



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:44 AM UTC

PDB ID : 6PTN / pdb_00006ptn
EMDB ID : EMD-20472
Title : Structure of Ctf4 trimer in complex with two CMG helicases
Authors : Yuan, Z.; Georgescu, R.; Bai, L.; Santos, R.; Donnell, M.; Li, H.
Deposited on : 2019-07-16
Resolution : 5.80 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:

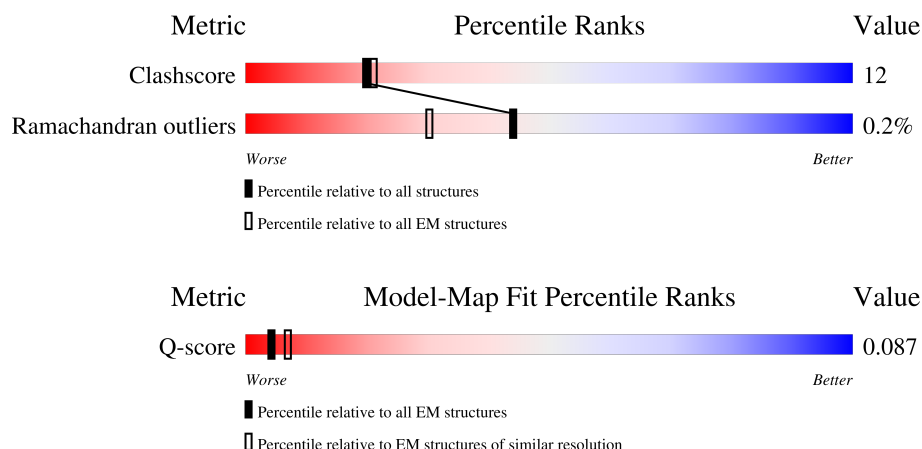
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 5.80 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	-
Q-score	-	25397	511 (5.30 - 6.30)

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	E	927	
1	F	927	
1	G	927	
2	A	208	
2	a	208	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	B	213	
3	b	213	
4	C	194	
4	c	194	
5	D	294	
5	d	294	
6	H	650	
6	h	650	
7	2	868	
7	i	868	
8	3	971	
8	j	971	
9	4	933	
9	k	933	
10	5	775	
10	l	775	
11	6	1017	
11	m	1017	
12	7	845	
12	n	845	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 91630 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA polymerase alpha-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	424	Total	C	N	O	S	1	0
			3416	2193	566	642	15		
1	F	431	Total	C	N	O	S	1	0
			3472	2227	576	653	16		
1	G	424	Total	C	N	O	S	1	0
			3416	2193	566	642	15		

- Molecule 2 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	208	Total	C	N	O	S	0	0
			1696	1065	290	331	10		
2	A	208	Total	C	N	O	S	0	0
			1696	1065	290	331	10		

- Molecule 3 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	181	Total	C	N	O	S	0	0
			1513	978	261	270	4		
3	B	181	Total	C	N	O	S	0	0
			1513	978	261	270	4		

- Molecule 4 is a protein called DNA replication complex GINS protein PSF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	159	Total	C	N	O	S	0	0
			1288	843	207	232	6		
4	C	159	Total	C	N	O	S	0	0
			1288	843	207	232	6		

- Molecule 5 is a protein called DNA replication complex GINS protein SLD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	234	Total	C	N	O	S	0	0
			1924	1224	315	372	13		
5	D	234	Total	C	N	O	S	0	0
			1924	1224	315	372	13		

- Molecule 6 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	h	553	Total	C	N	O	S	0	0
			4482	2862	763	844	13		
6	H	553	Total	C	N	O	S	0	0
			4482	2862	763	844	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	634	Total	C	N	O	S	0	0
			4970	3122	897	934	17		
7	2	634	Total	C	N	O	S	0	0
			4970	3122	897	934	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	594	Total	C	N	O	S	0	0
			4659	2936	832	878	13		
8	3	594	Total	C	N	O	S	0	0
			4659	2936	832	878	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	k	682	Total	C	N	O	S	0	0
			5410	3397	946	1039	28		
9	4	682	Total	C	N	O	S	0	0
			5410	3397	946	1039	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1	597	Total	C	N	O	S	0	0
			4688	2946	808	910	24		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
10	5	597	Total	C	N	O	S	0	0
			4688	2946	808	910	24		

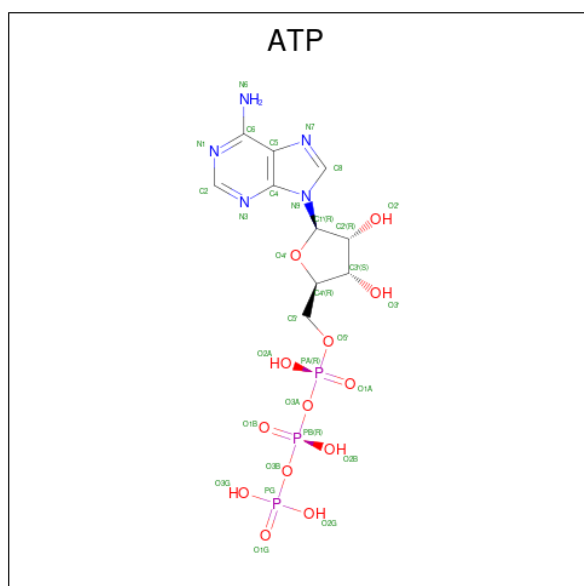
- Molecule 11 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	614	Total	C	N	O	S	0	0
			4720	2971	836	893	20		
11	6	614	Total	C	N	O	S	0	0
			4720	2971	836	893	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	n	663	Total	C	N	O	S	0	0
			5220	3290	904	996	30		
12	7	663	Total	C	N	O	S	0	0
			5220	3290	904	996	30		

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

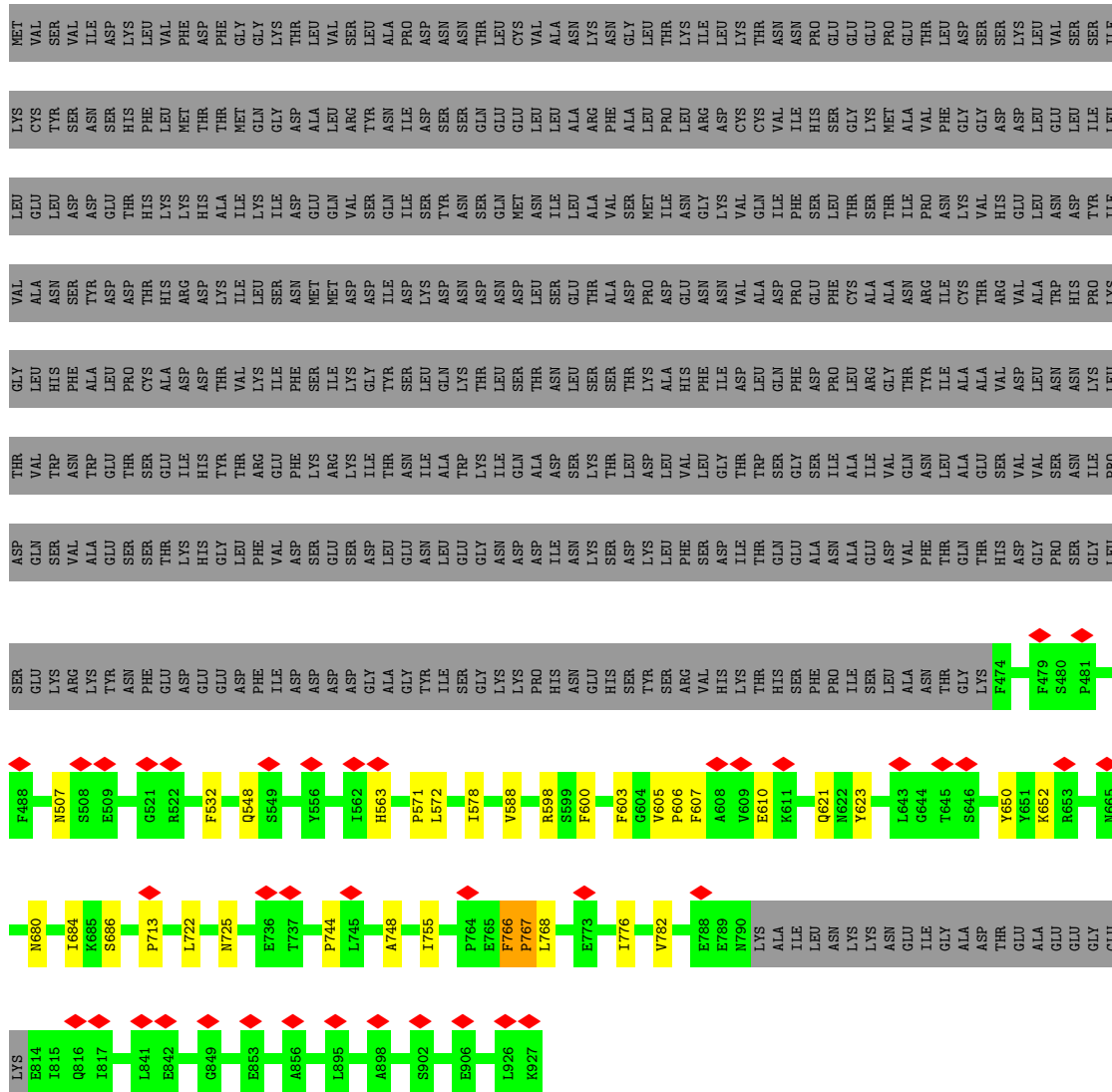


Mol	Chain	Residues	Atoms					AltConf
13	i	1	Total	C	N	O	P	0
			31	10	5	13	3	

Continued on next page...

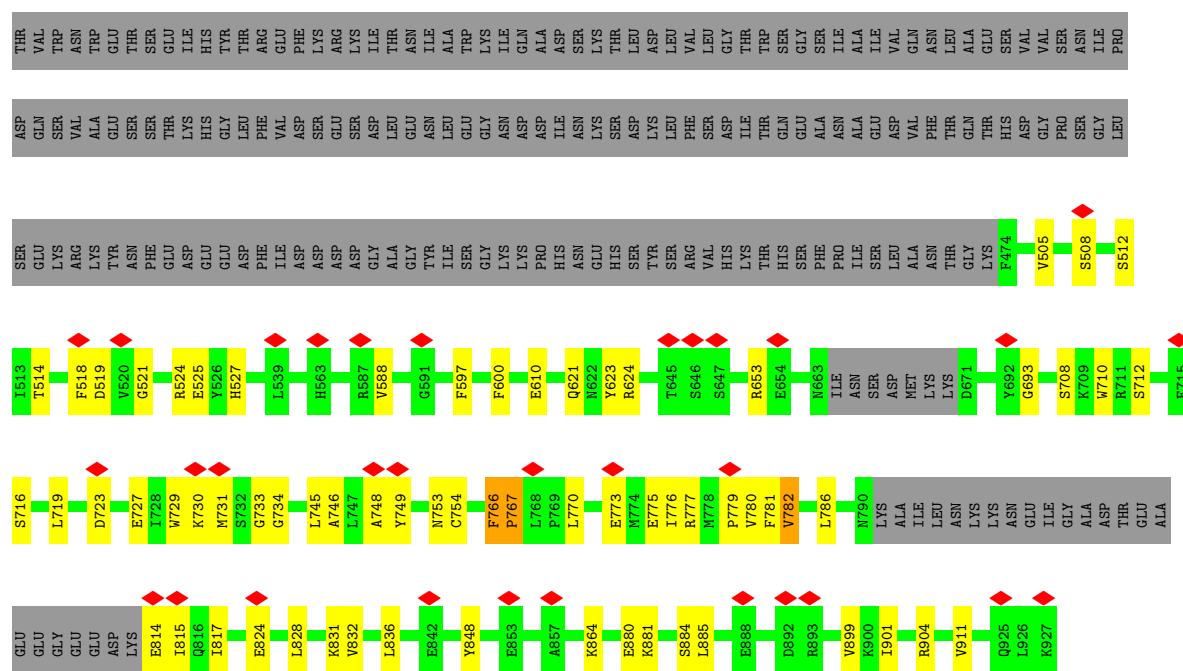
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
13	j	1	Total 31	C 10	N 5	O 13	P 3	0
13	1	1	Total 31	C 10	N 5	O 13	P 3	0
13	2	1	Total 31	C 10	N 5	O 13	P 3	0
13	3	1	Total 31	C 10	N 5	O 13	P 3	0
13	5	1	Total 31	C 10	N 5	O 13	P 3	0

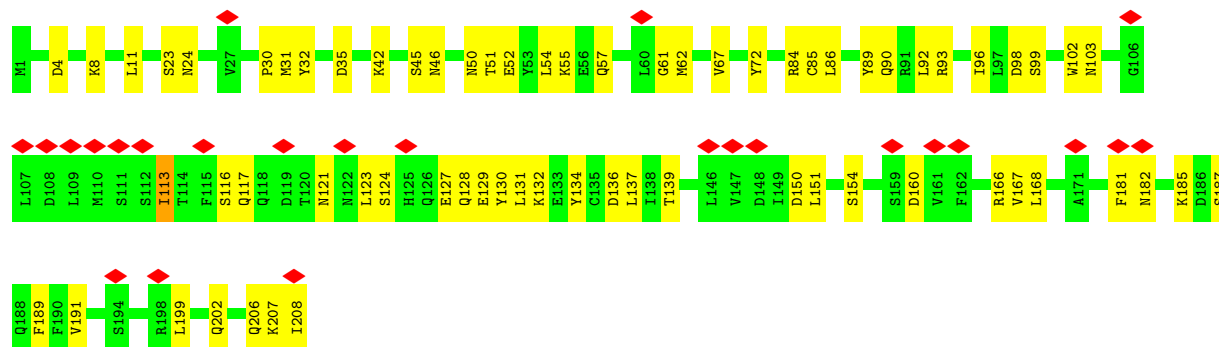


Chain G: 39% 7% 54%

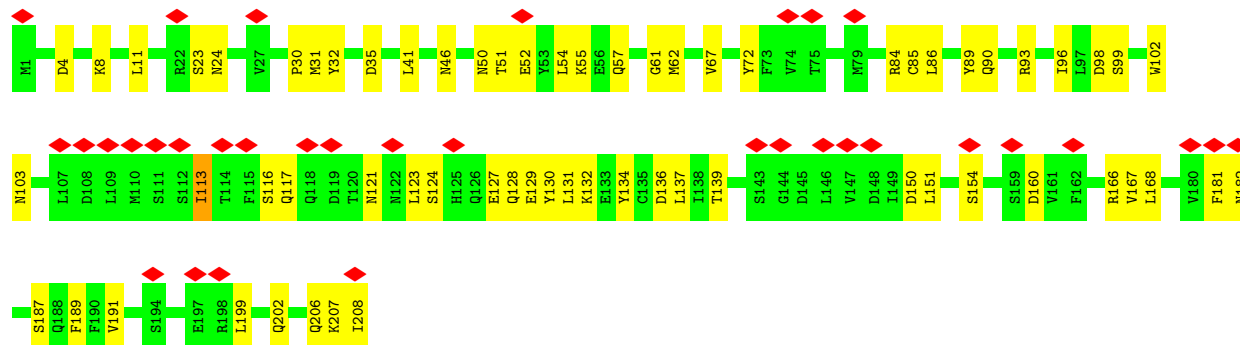




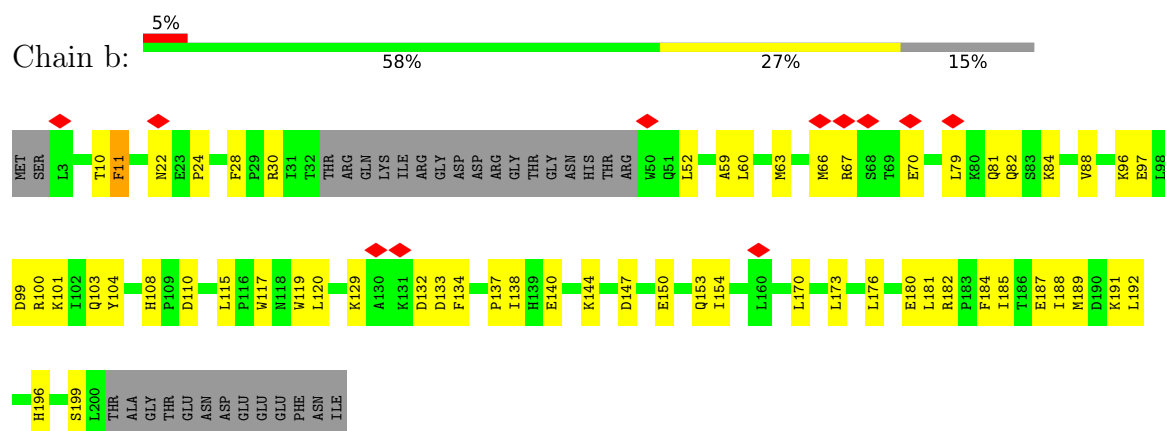
- Molecule 2: DNA replication complex GINS protein PSF1



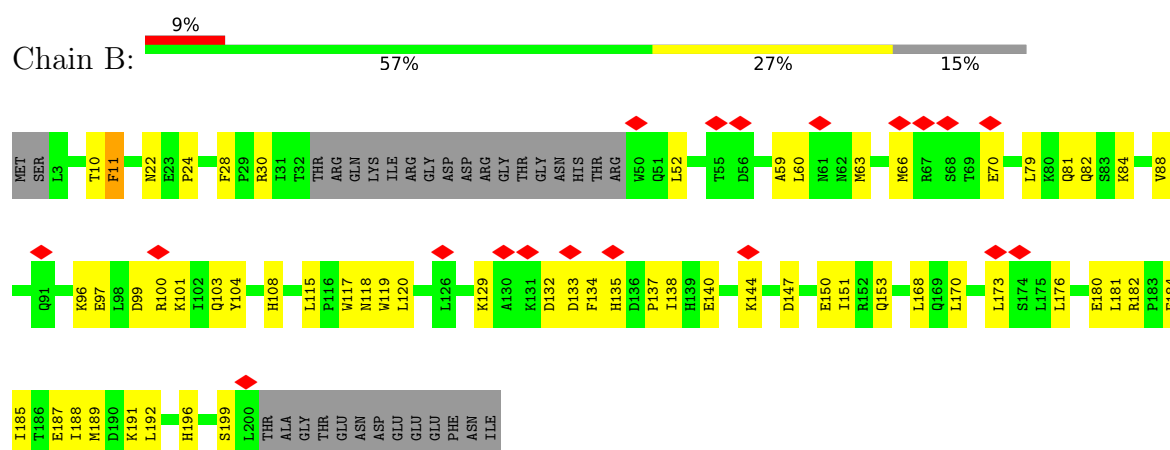
- Molecule 2: DNA replication complex GINS protein PSF1



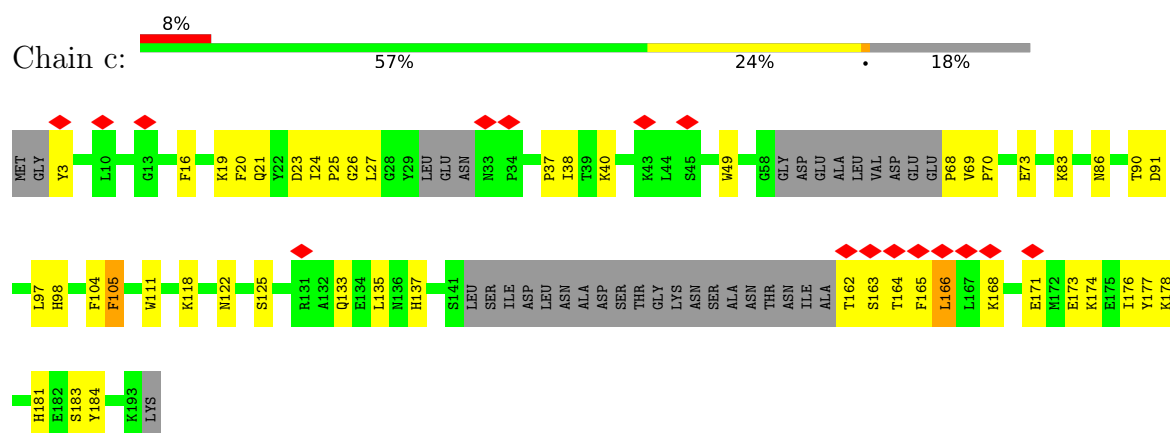
- Molecule 3: DNA replication complex GINS protein PSF2



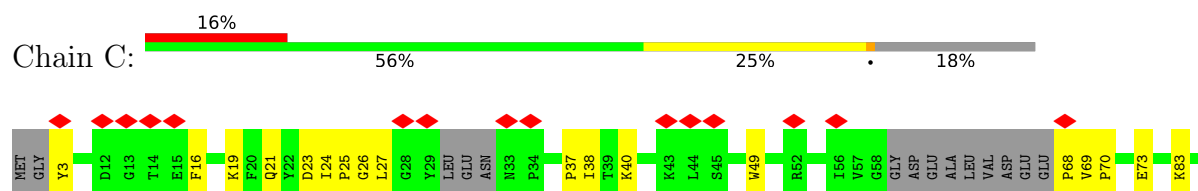
• Molecule 3: DNA replication complex GINS protein PSF2



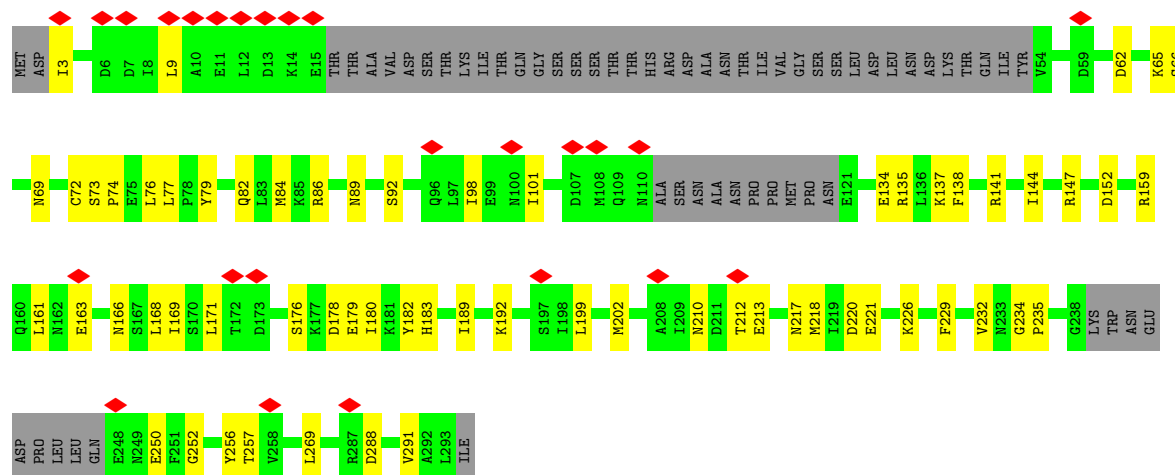
• Molecule 4: DNA replication complex GINS protein PSF3



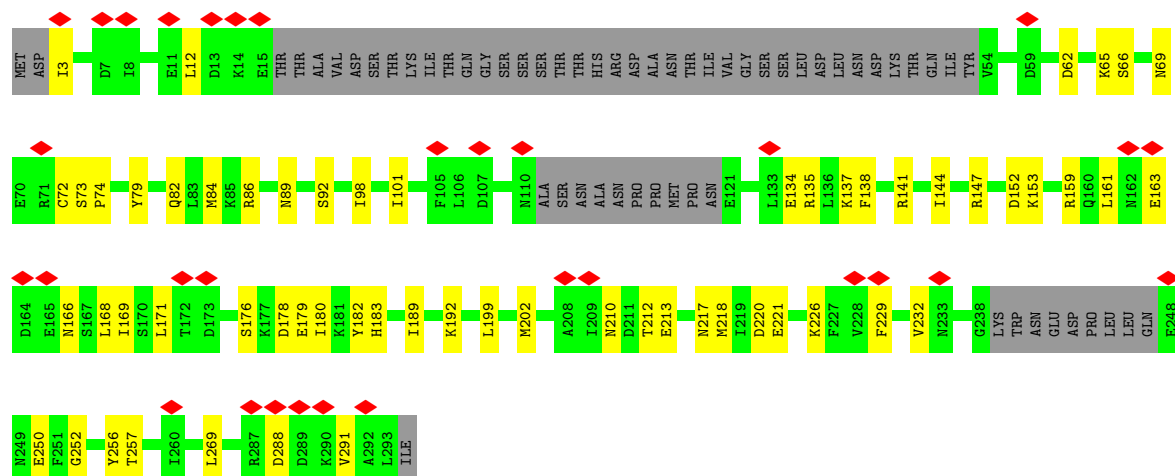
• Molecule 4: DNA replication complex GINS protein PSF3



- Molecule 5: DNA replication complex GINS protein SLD5

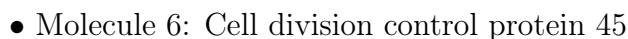


- Molecule 5: DNA replication complex GINS protein SLD5

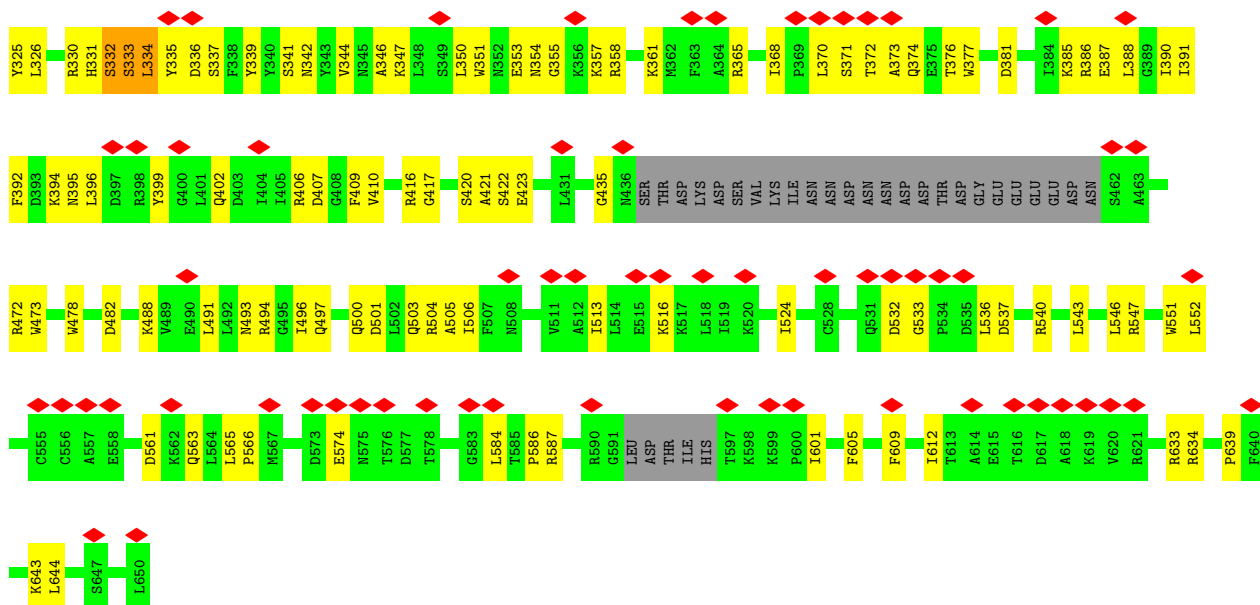


- Molecule 6: Cell division control protein 45

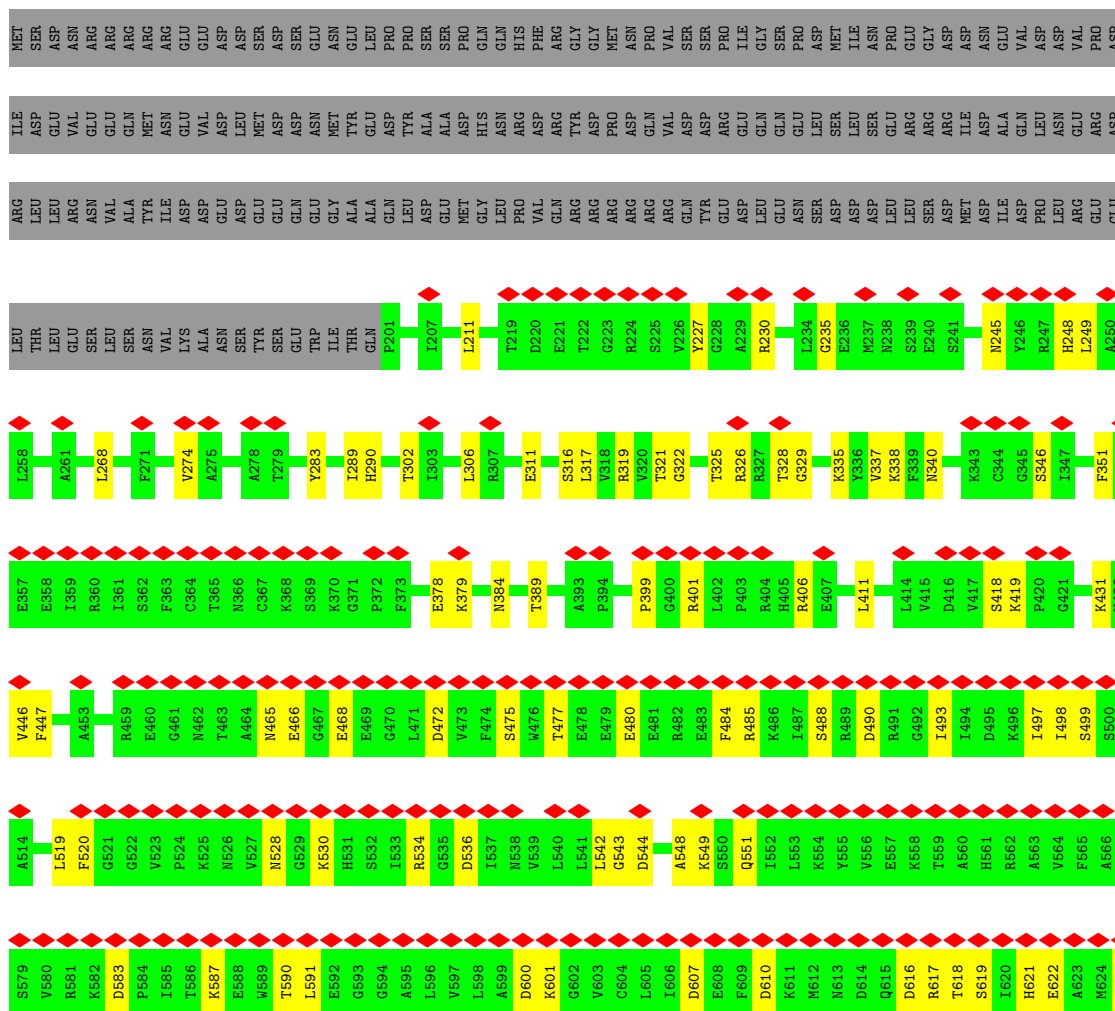


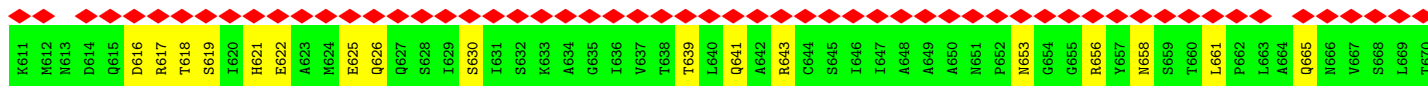


E232	E239	Y240	Y241	S242	Q243	T246	V247	V248	N249	Q254	S257	S260	A261	I262	G263	E264	T265	N266	L267	L270	W271	L272	N273	L274	L275	S279	L280	D281	I282	Y288	N289	R290	Q296	D297	K300	R301	L302	T303	S306	S309	D314	T315	P322	P323						
GLU	GLY	ASP	GLU	LEU	SER	GLY	ASP	GLU	ASN	ASP	GLY	GLY	GLY	ASP	GLU	ALA	THR	ASP	ALA	ASP	GLU	THR	ASP	GLU	GLU	ASP	GLU	ASP	GLU	THR	ILE	SER	ASN	ARG	GLY	ASN	SER	SER	ILE	GLY	PRO	W218	D219	L220	S221	K222	R226	K227	K228	
F95	Q101	E102	TYR	VAL	ILE	ASP	THR	GLU	LYS	SER	GLY	Q114	S115	F116	R117	R118	D119	I120	D124	R127	D132	N133	I134	F135	I139	I140	Q141	C142	F143	D144	D145	G146	T147	V148	D149	D150	T151	L152	Q155	K156	E157	A158	Y159	K161	L162	L163	E164	L165	ASP	GLU
MET	TYR	TYR	GLY	I5	S6	Q7	F8	S9	E10	N13	K14	I15	N18	S19	S20	S21	H22	S23	S24	C25	Q26	D37	K43	M44	L45	S46	L47	L48	Q52	Q55	R68	Y71	S72	Q73	L74	D75	D76	L81	L82	L83	V84	G85	F86	G87	G88	V89	I90	D91	A94	

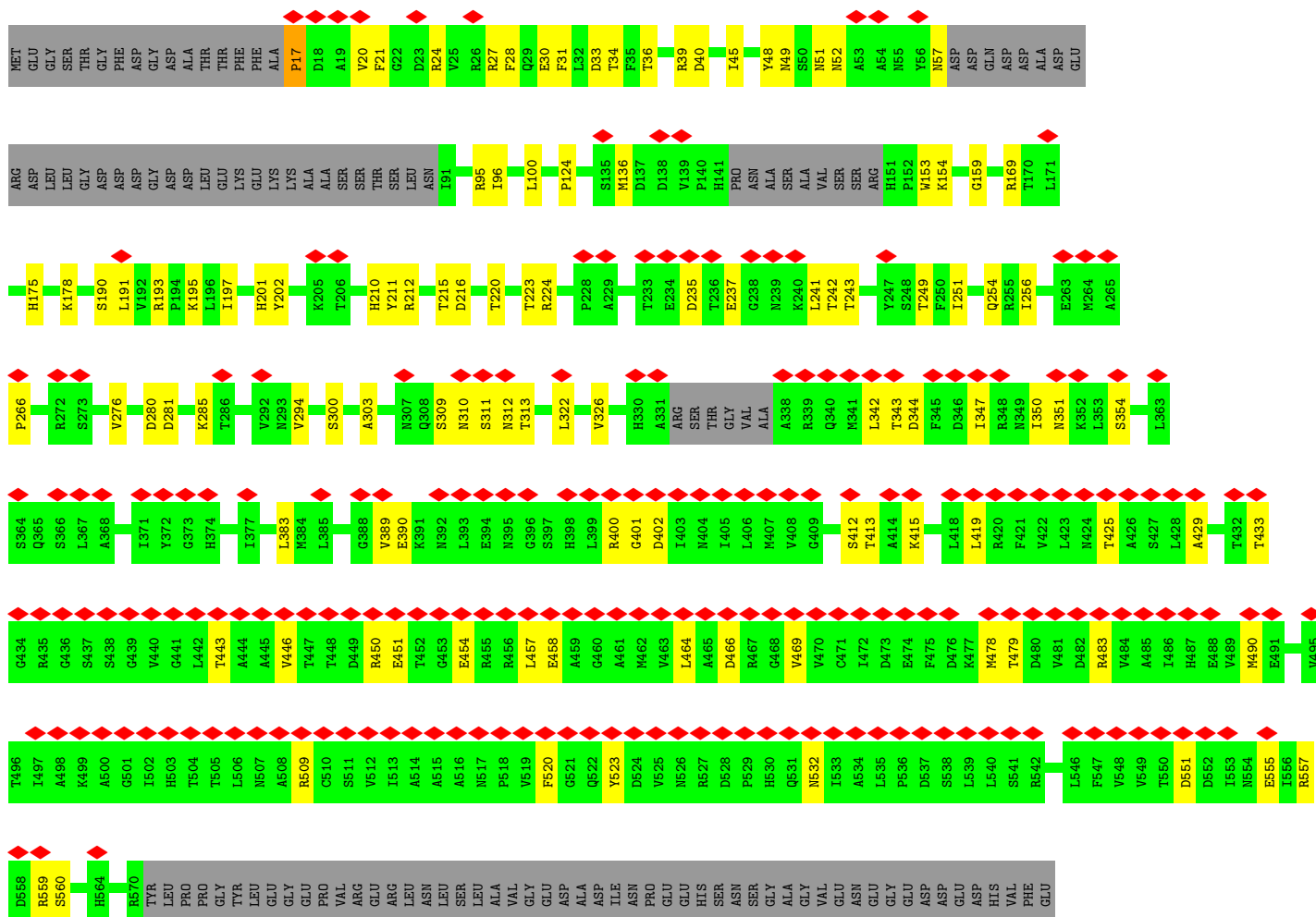


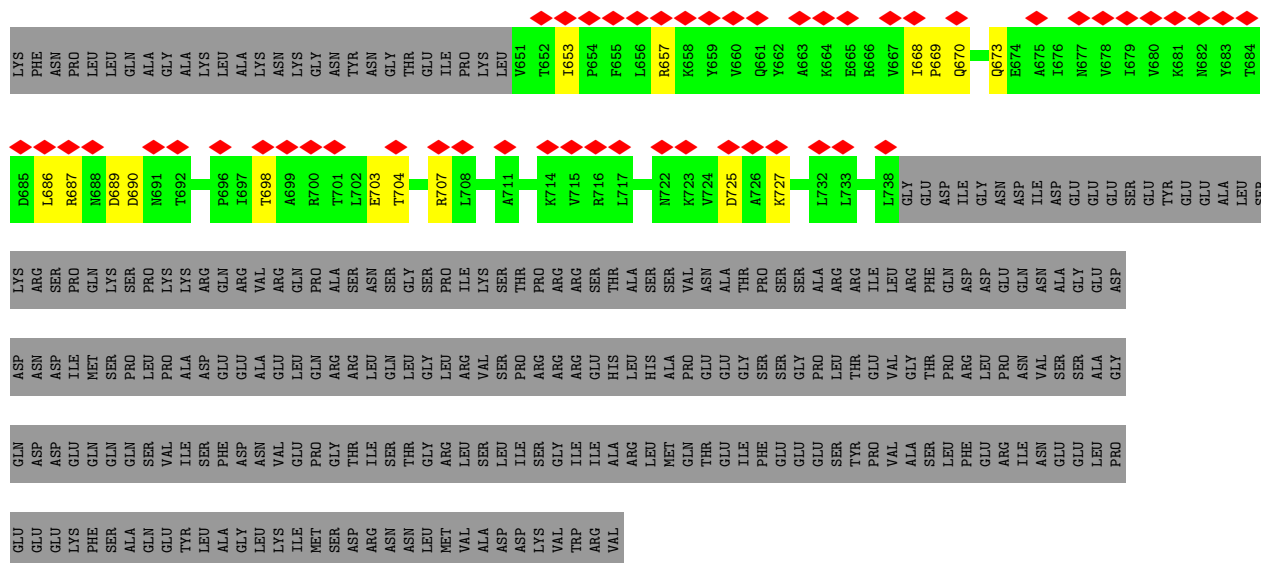
- Molecule 7: DNA replication licensing factor MCM2



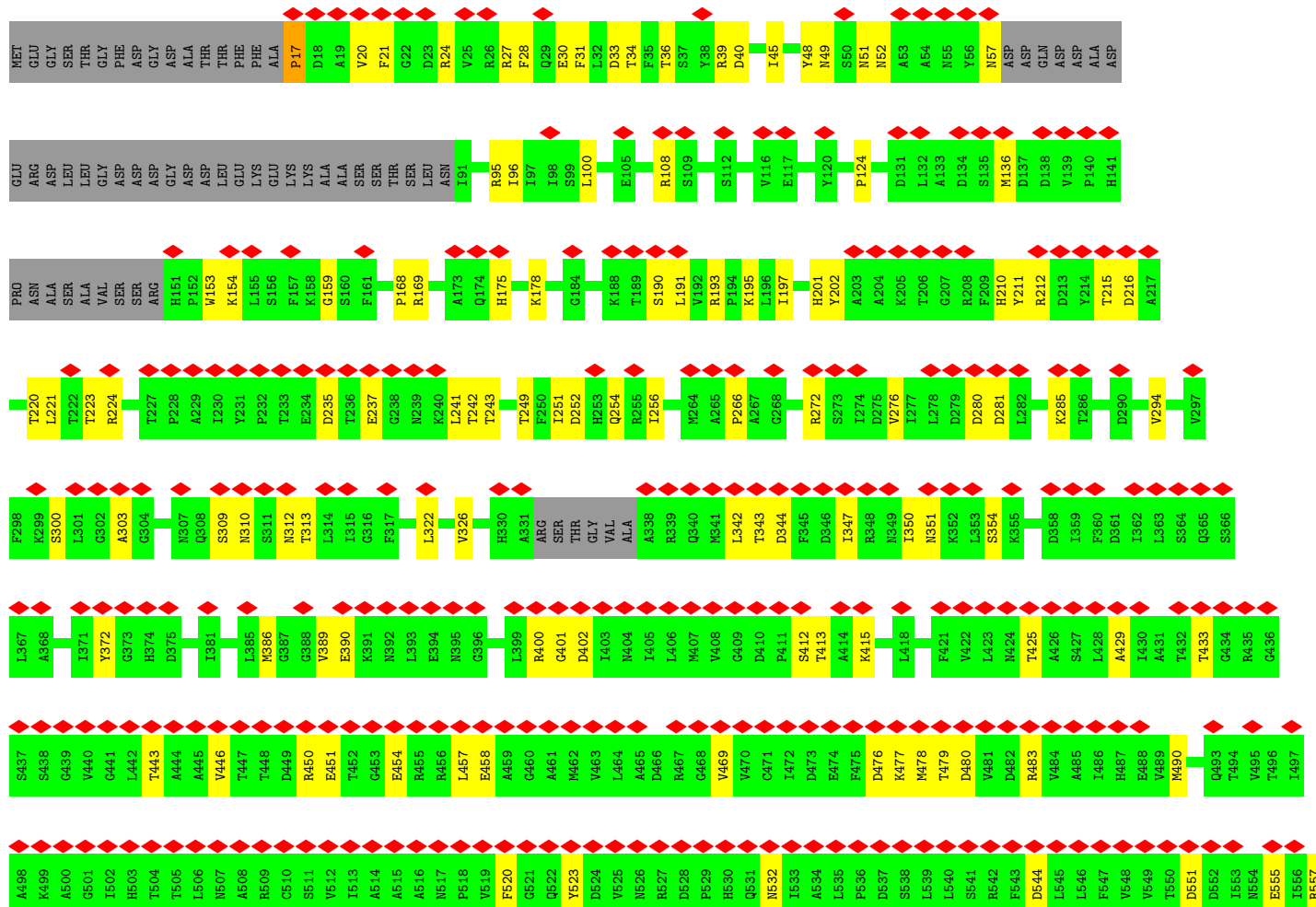


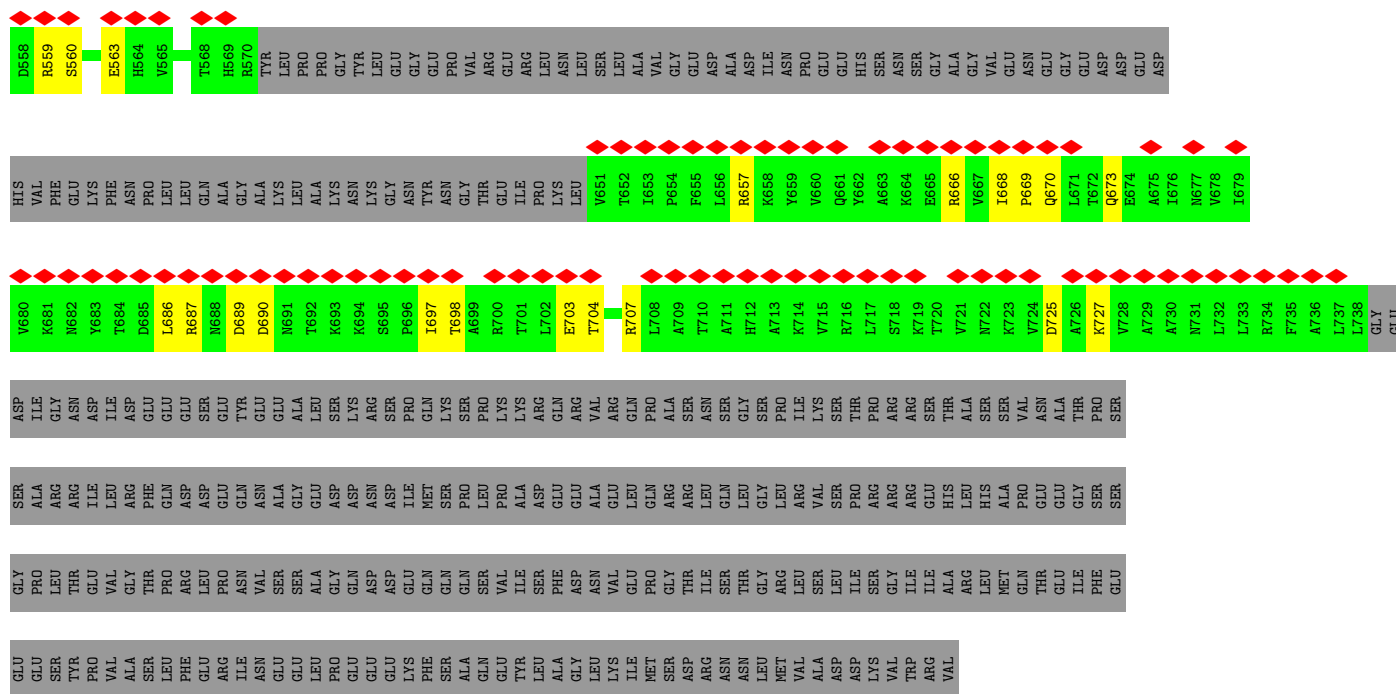
- Molecule 8: DNA replication licensing factor MCM3



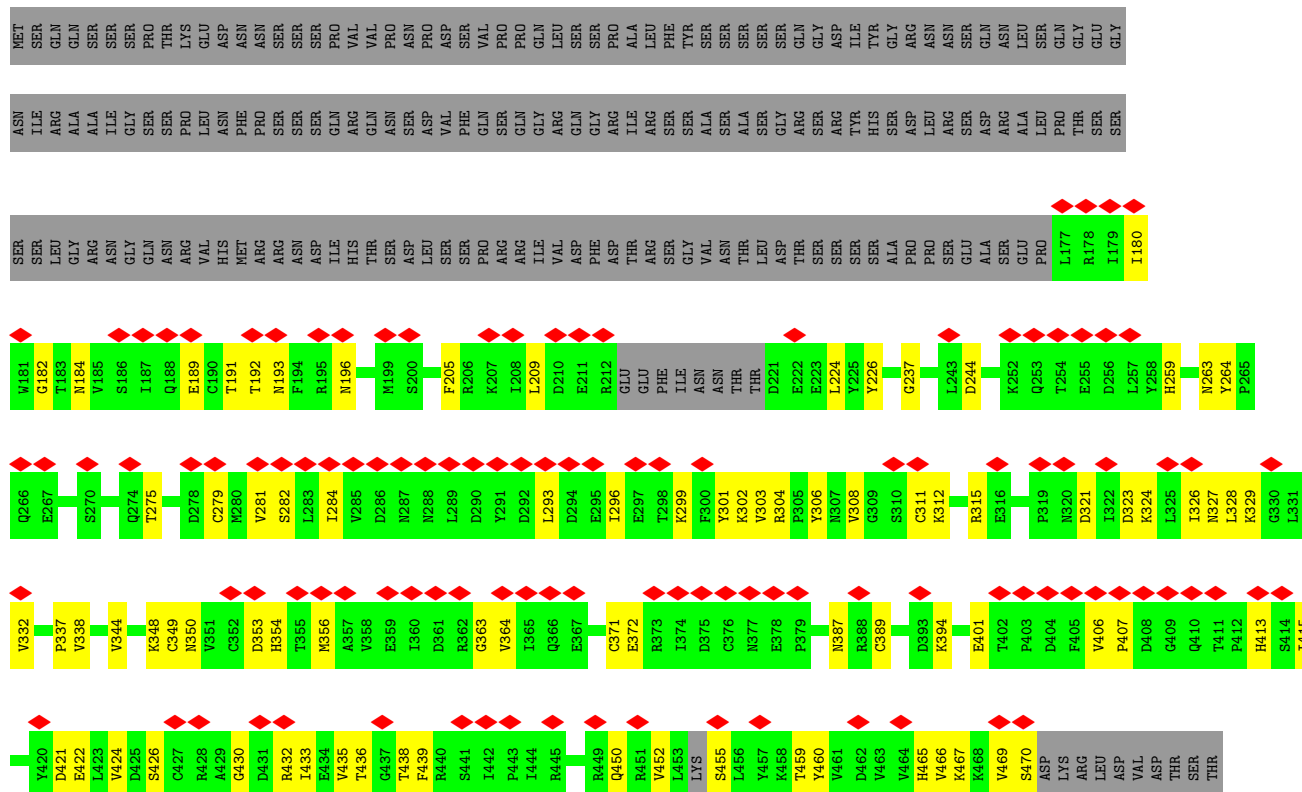


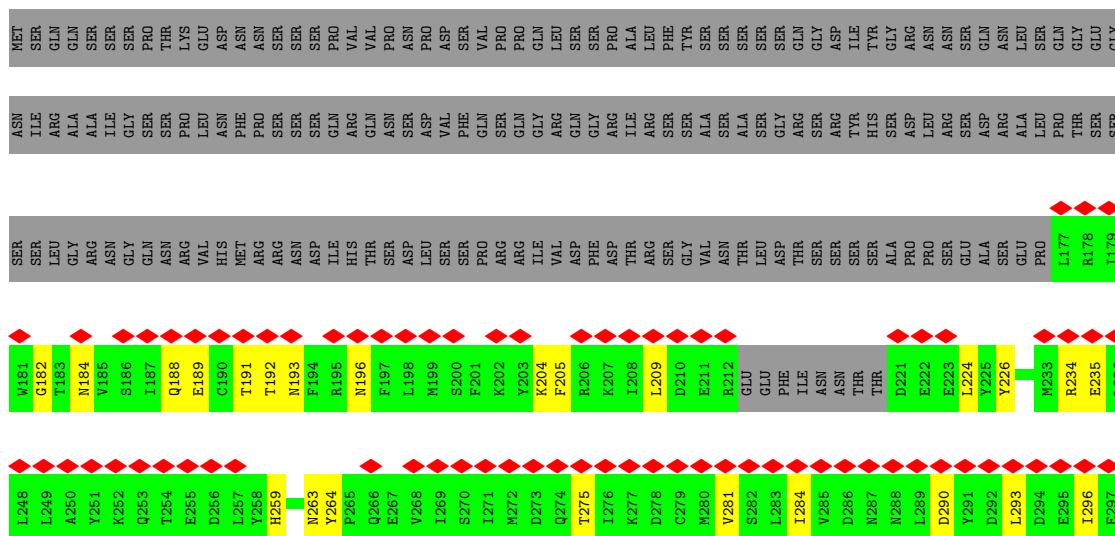
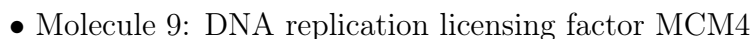
• Molecule 8: DNA replication licensing factor MCM3

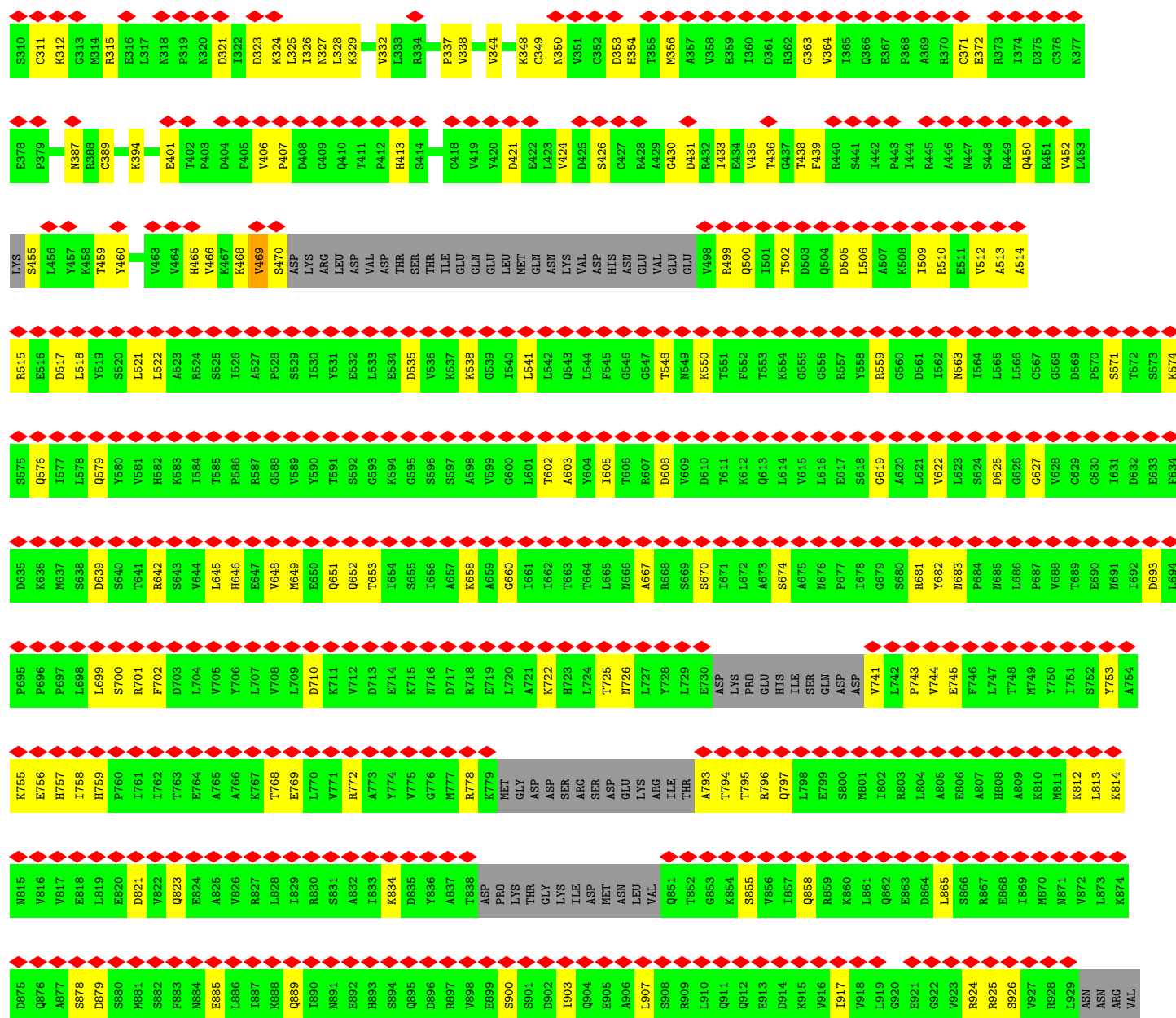




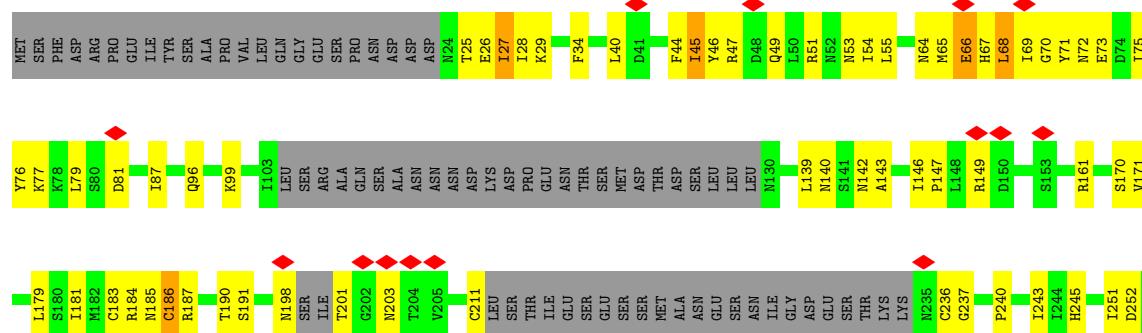
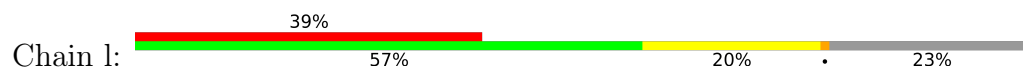
• Molecule 9: DNA replication licensing factor MCM4

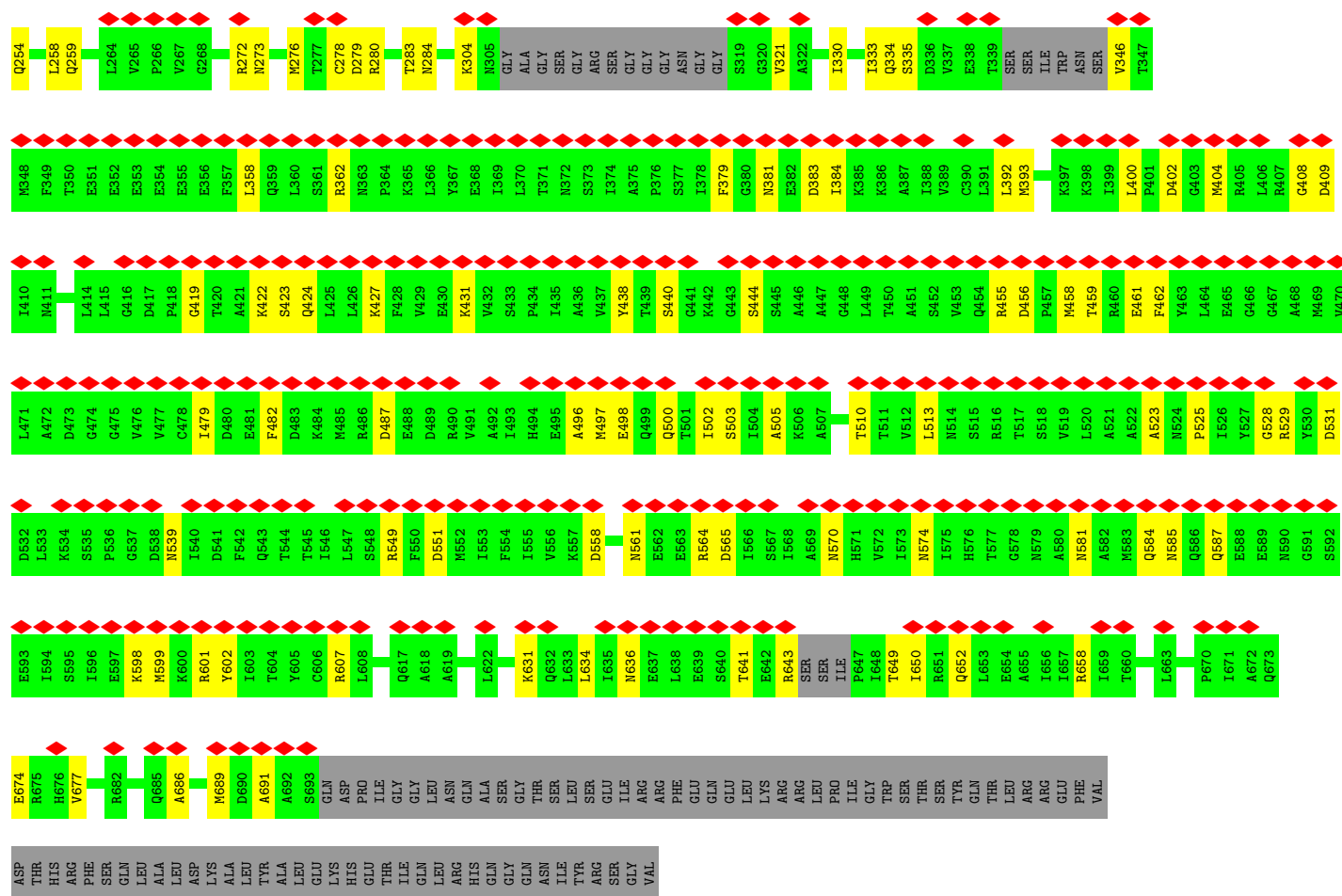




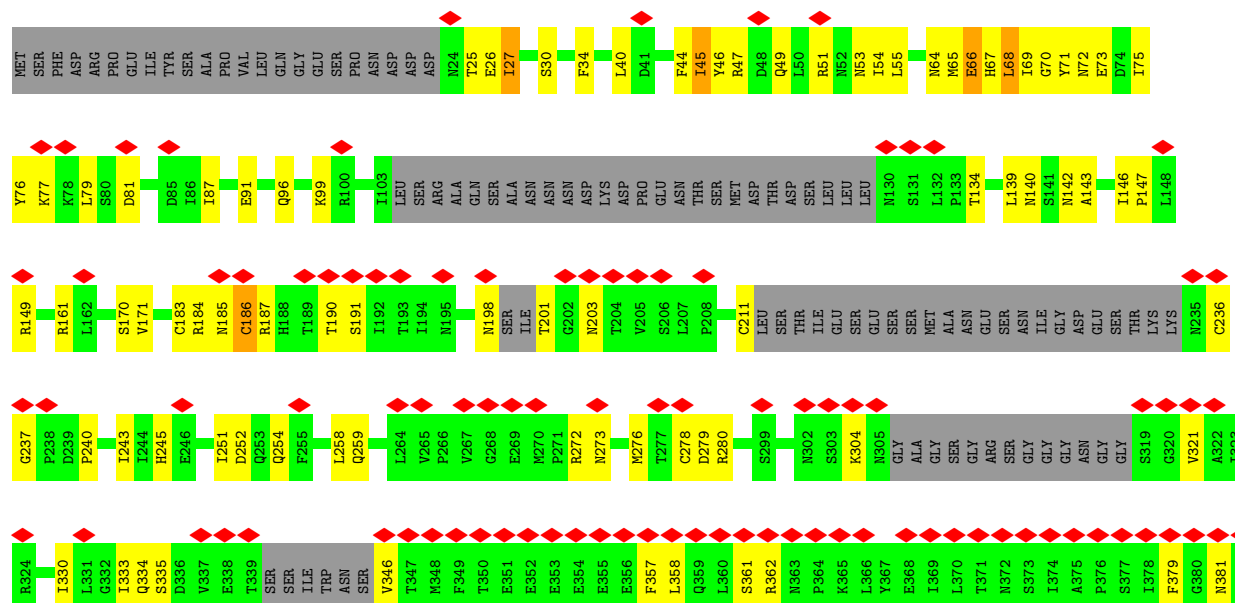
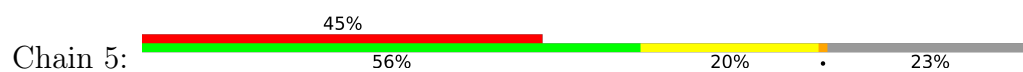


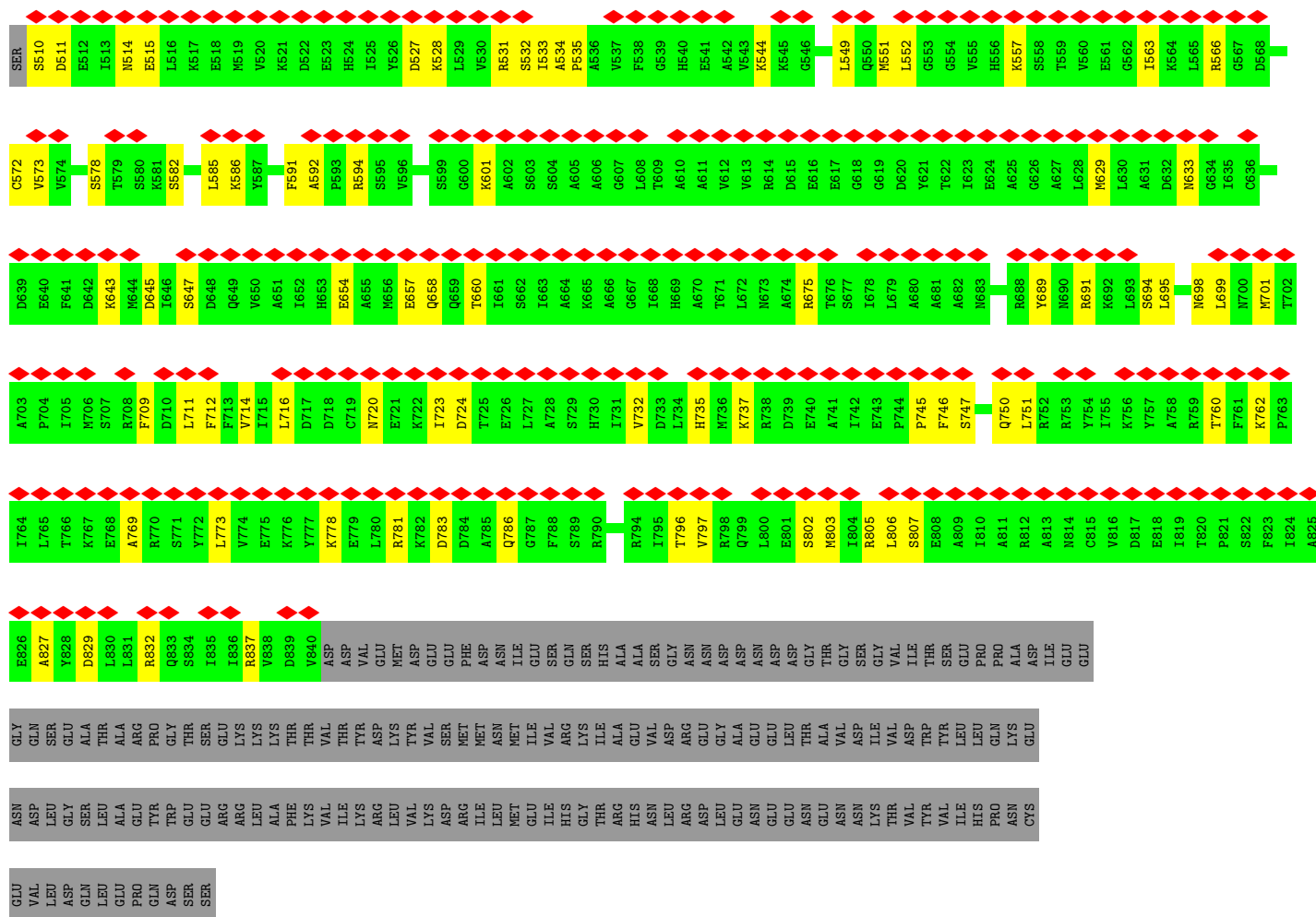
• Molecule 10: Minichromosome maintenance protein 5



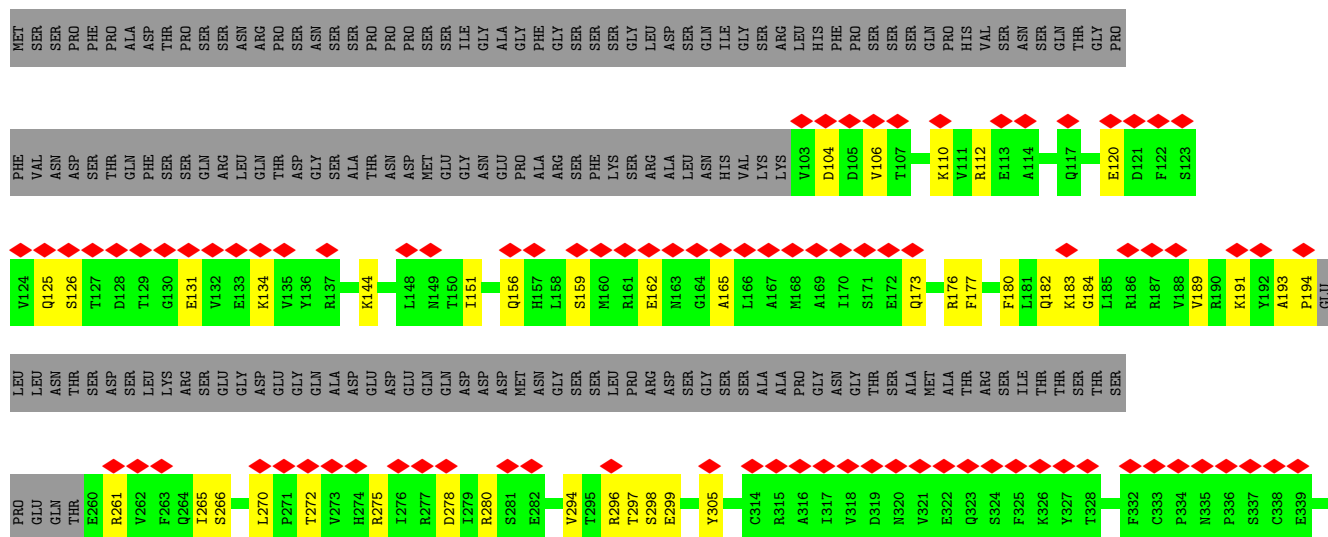


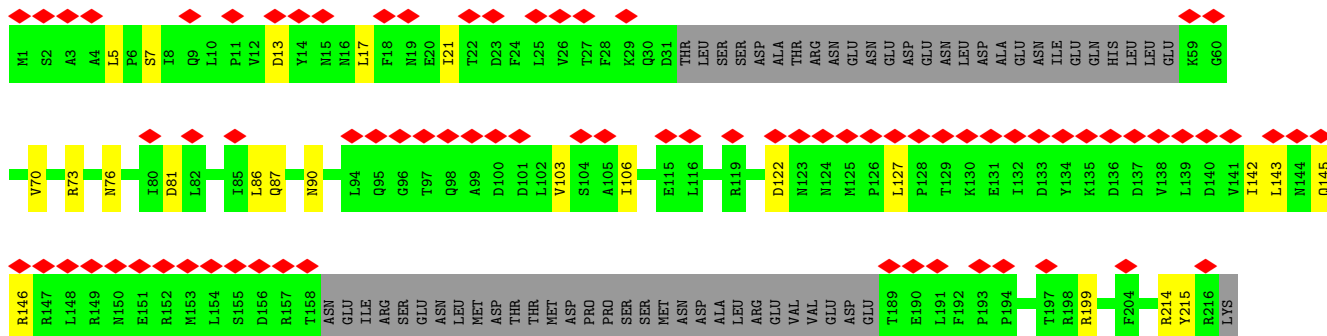
• Molecule 10: Minichromosome maintenance protein 5





● Molecule 11: DNA replication licensing factor MCM6





PRO	LYS	LEU	ALA	PRO	GLN	THR	THR	SER	K701	Y641	L581	I520	G460	R400	L331	Y267	T189
LEU	GLU	LEU	ALA	GLN	THR	THR	THR	THR	L702	I642	D582	C521	D461	V401	H334	E268	E190
ALA	ASN	ALA	ALA	VAL	ILE	ILE	THR	ASN	R703	N583	I523	C522	P462	M402	V335	V269	L191
GLN	VAL	GLN	VAL	VAL	THR	THR	THR	THR	L704	Y644	I584	I524	G463	E403	N336	F270	F192
THR	THR	THR	THR	THR	THR	THR	THR	THR	A705	A645	N585	D524	V464	L404	T337	Q271	P193
ALA	VAL	ALA	VAL	VAL	THR	THR	THR	THR	D706	K646	L586	E525	A465	I405	T338	E272	P194
SER	ARG	SER	ARG	SER	ARG	ARG	ARG	ARG	M707	T647	P587	F526	K466	T406	L339	V273	N195
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	V708	K648	A588	D527	Q468	S407	V340	N274	L196
ASN	ARG	ASN	ARG	ASN	ARG	ASN	ARG	ASN	D709	R649	A589	K528	L469	G408	R341	N275	T197
VAL	GLY	VAL	VAL	VAL	GLY	VAL	VAL	VAL	I710	P650	L590	M529	L469	D409	S342	R198	R199
ALA	THR	ALA	ALA	ALA	THR	ALA	ALA	ALA	D711	V651	L591	D530	K470	V410	L343	T277	Y200
THR	THR	THR	THR	THR	THR	THR	THR	THR	L712	M652	S592	E531	L471	Y411	S344	F278	F201
ASN	MET	ASN	GLN	ASN	THR	ASN	THR	ASN	V713	S653	R593	S532	A472	M412	P345	T279	L202
ASP	GLN	ASP	GLN	ASP	THR	ASP	GLN	ASP	E714	E654	F594	D533	I473	R413	G346	P280	L203
SER	LEU	SER	LEU	SER	LEU	SER	LEU	SER	E715	A655	D595	R534	C474	L414	D347	L281	F204
ASP	LEU	ASP	LEU	ASP	LEU	ASP	LEU	ASP	L716	V656	I596	T535	K475	A415	D350	S282	K205
GLN	SER	GLN	SER	GLN	SER	GLN	SER	GLN	V717	N657	L597	I537	I476	K416	F355	E283	P206
LEU	CYS	LEU	LEU	LEU	LEU	LEU	LEU	LEU	R718	D658	F598	I537	S477	S417	L356	C284	L207
ASP	GLN	ASP	GLN	ASP	GLN	ASP	GLN	ASP	L719	Y659	L599	H538	P478	I418	T285	S285	S208
ALA	GLU	ALA	GLU	ALA	GLU	ALA	GLU	ALA	V720	V660	M600	E539	R479	A419	P357	S286	R214
THR	THR	THR	THR	THR	THR	THR	THR	THR	R721	V661	L601	V540	G480	P420	A358	E287	Y215
THR	THR	THR	THR	THR	THR	THR	THR	THR	V722	Q662	D602	M541	V481	E421	P359	E288	R216
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	S723	L663	I603	E542	Y482	I422	T361	C289	LYS
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	L724	Y664	P604	Q543	T484	G424	G362	Q291	LYS
TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	E725	I665	S605	Q544	T484	M425	F363	Q292	ALA
HIS	HIS	LEU	LEU	ILE	ILE	ILE	ILE	ILE	S726	R666	R606	T545	G485	N425	K364	N292	T220
ILE	ILE	LEU	LEU	ILE	ILE	ILE	ILE	ILE	L727	L667	D607	I546	K486	L426	A365	Q293	P224
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	V728	R668	D608	I548	G487	D427	L366	T294	L225
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	Q729	Q669	D609	S549	S489	K429	K367	Q296	V227
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLU	D670	E610	S549	G490	K430	A368	Q297	R228
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	THR	D671	L611	K551	G491	K430	A368	M300	Q229
THR	THR	THR	THR	THR	THR	THR	THR	THR	ASN	S671	K611	A551	G490	K430	A368	S301	L235
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LYS	K672	L612	A551	G492	L432	L370	T302	G236
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	SER	R673	A613	G552	G492	L432	L370	Q237	G237
PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	LYS	E674	E614	I553	L493	L433	L371	L238	L238
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLU	M675	H615	N554	T494	L434	T372	R303	R303
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	D676	H616	N554	A495	L435	E373	S304	G236
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLU	S677	T617	T555	A496	L436	E377	S305	G237
THR	THR	THR	THR	THR	THR	THR	THR	THR	SER	K678	Y618	N558	A497	V437	A378	K306	L239
THR	THR	THR	THR	THR	THR	THR	THR	THR	PRO	F679	V619	A559	M498	V437	Q379	S308	L244
THR	THR	THR	THR	THR	THR	THR	THR	THR	LYS	H620	H620	R560	K499	G438	F310	A309	L245
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ILE	M621	M621	T561	D500	G439	Q383	S309	D250
GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	PHE	F681	H622	S562	P501	V440	H384	V251	K252
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	THR	G682	G623	I563	V502	K442	K386	V255	V255
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ILE	Q683	M623	L564	T503	R443	LYS	E256	E256
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	LYS	A684	Q625	A565	D504	V444	PHE	Q316	V255
SER	SER	SER	SER	SER	SER	SER	SER	SER	MET	P686	P626	A566	E505	G445	ALA	E317	E256
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	D627	D627	A567	M506	G445	ALA	S319	E256
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLN	T688	L628	N568	I507	D446	SER	S319	E258
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	L689	D629	P569	L508	G447	PHE	Q320	E259
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	F630	F630	L570	L508	M448	SER	Q321	V260
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	Y571	Y571	E509	E509	K449	LYS	Q321	V260
MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	T631	T631	G510	G510	K449	LYS	Q321	V260
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	G691	G691	G511	G511	K449	LYS	Q321	V260
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	I692	I692	G572	G572	K449	LYS	Q321	V260
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	I693	I693	R573	R573	K449	LYS	Q321	V260
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	R694	R694	Y574	L513	D453	E398	R329	S330
												N575	V514	D453	E398	R329	S330
												P576	L515	D453	E398	R329	S330
												R577	A516	D453	E398	R329	S330
												S579	D517	D453	E398	R329	S330
												L578	A516	D453	E398	R329	S330
												R579	A516	D453	E398	R329	S330
												P580	G519	D453	E398	R329	S330

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53853	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	0.087	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0246	Depositor
Map size (Å)	429.6, 429.6, 429.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	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: ATP

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	E	0.33	0/3501	0.99	9/4741 (0.2%)
1	F	0.33	0/3558	1.01	14/4817 (0.3%)
1	G	0.33	0/3500	1.04	14/4738 (0.3%)
2	A	0.42	0/1718	0.78	1/2314 (0.0%)
2	a	0.42	0/1718	0.78	1/2314 (0.0%)
3	B	0.49	1/1545 (0.1%)	0.76	0/2092
3	b	0.49	1/1545 (0.1%)	0.76	0/2092
4	C	0.47	0/1320	0.85	3/1784 (0.2%)
4	c	0.47	0/1320	0.85	3/1784 (0.2%)
5	D	0.40	0/1956	0.68	0/2638
5	d	0.40	0/1956	0.68	0/2638
6	H	0.43	0/4563	0.78	6/6173 (0.1%)
6	h	0.43	0/4563	0.78	6/6173 (0.1%)
7	2	0.43	0/5051	0.76	4/6821 (0.1%)
7	i	0.43	0/5051	0.76	4/6821 (0.1%)
8	3	0.43	0/4739	0.82	5/6425 (0.1%)
8	j	0.43	0/4739	0.82	5/6425 (0.1%)
9	4	0.35	0/5479	0.71	2/7392 (0.0%)
9	k	0.35	0/5479	0.71	1/7392 (0.0%)
10	5	0.47	0/4750	0.89	7/6412 (0.1%)
10	l	0.47	0/4750	0.89	7/6412 (0.1%)
11	6	0.40	0/4789	0.76	3/6466 (0.0%)
11	m	0.40	0/4789	0.76	3/6466 (0.0%)
12	7	0.34	0/5299	0.71	3/7160 (0.0%)
12	n	0.34	0/5299	0.71	3/7160 (0.0%)
All	All	0.40	2/92977 (0.0%)	0.80	104/125650 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
1	G	0	1
8	3	0	1
8	j	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	11	PHE	C-N	-7.84	1.22	1.33
3	b	11	PHE	C-N	-7.81	1.22	1.33

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	766	PHE	CA-C-N	30.20	157.59	119.84
1	G	766	PHE	C-N-CA	30.20	157.59	119.84
1	F	766	PHE	CA-C-N	29.60	156.84	119.84
1	F	766	PHE	C-N-CA	29.60	156.84	119.84
1	E	766	PHE	CA-C-N	28.90	155.96	119.84
1	E	766	PHE	C-N-CA	28.90	155.96	119.84
8	j	17	PRO	CA-C-O	-22.95	50.16	119.00
8	3	17	PRO	CA-C-O	-22.94	50.17	119.00
10	l	66	GLU	N-CA-C	14.44	127.02	111.28
10	5	66	GLU	N-CA-C	14.42	127.00	111.28
10	5	45	ILE	N-CA-C	13.99	124.89	110.62
10	l	45	ILE	N-CA-C	13.94	124.84	110.62
8	j	17	PRO	O-C-N	-13.25	101.80	123.00
8	3	17	PRO	O-C-N	-13.20	101.88	123.00
4	c	165	PHE	N-CA-C	12.11	124.56	111.36
4	C	165	PHE	N-CA-C	12.07	124.52	111.36
6	h	333	SER	N-CA-C	11.51	127.28	111.74
6	H	333	SER	N-CA-C	11.49	127.26	111.74
4	c	166	LEU	N-CA-C	10.91	123.17	111.28
4	C	166	LEU	N-CA-C	10.86	123.11	111.28
10	5	27	ILE	N-CA-C	-10.72	99.89	110.72
10	l	27	ILE	N-CA-C	-10.71	99.90	110.72
6	H	326	LEU	N-CA-C	-9.93	95.16	109.96
6	h	326	LEU	N-CA-C	-9.92	95.17	109.96
11	6	382	ARG	N-CA-C	9.41	126.21	112.94
11	m	382	ARG	N-CA-C	9.41	126.21	112.94
1	G	508	SER	N-CA-C	9.17	121.27	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	l	68	LEU	N-CA-C	-8.94	101.54	111.28
10	5	68	LEU	N-CA-C	-8.89	101.59	111.28
1	G	766	PHE	C-N-CD	-8.55	89.95	125.00
1	G	623	TYR	N-CA-C	7.74	119.71	111.28
1	G	624	ARG	N-CA-C	7.56	121.19	110.23
1	F	623	TYR	N-CA-C	7.45	123.11	114.62
4	C	105	PHE	N-CA-C	7.09	122.11	112.68
1	G	766	PHE	N-CA-C	7.07	122.45	108.59
4	c	105	PHE	N-CA-C	7.05	122.06	112.68
1	F	766	PHE	C-N-CD	-6.87	96.84	125.00
9	4	469	VAL	N-CA-C	6.86	118.74	112.29
1	G	766	PHE	CB-CA-C	-6.76	104.36	110.44
6	h	139	ILE	N-CA-C	-6.69	107.35	113.71
6	H	139	ILE	N-CA-C	-6.65	107.39	113.71
1	E	766	PHE	C-N-CD	-6.60	97.92	125.00
1	F	782	VAL	N-CA-C	-6.59	98.71	108.99
2	A	113	ILE	N-CA-C	-6.58	106.05	111.91
1	G	782	VAL	N-CA-C	-6.58	98.73	108.99
1	F	748	ALA	CA-C-N	6.57	134.09	121.54
1	F	748	ALA	C-N-CA	6.57	134.09	121.54
2	a	113	ILE	N-CA-C	-6.56	106.07	111.91
1	E	748	ALA	CA-C-N	6.55	134.04	121.54
1	E	748	ALA	C-N-CA	6.55	134.04	121.54
6	h	325	TYR	N-CA-C	-6.30	104.50	111.36
6	H	325	TYR	N-CA-C	-6.28	104.51	111.36
1	F	507	ASN	CA-C-N	6.11	133.21	121.54
1	F	507	ASN	C-N-CA	6.11	133.21	121.54
12	7	127	LEU	CA-C-N	-6.11	115.48	121.65
12	7	127	LEU	C-N-CA	-6.11	115.48	121.65
12	n	127	LEU	CA-C-N	-6.09	115.49	121.65
12	n	127	LEU	C-N-CA	-6.09	115.49	121.65
1	G	748	ALA	CA-C-N	6.06	133.11	121.54
1	G	748	ALA	C-N-CA	6.06	133.11	121.54
9	k	426	SER	N-CA-C	-5.96	106.99	114.56
7	2	433	ASN	N-CA-C	5.95	118.35	109.25
7	i	433	ASN	N-CA-C	5.93	118.32	109.25
9	4	426	SER	N-CA-C	-5.91	107.06	114.56
1	F	621	GLN	CA-C-N	5.88	132.78	121.54
1	F	621	GLN	C-N-CA	5.88	132.78	121.54
8	j	285	LYS	N-CA-C	-5.88	106.08	113.72
8	3	285	LYS	N-CA-C	-5.86	106.11	113.72
1	E	767	PRO	CA-N-CD	-5.83	103.84	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	767	PRO	CA-N-CD	-5.49	104.31	112.00
12	n	70	VAL	N-CA-C	-5.47	107.53	112.12
1	G	767	PRO	CA-N-CD	-5.42	104.42	112.00
12	7	70	VAL	N-CA-C	-5.41	107.58	112.12
1	F	766	PHE	CB-CA-C	5.37	117.92	109.27
1	G	754	CYS	N-CA-C	5.37	116.95	108.96
1	G	621	GLN	N-CA-C	-5.36	99.70	108.76
10	5	186	CYS	N-CA-C	-5.30	107.83	114.56
8	j	309	SER	CA-C-N	5.25	131.58	121.54
8	j	309	SER	C-N-CA	5.25	131.58	121.54
8	3	309	SER	CA-C-N	5.25	131.57	121.54
8	3	309	SER	C-N-CA	5.25	131.57	121.54
10	l	186	CYS	N-CA-C	-5.25	107.90	114.56
7	i	768	HIS	CA-C-N	-5.19	114.35	122.65
7	i	768	HIS	C-N-CA	-5.19	114.35	122.65
10	l	66	GLU	CA-C-N	-5.19	112.06	121.14
10	l	66	GLU	C-N-CA	-5.19	112.06	121.14
7	2	768	HIS	CA-C-N	-5.17	114.39	122.65
7	2	768	HIS	C-N-CA	-5.17	114.39	122.65
1	E	584	THR	N-CA-C	-5.16	101.15	109.82
7	2	755	ILE	N-CA-C	-5.16	108.09	113.10
10	5	66	GLU	CA-C-N	-5.16	112.11	121.14
10	5	66	GLU	C-N-CA	-5.16	112.11	121.14
1	F	725	ASN	N-CA-C	5.15	118.66	112.38
7	i	755	ILE	N-CA-C	-5.07	108.18	113.10
11	m	385	SER	CA-C-N	5.05	127.47	120.49
11	m	385	SER	C-N-CA	5.05	127.47	120.49
11	6	385	SER	CA-C-N	5.04	127.44	120.49
11	6	385	SER	C-N-CA	5.04	127.44	120.49
1	E	819	VAL	CA-C-N	5.03	127.27	120.38
1	E	819	VAL	C-N-CA	5.03	127.27	120.38
6	H	339	TYR	CA-C-N	-5.02	113.93	122.56
6	H	339	TYR	C-N-CA	-5.02	113.93	122.56
6	h	339	TYR	CA-C-N	-5.01	113.94	122.56
6	h	339	TYR	C-N-CA	-5.01	113.94	122.56

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	3	17	PRO	Mainchain
1	E	766	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	F	766	PHE	Peptide
1	G	766	PHE	Peptide
8	j	17	PRO	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3416	0	3353	83	0
1	F	3472	0	3418	59	0
1	G	3416	0	3352	201	0
2	A	1696	0	1698	52	0
2	a	1696	0	1698	53	0
3	B	1513	0	1558	77	0
3	b	1513	0	1557	85	0
4	C	1288	0	1298	47	0
4	c	1288	0	1298	44	0
5	D	1924	0	1926	48	0
5	d	1924	0	1926	59	0
6	H	4482	0	4499	167	0
6	h	4482	0	4498	157	0
7	2	4970	0	4981	112	0
7	i	4970	0	4981	119	0
8	3	4659	0	4720	98	0
8	j	4659	0	4720	93	0
9	4	5410	0	5490	146	0
9	k	5410	0	5490	138	0
10	5	4688	0	4750	190	0
10	l	4688	0	4750	192	0
11	6	4720	0	4663	104	0
11	m	4720	0	4663	102	0
12	7	5220	0	5296	104	0
12	n	5220	0	5296	98	0
13	2	31	0	12	1	0
13	3	31	0	12	5	0
13	5	31	0	12	5	0
13	i	31	0	12	1	0
13	j	31	0	12	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	l	31	0	12	5	0
All	All	91630	0	91951	2274	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 12.

All (2274) 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)
1:G:729:TRP:CH2	1:G:786:LEU:CD1	1.75	1.64
1:G:729:TRP:CH2	1:G:786:LEU:HD13	1.09	1.60
10:l:186:CYS:SG	10:l:236:CYS:HB2	1.44	1.57
10:5:186:CYS:SG	10:5:236:CYS:HB2	1.44	1.54
1:G:729:TRP:CZ3	1:G:786:LEU:HD13	1.48	1.46
1:G:727:GLU:OE2	1:G:777:ARG:CB	1.68	1.39
1:G:521:GLY:CA	3:b:84:LYS:HD3	1.54	1.37
1:F:603:PHE:CE1	1:G:880:GLU:O	1.79	1.34
1:G:729:TRP:CZ3	1:G:786:LEU:CD1	2.05	1.34
10:5:599:MET:HA	10:5:602:TYR:CE2	1.62	1.33
1:G:727:GLU:OE2	1:G:777:ARG:HB2	1.18	1.33
1:G:727:GLU:OE2	1:G:777:ARG:CG	1.76	1.31
10:l:599:MET:HA	10:l:602:TYR:CE2	1.62	1.31
10:5:68:LEU:O	10:5:72:ASN:HB2	1.13	1.31
1:E:518:PHE:O	3:B:30:ARG:NH1	1.63	1.29
10:l:68:LEU:O	10:l:72:ASN:HB2	1.14	1.28
10:l:186:CYS:SG	10:l:236:CYS:CB	2.22	1.28
10:5:186:CYS:SG	10:5:236:CYS:CB	2.22	1.27
11:m:381:LEU:HD13	11:m:385:SER:OG	1.15	1.26
10:l:66:GLU:O	10:l:69:ILE:CG1	1.84	1.26
1:G:770:LEU:HD12	3:b:134:PHE:CD1	1.71	1.25
1:E:527:HIS:CD2	6:H:301:ARG:HH22	1.54	1.25
11:6:381:LEU:HD13	11:6:385:SER:OG	1.15	1.25
10:5:66:GLU:O	10:5:69:ILE:CG1	1.84	1.24
1:F:571:PRO:CB	1:G:781:PHE:O	1.86	1.24
10:5:66:GLU:C	10:5:69:ILE:HG12	1.64	1.23
1:G:723:ASP:CB	1:G:779:PRO:HB3	1.69	1.23
1:G:525:GLU:O	6:h:263:GLY:HA3	1.31	1.23
1:F:603:PHE:CD1	1:G:881:LYS:HA	1.72	1.23
10:5:68:LEU:O	10:5:72:ASN:CB	1.87	1.22
1:G:770:LEU:HD21	3:b:133:ASP:CB	1.69	1.22
10:l:66:GLU:C	10:l:69:ILE:HG12	1.64	1.22

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:68:LEU:O	10:l:72:ASN:CB	1.88	1.21
1:F:571:PRO:HB3	1:G:781:PHE:O	1.38	1.21
11:6:381:LEU:CD1	11:6:385:SER:OG	1.90	1.20
11:m:381:LEU:CD1	11:m:385:SER:OG	1.90	1.19
1:G:729:TRP:HH2	1:G:786:LEU:CD1	1.26	1.19
1:G:770:LEU:CD2	3:b:133:ASP:HB2	1.73	1.18
9:4:431:ASP:OD2	9:4:468:LYS:HE2	1.44	1.18
1:E:525:GLU:O	6:H:263:GLY:HA3	1.43	1.17
1:E:527:HIS:CD2	6:H:301:ARG:HH12	1.63	1.17
1:G:521:GLY:HA3	3:b:84:LYS:CD	1.74	1.17
7:2:431:LYS:HD2	7:2:433:ASN:ND2	1.61	1.16
1:G:776:ILE:C	1:G:777:ARG:N	2.04	1.15
7:i:431:LYS:HD2	7:i:433:ASN:ND2	1.61	1.14
10:l:66:GLU:O	10:l:69:ILE:HG12	0.96	1.13
1:E:527:HIS:NE2	6:H:301:ARG:NH2	1.95	1.13
1:E:521:GLY:HA3	3:B:84:LYS:NZ	1.62	1.13
1:G:525:GLU:O	6:h:262:ILE:O	1.68	1.12
10:5:66:GLU:O	10:5:69:ILE:HG12	0.96	1.12
1:E:527:HIS:CD2	6:H:301:ARG:NH2	2.17	1.12
1:E:525:GLU:O	6:H:262:ILE:O	1.69	1.11
1:G:770:LEU:HD12	3:b:134:PHE:HD1	0.92	1.09
1:E:770:LEU:HD11	3:B:133:ASP:HB2	1.10	1.09
1:E:770:LEU:CD1	3:B:133:ASP:HB2	1.83	1.09
1:G:775:GLU:HG3	1:G:777:ARG:HH12	1.16	1.08
10:l:66:GLU:HA	10:l:69:ILE:CD1	1.85	1.07
1:G:729:TRP:CH2	1:G:786:LEU:HD12	1.78	1.07
10:5:66:GLU:HA	10:5:69:ILE:CD1	1.84	1.07
1:E:491:ARG:NH1	6:H:303:THR:HB	1.70	1.07
1:G:733:GLY:C	1:G:815:ILE:N	1.93	1.07
1:E:753[A]:ASN:HB3	3:B:66:MET:HE1	1.35	1.06
1:F:603:PHE:CD2	1:G:884:SER:HB3	1.90	1.06
1:E:527:HIS:CD2	6:H:301:ARG:NH1	2.24	1.06
1:F:603:PHE:CE1	1:G:880:GLU:C	2.32	1.06
1:G:775:GLU:CG	1:G:777:ARG:HH12	1.68	1.06
9:4:433:ILE:CD1	9:4:468:LYS:HB3	1.86	1.05
10:l:66:GLU:HA	10:l:69:ILE:HD13	1.36	1.02
9:k:432:ARG:CB	9:k:469:VAL:HB	1.90	1.02
1:G:904:ARG:NH1	5:d:3:ILE:HG23	1.74	1.02
10:5:66:GLU:HA	10:5:69:ILE:HD13	1.37	1.01
1:E:491:ARG:NH1	6:H:303:THR:O	1.92	1.01
10:l:186:CYS:CB	10:l:236:CYS:HB2	1.91	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:730:LYS:HD2	1:G:817:ILE:HD13	1.43	0.99
10:l:25:THR:OG1	10:l:26:GLU:OE2	1.79	0.99
10:5:186:CYS:CB	10:5:236:CYS:HB2	1.92	0.99
1:G:730:LYS:CD	1:G:817:ILE:HD11	1.92	0.99
1:G:525:GLU:HB3	6:h:263:GLY:O	1.62	0.99
1:G:775:GLU:HG3	1:G:777:ARG:NH1	1.78	0.99
1:G:770:LEU:CD1	3:b:134:PHE:HD1	1.74	0.98
10:5:27:ILE:HD12	10:5:27:ILE:H	1.22	0.98
10:l:27:ILE:H	10:l:27:ILE:HD12	1.22	0.98
1:G:723:ASP:HB2	1:G:779:PRO:HB3	1.41	0.98
10:l:66:GLU:CA	10:l:69:ILE:CD1	2.41	0.98
10:5:25:THR:OG1	10:5:26:GLU:OE2	1.79	0.98
3:B:28:PHE:CE2	3:B:88:VAL:HB	1.99	0.98
3:b:28:PHE:CE2	3:b:88:VAL:HB	1.98	0.98
6:h:370:LEU:HD13	10:l:161:ARG:HB3	1.43	0.98
1:G:770:LEU:HG	3:b:133:ASP:O	1.64	0.97
10:5:66:GLU:CA	10:5:69:ILE:CD1	2.41	0.97
10:5:186:CYS:HG	10:5:236:CYS:CB	1.69	0.97
1:E:527:HIS:HD2	6:H:301:ARG:HH12	1.09	0.96
6:H:370:LEU:HD13	10:5:161:ARG:HB3	1.43	0.96
1:E:524:ARG:NH2	6:H:13:ASN:HD21	1.62	0.96
1:E:746:ALA:HB3	3:B:66:MET:HE3	1.45	0.96
9:4:431:ASP:OD2	9:4:468:LYS:CE	2.13	0.96
1:G:525:GLU:O	6:h:263:GLY:CA	2.12	0.96
1:G:519:ASP:OD1	3:b:84:LYS:HE3	1.66	0.95
9:k:432:ARG:HB3	9:k:469:VAL:HB	1.48	0.95
10:l:66:GLU:CB	10:l:69:ILE:HD11	1.97	0.95
10:l:186:CYS:SG	10:l:236:CYS:CA	2.55	0.95
1:F:605:VAL:HG22	1:G:885:LEU:HD21	1.46	0.94
7:i:434:TYR:HD2	7:i:436:GLY:N	1.66	0.94
10:5:66:GLU:CB	10:5:69:ILE:HD11	1.97	0.94
10:5:186:CYS:SG	10:5:236:CYS:CA	2.55	0.94
1:G:733:GLY:O	1:G:815:ILE:HD13	1.68	0.94
1:F:571:PRO:CG	1:G:781:PHE:O	2.14	0.93
1:G:730:LYS:CD	1:G:817:ILE:CD1	2.46	0.93
1:G:773:GLU:OE2	3:b:66:MET:C	2.11	0.93
7:2:431:LYS:HD2	7:2:433:ASN:HD22	1.32	0.93
1:G:730:LYS:HD2	1:G:817:ILE:CD1	1.97	0.93
7:2:434:TYR:HD2	7:2:436:GLY:N	1.65	0.92
10:5:599:MET:HA	10:5:602:TYR:HE2	1.20	0.92
1:G:512:SER:OG	6:h:301:ARG:HG3	1.69	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:730:LYS:CG	1:G:817:ILE:HD11	2.00	0.92
1:G:770:LEU:HD21	3:b:133:ASP:HB2	0.92	0.92
10:l:599:MET:HA	10:l:602:TYR:HE2	1.20	0.92
1:E:521:GLY:HA3	3:B:84:LYS:HZ2	1.26	0.91
10:5:66:GLU:HA	10:5:69:ILE:CG1	2.01	0.91
1:E:491:ARG:HH11	6:H:303:THR:HB	1.23	0.90
1:E:527:HIS:CD2	6:H:301:ARG:CZ	2.53	0.90
10:l:186:CYS:HG	10:l:236:CYS:HB2	1.25	0.90
1:F:603:PHE:CE2	1:G:884:SER:HB3	2.06	0.90
10:l:66:GLU:HA	10:l:69:ILE:CG1	2.01	0.90
1:E:518:PHE:HD1	3:B:30:ARG:NH2	1.71	0.89
1:F:603:PHE:CD2	1:G:884:SER:CB	2.55	0.89
1:F:603:PHE:O	1:G:881:LYS:HE3	1.73	0.89
1:G:770:LEU:HG	3:b:134:PHE:HA	1.55	0.88
10:5:66:GLU:O	10:5:70:GLY:N	2.06	0.88
1:E:525:GLU:HB3	6:H:263:GLY:O	1.74	0.88
1:G:730:LYS:HG2	1:G:817:ILE:HD11	1.52	0.88
10:5:258:LEU:CD1	10:5:276:MET:HE1	2.03	0.88
10:5:258:LEU:HD13	10:5:276:MET:HE1	1.55	0.88
3:B:28:PHE:HE2	3:B:88:VAL:HB	1.39	0.88
10:l:186:CYS:HG	10:l:236:CYS:CB	1.77	0.88
10:l:258:LEU:HD13	10:l:276:MET:HE1	1.55	0.88
11:6:381:LEU:HD13	11:6:385:SER:CB	2.04	0.87
10:l:258:LEU:CD1	10:l:276:MET:HE1	2.03	0.87
10:l:66:GLU:O	10:l:70:GLY:N	2.06	0.87
11:m:381:LEU:HD13	11:m:385:SER:CB	2.04	0.87
10:5:66:GLU:CA	10:5:69:ILE:HD13	2.03	0.87
7:i:431:LYS:HD2	7:i:433:ASN:HD22	1.32	0.87
1:E:753[A]:ASN:HB3	3:B:66:MET:CE	2.03	0.86
1:G:525:GLU:O	6:h:262:ILE:C	2.18	0.86
10:5:186:CYS:HG	10:5:236:CYS:HB2	1.20	0.86
1:F:598:ARG:HH12	1:G:780:VAL:CG1	1.88	0.86
1:G:733:GLY:C	1:G:815:ILE:H	1.82	0.86
1:E:521:GLY:N	3:B:84:LYS:HD3	1.91	0.85
1:F:603:PHE:CD1	1:G:881:LYS:CA	2.56	0.85
1:G:723:ASP:HB2	1:G:779:PRO:CB	2.05	0.85
1:G:519:ASP:OD1	3:b:84:LYS:CE	2.25	0.85
9:k:432:ARG:HB2	9:k:469:VAL:HB	1.58	0.85
3:b:28:PHE:HE2	3:b:88:VAL:HB	1.39	0.84
11:6:806:LEU:HD11	11:6:827:ALA:HB1	1.59	0.84
1:E:525:GLU:O	6:H:263:GLY:CA	2.25	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:723:ASP:HB3	1:G:779:PRO:HB3	1.59	0.84
1:G:729:TRP:HZ3	1:G:786:LEU:CD1	1.86	0.84
1:G:525:GLU:C	6:h:263:GLY:HA3	2.01	0.84
10:l:66:GLU:CA	10:l:69:ILE:HD13	2.03	0.84
11:m:806:LEU:HD11	11:m:827:ALA:HB1	1.59	0.83
1:E:521:GLY:H	3:B:84:LYS:HE3	1.40	0.83
1:G:727:GLU:OE2	1:G:777:ARG:HG2	1.74	0.83
1:G:904:ARG:HH12	5:d:3:ILE:HG23	1.43	0.83
1:G:524:ARG:HD2	6:h:262:ILE:HG23	1.61	0.83
1:F:603:PHE:HD1	1:G:881:LYS:HA	1.42	0.82
1:G:729:TRP:HH2	1:G:786:LEU:CG	1.91	0.82
7:2:434:TYR:CD2	7:2:436:GLY:N	2.47	0.82
1:E:770:LEU:HD11	3:B:133:ASP:CB	2.03	0.82
1:E:505:VAL:HG11	6:H:300:LYS:O	1.80	0.82
10:l:66:GLU:CB	10:l:69:ILE:CD1	2.58	0.82
1:E:514:THR:OG1	6:H:301:ARG:HD3	1.80	0.82
10:5:66:GLU:CA	10:5:69:ILE:HG12	2.10	0.82
1:G:521:GLY:HA3	3:b:84:LYS:HD3	0.82	0.82
10:5:66:GLU:CB	10:5:69:ILE:CD1	2.58	0.82
7:i:434:TYR:CD2	7:i:436:GLY:N	2.48	0.81
1:G:727:GLU:OE2	1:G:777:ARG:HG3	1.78	0.81
10:l:66:GLU:CA	10:l:69:ILE:HG12	2.10	0.81
7:i:434:TYR:HD2	7:i:436:GLY:H	1.27	0.81
1:F:603:PHE:HE1	1:G:880:GLU:C	1.86	0.81
1:F:605:VAL:HG21	1:G:885:LEU:HD23	1.62	0.81
1:F:603:PHE:CZ	1:G:880:GLU:O	2.34	0.80
7:2:434:TYR:HD2	7:2:436:GLY:H	1.27	0.80
1:F:603:PHE:HB3	1:G:881:LYS:HG3	1.63	0.79
1:F:605:VAL:CG2	1:G:885:LEU:HD21	2.13	0.79
1:G:733:GLY:O	1:G:815:ILE:N	2.15	0.79
1:F:563:HIS:CE1	1:G:880:GLU:OE1	2.35	0.79
1:E:521:GLY:HA3	3:B:84:LYS:CE	2.11	0.79
10:5:598:LYS:O	10:5:602:TYR:HD2	1.66	0.78
1:G:514:THR:OG1	6:h:301:ARG:HD3	1.83	0.78
10:l:598:LYS:O	10:l:602:TYR:HD2	1.66	0.78
1:E:525:GLU:O	6:H:262:ILE:C	2.27	0.78
10:l:65:MET:O	10:l:69:ILE:HG23	1.83	0.78
1:G:512:SER:OG	6:h:301:ARG:CG	2.31	0.77
1:G:521:GLY:N	3:b:84:LYS:HD3	1.99	0.77
1:E:769:PRO:HB3	3:B:135:HIS:HB3	1.66	0.77
10:5:65:MET:O	10:5:69:ILE:HG23	1.83	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:770:LEU:HG	3:B:133:ASP:O	1.84	0.77
1:E:491:ARG:HH11	6:H:303:THR:CB	1.98	0.77
1:G:708:SER:HB2	1:G:836:LEU:HD21	1.67	0.77
1:G:729:TRP:CZ3	1:G:786:LEU:HD11	2.19	0.77
1:E:524:ARG:HH22	6:H:13:ASN:HD21	1.28	0.77
1:F:563:HIS:ND1	1:G:880:GLU:OE1	2.17	0.77
7:i:431:LYS:CD	7:i:433:ASN:HD22	1.97	0.76
9:k:602:THR:HG22	9:k:619:GLY:N	2.01	0.76
1:E:527:HIS:HE2	6:H:301:ARG:HH22	1.28	0.76
1:G:773:GLU:OE2	3:b:67:ARG:N	2.19	0.76
7:2:431:LYS:CD	7:2:433:ASN:HD22	1.97	0.76
9:4:433:ILE:HD12	9:4:468:LYS:HB3	1.66	0.76
9:4:602:THR:HG22	9:4:619:GLY:N	2.01	0.76
10:5:25:THR:C	10:5:27:ILE:HD12	2.11	0.76
10:l:25:THR:C	10:l:27:ILE:HD12	2.11	0.76
10:l:598:LYS:O	10:l:602:TYR:CD2	2.39	0.76
1:F:605:VAL:CG2	1:G:885:LEU:CD2	2.63	0.76
6:H:370:LEU:HD13	10:5:161:ARG:CB	2.16	0.76
1:F:606:PRO:HG3	1:G:824:GLU:HG3	1.67	0.75
1:G:864:LYS:HE3	5:d:9:LEU:CD1	2.15	0.75
1:G:770:LEU:CD1	3:b:134:PHE:HA	2.16	0.75
9:4:431:ASP:OD2	9:4:468:LYS:HB2	1.85	0.75
10:5:598:LYS:O	10:5:602:TYR:CD2	2.39	0.75
10:5:66:GLU:CA	10:5:69:ILE:CG1	2.65	0.75
1:E:521:GLY:CA	3:B:84:LYS:HZ2	1.99	0.75
1:G:770:LEU:CG	3:b:134:PHE:HA	2.16	0.75
1:F:607:PHE:O	1:G:828:LEU:HD22	1.86	0.74
1:G:770:LEU:CG	3:b:133:ASP:O	2.35	0.74
10:5:599:MET:CA	10:5:602:TYR:CE2	2.58	0.74
10:l:66:GLU:HB3	10:l:69:ILE:HD11	1.69	0.74
10:5:27:ILE:H	10:5:27:ILE:CD1	1.99	0.74
10:5:66:GLU:HB3	10:5:69:ILE:HD11	1.69	0.74
1:G:723:ASP:HB2	1:G:779:PRO:CG	2.18	0.74
6:h:370:LEU:CD1	10:l:161:ARG:HB3	2.18	0.74
1:E:491:ARG:NH1	6:H:303:THR:CB	2.50	0.74
10:l:599:MET:CA	10:l:602:TYR:CE2	2.58	0.74
6:h:370:LEU:HD13	10:l:161:ARG:CB	2.16	0.74
1:G:733:GLY:O	1:G:814:GLU:C	2.26	0.73
1:G:749:TYR:CE2	1:G:848:TYR:HE2	2.05	0.73
6:H:370:LEU:CD1	10:5:161:ARG:HB3	2.18	0.73
1:G:901:ILE:HG23	5:d:3:ILE:HD12	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5:64:ASN:CG	10:5:65:MET:HG3	2.13	0.73
10:l:64:ASN:CG	10:l:65:MET:HG3	2.13	0.73
1:E:769:PRO:CB	3:B:135:HIS:HB3	2.19	0.72
11:m:381:LEU:HD12	11:m:381:LEU:C	2.15	0.72
1:G:518:PHE:HB3	3:b:30:ARG:NH2	2.05	0.72
11:6:381:LEU:C	11:6:381:LEU:HD12	2.15	0.72
6:h:416:ARG:N	10:l:66:GLU:OE2	2.23	0.72
1:G:864:LYS:HE3	5:d:9:LEU:HD11	1.72	0.72
1:G:775:GLU:CG	1:G:777:ARG:NH1	2.44	0.71
7:2:431:LYS:HD2	7:2:433:ASN:HD21	1.53	0.71
1:G:770:LEU:HD21	3:b:133:ASP:C	2.14	0.71
1:G:775:GLU:HG2	1:G:777:ARG:HH12	1.53	0.71
9:4:433:ILE:CD1	9:4:468:LYS:CB	2.64	0.71
9:4:433:ILE:HD12	9:4:468:LYS:CB	2.21	0.71
10:l:66:GLU:CA	10:l:69:ILE:CG1	2.65	0.71
6:H:416:ARG:N	10:5:66:GLU:OE2	2.23	0.71
10:5:211:CYS:SG	10:5:236:CYS:HB3	2.31	0.71
1:G:770:LEU:HG	3:b:133:ASP:C	2.16	0.71
1:E:518:PHE:CD1	3:B:30:ARG:NH2	2.58	0.70
10:l:183:CYS:HB3	10:l:211:CYS:CB	2.22	0.70
1:F:598:ARG:HH12	1:G:780:VAL:HG12	1.56	0.70
1:G:770:LEU:CD2	3:b:133:ASP:C	2.65	0.70
4:c:177:TYR:CD2	4:c:181:HIS:HD2	2.10	0.70
10:5:183:CYS:HB3	10:5:211:CYS:CB	2.22	0.70
1:E:518:PHE:HD1	3:B:30:ARG:HH22	1.40	0.70
1:G:770:LEU:CD2	3:b:133:ASP:O	2.40	0.70
10:l:27:ILE:HD12	10:l:27:ILE:N	2.02	0.70
10:l:211:CYS:SG	10:l:236:CYS:HB3	2.31	0.70
4:C:177:TYR:CD2	4:C:181:HIS:HD2	2.10	0.70
4:c:24:ILE:HG22	4:c:26:GLY:H	1.56	0.69
1:G:864:LYS:CE	5:d:9:LEU:CD1	2.70	0.69
1:F:598:ARG:NH1	1:G:780:VAL:HG12	2.06	0.69
6:h:83:LEU:HD21	6:h:86:PHE:HB2	1.74	0.69
1:G:729:TRP:HH2	1:G:786:LEU:CB	2.05	0.69
4:C:24:ILE:HG22	4:C:26:GLY:H	1.57	0.69
10:l:72:ASN:O	10:l:76:TYR:N	2.25	0.69
1:E:521:GLY:H	3:B:84:LYS:CE	2.05	0.69
6:h:333:SER:O	6:h:335:TYR:N	2.26	0.69
6:H:416:ARG:CA	10:5:66:GLU:OE2	2.41	0.69
7:i:431:LYS:HD2	7:i:433:ASN:HD21	1.53	0.68
10:5:72:ASN:O	10:5:76:TYR:N	2.25	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:864:LYS:HD2	5:d:9:LEU:HD13	1.74	0.68
10:5:27:ILE:HD12	10:5:27:ILE:N	2.02	0.68
1:G:723:ASP:CG	1:G:779:PRO:HB3	2.18	0.68
1:E:521:GLY:N	3:B:84:LYS:HE3	2.09	0.68
6:h:416:ARG:CA	10:l:66:GLU:OE2	2.41	0.68
7:i:431:LYS:CD	7:i:433:ASN:ND2	2.49	0.68
6:H:83:LEU:HD21	6:H:86:PHE:HB2	1.74	0.68
12:n:228:ARG:HA	12:n:329:ARG:HH12	1.60	0.67
6:H:333:SER:O	6:H:335:TYR:N	2.26	0.67
12:7:228:ARG:HA	12:7:329:ARG:HH12	1.59	0.67
10:5:185:ASN:HB2	10:5:236:CYS:SG	2.34	0.67
1:G:525:GLU:CB	6:h:263:GLY:O	2.40	0.67
6:h:370:LEU:HA	10:l:143:ALA:HB3	1.77	0.67
10:l:185:ASN:HB2	10:l:236:CYS:SG	2.34	0.67
10:5:73:GLU:O	10:5:77:LYS:N	2.26	0.67
1:E:518:PHE:C	3:B:30:ARG:NH1	2.51	0.67
1:E:521:GLY:N	3:B:84:LYS:CD	2.58	0.67
6:h:488:LYS:HG3	6:h:491:LEU:HB3	1.76	0.67
6:H:488:LYS:HG3	6:H:491:LEU:HB3	1.76	0.67
6:H:370:LEU:HA	10:5:143:ALA:HB3	1.77	0.67
9:k:812:LYS:HG3	9:k:813:LEU:HG	1.77	0.67
7:2:630:SER:HB2	7:2:639:THR:HA	1.77	0.66
1:F:605:VAL:HG21	1:G:885:LEU:CD2	2.25	0.66
10:l:27:ILE:H	10:l:27:ILE:CD1	1.99	0.66
1:E:521:GLY:CA	3:B:84:LYS:CE	2.73	0.66
12:7:625:GLN:N	12:7:626:PRO:CD	2.57	0.66
8:j:100:LEU:HD13	8:j:159:GLY:HA3	1.77	0.66
10:l:73:GLU:O	10:l:77:LYS:N	2.26	0.66
6:H:337:SER:O	6:H:341:SER:N	2.28	0.66
10:5:44:PHE:CE2	10:5:47:ARG:HD3	2.31	0.66
10:l:44:PHE:CE2	10:l:47:ARG:HD3	2.31	0.66
12:n:625:GLN:N	12:n:626:PRO:HD2	2.09	0.66
9:4:812:LYS:HG3	9:4:813:LEU:HG	1.77	0.66
1:G:727:GLU:CD	1:G:777:ARG:CG	2.68	0.65
7:i:630:SER:HB2	7:i:639:THR:HA	1.77	0.65
9:4:328:LEU:HB2	9:4:435:VAL:HG12	1.78	0.65
9:k:605:ILE:O	9:k:605:ILE:HG12	1.97	0.65
6:H:342:ASN:ND2	6:H:351:TRP:O	2.29	0.65
8:3:390:GLU:HB2	8:3:401:GLY:HA3	1.79	0.65
12:7:625:GLN:N	12:7:626:PRO:HD2	2.09	0.65
12:n:625:GLN:N	12:n:626:PRO:CD	2.57	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:333:SER:C	6:H:335:TYR:N	2.54	0.65
8:j:450:ARG:NH2	8:j:451:GLU:OE2	2.30	0.65
1:G:730:LYS:O	1:G:814:GLU:CG	2.45	0.65
7:2:356:ASN:HA	10:5:321:VAL:HB	1.79	0.65
7:2:431:LYS:CD	7:2:433:ASN:ND2	2.49	0.65
8:3:450:ARG:NH2	8:3:451:GLU:OE2	2.30	0.65
1:E:512:SER:HB3	6:H:301:ARG:HG3	1.79	0.65
10:5:254:GLN:NE2	10:5:278:CYS:SG	2.70	0.65
7:i:356:ASN:HA	10:l:321:VAL:HB	1.79	0.65
10:l:254:GLN:NE2	10:l:278:CYS:SG	2.70	0.65
6:H:159:TYR:HA	6:H:162:LEU:HB2	1.78	0.65
8:3:100:LEU:HD13	8:3:159:GLY:HA3	1.77	0.65
6:h:333:SER:C	6:h:335:TYR:N	2.54	0.65
11:m:381:LEU:HD13	11:m:385:SER:HG	1.58	0.65
9:4:602:THR:HG22	9:4:619:GLY:CA	2.27	0.65
6:h:159:TYR:HA	6:h:162:LEU:HB2	1.78	0.64
8:j:390:GLU:HB2	8:j:401:GLY:HA3	1.79	0.64
9:4:605:ILE:O	9:4:605:ILE:HG12	1.97	0.64
6:h:22:HIS:HA	6:h:55:GLN:HE22	1.62	0.64
6:h:342:ASN:ND2	6:h:351:TRP:O	2.29	0.64
9:k:328:LEU:HB2	9:k:435:VAL:HG12	1.78	0.64
12:7:236:GLY:H	12:7:355:PHE:HB3	1.63	0.64
1:F:603:PHE:HE1	1:G:880:GLU:HB3	1.61	0.64
7:i:601:LYS:HG2	7:i:771:ARG:HE	1.63	0.64
1:E:521:GLY:N	3:B:84:LYS:CE	2.61	0.64
1:G:521:GLY:CA	3:b:84:LYS:CD	2.51	0.64
9:k:602:THR:HG22	9:k:619:GLY:CA	2.27	0.64
6:h:337:SER:O	6:h:341:SER:N	2.28	0.64
6:H:22:HIS:HA	6:H:55:GLN:HE22	1.62	0.64
10:5:186:CYS:SG	10:5:236:CYS:N	2.71	0.64
8:j:673:GLN:HE21	12:n:621:MET:HE1	1.62	0.64
11:6:714:VAL:O	11:6:837:ARG:NH1	2.31	0.64
11:6:806:LEU:HD11	11:6:827:ALA:CB	2.27	0.64
10:l:44:PHE:HE2	10:l:47:ARG:NE	1.96	0.64
10:5:44:PHE:HE2	10:5:47:ARG:NE	1.96	0.64
10:5:186:CYS:HB2	10:5:236:CYS:HB2	1.78	0.63
1:E:773:GLU:OE2	3:B:28:PHE:HE1	1.80	0.63
9:4:778:ARG:NH2	9:4:793:ALA:O	2.31	0.63
11:6:746:PHE:HA	11:6:750:GLN:HE21	1.62	0.63
1:E:525:GLU:C	6:H:263:GLY:HA3	2.22	0.63
1:G:518:PHE:CA	3:b:30:ARG:NH2	2.59	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:232:VAL:HA	5:d:291:VAL:HG23	1.80	0.63
10:l:186:CYS:SG	10:l:236:CYS:N	2.71	0.63
11:m:806:LEU:HD11	11:m:827:ALA:CB	2.27	0.63
5:D:152:ASP:N	5:D:152:ASP:OD1	2.30	0.63
1:G:749:TYR:HE2	1:G:848:TYR:HE2	1.46	0.63
7:2:601:LYS:HG2	7:2:771:ARG:HE	1.63	0.63
9:4:469:VAL:O	9:4:470:SER:CB	2.44	0.63
1:G:770:LEU:HG	3:b:134:PHE:CA	2.29	0.63
5:d:169:ILE:HB	5:d:171:LEU:HD23	1.81	0.63
8:3:673:GLN:HE21	12:7:621:MET:HE1	1.62	0.63
11:m:714:VAL:O	11:m:837:ARG:NH1	2.31	0.63
1:G:730:LYS:O	1:G:814:GLU:HG3	1.99	0.63
10:5:258:LEU:HD12	10:5:276:MET:HE1	1.79	0.63
5:D:169:ILE:HB	5:D:171:LEU:HD23	1.81	0.63
9:4:468:LYS:C	9:4:468:LYS:HD3	2.24	0.63
1:G:749:TYR:CE2	1:G:848:TYR:CE2	2.86	0.63
5:d:152:ASP:N	5:d:152:ASP:OD1	2.30	0.63
6:h:387:GLU:HA	6:h:390:ILE:HG12	1.81	0.63
10:l:186:CYS:HB2	10:l:236:CYS:HB2	1.78	0.63
11:m:746:PHE:HA	11:m:750:GLN:HE21	1.63	0.63
6:H:372:THR:O	6:H:376:THR:N	2.30	0.63
10:5:44:PHE:HE2	10:5:47:ARG:HE	1.47	0.63
9:k:778:ARG:NH2	9:k:793:ALA:O	2.31	0.62
10:l:68:LEU:O	10:l:72:ASN:CG	2.42	0.62
1:F:603:PHE:CD1	1:G:880:GLU:O	2.50	0.62
4:C:27:LEU:HD12	4:C:38:ILE:HG12	1.81	0.62
9:k:192:THR:O	9:k:196:ASN:ND2	2.33	0.62
10:l:183:CYS:SG	10:l:187:ARG:N	2.72	0.62
10:5:183:CYS:SG	10:5:187:ARG:N	2.72	0.62
8:j:39:ARG:NH1	8:j:136:MET:SD	2.73	0.62
10:l:44:PHE:HE2	10:l:47:ARG:HE	1.47	0.62
7:2:498:ILE:HD12	7:2:513:THR:HG22	1.81	0.62
7:2:843:ASP:OD1	7:2:843:ASP:N	2.31	0.62
8:3:39:ARG:NH1	8:3:136:MET:SD	2.73	0.62
9:4:433:ILE:HD11	9:4:468:LYS:HB3	1.78	0.62
7:i:789:VAL:HG13	7:i:863:ILE:HD12	1.81	0.62
5:D:79:TYR:HB2	5:D:147:ARG:HH22	1.64	0.62
9:4:192:THR:O	9:4:196:ASN:ND2	2.33	0.62
10:l:456:ASP:HB2	10:l:461:GLU:H	1.65	0.62
5:D:232:VAL:HA	5:D:291:VAL:HG23	1.80	0.62
9:4:363:GLY:HA2	11:6:437:VAL:HG22	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5:358:LEU:HB3	10:5:362:ARG:HH21	1.64	0.62
10:5:456:ASP:HB2	10:5:461:GLU:H	1.65	0.62
1:G:770:LEU:HD21	3:b:133:ASP:CA	2.27	0.62
5:d:79:TYR:HB2	5:d:147:ARG:HH22	1.64	0.62
12:n:465:ALA:HB3	12:n:468:GLN:HE21	1.65	0.62
10:5:68:LEU:O	10:5:72:ASN:CG	2.42	0.62
11:m:572:CYS:SG	11:m:573:VAL:N	2.73	0.62
7:2:789:VAL:HG13	7:2:863:ILE:HD12	1.81	0.62
1:G:723:ASP:HB2	1:G:779:PRO:HG3	1.80	0.61
4:c:27:LEU:HD12	4:c:38:ILE:HG12	1.81	0.61
5:d:250:GLU:HA	5:d:256:TYR:HB2	1.82	0.61
7:i:498:ILE:HD12	7:i:513:THR:HG22	1.81	0.61
8:j:45:ILE:O	8:j:49:ASN:ND2	2.33	0.61
6:H:387:GLU:HA	6:H:390:ILE:HG12	1.80	0.61
9:4:306:TYR:HB2	9:4:436:THR:HG21	1.82	0.61
1:F:605:VAL:HG22	1:G:885:LEU:CD2	2.21	0.61
6:h:331:HIS:O	6:h:332:SER:HB3	2.00	0.61
4:C:21:GLN:HE22	4:C:70:PRO:HG2	1.65	0.61
6:H:24:SER:HA	6:H:26:GLN:HE21	1.65	0.61
9:k:332:VAL:HG13	9:k:430:GLY:H	1.65	0.61
10:l:358:LEU:HB3	10:l:362:ARG:HH21	1.64	0.61
4:c:21:GLN:HE22	4:c:70:PRO:HG2	1.65	0.61
5:D:250:GLU:HA	5:D:256:TYR:HB2	1.82	0.61
9:4:469:VAL:O	9:4:469:VAL:HG12	2.00	0.61
11:6:390:LYS:NZ	11:6:391:PRO:O	2.34	0.61
1:G:770:LEU:CD1	3:b:134:PHE:CD1	2.60	0.61
12:n:236:GLY:H	12:n:355:PHE:HB3	1.63	0.61
10:5:186:CYS:SG	10:5:236:CYS:HA	2.41	0.61
10:5:581:ASN:HA	10:5:584:GLN:HB2	1.81	0.61
12:7:465:ALA:HB3	12:7:468:GLN:HE21	1.65	0.61
9:k:455:SER:N	12:n:276:ARG:O	2.34	0.61
10:l:186:CYS:SG	10:l:236:CYS:HA	2.41	0.61
2:A:127:GLU:HA	2:A:130:TYR:HD2	1.65	0.61
9:4:332:VAL:HG13	9:4:430:GLY:H	1.65	0.61
7:i:384:ASN:OD1	7:i:384:ASN:N	2.32	0.61
10:l:258:LEU:HD12	10:l:276:MET:HE1	1.79	0.61
11:6:796:THR:OG1	11:6:797:VAL:N	2.33	0.61
1:F:571:PRO:HG3	1:G:782:VAL:HG22	1.83	0.61
2:a:127:GLU:HA	2:a:130:TYR:HD2	1.65	0.61
7:i:843:ASP:N	7:i:843:ASP:OD1	2.31	0.61
9:k:284:ILE:HG23	9:k:293:LEU:HD22	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:472:ARG:HH11	6:H:473:TRP:HE1	1.49	0.61
7:2:790:TYR:OH	7:2:794:ARG:NH2	2.34	0.61
8:3:190:SER:OG	8:3:191:LEU:N	2.34	0.61
8:3:215:THR:HG21	8:3:224:ARG:HD2	1.82	0.61
3:b:191:LYS:HB3	4:c:105:PHE:CE1	2.35	0.61
9:k:363:GLY:HA2	11:m:437:VAL:HG22	1.82	0.61
10:l:581:ASN:HA	10:l:584:GLN:HB2	1.81	0.61
8:3:45:ILE:O	8:3:49:ASN:ND2	2.33	0.61
9:4:681:ARG:HG3	9:4:683:ASN:H	1.66	0.61
11:6:182:GLN:HB3	11:6:265:ILE:HD11	1.83	0.61
7:i:790:TYR:OH	7:i:794:ARG:NH2	2.34	0.61
9:k:306:TYR:HB2	9:k:436:THR:HG21	1.82	0.61
10:l:66:GLU:HA	10:l:69:ILE:HG12	1.70	0.61
3:B:191:LYS:HB3	4:C:105:PHE:CE1	2.35	0.61
10:5:66:GLU:HB3	10:5:69:ILE:CD1	2.29	0.61
11:6:572:CYS:SG	11:6:573:VAL:N	2.73	0.61
12:7:685:THR:HG23	12:7:688:THR:H	1.66	0.61
1:G:505:VAL:HG11	6:h:300:LYS:O	2.01	0.60
6:h:24:SER:HA	6:h:26:GLN:HE21	1.64	0.60
6:H:331:HIS:O	6:H:332:SER:HB3	2.00	0.60
7:2:325:THR:OG1	7:2:326:ARG:N	2.31	0.60
6:h:332:SER:HA	6:h:377:TRP:CZ3	2.37	0.60
10:l:64:ASN:ND2	10:l:65:MET:HG3	2.17	0.60
2:A:52:GLU:HA	2:A:55:LYS:HB2	1.84	0.60
9:4:191:THR:HG22	9:4:275:THR:HG22	1.83	0.60
9:4:758:ILE:HB	9:4:814:LYS:HE3	1.83	0.60
1:G:770:LEU:CG	3:b:133:ASP:C	2.75	0.60
8:j:190:SER:OG	8:j:191:LEU:N	2.34	0.60
9:k:758:ILE:HB	9:k:814:LYS:HE3	1.83	0.60
7:2:808:ARG:NH1	13:5:801:ATP:O1B	2.35	0.60
10:5:66:GLU:HB2	10:5:69:ILE:HD11	1.81	0.60
6:h:372:THR:O	6:h:376:THR:N	2.30	0.60
10:l:423:SER:OG	13:l:801:ATP:O1G	2.16	0.60
2:A:99:SER:O	2:A:103:ASN:ND2	2.34	0.60
6:h:333:SER:O	6:h:334:LEU:C	2.43	0.60
9:k:191:THR:HG22	9:k:275:THR:HG22	1.83	0.60
6:H:540:ARG:NH2	6:H:574:GLU:OE1	2.34	0.60
7:i:808:ARG:NH1	13:l:801:ATP:O1B	2.34	0.60
12:n:227:VAL:O	12:n:329:ARG:NH2	2.35	0.60
10:5:76:TYR:HA	10:5:79:LEU:HB2	1.83	0.60
11:6:689:TYR:HD1	11:6:698:ASN:HD22	1.50	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:5:ILE:N	6:h:144:ASP:O	2.34	0.60
6:h:540:ARG:NH2	6:h:574:GLU:OE1	2.34	0.60
9:k:681:ARG:HG3	9:k:683:ASN:H	1.66	0.60
4:C:177:TYR:CE2	4:C:181:HIS:CD2	2.90	0.60
6:H:73:GLN:HG2	6:H:74:LEU:HG	1.84	0.60
7:2:399:PRO:O	7:2:401:ARG:NH1	2.35	0.60
7:2:434:TYR:CZ	7:2:447:PHE:HA	2.17	0.60
9:4:455:SER:N	12:7:276:ARG:O	2.34	0.60
12:7:227:VAL:O	12:7:329:ARG:NH2	2.35	0.60
6:h:392:PHE:HA	6:h:395:ASN:HB2	1.83	0.60
11:m:182:GLN:HB3	11:m:265:ILE:HD11	1.83	0.60
6:H:332:SER:HA	6:H:377:TRP:CZ3	2.37	0.60
1:E:521:GLY:CA	3:B:84:LYS:NZ	2.51	0.60
4:c:177:TYR:CE2	4:c:181:HIS:CD2	2.90	0.60
10:l:66:GLU:HB2	10:l:69:ILE:HD11	1.81	0.60
10:l:183:CYS:HB3	10:l:211:CYS:HB3	1.84	0.60
6:H:5:ILE:N	6:H:144:ASP:O	2.34	0.60
6:H:333:SER:O	6:H:334:LEU:C	2.43	0.60
1:G:730:LYS:HD3	1:G:817:ILE:HD11	1.84	0.59
2:a:128:GLN:HA	2:a:131:LEU:HB3	1.84	0.59
4:c:3:TYR:O	5:d:217:ASN:ND2	2.35	0.59
8:j:215:THR:HG21	8:j:224:ARG:HD2	1.82	0.59
2:A:128:GLN:HA	2:A:131:LEU:HB3	1.84	0.59
9:k:702:PHE:O	9:k:796:ARG:NH2	2.35	0.59
7:2:689:GLU:O	11:6:778:LYS:NZ	2.36	0.59
9:4:702:PHE:O	9:4:796:ARG:NH2	2.35	0.59
10:5:183:CYS:HB3	10:5:211:CYS:HB3	1.84	0.59
7:i:399:PRO:O	7:i:401:ARG:NH1	2.35	0.59
7:i:641:GLN:OE1	7:i:643:ARG:NH2	2.35	0.59
11:m:390:LYS:NZ	11:m:391:PRO:O	2.34	0.59
6:H:132:ASP:OD1	6:H:132:ASP:N	2.35	0.59
1:F:603:PHE:CG	1:G:881:LYS:HA	2.34	0.59
10:l:76:TYR:HA	10:l:79:LEU:HB2	1.82	0.59
7:2:641:GLN:OE1	7:2:643:ARG:NH2	2.35	0.59
9:4:284:ILE:HG23	9:4:293:LEU:HD22	1.83	0.59
1:F:607:PHE:O	1:G:828:LEU:CD2	2.50	0.59
2:a:99:SER:O	2:a:103:ASN:ND2	2.34	0.59
6:h:472:ARG:HH11	6:h:473:TRP:HE1	1.49	0.59
2:A:31:MET:O	2:A:93:ARG:NH2	2.36	0.59
4:C:3:TYR:O	5:D:217:ASN:ND2	2.35	0.59
6:h:73:GLN:HG2	6:h:74:LEU:HG	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:434:TYR:CZ	7:i:446:VAL:O	2.55	0.59
6:H:48:LEU:O	6:H:52:GLN:NE2	2.36	0.59
8:3:668:ILE:HB	8:3:670:GLN:HE22	1.68	0.59
6:h:417:GLY:N	10:l:66:GLU:OE2	2.36	0.59
7:i:689:GLU:O	11:m:778:LYS:NZ	2.36	0.59
12:7:433:LEU:HA	12:7:436:LEU:HD12	1.85	0.59
2:a:4:ASP:N	2:a:4:ASP:OD1	2.36	0.59
6:h:71:TYR:OH	6:h:118:ARG:NH1	2.35	0.59
6:h:132:ASP:OD1	6:h:132:ASP:N	2.35	0.59
8:j:446:VAL:HG13	8:j:458:GLU:HB3	1.85	0.59
10:5:64:ASN:ND2	10:5:65:MET:HG3	2.16	0.59
1:G:518:PHE:HA	3:b:30:ARG:HH22	1.68	0.59
12:n:330:SER:OG	12:n:331:LEU:N	2.36	0.59
12:n:411:TYR:O	12:n:430:LYS:NZ	2.33	0.59
6:H:71:TYR:OH	6:H:118:ARG:NH1	2.35	0.59
1:G:518:PHE:CB	3:b:30:ARG:NH2	2.66	0.58
3:b:99:ASP:OD1	3:b:99:ASP:N	2.35	0.58
6:h:344:VAL:HA	6:h:347:LYS:HE2	1.83	0.58
6:H:417:GLY:N	10:5:66:GLU:OE2	2.36	0.58
1:E:527:HIS:CE1	6:H:301:ARG:NH2	2.68	0.58
8:j:668:ILE:HB	8:j:670:GLN:HE22	1.68	0.58
10:l:183:CYS:CB	10:l:211:CYS:HB2	2.33	0.58
11:m:802:SER:HA	11:m:805:ARG:HG2	1.85	0.58
12:n:685:THR:HG23	12:n:688:THR:H	1.67	0.58
2:A:207:LYS:NZ	2:A:208:ILE:O	2.36	0.58
6:H:392:PHE:HA	6:H:395:ASN:HB2	1.83	0.58
7:2:434:TYR:CZ	7:2:446:VAL:O	2.55	0.58
8:3:687:ARG:NH1	8:3:690:ASP:OD2	2.36	0.58
12:7:330:SER:OG	12:7:331:LEU:N	2.36	0.58
1:G:901:ILE:HG23	5:d:3:ILE:CD1	2.34	0.58
3:b:181:LEU:HD13	3:b:184:PHE:HZ	1.68	0.58
6:h:48:LEU:O	6:h:52:GLN:NE2	2.36	0.58
8:j:687:ARG:NH1	8:j:690:ASP:OD2	2.36	0.58
11:m:441:ARG:NH1	11:m:444:GLY:O	2.36	0.58
3:B:79:LEU:O	3:B:82:GLN:NE2	2.35	0.58
6:H:344:VAL:HA	6:H:347:LYS:HE2	1.83	0.58
6:H:358:ARG:NH2	6:H:399:TYR:OH	2.37	0.58
8:3:415:LYS:NZ	13:3:1001:ATP:O3B	2.36	0.58
2:a:207:LYS:NZ	2:a:208:ILE:O	2.36	0.58
4:c:166:LEU:HD22	4:c:166:LEU:N	2.18	0.58
8:j:216:ASP:OD1	8:j:216:ASP:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:433:LEU:HA	12:n:436:LEU:HD12	1.85	0.58
8:3:446:VAL:HG13	8:3:458:GLU:HB3	1.85	0.58
3:B:181:LEU:HD13	3:B:184:PHE:HZ	1.68	0.58
10:5:423:SER:OG	13:5:801:ATP:O1G	2.16	0.58
11:6:441:ARG:NH1	11:6:444:GLY:O	2.36	0.58
6:h:7:GLN:HB3	6:h:10:GLU:HG2	1.86	0.58
9:k:302:LYS:NZ	9:k:303:VAL:O	2.37	0.58
10:l:183:CYS:CB	10:l:211:CYS:CB	2.82	0.58
9:4:302:LYS:NZ	9:4:303:VAL:O	2.37	0.58
9:4:753:TYR:O	9:4:757:HIS:ND1	2.37	0.58
2:a:52:GLU:HA	2:a:55:LYS:HB2	1.84	0.58
6:h:390:ILE:O	6:h:394:LYS:NZ	2.37	0.58
6:H:7:GLN:HB3	6:H:10:GLU:HG2	1.86	0.58
10:5:183:CYS:CB	10:5:211:CYS:HB2	2.34	0.58
12:7:73:ARG:NH2	12:7:76:ASN:OD1	2.37	0.58
7:i:782:ASP:OD1	7:i:782:ASP:N	2.33	0.58
10:l:69:ILE:CG1	10:l:70:GLY:N	2.67	0.58
10:l:458:MET:HG3	10:l:459:THR:HG23	1.86	0.58
2:A:4:ASP:N	2:A:4:ASP:OD1	2.36	0.58
7:2:384:ASN:OD1	7:2:384:ASN:N	2.32	0.58
9:k:744:VAL:HG23	9:k:745:GLU:HG2	1.85	0.58
11:m:654:GLU:OE2	11:m:658:GLN:NE2	2.37	0.58
3:B:99:ASP:N	3:B:99:ASP:OD1	2.35	0.58
4:C:166:LEU:N	4:C:166:LEU:HD22	2.18	0.58
9:4:281:VAL:HA	9:4:284:ILE:HB	1.86	0.58
10:5:458:MET:HG3	10:5:459:THR:HG23	1.86	0.58
1:G:729:TRP:HZ3	1:G:786:LEU:HD11	1.61	0.57
4:c:135:LEU:HD21	4:c:177:TYR:HB3	1.86	0.57
5:d:65:LYS:O	5:d:69:ASN:ND2	2.35	0.57
9:k:281:VAL:HA	9:k:284:ILE:HB	1.86	0.57
10:l:140:ASN:HB3	10:l:334:GLN:HE22	1.69	0.57
11:m:689:TYR:HD1	11:m:698:ASN:HD22	1.50	0.57
10:5:183:CYS:CB	10:5:211:CYS:CB	2.82	0.57
11:6:802:SER:HA	11:6:805:ARG:HG2	1.85	0.57
1:G:776:ILE:CA	1:G:777:ARG:N	2.66	0.57
5:d:161:LEU:O	5:d:166:ASN:ND2	2.32	0.57
7:i:508:HIS:O	7:i:512:LYS:NZ	2.37	0.57
12:n:73:ARG:NH2	12:n:76:ASN:OD1	2.37	0.57
5:D:65:LYS:O	5:D:69:ASN:ND2	2.35	0.57
9:4:744:VAL:HG23	9:4:745:GLU:HG2	1.85	0.57
11:6:381:LEU:HD12	11:6:381:LEU:O	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:864:LYS:HD2	5:d:9:LEU:CD1	2.32	0.57
10:l:525:PRO:HG2	10:l:528:GLY:HA2	1.86	0.57
4:C:135:LEU:HD21	4:C:177:TYR:HB3	1.86	0.57
5:D:72:CYS:O	5:D:226:LYS:NZ	2.37	0.57
5:D:161:LEU:O	5:D:166:ASN:ND2	2.32	0.57
7:2:621:HIS:HD2	7:2:676:ARG:HH21	1.52	0.57
5:d:72:CYS:O	5:d:226:LYS:NZ	2.37	0.57
6:h:358:ARG:NH2	6:h:399:TYR:OH	2.37	0.57
6:h:435:GLY:HA2	6:h:494:ARG:HH22	1.69	0.57
7:i:227:TYR:HA	7:i:230:ARG:HE	1.69	0.57
7:2:508:HIS:O	7:2:512:LYS:NZ	2.37	0.57
10:5:649:THR:H	10:5:652:GLN:HE22	1.52	0.57
12:7:685:THR:O	12:7:688:THR:OG1	2.22	0.57
3:b:79:LEU:O	3:b:82:GLN:NE2	2.35	0.57
4:c:168:LYS:HA	4:c:171:GLU:HB3	1.86	0.57
7:i:325:THR:OG1	7:i:326:ARG:N	2.31	0.57
8:j:415:LYS:NZ	13:j:1001:ATP:O3B	2.36	0.57
11:m:112:ARG:HH12	11:m:183:LYS:HZ2	1.53	0.57
11:m:381:LEU:HD12	11:m:381:LEU:O	2.05	0.57
10:5:140:ASN:HB3	10:5:334:GLN:HE22	1.69	0.57
12:7:411:TYR:O	12:7:430:LYS:NZ	2.33	0.57
2:a:31:MET:O	2:a:93:ARG:NH2	2.36	0.57
7:i:621:HIS:HD2	7:i:676:ARG:HH21	1.52	0.57
6:H:335:TYR:OH	6:H:368:ILE:O	2.23	0.57
10:5:529:ARG:NH1	10:5:558:ASP:OD1	2.38	0.57
6:h:246:THR:OG1	6:h:247:VAL:N	2.38	0.57
7:i:490:ASP:H	7:i:493:ILE:HD11	1.69	0.57
9:k:900:SER:HA	9:k:903:ILE:HG12	1.86	0.57
6:H:435:GLY:HA2	6:H:494:ARG:HH22	1.69	0.57
10:5:383:ASP:N	10:5:383:ASP:OD1	2.38	0.57
11:6:112:ARG:HH12	11:6:183:LYS:HZ2	1.52	0.57
9:k:505:ASP:N	9:k:505:ASP:OD1	2.37	0.57
10:l:529:ARG:NH1	10:l:558:ASP:OD1	2.38	0.57
9:4:900:SER:HA	9:4:903:ILE:HG12	1.86	0.57
12:7:658:ASP:O	12:7:662:GLN:NE2	2.36	0.57
6:H:390:ILE:O	6:H:394:LYS:NZ	2.37	0.57
8:3:216:ASP:N	8:3:216:ASP:OD1	2.36	0.57
10:l:183:CYS:HB3	10:l:211:CYS:HB2	1.86	0.56
10:l:649:THR:H	10:l:652:GLN:HE22	1.52	0.56
12:n:685:THR:O	12:n:688:THR:OG1	2.22	0.56
2:A:89:TYR:OH	2:A:93:ARG:NH2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:168:LYS:HA	4:C:171:GLU:HB3	1.86	0.56
10:5:66:GLU:HA	10:5:69:ILE:HG12	1.70	0.56
1:G:719:LEU:HD13	1:G:832:VAL:HG13	1.87	0.56
8:j:280:ASP:N	8:j:280:ASP:OD1	2.38	0.56
10:l:531:ASP:OD2	10:l:539:ASN:ND2	2.39	0.56
11:m:724:ASP:N	11:m:724:ASP:OD1	2.36	0.56
11:m:796:THR:OG1	11:m:797:VAL:N	2.33	0.56
1:E:746:ALA:CB	3:B:66:MET:HE3	2.29	0.56
1:G:731:MET:C	1:G:814:GLU:HG3	2.30	0.56
1:G:770:LEU:CD1	3:b:134:PHE:CA	2.81	0.56
8:j:402:ASP:O	8:j:707:ARG:NH1	2.39	0.56
9:k:522:LEU:HB3	9:k:541:LEU:HD11	1.87	0.56
6:H:14:LYS:O	6:H:18:ASN:ND2	2.38	0.56
9:k:652:GLN:O	9:k:667:ALA:N	2.38	0.56
12:n:462:PRO:HB2	12:n:464:VAL:HG22	1.88	0.56
2:A:182:ASN:HD21	6:H:74:LEU:HB3	1.70	0.56
6:H:586:PRO:HG2	6:H:601:ILE:HD12	1.88	0.56
7:2:227:TYR:HA	7:2:230:ARG:HE	1.69	0.56
7:2:490:ASP:H	7:2:493:ILE:HD11	1.69	0.56
9:4:469:VAL:O	9:4:470:SER:HB2	2.06	0.56
10:5:69:ILE:CG1	10:5:70:GLY:N	2.67	0.56
6:h:14:LYS:O	6:h:18:ASN:ND2	2.38	0.56
8:j:300:SER:HG	10:l:245:HIS:HD1	1.51	0.56
9:k:424:VAL:HG21	11:m:280:ARG:NE	2.21	0.56
8:3:402:ASP:O	8:3:707:ARG:NH1	2.39	0.56
9:4:468:LYS:HE2	9:4:468:LYS:O	2.04	0.56
10:5:183:CYS:HB3	10:5:211:CYS:HB2	1.86	0.56
8:j:443:THR:HG21	8:j:457:LEU:HG	1.88	0.56
10:l:505:ALA:HA	10:l:510:THR:HG22	1.88	0.56
8:3:190:SER:O	8:3:254:GLN:NE2	2.38	0.56
10:5:273:ASN:N	10:5:273:ASN:OD1	2.38	0.56
10:5:525:PRO:HG2	10:5:528:GLY:HA2	1.86	0.56
6:h:335:TYR:OH	6:h:368:ILE:O	2.23	0.56
6:h:586:PRO:HG2	6:h:601:ILE:HD12	1.88	0.56
9:k:753:TYR:O	9:k:757:HIS:ND1	2.37	0.56
7:2:625:GLU:OE1	7:2:676:ARG:NH2	2.39	0.56
11:6:106:VAL:O	11:6:110:LYS:N	2.39	0.56
11:6:144:LYS:NZ	11:6:194:PRO:O	2.39	0.56
12:7:339:LEU:O	12:7:342:SER:OG	2.23	0.56
12:7:342:SER:O	12:7:383:GLN:NE2	2.39	0.56
2:a:89:TYR:OH	2:a:93:ARG:NH2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:190:SER:O	8:j:254:GLN:NE2	2.38	0.56
9:4:296:ILE:O	9:4:301:TYR:OH	2.24	0.56
9:4:424:VAL:HG21	11:6:280:ARG:NE	2.21	0.56
9:4:652:GLN:O	9:4:667:ALA:N	2.38	0.56
11:6:724:ASP:OD1	11:6:724:ASP:N	2.36	0.56
1:E:521:GLY:HA3	3:B:84:LYS:HZ1	1.65	0.56
9:k:296:ILE:O	9:k:301:TYR:OH	2.24	0.56
12:n:342:SER:O	12:n:383:GLN:NE2	2.39	0.56
2:A:32:TYR:OH	2:A:90:GLN:NE2	2.39	0.56
10:5:142:ASN:N	10:5:142:ASN:OD1	2.39	0.56
11:6:658:GLN:NE2	11:6:660:THR:O	2.39	0.56
6:h:387:GLU:O	6:h:391:ILE:N	2.39	0.55
8:j:402:ASP:OD1	8:j:402:ASP:N	2.39	0.55
1:E:773:GLU:OE2	3:B:28:PHE:CE1	2.58	0.55
1:G:723:ASP:CB	1:G:779:PRO:CB	2.59	0.55
10:l:383:ASP:OD1	10:l:383:ASP:N	2.38	0.55
8:3:294:VAL:HG23	8:3:326:VAL:HG12	1.88	0.55
10:5:531:ASP:OD2	10:5:539:ASN:ND2	2.39	0.55
12:7:462:PRO:HB2	12:7:464:VAL:HG22	1.88	0.55
1:F:571:PRO:HG2	1:G:781:PHE:O	2.06	0.55
2:a:182:ASN:HD21	6:h:74:LEU:HB3	1.70	0.55
8:j:169:ARG:NH1	8:j:266:PRO:O	2.36	0.55
8:j:725:ASP:N	8:j:725:ASP:OD1	2.39	0.55
6:H:246:THR:OG1	6:H:247:VAL:N	2.38	0.55
6:H:353:GLU:O	6:H:357:LYS:NZ	2.40	0.55
7:2:625:GLU:OE2	10:5:422:LYS:NZ	2.40	0.55
9:4:505:ASP:OD1	9:4:505:ASP:N	2.38	0.55
12:7:484:THR:OG1	12:7:525:GLU:OE1	2.24	0.55
1:G:527:HIS:CG	6:h:301:ARG:NH1	2.39	0.55
7:i:625:GLU:OE1	7:i:676:ARG:NH2	2.39	0.55
9:k:371:CYS:SG	9:k:372:GLU:N	2.79	0.55
9:k:518:LEU:HG	9:k:522:LEU:HD13	1.88	0.55
9:k:925:ARG:NH1	9:k:926:SER:O	2.40	0.55
6:H:334:LEU:O	6:H:337:SER:OG	2.24	0.55
7:2:253:LYS:O	7:2:257:ALA:N	2.40	0.55
8:3:280:ASP:OD1	8:3:280:ASP:N	2.38	0.55
3:b:134:PHE:HB3	3:b:137:PRO:HG3	1.89	0.55
9:k:337:PRO:HG3	11:m:375:ARG:HE	1.72	0.55
12:n:300:MET:HE3	12:n:301:SER:H	1.71	0.55
4:C:162:THR:HG21	10:5:346:VAL:HG22	1.89	0.55
11:6:297:THR:HA	11:6:359:VAL:HG12	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:6:654:GLU:OE2	11:6:658:GLN:NE2	2.37	0.55
8:j:193:ARG:HH22	8:j:454:GLU:HG2	1.71	0.55
10:l:64:ASN:OD1	10:l:65:MET:HG3	2.07	0.55
10:l:68:LEU:C	10:l:72:ASN:HB2	2.17	0.55
10:l:455:ARG:HG2	10:l:462:PHE:HE1	1.71	0.55
11:m:297:THR:HA	11:m:359:VAL:HG12	1.89	0.55
2:A:85:CYS:SG	2:A:86:LEU:N	2.80	0.55
6:H:387:GLU:O	6:H:391:ILE:N	2.39	0.55
12:7:300:MET:HE3	12:7:301:SER:H	1.71	0.55
2:a:85:CYS:SG	2:a:86:LEU:N	2.80	0.55
6:h:370:LEU:HD12	6:h:371:SER:N	2.22	0.55
6:H:355:GLY:HA2	6:H:358:ARG:HB2	1.89	0.55
8:3:400:ARG:NH1	8:3:490:MET:O	2.40	0.55
1:F:603:PHE:CD2	1:G:884:SER:OG	2.59	0.55
6:h:355:GLY:HA2	6:h:358:ARG:HB2	1.89	0.55
6:h:493:ASN:HA	6:h:496:ILE:HD12	1.89	0.55
7:i:253:LYS:O	7:i:257:ALA:N	2.40	0.55
8:j:294:VAL:HG23	8:j:326:VAL:HG12	1.87	0.55
12:n:399:GLU:OE2	12:n:400:ARG:NH2	2.40	0.55
5:D:62:ASP:OD1	5:D:62:ASP:N	2.37	0.55
9:4:522:LEU:HB3	9:4:541:LEU:HD11	1.87	0.55
10:5:68:LEU:C	10:5:72:ASN:HB2	2.17	0.55
6:h:537:ASP:OD1	10:l:587:GLN:NE2	2.40	0.55
9:k:722:LYS:O	9:k:726:ASN:ND2	2.40	0.55
11:m:557:LYS:HD3	11:m:762:LYS:HE3	1.89	0.55
3:B:82:GLN:HE22	3:B:84:LYS:HB2	1.71	0.55
6:H:370:LEU:HD12	6:H:371:SER:N	2.22	0.55
2:a:32:TYR:OH	2:a:90:GLN:NE2	2.39	0.55
6:h:370:LEU:HD22	10:l:161:ARG:HB3	1.89	0.55
9:k:224:LEU:HG	9:k:226:TYR:H	1.72	0.55
10:l:146:ILE:HD11	10:l:149:ARG:HB2	1.89	0.55
11:m:106:VAL:O	11:m:110:LYS:N	2.39	0.55
11:m:298:SER:OG	11:m:299:GLU:N	2.40	0.55
9:4:925:ARG:NH1	9:4:926:SER:O	2.40	0.55
10:5:455:ARG:HG2	10:5:462:PHE:HE1	1.71	0.55
11:6:557:LYS:HD3	11:6:762:LYS:HE3	1.89	0.55
12:7:399:GLU:OE2	12:7:400:ARG:NH2	2.40	0.55
3:b:22:ASN:OD1	5:d:135:ARG:NH1	2.40	0.54
10:l:424:GLN:NE2	13:l:801:ATP:O5'	2.40	0.54
11:m:658:GLN:NE2	11:m:660:THR:O	2.39	0.54
12:n:505:GLU:HB3	12:n:506:MET:HE2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:22:ASN:OD1	5:D:135:ARG:NH1	2.40	0.54
3:B:134:PHE:HB3	3:B:137:PRO:HG3	1.89	0.54
7:2:399:PRO:CB	11:6:629:MET:HE2	2.38	0.54
9:4:337:PRO:HG3	11:6:375:ARG:HE	1.71	0.54
7:i:340:ASN:HD22	7:i:346:SER:HB3	1.73	0.54
10:l:66:GLU:HB3	10:l:69:ILE:CD1	2.28	0.54
11:m:532:SER:HB3	11:m:745:PRO:HD2	1.90	0.54
10:5:505:ALA:HA	10:5:510:THR:HG22	1.88	0.54
7:i:625:GLU:OE2	10:l:422:LYS:NZ	2.39	0.54
12:n:339:LEU:O	12:n:342:SER:OG	2.24	0.54
8:3:193:ARG:HH22	8:3:454:GLU:HG2	1.72	0.54
10:5:64:ASN:OD1	10:5:65:MET:HG3	2.07	0.54
1:G:864:LYS:CD	5:d:9:LEU:CD1	2.85	0.54
6:h:353:GLU:O	6:h:357:LYS:NZ	2.40	0.54
10:l:68:LEU:O	10:l:72:ASN:N	2.41	0.54
12:n:484:THR:OG1	12:n:525:GLU:OE1	2.24	0.54
9:4:387:ASN:HD22	11:6:402:ILE:HD11	1.72	0.54
9:4:518:LEU:HG	9:4:522:LEU:HD13	1.89	0.54
11:6:532:SER:HB3	11:6:745:PRO:HD2	1.90	0.54
3:b:96:LYS:O	3:b:100:ARG:NH1	2.40	0.54
10:l:142:ASN:N	10:l:142:ASN:OD1	2.39	0.54
12:n:658:ASP:O	12:n:662:GLN:NE2	2.36	0.54
3:B:181:LEU:HD13	3:B:184:PHE:CZ	2.43	0.54
6:H:537:ASP:OD1	10:5:587:GLN:NE2	2.40	0.54
7:2:434:TYR:CD2	7:2:434:TYR:C	2.85	0.54
1:G:749:TYR:HE2	1:G:848:TYR:CE2	2.22	0.54
4:c:162:THR:HG21	10:l:346:VAL:HG22	1.89	0.54
6:h:482:ASP:OD1	6:h:482:ASP:N	2.33	0.54
8:j:400:ARG:NH1	8:j:490:MET:O	2.40	0.54
8:3:443:THR:HG21	8:3:457:LEU:HG	1.88	0.54
9:4:224:LEU:HG	9:4:226:TYR:H	1.72	0.54
9:4:885:GLU:OE2	9:4:889:GLN:NE2	2.41	0.54
10:5:146:ILE:HD11	10:5:149:ARG:HB2	1.89	0.54
10:5:258:LEU:HB2	10:5:276:MET:HE3	1.90	0.54
6:h:388:LEU:HA	6:h:391:ILE:HB	1.90	0.54
7:i:434:TYR:CD2	7:i:434:TYR:C	2.85	0.54
8:j:197:ILE:HG23	8:j:249:THR:HG23	1.90	0.54
2:A:23:SER:OG	2:A:24:ASN:N	2.40	0.54
7:2:340:ASN:HD22	7:2:346:SER:HB3	1.72	0.54
2:a:136:ASP:O	2:a:139:THR:OG1	2.26	0.54
4:c:104:PHE:C	4:c:104:PHE:CD2	2.85	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:321:THR:OG1	7:i:322:GLY:N	2.41	0.54
7:i:399:PRO:CB	11:m:629:MET:HE2	2.38	0.54
10:l:258:LEU:HB2	10:l:276:MET:HE3	1.90	0.54
12:n:103:VAL:HA	12:n:106:ILE:HG12	1.90	0.54
7:2:477:THR:N	7:2:480:GLU:OE1	2.41	0.54
9:4:431:ASP:OD2	9:4:468:LYS:HE3	2.06	0.54
9:4:722:LYS:O	9:4:726:ASN:ND2	2.40	0.54
9:4:794:THR:OG1	9:4:795:THR:N	2.41	0.54
1:G:525:GLU:O	6:h:263:GLY:N	2.40	0.54
2:a:23:SER:OG	2:a:24:ASN:N	2.40	0.54
3:b:181:LEU:HD13	3:b:184:PHE:CZ	2.43	0.54
6:h:342:ASN:O	6:h:346:ALA:N	2.40	0.54
9:k:907:LEU:HD22	9:k:924:ARG:HH12	1.73	0.54
11:m:381:LEU:HD12	11:m:385:SER:OG	2.00	0.54
4:C:177:TYR:CE2	4:C:181:HIS:HD2	2.24	0.54
6:H:249:ASN:OD1	6:H:290:ARG:NH2	2.40	0.54
6:H:342:ASN:O	6:H:346:ALA:N	2.40	0.54
6:H:493:ASN:HA	6:H:496:ILE:HD12	1.89	0.54
7:2:695:LEU:HD23	11:6:797:VAL:HG11	1.90	0.54
8:3:197:ILE:HG23	8:3:249:THR:HG23	1.90	0.54
12:7:505:GLU:HB3	12:7:506:MET:HE2	1.89	0.54
1:G:521:GLY:N	3:b:84:LYS:CD	2.70	0.53
7:i:695:LEU:HD23	11:m:797:VAL:HG11	1.90	0.53
6:H:493:ASN:O	6:H:497:GLN:NE2	2.41	0.53
7:2:434:TYR:OH	7:2:446:VAL:O	2.26	0.53
7:2:499:SER:HB3	7:2:509:ARG:HH12	1.72	0.53
8:3:725:ASP:OD1	8:3:725:ASP:N	2.38	0.53
10:5:424:GLN:NE2	13:5:801:ATP:O5'	2.40	0.53
1:G:521:GLY:H	3:b:84:LYS:CD	2.21	0.53
3:b:147:ASP:N	3:b:147:ASP:OD1	2.41	0.53
7:i:543:GLY:HA3	7:i:549:LYS:HD3	1.91	0.53
8:3:402:ASP:OD1	8:3:402:ASP:N	2.40	0.53
1:F:606:PRO:HG3	1:G:824:GLU:CG	2.38	0.53
3:b:82:GLN:HE22	3:b:84:LYS:HB2	1.71	0.53
7:i:499:SER:HB3	7:i:509:ARG:HH12	1.72	0.53
9:k:344:VAL:HG13	9:k:389:CYS:HB2	1.91	0.53
3:B:96:LYS:O	3:B:100:ARG:NH1	2.40	0.53
6:H:407:ASP:N	6:H:407:ASP:OD1	2.39	0.53
1:F:603:PHE:HD1	1:G:881:LYS:CA	2.10	0.53
4:c:177:TYR:CE2	4:c:181:HIS:HD2	2.24	0.53
6:h:493:ASN:O	6:h:497:GLN:NE2	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:387:ASN:HD22	11:m:402:ILE:HD11	1.72	0.53
7:2:338:LYS:NZ	7:2:378:GLU:O	2.41	0.53
9:4:793:ALA:O	9:4:797:GLN:NE2	2.41	0.53
12:7:664:TYR:OH	12:7:668:ARG:NH2	2.42	0.53
1:F:603:PHE:CD1	1:G:880:GLU:C	2.84	0.53
9:k:885:GLU:OE2	9:k:889:GLN:NE2	2.41	0.53
12:n:609:ASP:O	12:n:613:ALA:N	2.42	0.53
6:H:370:LEU:HD22	10:5:161:ARG:HB3	1.89	0.53
7:2:543:GLY:HA3	7:2:549:LYS:HD3	1.91	0.53
8:3:425:THR:HA	8:3:657:ARG:HH22	1.73	0.53
10:l:570:ASN:O	10:l:574:ASN:ND2	2.42	0.53
8:3:235:ASP:H	8:3:241:LEU:HD11	1.73	0.53
8:3:281:ASP:OD1	8:3:281:ASP:N	2.42	0.53
9:4:693:ASP:OD1	9:4:693:ASP:N	2.41	0.53
10:5:570:ASN:O	10:5:574:ASN:ND2	2.42	0.53
11:6:783:ASP:O	11:6:786:GLN:NE2	2.42	0.53
12:7:103:VAL:HA	12:7:106:ILE:HG12	1.90	0.53
12:n:664:TYR:OH	12:n:668:ARG:NH2	2.42	0.53
9:4:344:VAL:HG13	9:4:389:CYS:HB2	1.91	0.53
10:5:45:ILE:HG13	10:5:46:TYR:CD1	2.44	0.53
8:j:235:ASP:H	8:j:241:LEU:HD11	1.73	0.53
9:k:793:ALA:O	9:k:797:GLN:NE2	2.41	0.53
10:l:273:ASN:OD1	10:l:273:ASN:N	2.38	0.53
2:A:35:ASP:N	2:A:35:ASP:OD1	2.41	0.53
3:B:187:GLU:O	3:B:191:LYS:NZ	2.36	0.53
11:6:694:SER:OG	11:6:695:LEU:N	2.42	0.53
1:E:524:ARG:HD3	6:H:262:ILE:HG23	1.91	0.53
1:F:598:ARG:NH1	1:G:780:VAL:CG1	2.60	0.53
6:h:416:ARG:HH21	10:l:40:LEU:HD13	1.73	0.53
7:i:399:PRO:HB2	11:m:629:MET:HE2	1.90	0.53
7:i:434:TYR:OH	7:i:446:VAL:O	2.26	0.53
7:i:477:THR:N	7:i:480:GLU:OE1	2.41	0.53
9:k:878:SER:OG	9:k:879:ASP:N	2.40	0.53
12:n:122:ASP:OD1	12:n:122:ASP:N	2.38	0.53
2:A:136:ASP:O	2:A:139:THR:OG1	2.26	0.53
3:B:147:ASP:N	3:B:147:ASP:OD1	2.41	0.53
6:H:85:GLY:HA2	6:H:124:ASP:HA	1.91	0.53
8:3:300:SER:OG	10:5:245:HIS:ND1	2.39	0.53
10:5:427:LYS:O	10:5:431:LYS:NZ	2.42	0.53
11:m:151:ILE:O	11:m:266:SER:OG	2.27	0.53
11:m:694:SER:OG	11:m:695:LEU:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:544:GLN:OE1	12:n:559:ALA:N	2.41	0.53
2:A:46:ASN:O	2:A:50:ASN:ND2	2.41	0.53
2:A:96:ILE:O	2:A:99:SER:OG	2.25	0.53
2:A:129:GLU:HA	2:A:132:LYS:HG2	1.91	0.53
6:H:416:ARG:HH21	10:5:40:LEU:HD13	1.73	0.53
9:4:438:THR:OG1	9:4:439:PHE:N	2.41	0.53
4:c:23:ASP:OD1	4:c:40:LYS:N	2.41	0.52
7:i:340:ASN:ND2	7:i:346:SER:O	2.42	0.52
7:i:693:GLU:HA	7:i:696:ALA:HB3	1.90	0.52
10:l:45:ILE:HG13	10:l:46:TYR:CD1	2.44	0.52
12:n:499:LYS:NZ	12:n:505:GLU:OE2	2.42	0.52
12:7:499:LYS:NZ	12:7:505:GLU:OE2	2.42	0.52
8:j:425:THR:HA	8:j:657:ARG:HH22	1.74	0.52
10:l:185:ASN:CB	10:l:236:CYS:SG	2.98	0.52
12:n:494:THR:OG1	12:n:495:ALA:N	2.42	0.52
12:n:627:ASP:N	12:n:627:ASP:OD1	2.42	0.52
6:H:76:ASP:N	6:H:76:ASP:OD1	2.42	0.52
10:5:68:LEU:O	10:5:72:ASN:N	2.41	0.52
2:a:129:GLU:HA	2:a:132:LYS:HG2	1.91	0.52
7:i:434:TYR:CZ	7:i:447:PHE:HA	2.17	0.52
10:l:258:LEU:CD1	10:l:276:MET:CE	2.84	0.52
8:3:686:LEU:HA	8:3:689:ASP:HB2	1.92	0.52
11:6:120:GLU:O	11:6:134:LYS:NZ	2.42	0.52
11:6:533:ILE:HD12	11:6:544:LYS:HB3	1.92	0.52
12:7:494:THR:OG1	12:7:495:ALA:N	2.42	0.52
1:E:904:ARG:NH1	5:D:3:ILE:HG23	2.24	0.52
3:b:60:LEU:HB2	3:b:63:MET:HE2	1.91	0.52
13:j:1001:ATP:O2G	10:l:549:ARG:NH1	2.43	0.52
9:k:658:LYS:HG3	9:k:660:GLY:H	1.73	0.52
11:m:783:ASP:O	11:m:786:GLN:NE2	2.42	0.52
6:H:388:LEU:HA	6:H:391:ILE:HB	1.90	0.52
7:2:399:PRO:HB2	11:6:629:MET:HE2	1.90	0.52
1:G:524:ARG:HD2	6:h:262:ILE:CG2	2.37	0.52
9:k:535:ASP:OD1	9:k:535:ASP:N	2.43	0.52
10:l:631:LYS:HA	10:l:634:LEU:HB2	1.91	0.52
10:l:643:ARG:NH2	10:l:691:ALA:O	2.43	0.52
4:C:122:ASN:O	4:C:125:SER:OG	2.26	0.52
9:4:658:LYS:HG3	9:4:660:GLY:H	1.73	0.52
9:4:700:SER:OG	9:4:701:ARG:NH1	2.43	0.52
10:5:185:ASN:N	10:5:236:CYS:SG	2.81	0.52
11:6:378:ASP:OD2	11:6:378:ASP:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:491:ARG:NH1	6:H:303:THR:C	2.65	0.52
1:E:514:THR:HG1	6:H:301:ARG:HD3	1.71	0.52
5:d:178:ASP:N	5:d:178:ASP:OD1	2.41	0.52
7:i:519:LEU:O	7:i:771:ARG:NH1	2.43	0.52
8:j:412:SER:O	8:j:412:SER:OG	2.27	0.52
10:l:185:ASN:N	10:l:236:CYS:SG	2.81	0.52
11:m:120:GLU:O	11:m:134:LYS:NZ	2.42	0.52
12:n:461:ASP:OD1	12:n:461:ASP:N	2.42	0.52
6:H:493:ASN:OD1	6:H:493:ASN:N	2.42	0.52
7:2:528:ASN:H	7:2:530:LYS:HZ3	1.56	0.52
7:2:693:GLU:HA	7:2:696:ALA:HB3	1.90	0.52
8:3:523:TYR:OH	8:3:532:ASN:O	2.24	0.52
13:3:1001:ATP:O2G	10:5:549:ARG:NH1	2.43	0.52
12:7:495:ALA:HA	12:7:510:GLY:HA2	1.92	0.52
6:h:85:GLY:HA2	6:h:124:ASP:HA	1.91	0.52
8:j:686:LEU:HA	8:j:689:ASP:HB2	1.92	0.52
9:k:435:VAL:HG23	9:k:466:VAL:HG23	1.92	0.52
10:l:487:ASP:N	10:l:487:ASP:OD1	2.43	0.52
10:l:561:ASN:HB2	10:l:564:ARG:HG2	1.92	0.52
3:B:60:LEU:HB2	3:B:63:MET:HE2	1.91	0.52
4:C:23:ASP:OD1	4:C:40:LYS:N	2.41	0.52
7:2:321:THR:OG1	7:2:322:GLY:N	2.41	0.52
7:2:519:LEU:O	7:2:771:ARG:NH1	2.43	0.52
7:2:551:GLN:HE21	11:6:563:ILE:HG12	1.75	0.52
9:4:878:SER:OG	9:4:879:ASP:N	2.40	0.52
10:5:185:ASN:CB	10:5:236:CYS:SG	2.98	0.52
11:6:151:ILE:O	11:6:266:SER:OG	2.26	0.52
12:7:461:ASP:OD1	12:7:461:ASP:N	2.42	0.52
12:7:627:ASP:N	12:7:627:ASP:OD1	2.42	0.52
2:a:96:ILE:O	2:a:99:SER:OG	2.25	0.52
2:a:151:LEU:HD11	5:d:144:ILE:HD11	1.92	0.52
6:h:533:GLY:H	6:h:536:LEU:HD21	1.75	0.52
7:i:551:GLN:HE21	11:m:563:ILE:HG12	1.75	0.52
7:i:794:ARG:HE	7:i:798:ILE:HD11	1.75	0.52
9:k:259:HIS:O	9:k:263:ASN:ND2	2.43	0.52
11:m:144:LYS:NZ	11:m:194:PRO:O	2.39	0.52
5:D:82:GLN:OE1	5:D:86:ARG:NH1	2.42	0.52
9:4:907:LEU:HD22	9:4:924:ARG:HH12	1.73	0.52
10:5:631:LYS:HA	10:5:634:LEU:HB2	1.91	0.52
1:G:745:LEU:HB2	3:b:66:MET:HE1	1.90	0.52
5:d:62:ASP:OD1	5:d:62:ASP:N	2.37	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:379:PHE:N	13:l:801:ATP:N1	2.49	0.52
11:m:533:ILE:HD12	11:m:544:LYS:HB3	1.92	0.52
5:D:178:ASP:N	5:D:178:ASP:OD1	2.41	0.52
9:4:323:ASP:OD2	12:7:303:ARG:HG2	2.10	0.52
9:k:308:VAL:O	9:k:327:ASN:ND2	2.42	0.52
12:7:500:ASP:HB2	12:7:505:GLU:HA	1.92	0.52
1:E:722:LEU:HD13	1:E:776:ILE:HA	1.92	0.51
7:i:699:VAL:O	7:i:702:SER:OG	2.28	0.51
9:k:353:ASP:OD1	9:k:353:ASP:N	2.43	0.51
10:l:498:GLU:OE1	10:l:549:ARG:NE	2.44	0.51
4:C:104:PHE:CD2	4:C:104:PHE:C	2.85	0.51
10:5:643:ARG:NH2	10:5:691:ALA:O	2.43	0.51
11:6:125:GLN:NE2	11:6:131:GLU:OE1	2.43	0.51
11:6:381:LEU:CD1	11:6:385:SER:HG	2.19	0.51
11:6:711:LEU:HG	11:6:712:PHE:H	1.76	0.51
12:7:609:ASP:O	12:7:613:ALA:N	2.42	0.51
1:G:773:GLU:OE2	3:b:67:ARG:CA	2.58	0.51
3:b:132:ASP:N	3:b:132:ASP:OD1	2.43	0.51
6:h:68:ARG:NH1	6:h:95:PHE:O	2.44	0.51
9:k:323:ASP:OD2	12:n:303:ARG:HG2	2.10	0.51
3:B:132:ASP:N	3:B:132:ASP:OD1	2.43	0.51
9:4:259:HIS:O	9:4:263:ASN:ND2	2.43	0.51
9:4:699:LEU:O	9:4:796:ARG:NH2	2.39	0.51
10:5:259:GLN:NE2	10:5:272:ARG:O	2.41	0.51
10:5:561:ASN:HB2	10:5:564:ARG:HG2	1.92	0.51
11:6:298:SER:OG	11:6:299:GLU:N	2.40	0.51
5:d:82:GLN:OE1	5:d:86:ARG:NH1	2.42	0.51
5:d:189:ILE:HD12	5:d:192:LYS:HB2	1.93	0.51
6:h:407:ASP:OD1	6:h:407:ASP:N	2.39	0.51
7:i:528:ASN:H	7:i:530:LYS:HZ3	1.56	0.51
9:k:700:SER:OG	9:k:701:ARG:NH1	2.43	0.51
11:m:125:GLN:NE2	11:m:131:GLU:OE1	2.43	0.51
5:D:179:GLU:HA	5:D:182:TYR:HB3	1.92	0.51
9:4:180:ILE:HG22	9:4:182:GLY:H	1.75	0.51
11:6:747:SER:H	11:6:750:GLN:HG2	1.76	0.51
5:d:210:ASN:C	5:d:218:MET:SD	2.94	0.51
9:k:180:ILE:HG22	9:k:182:GLY:H	1.75	0.51
9:k:323:ASP:OD2	12:n:303:ARG:CG	2.59	0.51
9:k:794:THR:OG1	9:k:795:THR:N	2.40	0.51
12:n:364:LYS:HA	12:n:368:ALA:HB3	1.93	0.51
6:H:533:GLY:H	6:H:536:LEU:HD21	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:514:THR:OG1	6:h:301:ARG:CD	2.56	0.51
5:d:179:GLU:HA	5:d:182:TYR:HB3	1.92	0.51
6:h:249:ASN:OD1	6:h:290:ARG:NH2	2.40	0.51
6:h:334:LEU:O	6:h:337:SER:OG	2.24	0.51
2:A:67:VAL:HG13	4:C:24:ILE:HG23	1.92	0.51
2:A:137:LEU:HD21	5:D:182:TYR:HD1	1.76	0.51
3:B:185:ILE:HD12	3:B:188:ILE:HD11	1.93	0.51
7:2:340:ASN:ND2	7:2:346:SER:O	2.43	0.51
8:3:169:ARG:NH1	8:3:266:PRO:O	2.36	0.51
10:5:258:LEU:CD1	10:5:276:MET:CE	2.84	0.51
11:6:601:LYS:HG2	11:6:643:LYS:HD3	1.93	0.51
9:k:769:GLU:OE2	9:k:823:GLN:NE2	2.43	0.51
11:m:711:LEU:HG	11:m:712:PHE:H	1.75	0.51
8:3:413:THR:H	8:3:415:LYS:HZ1	1.59	0.51
10:5:381:ASN:HD21	10:5:384:ILE:HD12	1.75	0.51
10:5:498:GLU:OE1	10:5:549:ARG:NE	2.44	0.51
12:7:534:ARG:HG2	12:7:586:LEU:HD11	1.93	0.51
5:D:210:ASN:C	5:D:218:MET:SD	2.94	0.51
6:H:68:ARG:NH1	6:H:95:PHE:O	2.44	0.51
7:2:583:ASP:HB2	7:2:587:LYS:HB2	1.93	0.51
8:3:313:THR:N	10:5:201:THR:O	2.39	0.51
12:n:495:ALA:HA	12:n:510:GLY:HA2	1.92	0.51
6:H:381:ASP:O	6:H:385:LYS:N	2.30	0.51
7:2:235:GLY:HA3	7:2:283:TYR:HE2	1.76	0.51
9:4:315:ARG:NH2	12:7:250:ASP:OD1	2.44	0.51
9:4:769:GLU:OE2	9:4:823:GLN:NE2	2.44	0.51
1:G:730:LYS:CD	1:G:817:ILE:HD13	2.20	0.51
2:a:35:ASP:N	2:a:35:ASP:OD1	2.41	0.51
3:b:150:GLU:HA	3:b:153:GLN:HG2	1.93	0.51
6:h:516:LYS:HE2	7:i:779:HIS:HE1	1.76	0.51
10:l:427:LYS:O	10:l:431:LYS:NZ	2.42	0.51
12:n:534:ARG:HG2	12:n:586:LEU:HD11	1.93	0.51
6:H:516:LYS:HE2	7:2:779:HIS:HE1	1.76	0.51
9:4:364:VAL:HG13	11:6:440:LEU:HD21	1.92	0.51
6:h:127:ARG:O	6:h:127:ARG:NH1	2.39	0.51
7:i:583:ASP:HB2	7:i:587:LYS:HB2	1.93	0.51
4:C:86:ASN:OD1	4:C:86:ASN:N	2.44	0.51
8:3:412:SER:O	8:3:412:SER:OG	2.27	0.51
9:4:917:ILE:HG22	9:4:925:ARG:HB3	1.93	0.51
3:b:187:GLU:O	3:b:191:LYS:NZ	2.36	0.50
4:c:122:ASN:O	4:c:125:SER:OG	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:282:ILE:O	6:h:587:ARG:NH1	2.42	0.50
8:j:281:ASP:OD1	8:j:281:ASP:N	2.42	0.50
10:l:599:MET:CA	10:l:602:TYR:HE2	2.08	0.50
7:2:699:VAL:O	7:2:702:SER:OG	2.28	0.50
9:4:184:ASN:ND2	9:4:264:TYR:OH	2.43	0.50
10:5:68:LEU:O	10:5:72:ASN:CA	2.56	0.50
12:7:73:ARG:NH2	12:7:199:ARG:O	2.44	0.50
12:7:544:GLN:OE1	12:7:559:ALA:N	2.41	0.50
9:k:184:ASN:ND2	9:k:264:TYR:OH	2.43	0.50
9:k:327:ASN:O	9:k:329:LYS:NZ	2.45	0.50
9:k:364:VAL:HG13	11:m:440:LEU:HD21	1.92	0.50
9:k:917:ILE:HG22	9:k:925:ARG:HB3	1.93	0.50
12:n:500:ASP:HB2	12:n:505:GLU:HA	1.92	0.50
5:D:176:SER:N	5:D:179:GLU:OE2	2.40	0.50
6:H:551:TRP:HE3	6:H:552:LEU:HD22	1.76	0.50
7:2:794:ARG:HE	7:2:798:ILE:HD11	1.75	0.50
8:3:95:ARG:HH22	8:3:154:LYS:HG3	1.76	0.50
9:4:535:ASP:N	9:4:535:ASP:OD1	2.43	0.50
9:4:563:ASN:ND2	9:4:701:ARG:O	2.36	0.50
10:5:392:LEU:O	10:5:607:ARG:NH2	2.44	0.50
1:G:864:LYS:CE	5:d:9:LEU:HD11	2.36	0.50
2:a:137:LEU:HD21	5:d:182:TYR:HD1	1.76	0.50
8:j:429:ALA:HB1	8:j:469:VAL:H	1.76	0.50
9:k:563:ASN:ND2	9:k:701:ARG:O	2.36	0.50
10:l:381:ASN:HD21	10:l:384:ILE:HD12	1.75	0.50
7:2:316:SER:OG	7:2:317:LEU:N	2.43	0.50
9:4:435:VAL:HG23	9:4:466:VAL:HG23	1.92	0.50
4:c:174:LYS:O	4:c:178:LYS:N	2.44	0.50
6:h:416:ARG:HA	10:l:66:GLU:OE2	2.11	0.50
8:j:195:LYS:N	8:j:251:ILE:O	2.44	0.50
11:m:378:ASP:OD2	11:m:378:ASP:N	2.42	0.50
5:D:189:ILE:HD12	5:D:192:LYS:HB2	1.93	0.50
2:a:67:VAL:HG13	4:c:24:ILE:HG23	1.92	0.50
6:h:639:PRO:O	6:h:643:LYS:NZ	2.43	0.50
10:l:392:LEU:O	10:l:607:ARG:NH2	2.44	0.50
6:H:420:SER:N	6:H:423:GLU:OE2	2.45	0.50
10:5:599:MET:CA	10:5:602:TYR:HE2	2.08	0.50
1:E:704:LEU:HD22	1:E:752:LEU:HD22	1.94	0.50
1:G:731:MET:HA	1:G:814:GLU:OE2	2.12	0.50
2:a:8:LYS:HA	2:a:11:LEU:HB2	1.94	0.50
7:i:625:GLU:OE2	10:l:423:SER:OG	2.30	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:706:SER:O	11:m:762:LYS:NZ	2.34	0.50
12:n:73:ARG:NH2	12:n:199:ARG:O	2.44	0.50
3:B:150:GLU:HA	3:B:153:GLN:HG2	1.93	0.50
8:3:195:LYS:N	8:3:251:ILE:O	2.44	0.50
8:3:310:ASN:O	8:3:312:ASN:ND2	2.45	0.50
9:4:327:ASN:O	9:4:329:LYS:NZ	2.45	0.50
9:4:509:ILE:O	9:4:513:ALA:N	2.39	0.50
7:i:316:SER:OG	7:i:317:LEU:N	2.43	0.50
8:j:40:ASP:OD1	8:j:40:ASP:N	2.44	0.50
9:k:304:ARG:HG2	9:k:465:HIS:HB2	1.93	0.50
9:k:315:ARG:NH2	12:n:250:ASP:OD1	2.44	0.50
9:4:646:HIS:CD2	9:4:646:HIS:H	2.30	0.50
1:E:518:PHE:HB3	3:B:30:ARG:CZ	2.42	0.50
1:F:607:PHE:HD1	1:G:831:LYS:NZ	2.10	0.50
1:G:904:ARG:HH11	5:d:3:ILE:HG12	1.77	0.50
5:d:98:ILE:HA	5:d:101:ILE:HG22	1.93	0.50
8:j:95:ARG:HH22	8:j:154:LYS:HG3	1.76	0.50
9:k:226:TYR:OH	9:k:244:ASP:N	2.42	0.50
11:m:297:THR:OG1	11:m:298:SER:N	2.45	0.50
11:m:566:ARG:NH1	11:m:657:GLU:O	2.44	0.50
2:A:150:ASP:OD1	5:D:137:LYS:NZ	2.45	0.50
6:H:6:SER:OG	6:H:141:GLN:OE1	2.27	0.50
6:H:416:ARG:HA	10:5:66:GLU:OE2	2.11	0.50
7:2:328:THR:OG1	7:2:329:GLY:N	2.45	0.50
7:2:686:LEU:O	11:6:781:ARG:NH1	2.44	0.50
9:4:323:ASP:OD2	12:7:303:ARG:CG	2.59	0.50
9:4:517:ASP:O	9:4:521:LEU:N	2.36	0.50
10:5:400:LEU:O	10:5:402:ASP:N	2.42	0.50
11:6:297:THR:OG1	11:6:298:SER:N	2.45	0.50
1:G:708:SER:CB	1:G:836:LEU:HD21	2.41	0.50
5:d:288:ASP:OD1	5:d:288:ASP:N	2.43	0.50
8:j:523:TYR:OH	8:j:532:ASN:O	2.24	0.50
9:k:401:GLU:OE2	9:k:413:HIS:N	2.45	0.50
10:l:184:ARG:H	10:l:240:PRO:HB2	1.77	0.50
6:H:91:ASP:OD2	6:H:94:ALA:N	2.43	0.50
10:5:96:GLN:HA	10:5:99:LYS:HE2	1.93	0.50
10:5:251:ILE:HA	10:5:280:ARG:HE	1.77	0.50
1:E:904:ARG:HH11	5:D:3:ILE:HG23	1.77	0.49
6:h:561:ASP:OD1	6:h:561:ASP:N	2.42	0.49
7:i:235:GLY:HA3	7:i:283:TYR:HE2	1.76	0.49
12:n:427:ASP:N	12:n:427:ASP:OD1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3:429:ALA:HB1	8:3:469:VAL:H	1.76	0.49
9:4:304:ARG:HG2	9:4:465:HIS:HB2	1.93	0.49
9:4:353:ASP:N	9:4:353:ASP:OD1	2.43	0.49
9:4:433:ILE:HD12	9:4:468:LYS:CA	2.41	0.49
9:4:468:LYS:C	9:4:468:LYS:CD	2.86	0.49
9:4:651:GLN:HG2	11:6:586:LYS:HZ1	1.75	0.49
10:5:258:LEU:HD12	10:5:276:MET:CE	2.42	0.49
10:5:276:MET:SD	10:5:330:ILE:HG21	2.52	0.49
10:5:379:PHE:N	13:5:801:ATP:N1	2.49	0.49
1:G:770:LEU:HD12	3:b:134:PHE:HA	1.93	0.49
2:a:150:ASP:OD1	5:d:137:LYS:NZ	2.45	0.49
7:i:328:THR:OG1	7:i:329:GLY:N	2.45	0.49
7:i:338:LYS:NZ	7:i:378:GLU:O	2.42	0.49
7:i:686:LEU:O	11:m:781:ARG:NH1	2.44	0.49
8:j:212:ARG:HH21	12:n:5:LEU:HD21	1.77	0.49
9:k:622:VAL:HG22	9:k:667:ALA:HB2	1.94	0.49
3:B:153:GLN:HE21	10:5:51:ARG:HE	1.61	0.49
10:5:198:ASN:N	10:5:198:ASN:OD1	2.45	0.49
1:E:527:HIS:CG	6:H:301:ARG:NH1	2.76	0.49
6:h:76:ASP:OD1	6:h:76:ASP:N	2.42	0.49
10:l:96:GLN:HA	10:l:99:LYS:HE2	1.93	0.49
10:l:259:GLN:NE2	10:l:272:ARG:O	2.41	0.49
11:m:747:SER:H	11:m:750:GLN:HG2	1.76	0.49
12:n:87:GLN:HA	12:n:90:ASN:HB2	1.94	0.49
12:n:517:ASP:OD2	12:n:560:ARG:NH2	2.46	0.49
2:A:151:LEU:HD11	5:D:144:ILE:HD11	1.92	0.49
6:H:282:ILE:O	6:H:587:ARG:NH1	2.43	0.49
10:5:69:ILE:HG13	10:5:70:GLY:N	2.26	0.49
10:5:487:ASP:OD1	10:5:487:ASP:N	2.43	0.49
1:E:521:GLY:H	3:B:84:LYS:CD	2.23	0.49
3:b:185:ILE:HD12	3:b:188:ILE:HD11	1.92	0.49
9:k:512:VAL:HG22	9:k:515:ARG:HH12	1.77	0.49
9:k:651:GLN:HG2	11:m:586:LYS:HZ1	1.78	0.49
6:H:386:ARG:O	6:H:390:ILE:N	2.45	0.49
9:4:512:VAL:HG22	9:4:515:ARG:HH12	1.77	0.49
12:7:595:ASP:OD1	12:7:595:ASP:N	2.46	0.49
10:l:276:MET:SD	10:l:330:ILE:HG21	2.52	0.49
10:l:444:SER:O	10:l:444:SER:OG	2.30	0.49
11:m:275:ARG:NH1	11:m:278:ASP:OD2	2.46	0.49
12:n:690:LEU:HA	12:n:693:ILE:HD12	1.93	0.49
6:H:75:ASP:HB3	6:H:118:ARG:HH22	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:625:GLU:OE2	10:5:423:SER:OG	2.30	0.49
8:3:480:ASP:OD1	8:3:480:ASP:N	2.44	0.49
9:4:515:ARG:HG2	9:4:517:ASP:H	1.78	0.49
2:a:62:MET:N	2:a:62:MET:SD	2.86	0.49
2:a:67:VAL:HG22	4:c:24:ILE:HD12	1.95	0.49
4:c:86:ASN:OD1	4:c:86:ASN:N	2.44	0.49
5:d:74:PRO:HB3	5:d:226:LYS:HE3	1.94	0.49
6:h:228:LYS:O	6:h:232:GLU:N	2.41	0.49
11:m:601:LYS:HG2	11:m:643:LYS:HD3	1.93	0.49
2:A:67:VAL:HG22	4:C:24:ILE:HD12	1.95	0.49
2:A:124:SER:O	2:A:128:GLN:N	2.46	0.49
6:H:239:GLU:O	6:H:243:GLN:NE2	2.46	0.49
6:H:254:GLN:O	6:H:257:SER:OG	2.28	0.49
7:2:739:ASN:O	7:2:743:ARG:N	2.43	0.49
8:3:212:ARG:HH21	12:7:5:LEU:HD21	1.77	0.49
9:4:622:VAL:HG22	9:4:667:ALA:HB2	1.94	0.49
12:7:517:ASP:OD2	12:7:560:ARG:NH2	2.46	0.49
2:a:46:ASN:O	2:a:50:ASN:ND2	2.41	0.49
6:h:75:ASP:HB3	6:h:118:ARG:HH22	1.78	0.49
6:h:323:ASP:OD2	6:h:406:ARG:NH1	2.45	0.49
6:h:420:SER:N	6:h:423:GLU:OE2	2.45	0.49
6:h:493:ASN:OD1	6:h:493:ASN:N	2.42	0.49
7:i:466:GLU:OE1	7:i:741:ARG:NH1	2.46	0.49
10:l:69:ILE:HG13	10:l:70:GLY:N	2.27	0.49
10:l:400:LEU:O	10:l:402:ASP:N	2.42	0.49
12:n:673:ARG:NH1	12:n:674:GLU:OE1	2.45	0.49
2:A:62:MET:SD	2:A:62:MET:N	2.86	0.49
7:2:782:ASP:OD1	7:2:782:ASP:N	2.33	0.49
8:3:24:ARG:HD3	8:3:124:PRO:HG3	1.95	0.49
10:5:184:ARG:H	10:5:240:PRO:HB2	1.77	0.49
12:7:364:LYS:HA	12:7:368:ALA:HB3	1.93	0.49
12:7:690:LEU:HA	12:7:693:ILE:HD12	1.93	0.49
2:a:124:SER:O	2:a:128:GLN:N	2.46	0.49
7:i:434:TYR:CZ	7:i:447:PHE:CA	2.83	0.49
10:l:598:LYS:HG2	10:l:601:ARG:HH22	1.78	0.49
12:n:13:ASP:OD1	12:n:13:ASP:N	2.46	0.49
6:H:377:TRP:HA	6:H:381:ASP:HB3	1.95	0.49
6:H:612:ILE:HD11	6:H:644:LEU:HD21	1.94	0.49
11:6:275:ARG:NH1	11:6:278:ASP:OD2	2.46	0.49
11:6:645:ASP:OD1	11:6:647:SER:OG	2.29	0.49
1:F:571:PRO:CG	1:G:781:PHE:C	2.86	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:512:SER:OG	6:h:301:ARG:HG2	2.13	0.49
6:h:377:TRP:HA	6:h:381:ASP:HB3	1.94	0.49
8:j:313:THR:N	10:l:201:THR:O	2.39	0.49
9:k:506:LEU:HD23	9:k:509:ILE:HD11	1.94	0.49
9:k:509:ILE:O	9:k:513:ALA:N	2.39	0.49
9:k:515:ARG:HG2	9:k:517:ASP:H	1.78	0.49
10:l:251:ILE:HA	10:l:280:ARG:HE	1.77	0.49
4:C:25:PRO:HA	4:C:37:PRO:HA	1.95	0.49
6:H:37:ASP:OD1	6:H:37:ASP:N	2.45	0.49
6:H:323:ASP:OD2	6:H:406:ARG:NH1	2.46	0.49
6:H:409:PHE:O	6:H:420:SER:OG	2.28	0.49
6:H:503:GLN:HA	6:H:506:ILE:HG22	1.95	0.49
11:6:173:GLN:O	11:6:177:PHE:N	2.34	0.49
12:7:90:ASN:OD1	12:7:214:ARG:NH1	2.42	0.49
1:G:527:HIS:HB2	6:h:301:ARG:NH1	2.28	0.49
3:b:153:GLN:HE21	10:l:51:ARG:HE	1.61	0.49
6:h:386:ARG:O	6:h:390:ILE:N	2.45	0.49
6:h:551:TRP:HE3	6:h:552:LEU:HD22	1.76	0.49
7:i:245:ASN:HD21	7:i:248:HIS:HB2	1.77	0.49
8:j:201:HIS:HB2	8:j:210:HIS:HB2	1.95	0.49
12:n:90:ASN:OD1	12:n:214:ARG:NH1	2.42	0.49
7:2:617:ARG:O	7:2:621:HIS:ND1	2.38	0.49
9:4:308:VAL:O	9:4:327:ASN:ND2	2.42	0.49
9:4:371:CYS:SG	9:4:372:GLU:N	2.79	0.49
9:4:768:THR:HG22	9:4:772:ARG:HH21	1.78	0.49
11:6:381:LEU:HD12	11:6:385:SER:OG	2.00	0.49
12:7:287:GLU:O	12:7:291:GLN:NE2	2.43	0.49
2:a:113:ILE:O	2:a:116:SER:OG	2.30	0.48
6:h:267:LEU:O	6:h:271:TRP:N	2.44	0.48
6:h:503:GLN:HA	6:h:506:ILE:HG22	1.95	0.48
6:h:612:ILE:HD11	6:h:644:LEU:HD21	1.94	0.48
5:D:66:SER:O	5:D:69:ASN:ND2	2.46	0.48
5:D:74:PRO:HB3	5:D:226:LYS:HE3	1.94	0.48
6:H:331:HIS:O	6:H:332:SER:CB	2.61	0.48
1:E:527:HIS:HD2	6:H:301:ARG:NH1	1.86	0.48
6:h:37:ASP:OD1	6:h:37:ASP:N	2.45	0.48
6:h:331:HIS:O	6:h:332:SER:CB	2.61	0.48
8:j:310:ASN:O	8:j:312:ASN:ND2	2.45	0.48
9:k:438:THR:OG1	9:k:439:PHE:N	2.41	0.48
5:D:159:ARG:O	5:D:163:GLU:N	2.46	0.48
5:D:161:LEU:HD21	5:D:168:LEU:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:257:THR:OG1	5:D:269:LEU:O	2.27	0.48
9:4:401:GLU:OE2	9:4:413:HIS:N	2.45	0.48
9:4:674:SER:O	9:4:674:SER:OG	2.31	0.48
12:7:290:SER:HA	12:7:295:LYS:HG3	1.95	0.48
4:c:25:PRO:HA	4:c:37:PRO:HA	1.95	0.48
5:d:66:SER:O	5:d:69:ASN:ND2	2.46	0.48
5:d:159:ARG:O	5:d:163:GLU:N	2.46	0.48
6:h:6:SER:OG	6:h:141:GLN:OE1	2.27	0.48
9:k:311:CYS:SG	9:k:312:LYS:N	2.85	0.48
9:k:699:LEU:O	9:k:796:ARG:NH2	2.39	0.48
12:n:287:GLU:O	12:n:291:GLN:NE2	2.43	0.48
12:n:595:ASP:OD1	12:n:595:ASP:N	2.46	0.48
5:D:98:ILE:HA	5:D:101:ILE:HG22	1.93	0.48
6:H:482:ASP:OD1	6:H:482:ASP:N	2.33	0.48
7:2:466:GLU:OE1	7:2:741:ARG:NH1	2.46	0.48
10:5:440:SER:HA	10:5:479:ILE:HA	1.95	0.48
10:5:444:SER:O	10:5:444:SER:OG	2.30	0.48
1:G:525:GLU:CG	6:h:263:GLY:O	2.62	0.48
1:G:864:LYS:CD	5:d:9:LEU:HD11	2.43	0.48
6:h:239:GLU:O	6:h:243:GLN:NE2	2.46	0.48
9:k:674:SER:O	9:k:674:SER:OG	2.31	0.48
9:k:768:THR:HG22	9:k:772:ARG:HH21	1.78	0.48
5:D:288:ASP:N	5:D:288:ASP:OD1	2.43	0.48
9:4:311:CYS:SG	9:4:312:LYS:N	2.85	0.48
12:7:142:ILE:HA	12:7:145:GLN:HB2	1.95	0.48
1:E:527:HIS:CE1	6:H:260:SER:HB2	2.48	0.48
3:b:52:LEU:HB2	3:b:59:ALA:HB2	1.96	0.48
7:i:465:ASN:OD1	7:i:465:ASN:N	2.43	0.48
7:i:610:ASP:N	7:i:610:ASP:OD1	2.45	0.48
8:j:27:ARG:HA	8:j:30:GLU:HB3	1.96	0.48
9:k:646:HIS:H	9:k:646:HIS:CD2	2.30	0.48
3:B:24:PRO:HB2	3:B:70:GLU:HG3	1.94	0.48
4:C:174:LYS:O	4:C:178:LYS:N	2.44	0.48
6:H:127:ARG:O	6:H:127:ARG:NH1	2.40	0.48
9:4:506:LEU:HD23	9:4:509:ILE:HD11	1.94	0.48
10:5:333:ILE:HG22	10:5:335:SER:HB3	1.96	0.48
1:G:729:TRP:CZ2	1:G:815:ILE:HG21	2.48	0.48
3:b:24:PRO:HB2	3:b:70:GLU:HG3	1.94	0.48
4:c:16:PHE:HZ	4:c:111:TRP:HZ3	1.62	0.48
6:h:396:LEU:HD11	6:h:402:GLN:HE22	1.79	0.48
7:i:835:ASP:OD1	7:i:835:ASP:N	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:n:290:SER:HA	12:n:295:LYS:HG3	1.95	0.48
7:2:245:ASN:HD21	7:2:248:HIS:HB2	1.77	0.48
9:4:571:SER:O	9:4:571:SER:OG	2.30	0.48
12:7:87:GLN:HA	12:7:90:ASN:HB2	1.94	0.48
1:E:524:ARG:NH2	6:H:13:ASN:ND2	2.46	0.48
2:a:168:LEU:N	2:a:206:GLN:OE1	2.45	0.48
8:j:343:THR:OG1	8:j:344:ASP:N	2.47	0.48
8:j:415:LYS:N	13:j:1001:ATP:O2B	2.46	0.48
9:k:354:HIS:CE1	9:k:356:MET:HB3	2.49	0.48
10:l:44:PHE:CE2	10:l:47:ARG:CD	2.97	0.48
12:n:264:GLN:OE1	12:n:296:GLY:N	2.47	0.48
7:2:439:ASN:OD1	7:2:439:ASN:N	2.47	0.48
8:3:27:ARG:HA	8:3:30:GLU:HB3	1.96	0.48
8:3:31:PHE:HA	8:3:34:THR:HG23	1.95	0.48
8:3:40:ASP:OD1	8:3:40:ASP:N	2.44	0.48
12:7:293:GLN:NE2	12:7:294:THR:OG1	2.47	0.48
12:7:441:ASP:OD1	12:7:441:ASP:N	2.46	0.48
6:h:381:ASP:O	6:h:385:LYS:N	2.30	0.48
7:i:653:ASN:O	7:i:658:ASN:ND2	2.47	0.48
9:k:237:GLY:O	9:k:299:LYS:NZ	2.43	0.48
10:l:565:ASP:N	10:l:565:ASP:OD1	2.47	0.48
5:D:134:GLU:O	5:D:138:PHE:N	2.46	0.48
6:H:354:ASN:O	6:H:358:ARG:N	2.38	0.48
6:H:396:LEU:HD11	6:H:402:GLN:HE22	1.79	0.48
7:2:653:ASN:O	7:2:658:ASN:ND2	2.47	0.48
7:2:835:ASP:N	7:2:835:ASP:OD1	2.45	0.48
8:3:415:LYS:N	13:3:1001:ATP:O2B	2.46	0.48
11:6:566:ARG:NH1	11:6:657:GLU:O	2.44	0.48
2:a:160:ASP:OD1	2:a:160:ASP:N	2.47	0.48
3:b:196:HIS:O	3:b:199:SER:OG	2.32	0.48
8:j:303:ALA:HA	10:l:243:ILE:HD12	1.95	0.48
11:m:829:ASP:HA	11:m:832:ARG:HB2	1.96	0.48
12:n:441:ASP:N	12:n:441:ASP:OD1	2.46	0.48
2:A:8:LYS:HA	2:A:11:LEU:HB2	1.94	0.48
2:A:150:ASP:OD1	2:A:150:ASP:N	2.47	0.48
10:5:598:LYS:HG2	10:5:601:ARG:HH22	1.78	0.48
11:6:829:ASP:HA	11:6:832:ARG:HB2	1.96	0.48
12:7:427:ASP:OD1	12:7:427:ASP:N	2.45	0.48
10:l:68:LEU:O	10:l:72:ASN:CA	2.56	0.48
11:m:732:VAL:HA	11:m:735:HIS:CE1	2.49	0.48
3:B:196:HIS:O	3:B:199:SER:OG	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:250:GLU:OE2	5:D:252:GLY:N	2.41	0.48
9:4:421:ASP:N	9:4:421:ASP:OD1	2.47	0.48
10:5:44:PHE:CE2	10:5:47:ARG:NE	2.81	0.48
1:E:588:VAL:HB	1:E:600:PHE:HB2	1.96	0.47
6:h:331:HIS:HD2	6:h:423:GLU:HG3	1.78	0.47
8:j:31:PHE:HA	8:j:34:THR:HG23	1.96	0.47
8:j:478:MET:O	8:j:483:ARG:NH1	2.47	0.47
7:2:465:ASN:N	7:2:465:ASN:OD1	2.43	0.47
7:2:610:ASP:OD1	7:2:610:ASP:N	2.45	0.47
9:4:237:GLY:O	9:4:299:LYS:NZ	2.43	0.47
9:4:625:ASP:OD1	9:4:625:ASP:N	2.47	0.47
11:6:732:VAL:HA	11:6:735:HIS:CE1	2.49	0.47
12:7:286:SER:OG	12:7:289:CYS:SG	2.68	0.47
12:7:673:ARG:NH1	12:7:674:GLU:OE1	2.45	0.47
6:h:272:LEU:HA	6:h:275:LEU:HD12	1.96	0.47
9:k:421:ASP:OD1	9:k:421:ASP:N	2.47	0.47
10:l:333:ILE:HG22	10:l:335:SER:HB3	1.95	0.47
10:l:496:ALA:O	10:l:500:GLN:NE2	2.47	0.47
12:n:293:GLN:NE2	12:n:294:THR:OG1	2.47	0.47
5:D:89:ASN:O	5:D:92:SER:OG	2.27	0.47
8:3:201:HIS:HB2	8:3:210:HIS:HB2	1.95	0.47
10:5:44:PHE:CE2	10:5:47:ARG:CD	2.97	0.47
10:5:496:ALA:O	10:5:500:GLN:NE2	2.47	0.47
11:6:769:ALA:O	11:6:773:LEU:N	2.48	0.47
12:7:122:ASP:OD1	12:7:122:ASP:N	2.38	0.47
1:E:540:ASN:ND2	1:E:583:ALA:O	2.47	0.47
6:h:254:GLN:O	6:h:257:SER:OG	2.28	0.47
11:m:528:LYS:HE2	11:m:745:PRO:HG3	1.96	0.47
3:B:104:TYR:O	3:B:108:HIS:ND1	2.47	0.47
6:H:331:HIS:HD2	6:H:423:GLU:HG3	1.79	0.47
7:2:616:ASP:O	7:2:619:SER:OG	2.30	0.47
9:4:651:GLN:HB2	9:4:653:THR:HG22	1.97	0.47
1:F:603:PHE:HE1	1:G:880:GLU:CB	2.26	0.47
3:b:150:GLU:O	3:b:154:ILE:N	2.43	0.47
8:j:24:ARG:HD3	8:j:124:PRO:HG3	1.95	0.47
8:j:557:ARG:O	8:j:560:SER:OG	2.31	0.47
10:l:440:SER:HA	10:l:479:ILE:HA	1.95	0.47
3:B:52:LEU:HB2	3:B:59:ALA:HB2	1.96	0.47
6:H:639:PRO:O	6:H:643:LYS:NZ	2.43	0.47
8:3:201:HIS:O	8:3:210:HIS:N	2.47	0.47
1:G:776:ILE:C	1:G:777:ARG:CA	2.86	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:104:TYR:O	3:b:108:HIS:ND1	2.47	0.47
3:b:180:GLU:HB3	4:c:184:TYR:HE1	1.80	0.47
5:d:161:LEU:HD21	5:d:168:LEU:HB3	1.95	0.47
9:k:338:VAL:HG13	9:k:394:LYS:H	1.79	0.47
7:2:590:THR:OG1	7:2:591:LEU:N	2.45	0.47
8:3:303:ALA:HA	10:5:243:ILE:HD12	1.95	0.47
12:7:143:LEU:HD23	12:7:146:ARG:HE	1.79	0.47
12:7:264:GLN:OE1	12:7:296:GLY:N	2.47	0.47
12:7:418:ILE:HD11	12:7:473:ILE:HG23	1.97	0.47
6:h:314:ASP:OD2	6:h:314:ASP:N	2.36	0.47
7:i:439:ASN:OD1	7:i:439:ASN:N	2.46	0.47
7:i:544:ASP:HB2	7:i:656:ARG:HE	1.80	0.47
9:k:594:LYS:NZ	9:k:636:LYS:O	2.45	0.47
9:k:651:GLN:HB2	9:k:653:THR:HG22	1.97	0.47
9:k:700:SER:HB2	11:m:578:SER:HB2	1.96	0.47
11:m:194:PRO:O	11:m:261:ARG:NH2	2.48	0.47
7:2:419:LYS:N	7:2:422:GLU:OE2	2.42	0.47
10:5:581:ASN:O	10:5:585:ASN:ND2	2.47	0.47
1:G:773:GLU:HG3	3:b:28:PHE:HE1	1.78	0.47
6:h:373:ALA:HB1	6:h:377:TRP:NE1	2.30	0.47
7:i:245:ASN:O	7:i:249:LEU:N	2.48	0.47
9:k:625:ASP:OD1	9:k:625:ASP:N	2.47	0.47
10:l:581:ASN:O	10:l:585:ASN:ND2	2.48	0.47
12:n:437:VAL:HG23	12:n:642:ILE:HG23	1.97	0.47
7:2:434:TYR:CE2	7:2:436:GLY:HA2	2.50	0.47
8:3:343:THR:OG1	8:3:344:ASP:N	2.47	0.47
9:4:338:VAL:HG13	9:4:394:LYS:H	1.79	0.47
9:4:354:HIS:CE1	9:4:356:MET:HB3	2.49	0.47
10:5:482:PHE:HB2	10:5:523:ALA:HB2	1.97	0.47
11:6:126:SER:OG	11:6:131:GLU:OE1	2.25	0.47
11:6:398:THR:OG1	11:6:458:HIS:N	2.48	0.47
11:6:528:LYS:HE2	11:6:745:PRO:HG3	1.96	0.47
1:F:680:ASN:ND2	1:F:684:ILE:O	2.48	0.47
1:G:733:GLY:O	1:G:815:ILE:CD1	2.43	0.47
2:a:67:VAL:HG11	4:c:25:PRO:HD2	1.97	0.47
6:h:333:SER:C	6:h:335:TYR:H	2.21	0.47
8:j:703:GLU:HB3	8:j:707:ARG:HH21	1.79	0.47
9:k:682:TYR:OH	9:k:710:ASP:N	2.47	0.47
10:l:258:LEU:HD12	10:l:276:MET:CE	2.42	0.47
12:n:451:ARG:O	12:n:694:ARG:NH2	2.48	0.47
4:C:16:PHE:HZ	4:C:111:TRP:HZ3	1.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:333:SER:C	6:H:335:TYR:H	2.21	0.47
6:H:373:ALA:HB1	6:H:377:TRP:NE1	2.30	0.47
11:6:510:SER:O	11:6:514:ASN:ND2	2.48	0.47
11:6:551:MET:HE1	11:6:592:ALA:HA	1.97	0.47
1:F:532:PHE:O	1:F:548:GLN:NE2	2.47	0.47
9:k:602:THR:CG2	9:k:619:GLY:HA3	2.45	0.47
10:l:190:THR:OG1	10:l:191:SER:N	2.48	0.47
11:m:112:ARG:HE	11:m:184:GLY:HA2	1.80	0.47
11:m:511:ASP:O	11:m:515:GLU:N	2.48	0.47
12:n:724:LYS:HD2	12:n:724:LYS:HA	1.65	0.47
3:B:81:GLN:HA	3:B:129:LYS:HE3	1.97	0.47
3:B:180:GLU:HB3	4:C:184:TYR:HE1	1.80	0.47
8:3:478:MET:O	8:3:483:ARG:NH1	2.48	0.47
10:5:45:ILE:HG13	10:5:46:TYR:N	2.29	0.47
11:6:194:PRO:O	11:6:261:ARG:NH2	2.48	0.47
11:6:511:ASP:O	11:6:515:GLU:N	2.48	0.47
1:E:521:GLY:CA	3:B:84:LYS:HD3	2.45	0.47
6:h:91:ASP:OD2	6:h:94:ALA:N	2.43	0.47
7:i:434:TYR:CE2	7:i:436:GLY:HA2	2.50	0.47
10:l:482:PHE:HB2	10:l:523:ALA:HB2	1.97	0.47
12:n:143:LEU:HD23	12:n:146:ARG:HE	1.79	0.47
12:n:302:THR:O	12:n:305:SER:OG	2.30	0.47
2:A:54:LEU:O	2:A:72:TYR:OH	2.33	0.47
8:3:703:GLU:HB3	8:3:707:ARG:HH21	1.79	0.47
9:4:226:TYR:OH	9:4:244:ASP:N	2.42	0.47
11:6:112:ARG:HE	11:6:184:GLY:HA2	1.80	0.47
1:F:686:SER:HB3	1:F:744:PRO:HG2	1.97	0.46
8:3:235:ASP:O	8:3:237:GLU:N	2.48	0.46
9:4:602:THR:CG2	9:4:619:GLY:HA3	2.45	0.46
9:4:639:ASP:OD1	9:4:642:ARG:NH2	2.48	0.46
1:F:606:PRO:HB2	1:G:828:LEU:HD21	1.97	0.46
1:F:652:LYS:NZ	1:F:713:PRO:O	2.49	0.46
2:a:42:LYS:O	2:a:45:SER:OG	2.28	0.46
7:i:739:ASN:O	7:i:743:ARG:N	2.43	0.46
2:A:113:ILE:O	2:A:116:SER:OG	2.30	0.46
8:3:433:THR:OG1	10:5:503:SER:O	2.33	0.46
10:5:26:GLU:OE1	10:5:26:GLU:HA	2.16	0.46
12:7:437:VAL:HG23	12:7:642:ILE:HG23	1.97	0.46
12:7:451:ARG:O	12:7:694:ARG:NH2	2.48	0.46
6:h:633:ARG:HH11	6:h:634:ARG:H	1.62	0.46
7:i:590:THR:OG1	7:i:591:LEU:N	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:21:PHE:HA	8:j:24:ARG:HE	1.79	0.46
6:H:561:ASP:OD1	6:H:561:ASP:N	2.42	0.46
7:2:245:ASN:O	7:2:249:LEU:N	2.48	0.46
8:3:21:PHE:HA	8:3:24:ARG:HE	1.79	0.46
8:3:666:ARG:HD3	8:3:666:ARG:HA	1.80	0.46
10:5:190:THR:OG1	10:5:191:SER:N	2.48	0.46
1:G:730:LYS:CG	1:G:817:ILE:CD1	2.83	0.46
1:G:730:LYS:HD3	1:G:817:ILE:CD1	2.38	0.46
5:d:69:ASN:O	5:d:73:SER:OG	2.34	0.46
5:d:257:THR:OG1	5:d:269:LEU:O	2.27	0.46
8:j:57:ASN:HD21	12:n:220:ILE:HD11	1.81	0.46
9:k:517:ASP:O	9:k:521:LEU:N	2.36	0.46
6:H:272:LEU:HA	6:H:275:LEU:HD12	1.96	0.46
9:4:436:THR:O	9:4:436:THR:OG1	2.32	0.46
1:G:519:ASP:HA	3:b:30:ARG:HH11	1.79	0.46
7:i:534:ARG:HH11	7:i:815:ARG:HH22	1.63	0.46
13:j:1001:ATP:C8	10:l:650:ILE:HD11	2.50	0.46
9:k:436:THR:OG1	9:k:436:THR:O	2.32	0.46
9:k:576:GLN:HA	9:k:579:GLN:HB2	1.97	0.46
11:m:294:VAL:HG13	11:m:391:PRO:HA	1.97	0.46
11:m:510:SER:O	11:m:514:ASN:ND2	2.48	0.46
9:4:700:SER:HB2	11:6:578:SER:HB2	1.96	0.46
1:E:525:GLU:CB	6:H:263:GLY:O	2.56	0.46
1:E:713:PRO:O	1:G:653:ARG:NH2	2.48	0.46
1:G:729:TRP:CH2	1:G:786:LEU:CB	2.91	0.46
2:a:117:GLN:O	2:a:121:ASN:N	2.48	0.46
3:b:191:LYS:HB3	4:c:105:PHE:HE1	1.79	0.46
6:h:152:LEU:HD12	6:h:152:LEU:HA	1.83	0.46
6:h:370:LEU:HD21	10:l:161:ARG:H	1.81	0.46
7:i:510:ASP:OD1	7:i:510:ASP:N	2.49	0.46
8:j:389:VAL:HG21	8:j:668:ILE:HD13	1.97	0.46
12:n:418:ILE:HD11	12:n:473:ILE:HG23	1.97	0.46
2:A:67:VAL:HG11	4:C:25:PRO:HD2	1.97	0.46
4:C:166:LEU:N	4:C:166:LEU:CD2	2.79	0.46
7:2:544:ASP:HB2	7:2:656:ARG:HE	1.79	0.46
8:3:415:LYS:HZ3	13:3:1001:ATP:PG	2.38	0.46
9:4:354:HIS:CE1	9:4:372:GLU:HG3	2.51	0.46
9:4:699:LEU:HA	9:4:702:PHE:CZ	2.51	0.46
3:b:182:ARG:HH12	5:d:229:PHE:H	1.64	0.46
7:i:418:SER:OG	7:i:419:LYS:N	2.48	0.46
8:j:310:ASN:OD1	10:l:304:LYS:NZ	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:450:GLN:HB2	9:k:452:VAL:HG22	1.97	0.46
12:n:142:ILE:HA	12:n:145:GLN:HB2	1.96	0.46
12:n:229:GLN:OE1	12:n:229:GLN:N	2.49	0.46
12:n:657:ASN:HA	12:n:660:VAL:HG22	1.97	0.46
7:2:548:ALA:HB2	13:2:901:ATP:C5	2.51	0.46
7:2:745:LEU:O	7:2:749:ARG:N	2.49	0.46
9:4:349:CYS:SG	9:4:350:ASN:N	2.89	0.46
1:G:693:GLY:O	1:G:710:TRP:NE1	2.49	0.46
3:b:97:GLU:OE2	3:b:101:LYS:NZ	2.49	0.46
7:i:548:ALA:HB2	13:i:901:ATP:C5	2.51	0.46
7:i:607:ASP:OD1	7:i:607:ASP:N	2.39	0.46
11:m:551:MET:HE1	11:m:592:ALA:HA	1.97	0.46
12:n:530:ASP:HA	12:n:533:ASP:HB2	1.98	0.46
6:H:89:VAL:HG13	6:H:90:ILE:HD12	1.97	0.46
9:4:450:GLN:HB2	9:4:452:VAL:HG22	1.98	0.46
10:5:25:THR:O	10:5:27:ILE:HD12	2.16	0.46
11:6:582:SER:HA	11:6:585:LEU:HD12	1.97	0.46
12:7:570:LEU:HG	12:7:571:TYR:H	1.80	0.46
1:G:734:GLY:N	1:G:815:ILE:H	2.11	0.46
3:b:81:GLN:HA	3:b:129:LYS:HE3	1.97	0.46
3:b:110:ASP:OD1	3:b:110:ASP:N	2.48	0.46
5:d:176:SER:N	5:d:179:GLU:OE2	2.40	0.46
5:d:199:LEU:HD22	5:d:202:MET:HB2	1.97	0.46
6:h:9:SER:OG	6:h:10:GLU:OE2	2.34	0.46
6:h:322:PRO:O	6:h:330:ARG:NH2	2.48	0.46
9:k:917:ILE:HB	9:k:925:ARG:HH21	1.80	0.46
10:l:45:ILE:HG13	10:l:46:TYR:N	2.29	0.46
6:H:322:PRO:O	6:H:330:ARG:NH2	2.48	0.46
6:H:633:ARG:HH11	6:H:634:ARG:H	1.62	0.46
7:2:626:GLN:OE1	10:5:438:TYR:OH	2.33	0.46
8:3:476:ASP:HB3	8:3:477:LYS:HZ2	1.79	0.46
9:4:821:ASP:N	9:4:821:ASP:OD1	2.49	0.46
10:5:565:ASP:OD1	10:5:565:ASP:N	2.47	0.46
8:j:433:THR:OG1	10:l:503:SER:O	2.33	0.46
9:k:548:THR:O	9:k:550:LYS:NZ	2.49	0.46
9:k:559:ARG:HD3	9:k:652:GLN:HG3	1.97	0.46
9:k:699:LEU:HA	9:k:702:PHE:CZ	2.51	0.46
10:l:170:SER:OG	10:l:171:VAL:N	2.49	0.46
3:B:97:GLU:OE2	3:B:101:LYS:NZ	2.49	0.46
4:C:19:LYS:O	4:C:73:GLU:N	2.45	0.46
8:3:389:VAL:HG21	8:3:668:ILE:HD13	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3:479:THR:O	8:3:483:ARG:NE	2.49	0.46
10:5:26:GLU:CD	10:5:26:GLU:N	2.73	0.46
10:5:419:GLY:H	13:5:801:ATP:PG	2.38	0.46
11:6:294:VAL:HG13	11:6:391:PRO:HA	1.97	0.46
1:G:730:LYS:O	1:G:814:GLU:HG2	2.16	0.45
1:G:746:ALA:HB3	1:G:753[B]:ASN:HD22	1.82	0.45
2:a:54:LEU:O	2:a:72:TYR:OH	2.33	0.45
4:c:166:LEU:N	4:c:166:LEU:CD2	2.79	0.45
5:d:134:GLU:O	5:d:138:PHE:N	2.46	0.45
6:h:350:LEU:HD22	6:h:354:ASN:HB3	1.97	0.45
10:l:198:ASN:OD1	10:l:198:ASN:N	2.45	0.45
10:l:551:ASP:N	10:l:551:ASP:OD1	2.41	0.45
10:l:636:ASN:O	10:l:641:THR:OG1	2.27	0.45
12:n:483:THR:OG1	12:n:484:THR:N	2.49	0.45
8:3:551:ASP:N	8:3:551:ASP:OD1	2.48	0.45
12:7:302:THR:O	12:7:305:SER:OG	2.30	0.45
1:E:753[A]:ASN:CB	3:B:66:MET:CE	2.51	0.45
9:k:354:HIS:CE1	9:k:372:GLU:HG3	2.51	0.45
9:k:639:ASP:OD1	9:k:642:ARG:NH2	2.48	0.45
9:k:821:ASP:OD1	9:k:821:ASP:N	2.49	0.45
10:l:561:ASN:HD22	10:l:564:ARG:HD2	1.82	0.45
12:n:350:ASP:N	12:n:350:ASP:OD1	2.49	0.45
12:n:575:ASN:HB3	12:n:578:LEU:HB2	1.99	0.45
2:A:117:GLN:O	2:A:121:ASN:N	2.49	0.45
8:3:310:ASN:OD1	10:5:304:LYS:NZ	2.49	0.45
9:4:576:GLN:HA	9:4:579:GLN:HB2	1.97	0.45
9:4:627:GLY:O	9:4:670:SER:OG	2.34	0.45
9:4:855:SER:HA	9:4:858:GLN:HB2	1.98	0.45
1:F:603:PHE:O	1:G:881:LYS:CE	2.54	0.45
6:h:43:LYS:O	6:h:46:SER:OG	2.35	0.45
7:i:311:GLU:N	11:m:355:ASP:OD2	2.50	0.45
7:i:626:GLN:OE1	10:l:438:TYR:OH	2.33	0.45
7:i:745:LEU:O	7:i:749:ARG:N	2.49	0.45
8:j:20:VAL:HG13	8:j:24:ARG:HH21	1.81	0.45
8:j:235:ASP:O	8:j:237:GLU:N	2.48	0.45
8:j:551:ASP:OD1	8:j:551:ASP:N	2.47	0.45
9:k:349:CYS:SG	9:k:350:ASN:N	2.89	0.45
2:A:51:THR:OG1	2:A:55:LYS:NZ	2.34	0.45
6:H:350:LEU:HD22	6:H:354:ASN:HB3	1.97	0.45
13:3:1001:ATP:C8	10:5:650:ILE:HD11	2.50	0.45
12:7:657:ASN:HA	12:7:660:VAL:HG22	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:527:HIS:CB	6:h:301:ARG:NH1	2.78	0.45
6:h:39:LEU:O	6:h:42:THR:OG1	2.30	0.45
6:h:410:VAL:HG23	6:h:420:SER:HB2	1.98	0.45
9:k:725:THR:HG23	12:n:657:ASN:HB2	1.99	0.45
10:l:419:GLY:H	13:l:801:ATP:PG	2.38	0.45
11:m:173:GLN:O	11:m:177:PHE:N	2.35	0.45
12:n:90:ASN:ND2	12:n:215:TYR:OH	2.49	0.45
12:n:255:VAL:HG23	12:n:307:PHE:HE1	1.82	0.45
4:C:171:GLU:HA	4:C:174:LYS:HG2	1.98	0.45
5:D:69:ASN:O	5:D:73:SER:OG	2.34	0.45
5:D:199:LEU:HD22	5:D:202:MET:HB2	1.96	0.45
7:2:418:SER:OG	7:2:419:LYS:N	2.48	0.45
7:2:501:MET:HE3	7:2:501:MET:HB3	1.77	0.45
8:3:202:TYR:O	8:3:242:THR:OG1	2.30	0.45
9:4:834:LYS:HD3	9:4:834:LYS:HA	1.72	0.45
10:5:170:SER:OG	10:5:171:VAL:N	2.49	0.45
4:c:171:GLU:HA	4:c:174:LYS:HG2	1.98	0.45
8:j:201:HIS:O	8:j:210:HIS:N	2.46	0.45
9:k:433:ILE:HD12	9:k:433:ILE:HA	1.87	0.45
3:B:180:GLU:OE1	4:C:183:SER:OG	2.32	0.45
8:3:57:ASN:HD21	12:7:220:ILE:HD11	1.81	0.45
9:4:559:ARG:HD3	9:4:652:GLN:HG3	1.97	0.45
10:5:498:GLU:N	10:5:500:GLN:OE1	2.49	0.45
7:i:520:PHE:HE1	7:i:767:ILE:HG23	1.82	0.45
7:i:616:ASP:O	7:i:619:SER:OG	2.30	0.45
9:k:602:THR:CG2	9:k:619:GLY:CA	2.95	0.45
10:l:25:THR:O	10:l:27:ILE:HD12	2.16	0.45
11:m:381:LEU:CD1	11:m:385:SER:HG	2.20	0.45
11:m:527:ASP:OD2	11:m:531:ARG:NH1	2.36	0.45
12:n:570:LEU:HG	12:n:571:TYR:H	1.80	0.45
6:H:370:LEU:HD21	10:5:161:ARG:H	1.81	0.45
7:2:520:PHE:HE1	7:2:767:ILE:HG23	1.82	0.45
8:3:33:ASP:HA	8:3:36:THR:HG23	1.99	0.45
12:7:350:ASP:OD1	12:7:350:ASP:N	2.49	0.45
1:F:607:PHE:CD1	1:G:831:LYS:NZ	2.85	0.45
2:a:32:TYR:H	2:a:123:LEU:HD11	1.82	0.45
5:d:250:GLU:OE2	5:d:252:GLY:N	2.41	0.45
6:h:297:ASP:OD1	6:h:297:ASP:N	2.47	0.45
8:j:415:LYS:HZ3	13:j:1001:ATP:PG	2.39	0.45
11:m:582:SER:HA	11:m:585:LEU:HD12	1.97	0.45
4:C:68:PRO:HB2	4:C:69:VAL:H	1.61	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:9:SER:OG	6:H:10:GLU:OE2	2.34	0.45
6:H:410:VAL:HG23	6:H:420:SER:HB2	1.98	0.45
8:3:557:ARG:O	8:3:560:SER:OG	2.31	0.45
11:6:591:PHE:HZ	11:6:751:LEU:HD22	1.81	0.45
12:7:13:ASP:OD1	12:7:13:ASP:N	2.46	0.45
12:7:90:ASN:ND2	12:7:215:TYR:OH	2.49	0.45
1:E:893:ARG:HE	5:D:12:LEU:CD1	2.29	0.45
1:G:733:GLY:O	1:G:815:ILE:CA	2.64	0.45
2:a:166:ARG:HE	6:h:478:TRP:HE1	1.65	0.45
7:i:571:ALA:HB1	7:i:576:LEU:HD11	1.99	0.45
8:j:33:ASP:HA	8:j:36:THR:HG23	1.99	0.45
8:j:223:THR:HG21	10:l:245:HIS:H	1.82	0.45
8:j:686:LEU:O	8:j:690:ASP:N	2.50	0.45
10:l:26:GLU:N	10:l:26:GLU:CD	2.73	0.45
11:m:699:LEU:HD12	11:m:701:MET:H	1.82	0.45
12:n:252:LYS:HE2	12:n:252:LYS:HB2	1.82	0.45
12:n:652:MET:HB3	12:n:656:VAL:HG21	1.99	0.45
2:A:32:TYR:H	2:A:123:LEU:HD11	1.82	0.45
3:B:120:LEU:HD23	3:B:176:LEU:HD13	1.99	0.45
3:B:140:GLU:OE2	3:B:144:LYS:NZ	2.50	0.45
7:2:796:GLU:O	7:2:800:THR:OG1	2.27	0.45
12:7:229:GLN:OE1	12:7:229:GLN:N	2.49	0.45
12:7:652:MET:HB3	12:7:656:VAL:HG21	1.99	0.45
1:G:518:PHE:HB3	3:b:30:ARG:CZ	2.47	0.45
1:G:727:GLU:CD	1:G:777:ARG:HG3	2.39	0.45
3:b:140:GLU:OE2	3:b:144:LYS:NZ	2.50	0.45
4:c:68:PRO:HB2	4:c:69:VAL:H	1.61	0.45
4:c:97:LEU:HD23	4:c:98:HIS:HD2	1.82	0.45
6:h:545:LEU:HD13	6:h:545:LEU:HA	1.83	0.45
8:j:479:THR:O	8:j:483:ARG:NE	2.49	0.45
9:k:189:GLU:O	9:k:193:ASN:N	2.43	0.45
2:A:168:LEU:N	2:A:206:GLN:OE1	2.45	0.45
3:B:99:ASP:O	3:B:103:GLN:NE2	2.50	0.45
6:H:297:ASP:OD1	6:H:297:ASP:N	2.47	0.45
8:3:20:VAL:HG13	8:3:24:ARG:HH21	1.81	0.45
9:4:348:LYS:HB3	9:4:348:LYS:HE2	1.66	0.45
9:4:548:THR:O	9:4:550:LYS:NZ	2.49	0.45
10:5:561:ASN:HD22	10:5:564:ARG:HD2	1.82	0.45
1:E:491:ARG:NH1	6:H:303:THR:CA	2.80	0.45
3:b:180:GLU:OE1	4:c:183:SER:OG	2.32	0.45
4:c:90:THR:OG1	4:c:91:ASP:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:422:SER:OG	6:h:423:GLU:N	2.49	0.45
6:h:524:ILE:O	6:h:563:GLN:NE2	2.50	0.45
10:l:26:GLU:OE1	10:l:26:GLU:HA	2.16	0.45
2:A:52:GLU:HA	2:A:55:LYS:HD2	1.99	0.45
4:C:104:PHE:CD2	4:C:104:PHE:O	2.70	0.45
6:H:422:SER:OG	6:H:423:GLU:N	2.49	0.45
7:2:534:ARG:HH11	7:2:815:ARG:HH22	1.63	0.45
9:4:315:ARG:HA	12:7:341:ARG:HH21	1.82	0.45
9:4:917:ILE:HB	9:4:925:ARG:HH21	1.81	0.45
12:7:252:LYS:HE2	12:7:252:LYS:HB2	1.82	0.45
12:7:530:ASP:HA	12:7:533:ASP:HB2	1.98	0.45
12:7:575:ASN:HB3	12:7:578:LEU:HB2	1.99	0.45
2:a:199:LEU:HA	2:a:202:GLN:HB3	1.98	0.44
6:h:150:ASP:O	6:h:152:LEU:N	2.50	0.44
6:h:524:ILE:HG22	6:h:565:LEU:HD22	2.00	0.44
8:j:350:ILE:O	8:j:354:SER:OG	2.24	0.44
8:j:698:THR:HB	12:n:463:GLY:HA3	1.99	0.44
9:k:387:ASN:N	9:k:387:ASN:OD1	2.50	0.44
9:k:855:SER:HA	9:k:858:GLN:HB2	1.98	0.44
10:l:139:LEU:O	10:l:334:GLN:NE2	2.50	0.44
10:l:409:ASP:O	10:l:658:ARG:NH1	2.50	0.44
10:l:498:GLU:N	10:l:500:GLN:OE1	2.49	0.44
11:m:296:ARG:NH1	11:m:297:THR:O	2.50	0.44
11:m:591:PHE:HZ	11:m:751:LEU:HD22	1.81	0.44
4:C:49:TRP:CD1	4:C:49:TRP:H	2.35	0.44
4:C:90:THR:OG1	4:C:91:ASP:N	2.50	0.44
6:H:524:ILE:HG22	6:H:565:LEU:HD22	1.99	0.44
11:6:296:ARG:NH1	11:6:297:THR:O	2.50	0.44
11:6:699:LEU:HD12	11:6:701:MET:H	1.82	0.44
12:7:255:VAL:HG23	12:7:307:PHE:HE1	1.82	0.44
12:7:483:THR:OG1	12:7:484:THR:N	2.49	0.44
6:h:89:VAL:HG13	6:h:90:ILE:HD12	1.97	0.44
6:h:273:ASN:N	6:h:273:ASN:OD1	2.48	0.44
6:h:354:ASN:O	6:h:358:ARG:N	2.38	0.44
9:k:321:ASP:HA	9:k:324:LYS:HD3	1.99	0.44
11:m:769:ALA:O	11:m:773:LEU:N	2.48	0.44
2:A:199:LEU:HA	2:A:202:GLN:HB3	1.98	0.44
6:H:420:SER:OG	6:H:421:ALA:N	2.50	0.44
8:3:201:HIS:HD1	8:3:243:THR:HG23	1.82	0.44
3:b:99:ASP:O	3:b:103:GLN:NE2	2.50	0.44
3:b:120:LEU:HD23	3:b:176:LEU:HD13	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:19:LYS:O	4:c:73:GLU:N	2.45	0.44
6:h:361:LYS:HE3	6:h:365:ARG:HH22	1.82	0.44
7:i:617:ARG:O	7:i:621:HIS:ND1	2.38	0.44
8:j:48:TYR:HA	8:j:51:ASN:HB2	1.98	0.44
9:k:627:GLY:O	9:k:670:SER:OG	2.34	0.44
9:k:649:MET:HG2	9:k:701:ARG:HB3	2.00	0.44
10:l:44:PHE:CE2	10:l:47:ARG:NE	2.81	0.44
11:m:803:MET:O	11:m:807:SER:OG	2.32	0.44
3:B:182:ARG:HH12	5:D:229:PHE:H	1.64	0.44
6:H:361:LYS:HE3	6:H:365:ARG:HH22	1.82	0.44
8:3:48:TYR:HA	8:3:51:ASN:HB2	1.98	0.44
10:5:71:TYR:O	10:5:75:ILE:HD12	2.18	0.44
12:7:724:LYS:HD2	12:7:724:LYS:HA	1.65	0.44
2:a:98:ASP:OD1	2:a:98:ASP:N	2.50	0.44
4:c:104:PHE:CD2	4:c:104:PHE:O	2.70	0.44
7:i:501:MET:HE3	7:i:501:MET:HB3	1.77	0.44
9:k:315:ARG:HA	12:n:341:ARG:HH21	1.82	0.44
11:m:398:THR:OG1	11:m:458:HIS:N	2.48	0.44
3:B:191:LYS:HB3	4:C:105:PHE:HE1	1.79	0.44
4:C:173:GLU:HA	4:C:176:ILE:HD12	1.99	0.44
7:2:311:GLU:N	11:6:355:ASP:OD2	2.49	0.44
7:2:458:ARG:HE	7:2:458:ARG:HB3	1.64	0.44
7:2:790:TYR:O	7:2:794:ARG:N	2.50	0.44
8:3:108:ARG:HA	8:3:108:ARG:HD2	1.85	0.44
10:5:409:ASP:O	10:5:658:ARG:NH1	2.50	0.44
11:6:594:ARG:NH1	11:6:633:ASN:OD1	2.49	0.44
7:i:600:ASP:OD2	7:i:601:LYS:NZ	2.36	0.44
9:k:828:LEU:O	9:k:831:SER:OG	2.32	0.44
12:n:265:CYS:HB3	12:n:289:CYS:HB3	1.71	0.44
6:H:147:THR:OG1	6:H:148:VAL:N	2.51	0.44
6:H:150:ASP:O	6:H:152:LEU:N	2.50	0.44
6:H:267:LEU:O	6:H:271:TRP:N	2.44	0.44
8:3:313:THR:N	10:5:201:THR:OG1	2.51	0.44
8:3:686:LEU:O	8:3:690:ASP:N	2.50	0.44
9:4:725:THR:HG23	12:7:657:ASN:HB2	1.99	0.44
10:5:636:ASN:O	10:5:641:THR:OG1	2.28	0.44
12:7:413:ARG:O	12:7:417:SER:OG	2.35	0.44
7:i:796:GLU:O	7:i:800:THR:OG1	2.27	0.44
10:5:139:LEU:O	10:5:334:GLN:NE2	2.50	0.44
2:a:51:THR:OG1	2:a:55:LYS:NZ	2.34	0.44
7:i:778:LEU:HD13	7:i:829:VAL:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:313:THR:N	10:l:201:THR:OG1	2.51	0.44
8:j:690:ASP:N	8:j:690:ASP:OD1	2.51	0.44
10:l:404:MET:HE2	10:l:404:MET:HB3	1.91	0.44
11:m:691:ARG:HH12	11:m:716:LEU:HB2	1.83	0.44
2:A:166:ARG:HE	6:H:478:TRP:HE1	1.64	0.44
6:H:273:ASN:N	6:H:273:ASN:OD1	2.48	0.44
7:2:472:ASP:N	7:2:472:ASP:OD1	2.50	0.44
7:2:536:ASP:O	7:2:815:ARG:NH1	2.50	0.44
8:3:223:THR:HG21	10:5:245:HIS:H	1.82	0.44
8:3:698:THR:HB	12:7:463:GLY:HA3	2.00	0.44
11:6:747:SER:HG	11:6:750:GLN:H	1.65	0.44
12:7:86:LEU:O	12:7:90:ASN:N	2.51	0.44
1:F:722:LEU:HD22	1:F:776:ILE:HG22	2.00	0.44
4:c:173:GLU:HA	4:c:176:ILE:HD12	1.99	0.44
7:i:302:THR:O	7:i:319:ARG:NH2	2.47	0.44
8:j:310:ASN:HA	10:l:203:ASN:HD22	1.83	0.44
9:k:326:ILE:HD11	9:k:439:PHE:HB2	2.00	0.44
10:l:49:GLN:O	10:l:53:ASN:ND2	2.51	0.44
10:l:54:ILE:HD12	10:l:54:ILE:HA	1.90	0.44
6:H:228:LYS:O	6:H:232:GLU:N	2.41	0.44
8:3:310:ASN:HA	10:5:203:ASN:HD22	1.83	0.44
11:6:527:ASP:OD2	11:6:531:ARG:NH1	2.36	0.44
11:6:533:ILE:HD12	11:6:544:LYS:HE2	2.00	0.44
3:B:170:LEU:HB3	3:B:173:LEU:HD23	2.00	0.44
6:H:314:ASP:OD2	6:H:314:ASP:N	2.37	0.44
6:H:524:ILE:O	6:H:563:GLN:NE2	2.50	0.44
10:5:27:ILE:O	10:5:30:SER:OG	2.26	0.44
11:6:691:ARG:HH12	11:6:716:LEU:HB2	1.83	0.44
5:d:89:ASN:O	5:d:92:SER:OG	2.28	0.43
8:j:347:ILE:O	8:j:351:ASN:ND2	2.51	0.43
10:l:181:ILE:HD13	10:l:181:ILE:HA	1.88	0.43
11:m:191:LYS:HE2	11:m:191:LYS:HB3	1.70	0.43
4:C:83:LYS:HA	4:C:83:LYS:HD2	1.76	0.43
4:C:176:ILE:H	4:C:176:ILE:HG13	1.64	0.43
5:D:134:GLU:HA	5:D:137:LYS:HB3	2.00	0.43
9:4:682:TYR:OH	9:4:710:ASP:N	2.47	0.43
2:a:150:ASP:OD1	2:a:150:ASP:N	2.47	0.43
6:h:21:SER:HG	6:h:23:SER:HG	1.66	0.43
9:k:348:LYS:HB3	9:k:348:LYS:HE2	1.66	0.43
10:l:497:MET:HA	10:l:500:GLN:HE22	1.83	0.43
4:C:97:LEU:HD23	4:C:98:HIS:HD2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:14:LYS:HE2	6:H:14:LYS:HB3	1.83	0.43
8:3:386:MET:HB3	8:3:386:MET:HE3	1.64	0.43
10:5:358:LEU:O	10:5:362:ARG:NE	2.51	0.43
10:5:497:MET:HA	10:5:500:GLN:HE22	1.83	0.43
11:6:270:LEU:HD23	11:6:272:THR:H	1.84	0.43
1:F:603:PHE:O	1:G:881:LYS:HG3	2.18	0.43
5:d:134:GLU:HA	5:d:137:LYS:HB3	2.00	0.43
8:j:464:LEU:H	8:j:464:LEU:HG	1.68	0.43
9:k:632:ASP:OD1	9:k:674:SER:OG	2.29	0.43
11:m:189:VAL:O	11:m:193:ALA:N	2.41	0.43
12:n:697:GLN:HA	12:n:700:ALA:HB3	2.01	0.43
2:A:57:GLN:HG2	2:A:61:GLY:HA3	2.00	0.43
7:2:685:ASP:OD1	7:2:685:ASP:N	2.51	0.43
9:4:649:MET:HG2	9:4:701:ARG:HB3	2.00	0.43
10:5:49:GLN:O	10:5:53:ASN:ND2	2.51	0.43
10:5:258:LEU:HB2	10:5:276:MET:CE	2.48	0.43
12:7:672:LYS:HD2	12:7:672:LYS:HA	1.81	0.43
12:7:697:GLN:HA	12:7:700:ALA:HB3	2.01	0.43
2:a:11:LEU:HD23	2:a:11:LEU:HA	1.83	0.43
5:d:210:ASN:O	5:d:218:MET:SD	2.76	0.43
6:h:147:THR:OG1	6:h:148:VAL:N	2.50	0.43
6:h:501:ASP:O	6:h:505:ALA:N	2.50	0.43
8:j:201:HIS:HD1	8:j:243:THR:HG23	1.82	0.43
9:k:205:PHE:HD2	9:k:209:LEU:HD21	1.83	0.43
10:l:71:TYR:O	10:l:75:ILE:HD12	2.18	0.43
10:l:393:MET:HE2	10:l:393:MET:HB3	1.93	0.43
9:4:326:ILE:HD11	9:4:439:PHE:HB2	2.00	0.43
10:5:686:ALA:HA	10:5:689:MET:HE2	2.01	0.43
11:6:720:ASN:HB3	11:6:723:ILE:HG12	2.01	0.43
2:a:131:LEU:HA	2:a:134:TYR:HD2	1.83	0.43
6:h:420:SER:OG	6:h:421:ALA:N	2.49	0.43
8:j:413:THR:H	8:j:415:LYS:HZ1	1.66	0.43
10:l:674:GLU:HA	10:l:677:VAL:HG12	2.01	0.43
2:A:167:VAL:HG12	2:A:187:SER:H	1.83	0.43
6:H:370:LEU:CD2	10:5:161:ARG:HB3	2.47	0.43
7:2:510:ASP:OD1	7:2:510:ASP:N	2.49	0.43
9:4:188:GLN:H	9:4:188:GLN:HG3	1.47	0.43
11:6:189:VAL:O	11:6:193:ALA:N	2.41	0.43
11:6:658:GLN:H	11:6:658:GLN:HG3	1.72	0.43
12:7:625:GLN:H	12:7:626:PRO:CD	2.31	0.43
1:G:729:TRP:CZ3	1:G:786:LEU:HD12	2.22	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:179:GLU:O	5:d:183:HIS:N	2.47	0.43
7:i:248:HIS:O	7:i:252:SER:OG	2.26	0.43
7:i:790:TYR:O	7:i:794:ARG:N	2.50	0.43
10:l:25:THR:C	10:l:26:GLU:CG	2.91	0.43
10:l:25:THR:O	10:l:26:GLU:CB	2.67	0.43
2:A:98:ASP:OD1	2:A:98:ASP:N	2.50	0.43
7:2:706:SER:O	11:6:762:LYS:NZ	2.34	0.43
8:3:727:LYS:HD3	8:3:727:LYS:HA	1.80	0.43
9:4:321:ASP:HA	9:4:324:LYS:HD3	1.99	0.43
10:5:279:ASP:OD2	10:5:280:ARG:N	2.51	0.43
11:6:177:PHE:HB3	11:6:180:PHE:HB2	2.01	0.43
11:6:373:MET:HE3	11:6:373:MET:HB2	1.92	0.43
12:7:258:ILE:HD12	12:7:258:ILE:HA	1.91	0.43
1:E:823:ALA:HB2	1:E:868:ARG:HD2	2.00	0.43
2:a:52:GLU:HA	2:a:55:LYS:HD2	2.00	0.43
7:i:411:LEU:HD23	7:i:411:LEU:HA	1.80	0.43
7:i:536:ASP:O	7:i:815:ARG:NH1	2.50	0.43
8:j:28:PHE:HA	8:j:31:PHE:CZ	2.54	0.43
8:j:211:TYR:HB2	12:n:7:SER:HB3	2.01	0.43
9:k:834:LYS:HA	9:k:834:LYS:HD3	1.72	0.43
12:n:86:LEU:O	12:n:90:ASN:N	2.51	0.43
7:2:325:THR:HG23	7:2:389:THR:HG23	2.00	0.43
7:2:335:LYS:HE2	7:2:335:LYS:HB3	1.76	0.43
8:3:347:ILE:O	8:3:351:ASN:ND2	2.51	0.43
9:4:602:THR:CG2	9:4:619:GLY:CA	2.95	0.43
10:5:54:ILE:HD12	10:5:54:ILE:HA	1.90	0.43
11:6:576:ASP:O	11:6:579:THR:OG1	2.29	0.43
12:7:711:ASP:OD1	12:7:711:ASP:N	2.52	0.43
2:a:57:GLN:HG2	2:a:61:GLY:HA3	2.00	0.43
7:i:794:ARG:HA	7:i:805:ILE:HD11	2.01	0.43
10:l:149:ARG:HD3	10:l:149:ARG:HA	1.82	0.43
10:l:258:LEU:HB2	10:l:276:MET:CE	2.48	0.43
10:l:279:ASP:OD2	10:l:280:ARG:N	2.51	0.43
8:3:211:TYR:HB2	12:7:7:SER:HB3	2.01	0.43
9:4:741:VAL:HG12	9:4:743:PRO:HD3	2.01	0.43
10:5:51:ARG:HH12	10:5:55:LEU:HD22	1.84	0.43
1:G:519:ASP:OD1	3:b:84:LYS:HE2	2.14	0.43
3:b:138:ILE:HD12	3:b:138:ILE:HA	1.85	0.43
6:h:346:ALA:HA	6:h:350:LEU:O	2.19	0.43
6:h:370:LEU:CD2	10:l:161:ARG:HB3	2.47	0.43
8:j:653:ILE:HD13	8:j:653:ILE:HA	1.89	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:315:ARG:HH12	9:k:413:HIS:HD2	1.67	0.43
9:k:693:ASP:N	9:k:693:ASP:OD1	2.41	0.43
11:m:720:ASN:HB3	11:m:723:ILE:HG12	2.01	0.43
12:n:258:ILE:HD12	12:n:258:ILE:HA	1.91	0.43
8:3:687:ARG:HD2	8:3:687:ARG:HA	1.84	0.43
10:5:25:THR:O	10:5:26:GLU:CB	2.67	0.43
12:7:226:SER:OG	12:7:229:GLN:OE1	2.32	0.43
12:7:383:GLN:O	12:7:384:HIS:ND1	2.52	0.43
2:a:181:PHE:HB3	2:a:189:PHE:HE1	1.84	0.43
3:b:170:LEU:HB3	3:b:173:LEU:HD23	2.00	0.43
7:i:289:ILE:HG12	7:i:290:HIS:CD2	2.54	0.43
7:i:325:THR:HG23	7:i:389:THR:HG23	2.00	0.43
8:j:419:LEU:HD13	8:j:419:LEU:HA	1.84	0.43
3:B:138:ILE:HD12	3:B:138:ILE:HA	1.85	0.43
6:H:323:ASP:OD1	6:H:323:ASP:N	2.52	0.43
9:4:315:ARG:HH12	9:4:413:HIS:HD2	1.67	0.43
9:4:603:ALA:O	9:4:658:LYS:NZ	2.52	0.43
12:7:81:ASP:OD1	12:7:81:ASP:N	2.52	0.43
7:i:685:ASP:N	7:i:685:ASP:OD1	2.51	0.42
8:j:256:ILE:HG13	8:j:276:VAL:HG13	2.01	0.42
9:k:510:ARG:O	9:k:514:ALA:N	2.52	0.42
12:n:81:ASP:OD1	12:n:81:ASP:N	2.52	0.42
4:C:83:LYS:HD2	4:C:86:ASN:HD21	1.84	0.42
5:D:210:ASN:O	5:D:218:MET:SD	2.77	0.42
6:H:43:LYS:O	6:H:46:SER:OG	2.35	0.42
6:H:346:ALA:HA	6:H:350:LEU:O	2.19	0.42
7:2:302:THR:O	7:2:319:ARG:NH2	2.47	0.42
7:2:571:ALA:HB1	7:2:576:LEU:HD11	1.99	0.42
7:2:778:LEU:HD13	7:2:829:VAL:HG21	2.00	0.42
9:4:205:PHE:HD2	9:4:209:LEU:HD21	1.83	0.42
9:4:563:ASN:OD1	9:4:563:ASN:N	2.52	0.42
10:5:357:PHE:O	10:5:361:SER:OG	2.34	0.42
11:6:803:MET:HE3	11:6:803:MET:HB2	1.86	0.42
1:E:521:GLY:CA	3:B:84:LYS:HE3	2.46	0.42
6:h:547:ARG:HE	6:h:547:ARG:HB3	1.58	0.42
9:k:432:ARG:HB3	9:k:469:VAL:CB	2.34	0.42
9:k:469:VAL:HG13	9:k:470:SER:N	2.34	0.42
10:l:140:ASN:HB3	10:l:334:GLN:NE2	2.33	0.42
10:l:358:LEU:O	10:l:362:ARG:NE	2.51	0.42
11:m:534:ALA:HA	11:m:535:PRO:HD3	1.89	0.42
2:A:131:LEU:HA	2:A:134:TYR:HD2	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2:337:VAL:HB	7:2:351:PHE:HB2	2.00	0.42
8:3:256:ILE:HG13	8:3:276:VAL:HG13	2.01	0.42
9:4:510:ARG:O	9:4:514:ALA:N	2.52	0.42
9:4:879:ASP:HB3	9:4:926:SER:H	1.84	0.42
10:5:252:ASP:HB3	10:5:280:ARG:HG2	2.01	0.42
10:5:408:GLY:HA2	10:5:658:ARG:HD3	2.01	0.42
12:7:670:ASP:N	12:7:670:ASP:OD1	2.52	0.42
4:c:83:LYS:HD2	4:c:86:ASN:HD21	1.84	0.42
4:c:168:LYS:HE3	4:c:168:LYS:HB2	1.89	0.42
6:h:323:ASP:N	6:h:323:ASP:OD1	2.52	0.42
6:h:373:ALA:HB1	6:h:377:TRP:CD1	2.54	0.42
7:i:306:LEU:HD11	7:i:406:ARG:HG3	2.01	0.42
11:m:381:LEU:CD1	11:m:381:LEU:C	2.85	0.42
12:n:222:SER:O	12:n:222:SER:OG	2.30	0.42
12:n:383:GLN:O	12:n:384:HIS:ND1	2.52	0.42
4:C:112:ILE:HD12	4:C:112:ILE:HA	1.85	0.42
6:H:101:GLN:H	6:H:116:PHE:HE1	1.67	0.42
7:2:232:ARG:O	7:2:283:TYR:OH	2.32	0.42
7:2:485:ARG:O	7:2:488:SER:OG	2.29	0.42
10:5:25:THR:C	10:5:26:GLU:CG	2.91	0.42
11:6:359:VAL:HG23	11:6:379:VAL:HG13	2.01	0.42
6:h:101:GLN:H	6:h:116:PHE:HE1	1.67	0.42
9:k:193:ASN:HA	9:k:196:ASN:HD21	1.84	0.42
9:k:538:LYS:HA	9:k:538:LYS:HD3	1.84	0.42
9:k:661:ILE:HD12	9:k:661:ILE:HA	1.90	0.42
10:l:34:PHE:HZ	10:l:67:HIS:CD2	2.38	0.42
11:m:533:ILE:HD12	11:m:544:LYS:HE2	2.01	0.42
11:m:633:ASN:H	11:m:675:ARG:NH2	2.18	0.42
2:A:41:LEU:HD23	2:A:41:LEU:HA	1.87	0.42
3:B:151:ILE:HD13	3:B:151:ILE:HA	1.91	0.42
8:3:28:PHE:HA	8:3:31:PHE:CZ	2.54	0.42
8:3:221:LEU:HD23	8:3:221:LEU:HA	1.80	0.42
9:4:234:ARG:NH1	9:4:290:ASP:OD2	2.38	0.42
9:4:645:LEU:HA	9:4:648:VAL:HG12	2.01	0.42
10:5:674:GLU:HA	10:5:677:VAL:HG12	2.01	0.42
11:6:104:ASP:OD2	11:6:176:ARG:NH1	2.44	0.42
1:E:704:LEU:HD21	1:E:747:LEU:HD22	2.01	0.42
2:a:166:ARG:HD2	2:a:207:LYS:HE3	2.02	0.42
4:c:49:TRP:CD1	4:c:49:TRP:H	2.35	0.42
6:h:396:LEU:HD12	6:h:396:LEU:HA	1.91	0.42
8:j:520:PHE:HB3	8:j:523:TYR:CG	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:k:741:VAL:HG12	9:k:743:PRO:HD3	2.01	0.42
12:n:444:VAL:HB	12:n:448:MET:HG3	2.01	0.42
2:A:189:PHE:HB3	2:A:191:VAL:HG13	2.02	0.42
4:C:133:GLN:O	4:C:137:HIS:ND1	2.53	0.42
4:C:163:SER:OG	4:C:164:THR:N	2.53	0.42
7:2:306:LEU:HD11	7:2:406:ARG:HG3	2.01	0.42
8:3:342:LEU:HD21	8:3:347:ILE:HD12	2.02	0.42
9:4:193:ASN:HA	9:4:196:ASN:HD21	1.84	0.42
9:4:325:LEU:HD13	9:4:325:LEU:HA	1.92	0.42
10:5:34:PHE:HZ	10:5:67:HIS:CD2	2.38	0.42
10:5:66:GLU:HA	10:5:69:ILE:CG2	2.49	0.42
10:5:599:MET:HG2	10:5:602:TYR:OH	2.20	0.42
11:6:633:ASN:H	11:6:675:ARG:NH2	2.18	0.42
12:7:444:VAL:HB	12:7:448:MET:HG3	2.01	0.42
1:F:755:ILE:HG13	1:F:768:LEU:HD11	2.02	0.42
6:h:294:LEU:HD23	6:h:294:LEU:HA	1.89	0.42
7:i:485:ARG:O	7:i:488:SER:OG	2.29	0.42
7:2:839:LYS:HA	7:2:839:LYS:HD2	1.91	0.42
10:5:659:ILE:HD13	10:5:659:ILE:HA	1.91	0.42
11:6:361:ILE:O	11:6:376:THR:OG1	2.26	0.42
12:7:455:ASN:HB3	12:7:563:ILE:HB	2.01	0.42
1:F:603:PHE:CE1	1:G:880:GLU:HB3	2.49	0.42
2:a:92:LEU:HD12	2:a:92:LEU:HA	1.82	0.42
7:i:472:ASP:OD1	7:i:472:ASP:N	2.50	0.42
8:j:342:LEU:HD21	8:j:347:ILE:HD12	2.02	0.42
8:j:707:ARG:HE	8:j:707:ARG:HB2	1.73	0.42
9:k:756:GLU:O	9:k:759:HIS:NE2	2.53	0.42
9:k:865:LEU:HD23	9:k:865:LEU:HA	1.91	0.42
11:m:747:SER:HG	11:m:750:GLN:H	1.65	0.42
2:A:166:ARG:HD2	2:A:207:LYS:HE3	2.02	0.42
7:2:289:ILE:HG12	7:2:290:HIS:CD2	2.54	0.42
7:2:794:ARG:HA	7:2:805:ILE:HD11	2.01	0.42
9:4:538:LYS:HA	9:4:538:LYS:HD3	1.85	0.42
9:4:755:LYS:HB3	9:4:755:LYS:HE2	1.77	0.42
11:6:549:LEU:HD13	11:6:552:LEU:HD21	2.02	0.42
12:7:664:TYR:O	12:7:668:ARG:N	2.53	0.42
2:a:167:VAL:HG12	2:a:187:SER:H	1.83	0.42
7:i:337:VAL:HB	7:i:351:PHE:HB2	2.00	0.42
7:i:484:PHE:HD1	7:i:484:PHE:HA	1.77	0.42
8:j:251:ILE:HD12	8:j:251:ILE:HA	1.80	0.42
9:k:459:THR:OG1	9:k:460:TYR:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:m:645:ASP:OD1	11:m:647:SER:OG	2.29	0.42
12:n:371:LEU:HD23	12:n:371:LEU:HA	1.89	0.42
12:n:711:ASP:OD1	12:n:711:ASP:N	2.52	0.42
4:C:89:LYS:HD2	4:C:89:LYS:HA	1.78	0.42
8:3:520:PHE:HB3	8:3:523:TYR:CG	2.54	0.42
1:E:478:PRO:HB2	1:E:536:LEU:HD21	2.01	0.42
1:E:660:SER:HB2	1:E:701:ASP:HB3	2.02	0.42
6:h:237:LEU:HD13	6:h:237:LEU:HA	1.92	0.42
6:h:469:LEU:HD12	6:h:469:LEU:HA	1.86	0.42
8:j:48:TYR:O	8:j:52:ASN:ND2	2.53	0.42
8:j:220:THR:HA	8:j:322:LEU:HD22	2.02	0.42
8:j:300:SER:OG	10:l:245:HIS:ND1	2.39	0.42
9:k:879:ASP:HB3	9:k:926:SER:H	1.84	0.42
11:m:270:LEU:HD23	11:m:272:THR:H	1.84	0.42
2:A:84:ARG:NH2	5:D:217:ASN:OD1	2.53	0.42
2:A:181:PHE:HB3	2:A:189:PHE:HE1	1.84	0.42
3:B:119:TRP:CD1	3:B:119:TRP:H	2.38	0.42
4:C:193:LYS:HE3	4:C:193:LYS:HB2	1.88	0.42
6:H:500:GLN:O	6:H:504:ARG:NH2	2.53	0.42
6:H:501:ASP:O	6:H:505:ALA:N	2.50	0.42
8:3:175:HIS:HB2	8:3:178:LYS:HB2	2.02	0.42
9:4:189:GLU:O	9:4:193:ASN:N	2.43	0.42
9:4:204:LYS:HD2	9:4:204:LYS:HA	1.88	0.42
9:4:433:ILE:HD12	9:4:468:LYS:HA	2.02	0.42
9:4:459:THR:OG1	9:4:460:TYR:N	2.53	0.42
11:6:534:ALA:HA	11:6:535:PRO:HD3	1.90	0.42
1:F:607:PHE:HD1	1:G:831:LYS:HZ1	1.67	0.42
4:c:105:PHE:CD2	4:c:105:PHE:C	2.98	0.42
6:h:145:ASP:O	6:h:147:THR:N	2.49	0.42
8:j:727:LYS:HA	8:j:727:LYS:HD3	1.80	0.42
9:k:571:SER:H	9:k:574:LYS:HE3	1.84	0.42
10:l:51:ARG:HH12	10:l:55:LEU:HD22	1.84	0.42
10:l:599:MET:HG2	10:l:602:TYR:OH	2.20	0.42
12:n:625:GLN:H	12:n:626:PRO:CD	2.31	0.42
12:n:664:TYR:O	12:n:668:ARG:N	2.53	0.42
2:A:98:ASP:O	2:A:102:TRP:N	2.53	0.42
9:4:756:GLU:O	9:4:759:HIS:NE2	2.53	0.42
12:7:265:CYS:HB3	12:7:289:CYS:HB3	1.71	0.42
1:F:603:PHE:CD1	1:G:881:LYS:N	2.87	0.41
1:G:776:ILE:HA	1:G:777:ARG:N	2.35	0.41
2:a:32:TYR:N	2:a:123:LEU:HD11	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:81:LEU:HB3	6:h:120:ILE:HG22	2.02	0.41
8:j:202:TYR:N	8:j:242:THR:O	2.49	0.41
8:j:555:GLU:O	8:j:559:ARG:NH1	2.53	0.41
9:k:499:ARG:HH22	9:k:502:THR:HG23	1.85	0.41
9:k:499:ARG:NH2	9:k:500:GLN:O	2.53	0.41
10:l:66:GLU:HA	10:l:69:ILE:CG2	2.49	0.41
11:m:359:VAL:HG23	11:m:379:VAL:HG13	2.01	0.41
6:H:543:LEU:HD13	6:H:546:LEU:HD21	2.01	0.41
8:3:555:GLU:O	8:3:559:ARG:NH1	2.53	0.41
4:c:163:SER:OG	4:c:164:THR:N	2.53	0.41
5:d:84:MET:HE3	5:d:84:MET:HB2	1.79	0.41
6:h:14:LYS:HB3	6:h:14:LYS:HE2	1.83	0.41
6:h:281:ASP:HA	6:h:288:TYR:CE1	2.56	0.41
6:h:376:THR:O	6:h:381:ASP:N	2.54	0.41
7:i:268:LEU:HD23	7:i:268:LEU:HA	1.87	0.41
8:j:175:HIS:HB2	8:j:178:LYS:HB2	2.02	0.41
8:j:466:ASP:OD1	8:j:509:ARG:N	2.48	0.41
9:k:422:GLU:H	9:k:422:GLU:CD	2.28	0.41
11:m:572:CYS:H	11:m:709:PHE:HE2	1.68	0.41
12:n:237:GLN:HB2	12:n:239:ILE:HD11	2.03	0.41
12:n:672:LYS:HA	12:n:672:LYS:HD2	1.81	0.41
2:A:154:SER:OG	5:D:141:ARG:NE	2.54	0.41
3:B:10:THR:OG1	3:B:11:PHE:N	2.53	0.41
3:B:191:LYS:HD2	4:C:105:PHE:CE1	2.56	0.41
6:H:21:SER:HG	6:H:23:SER:HG	1.66	0.41
7:2:622:GLU:OE1	7:2:622:GLU:N	2.53	0.41
10:5:464:LEU:HD13	10:5:464:LEU:HA	1.87	0.41
11:6:191:LYS:HB3	11:6:191:LYS:HE2	1.70	0.41
12:7:371:LEU:HD23	12:7:371:LEU:HA	1.89	0.41
6:h:333:SER:O	6:h:336:ASP:N	2.53	0.41
9:k:279:CYS:O	9:k:282:SER:OG	2.32	0.41
11:m:361:ILE:O	11:m:376:THR:OG1	2.26	0.41
6:H:333:SER:O	6:H:336:ASP:N	2.53	0.41
6:H:373:ALA:HB1	6:H:377:TRP:CD1	2.54	0.41
8:3:350:ILE:O	8:3:354:SER:OG	2.23	0.41
10:5:87:ILE:HD13	10:5:87:ILE:HA	1.88	0.41
11:6:643:LYS:HE2	11:6:643:LYS:HB2	1.88	0.41
12:7:581:LEU:HD12	12:7:584:ILE:HB	2.03	0.41
6:h:500:GLN:O	6:h:504:ARG:NH2	2.53	0.41
6:h:543:LEU:HD13	6:h:546:LEU:HD21	2.01	0.41
9:k:563:ASN:N	9:k:563:ASN:OD1	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:81:ASP:OD2	10:l:81:ASP:N	2.53	0.41
11:m:177:PHE:HB3	11:m:180:PHE:HB2	2.01	0.41
12:n:338:THR:O	12:n:338:THR:OG1	2.34	0.41
12:n:455:ASN:HB3	12:n:563:ILE:HB	2.01	0.41
3:B:189:MET:HA	3:B:192:LEU:HG	2.02	0.41
6:H:374:GLN:HE22	10:5:142:ASN:C	2.28	0.41
9:4:235:GLU:H	9:4:235:GLU:HG3	1.78	0.41
10:5:412:VAL:HG12	10:5:552:MET:HB3	2.02	0.41
12:7:19:ASN:O	12:7:22:THR:OG1	2.31	0.41
1:F:603:PHE:HD2	1:G:884:SER:CB	2.26	0.41
5:d:212:THR:OG1	5:d:213:GLU:N	2.54	0.41
6:h:370:LEU:HD12	6:h:371:SER:CB	2.51	0.41
7:i:379:LYS:HA	7:i:379:LYS:HD2	1.90	0.41
7:i:520:PHE:O	7:i:771:ARG:NH1	2.54	0.41
10:l:34:PHE:HZ	10:l:67:HIS:HD2	1.68	0.41
10:l:236:CYS:SG	10:l:237:GLY:N	2.88	0.41
10:l:252:ASP:HB3	10:l:280:ARG:HG2	2.01	0.41
10:l:408:GLY:HA2	10:l:658:ARG:HD3	2.02	0.41
12:n:446:ASP:OD1	12:n:447:GLY:N	2.53	0.41
2:A:96:ILE:HA	2:A:96:ILE:HD12	1.82	0.41
3:B:118:ASN:OD1	3:B:118:ASN:N	2.53	0.41
9:4:571:SER:H	9:4:574:LYS:HE3	1.84	0.41
10:5:91:GLU:OE2	10:5:134:THR:OG1	2.39	0.41
3:b:189:MET:HA	3:b:192:LEU:HG	2.02	0.41
4:c:83:LYS:HD2	4:c:83:LYS:HA	1.76	0.41
7:i:497:ILE:HD13	7:i:497:ILE:HA	1.86	0.41
7:i:818:GLU:H	7:i:818:GLU:HG3	1.68	0.41
11:m:381:LEU:HD11	11:m:386:VAL:N	2.36	0.41
12:n:581:LEU:HD12	12:n:584:ILE:HB	2.02	0.41
2:A:32:TYR:N	2:A:123:LEU:HD11	2.35	0.41
6:H:376:THR:O	6:H:381:ASP:N	2.53	0.41
7:2:520:PHE:O	7:2:771:ARG:NH1	2.54	0.41
8:3:372:TYR:HD1	8:3:372:TYR:HA	1.75	0.41
9:4:499:ARG:NH2	9:4:500:GLN:O	2.53	0.41
10:5:34:PHE:HZ	10:5:67:HIS:HD2	1.68	0.41
10:5:81:ASP:OD2	10:5:81:ASP:N	2.53	0.41
12:7:496:ALA:HB3	12:7:498:MET:HE2	2.02	0.41
1:G:588:VAL:HB	1:G:600:PHE:HB2	2.02	0.41
1:G:729:TRP:HH2	1:G:786:LEU:HB3	1.83	0.41
7:i:211:LEU:HD11	7:i:274:VAL:HG11	2.03	0.41
7:i:622:GLU:OE1	7:i:622:GLU:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:96:ILE:HD11	8:j:153:TRP:HE3	1.86	0.41
9:k:760:PRO:O	11:m:737:LYS:NZ	2.36	0.41
11:m:162:GLU:HB3	11:m:165:ALA:HB3	2.03	0.41
11:m:803:MET:HE3	11:m:803:MET:HB2	1.86	0.41
2:A:150:ASP:H	5:D:137:LYS:NZ	2.19	0.41
5:D:179:GLU:O	5:D:183:HIS:N	2.47	0.41
1:E:685:LYS:HD2	1:E:698:PHE:HE2	1.85	0.41
1:E:893:ARG:HE	5:D:12:LEU:HD11	1.85	0.41
2:a:185:LYS:HZ2	2:a:185:LYS:HG3	1.60	0.41
3:b:119:TRP:CD1	3:b:119:TRP:H	2.38	0.41
7:i:335:LYS:HB3	7:i:335:LYS:HE2	1.76	0.41
7:i:751:LYS:HB3	7:i:751:LYS:HE3	1.94	0.41
8:j:202:TYR:O	8:j:242:THR:OG1	2.30	0.41
9:k:645:LEU:HA	9:k:648:VAL:HG12	2.01	0.41
10:l:28:ILE:H	10:l:28:ILE:HG13	1.55	0.41
12:n:496:ALA:HB3	12:n:498:MET:HE2	2.02	0.41
3:B:168:LEU:HD13	3:B:168:LEU:HA	1.87	0.41
3:B:199:SER:HB2	4:C:118:LYS:HD3	2.03	0.41
4:C:174:LYS:HD3	4:C:177:TYR:CE1	2.56	0.41
5:D:212:THR:OG1	5:D:213:GLU:N	2.54	0.41
6:H:281:ASP:HA	6:H:288:TYR:CE1	2.56	0.41
10:5:236:CYS:SG	10:5:237:GLY:N	2.88	0.41
11:6:156:GLN:O	11:6:159:SER:OG	2.29	0.41
11:6:381:LEU:HD11	11:6:386:VAL:N	2.36	0.41
1:G:712:SER:O	1:G:716:SER:OG	2.38	0.41
1:G:899:VAL:HG13	1:G:911:VAL:HG13	2.03	0.41
3:b:10:THR:OG1	3:b:11:PHE:N	2.52	0.41
3:b:79:LEU:HD12	3:b:79:LEU:HA	1.93	0.41
3:b:191:LYS:HD2	4:c:105:PHE:CE1	2.56	0.41
4:c:133:GLN:O	4:c:137:HIS:ND1	2.53	0.41
6:h:368:ILE:HA	6:h:369:PRO:HD3	1.84	0.41
6:h:374:GLN:HE22	10:l:142:ASN:C	2.29	0.41
6:h:532:ASP:OD2	7:i:780:GLN:NE2	2.54	0.41
7:i:399:PRO:HB3	11:m:629:MET:HE2	2.03	0.41
7:i:618:THR:HA	7:i:621:HIS:CE1	2.56	0.41
7:i:838:ILE:HD13	7:i:838:ILE:HA	1.82	0.41
9:k:406:VAL:HA	9:k:407:PRO:HD3	1.94	0.41
9:k:641:THR:OG1	9:k:642:ARG:N	2.53	0.41
9:k:653:THR:OG1	9:k:654:ILE:N	2.54	0.41
10:l:686:ALA:HA	10:l:689:MET:HE2	2.01	0.41
4:C:105:PHE:CD2	4:C:105:PHE:C	2.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:168:LYS:HE3	4:C:168:LYS:HB2	1.89	0.41
5:D:153:LYS:HB3	5:D:153:LYS:HE2	1.88	0.41
5:D:180:ILE:HA	5:D:183:HIS:HB3	2.03	0.41
5:D:220:ASP:OD1	5:D:221:GLU:N	2.54	0.41
6:H:513:ILE:HD12	6:H:513:ILE:HA	1.91	0.41
6:H:547:ARG:HE	6:H:547:ARG:HB3	1.58	0.41
6:H:566:PRO:HB2	6:H:584:LEU:HB2	2.03	0.41
7:2:201:PRO:HB2	7:2:202:ASN:H	1.76	0.41
7:2:434:TYR:CE2	7:2:436:GLY:CA	3.04	0.41
7:2:607:ASP:OD1	7:2:607:ASP:N	2.38	0.41
7:2:695:LEU:HD12	7:2:695:LEU:HA	1.92	0.41
8:3:48:TYR:O	8:3:52:ASN:ND2	2.53	0.41
8:3:252:ASP:OD1	8:3:252:ASP:N	2.51	0.41
8:3:690:ASP:N	8:3:690:ASP:OD1	2.51	0.41
9:4:406:VAL:HA	9:4:407:PRO:HD3	1.94	0.41
11:6:162:GLU:HB3	11:6:165:ALA:HB3	2.03	0.41
11:6:572:CYS:H	11:6:709:PHE:HE2	1.68	0.41
11:6:738:ARG:HD3	11:6:738:ARG:HA	1.90	0.41
1:F:572:LEU:HD11	1:F:578:ILE:HG13	2.03	0.41
2:a:189:PHE:HB3	2:a:191:VAL:HG13	2.02	0.41
6:h:644:LEU:HD23	6:h:644:LEU:HA	1.89	0.41
7:i:465:ASN:ND2	7:i:468:GLU:O	2.51	0.41
8:j:704:THR:O	8:j:707:ARG:N	2.54	0.41
9:k:415:ILE:HD12	9:k:415:ILE:HA	1.87	0.41
11:m:125:GLN:H	11:m:125:GLN:HG3	1.69	0.41
11:m:126:SER:OG	11:m:131:GLU:OE1	2.25	0.41
11:m:549:LEU:HD13	11:m:552:LEU:HD21	2.02	0.41
6:H:605:PHE:O	6:H:609:PHE:N	2.51	0.41
8:3:220:THR:HA	8:3:322:LEU:HD22	2.02	0.41
8:3:563:GLU:H	8:3:563:GLU:HG3	1.74	0.41
9:4:499:ARG:HH22	9:4:502:THR:HG23	1.84	0.41
10:5:558:ASP:OD1	10:5:558:ASP:N	2.54	0.41
11:6:558:SER:HB3	11:6:565:LEU:HD23	2.03	0.41
12:7:23:ASP:HA	12:7:25:LEU:HD22	2.03	0.41
1:F:610:GLU:OE2	1:F:650:TYR:OH	2.39	0.40
1:G:597:PHE:HB3	1:G:610:GLU:HB3	2.03	0.40
2:a:32:TYR:HA	2:a:93:ARG:HH22	1.86	0.40
2:a:84:ARG:NH2	5:d:217:ASN:OD1	2.53	0.40
3:b:60:LEU:HD13	3:b:60:LEU:HA	1.95	0.40
7:i:475:SER:O	7:i:475:SER:OG	2.38	0.40
8:j:383:LEU:HD12	8:j:383:LEU:HA	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:l:29:LYS:HE2	10:l:29:LYS:HB2	1.95	0.40
10:l:283:THR:OG1	10:l:284:ASN:N	2.54	0.40
11:m:594:ARG:NH1	11:m:633:ASN:OD1	2.49	0.40
11:m:760:THR:O	11:m:760:THR:OG1	2.38	0.40
12:n:17:LEU:O	12:n:21:ILE:HG12	2.21	0.40
12:n:652:MET:HA	12:n:708:VAL:HG21	2.04	0.40
5:D:84:MET:HE3	5:D:84:MET:HB2	1.79	0.40
6:H:81:LEU:HB3	6:H:120:ILE:HG22	2.02	0.40
6:H:161:LYS:HA	6:H:161:LYS:HD3	1.86	0.40
6:H:370:LEU:HD12	6:H:371:SER:CB	2.51	0.40
6:H:532:ASP:OD2	7:2:780:GLN:NE2	2.54	0.40
7:2:618:THR:HA	7:2:621:HIS:CE1	2.56	0.40
8:3:168:PRO:O	8:3:272:ARG:NH2	2.32	0.40
9:4:608:ASP:OD1	9:4:608:ASP:N	2.54	0.40
10:5:399:ILE:HD12	10:5:399:ILE:HA	1.95	0.40
12:7:17:LEU:O	12:7:21:ILE:HG12	2.21	0.40
12:7:24:PHE:O	12:7:63:TYR:OH	2.24	0.40
12:7:654:GLU:HA	12:7:657:ASN:HD21	1.86	0.40
2:a:154:SER:OG	5:d:141:ARG:NE	2.54	0.40
3:b:199:SER:HB2	4:c:118:LYS:HD3	2.03	0.40
4:c:20:PHE:HD1	4:c:20:PHE:HA	1.72	0.40
6:h:566:PRO:HB2	6:h:584:LEU:HB2	2.03	0.40
7:i:542:LEU:HD12	7:i:542:LEU:HA	1.89	0.40
12:n:649:ARG:H	12:n:701:LYS:HZ3	1.70	0.40
2:A:160:ASP:OD1	2:A:160:ASP:N	2.47	0.40
8:3:687:ARG:NH1	8:3:697:ILE:O	2.49	0.40
11:6:803:MET:O	11:6:807:SER:OG	2.32	0.40
12:7:23:ASP:O	12:7:88:TYR:OH	2.25	0.40
1:F:588:VAL:HB	1:F:600:PHE:HB2	2.02	0.40
5:d:77:LEU:HD13	5:d:77:LEU:HA	1.95	0.40
5:d:180:ILE:HA	5:d:183:HIS:HB3	2.03	0.40
5:d:220:ASP:OD1	5:d:221:GLU:N	2.54	0.40
5:d:234:GLY:HA2	5:d:235:PRO:HD3	1.94	0.40
7:i:813:ILE:HD13	7:i:813:ILE:HA	1.91	0.40
10:l:87:ILE:HD13	10:l:87:ILE:HA	1.88	0.40
10:l:179:LEU:HD23	10:l:179:LEU:HA	1.88	0.40
10:l:502:ILE:HD11	10:l:513:LEU:HD11	2.04	0.40
11:m:104:ASP:OD2	11:m:176:ARG:NH1	2.44	0.40
7:2:399:PRO:HB3	11:6:629:MET:HE2	2.03	0.40
8:3:96:ILE:HD11	8:3:153:TRP:HE3	1.85	0.40
8:3:704:THR:O	8:3:707:ARG:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5:533:LEU:HD23	10:5:533:LEU:HA	1.93	0.40
12:7:237:GLN:HB2	12:7:239:ILE:HD11	2.02	0.40
2:a:98:ASP:O	2:a:102:TRP:N	2.53	0.40
4:c:174:LYS:HD3	4:c:177:TYR:CE1	2.56	0.40
5:d:76:LEU:HA	5:d:76:LEU:HD12	1.89	0.40
6:h:73:GLN:HE21	6:h:74:LEU:HD12	1.87	0.40
9:k:467:LYS:HD3	9:k:467:LYS:HA	1.84	0.40
11:m:373:MET:HE3	11:m:373:MET:HB2	1.92	0.40
3:B:115:LEU:HG	3:B:117:TRP:H	1.86	0.40
6:H:15:ILE:HD12	6:H:15:ILE:HA	1.95	0.40
6:H:543:LEU:HD13	6:H:543:LEU:HA	1.93	0.40
7:2:661:LEU:HB3	7:2:665:GLN:HG3	2.03	0.40
8:3:202:TYR:N	8:3:242:THR:O	2.49	0.40
9:4:865:LEU:HD23	9:4:865:LEU:HA	1.91	0.40
12:7:72:ASN:OD1	12:7:72:ASN:N	2.55	0.40
12:7:703:ARG:NH1	12:7:707:MET:SD	2.94	0.40
3:b:115:LEU:HG	3:b:117:TRP:H	1.87	0.40
5:d:178:ASP:O	5:d:182:TYR:N	2.49	0.40
7:i:600:ASP:HB3	7:i:601:LYS:HD2	2.03	0.40
7:i:839:LYS:HA	7:i:839:LYS:HD2	1.91	0.40
2:A:151:LEU:HD13	2:A:151:LEU:HA	1.96	0.40
6:H:155:GLN:HE22	6:H:158:ALA:HB3	1.86	0.40
7:2:211:LEU:HD11	7:2:274:VAL:HG11	2.02	0.40
7:2:411:LEU:HA	7:2:411:LEU:HD23	1.80	0.40
7:2:680:LEU:HD13	7:2:680:LEU:HA	1.97	0.40
8:3:544:ASP:OD1	8:3:544:ASP:N	2.54	0.40
10:5:404:MET:HE2	10:5:404:MET:HB3	1.92	0.40
11:6:702:THR:OG1	11:6:703:ALA:N	2.54	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	E	419/927 (45%)	407 (97%)	11 (3%)	1 (0%)	43	78
1	F	428/927 (46%)	415 (97%)	12 (3%)	1 (0%)	43	78
1	G	417/927 (45%)	407 (98%)	9 (2%)	1 (0%)	43	78
2	A	41/208 (20%)	34 (83%)	6 (15%)	1 (2%)	4	26
2	a	206/208 (99%)	180 (87%)	25 (12%)	1 (0%)	24	63
3	b	177/213 (83%)	150 (85%)	27 (15%)	0	100	100
4	C	56/194 (29%)	51 (91%)	5 (9%)	0	100	100
4	c	151/194 (78%)	139 (92%)	12 (8%)	0	100	100
5	D	213/294 (72%)	189 (89%)	24 (11%)	0	100	100
5	d	226/294 (77%)	202 (89%)	24 (11%)	0	100	100
6	H	517/650 (80%)	454 (88%)	60 (12%)	3 (1%)	21	59
6	h	543/650 (84%)	476 (88%)	64 (12%)	3 (1%)	21	59
7	2	630/868 (73%)	537 (85%)	93 (15%)	0	100	100
7	i	630/868 (73%)	537 (85%)	93 (15%)	0	100	100
8	3	584/971 (60%)	506 (87%)	77 (13%)	1 (0%)	43	78
8	j	584/971 (60%)	506 (87%)	76 (13%)	2 (0%)	36	72
9	4	668/933 (72%)	579 (87%)	89 (13%)	0	100	100
9	k	668/933 (72%)	578 (86%)	90 (14%)	0	100	100
10	5	583/775 (75%)	493 (85%)	89 (15%)	1 (0%)	43	78
10	l	583/775 (75%)	493 (85%)	89 (15%)	1 (0%)	43	78
11	6	606/1017 (60%)	506 (84%)	99 (16%)	1 (0%)	43	78
11	m	606/1017 (60%)	506 (84%)	99 (16%)	1 (0%)	43	78
12	7	653/845 (77%)	556 (85%)	97 (15%)	0	100	100
12	n	653/845 (77%)	554 (85%)	99 (15%)	0	100	100
All	All	10842/16504 (66%)	9455 (87%)	1369 (13%)	18 (0%)	44	78

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	h	334	LEU
6	H	334	LEU
1	G	767	PRO
6	h	332	SER
10	l	147	PRO
11	m	305	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	H	332	SER
10	5	147	PRO
11	6	305	TYR
1	E	767	PRO
2	a	30	PRO
2	A	30	PRO
8	j	311	SER
8	j	669	PRO
8	3	669	PRO
1	F	767	PRO
6	h	146	GLY
6	H	146	GLY

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
13	ATP	5	801	-	32,33,33	1.26	5 (15%)	48,52,52	1.91	12 (25%)
13	ATP	j	1001	-	32,33,33	1.33	5 (15%)	48,52,52	1.78	11 (22%)
13	ATP	i	901	-	32,33,33	1.30	6 (18%)	48,52,52	1.77	10 (20%)
13	ATP	1	801	-	32,33,33	1.25	5 (15%)	48,52,52	1.93	12 (25%)
13	ATP	3	1001	-	32,33,33	1.32	5 (15%)	48,52,52	1.78	11 (22%)
13	ATP	2	901	-	32,33,33	1.29	6 (18%)	48,52,52	1.77	10 (20%)

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
13	ATP	5	801	-	-	4/22/38/38	0/3/3/3
13	ATP	j	1001	-	-	5/22/38/38	0/3/3/3
13	ATP	i	901	-	-	6/22/38/38	0/3/3/3
13	ATP	1	801	-	-	4/22/38/38	0/3/3/3
13	ATP	3	1001	-	-	4/22/38/38	0/3/3/3
13	ATP	2	901	-	-	6/22/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	i	901	ATP	C5-C4	4.26	1.46	1.39
13	2	901	ATP	C5-C4	4.18	1.46	1.39
13	j	1001	ATP	C5-C4	4.18	1.46	1.39
13	3	1001	ATP	C5-C4	4.09	1.46	1.39
13	1	801	ATP	C5-C4	4.02	1.46	1.39
13	5	801	ATP	C5-C4	4.01	1.46	1.39
13	j	1001	ATP	C4-N9	-2.63	1.32	1.37
13	3	1001	ATP	C4-N9	-2.62	1.32	1.37
13	2	901	ATP	C5-N7	-2.58	1.34	1.39
13	j	1001	ATP	C5-N7	-2.56	1.34	1.39
13	i	901	ATP	C5-N7	-2.55	1.34	1.39
13	3	1001	ATP	C5-N7	-2.54	1.34	1.39
13	1	801	ATP	C5-C6	2.54	1.48	1.41
13	5	801	ATP	C5-C6	2.54	1.48	1.41
13	1	801	ATP	C5-N7	-2.49	1.34	1.39
13	5	801	ATP	C5-N7	-2.47	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	i	901	ATP	C4-N9	-2.41	1.32	1.37
13	2	901	ATP	C5-C6	2.41	1.47	1.41
13	2	901	ATP	C4-N9	-2.40	1.32	1.37
13	j	1001	ATP	C5-C6	2.40	1.47	1.41
13	3	1001	ATP	C5-C6	2.39	1.47	1.41
13	i	901	ATP	C5-C6	2.35	1.47	1.41
13	5	801	ATP	C8-N7	2.22	1.36	1.31
13	1	801	ATP	C4-N9	-2.15	1.33	1.37
13	1	801	ATP	C8-N7	2.14	1.35	1.31
13	5	801	ATP	C4-N9	-2.08	1.33	1.37
13	2	901	ATP	C8-N7	2.07	1.35	1.31
13	3	1001	ATP	C8-N7	2.06	1.35	1.31
13	i	901	ATP	C8-N7	2.05	1.35	1.31
13	j	1001	ATP	C8-N7	2.05	1.35	1.31
13	2	901	ATP	C8-N9	-2.04	1.34	1.37
13	i	901	ATP	C8-N9	-2.04	1.34	1.37

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	801	ATP	C5-C4-N3	-5.78	118.76	126.72
13	5	801	ATP	C5-C4-N3	-5.75	118.80	126.72
13	i	901	ATP	C5-C4-N3	-5.53	119.10	126.72
13	2	901	ATP	C5-C4-N3	-5.53	119.10	126.72
13	3	1001	ATP	C5-C4-N3	-5.30	119.42	126.72
13	j	1001	ATP	C5-C4-N3	-5.27	119.46	126.72
13	1	801	ATP	N3-C4-N9	4.51	134.83	127.17
13	i	901	ATP	N3-C4-N9	4.49	134.81	127.17
13	3	1001	ATP	N3-C4-N9	4.49	134.81	127.17
13	5	801	ATP	N3-C4-N9	4.48	134.79	127.17
13	2	901	ATP	N3-C4-N9	4.48	134.79	127.17
13	j	1001	ATP	N3-C4-N9	4.48	134.78	127.17
13	1	801	ATP	C2-N3-C4	3.92	121.41	111.83
13	5	801	ATP	C2-N3-C4	3.92	121.40	111.83
13	5	801	ATP	N3-C2-N1	-3.76	122.89	128.58
13	1	801	ATP	C4-C5-N7	-3.76	106.28	110.58
13	1	801	ATP	N3-C2-N1	-3.74	122.92	128.58
13	5	801	ATP	C4-C5-N7	-3.70	106.35	110.58
13	i	901	ATP	C4-C5-N7	-3.55	106.52	110.58
13	3	1001	ATP	C4-N9-C8	3.52	109.43	105.74
13	3	1001	ATP	C2-N3-C4	3.51	120.41	111.83
13	2	901	ATP	C4-C5-N7	-3.50	106.58	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	j	1001	ATP	C4-N9-C8	3.50	109.41	105.74
13	j	1001	ATP	C2-N3-C4	3.49	120.36	111.83
13	2	901	ATP	C2-N3-C4	3.40	120.15	111.83
13	i	901	ATP	C2-N3-C4	3.38	120.08	111.83
13	i	901	ATP	C4-N9-C8	3.30	109.20	105.74
13	2	901	ATP	C4-N9-C8	3.26	109.16	105.74
13	3	1001	ATP	N3-C2-N1	-3.16	123.80	128.58
13	j	1001	ATP	N3-C2-N1	-3.13	123.84	128.58
13	l	801	ATP	C4-N9-C8	3.13	109.03	105.74
13	5	801	ATP	C4-N9-C8	3.08	108.97	105.74
13	l	801	ATP	O4'-C1'-N9	3.04	113.93	108.09
13	3	1001	ATP	C4-C5-N7	-3.03	107.12	110.58
13	5	801	ATP	O4'-C1'-N9	3.02	113.90	108.09
13	j	1001	ATP	C4-C5-N7	-3.01	107.14	110.58
13	2	901	ATP	N3-C2-N1	-2.96	124.10	128.58
13	l	801	ATP	C5-N7-C8	2.91	108.03	103.45
13	i	901	ATP	N3-C2-N1	-2.89	124.20	128.58
13	5	801	ATP	C5-N7-C8	2.83	107.90	103.45
13	i	901	ATP	C5-N7-C8	2.63	107.59	103.45
13	l	801	ATP	C6-C5-N7	2.61	137.12	132.09
13	2	901	ATP	C5-N7-C8	2.60	107.54	103.45
13	l	801	ATP	N9-C8-N7	-2.60	110.25	113.94
13	5	801	ATP	C6-C5-N7	2.59	137.08	132.09
13	5	801	ATP	N9-C8-N7	-2.52	110.36	113.94
13	3	1001	ATP	N9-C8-N7	-2.36	110.58	113.94
13	i	901	ATP	N9-C8-N7	-2.35	110.60	113.94
13	2	901	ATP	N9-C8-N7	-2.35	110.60	113.94
13	j	1001	ATP	N9-C8-N7	-2.35	110.61	113.94
13	i	901	ATP	C3'-C2'-C1'	2.33	105.86	101.46
13	5	801	ATP	C2-N1-C6	2.32	122.54	118.73
13	j	1001	ATP	C5-N7-C8	2.31	107.09	103.45
13	2	901	ATP	C3'-C2'-C1'	2.31	105.83	101.46
13	3	1001	ATP	C5-N7-C8	2.31	107.08	103.45
13	l	801	ATP	C2-N1-C6	2.30	122.51	118.73
13	l	801	ATP	O3G-PG-O2G	2.26	116.29	107.80
13	5	801	ATP	O3G-PG-O2G	2.26	116.26	107.80
13	j	1001	ATP	C2'-C1'-N9	-2.21	107.80	113.30
13	3	1001	ATP	C2'-C1'-N9	-2.19	107.87	113.30
13	j	1001	ATP	C2'-C3'-C4'	2.16	106.79	102.61
13	3	1001	ATP	C2'-C3'-C4'	2.12	106.70	102.61
13	3	1001	ATP	C3'-C2'-C1'	2.10	105.43	101.46
13	j	1001	ATP	C3'-C2'-C1'	2.09	105.42	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	i	901	ATP	O2A-PA-O1A	2.04	121.95	112.44
13	2	901	ATP	O2A-PA-O1A	2.02	121.86	112.44

There are no chirality outliers.

All (29) torsion outliers are listed below:

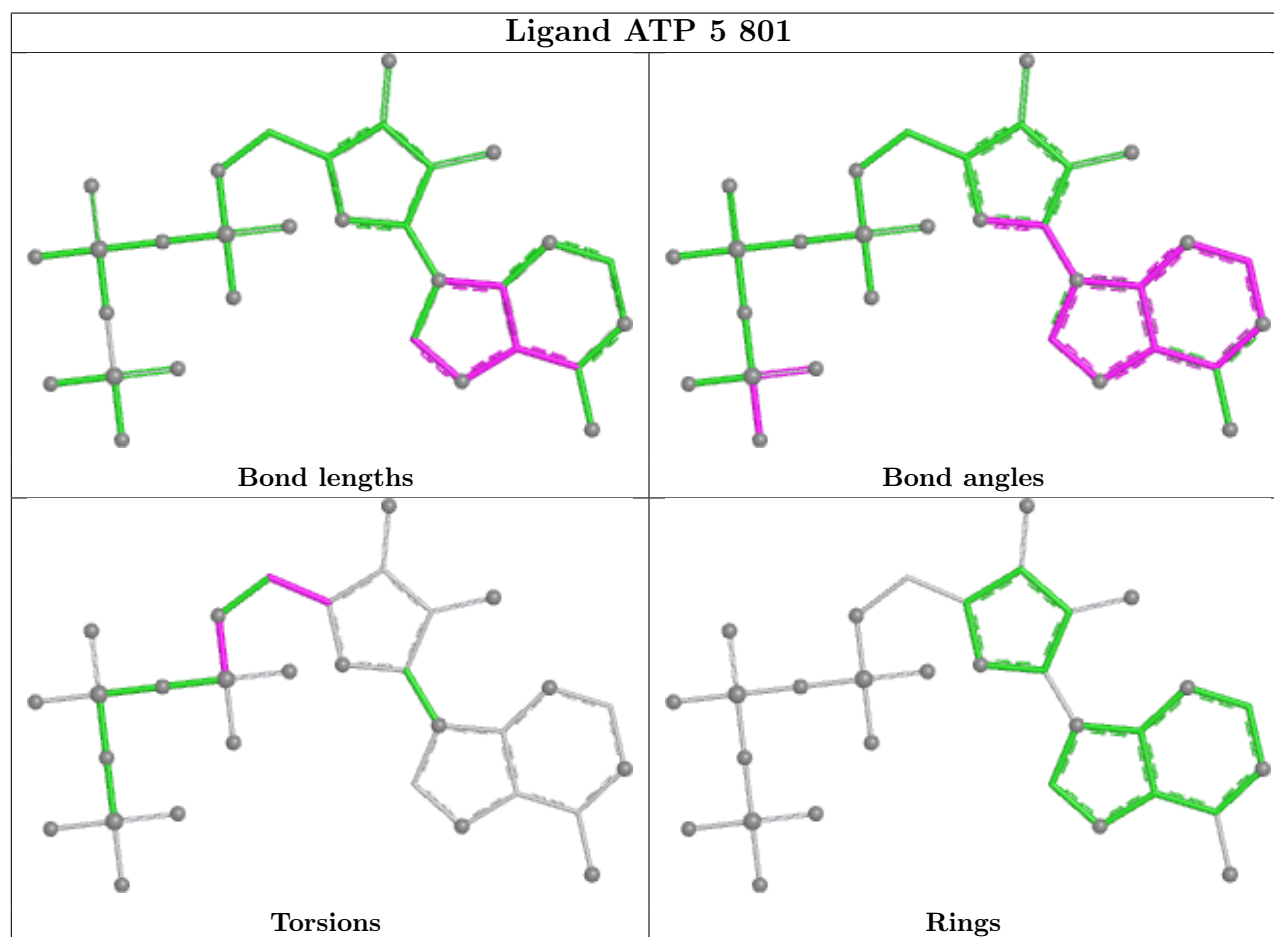
Mol	Chain	Res	Type	Atoms
13	i	901	ATP	C5'-O5'-PA-O1A
13	i	901	ATP	C5'-O5'-PA-O2A
13	i	901	ATP	C5'-O5'-PA-O3A
13	j	1001	ATP	C5'-O5'-PA-O2A
13	j	1001	ATP	C5'-O5'-PA-O3A
13	1	801	ATP	C5'-O5'-PA-O2A
13	2	901	ATP	C5'-O5'-PA-O1A
13	2	901	ATP	C5'-O5'-PA-O2A
13	2	901	ATP	C5'-O5'-PA-O3A
13	3	1001	ATP	C5'-O5'-PA-O2A
13	3	1001	ATP	C5'-O5'-PA-O3A
13	5	801	ATP	C5'-O5'-PA-O2A
13	i	901	ATP	C3'-C4'-C5'-O5'
13	2	901	ATP	C3'-C4'-C5'-O5'
13	i	901	ATP	O4'-C4'-C5'-O5'
13	2	901	ATP	O4'-C4'-C5'-O5'
13	j	1001	ATP	O4'-C4'-C5'-O5'
13	3	1001	ATP	O4'-C4'-C5'-O5'
13	1	801	ATP	O4'-C4'-C5'-O5'
13	5	801	ATP	O4'-C4'-C5'-O5'
13	j	1001	ATP	C3'-C4'-C5'-O5'
13	3	1001	ATP	C3'-C4'-C5'-O5'
13	1	801	ATP	C5'-O5'-PA-O3A
13	5	801	ATP	C5'-O5'-PA-O3A
13	i	901	ATP	C4'-C5'-O5'-PA
13	2	901	ATP	C4'-C5'-O5'-PA
13	1	801	ATP	C3'-C4'-C5'-O5'
13	5	801	ATP	C3'-C4'-C5'-O5'
13	j	1001	ATP	PG-O3B-PB-O2B

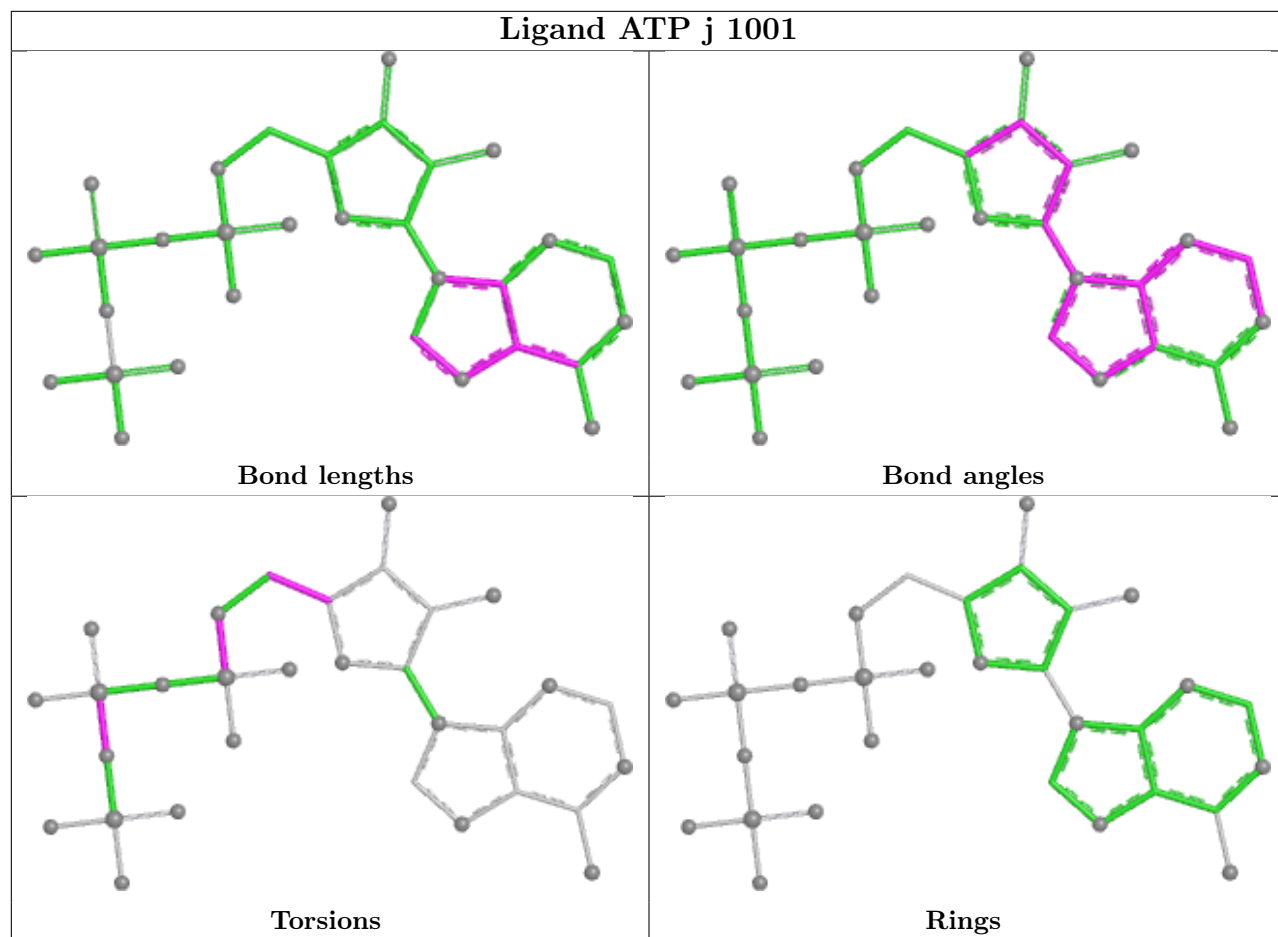
There are no ring outliers.

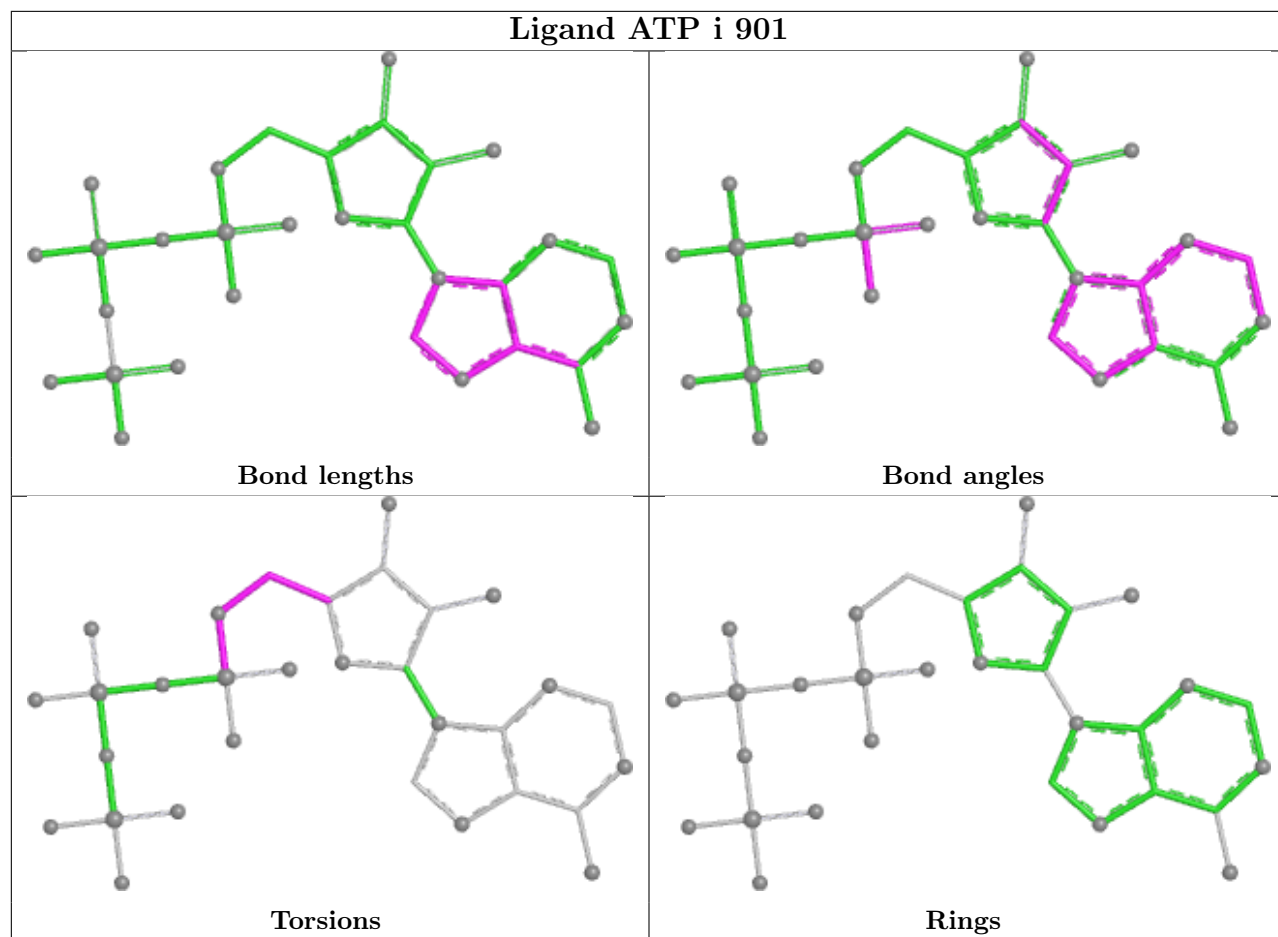
6 monomers are involved in 22 short contacts:

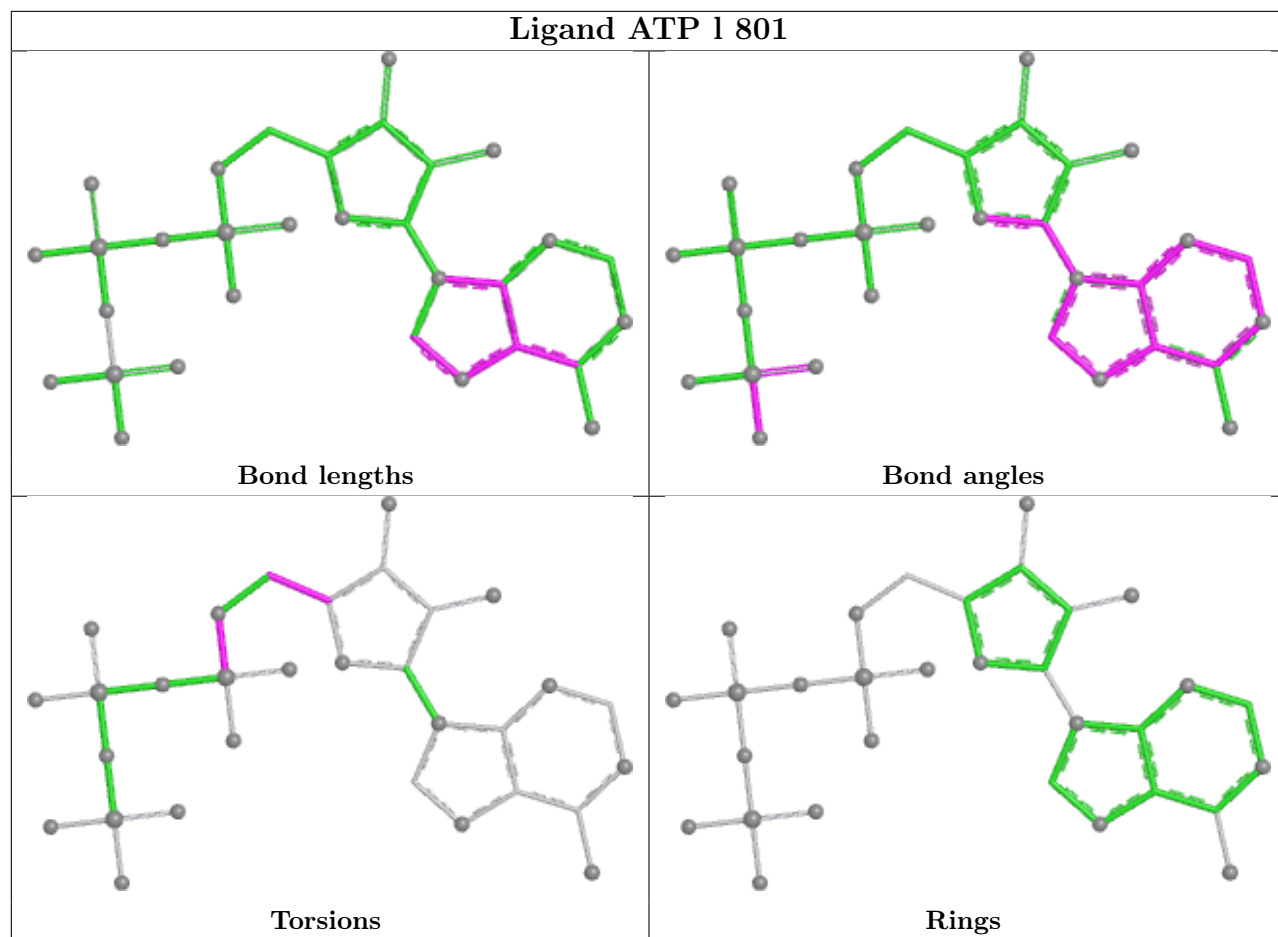
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	5	801	ATP	5	0
13	j	1001	ATP	5	0
13	i	901	ATP	1	0
13	l	801	ATP	5	0
13	3	1001	ATP	5	0
13	2	901	ATP	1	0

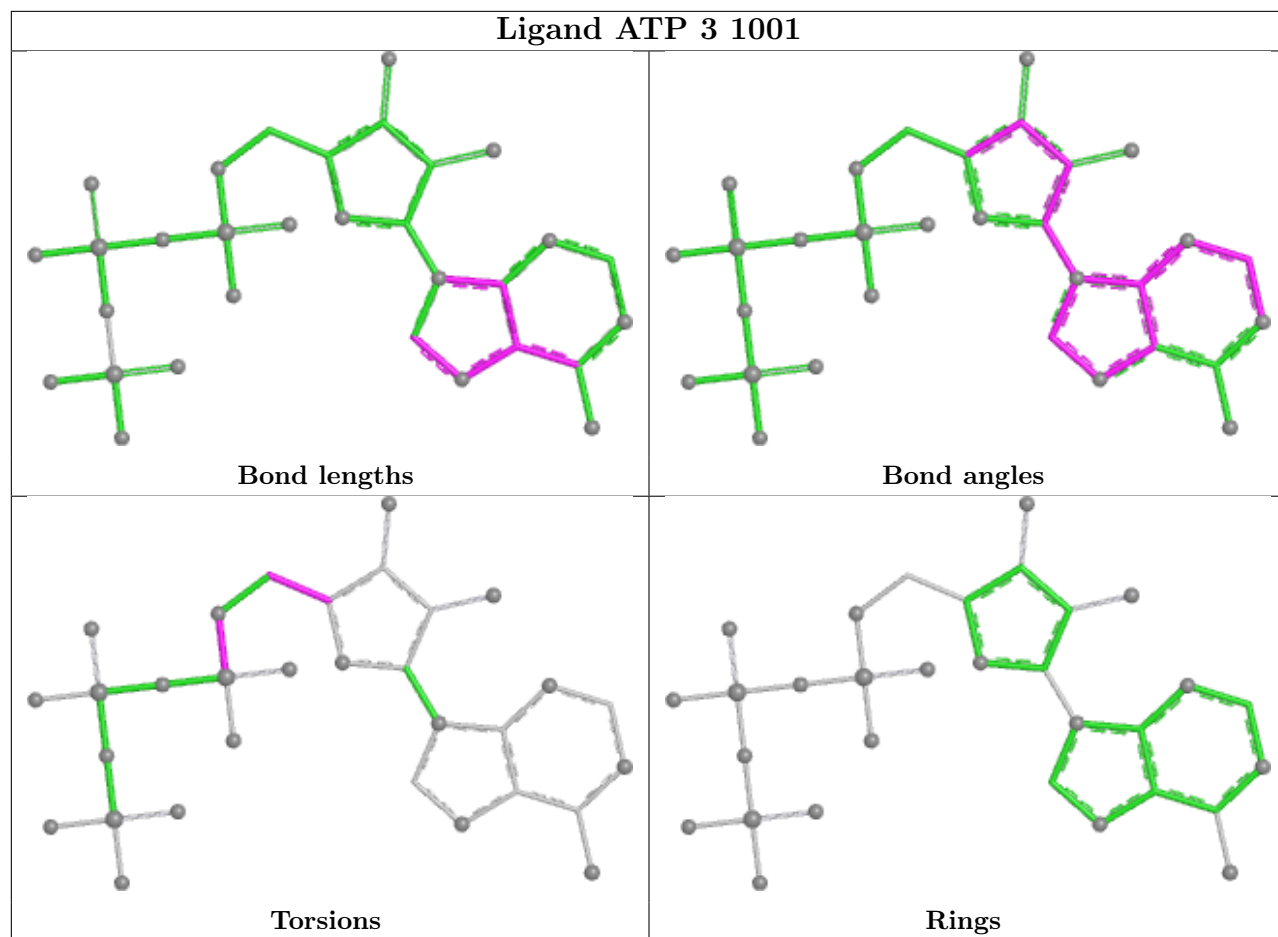
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

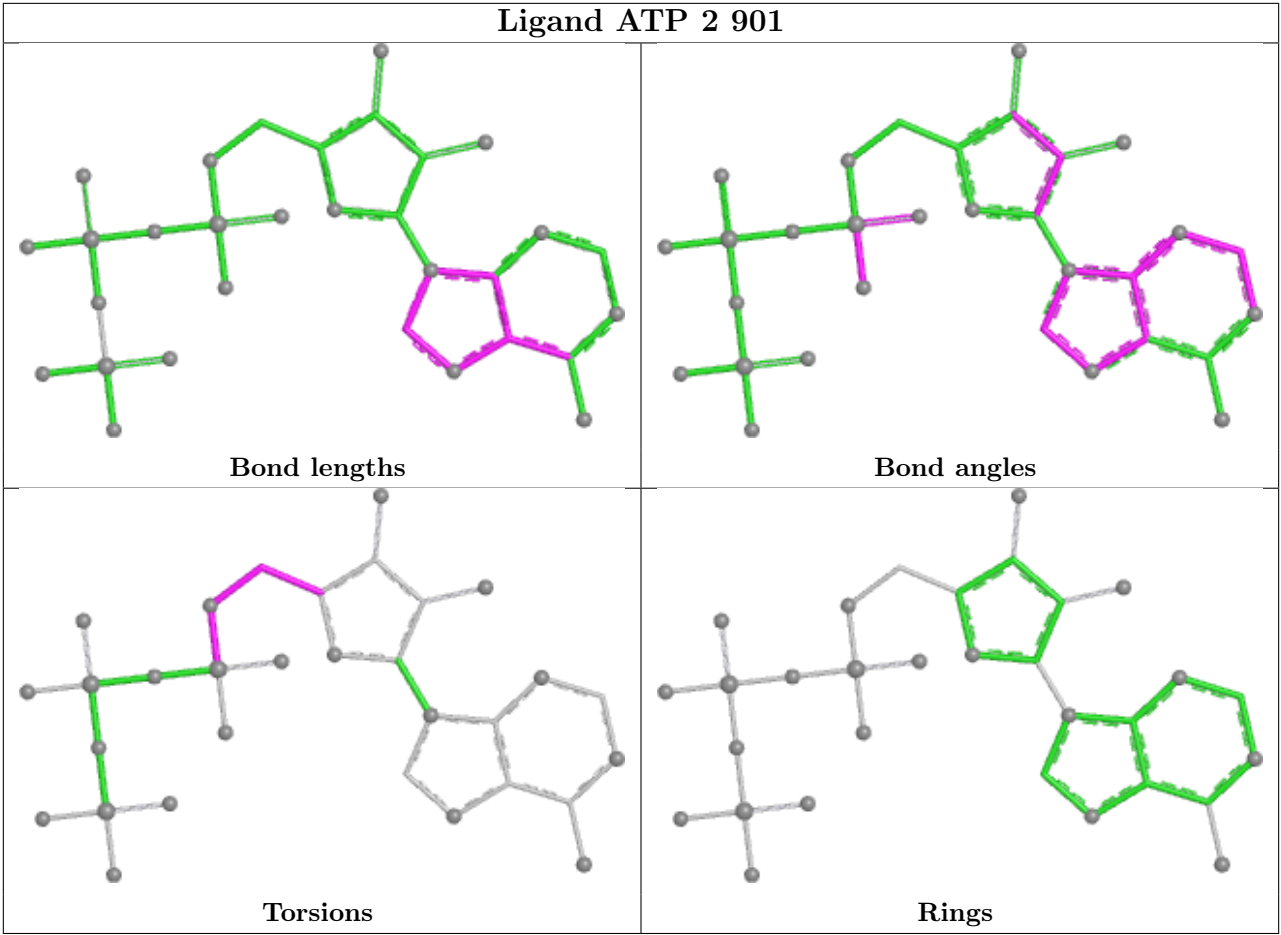












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	776:ILE	C	777:ARG	N	2.04

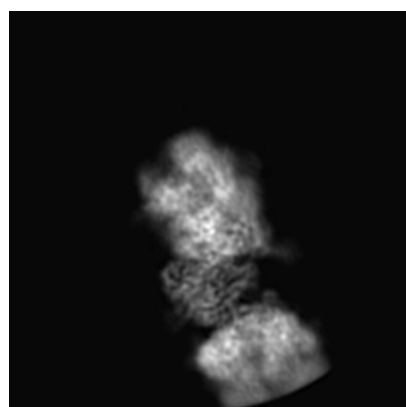
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20472. These allow visual inspection of the internal detail of the map and identification of artifacts.

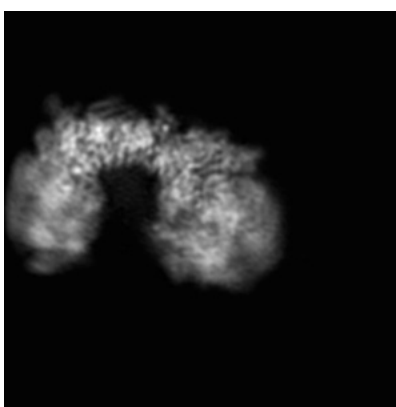
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

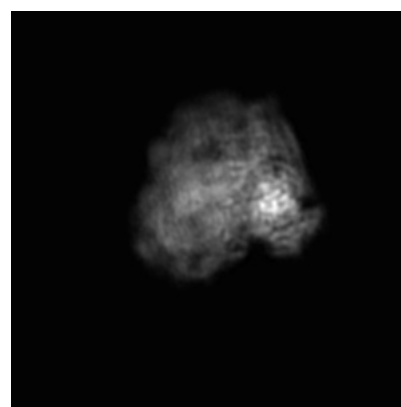
6.1.1 Primary map



X



Y

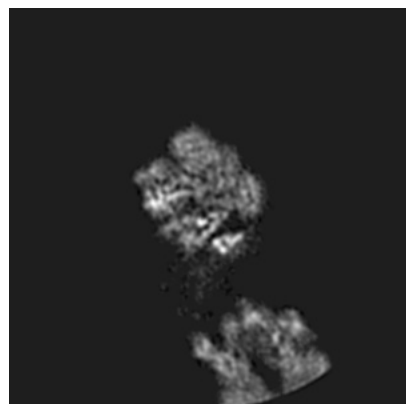


Z

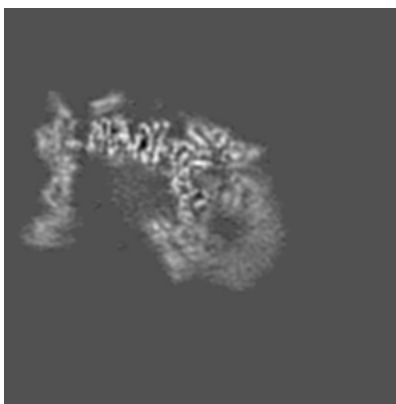
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

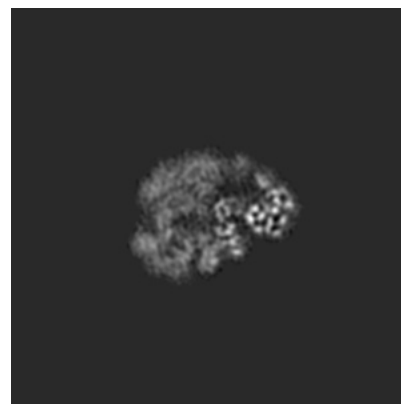
6.2.1 Primary map



X Index: 200



Y Index: 200

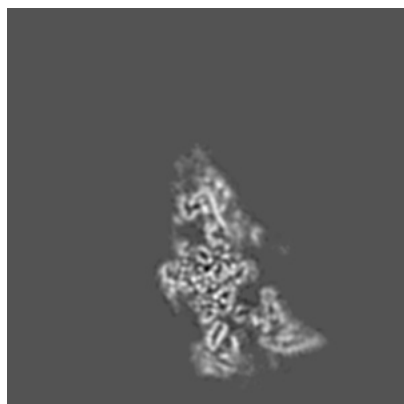


Z Index: 200

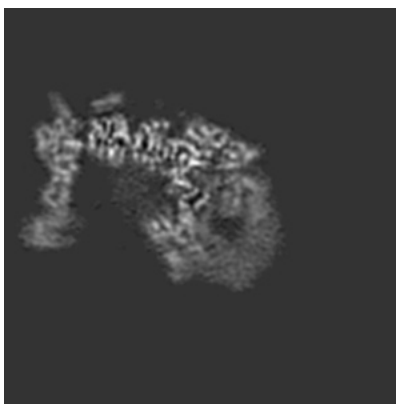
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

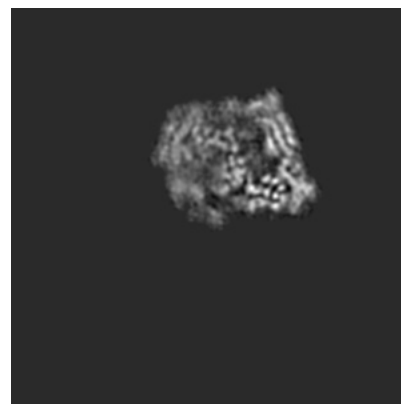
6.3.1 Primary map



X Index: 264



Y Index: 202



Z Index: 68

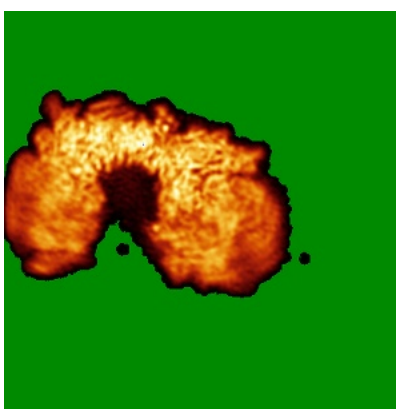
The images above show the largest variance slices of the map in three orthogonal directions.

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

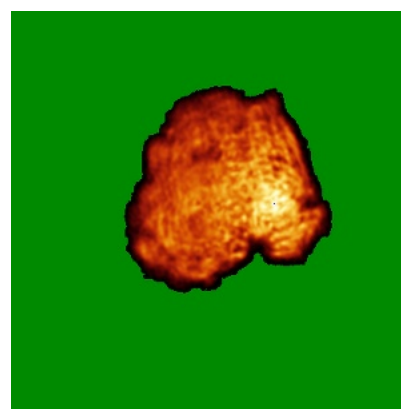
6.4.1 Primary map



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

This section was not generated.

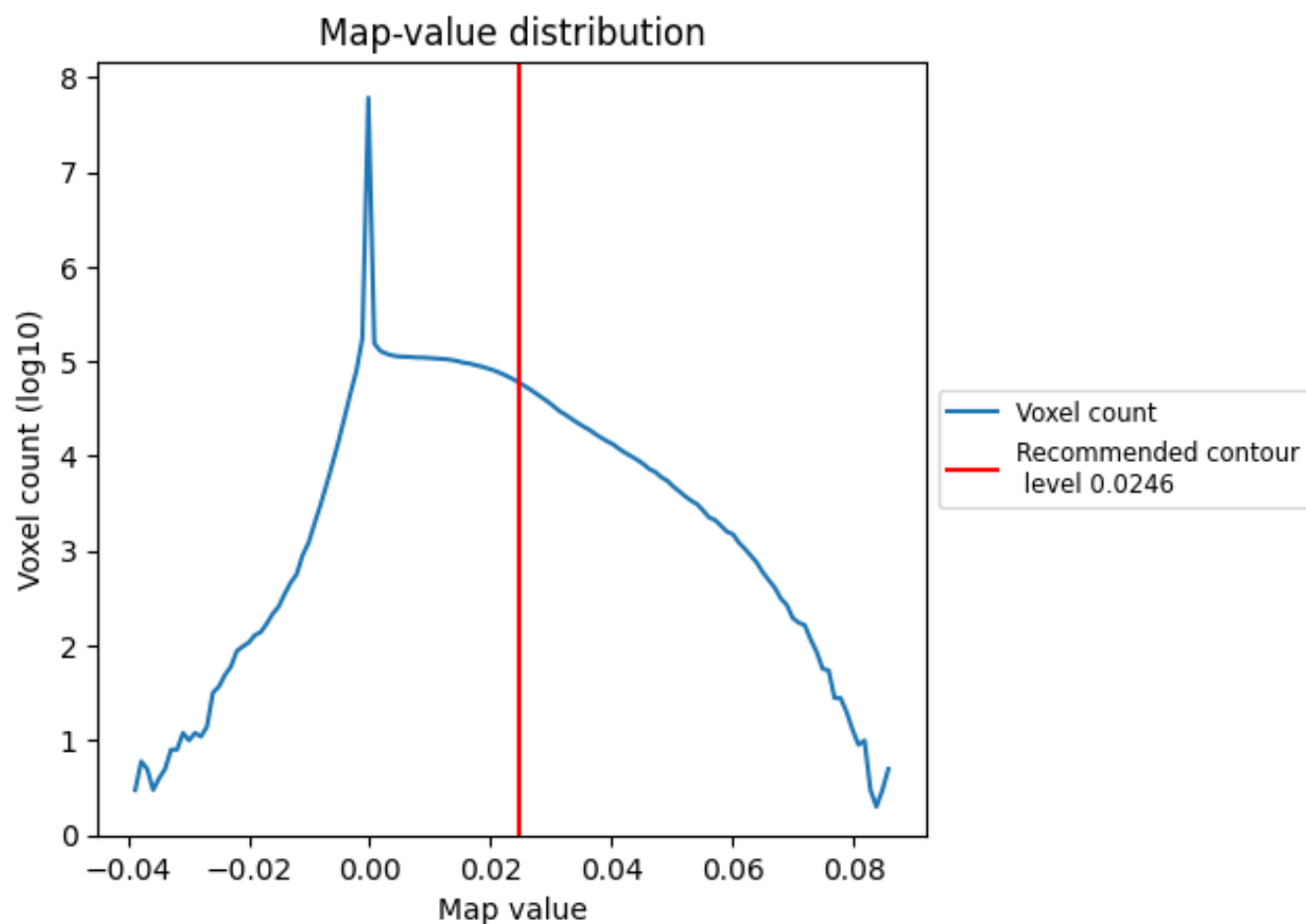
6.6 Mask visualisation

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

7 Map analysis [i](#)

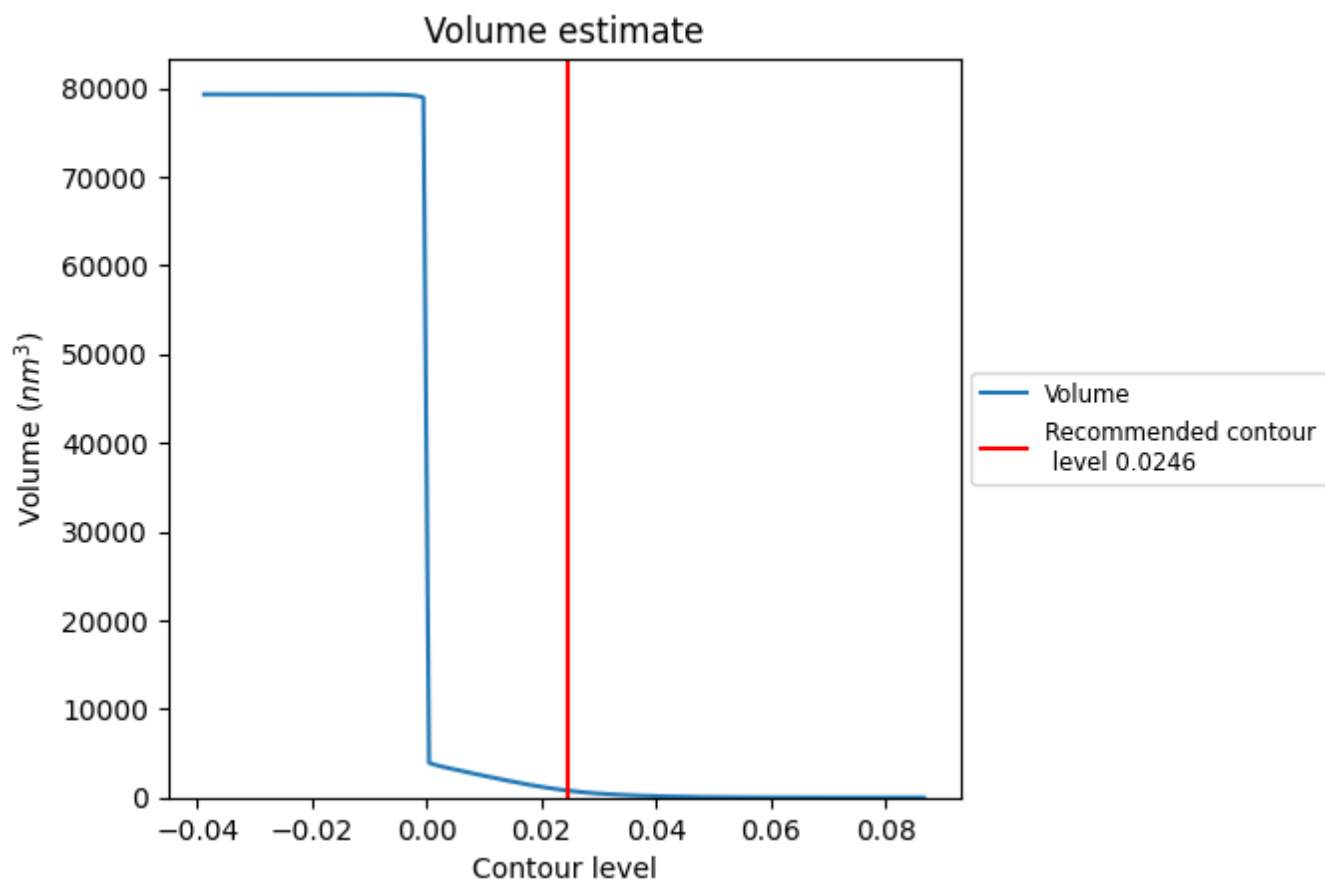
This section contains the results of statistical analysis of the map.

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.

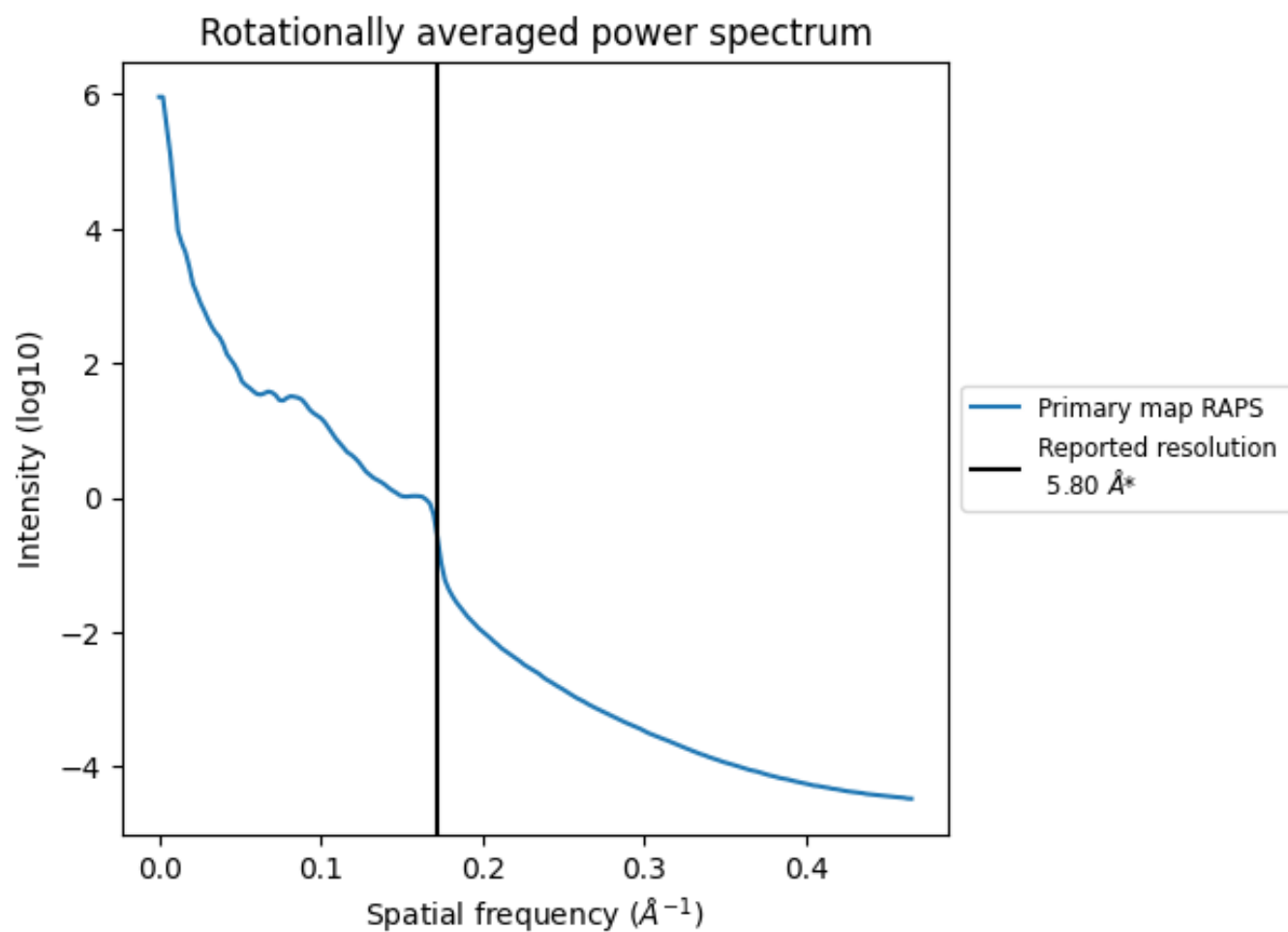
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 790 nm^3 ; this corresponds to an approximate mass of 713 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 0.172 Å⁻¹

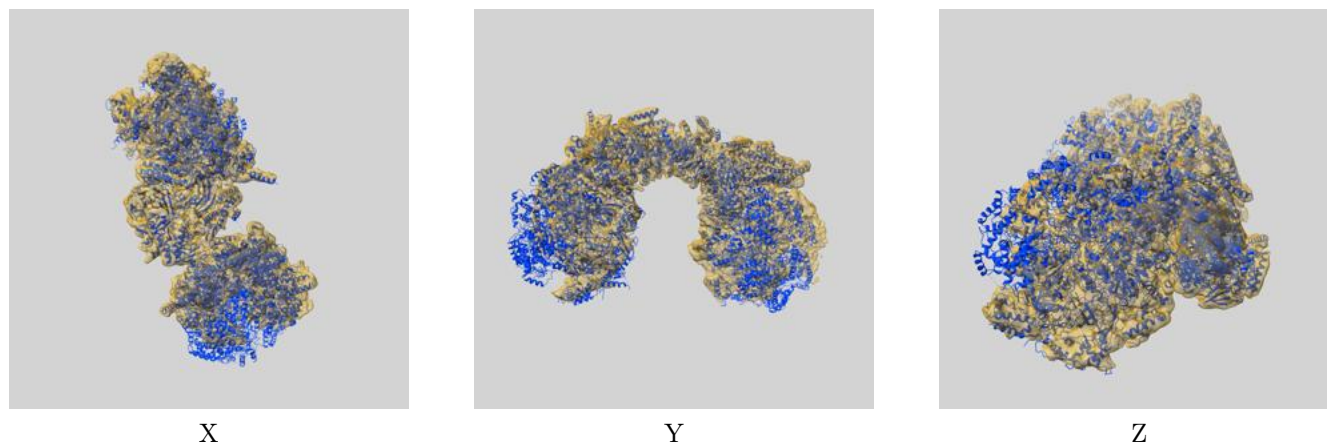
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

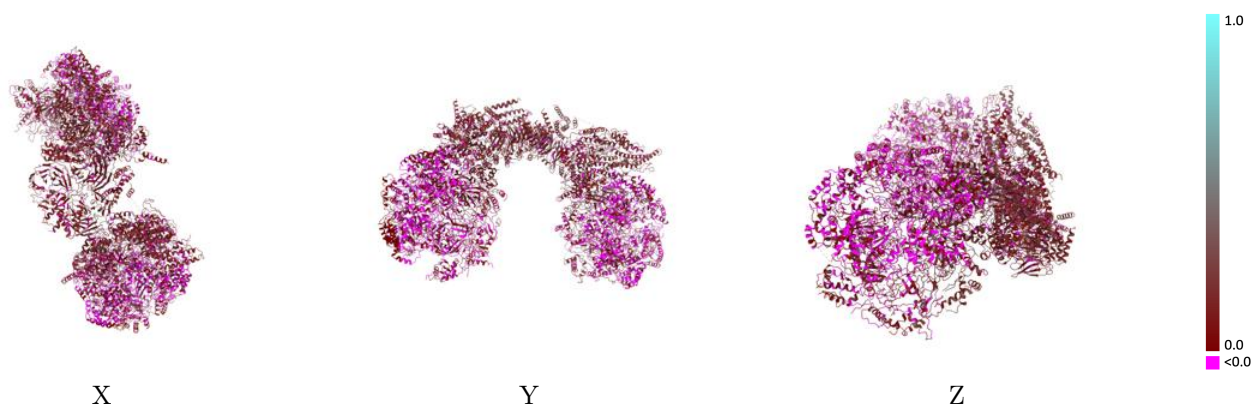
This section contains information regarding the fit between EMDB map EMD-20472 and PDB model 6PTN. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



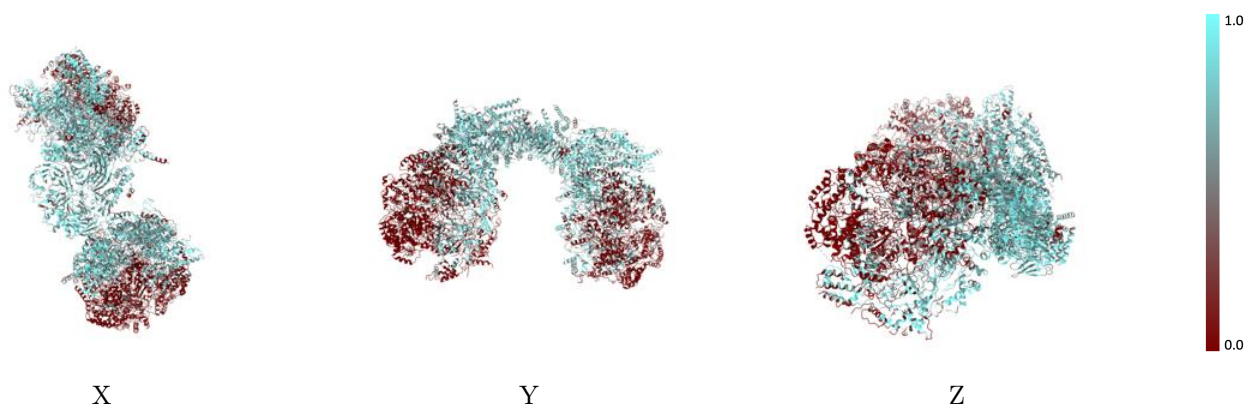
The images above show the 3D surface view of the map at the recommended contour level 0.0246 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



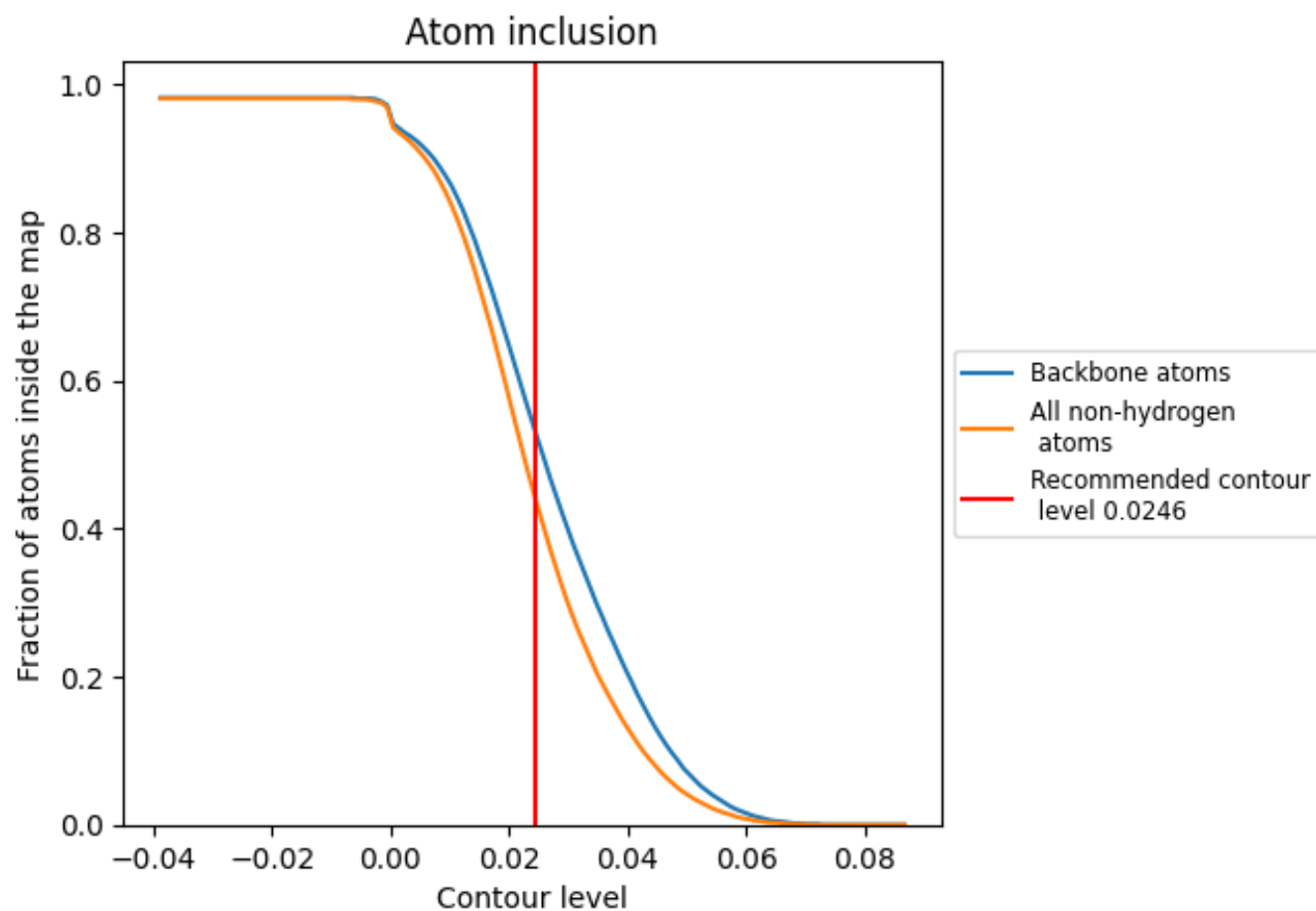
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0246).

9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 44% 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 (0.0246) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4360	 0.0870
2	 0.2410	 0.0390
3	 0.3320	 0.0510
4	 0.1460	 0.0300
5	 0.3520	 0.0660
6	 0.1940	 0.0320
7	 0.1580	 0.0300
A	 0.6820	 0.1640
B	 0.6730	 0.1620
C	 0.6840	 0.1410
D	 0.7090	 0.1630
E	 0.7120	 0.1720
F	 0.7070	 0.1510
G	 0.7170	 0.1680
H	 0.6800	 0.1390
a	 0.7450	 0.1660
b	 0.7480	 0.1750
c	 0.7360	 0.1620
d	 0.7480	 0.1740
h	 0.6770	 0.1390
i	 0.3080	 0.0380
j	 0.4640	 0.0880
k	 0.2590	 0.0460
l	 0.4060	 0.0750
m	 0.3480	 0.0570
n	 0.3290	 0.0540

