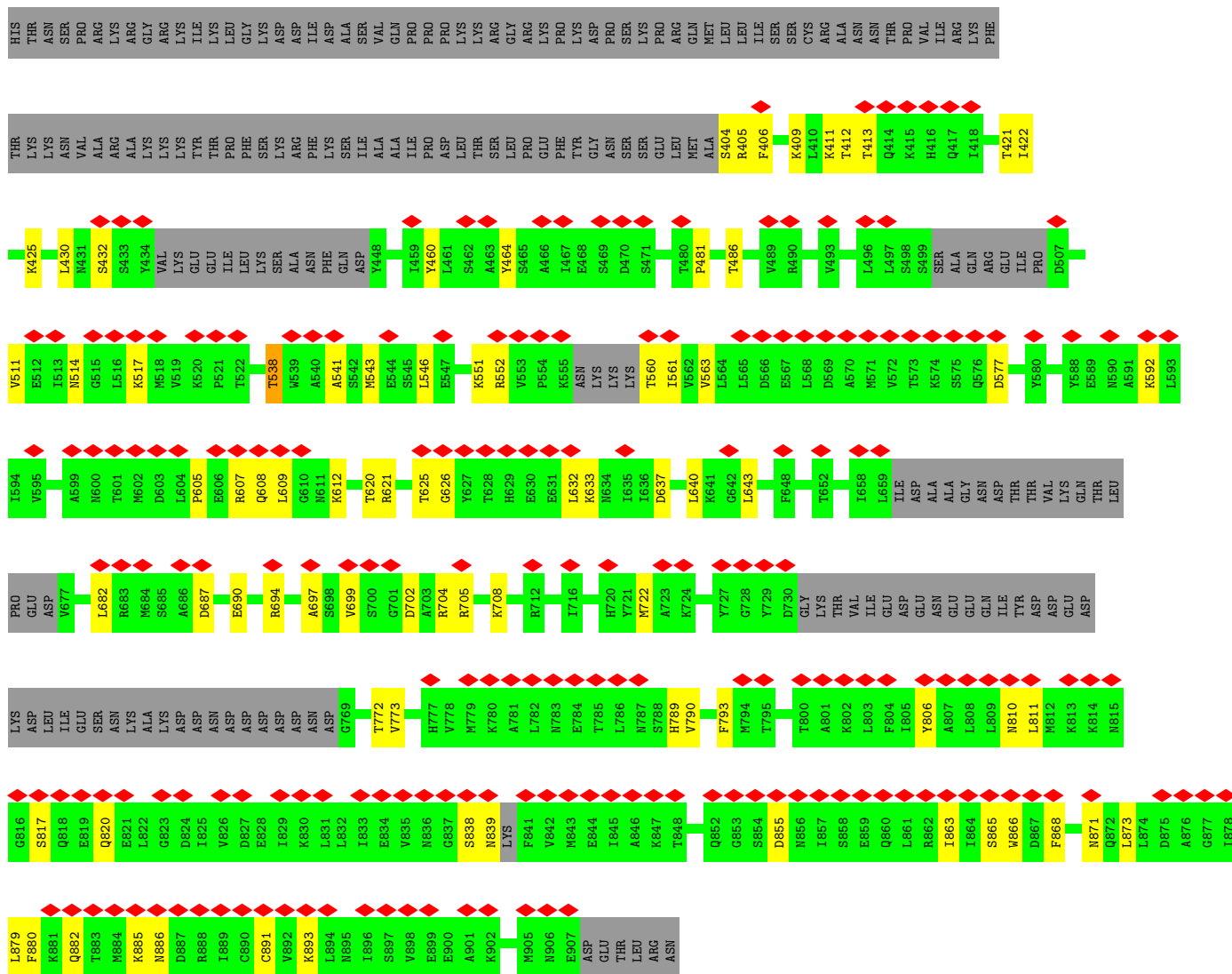
Mol	Chain	Residues	Atoms						AltConf
17	9	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
17	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 2: Cell division control protein 6

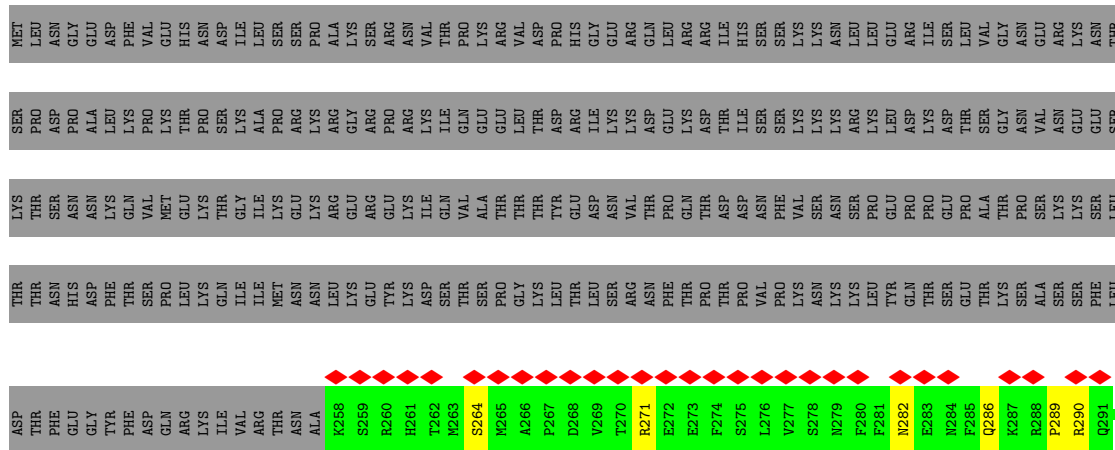
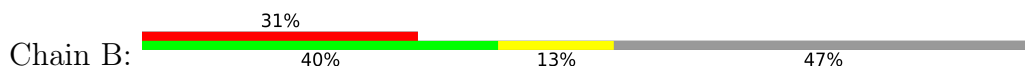


- Molecule 3: Origin recognition complex subunit 1





• Molecule 4: Origin recognition complex subunit 2

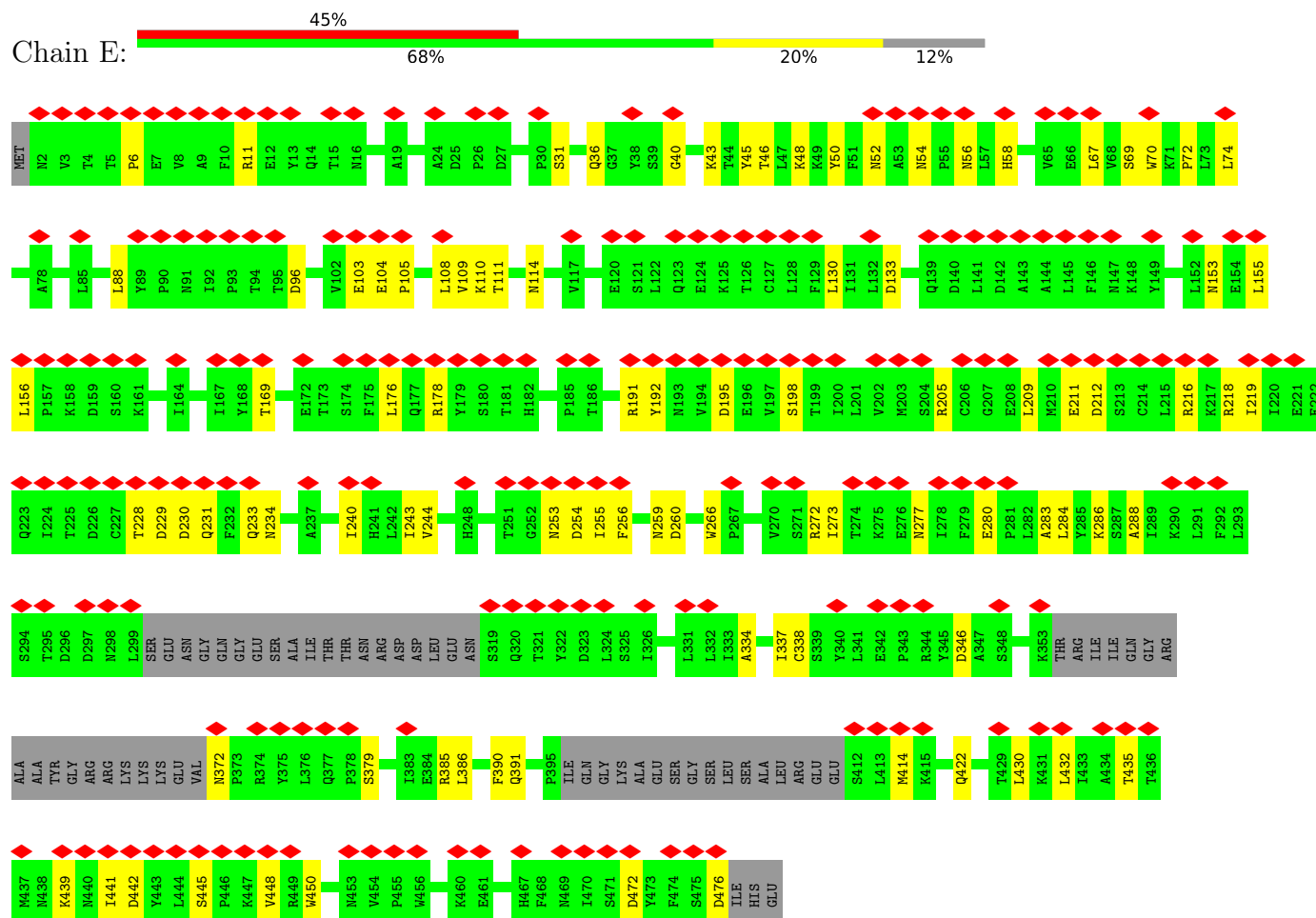




L569	L570	E571	T572	P573	D574	A575	F576	D577	K578	V579	A580	L581	M585	Q586	A587	I588	F589	E592	N593	M594	G595	L596	I597	K598	F599	Q600	S601	T602	K603	S604	Y605	V608	E609	K610	C611	V612	W613	R614	G615	I616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	E568
F499	SER	LEU	ASP	LYS	GLU	ASN	ASP	THR	L509	S510	G511	D512	L513	D514	K515	L516	M517	A518	F519	V520	L521	G522	O523	L524	F525	Y528	A531	M532	M533	T534	L535	M536	R452	L453	H454	F455	P456	P457	L458	D459	L468	D469	L479	K484	L487	D488	D489	H490	L491	W494	L498	L507	E568																													
F412	L413	E414	E415	E416	L417	M418	L419	L420	N421	F422	N423	E426	H429	L433	L436	D437	Y439	L440	D441	R442	W443	S444	A445	C446	K447	E448	Y449	K450	D451	R452	L453	H454	F455	P456	P457	L458	D459	L468	D469	L479	K484	L487	D488	D489	H490	L491	W494	L498	L507	E568																																
T310	N311	H312	Y328	P340	V341	N342	V343	D344	F345	L346	N347	D348	D349	Y350	L351	K352	L353	G356	C357	P358	F362	F363	V364	E365	G366	L367	I368	K369	Q370	H371	A372	P373	A374	D375	E376	L377	L378	S379	L380	L381	T382	N383	K384	N385	R386	G387	L388	E389	E390	F391	F392	V393	L396																													
A226	F227	K228	Y229	D230	H231	V232	L236	L237	F238	N241	T242	N243	N246	N250	L251	R252	L258	R261	L266	D267	V268	N271	K272	G273	F274	K275	Y276	G277	N278	Q279	L285	K286	D287	D289	G290	D296	R297	F298	V299	E300	F301	L302	L303	S304	K305	M306	A307	K324	S225	N309																																
A153	A154	D155	A156	E157	E158	H159	THR	THR	I1E	L1E	ASP	ASN	ASP	GLU	GLY	ASP	PHE	THR	GLU	GLN	ASN	D180	L181	S182	R193	L194	E197	G196	K197	D198	L199	A200	F205	K206	D207	V208	L128	D209	S210	E211	N212	F213	N214	T215	N218	F219	I220	L221	L222	L223	K224	S225																														
Q63	N78	I79	D82	A85	E86	I87	S88	D89	Y92	S93	E94	T95	T96	Q97	K98	R99	R100	C101	D111	S112	T113	T114	K115	I116	E117	L118	K119	D120	E121	S122	S123	R124	Y125	N126	Y127	L128	I129	E130	L131	T132	P133	K134	E135	Y136	V139	R140	M141	M142	L143	R144	R145	S146																														
MET	SER	ASP	LEU	ASN	GLN	SER	LYS	LYS	MET	ASN	VAL	SER	GLU	PHE	A16	Q19	R20	S21	H22	Y23	T24	V25	Y26	P27	SER	LEU	PRO	GLN	SER	ASN	LYS	ASN	ASP	LYS	HIS	ILE	PRO	PHE	VAL	LYS	LEU	LEU	SER	GLY	LYS	GLU	SER	GLU	GLU	VAL	ASN	VAL	E55	W58	E59	L60	Y61	H62																								

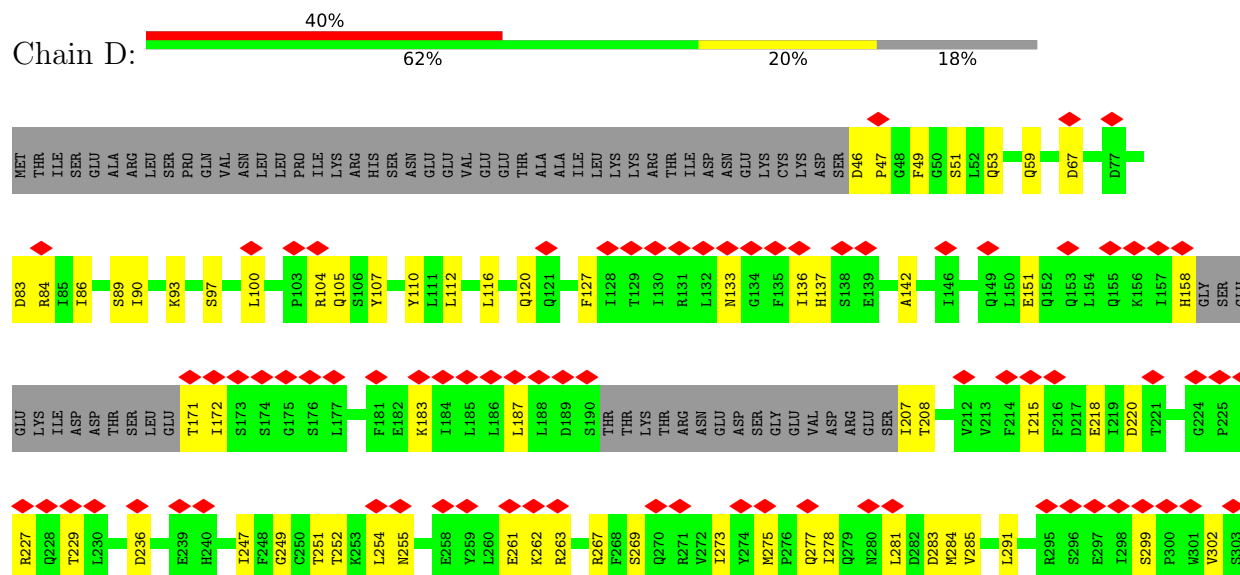
• Molecule 6: Origin recognition complex subunit 5

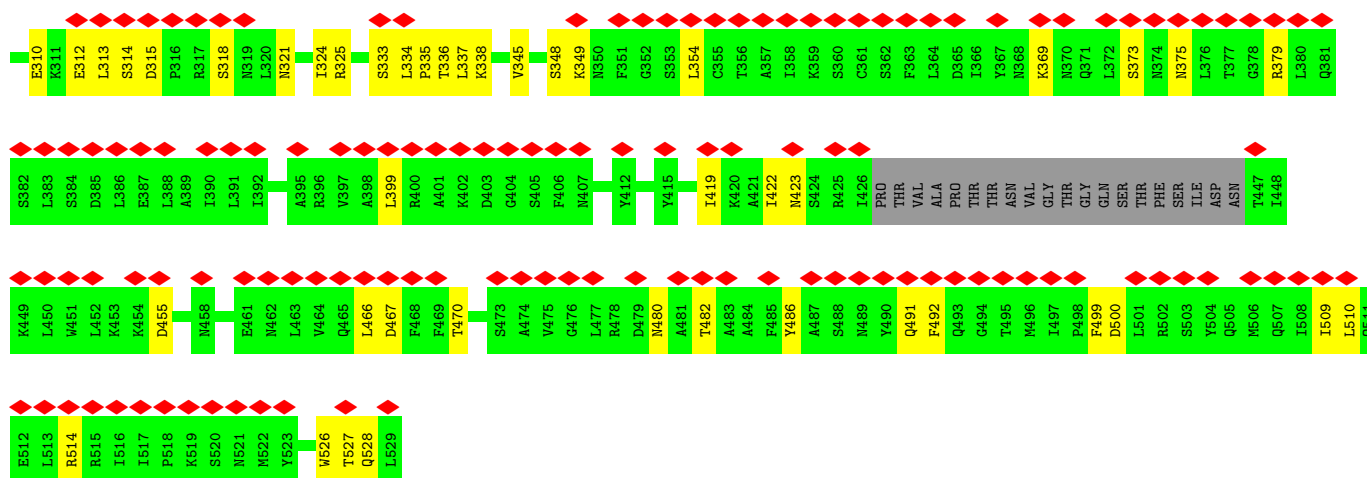
Chain E:



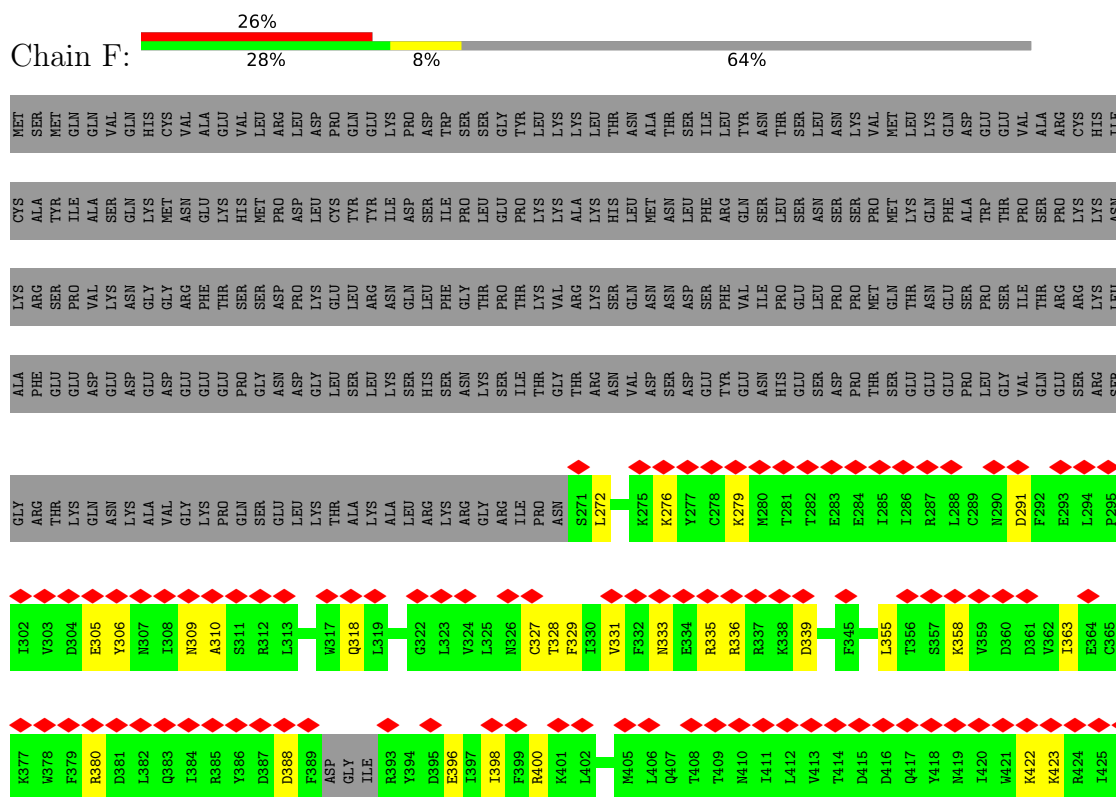
• Molecule 7: Origin recognition complex subunit 4

Chain D:

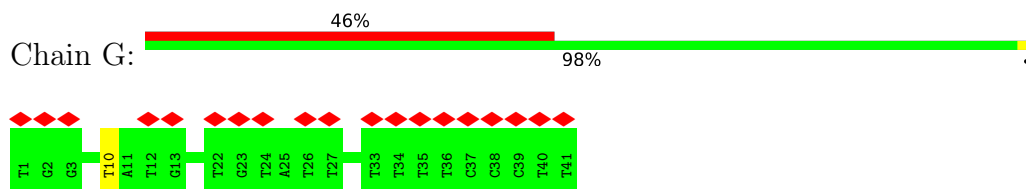




• Molecule 8: Origin recognition complex subunit 6

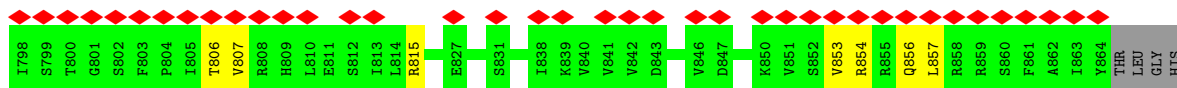


• Molecule 9: DNA (41-MER)



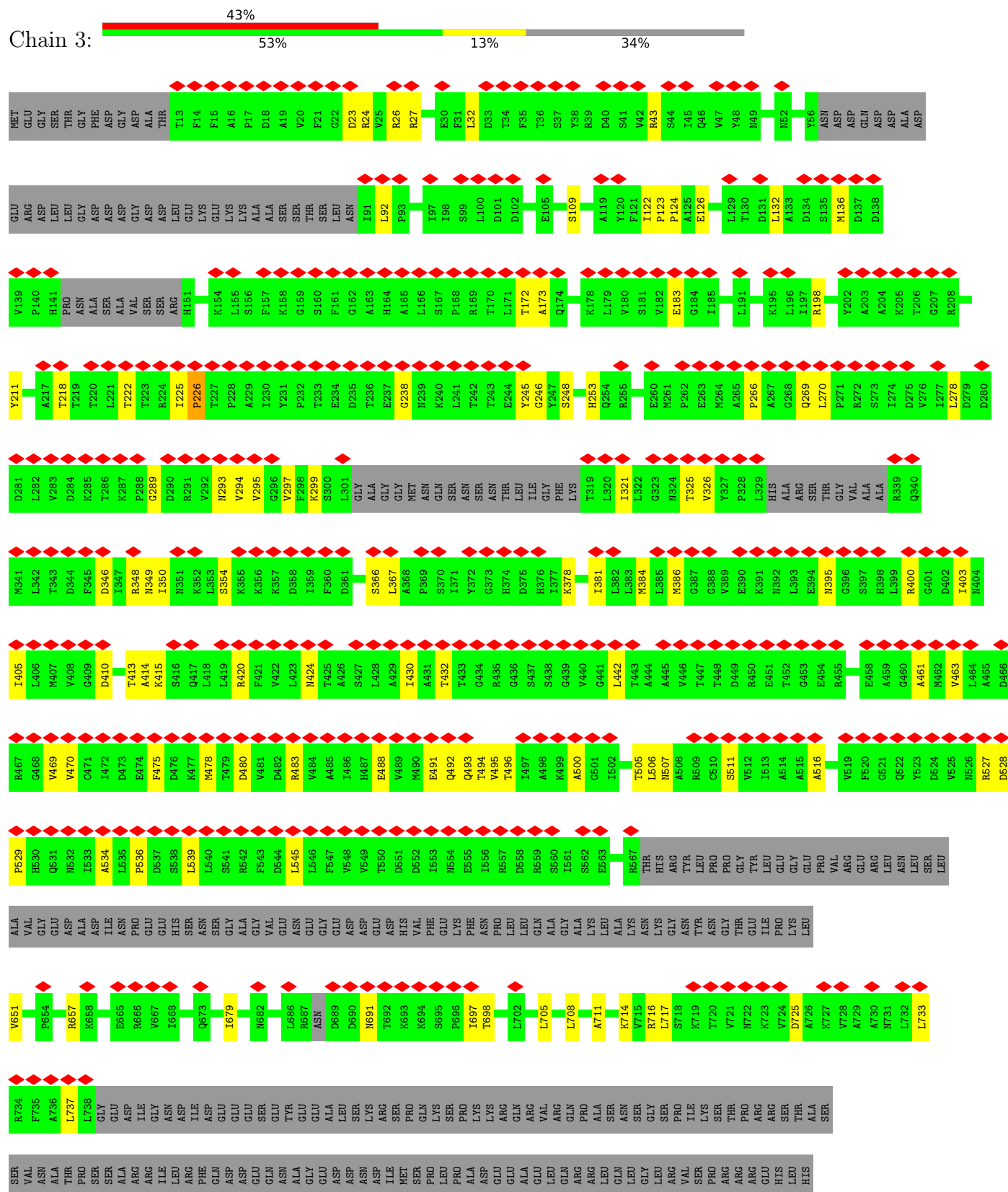
• Molecule 10: DNA (41-MER)

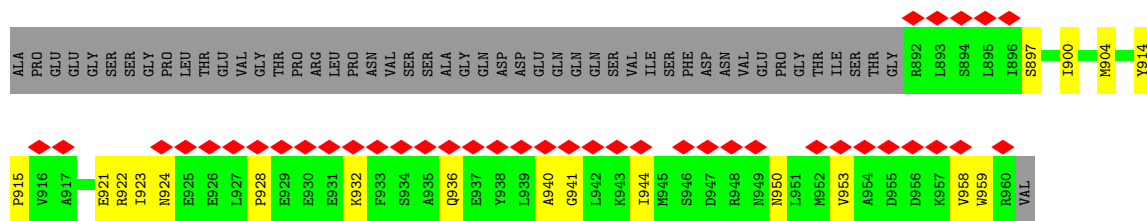




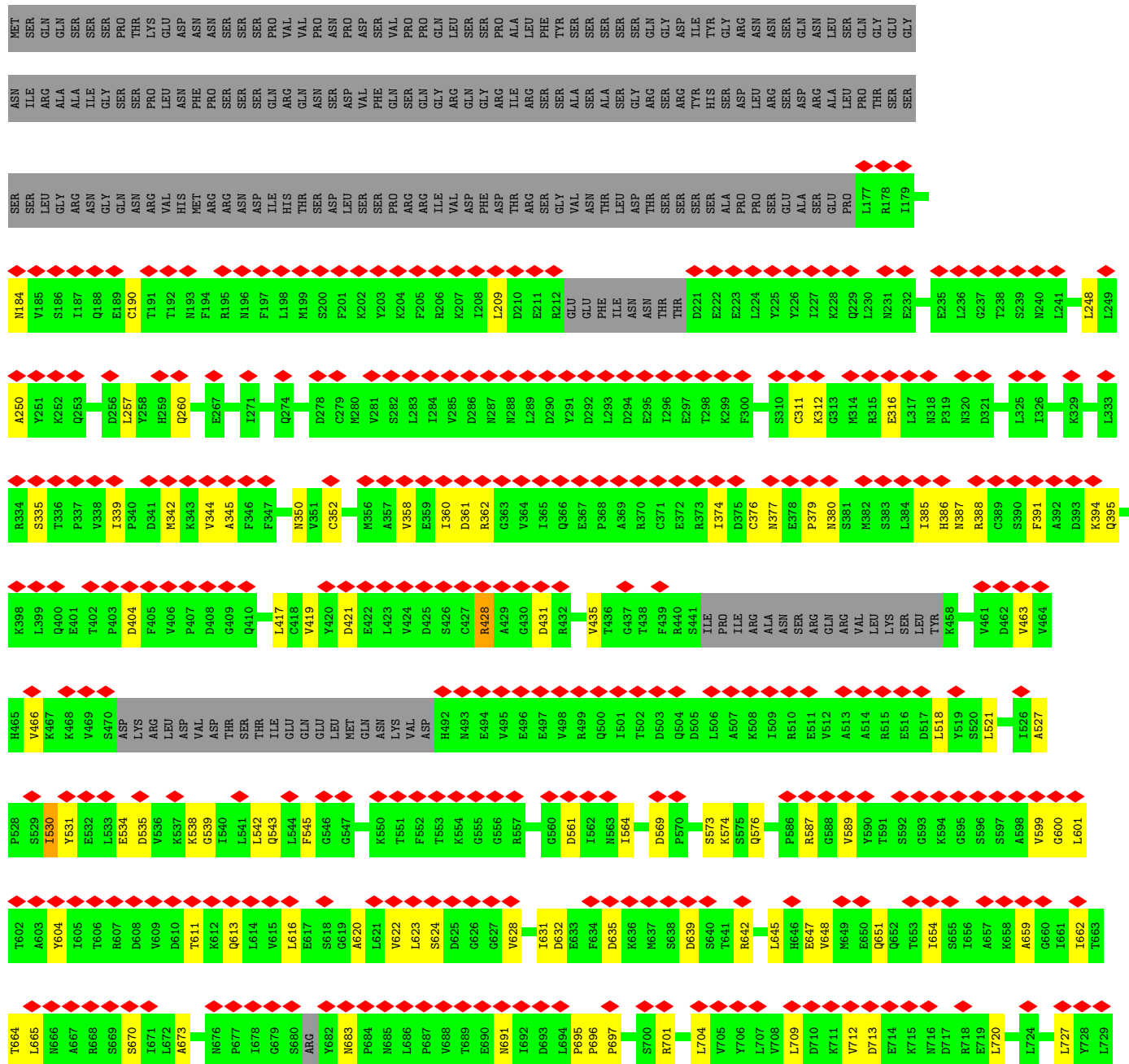
• Molecule 12: DNA replication licensing factor MCM3

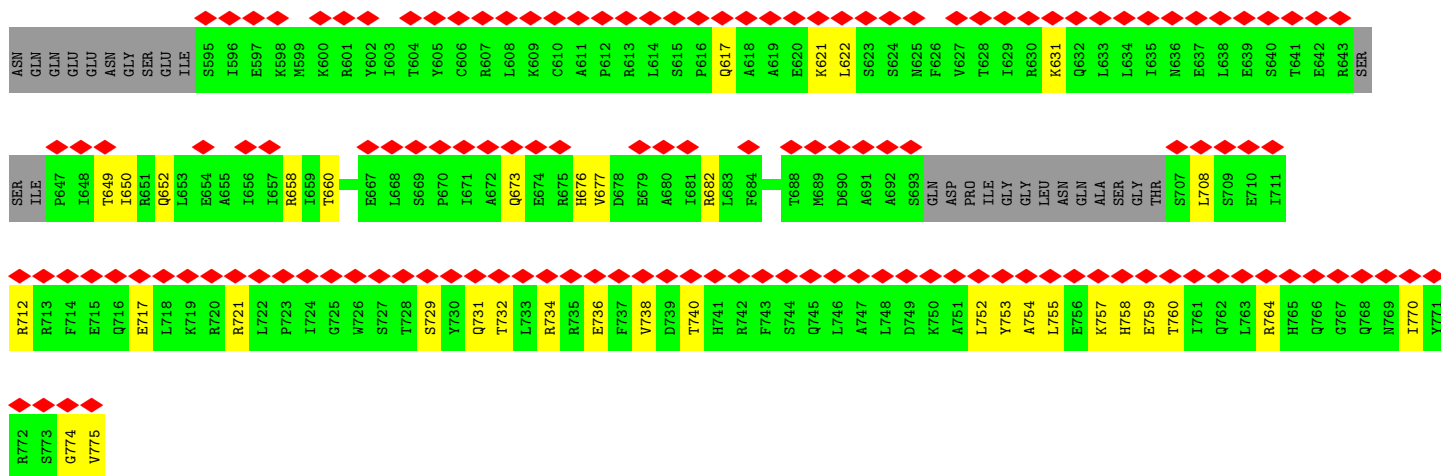
Chain 3:



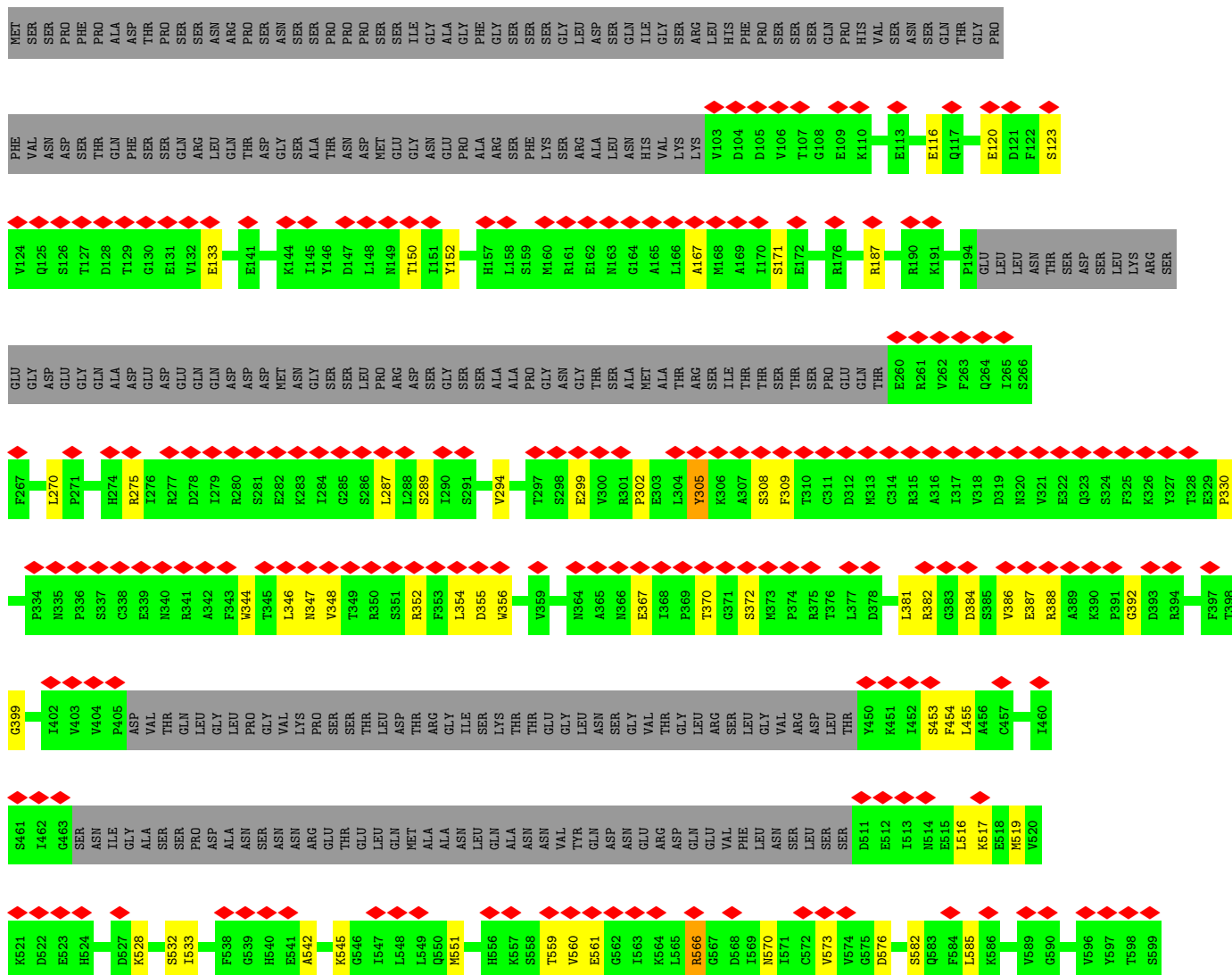


• Molecule 13: DNA replication licensing factor MCM4





- Molecule 15: DNA replication licensing factor MCM6



LEU	ILE	GLU	THR	ASN	GLY	GLU	ASN	SER	THR	LYS	GLU	ASP	GLU	ASP	SER	PHE	VAL	ASP	ASP	GLN	GLU	ASP	SER	LEU	VAL	SER	THR	PRO	LYS	LEU	ALA	PRO	GLN	THR	THR	THR	ALA	SER	ALA	ASN	VAL	SER	SER	ALA	GLN	ASP	ASP	ILE	ASP	LEU	GLN	ASP	ALA					
Q729	GLU	THR	ASN	LYS	ASN	SER	THR	LYS	GLU	ASP	GLU	ASP	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	I783	Q784	E785	Y786	S787	Y788	L789	N790	V791	TRP	HIS
R668	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	N657	D658	Y659	V660	V661	Q662	A663	Y664	I665	R666	L667						
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
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	T503	D504	E505	M506	L507	L508	E509	G510	V514	L515	A516	D517	N518	G519	I520	C521	C522	I523	D524	E525	F526	D527	K528	M529	D530	E531	S532			

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 (\AA)	335.36, 335.36, 335.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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 ⓘ

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

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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

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Mol	Chain	Res	Type
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:

Mol	Chain	Res	Type
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

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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	E	2001	-	26,33,33	0.68	0	26,52,52	1.33	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%)

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	E	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

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

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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:

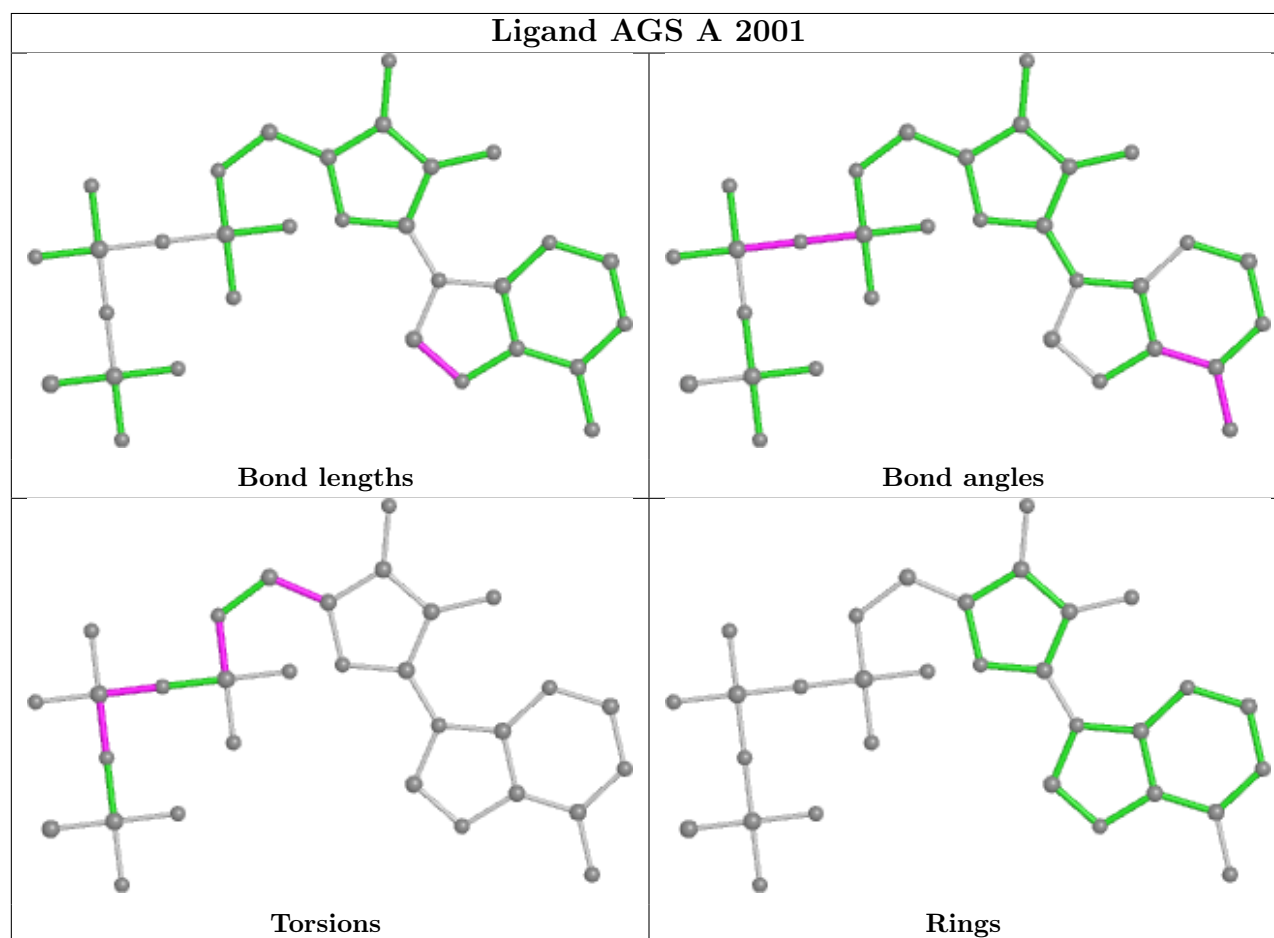
Mol	Chain	Res	Type	Atoms
17	9	2001	AGS	C5'-O5'-PA-O2A
17	9	2001	AGS	C5'-O5'-PA-O3A
17	A	2001	AGS	C5'-O5'-PA-O1A
17	A	2001	AGS	C5'-O5'-PA-O2A
17	A	2001	AGS	O4'-C4'-C5'-O5'
17	E	2001	AGS	C5'-O5'-PA-O1A
17	E	2001	AGS	C5'-O5'-PA-O2A
17	E	2001	AGS	C5'-O5'-PA-O3A
17	9	2001	AGS	O4'-C4'-C5'-O5'
17	E	2001	AGS	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'

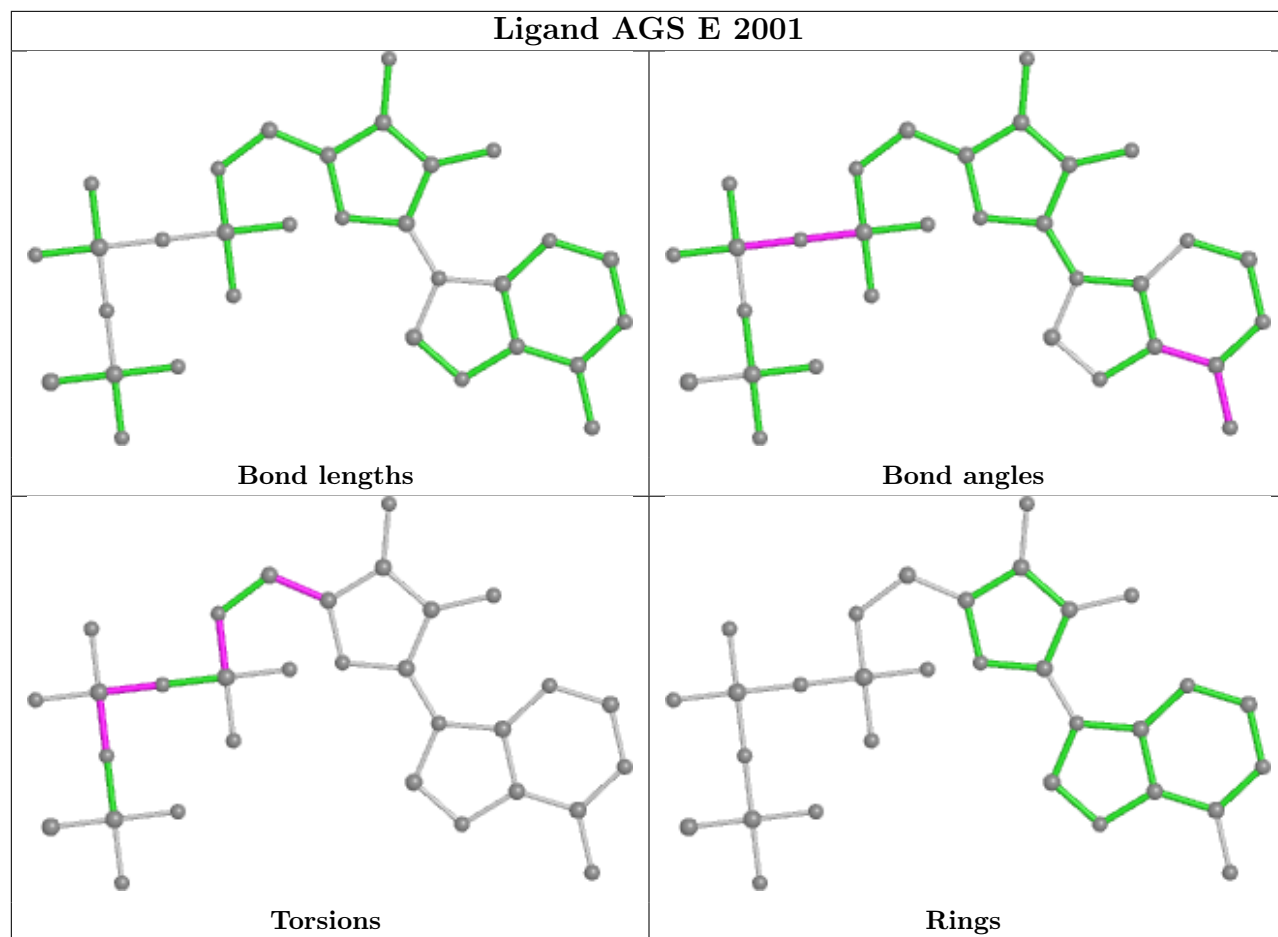
There are no ring outliers.

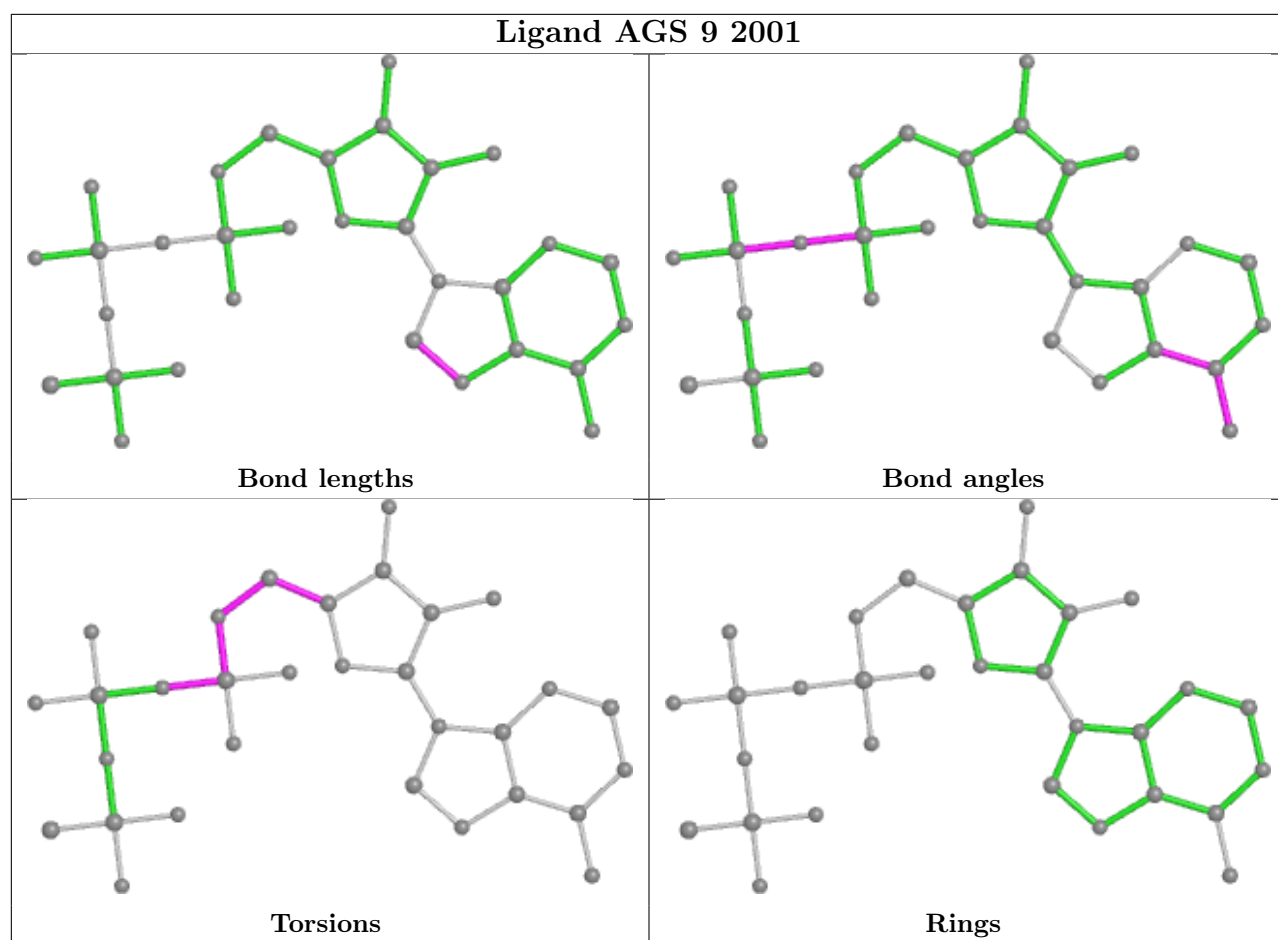
4 monomers are involved in 20 short contacts:

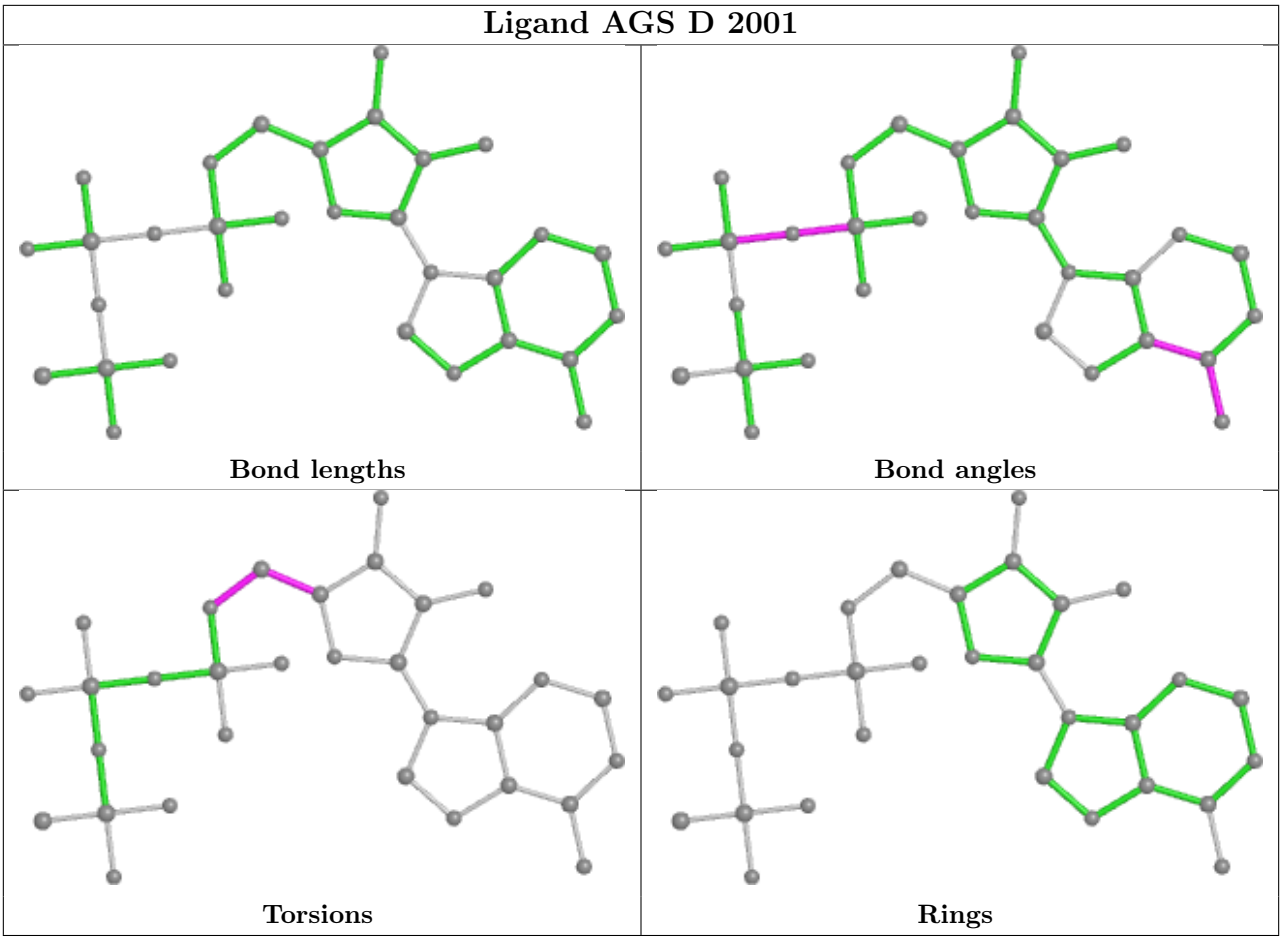
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	2001	AGS	7	0
17	E	2001	AGS	5	0
17	9	2001	AGS	4	0
17	D	2001	AGS	4	0

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

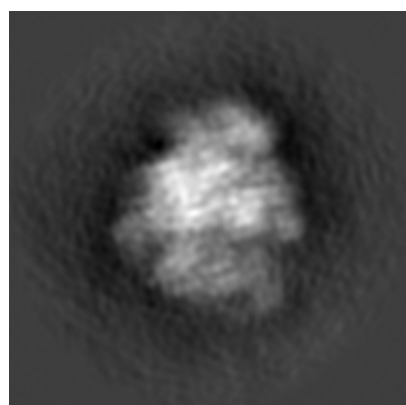
6 Map visualisation [i](#)

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.

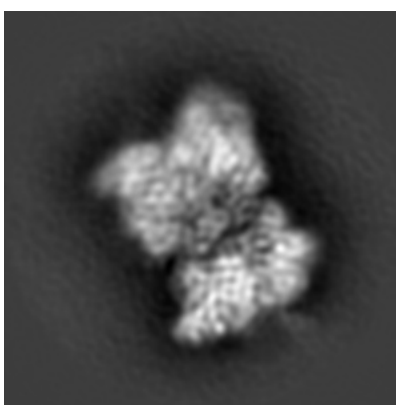
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

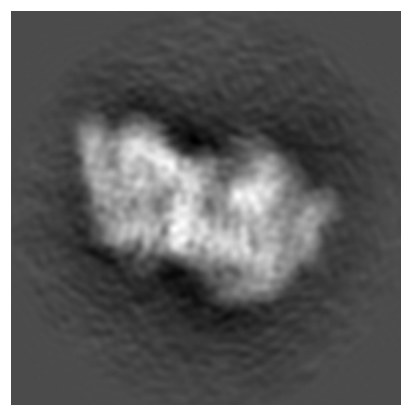
6.1.1 Primary map



X



Y

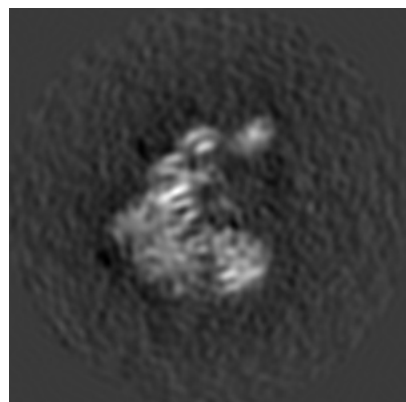


Z

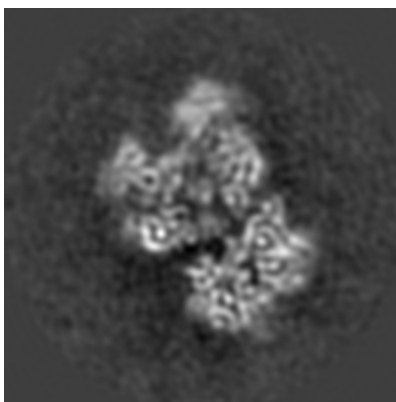
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

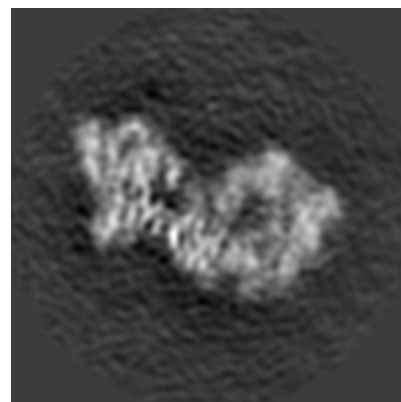
6.2.1 Primary map



X Index: 128



Y Index: 128

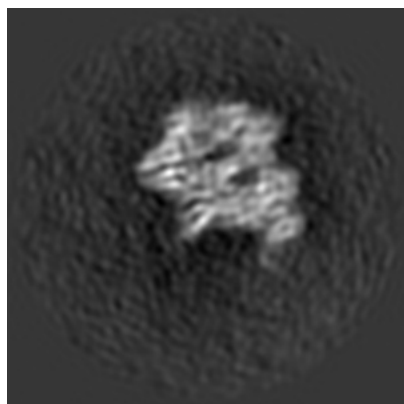


Z Index: 128

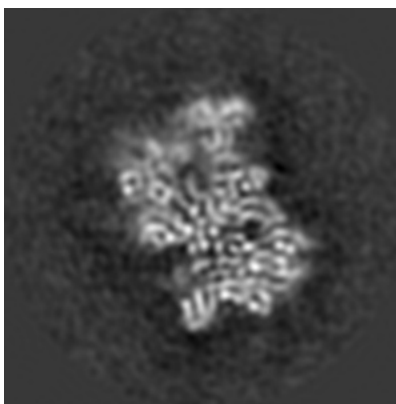
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

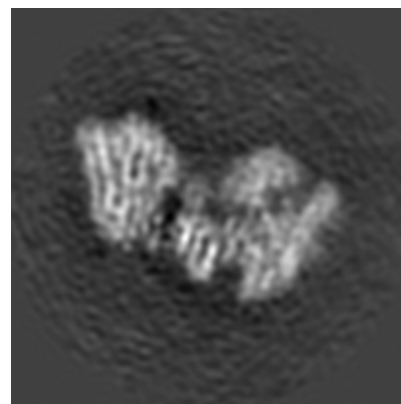
6.3.1 Primary map



X Index: 86



Y Index: 113

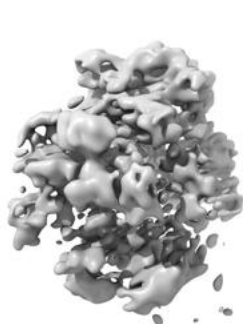


Z Index: 134

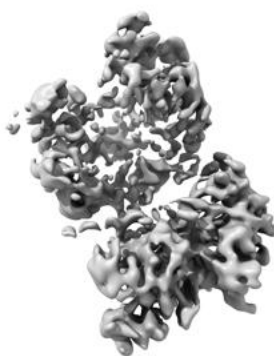
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

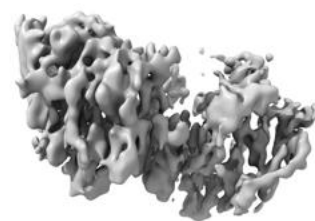
6.4.1 Primary map



X



Y



Z

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.

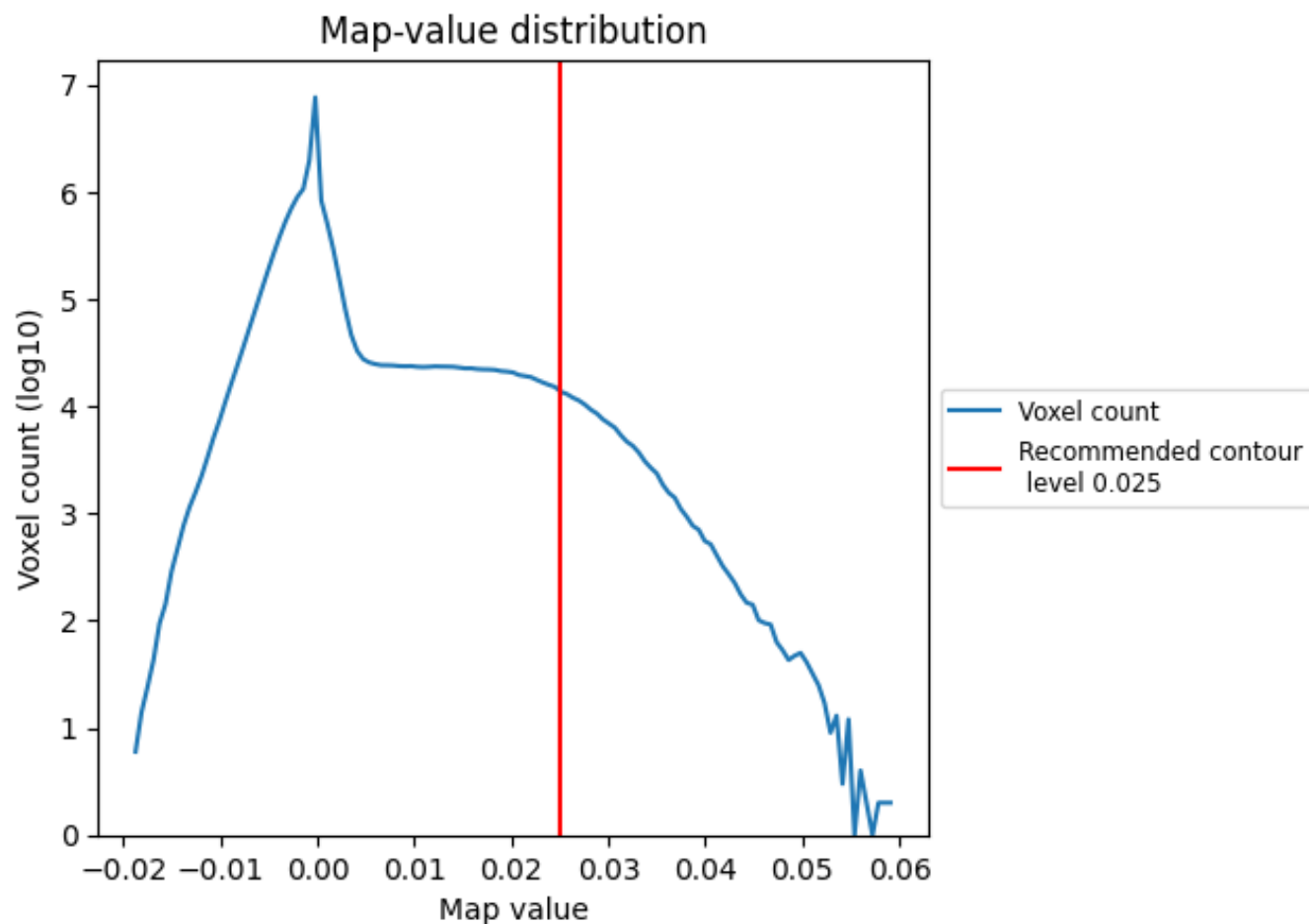
6.5 Mask visualisation

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

7 Map analysis [i](#)

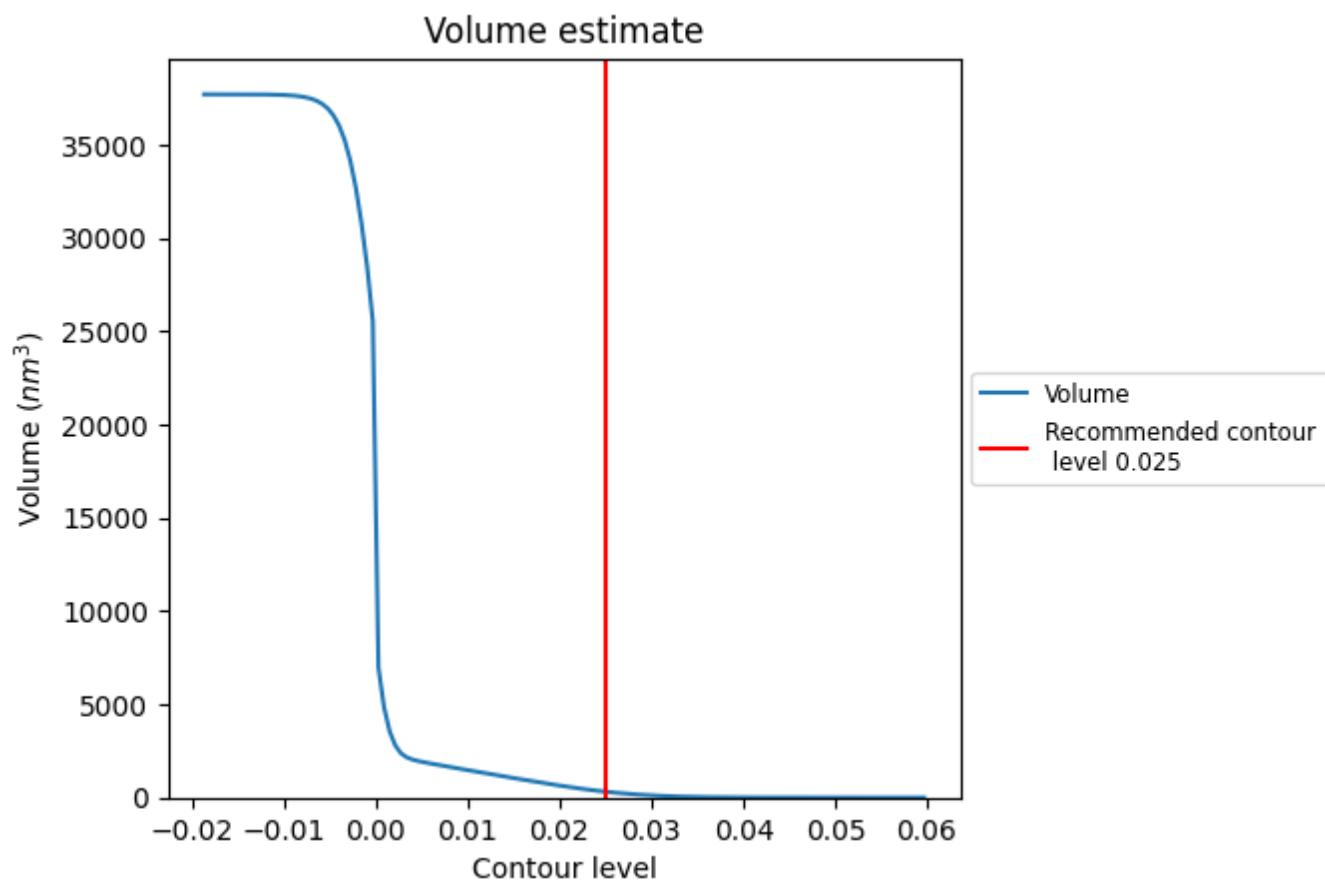
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

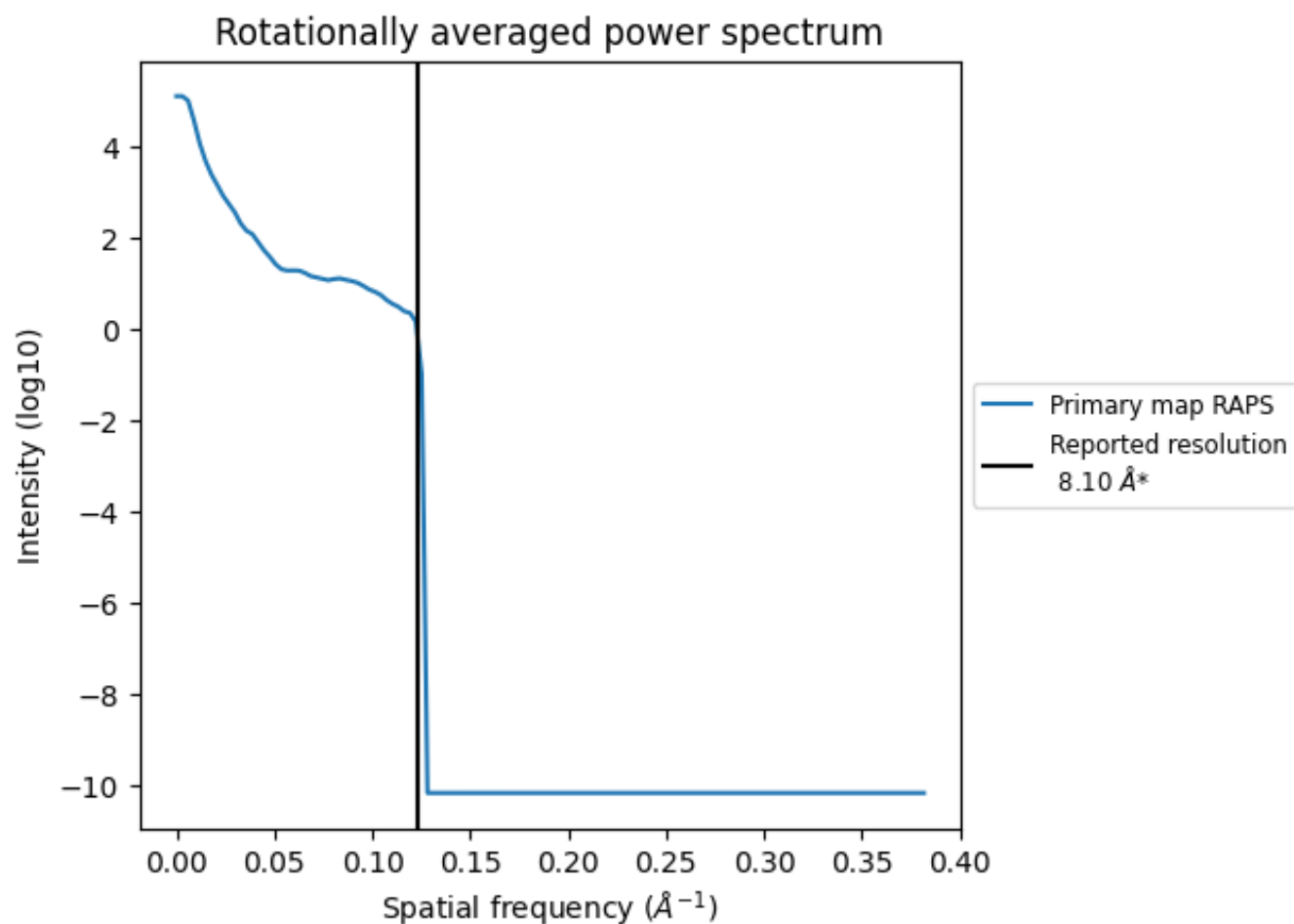
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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

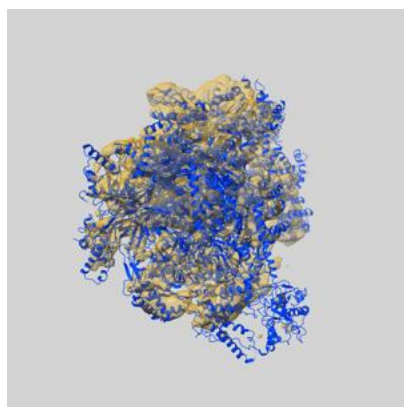
8 Fourier-Shell correlation

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

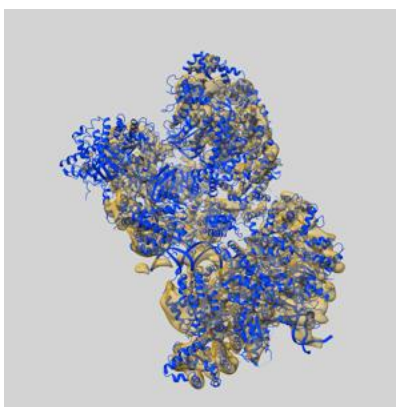
9 Map-model fit [i](#)

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.

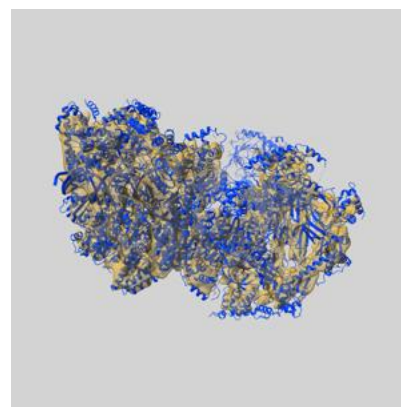
9.1 Map-model overlay [i](#)



X



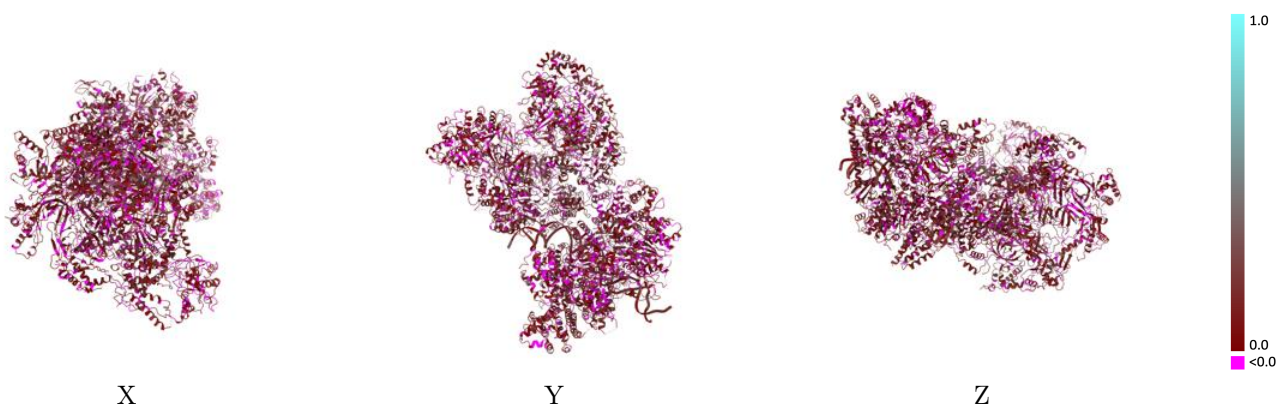
Y



Z

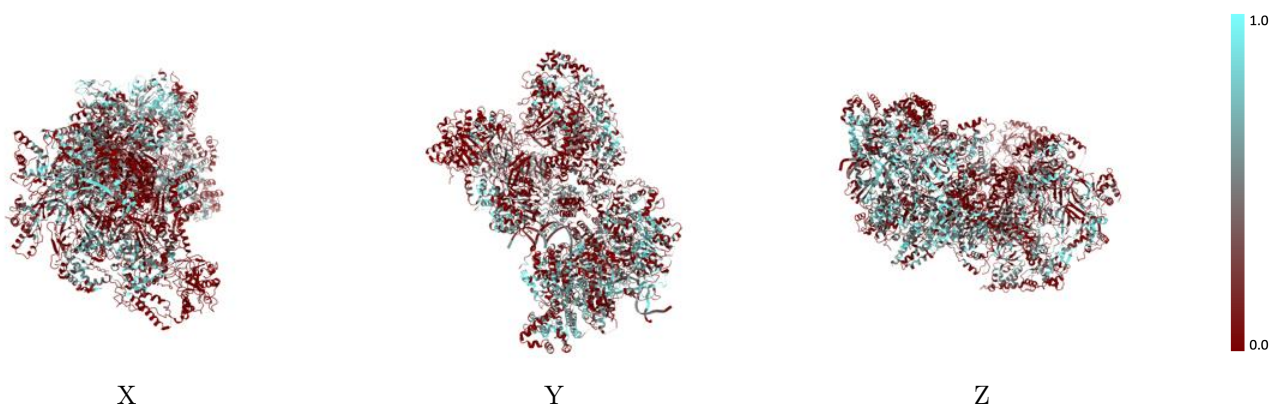
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



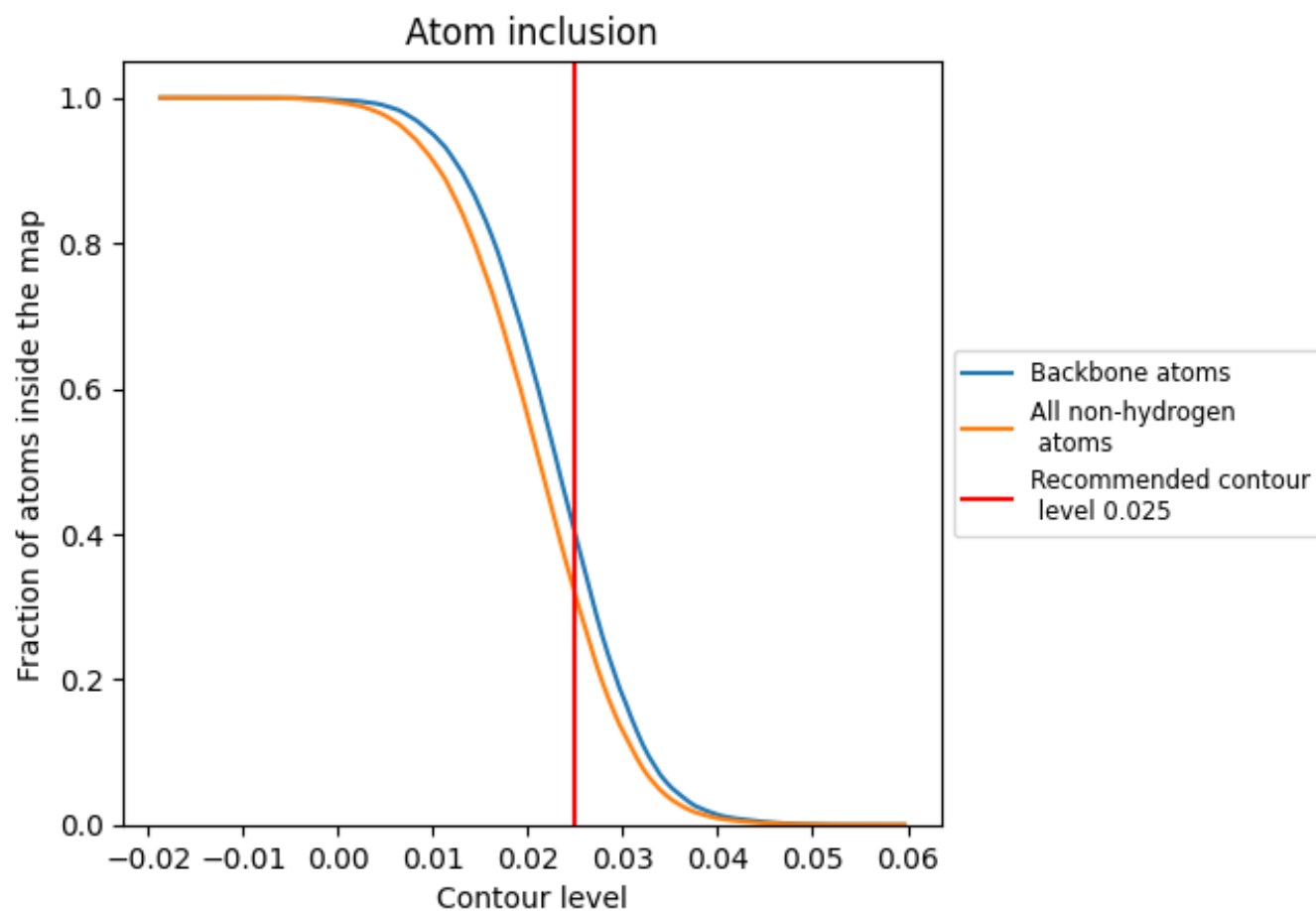
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.3162	<div></div> 0.1040
2	<div></div> 0.2791	<div></div> 0.1060
3	<div></div> 0.3103	<div></div> 0.1010
4	<div></div> 0.2853	<div></div> 0.1110
5	<div></div> 0.1860	<div></div> 0.0970
6	<div></div> 0.3390	<div></div> 0.1010
7	<div></div> 0.2474	<div></div> 0.1150
8	<div></div> 0.0376	<div></div> 0.0690
9	<div></div> 0.3418	<div></div> 0.0670
A	<div></div> 0.4343	<div></div> 0.1060
B	<div></div> 0.3385	<div></div> 0.0930
C	<div></div> 0.4401	<div></div> 0.1060
D	<div></div> 0.4253	<div></div> 0.1220
E	<div></div> 0.4012	<div></div> 0.1230
F	<div></div> 0.2363	<div></div> 0.0540
G	<div></div> 0.4320	<div></div> 0.1780
H	<div></div> 0.5573	<div></div> 0.2000

