



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 10:21 AM UTC

PDB ID : 6V6S / pdb_00006v6s
EMDB ID : EMD-21073
Title : Structure of the native human gamma-tubulin ring complex
Authors : Wieczorek, M.; Urnavicius, L.; Ti, S.; Molloy, K.R.; Chait, B.T.; Kapoor, T.M.
Deposited on : 2019-12-05
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

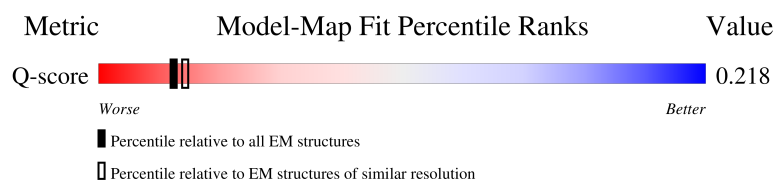
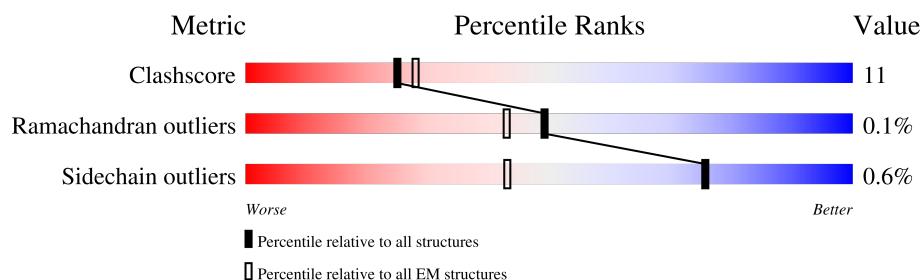
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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

Mol	Chain	Length	Quality of chain
1	A	930	5% 46% 11% 42%
1	C	930	45% 13% 42%
1	E	930	44% 14% 42%
1	G	930	5% 44% 14% 42%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	930	
2	B	907	
2	D	907	
2	F	907	
2	H	907	
2	T	907	
3	I	667	
3	K	667	
4	J	1024	
5	L	1819	
6	N	50	
6	O	50	
6	Q	50	
6	R	50	
6	S	50	
7	U	374	
8	V	66	
8	Y	66	
9	W	165	
10	X	263	
11	a	451	
11	b	451	
11	c	451	
11	d	451	
11	e	451	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
11	f	451	68%14%18%
11	g	451	63%19%18%
11	h	451	66%16%18%
11	i	451	62%20%18%
11	j	451	27%62%20%18%
11	k	451	23%62%20%18%
11	l	451	40%61%21%18%
11	m	451	78%66%16%18%
11	t	451	82%81%18%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 106422 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 Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	539	Total	C	N	O	S	0	0
			4371	2825	721	795	30		
1	C	539	Total	C	N	O	S	0	0
			4371	2825	721	795	30		
1	E	539	Total	C	N	O	S	0	0
			4371	2825	721	795	30		
1	G	539	Total	C	N	O	S	0	0
			4371	2825	721	795	30		
1	M	539	Total	C	N	O	S	0	0
			4371	2825	721	795	30		

- Molecule 2 is a protein called Gamma-tubulin complex component 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	572	Total	C	N	O	S	0	0
			4744	3034	832	853	25		
2	D	572	Total	C	N	O	S	0	0
			4744	3034	832	853	25		
2	F	572	Total	C	N	O	S	0	0
			4744	3034	832	853	25		
2	H	572	Total	C	N	O	S	0	0
			4744	3034	832	853	25		
2	T	572	Total	C	N	O		0	0
			2840	1696	572	572			

- Molecule 3 is a protein called Gamma-tubulin complex component 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	543	Total	C	N	O	S	2	0
			4376	2844	734	780	18		
3	K	543	Total	C	N	O	S	2	0
			4376	2844	734	780	18		

- Molecule 4 is a protein called Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	484	Total	C	N	O	S	0	0
			3977	2603	656	695	23		

- Molecule 5 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	497	Total	C	N	O	S	0	0
			4007	2630	667	690	20		

- Molecule 6 is a protein called Unassigned poly-alanine chain ("staple").

Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	35	Total	C	N	O	0	0
			175	105	35	35		
6	O	40	Total	C	N	O	0	0
			200	120	40	40		
6	Q	38	Total	C	N	O	0	0
			190	114	38	38		
6	R	39	Total	C	N	O	0	0
			195	117	39	39		
6	S	40	Total	C	N	O	0	0
			200	120	40	40		

- Molecule 7 is a protein called beta actin.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	U	364	Total	C	N	O	0	0
			1795	1067	364	364		

- Molecule 8 is a protein called Unassigned poly-alanine model ("CC").

Mol	Chain	Residues	Atoms				AltConf	Trace
8	V	62	Total	C	N	O	0	0
			310	186	62	62		
8	Y	57	Total	C	N	O	0	0
			285	171	57	57		

- Molecule 9 is a protein called Unassigned poly-alanine model ("HB").

Mol	Chain	Residues	Atoms				AltConf	Trace
9	W	155	Total	C	N	O	0	0
			775	465	155	155		

- Molecule 10 is a protein called Unassigned poly-alanine model ("Lumenal bridge helical bundles").

Mol	Chain	Residues	Atoms				AltConf	Trace
10	X	254	Total	C	N	O	0	0
			1270	762	254	254		

- Molecule 11 is a protein called Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	b	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	c	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	d	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	e	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	f	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	g	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	h	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	i	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	j	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	k	370	Total	C	N	O	S	0	0
			2955	1875	518	548	14		
11	l	370	Total	C	N	O	S	0	0
			2955	1875	518	548	14		
11	m	369	Total	C	N	O	S	0	0
			2951	1873	517	547	14		
11	t	370	Total	C	N	O		0	0
			1830	1090	370	370			

There are 28 discrepancies between the modelled and reference sequences:

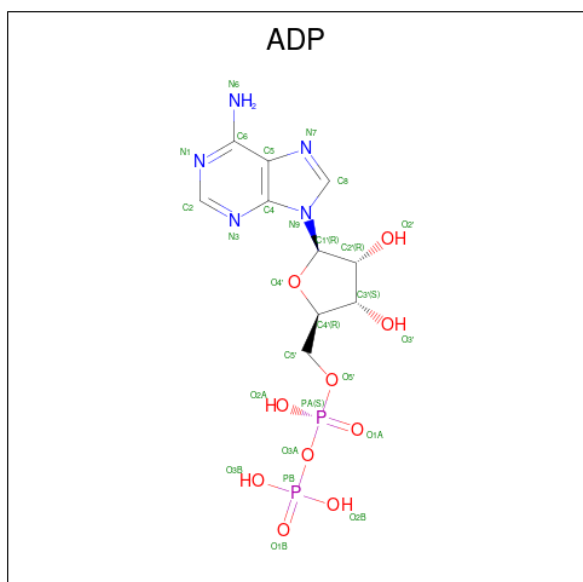
Chain	Residue	Modelled	Actual	Comment	Reference
a	35	ALA	GLY	conflict	UNP P23258
a	202	LEU	VAL	conflict	UNP P23258
b	35	ALA	GLY	conflict	UNP P23258

Continued on next page...

Continued from previous page...

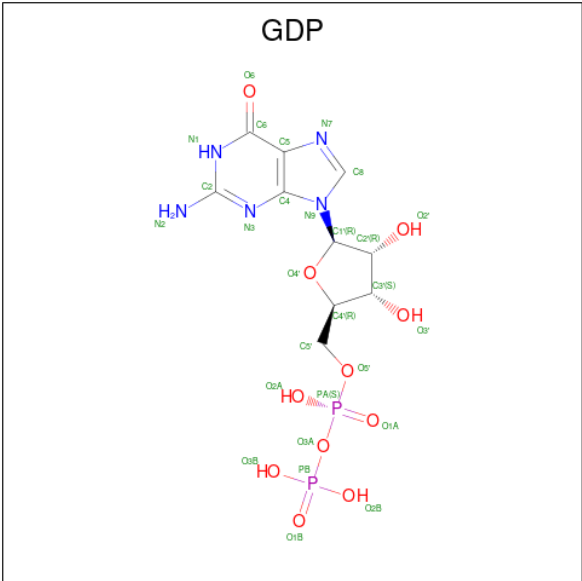
Chain	Residue	Modelled	Actual	Comment	Reference
b	202	LEU	VAL	conflict	UNP P23258
c	35	ALA	GLY	conflict	UNP P23258
c	202	LEU	VAL	conflict	UNP P23258
d	35	ALA	GLY	conflict	UNP P23258
d	202	LEU	VAL	conflict	UNP P23258
e	35	ALA	GLY	conflict	UNP P23258
e	202	LEU	VAL	conflict	UNP P23258
f	35	ALA	GLY	conflict	UNP P23258
f	202	LEU	VAL	conflict	UNP P23258
g	35	ALA	GLY	conflict	UNP P23258
g	202	LEU	VAL	conflict	UNP P23258
h	35	ALA	GLY	conflict	UNP P23258
h	202	LEU	VAL	conflict	UNP P23258
i	35	ALA	GLY	conflict	UNP P23258
i	202	LEU	VAL	conflict	UNP P23258
j	35	ALA	GLY	conflict	UNP P23258
j	202	LEU	VAL	conflict	UNP P23258
k	35	ALA	GLY	conflict	UNP P23258
k	202	LEU	VAL	conflict	UNP P23258
l	35	ALA	GLY	conflict	UNP P23258
l	202	LEU	VAL	conflict	UNP P23258
m	35	ALA	GLY	conflict	UNP P23258
m	202	LEU	VAL	conflict	UNP P23258
t	35	ALA	GLY	conflict	UNP P23258
t	202	LEU	VAL	conflict	UNP P23258

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
12	U	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 13 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



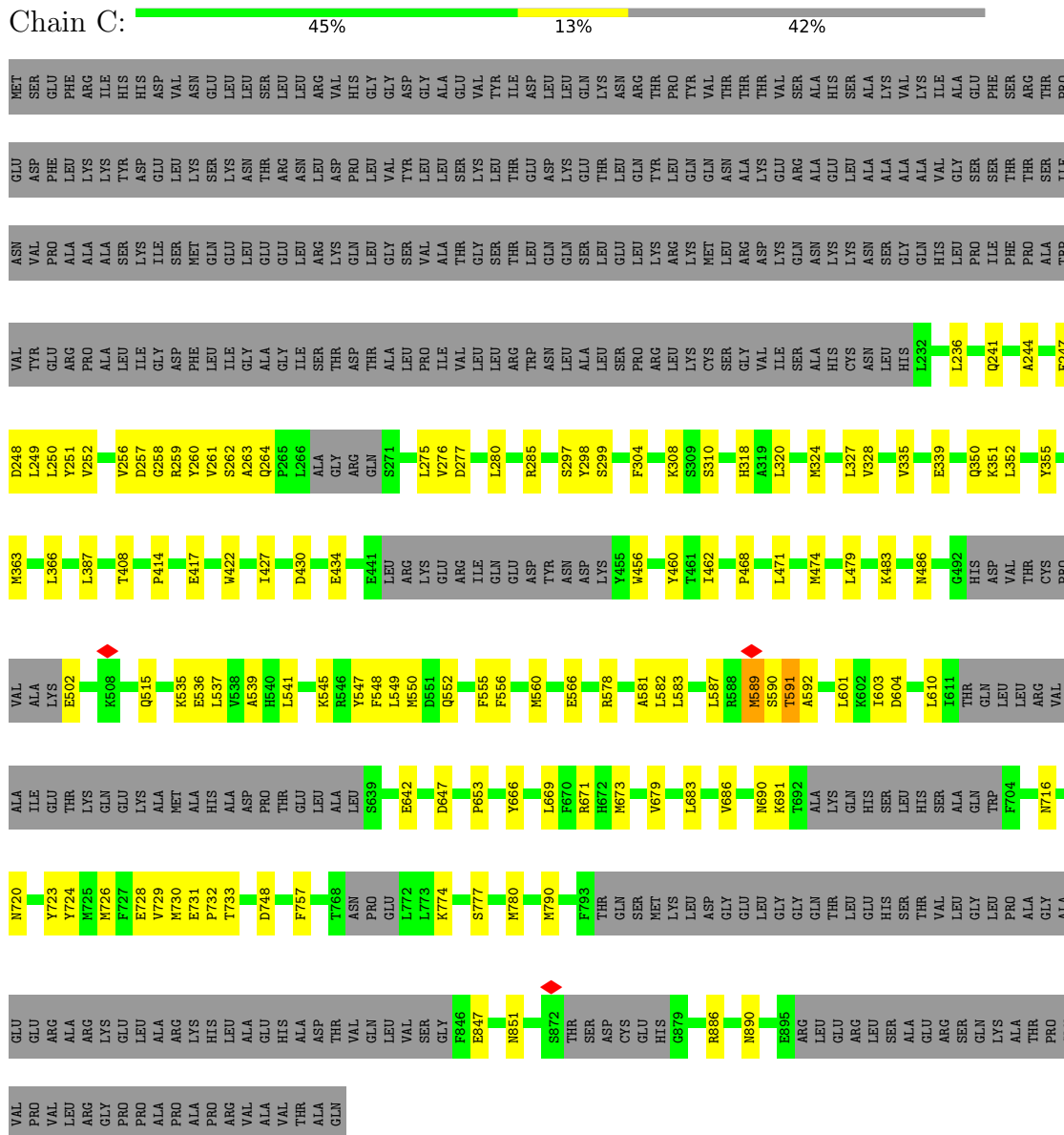
Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	b	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	c	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	d	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	e	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	f	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	g	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	h	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	i	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	j	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	k	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

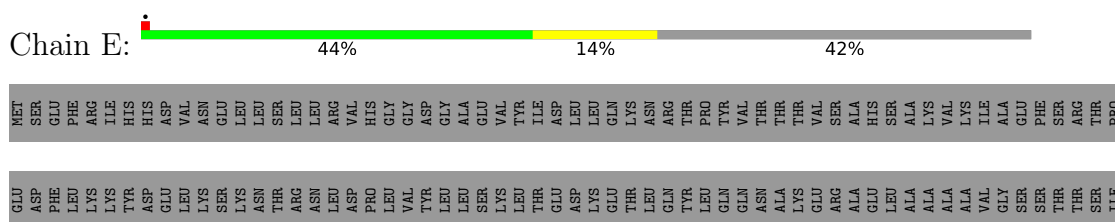
Continued from previous page...

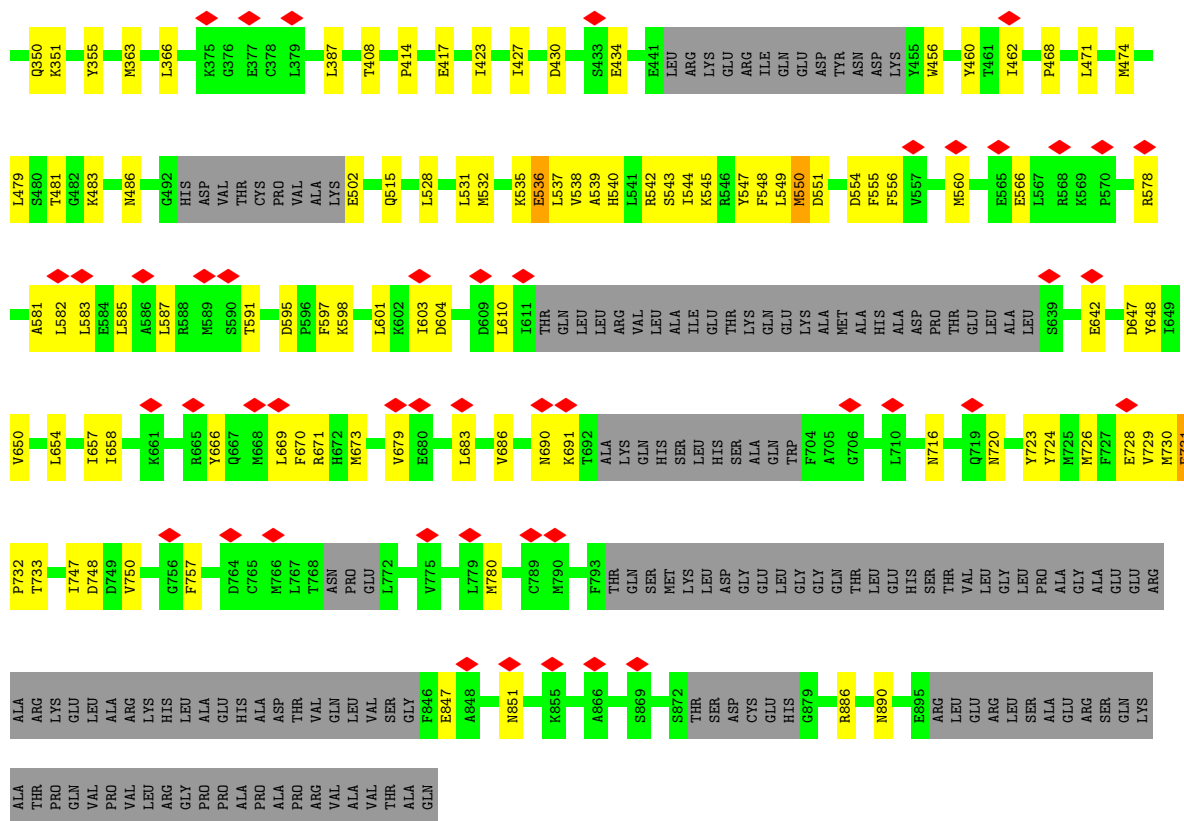
Mol	Chain	Residues	Atoms					AltConf
13	l	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	m	1	Total	C	N	O	P	0
			28	10	5	11	2	
13	t	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 1: Gamma-tubulin complex component 2

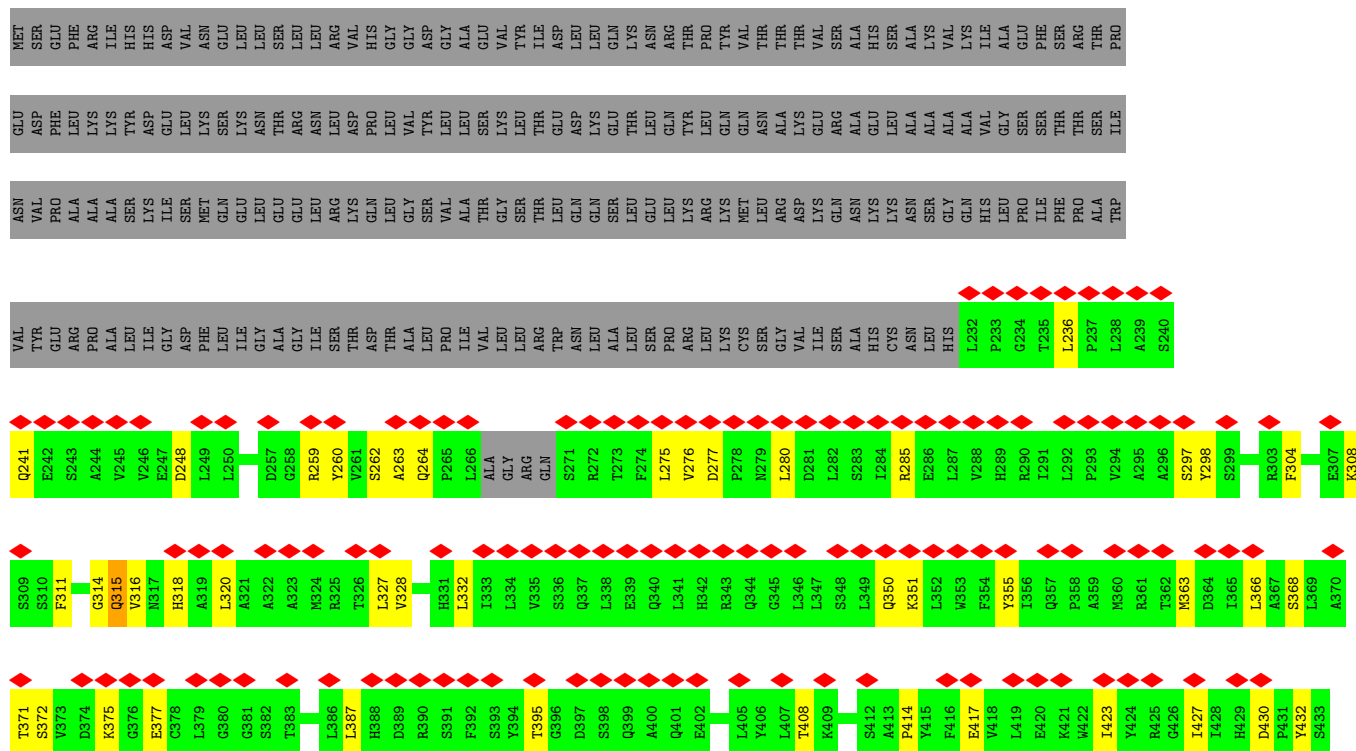


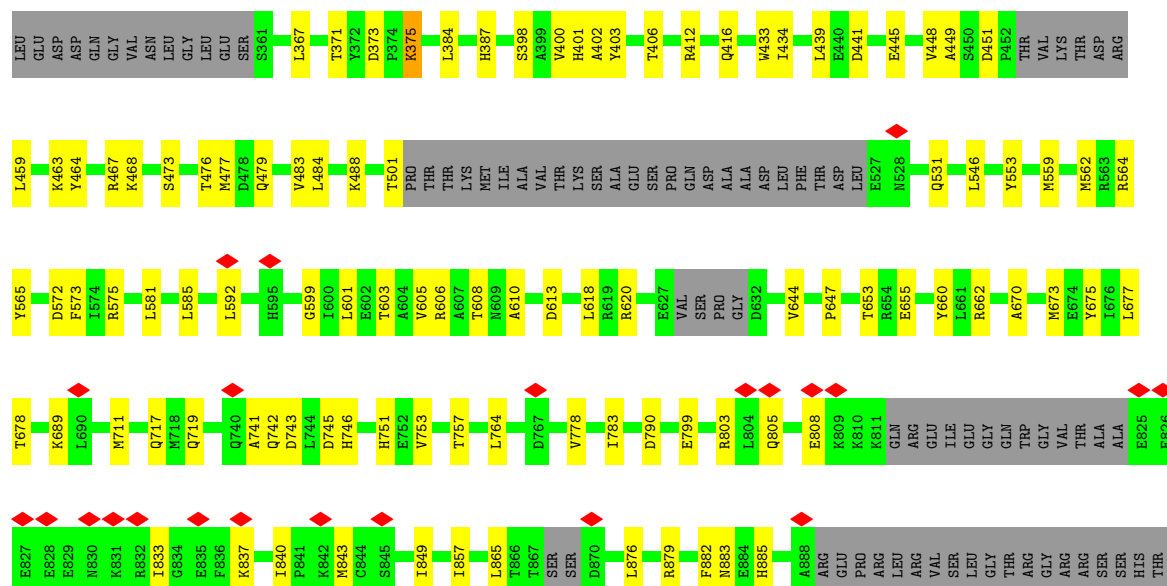
- Molecule 1: Gamma-tubulin complex component 2



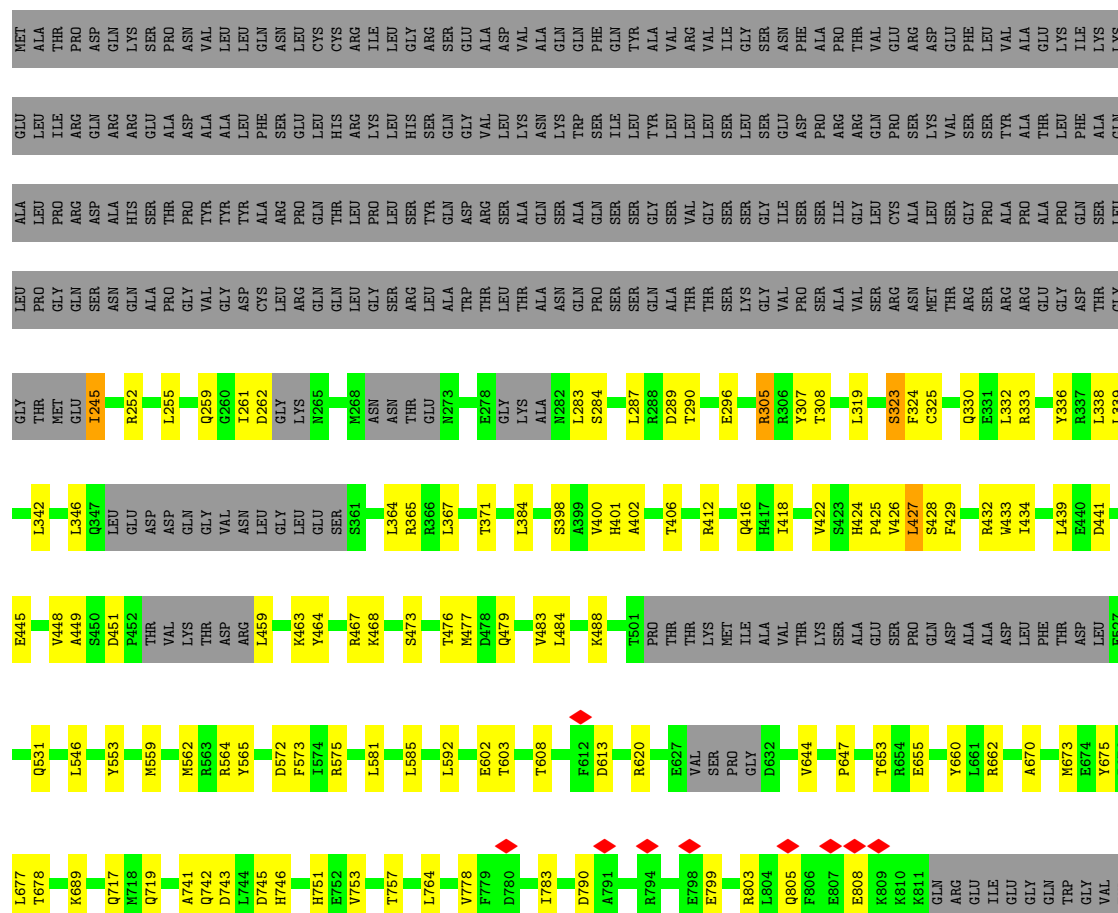


• Molecule 1: Gamma-tubulin complex component 2

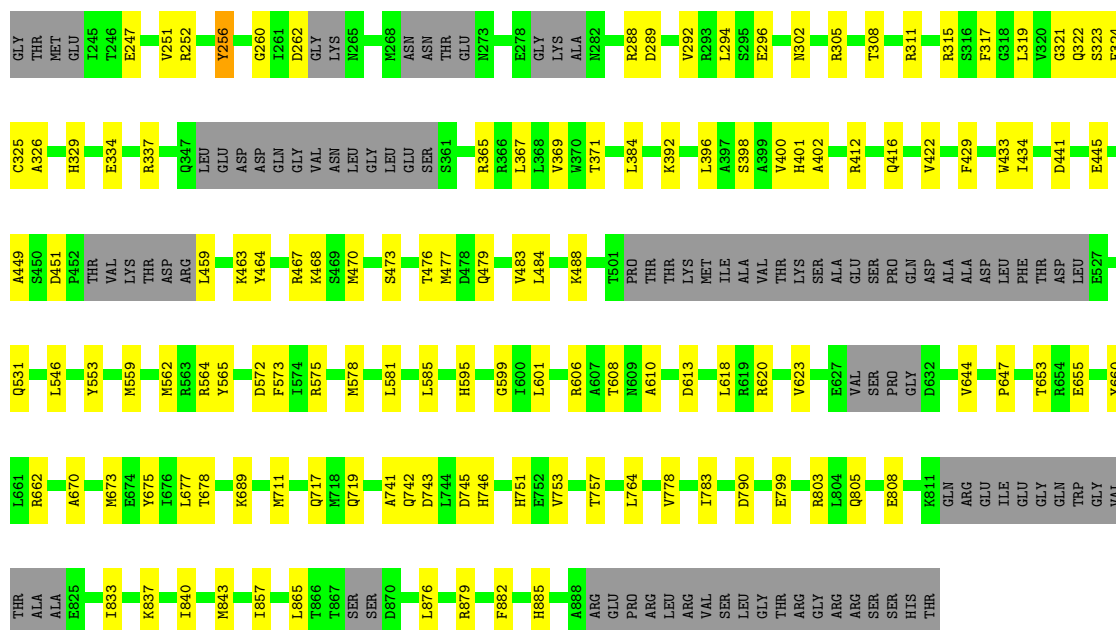




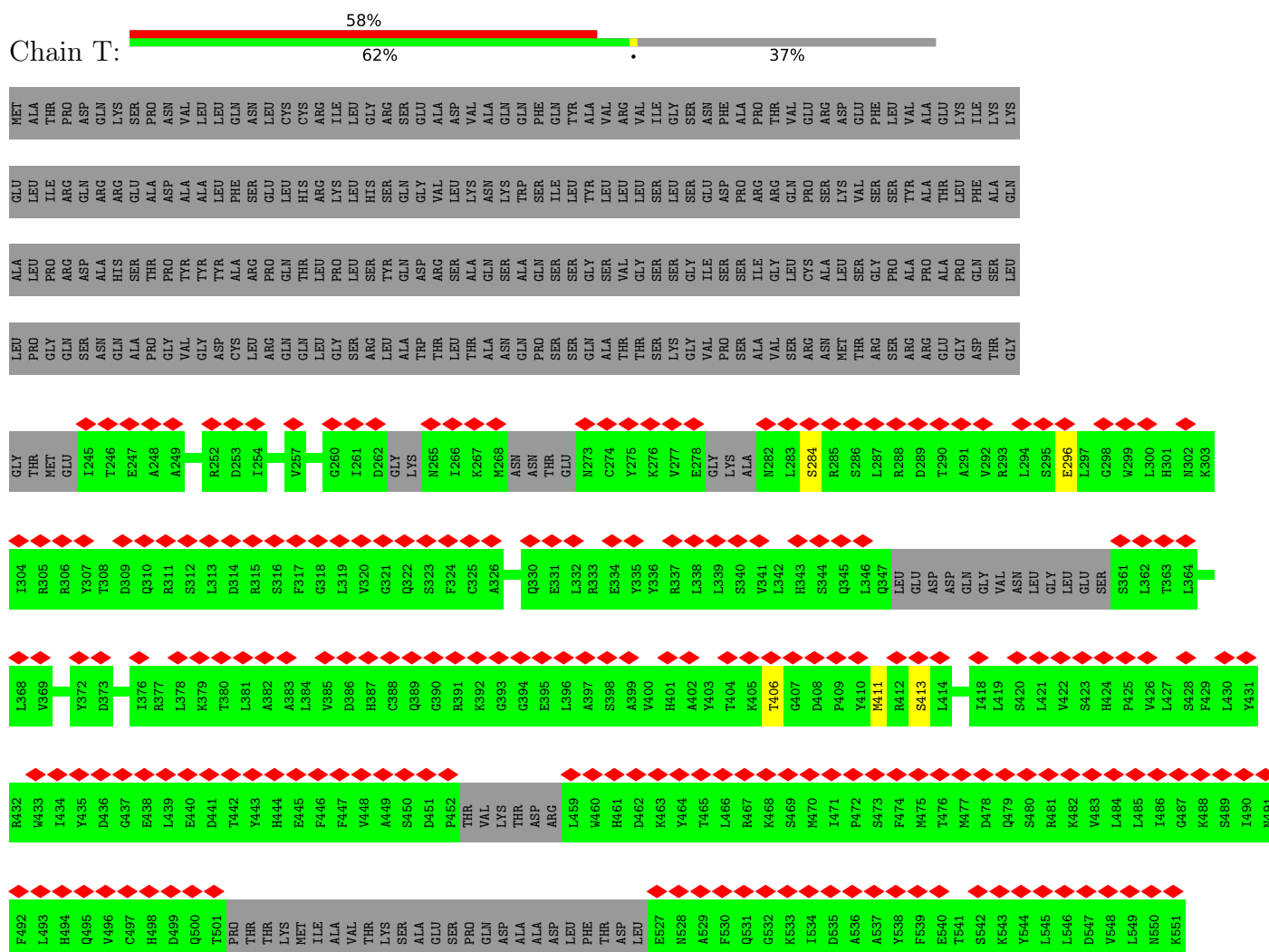
• Molecule 2: Gamma-tubulin complex component 3

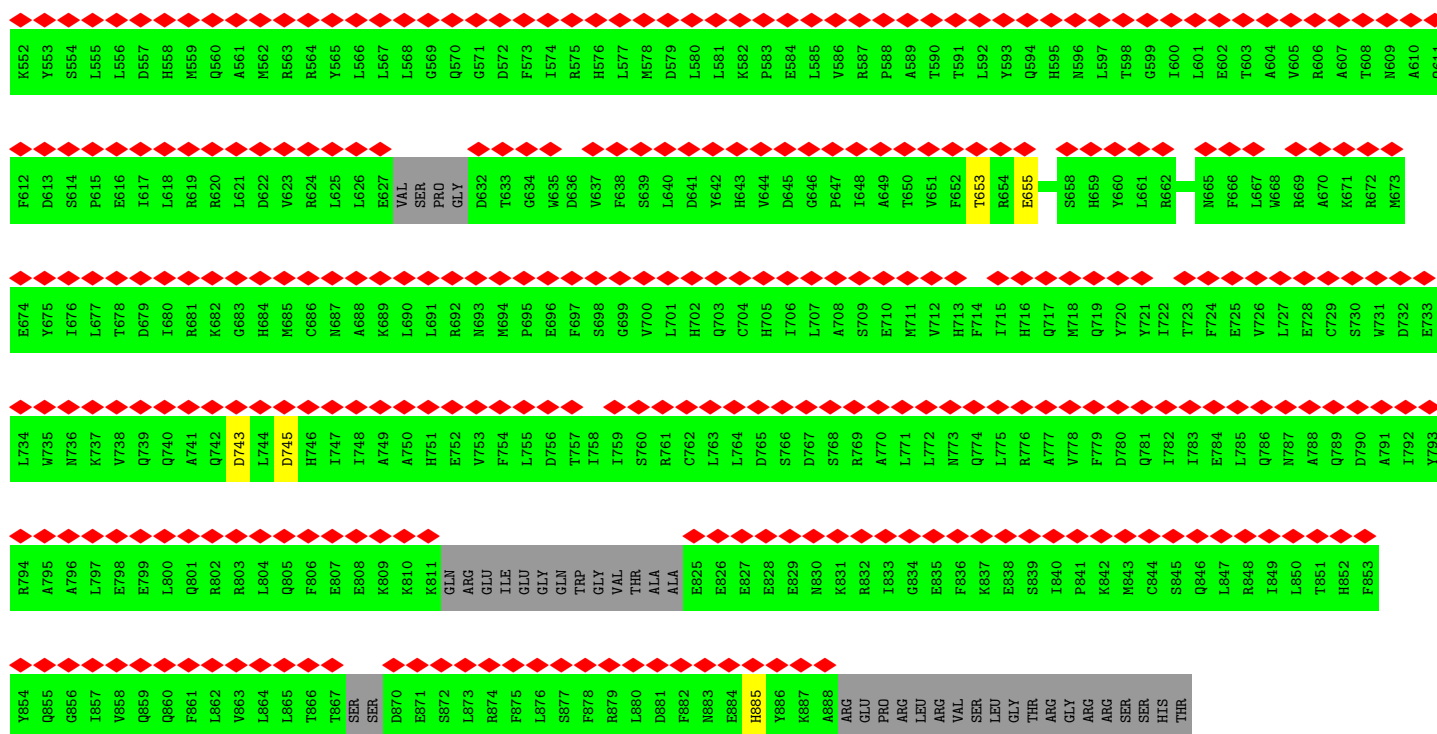




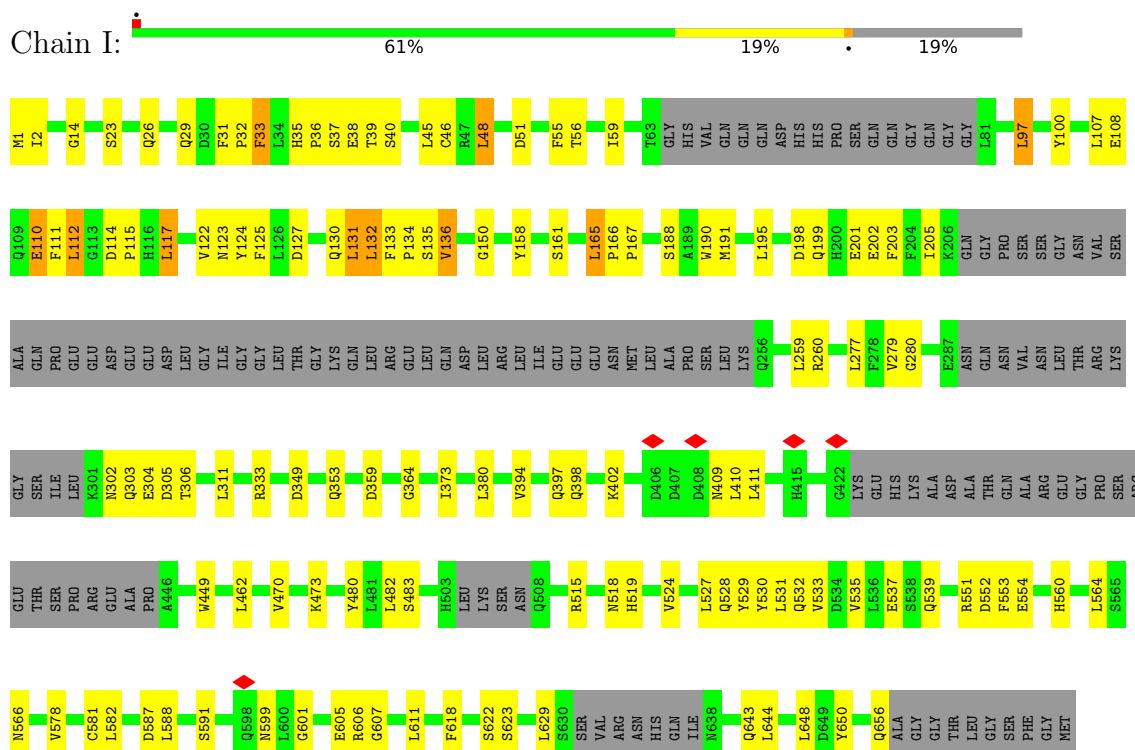


• Molecule 2: Gamma-tubulin complex component 3



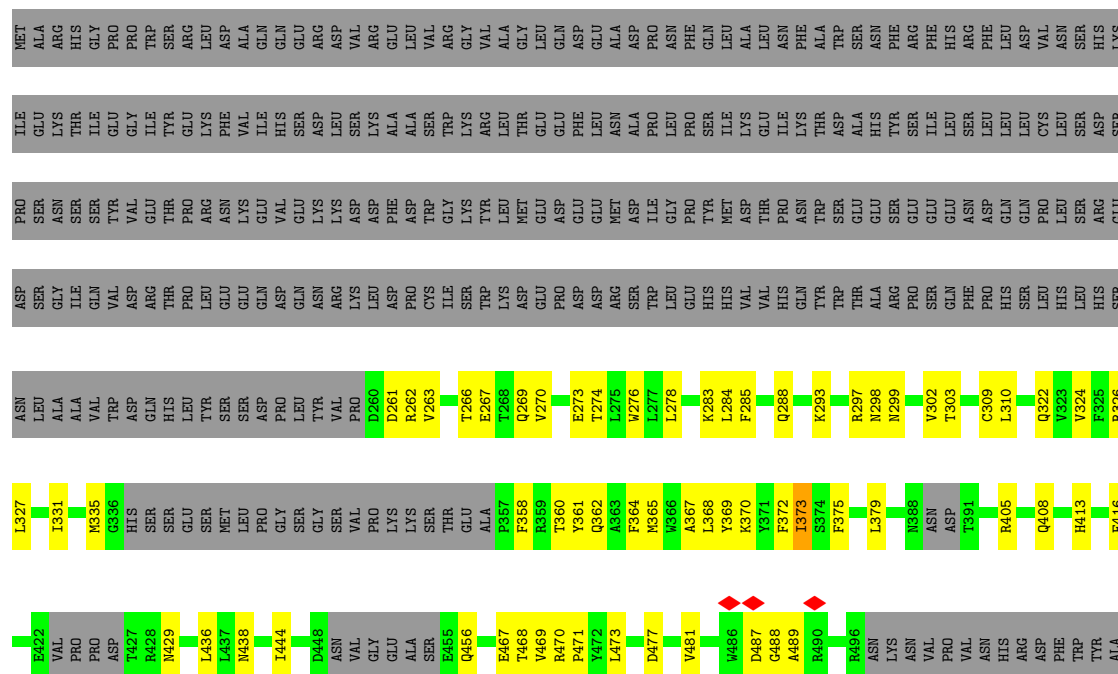


• Molecule 3: Gamma-tubulin complex component 4



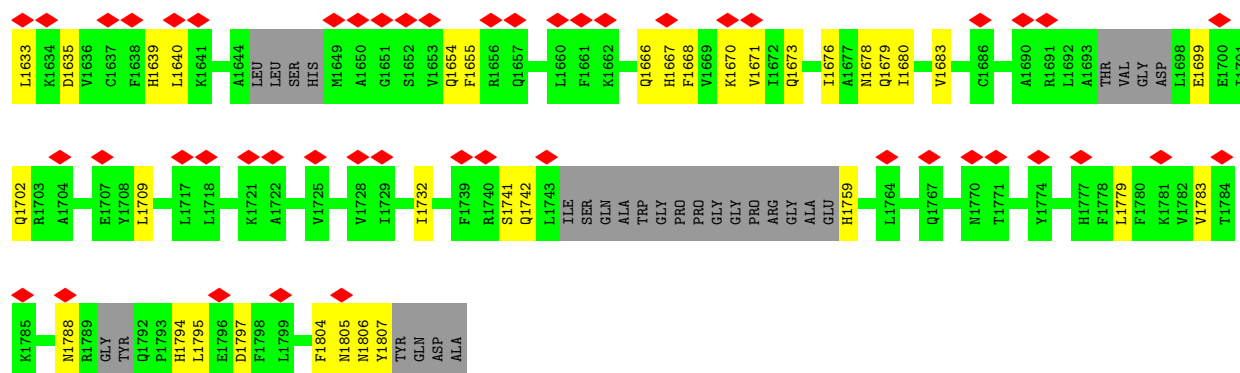
• Molecule 3: Gamma-tubulin complex component 4



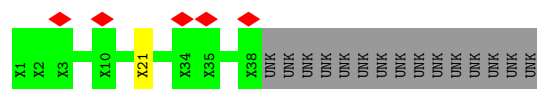




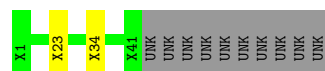




- Molecule 6: Unassigned poly-alanine chain ("staple")



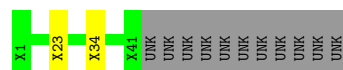
- Molecule 6: Unassigned poly-alanine chain ("staple")



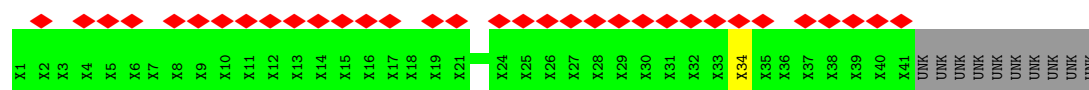
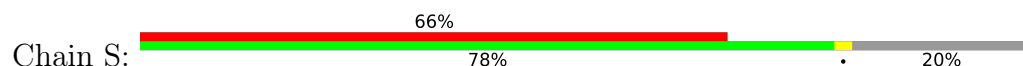
- Molecule 6: Unassigned poly-alanine chain ("staple")



- Molecule 6: Unassigned poly-alanine chain ("staple")

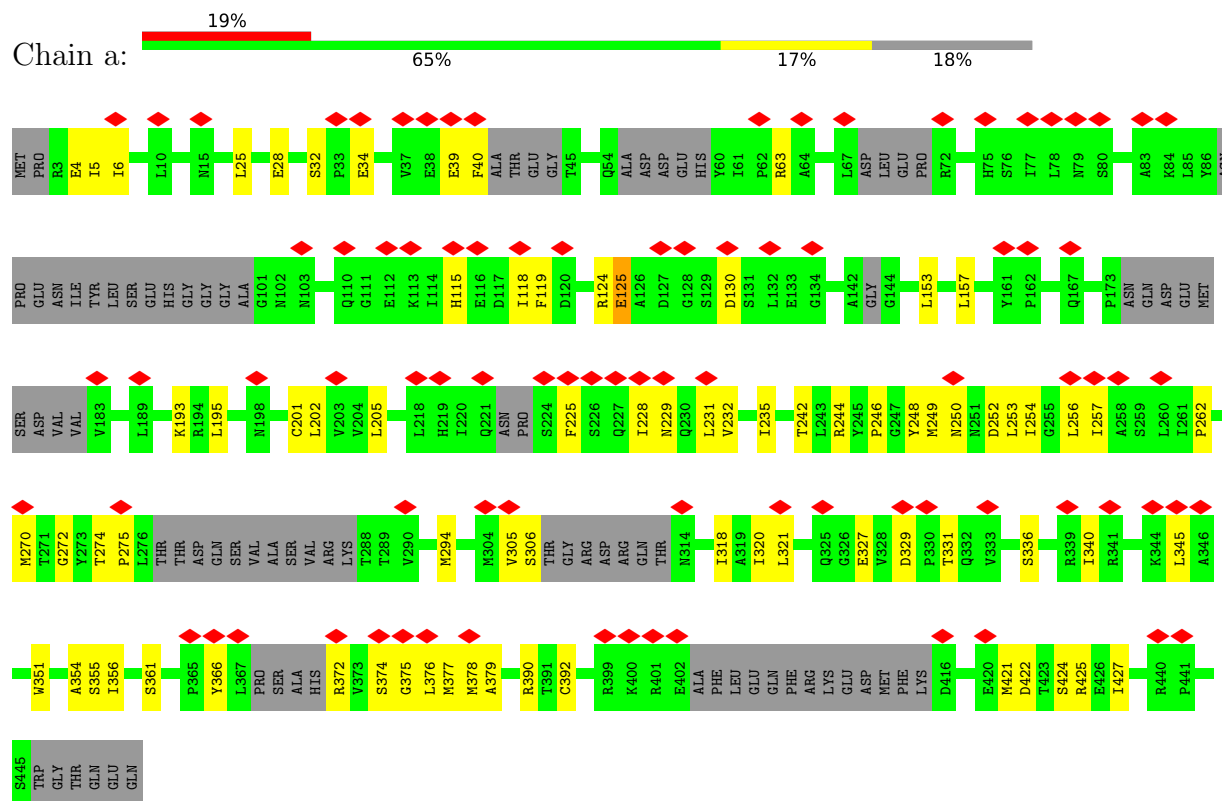


- Molecule 6: Unassigned poly-alanine chain ("staple")

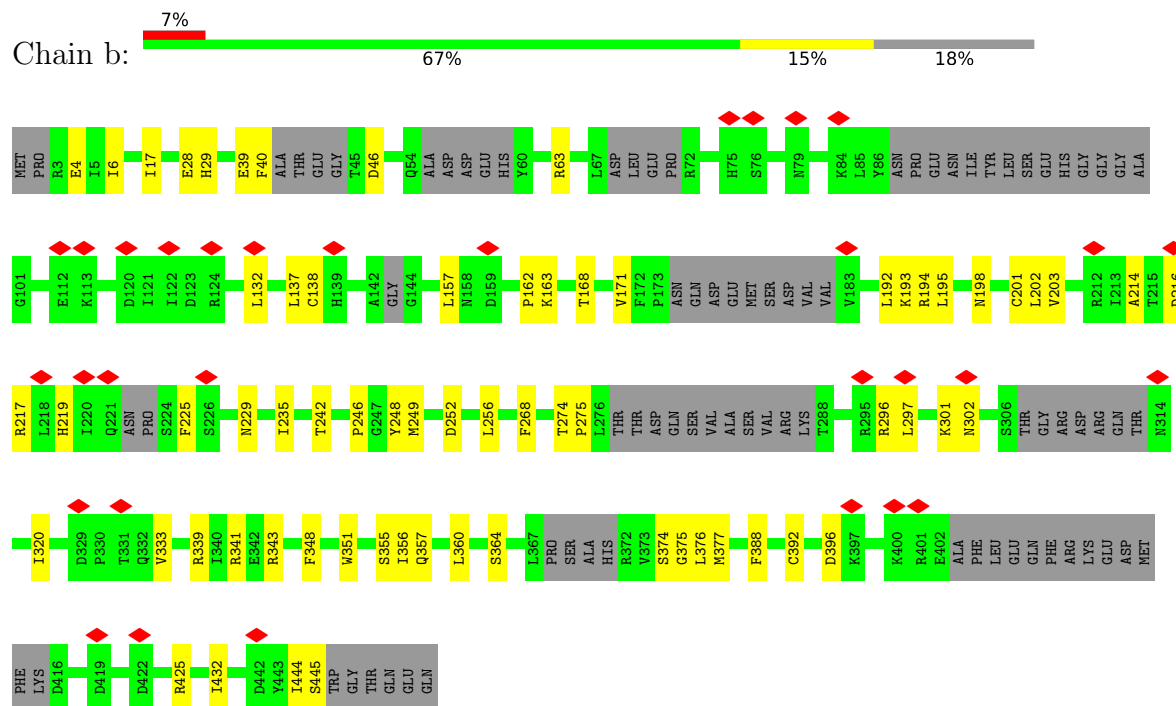


- Molecule 7: beta actin

- Molecule 11: Tubulin gamma-1 chain



- Molecule 11: Tubulin gamma-1 chain



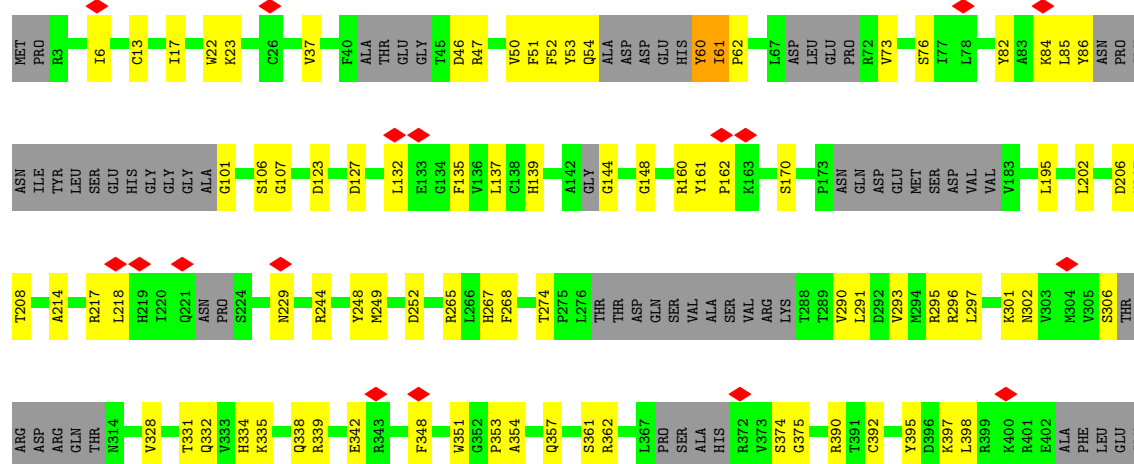
- Molecule 11: Tubulin gamma-1 chain

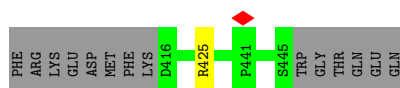


[illegible]

- Molecule 11: Tubulin gamma-1 chain

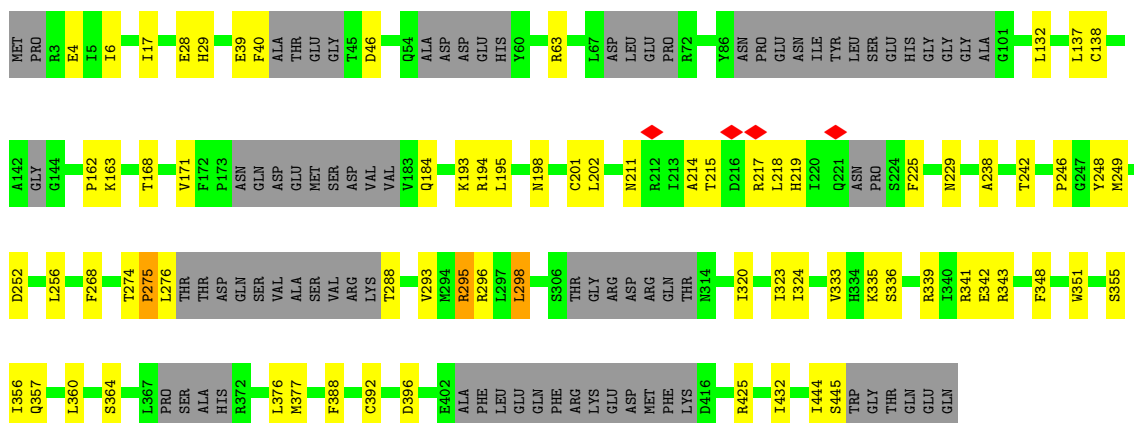
MET	PRO	R3	E4	I5	16	T7	L8	Q24	E28	S32	P33	E34	E39	F40	ALA	THR	GLU	GLY	T45	Q54	ALA	ASP	ASP	GLU	HIS	Y60	R63	A64	V65	L66	L67	ASP	LEU	LEU	GLU	PRO	R72	Y86	ASN	PRO	PRO	GLU	ASN	ASN	ILE	TYR	LEU	SER	GLU	GLY	HIS	GLY	GLY	ALA
-----	-----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----





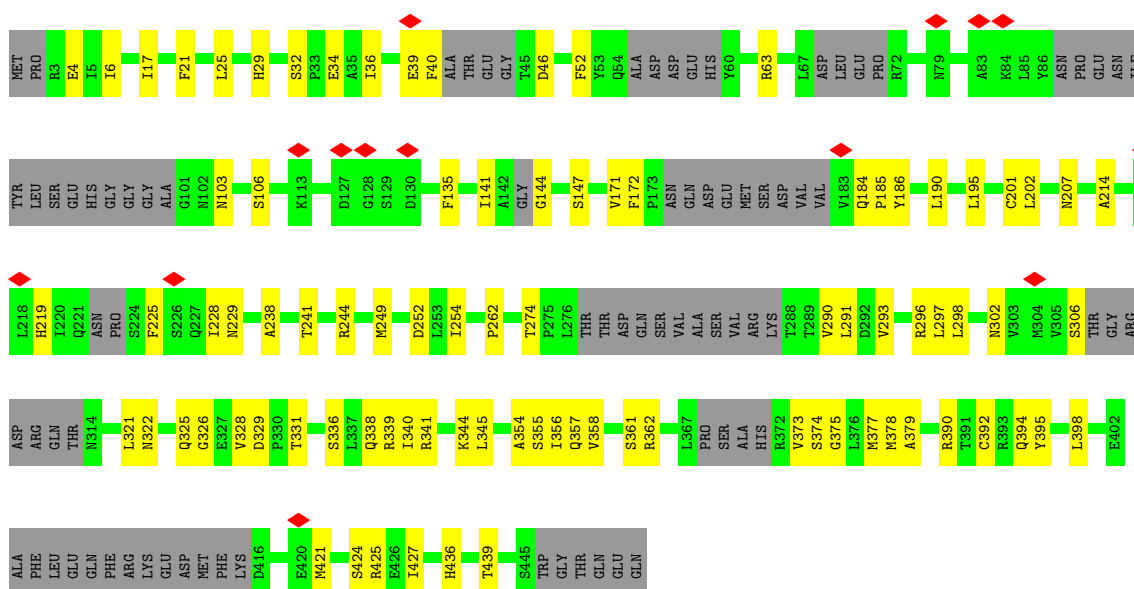
• Molecule 11: Tubulin gamma-1 chain

Chain h: 66% 16% 18%



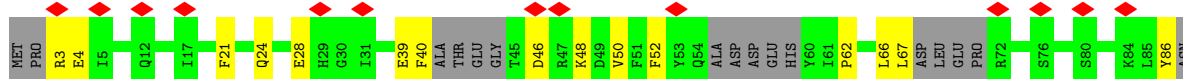
• Molecule 11: Tubulin gamma-1 chain

Chain i: 62% 20% 18%

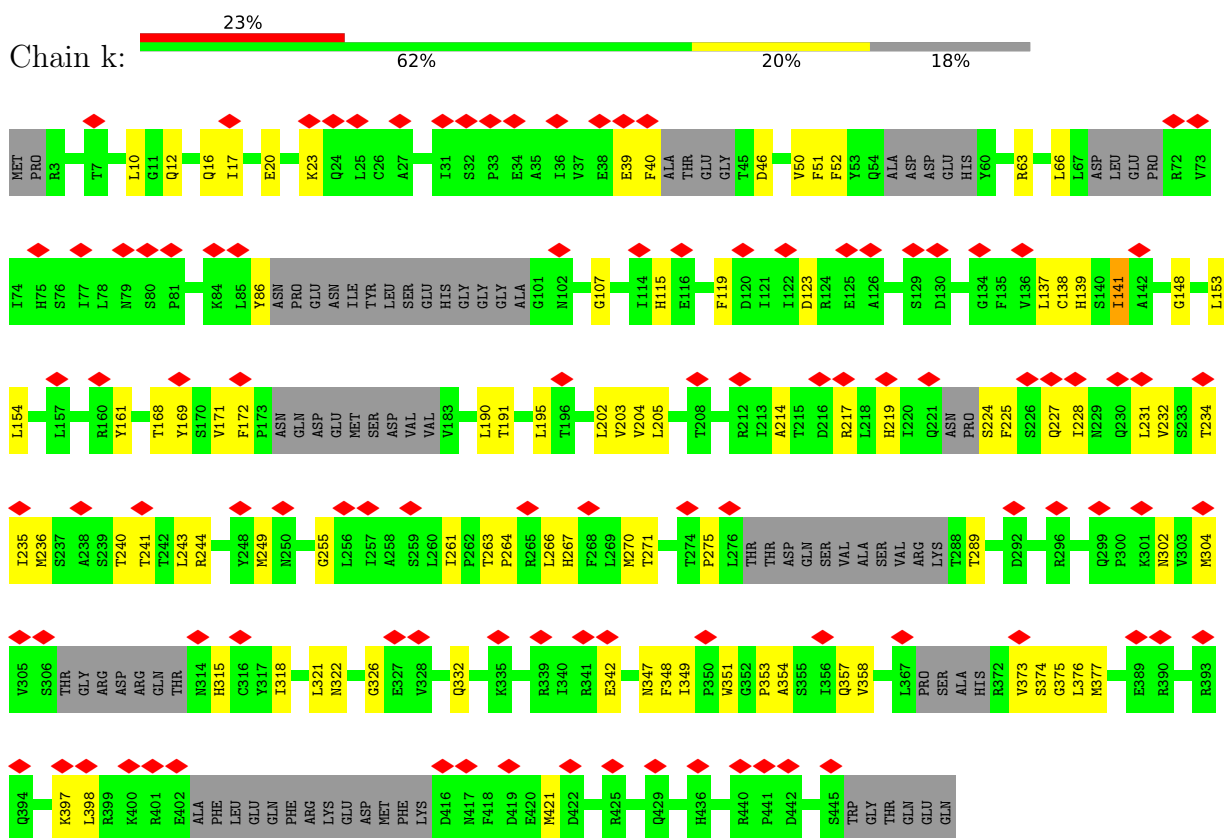


• Molecule 11: Tubulin gamma-1 chain

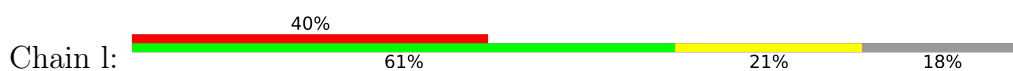
Chain j: 27% 62% 20% 18%



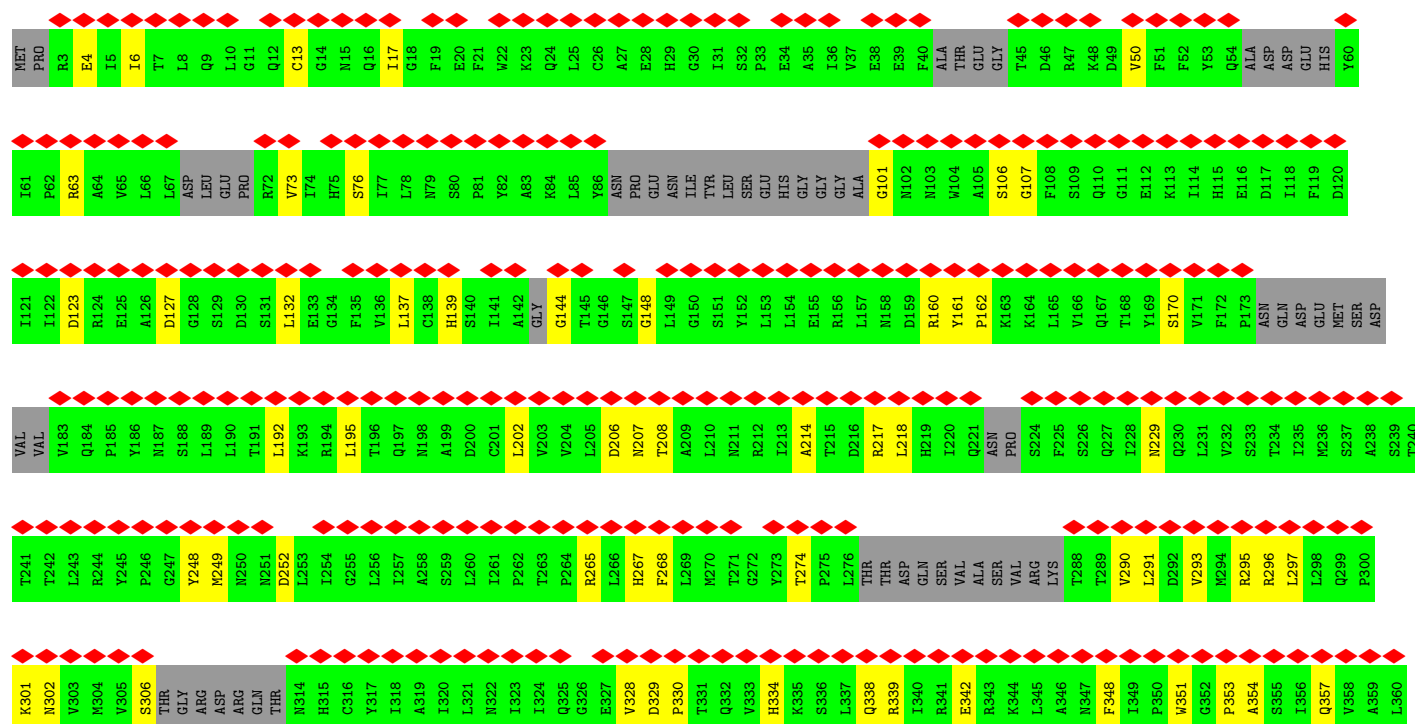
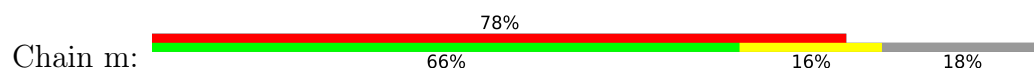
- Molecule 11: Tubulin gamma-1 chain

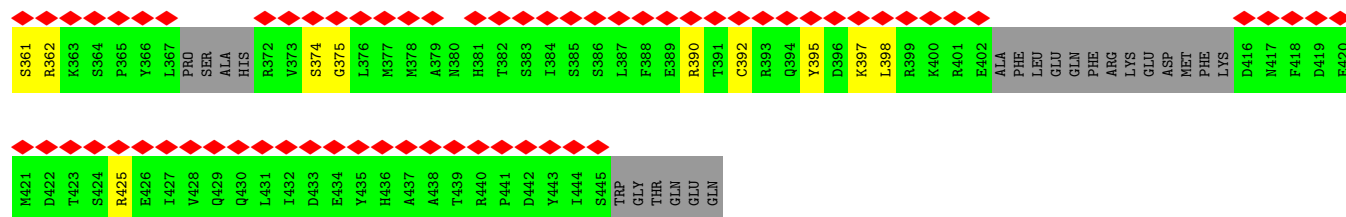


- Molecule 11: Tubulin gamma-1 chain

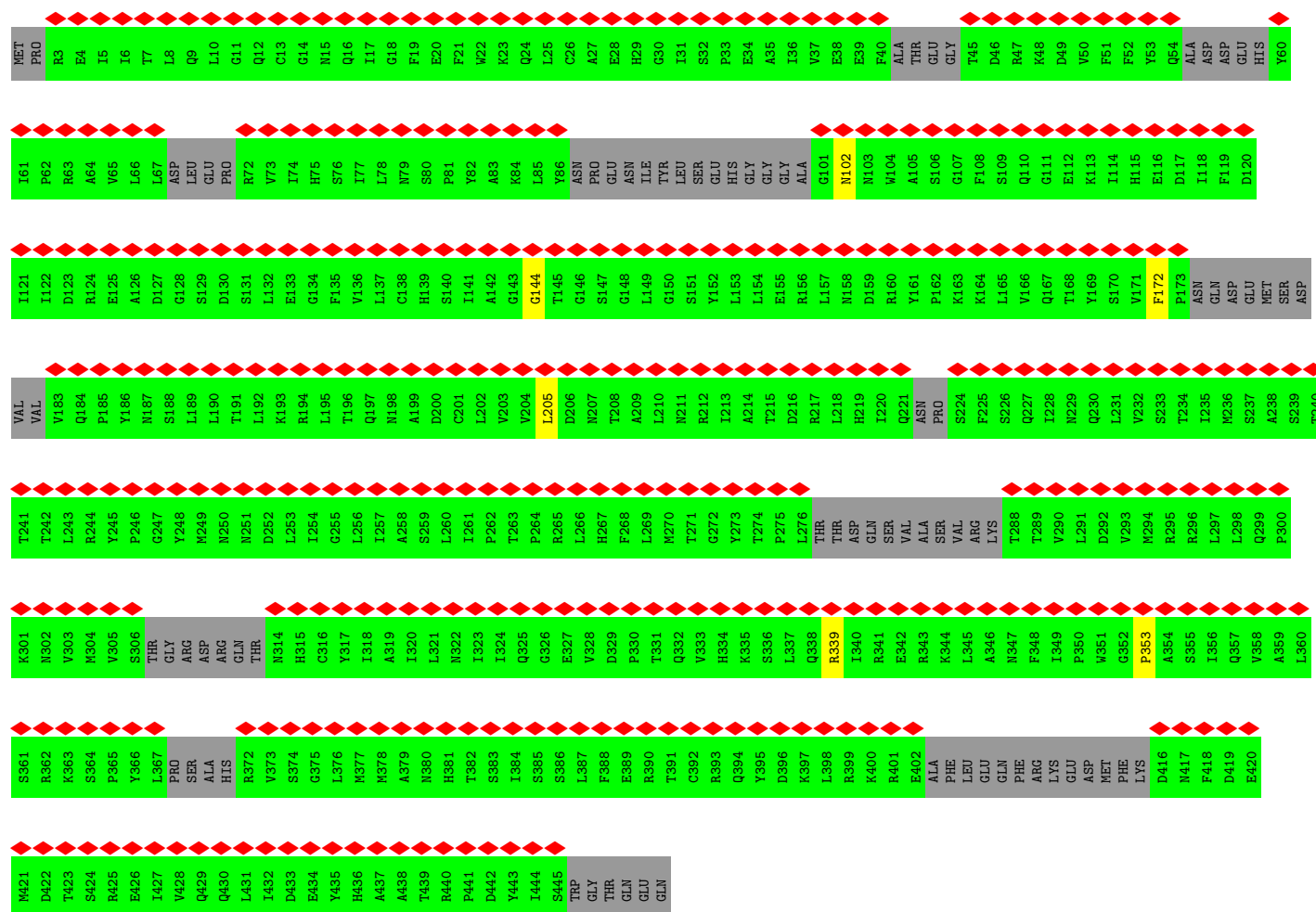
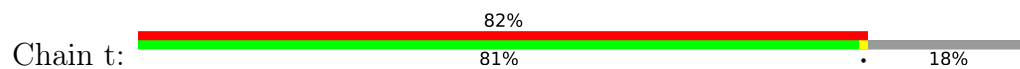


- Molecule 11: Tubulin gamma-1 chain





• Molecule 11: Tubulin gamma-1 chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103172	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 ($e^-/\text{\AA}^2$)	45	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	0.135	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	491.28003, 491.28003, 491.28003	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.335, 1.335, 1.335	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/4461	0.44	0/6020
1	C	0.38	0/4461	0.53	0/6020
1	E	0.40	0/4461	0.56	0/6020
1	G	0.40	0/4461	0.55	1/6020 (0.0%)
1	M	0.34	0/4461	0.47	0/6020
2	B	0.31	0/4839	0.45	1/6522 (0.0%)
2	D	0.39	0/4839	0.53	0/6522
2	F	0.35	0/4839	0.48	1/6522 (0.0%)
2	H	0.40	0/4839	0.54	1/6522 (0.0%)
2	T	0.24	0/2830	0.35	0/3934
3	I	0.35	0/4479	0.47	0/6073
3	K	0.23	0/4479	0.40	0/6073
4	J	0.31	0/4050	0.46	0/5466
5	L	0.22	0/4102	0.36	0/5545
7	U	0.41	0/1793	1.04	4/2492 (0.2%)
11	a	0.36	0/3001	0.50	0/4052
11	b	0.22	0/3001	0.40	0/4052
11	c	0.21	0/3001	0.38	0/4052
11	d	0.24	0/3001	0.42	0/4052
11	e	0.39	0/3001	0.54	0/4052
11	f	0.22	0/3001	0.40	0/4052
11	g	0.33	0/3001	0.48	1/4052 (0.0%)
11	h	0.34	0/3001	0.50	0/4052
11	i	0.27	0/3001	0.45	0/4052
11	j	0.15	0/3001	0.35	0/4052
11	k	0.31	0/3006	0.46	0/4060
11	l	0.22	0/3006	0.42	0/4060
11	m	0.21	0/3001	0.38	0/4052
11	t	0.20	0/1819	0.32	0/2517
All	All	0.32	0/104236	0.48	9/140980 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	163	VAL	N-CA-C	7.65	115.72	108.15
7	U	366	GLY	CA-C-N	6.10	126.27	119.32
7	U	366	GLY	C-N-CA	6.10	126.27	119.32
2	B	375	LYS	N-CA-C	-5.98	106.02	113.38
2	F	375	LYS	N-CA-C	-5.96	106.05	113.38
2	H	256	TYR	CB-CA-C	5.44	117.84	109.03
7	U	162	THR	N-CA-C	-5.28	99.80	108.41
1	G	750	VAL	N-CA-C	-5.24	105.39	110.42
11	g	331	THR	N-CA-C	-5.02	108.90	114.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4371	0	4360	83	0
1	C	4371	0	4360	142	0
1	E	4371	0	4360	142	0
1	G	4371	0	4360	154	0
1	M	4371	0	4360	115	0
2	B	4744	0	4722	92	0
2	D	4744	0	4722	137	0
2	F	4744	0	4722	97	0
2	H	4744	0	4722	122	0
2	T	2840	0	1242	12	0
3	I	4376	0	4314	125	0
3	K	4376	0	4314	97	0
4	J	3977	0	4067	121	0
5	L	4007	0	4022	82	0
6	N	175	0	39	1	0
6	O	200	0	45	5	0
6	Q	190	0	42	6	0
6	R	195	0	43	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	200	0	45	1	0
7	U	1795	0	820	2	0
8	V	310	0	66	1	0
8	Y	285	0	61	4	0
9	W	775	0	173	2	0
10	X	1270	0	287	3	0
11	a	2951	0	2939	80	0
11	b	2951	0	2939	50	0
11	c	2951	0	2939	58	0
11	d	2951	0	2939	55	0
11	e	2951	0	2939	93	0
11	f	2951	0	2939	48	0
11	g	2951	0	2939	85	0
11	h	2951	0	2939	79	0
11	i	2951	0	2939	77	0
11	j	2951	0	2939	59	0
11	k	2955	0	2943	67	0
11	l	2955	0	2943	76	0
11	m	2951	0	2939	56	0
11	t	1830	0	790	6	0
12	U	27	0	12	0	0
13	a	28	0	12	0	0
13	b	28	0	12	1	0
13	c	28	0	12	4	0
13	d	28	0	12	1	0
13	e	28	0	12	0	0
13	f	28	0	12	2	0
13	g	28	0	12	3	0
13	h	28	0	12	1	0
13	i	28	0	12	2	0
13	j	28	0	12	2	0
13	k	28	0	12	0	0
13	l	28	0	12	4	0
13	m	28	0	12	4	0
13	t	28	0	12	0	0
All	All	106422	0	99453	2163	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 11.

All (2163) 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:673:MET:CE	1:G:730:MET:HE1	1.42	1.49
1:C:673:MET:CE	1:C:730:MET:HE1	1.40	1.48
1:E:726:MET:SD	11:e:248:TYR:HB3	1.71	1.30
1:C:555:PHE:CE1	1:C:587:LEU:HD23	1.67	1.29
11:g:54:GLN:HG3	11:g:60:TYR:CE2	1.65	1.28
3:I:35:HIS:ND1	3:I:36:PRO:HD2	1.46	1.26
5:L:1548:LEU:HD21	1:M:881:ALA:CB	1.64	1.25
11:k:172:PHE:CD1	11:k:204:VAL:HG23	1.72	1.24
1:C:555:PHE:CE1	1:C:587:LEU:CD2	2.21	1.23
1:M:669:LEU:HD13	1:M:730:MET:CE	1.66	1.23
1:M:733:THR:HG22	1:M:757:PHE:CD1	1.76	1.21
1:E:723:TYR:CG	11:e:249:MET:HE1	1.76	1.20
1:G:545:LYS:HG3	1:G:549:LEU:HD22	1.23	1.18
4:J:716:LEU:HG	4:J:809:VAL:HG13	1.22	1.15
1:C:733:THR:HG22	1:C:757:PHE:CD1	1.82	1.15
1:G:585:LEU:HD21	11:h:343:ARG:HD3	1.25	1.15
1:G:583:LEU:HD22	1:G:603:ILE:HD11	1.18	1.14
1:C:259:ARG:NH1	2:D:284:SER:HB2	1.63	1.13
1:C:673:MET:HE2	1:C:730:MET:CE	1.78	1.12
1:G:733:THR:HG22	1:G:757:PHE:CD1	1.84	1.11
1:C:733:THR:HG22	1:C:757:PHE:HD1	0.97	1.11
1:E:326:THR:HG21	8:Y:6:UNK:CB	1.79	1.11
1:G:673:MET:HE2	1:G:730:MET:CE	1.79	1.11
2:H:296:GLU:CG	6:R:34:UNK:CB	2.29	1.10
1:M:669:LEU:HD13	1:M:730:MET:HE1	1.12	1.10
11:k:172:PHE:CE1	11:k:204:VAL:HG23	1.85	1.10
1:G:733:THR:HG22	1:G:757:PHE:HD1	0.98	1.09
1:C:555:PHE:CD1	1:C:587:LEU:HD23	1.88	1.08
4:J:362:GLN:HE21	3:K:165:LEU:HD22	1.17	1.08
1:C:673:MET:CE	1:C:730:MET:CE	2.30	1.08
1:G:341:LEU:CD2	1:G:346:LEU:HB2	1.84	1.07
1:M:733:THR:HG22	1:M:757:PHE:HD1	0.91	1.07
1:E:723:TYR:CD1	11:e:249:MET:HE1	1.90	1.07
11:k:172:PHE:CE1	11:k:204:VAL:CG2	2.37	1.07
1:G:673:MET:CE	1:G:730:MET:CE	2.32	1.06
1:G:585:LEU:HD21	11:h:343:ARG:CD	1.85	1.06
2:F:290:THR:O	2:F:294:LEU:HB2	1.54	1.05
1:E:552:GLN:NE2	1:E:591:THR:HG23	1.73	1.03
5:L:1548:LEU:HD21	1:M:881:ALA:HB2	1.36	1.03
1:M:733:THR:CG2	1:M:757:PHE:HD1	1.70	1.03
1:G:673:MET:HE1	1:G:730:MET:HE1	1.40	1.02
1:C:583:LEU:CD2	1:C:603:ILE:HD11	1.88	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:172:PHE:CD1	11:k:204:VAL:CG2	2.41	1.02
4:J:716:LEU:HG	4:J:809:VAL:CG1	1.90	1.01
1:C:583:LEU:HD22	1:C:603:ILE:HD11	1.02	1.01
1:C:673:MET:HE1	1:C:730:MET:HE1	1.39	1.00
1:C:583:LEU:HD22	1:C:603:ILE:CD1	1.91	0.99
1:E:552:GLN:NE2	1:E:591:THR:CG2	2.25	0.99
1:M:669:LEU:CD1	1:M:730:MET:HE1	1.92	0.98
1:G:341:LEU:HD21	1:G:346:LEU:CB	1.93	0.98
5:L:1548:LEU:HD21	1:M:881:ALA:HB1	1.45	0.97
2:F:374:PRO:O	2:F:378:LEU:HD23	1.65	0.97
11:i:141:ILE:HD13	11:i:172:PHE:CE1	2.00	0.96
4:J:270:VAL:O	4:J:274:THR:HG23	1.66	0.96
11:g:54:GLN:CG	11:g:60:TYR:CE2	2.49	0.96
1:C:545:LYS:HA	1:C:549:LEU:HD13	1.47	0.96
11:h:336:SER:HA	11:h:339:ARG:HE	1.31	0.95
11:a:40:PHE:HD2	11:a:366:TYR:CD1	1.84	0.95
1:A:723:TYR:CD2	11:a:249:MET:HE1	2.02	0.94
1:C:733:THR:CG2	1:C:757:PHE:HD1	1.79	0.94
1:E:723:TYR:CD1	11:e:249:MET:CE	2.51	0.94
1:C:259:ARG:HH11	2:D:284:SER:HB2	1.24	0.94
1:E:552:GLN:HE21	1:E:591:THR:CG2	1.80	0.94
1:G:555:PHE:CD1	1:G:587:LEU:HD23	2.02	0.94
3:I:111:PHE:CZ	3:I:122:VAL:CG2	2.50	0.94
1:M:545:LYS:HG3	1:M:549:LEU:HD22	1.49	0.94
1:G:733:THR:CG2	1:G:757:PHE:HD1	1.81	0.93
1:G:673:MET:HE2	1:G:730:MET:HE1	0.93	0.93
2:D:432:ARG:HE	1:E:508:LYS:NZ	1.65	0.93
1:M:545:LYS:HA	1:M:549:LEU:HD13	1.51	0.93
1:M:733:THR:CG2	1:M:757:PHE:CD1	2.49	0.93
3:I:31:PHE:HB3	3:I:33:PHE:CE1	2.02	0.93
1:G:341:LEU:HD23	1:G:346:LEU:HB2	1.51	0.92
1:G:545:LYS:HA	1:G:549:LEU:HD13	1.51	0.92
1:G:341:LEU:CD2	1:G:346:LEU:CB	2.47	0.92
1:E:726:MET:SD	11:e:248:TYR:CB	2.58	0.92
11:g:22:TRP:CD1	11:g:86:TYR:HH	1.87	0.92
1:G:555:PHE:CE1	1:G:587:LEU:CD2	2.53	0.91
2:D:305:ARG:HG2	2:D:305:ARG:HH11	1.32	0.91
11:a:40:PHE:CD2	11:a:366:TYR:HD1	1.88	0.91
1:C:339:GLU:OE1	2:D:365:ARG:HG2	1.70	0.91
1:C:673:MET:HE2	1:C:730:MET:HE1	0.91	0.91
2:D:296:GLU:HG3	6:O:34:UNK:CB	2.01	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:315:ARG:HH21	2:H:315:ARG:HG3	1.35	0.91
10:X:1317:UNK:CB	10:X:1401:UNK:CB	2.49	0.91
1:A:726:MET:SD	11:a:248:TYR:HB3	2.10	0.90
11:e:119:PHE:CE2	11:e:160:ARG:HD2	2.05	0.90
11:e:156:ARG:HG2	11:e:156:ARG:HH11	1.36	0.89
1:C:545:LYS:HG3	1:C:549:LEU:HD22	1.52	0.89
1:E:326:THR:CG2	8:Y:6:UNK:CB	2.50	0.89
11:k:172:PHE:HD1	11:k:204:VAL:HG23	1.32	0.89
1:G:341:LEU:HD21	1:G:346:LEU:HB3	1.53	0.89
1:C:555:PHE:CE1	1:C:587:LEU:HD21	2.05	0.89
1:G:585:LEU:CD2	11:h:343:ARG:HD3	2.02	0.88
11:e:24:GLN:O	11:e:28:GLU:HG3	1.73	0.88
4:J:716:LEU:HD11	4:J:812:VAL:HG21	1.55	0.88
11:i:141:ILE:HD13	11:i:172:PHE:CD1	2.08	0.88
11:l:12:GLN:HB3	13:l:501:GDP:O1A	1.74	0.87
1:G:583:LEU:CD2	1:G:603:ILE:HD11	2.04	0.86
1:C:339:GLU:CD	2:D:365:ARG:HG2	2.00	0.86
4:J:716:LEU:CG	4:J:809:VAL:HG13	2.02	0.86
3:I:111:PHE:HZ	3:I:122:VAL:HG23	1.38	0.86
1:C:731:GLU:HB3	1:C:732:PRO:HD3	1.57	0.86
1:E:710:LEU:HD22	1:E:786:PHE:CE1	2.10	0.86
11:h:274:THR:CG2	11:h:275:PRO:HD3	2.04	0.86
2:H:599:GLY:HA2	11:i:338:GLN:HE21	1.41	0.86
2:H:296:GLU:OE2	6:R:34:UNK:CB	2.24	0.85
11:e:40:PHE:HD2	11:e:366:TYR:CD1	1.93	0.85
1:M:669:LEU:HD13	1:M:730:MET:HE2	1.59	0.85
2:H:296:GLU:HG3	6:R:34:UNK:CB	2.06	0.85
3:I:108:GLU:OE1	3:I:112:LEU:HD21	1.76	0.85
11:k:171:VAL:HG12	11:k:205:LEU:HB2	1.56	0.85
1:G:247:GLU:O	1:G:251:TYR:CD2	2.30	0.85
1:G:545:LYS:HG3	1:G:549:LEU:CD2	2.07	0.85
1:G:555:PHE:CE1	1:G:587:LEU:HD21	2.12	0.85
2:H:296:GLU:HG2	6:R:34:UNK:CB	2.03	0.85
11:a:40:PHE:HB2	11:a:366:TYR:CE1	2.12	0.84
2:D:308:THR:HG1	2:D:325:CYS:HG	1.24	0.84
5:L:1548:LEU:CD2	1:M:881:ALA:HB2	2.06	0.84
1:C:566:GLU:OE1	1:C:582:LEU:HD11	1.76	0.84
1:E:723:TYR:CE1	11:e:249:MET:CE	2.60	0.84
1:G:550:MET:HB3	1:G:556:PHE:CE2	2.12	0.84
1:M:726:MET:HB3	11:m:248:TYR:CD1	2.13	0.84
11:g:54:GLN:NE2	11:g:60:TYR:OH	2.10	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:LEU:O	2:D:336:TYR:CD2	2.31	0.83
1:G:545:LYS:CG	1:G:549:LEU:HD22	2.07	0.83
1:G:583:LEU:HD22	1:G:603:ILE:CD1	2.06	0.83
11:i:141:ILE:CD1	11:i:172:PHE:CD1	2.62	0.83
1:G:733:THR:CG2	1:G:757:PHE:CD1	2.60	0.83
2:D:261:ILE:HG23	1:E:286:GLU:OE2	1.78	0.83
4:J:362:GLN:HE21	3:K:165:LEU:CD2	1.91	0.83
2:F:296:GLU:OE2	6:Q:34:UNK:CB	2.27	0.82
1:G:726:MET:HB3	11:g:248:TYR:CD2	2.15	0.82
1:C:733:THR:CG2	1:C:757:PHE:CD1	2.58	0.82
1:A:710:LEU:HD22	1:A:786:PHE:CE1	2.14	0.82
1:E:723:TYR:CE1	11:e:249:MET:HE3	2.14	0.82
11:a:40:PHE:HB2	11:a:366:TYR:HE1	1.44	0.82
3:I:111:PHE:HZ	3:I:122:VAL:CG2	1.91	0.82
2:T:885:HIS:CB	11:t:353:PRO:HA	2.10	0.82
11:k:137:LEU:HG	11:k:139:HIS:HD2	1.43	0.82
2:B:402:ALA:O	6:N:21:UNK:CB	2.28	0.82
11:a:153:LEU:O	11:a:157:LEU:HG	1.80	0.81
1:A:552:GLN:HG3	11:a:246:PRO:HB2	1.62	0.81
2:D:296:GLU:OE2	6:O:34:UNK:CB	2.27	0.81
3:I:35:HIS:HD1	3:I:36:PRO:HD2	1.42	0.81
1:C:555:PHE:CZ	1:C:587:LEU:HD21	2.13	0.81
2:F:484:LEU:O	2:F:484:LEU:HD23	1.81	0.81
1:G:550:MET:HG2	1:G:556:PHE:CZ	2.16	0.81
1:E:306:GLU:OE2	6:Q:36:UNK:HA	1.81	0.81
4:J:362:GLN:HE22	3:K:164:GLY:HA3	1.44	0.81
2:B:484:LEU:HD23	2:B:484:LEU:O	1.81	0.80
1:E:723:TYR:CD2	11:e:249:MET:HE1	2.15	0.80
1:G:333:ILE:HG12	2:H:369:VAL:CG2	2.11	0.80
2:H:484:LEU:HD23	2:H:484:LEU:O	1.81	0.80
3:I:529:TYR:HE2	11:i:249:MET:HB3	1.47	0.80
3:I:35:HIS:CE1	3:I:36:PRO:HD2	2.16	0.80
2:D:484:LEU:O	2:D:484:LEU:HD23	1.81	0.80
11:a:124:ARG:HH22	11:b:301:LYS:HD3	1.47	0.80
1:G:566:GLU:OE1	1:G:582:LEU:HD11	1.82	0.79
1:G:548:PHE:CE1	1:G:648:TYR:HB2	2.17	0.79
4:J:278:LEU:HB3	4:J:379:LEU:CD2	2.12	0.79
11:k:141:ILE:HD11	11:k:172:PHE:HA	1.64	0.79
11:m:290:VAL:HG13	11:m:328:VAL:HG21	1.64	0.79
4:J:375:PHE:HE1	4:J:405:ARG:HB3	1.45	0.79
5:L:1571:ASN:HB3	5:L:1599:LYS:HB3	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:595:HIS:HE1	3:I:648:LEU:HD23	1.47	0.79
3:I:35:HIS:CG	3:I:36:PRO:HD2	2.18	0.79
11:e:119:PHE:HE2	11:e:160:ARG:CD	1.95	0.79
11:h:274:THR:HG23	11:h:275:PRO:HD3	1.63	0.79
1:A:723:TYR:CD2	11:a:249:MET:CE	2.64	0.79
2:D:332:LEU:O	2:D:336:TYR:HD2	1.65	0.79
11:e:119:PHE:HE2	11:e:160:ARG:HD2	1.48	0.78
3:K:34:LEU:O	3:K:34:LEU:HD12	1.83	0.78
11:c:329:ASP:OD1	11:c:330:PRO:HD2	1.83	0.78
2:D:296:GLU:CG	6:O:34:UNK:CB	2.61	0.78
1:E:723:TYR:CZ	11:e:249:MET:HE3	2.17	0.78
2:H:296:GLU:CD	6:R:34:UNK:CB	2.57	0.78
11:e:40:PHE:CD2	11:e:366:TYR:CD1	2.72	0.78
11:m:329:ASP:OD1	11:m:330:PRO:HD2	1.84	0.78
2:D:402:ALA:O	6:O:23:UNK:CB	2.31	0.77
1:C:244:ALA:O	1:C:247:GLU:HG3	1.84	0.77
2:D:296:GLU:CD	6:O:34:UNK:CB	2.58	0.77
1:M:314:GLY:C	1:M:318:HIS:CE1	2.62	0.77
4:J:278:LEU:HB3	4:J:379:LEU:HD21	1.64	0.77
2:H:321:GLY:HA2	2:H:396:LEU:HD23	1.64	0.77
1:C:244:ALA:HA	1:C:247:GLU:OE2	1.85	0.77
1:E:462:ILE:HG12	1:E:479:LEU:HD22	1.67	0.77
1:G:247:GLU:O	1:G:251:TYR:CE2	2.37	0.76
1:G:673:MET:HE1	1:G:730:MET:CE	2.09	0.76
3:I:111:PHE:CE1	3:I:122:VAL:HG22	2.20	0.76
11:k:172:PHE:CE1	11:k:204:VAL:HG21	2.18	0.76
1:E:311:PHE:HB3	1:E:432:TYR:OH	1.86	0.76
1:E:555:PHE:CZ	1:E:583:LEU:HD12	2.21	0.76
1:G:333:ILE:HG12	2:H:369:VAL:HG21	1.65	0.76
1:C:259:ARG:NH1	2:D:284:SER:CB	2.48	0.76
2:F:608:THR:HG23	2:F:610:ALA:H	1.50	0.76
2:H:296:GLU:HG3	6:R:34:UNK:C	2.15	0.76
3:I:107:LEU:HD21	3:I:125:PHE:CG	2.21	0.76
11:a:6:ILE:HD12	11:a:125:GLU:HG3	1.68	0.76
2:H:608:THR:HG23	2:H:610:ALA:H	1.50	0.76
1:C:578:ARG:HD3	11:d:342:GLU:OE1	1.86	0.75
11:g:54:GLN:HG3	11:g:60:TYR:CD2	2.21	0.75
2:B:288:ARG:O	2:B:292:VAL:HG23	1.86	0.75
1:A:462:ILE:HG12	1:A:479:LEU:HD22	1.67	0.75
1:A:723:TYR:CG	11:a:249:MET:HE1	2.21	0.75
1:C:256:VAL:HG21	2:D:290:THR:OG1	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:MET:HG2	1:C:556:PHE:CZ	2.22	0.75
11:h:295:ARG:CB	11:h:295:ARG:HH11	1.99	0.75
11:l:146:GLY:HA2	11:l:149:LEU:HB2	1.68	0.75
11:g:22:TRP:HD1	11:g:86:TYR:HH	1.34	0.75
11:h:295:ARG:HH11	11:h:295:ARG:HB3	1.51	0.75
1:E:318:HIS:ND1	2:F:406:THR:O	2.20	0.75
2:F:257:VAL:O	2:F:298:GLY:HA3	1.85	0.75
1:E:555:PHE:CZ	1:E:583:LEU:CD1	2.70	0.74
11:a:40:PHE:CD2	11:a:366:TYR:CD1	2.66	0.74
11:k:172:PHE:HE1	11:k:204:VAL:CG2	2.00	0.74
1:G:555:PHE:CE1	1:G:587:LEU:HD23	2.21	0.74
1:G:731:GLU:HB3	1:G:732:PRO:HD3	1.68	0.74
4:J:904:ARG:NH1	11:j:330:PRO:O	2.20	0.74
3:I:165:LEU:N	3:I:165:LEU:HD23	2.01	0.74
1:A:723:TYR:CG	11:a:249:MET:CE	2.71	0.74
2:B:608:THR:HG23	2:B:610:ALA:H	1.50	0.74
1:A:237:PRO:HG2	1:A:240:SER:HB3	1.70	0.73
2:D:432:ARG:HE	1:E:508:LYS:HZ2	1.34	0.73
1:E:237:PRO:HG2	1:E:240:SER:HB3	1.70	0.73
1:E:555:PHE:HZ	1:E:583:LEU:CD1	2.01	0.73
2:H:308:THR:HG1	2:H:325:CYS:HG	1.27	0.73
11:j:392:CYS:SG	11:j:425:ARG:NH1	2.61	0.73
2:B:387:HIS:CD2	2:B:403:TYR:HE1	2.06	0.73
3:I:33:PHE:H	3:I:33:PHE:HD1	1.35	0.73
5:L:1676:ILE:HG23	5:L:1680:ILE:HD12	1.71	0.73
1:M:724:TYR:O	1:M:729:VAL:HG23	1.88	0.73
11:g:37:VAL:HB	11:g:60:TYR:HE1	1.51	0.73
11:e:156:ARG:HG2	11:e:156:ARG:NH1	1.97	0.73
2:B:245:ILE:HD12	2:B:245:ILE:N	2.03	0.73
2:D:245:ILE:HD12	2:D:245:ILE:N	2.03	0.73
2:D:432:ARG:NE	1:E:508:LYS:NZ	2.37	0.73
1:G:341:LEU:HD21	1:G:346:LEU:HB2	1.60	0.73
1:M:731:GLU:HB3	1:M:732:PRO:HD3	1.69	0.73
2:F:259:GLN:NE2	1:G:350:GLN:OE1	2.22	0.73
2:F:387:HIS:HB2	2:F:403:TYR:OH	1.89	0.73
1:G:544:ILE:HG12	1:G:648:TYR:CE2	2.24	0.73
1:M:377:GLU:N	1:M:377:GLU:OE1	2.21	0.73
2:F:245:ILE:N	2:F:245:ILE:HD12	2.03	0.72
4:J:362:GLN:HE22	3:K:164:GLY:CA	2.01	0.72
11:k:217:ARG:NH1	11:k:302:ASN:OD1	2.22	0.72
2:D:346:LEU:HD23	2:D:346:LEU:O	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:595:ILE:HD11	5:L:1484:LEU:HD21	1.71	0.72
2:B:259:GLN:NE2	1:C:350:GLN:OE1	2.22	0.72
1:C:566:GLU:OE1	1:C:582:LEU:CD1	2.38	0.71
1:G:731:GLU:HA	1:G:731:GLU:OE2	1.89	0.71
1:E:330:GLU:OE1	1:E:333:ILE:HD12	1.89	0.71
1:G:536:GLU:H	1:G:536:GLU:CD	1.97	0.71
3:I:132:LEU:C	3:I:132:LEU:HD12	2.15	0.71
4:J:716:LEU:HD23	4:J:716:LEU:C	2.15	0.71
5:L:546:ARG:HE	1:M:395:THR:HG23	1.54	0.71
5:L:1548:LEU:CD2	1:M:881:ALA:CB	2.57	0.71
3:I:111:PHE:CZ	3:I:122:VAL:HG22	2.26	0.70
3:K:401:HIS:HD2	11:I:339:ARG:HH21	1.39	0.70
1:M:550:MET:HG2	1:M:556:PHE:CZ	2.26	0.70
11:h:211:ASN:O	11:h:215:THR:HG23	1.90	0.70
11:k:107:GLY:HA3	11:k:148:GLY:HA3	1.73	0.70
11:e:6:ILE:HD12	11:e:125:GLU:HG2	1.73	0.70
11:k:50:VAL:HG13	11:k:51:PHE:HD1	1.56	0.70
1:G:585:LEU:CD2	11:h:343:ARG:HB2	2.22	0.70
3:I:132:LEU:HD12	3:I:132:LEU:O	1.91	0.70
11:h:214:ALA:HA	11:h:218:LEU:HB2	1.73	0.70
11:k:190:LEU:HD21	11:k:421:MET:HG2	1.72	0.70
1:C:673:MET:HE1	1:C:730:MET:CE	2.08	0.70
11:g:23:LYS:NZ	11:g:82:TYR:CE1	2.58	0.70
3:I:117:LEU:N	3:I:117:LEU:HD23	2.07	0.70
3:K:34:LEU:HD12	3:K:34:LEU:C	2.17	0.70
1:A:552:GLN:NE2	1:A:591:THR:HG23	2.06	0.69
1:E:552:GLN:HE22	1:E:591:THR:HG23	1.53	0.69
1:E:397:ASP:OD2	1:E:400:ALA:HB3	1.92	0.69
1:G:548:PHE:HE1	1:G:648:TYR:HB2	1.55	0.69
4:J:284:LEU:HA	3:K:37:SER:HB2	1.74	0.69
11:g:54:GLN:NE2	11:g:60:TYR:CE2	2.61	0.69
1:A:536:GLU:HG3	1:A:539:ALA:HB3	1.74	0.69
1:C:251:TYR:CE1	2:D:365:ARG:NE	2.61	0.69
3:I:131:LEU:HD23	3:I:131:LEU:C	2.18	0.69
4:J:362:GLN:NE2	3:K:165:LEU:HD22	2.01	0.69
11:g:22:TRP:HD1	11:g:86:TYR:OH	1.75	0.69
11:a:242:THR:HG21	11:a:256:LEU:HD11	1.73	0.69
1:C:318:HIS:ND1	2:D:406:THR:O	2.21	0.69
2:H:319:LEU:N	2:H:319:LEU:HD12	2.07	0.69
4:J:283:LYS:O	3:K:37:SER:HB2	1.92	0.69
3:K:16:ILE:HG23	3:K:31:PHE:CE2	2.28	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:368:SER:HA	1:M:371:THR:HG22	1.73	0.69
1:E:287:LEU:O	1:E:287:LEU:HD23	1.93	0.69
1:E:289:HIS:CD2	1:E:292:LEU:HD12	2.28	0.69
1:A:552:GLN:HG3	11:a:246:PRO:CB	2.22	0.69
1:M:368:SER:HA	1:M:371:THR:CG2	2.23	0.69
11:e:205:LEU:HD22	11:e:232:VAL:HG23	1.75	0.68
1:G:585:LEU:HD21	11:h:343:ARG:CB	2.23	0.68
1:M:549:LEU:N	1:M:549:LEU:HD12	2.08	0.68
1:E:390:ARG:NH2	1:E:394:TYR:OH	2.26	0.68
1:E:536:GLU:HG3	1:E:539:ALA:HB3	1.75	0.68
11:a:205:LEU:HD22	11:a:232:VAL:HG23	1.75	0.68
1:A:312:GLU:OE1	1:A:312:GLU:N	2.21	0.68
11:d:291:LEU:HD22	11:d:339:ARG:HH21	1.58	0.68
1:M:460:TYR:OH	1:M:486:ASN:ND2	2.27	0.68
11:a:125:GLU:OE1	11:a:125:GLU:HA	1.93	0.68
1:C:250:LEU:HD11	1:C:335:VAL:HG13	1.76	0.68
11:h:217:ARG:HH11	11:h:276:LEU:HB2	1.58	0.68
1:C:250:LEU:CD1	1:C:335:VAL:HG13	2.23	0.68
1:A:723:TYR:CE2	11:a:249:MET:HE3	2.29	0.67
1:M:259:ARG:NH1	2:T:284:SER:CB	2.57	0.67
1:G:236:LEU:HD22	1:G:241:GLN:HB3	1.77	0.67
3:I:519:HIS:NE2	11:i:262:PRO:O	2.26	0.67
1:C:460:TYR:OH	1:C:486:ASN:ND2	2.27	0.67
11:i:184:GLN:H	11:i:184:GLN:CD	2.03	0.67
1:A:390:ARG:NH2	1:A:394:TYR:OH	2.26	0.67
1:G:460:TYR:OH	1:G:486:ASN:ND2	2.27	0.67
2:B:401:HIS:HD2	2:B:473:SER:HB3	1.60	0.67
1:G:550:MET:HE3	1:G:670:PHE:CE1	2.30	0.67
1:C:549:LEU:HD12	1:C:549:LEU:N	2.09	0.67
1:E:460:TYR:OH	1:E:486:ASN:ND2	2.28	0.67
1:M:236:LEU:HD22	1:M:241:GLN:HB3	1.77	0.67
11:c:296:ARG:O	11:c:302:ASN:ND2	2.28	0.67
3:K:38:GLU:OE1	3:K:41:VAL:CG1	2.43	0.67
11:d:28:GLU:HG3	11:d:364:SER:HB3	1.77	0.67
1:C:236:LEU:HD22	1:C:241:GLN:HB3	1.77	0.66
11:g:61:ILE:N	11:g:61:ILE:HD12	2.10	0.66
11:i:321:LEU:HB3	11:i:378:MET:HB2	1.75	0.66
4:J:947:VAL:HA	4:J:951:LYS:HB3	1.77	0.66
11:f:28:GLU:HG3	11:f:364:SER:HB3	1.77	0.66
1:A:722:GLN:HB3	11:a:249:MET:SD	2.36	0.66
1:E:554:ASP:OD2	1:E:591:THR:CG2	2.43	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:885:HIS:CB	11:t:353:PRO:CA	2.74	0.66
2:H:595:HIS:HE1	3:I:648:LEU:CD2	2.08	0.66
3:I:114:ASP:OD1	3:I:115:PRO:HD2	1.94	0.66
11:m:290:VAL:CG1	11:m:328:VAL:HG21	2.25	0.66
11:c:214:ALA:HA	11:c:218:LEU:HD12	1.78	0.66
11:l:297:LEU:HD13	11:l:377:MET:HB2	1.78	0.66
1:A:460:TYR:OH	1:A:486:ASN:ND2	2.28	0.66
11:d:291:LEU:HD22	11:d:339:ARG:NH2	2.11	0.66
1:G:581:ALA:HB1	11:h:342:GLU:HG3	1.75	0.66
1:E:311:PHE:O	1:E:432:TYR:CZ	2.49	0.66
11:i:141:ILE:HG12	11:i:171:VAL:O	1.96	0.66
2:D:401:HIS:HD2	2:D:473:SER:HB3	1.60	0.65
11:g:296:ARG:O	11:g:302:ASN:ND2	2.28	0.65
1:E:552:GLN:HE21	1:E:591:THR:HG22	1.61	0.65
11:a:124:ARG:NH2	11:b:301:LYS:HD3	2.12	0.65
2:D:432:ARG:HE	1:E:508:LYS:HZ1	1.43	0.65
1:E:312:GLU:H	1:E:312:GLU:CD	2.04	0.65
2:H:595:HIS:CE1	3:I:648:LEU:CD2	2.80	0.65
11:i:39:GLU:HG2	11:i:40:PHE:H	1.61	0.65
1:C:259:ARG:HH12	2:D:284:SER:HB2	1.59	0.65
1:E:329:LYS:O	1:E:333:ILE:HG13	1.95	0.65
11:b:28:GLU:HG3	11:b:364:SER:HB3	1.77	0.65
11:e:242:THR:HG21	11:e:256:LEU:HD11	1.79	0.65
11:h:295:ARG:HB3	11:h:295:ARG:NH1	2.10	0.65
1:E:298:TYR:O	1:E:302:THR:HG22	1.97	0.65
1:G:585:LEU:HD21	11:h:343:ARG:CG	2.26	0.65
5:L:1805:ASN:HD22	11:l:348:PHE:HB2	1.62	0.65
11:h:238:ALA:HB3	11:h:376:LEU:HD12	1.78	0.65
11:g:214:ALA:HA	11:g:218:LEU:HD12	1.78	0.65
1:G:566:GLU:OE1	1:G:582:LEU:CD1	2.45	0.65
11:m:296:ARG:O	11:m:302:ASN:ND2	2.28	0.65
2:D:675:TYR:HA	2:D:678:THR:HG22	1.79	0.65
11:e:320:ILE:HG23	11:e:379:ALA:HB2	1.78	0.65
1:G:585:LEU:HD21	11:h:343:ARG:HB2	1.76	0.65
1:G:547:TYR:CG	1:G:601:LEU:HD11	2.32	0.65
1:C:259:ARG:HH11	2:D:284:SER:CB	2.05	0.64
2:D:261:ILE:HG21	1:E:283:SER:HA	1.79	0.64
2:F:675:TYR:HA	2:F:678:THR:HG22	1.79	0.64
2:H:401:HIS:HD2	2:H:473:SER:HB3	1.60	0.64
11:m:214:ALA:HA	11:m:218:LEU:HD12	1.78	0.64
1:E:306:GLU:CD	6:Q:36:UNK:HA	2.22	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:137:LEU:HG	11:k:139:HIS:CD2	2.30	0.64
1:A:584:GLU:OE2	11:b:339:ARG:NH1	2.30	0.64
2:H:675:TYR:HA	2:H:678:THR:HG22	1.79	0.64
2:B:885:HIS:NE2	11:b:351:TRP:O	2.28	0.64
4:J:429:ASN:ND2	4:J:489:ALA:O	2.29	0.64
1:M:536:GLU:HG3	1:M:539:ALA:HB3	1.79	0.64
3:I:259:LEU:HB2	3:I:277:LEU:HD22	1.80	0.64
4:J:921:LYS:H	4:J:925:GLN:HE21	1.46	0.64
1:G:673:MET:HE1	1:G:730:MET:SD	2.38	0.64
11:h:28:GLU:HG3	11:h:364:SER:HB3	1.77	0.64
11:l:207:ASN:OD1	13:l:501:GDP:N2	2.30	0.64
1:C:673:MET:HE1	1:C:730:MET:SD	2.38	0.64
1:E:584:GLU:OE2	11:f:339:ARG:NH1	2.31	0.64
2:H:322:GLN:HG2	3:I:165:LEU:HD21	1.79	0.64
3:I:29:GLN:O	3:I:31:PHE:CE1	2.49	0.64
3:I:38:GLU:OE1	3:I:38:GLU:HA	1.96	0.64
4:J:284:LEU:HA	3:K:37:SER:CB	2.28	0.64
11:a:320:ILE:HG23	11:a:379:ALA:HB2	1.78	0.64
2:H:885:HIS:NE2	11:h:351:TRP:O	2.28	0.64
11:c:101:GLY:N	11:c:106:SER:HG	1.94	0.64
1:E:312:GLU:OE1	1:E:312:GLU:N	2.20	0.64
11:l:168:THR:HG23	11:l:202:LEU:HD13	1.79	0.64
1:M:368:SER:C	1:M:371:THR:HG22	2.23	0.64
11:g:101:GLY:N	11:g:106:SER:HG	1.95	0.64
11:i:290:VAL:HG13	11:i:328:VAL:HG21	1.80	0.64
2:D:346:LEU:HD23	2:D:346:LEU:C	2.23	0.63
2:F:387:HIS:CB	2:F:403:TYR:OH	2.46	0.63
1:G:536:GLU:OE1	1:G:536:GLU:N	2.22	0.63
11:m:101:GLY:N	11:m:106:SER:HG	1.96	0.63
1:E:679:VAL:HG21	1:E:780:MET:CE	2.28	0.63
5:L:1635:ASP:O	5:L:1639:HIS:N	2.30	0.63
11:d:275:PRO:HG3	11:d:374:SER:HA	1.80	0.63
1:C:536:GLU:HG3	1:C:539:ALA:HB3	1.79	0.63
3:K:523:LEU:HG	3:K:527:LEU:HD23	1.80	0.63
11:j:201:CYS:SG	11:j:202:LEU:N	2.71	0.63
2:B:257:VAL:O	2:B:298:GLY:HA3	1.99	0.63
11:j:67:LEU:HD13	11:j:149:LEU:HD21	1.81	0.63
2:D:262:ASP:OD1	2:D:262:ASP:N	2.31	0.63
2:F:400:VAL:HG13	2:F:419:LEU:HD13	1.79	0.63
2:H:365:ARG:N	2:H:365:ARG:HD2	2.13	0.63
4:J:688:ARG:HH11	4:J:691:LEU:HD22	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:e:306:SER:OG	11:e:390:ARG:NH1	2.32	0.63
11:h:376:LEU:HD23	11:h:376:LEU:C	2.23	0.63
11:h:323:ILE:HB	11:h:376:LEU:HB3	1.81	0.63
1:A:277:ASP:O	1:A:285:ARG:NH1	2.31	0.63
1:G:550:MET:CB	1:G:556:PHE:CE2	2.82	0.63
11:a:306:SER:OG	11:a:390:ARG:NH1	2.32	0.63
1:C:724:TYR:O	1:C:729:VAL:HG23	1.99	0.62
2:D:305:ARG:HH11	2:D:305:ARG:CG	2.09	0.62
1:G:276:VAL:HG23	1:G:277:ASP:H	1.64	0.62
1:A:312:GLU:H	1:A:312:GLU:CD	2.06	0.62
1:G:555:PHE:CD1	1:G:587:LEU:CD2	2.73	0.62
4:J:723:MET:CE	4:J:821:TYR:CZ	2.82	0.62
5:L:513:CYS:SG	5:L:514:SER:N	2.71	0.62
1:C:244:ALA:O	1:C:247:GLU:CG	2.46	0.62
1:G:720:ASN:OD1	11:g:357:GLN:NE2	2.30	0.62
2:H:319:LEU:HD22	2:H:429:PHE:HZ	1.62	0.62
5:L:1590:VAL:O	5:L:1625:GLN:NE2	2.30	0.62
11:b:275:PRO:HG3	11:b:374:SER:HA	1.80	0.62
11:f:275:PRO:HG3	11:f:374:SER:HA	1.80	0.62
11:i:274:THR:HB	11:i:297:LEU:HD23	1.80	0.62
1:A:723:TYR:CZ	11:a:249:MET:HE3	2.34	0.62
1:C:276:VAL:HG23	1:C:277:ASP:H	1.64	0.62
1:E:502:GLU:O	1:E:515:GLN:NE2	2.32	0.62
1:G:256:VAL:HG23	2:H:289:ASP:HB3	1.80	0.62
4:J:716:LEU:HD11	4:J:812:VAL:CG2	2.29	0.62
2:B:675:TYR:HA	2:B:678:THR:HG22	1.79	0.62
3:K:344:MET:O	3:K:350:LEU:HB2	1.98	0.62
11:a:40:PHE:CB	11:a:366:TYR:CE1	2.83	0.62
11:g:54:GLN:CG	11:g:60:TYR:HE2	2.08	0.62
2:F:885:HIS:NE2	11:f:351:TRP:O	2.28	0.62
3:K:524:VAL:O	3:K:647:ARG:NH1	2.32	0.62
1:E:710:LEU:CD2	1:E:786:PHE:CE1	2.83	0.62
2:H:334:GLU:OE1	2:H:334:GLU:HA	2.00	0.62
2:D:434:ILE:HD11	2:D:483:VAL:HG12	1.82	0.62
5:L:1678:ASN:ND2	5:L:1679:GLN:OE1	2.33	0.62
11:h:274:THR:HG22	11:h:275:PRO:HD3	1.81	0.62
1:A:502:GLU:O	1:A:515:GLN:NE2	2.32	0.62
2:H:434:ILE:HD11	2:H:483:VAL:HG12	1.82	0.62
11:c:229:ASN:ND2	13:c:501:GDP:O6	2.33	0.62
2:B:262:ASP:OD1	2:B:262:ASP:N	2.31	0.61
2:D:261:ILE:CG2	1:E:283:SER:HA	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:LEU:HD23	1:E:287:LEU:C	2.24	0.61
1:G:549:LEU:HD11	1:G:666:TYR:CE1	2.35	0.61
1:G:724:TYR:O	1:G:729:VAL:HG23	2.00	0.61
3:K:648:LEU:HD13	3:K:653:TYR:HB2	1.82	0.61
1:M:720:ASN:OD1	11:m:357:GLN:NE2	2.30	0.61
11:k:315:HIS:O	11:k:347:ASN:ND2	2.33	0.61
1:G:549:LEU:HD11	1:G:666:TYR:HE1	1.65	0.61
1:M:368:SER:O	1:M:371:THR:CG2	2.49	0.61
11:l:3:ARG:HB3	11:l:133:GLU:HB2	1.82	0.61
1:G:543:SER:OG	1:G:597:PHE:HB2	2.00	0.61
2:H:315:ARG:HH21	2:H:315:ARG:CG	2.10	0.61
3:I:136:VAL:HG13	3:I:136:VAL:O	2.01	0.61
1:M:276:VAL:HG23	1:M:277:ASP:H	1.64	0.61
11:i:141:ILE:HD11	11:i:172:PHE:CD1	2.35	0.61
1:A:682:GLN:HE22	1:A:784:VAL:HG23	1.64	0.61
3:I:35:HIS:ND1	3:I:36:PRO:CD	2.41	0.61
2:B:434:ILE:HD11	2:B:483:VAL:HG12	1.82	0.61
11:a:25:LEU:HD11	11:a:244:ARG:CD	2.30	0.61
4:J:566:MET:HE3	4:J:570:LYS:HE2	1.82	0.61
2:D:432:ARG:NE	1:E:508:LYS:HZ1	1.99	0.61
2:F:262:ASP:N	2:F:262:ASP:OD1	2.31	0.61
1:G:462:ILE:HG12	1:G:479:LEU:HD22	1.82	0.61
3:I:166:PRO:N	3:I:167:PRO:HD2	2.16	0.61
1:C:350:GLN:O	1:C:350:GLN:NE2	2.34	0.61
3:K:498:GLN:HB3	3:K:515:ARG:HE	1.65	0.61
1:M:368:SER:CA	1:M:371:THR:HG22	2.31	0.61
1:C:249:LEU:HD23	1:C:352:LEU:HD23	1.81	0.61
2:H:262:ASP:N	2:H:262:ASP:OD1	2.31	0.61
11:i:186:TYR:CE1	11:i:398:LEU:HD13	2.36	0.61
11:j:264:PRO:O	11:j:267:HIS:ND1	2.33	0.61
11:l:146:GLY:O	11:l:150:GLY:N	2.33	0.61
11:l:425:ARG:NH1	11:l:429:GLN:OE1	2.34	0.61
5:L:1545:LEU:HD11	5:L:1580:PRO:HD2	1.83	0.61
1:A:304:PHE:CE1	1:A:308:LYS:HG3	2.36	0.60
1:G:350:GLN:NE2	1:G:350:GLN:O	2.34	0.60
11:b:225:PHE:O	11:b:229:ASN:ND2	2.35	0.60
11:j:4:GLU:HA	11:j:50:VAL:HG13	1.83	0.60
1:A:679:VAL:HG21	1:A:780:MET:CE	2.31	0.60
2:F:434:ILE:HD11	2:F:483:VAL:HG12	1.82	0.60
11:h:238:ALA:CB	11:h:376:LEU:HD12	2.31	0.60
1:E:311:PHE:HE2	2:F:406:THR:HB	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:285:PHE:O	4:J:297:ARG:NH2	2.32	0.60
11:k:224:SER:N	11:k:227:GLN:OE1	2.34	0.60
1:C:310:SER:O	1:C:318:HIS:NE2	2.35	0.60
3:I:629:LEU:HD12	3:I:644:LEU:HD13	1.83	0.60
5:L:532:TYR:HA	5:L:535:PHE:HD2	1.65	0.60
1:M:502:GLU:O	1:M:515:GLN:NE2	2.35	0.60
11:h:225:PHE:O	11:h:229:ASN:ND2	2.35	0.60
4:J:723:MET:HE2	4:J:821:TYR:CZ	2.37	0.60
1:M:350:GLN:O	1:M:350:GLN:NE2	2.34	0.60
1:C:339:GLU:OE2	2:D:365:ARG:HG2	2.00	0.60
1:C:462:ILE:HG12	1:C:479:LEU:HD22	1.82	0.60
11:i:241:THR:OG1	11:i:325:GLN:NE2	2.34	0.60
11:j:193:LYS:HD3	11:j:194:ARG:HD2	1.83	0.60
1:C:252:VAL:HG21	1:C:261:VAL:CG1	2.32	0.60
2:F:293:ARG:O	2:F:293:ARG:HG2	2.00	0.60
1:M:462:ILE:HG12	1:M:479:LEU:HD22	1.82	0.60
11:h:29:HIS:ND1	11:h:46:ASP:OD2	2.35	0.60
4:J:830:GLN:HE22	4:J:955:MET:HE1	1.67	0.60
11:f:225:PHE:O	11:f:229:ASN:ND2	2.35	0.60
1:G:642:GLU:O	1:G:671:ARG:NH1	2.35	0.59
2:H:365:ARG:CD	2:H:365:ARG:H	2.15	0.59
3:K:599:ASN:ND2	3:K:601:GLY:O	2.34	0.59
11:d:225:PHE:O	11:d:229:ASN:ND2	2.35	0.59
2:B:330:GLN:OE1	2:B:333:ARG:NH1	2.35	0.59
1:C:720:ASN:OD1	11:c:357:GLN:NE2	2.30	0.59
2:D:573:PHE:HB2	2:D:608:THR:HG21	1.85	0.59
4:J:278:LEU:CB	4:J:379:LEU:HD23	2.31	0.59
1:A:311:PHE:O	1:A:313:TYR:N	2.32	0.59
1:A:468:PRO:HG2	1:A:471:LEU:HD12	1.84	0.59
2:B:290:THR:O	2:B:294:LEU:HG	2.02	0.59
1:E:281:ASP:HB2	1:E:284:ILE:HB	1.83	0.59
1:G:502:GLU:O	1:G:515:GLN:NE2	2.35	0.59
1:C:548:PHE:CD2	1:C:666:TYR:HB3	2.37	0.59
11:k:137:LEU:HB3	11:k:168:THR:HG22	1.83	0.59
2:F:330:GLN:OE1	2:F:333:ARG:NH1	2.35	0.59
1:G:333:ILE:HG12	2:H:369:VAL:HG23	1.85	0.59
5:L:1670:LYS:O	11:l:357:GLN:NE2	2.34	0.59
1:A:848:ALA:HA	1:A:851:ASN:HD21	1.68	0.59
1:G:312:GLU:OE1	1:G:312:GLU:N	2.34	0.59
11:a:40:PHE:CB	11:a:366:TYR:CD1	2.86	0.59
11:e:245:TYR:CZ	11:e:362:ARG:O	2.55	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:39:GLU:HG2	11:k:40:PHE:H	1.65	0.59
6:S:34:UNK:CB	2:T:296:GLU:CB	2.80	0.59
11:i:201:CYS:SG	11:i:202:LEU:N	2.75	0.59
2:H:620:ARG:HH11	2:H:644:VAL:HA	1.68	0.59
3:I:397:GLN:HE22	3:I:411:LEU:HG	1.66	0.59
1:M:264:GLN:HE21	1:M:275:LEU:HB3	1.67	0.59
11:e:40:PHE:CD2	11:e:366:TYR:HD1	2.18	0.59
11:i:306:SER:OG	11:i:390:ARG:NH1	2.34	0.59
2:B:620:ARG:HH11	2:B:644:VAL:HA	1.68	0.59
1:C:339:GLU:OE2	2:D:365:ARG:HB2	2.03	0.59
1:E:723:TYR:CZ	11:e:249:MET:CE	2.85	0.59
1:E:848:ALA:HA	1:E:851:ASN:HD21	1.68	0.59
5:L:445:ALA:O	5:L:449:SER:OG	2.20	0.59
1:E:320:LEU:HD12	1:E:320:LEU:O	2.02	0.59
2:F:451:ASP:HB3	2:F:463:LYS:HA	1.85	0.59
1:G:264:GLN:HE21	1:G:275:LEU:HB3	1.67	0.59
3:K:587:ASP:HA	3:K:590:HIS:HD2	1.67	0.59
5:L:427:LEU:HD23	5:L:535:PHE:HZ	1.67	0.59
11:d:296:ARG:O	11:d:302:ASN:ND2	2.36	0.59
2:B:673:MET:HE1	2:B:783:ILE:HD11	1.85	0.58
1:C:264:GLN:HE21	1:C:275:LEU:HB3	1.67	0.58
2:D:603:THR:HG21	11:e:343:ARG:NH1	2.18	0.58
2:D:673:MET:HE1	2:D:783:ILE:HD11	1.85	0.58
2:D:885:HIS:NE2	11:d:351:TRP:O	2.28	0.58
1:G:256:VAL:CG2	2:H:289:ASP:HB3	2.33	0.58
4:J:358:PHE:HD2	4:J:361:TYR:H	1.51	0.58
11:d:29:HIS:ND1	11:d:46:ASP:OD2	2.35	0.58
11:l:270:MET:HE2	11:l:305:VAL:HG21	1.85	0.58
2:D:424:HIS:N	2:D:425:PRO:HD2	2.18	0.58
2:D:620:ARG:HH11	2:D:644:VAL:HA	1.68	0.58
1:E:555:PHE:CE1	1:E:583:LEU:HD12	2.38	0.58
2:F:620:ARG:HH11	2:F:644:VAL:HA	1.68	0.58
3:K:269:PRO:HD3	3:K:322:LEU:HD21	1.85	0.58
11:d:171:VAL:HG11	13:d:501:GDP:HN22	1.68	0.58
5:L:427:LEU:HB3	5:L:551:GLU:OE1	2.04	0.58
11:h:336:SER:HA	11:h:339:ARG:NE	2.11	0.58
1:M:259:ARG:HH12	2:T:284:SER:CB	2.16	0.58
11:i:141:ILE:CD1	11:i:172:PHE:CE1	2.80	0.58
11:k:275:PRO:HG3	11:k:374:SER:HA	1.84	0.58
2:D:330:GLN:OE1	2:D:333:ARG:NH1	2.35	0.58
3:I:201:GLU:HG2	3:I:260:ARG:HH22	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:922:ASP:HB3	4:J:925:GLN:HG2	1.86	0.58
11:b:296:ARG:O	11:b:302:ASN:ND2	2.36	0.58
11:f:29:HIS:ND1	11:f:46:ASP:OD2	2.35	0.58
11:f:296:ARG:O	11:f:302:ASN:ND2	2.36	0.58
2:D:255:LEU:CD1	2:D:346:LEU:HD12	2.34	0.58
1:G:847:GLU:O	1:G:851:ASN:ND2	2.37	0.58
1:M:315:GLN:HA	1:M:318:HIS:ND1	2.18	0.58
1:M:550:MET:HE1	1:M:677:LYS:HG2	1.85	0.58
11:b:29:HIS:ND1	11:b:46:ASP:OD2	2.35	0.58
1:C:339:GLU:CD	2:D:365:ARG:CG	2.76	0.58
2:H:564:ARG:NH2	2:H:565:TYR:OH	2.37	0.58
1:C:590:SER:C	1:C:592:ALA:H	2.12	0.58
1:C:847:GLU:O	1:C:851:ASN:ND2	2.37	0.58
1:E:723:TYR:CG	11:e:249:MET:CE	2.69	0.58
2:H:365:ARG:HD2	2:H:365:ARG:H	1.68	0.58
3:I:108:GLU:O	3:I:112:LEU:HD23	2.04	0.58
1:M:847:GLU:O	1:M:851:ASN:ND2	2.37	0.58
11:k:141:ILE:HG22	11:k:191:THR:HG21	1.85	0.58
2:F:378:LEU:HD22	2:F:378:LEU:N	2.19	0.58
1:G:544:ILE:HD11	1:G:658:ILE:CD1	2.34	0.58
2:H:451:ASP:HB3	2:H:463:LYS:HA	1.84	0.58
1:M:890:ASN:ND2	11:m:354:ALA:O	2.37	0.58
2:B:387:HIS:CD2	2:B:403:TYR:CE1	2.91	0.58
1:C:355:TYR:CE1	8:Y:56:UNK:O	2.56	0.58
1:C:578:ARG:CD	11:d:342:GLU:OE1	2.52	0.58
1:E:468:PRO:HG2	1:E:471:LEU:HD12	1.84	0.58
1:E:551:ASP:HA	11:e:248:TYR:CE1	2.38	0.58
2:H:673:MET:HE1	2:H:783:ILE:HD11	1.85	0.58
11:e:245:TYR:OH	11:e:364:SER:N	2.36	0.58
11:j:436:HIS:O	11:j:440:ARG:NH2	2.36	0.58
2:F:673:MET:HE1	2:F:783:ILE:HD11	1.85	0.57
1:G:540:HIS:HE1	1:G:650:VAL:HG12	1.68	0.57
11:i:186:TYR:OH	11:i:398:LEU:HB3	2.04	0.57
11:k:270:MET:HE3	11:k:271:THR:H	1.69	0.57
2:D:261:ILE:HG23	1:E:286:GLU:CD	2.29	0.57
1:G:554:ASP:HB3	1:G:591:THR:HG22	1.86	0.57
11:g:54:GLN:HA	11:g:60:TYR:CD2	2.39	0.57
11:e:113:LYS:HB2	11:e:113:LYS:NZ	2.18	0.57
11:l:139:HIS:HE1	11:l:141:ILE:HG22	1.69	0.57
11:m:329:ASP:OD1	11:m:330:PRO:CD	2.53	0.57
2:B:451:ASP:HB3	2:B:463:LYS:HA	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:f:171:VAL:HG11	13:f:501:GDP:HN22	1.69	0.57
1:C:642:GLU:O	1:C:671:ARG:NH1	2.35	0.57
11:g:229:ASN:ND2	13:g:501:GDP:O6	2.33	0.57
11:h:335:LYS:O	11:h:339:ARG:HD3	2.05	0.57
2:B:564:ARG:NH2	2:B:565:TYR:OH	2.37	0.57
1:G:423:ILE:HG23	1:G:481:THR:HG21	1.87	0.57
4:J:278:LEU:HB3	4:J:379:LEU:HD23	1.87	0.57
5:L:608:CYS:SG	5:L:1498:TYR:OH	2.58	0.57
1:M:423:ILE:HG23	1:M:481:THR:HG21	1.87	0.57
11:l:132:LEU:O	11:l:164:LYS:NZ	2.36	0.57
3:K:12:TYR:OH	5:L:399:GLU:OE1	2.20	0.57
3:K:331:ARG:O	3:K:335:THR:OG1	2.21	0.57
1:M:642:GLU:O	1:M:671:ARG:NH1	2.35	0.57
11:l:28:GLU:OE1	11:l:244:ARG:NH1	2.36	0.57
1:G:890:ASN:ND2	11:g:354:ALA:O	2.37	0.57
3:I:552:ASP:OD1	3:I:553:PHE:N	2.38	0.57
3:K:532:GLN:HA	3:K:535:VAL:HG12	1.86	0.57
11:l:264:PRO:O	11:l:267:HIS:ND1	2.37	0.57
4:J:562:ALA:HB2	4:J:699:TYR:HD1	1.68	0.57
4:J:716:LEU:HB2	4:J:809:VAL:HG22	1.87	0.57
11:a:195:LEU:HD13	11:a:202:LEU:HD11	1.87	0.57
11:h:274:THR:HG23	11:h:275:PRO:CD	2.34	0.57
3:I:33:PHE:CD1	3:I:33:PHE:N	2.73	0.56
11:c:329:ASP:OD1	11:c:330:PRO:CD	2.52	0.56
11:m:229:ASN:ND2	13:m:501:GDP:O6	2.33	0.56
1:A:603:ILE:HD12	1:A:644:PHE:HE1	1.70	0.56
2:D:564:ARG:NH2	2:D:565:TYR:OH	2.37	0.56
1:G:310:SER:O	1:G:318:HIS:NE2	2.35	0.56
2:D:319:LEU:HD12	2:D:319:LEU:N	2.19	0.56
1:G:339:GLU:HG2	2:H:365:ARG:HG2	1.87	0.56
2:H:606:ARG:HB3	11:i:339:ARG:NH1	2.19	0.56
3:I:23:SER:OG	3:I:26:GLN:NE2	2.39	0.56
3:I:165:LEU:HD23	3:I:165:LEU:H	1.69	0.56
11:h:201:CYS:SG	11:h:202:LEU:N	2.78	0.56
11:h:298:LEU:N	11:h:298:LEU:HD23	2.20	0.56
3:I:111:PHE:CZ	3:I:122:VAL:HG23	2.23	0.56
11:b:39:GLU:HG2	11:b:40:PHE:H	1.71	0.56
11:g:23:LYS:HG3	11:g:82:TYR:OH	2.05	0.56
2:F:564:ARG:NH2	2:F:565:TYR:OH	2.37	0.56
1:G:669:LEU:HD13	1:G:730:MET:HE2	1.86	0.56
11:d:201:CYS:SG	11:d:202:LEU:N	2.78	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:319:LEU:HD23	1:E:395:THR:HG21	1.88	0.56
3:K:368:LEU:HD21	3:K:396:PHE:HE1	1.71	0.56
11:j:125:GLU:O	11:j:129:SER:N	2.37	0.56
11:k:321:LEU:HD12	11:k:357:GLN:HB2	1.87	0.56
1:C:327:LEU:HD12	1:C:366:LEU:HD11	1.87	0.56
5:L:1547:PRO:O	5:L:1551:ASN:HB3	2.05	0.56
11:b:201:CYS:SG	11:b:202:LEU:N	2.78	0.56
1:A:311:PHE:C	1:A:313:TYR:H	2.14	0.56
1:A:710:LEU:CD2	1:A:786:PHE:CE1	2.87	0.56
1:C:669:LEU:HD13	1:C:730:MET:HE2	1.88	0.56
3:I:480:TYR:O	3:I:483:SER:OG	2.20	0.56
4:J:370:LYS:O	4:J:373:ILE:CG2	2.54	0.56
1:M:585:LEU:HD22	11:t:339:ARG:CB	2.35	0.56
11:c:306:SER:OG	11:c:390:ARG:NH1	2.39	0.56
1:G:537:LEU:HD21	1:G:657:ILE:HG21	1.88	0.56
2:H:805:GLN:HA	2:H:808:GLU:HG2	1.88	0.56
11:j:46:ASP:O	11:j:48:LYS:NZ	2.38	0.56
1:A:311:PHE:HE1	2:B:406:THR:HB	1.71	0.56
2:D:338:LEU:HG	2:D:342:LEU:HD22	1.88	0.56
11:e:275:PRO:HG3	11:e:374:SER:HA	1.88	0.56
11:h:39:GLU:HG2	11:h:40:PHE:H	1.71	0.56
11:m:6:ILE:HG22	11:m:132:LEU:HD11	1.88	0.56
11:m:73:VAL:O	11:m:76:SER:OG	2.20	0.56
2:D:307:TYR:CE2	2:D:324:PHE:HE2	2.24	0.55
11:e:195:LEU:HD13	11:e:202:LEU:HD11	1.87	0.55
11:j:132:LEU:O	11:j:164:LYS:NZ	2.33	0.55
11:m:306:SER:OG	11:m:390:ARG:NH1	2.39	0.55
2:B:805:GLN:HA	2:B:808:GLU:HG2	1.88	0.55
11:c:6:ILE:HG22	11:c:132:LEU:HD11	1.88	0.55
11:d:39:GLU:HG2	11:d:40:PHE:H	1.70	0.55
11:e:156:ARG:HH11	11:e:156:ARG:CG	2.13	0.55
11:f:201:CYS:SG	11:f:202:LEU:N	2.78	0.55
11:g:306:SER:OG	11:g:390:ARG:NH1	2.39	0.55
1:M:320:LEU:HD13	1:M:387:LEU:HD11	1.89	0.55
11:i:172:PHE:O	11:i:207:ASN:ND2	2.40	0.55
11:i:214:ALA:O	11:i:219:HIS:N	2.38	0.55
11:j:141:ILE:HA	11:j:147:SER:HB3	1.86	0.55
1:A:723:TYR:CE2	11:a:249:MET:CE	2.88	0.55
1:E:603:ILE:HD12	1:E:644:PHE:HE1	1.70	0.55
2:F:805:GLN:HA	2:F:808:GLU:HG2	1.88	0.55
1:G:549:LEU:N	1:G:549:LEU:HD12	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:327:LEU:HD12	1:M:366:LEU:HD11	1.87	0.55
11:d:274:THR:HG23	11:d:275:PRO:HD3	1.88	0.55
11:h:293:VAL:HG11	11:h:324:ILE:HD12	1.88	0.55
1:A:552:GLN:NE2	1:A:591:THR:CG2	2.69	0.55
1:G:320:LEU:HD13	1:G:387:LEU:HD11	1.89	0.55
2:H:367:LEU:O	2:H:371:THR:HG22	2.07	0.55
1:M:298:TYR:HE1	1:M:328:VAL:HG13	1.72	0.55
11:f:39:GLU:HG2	11:f:40:PHE:H	1.71	0.55
11:l:252:ASP:N	11:l:252:ASP:OD1	2.38	0.55
2:D:451:ASP:HB3	2:D:463:LYS:HA	1.88	0.55
1:E:333:ILE:HG22	1:E:337:GLN:NE2	2.22	0.55
4:J:438:ASN:HB2	4:J:549:VAL:HG12	1.88	0.55
11:a:275:PRO:HG3	11:a:374:SER:HA	1.88	0.55
2:D:689:LYS:NZ	11:d:198:ASN:O	2.40	0.55
11:g:374:SER:OG	11:g:375:GLY:N	2.40	0.55
11:i:39:GLU:HG2	11:i:40:PHE:N	2.21	0.55
11:j:289:THR:N	11:j:292:ASP:OD2	2.35	0.55
11:l:206:ASP:OD2	11:l:306:SER:N	2.39	0.55
1:E:289:HIS:HA	1:E:292:LEU:HD12	1.89	0.55
5:L:1602:TRP:HB3	5:L:1603:PRO:HD3	1.89	0.55
1:E:555:PHE:HZ	1:E:583:LEU:HD12	1.64	0.55
1:E:716:ASN:O	1:E:720:ASN:ND2	2.40	0.55
1:E:890:ASN:HD21	11:e:354:ALA:HB3	1.72	0.55
2:H:575:ARG:NH2	11:h:252:ASP:OD2	2.40	0.55
3:I:166:PRO:CD	3:I:167:PRO:HD2	2.36	0.55
11:e:250:ASN:HB3	11:e:256:LEU:CD1	2.37	0.55
11:j:334:HIS:CE1	11:j:335:LYS:HG3	2.43	0.55
11:m:374:SER:OG	11:m:375:GLY:N	2.40	0.55
1:G:468:PRO:HG2	1:G:471:LEU:HD12	1.90	0.54
4:J:367:ALA:HB2	4:J:467:GLU:HB2	1.89	0.54
1:M:375:LYS:HD2	9:W:203:UNK:HA	1.87	0.54
11:f:274:THR:HG23	11:f:275:PRO:HD3	1.88	0.54
11:g:132:LEU:HD21	11:g:135:PHE:CE1	2.43	0.54
11:k:39:GLU:HG2	11:k:40:PHE:N	2.22	0.54
1:A:716:ASN:O	1:A:720:ASN:ND2	2.40	0.54
1:C:890:ASN:ND2	11:c:354:ALA:O	2.37	0.54
11:b:274:THR:HG23	11:b:275:PRO:HD3	1.88	0.54
11:b:374:SER:OG	11:b:375:GLY:N	2.40	0.54
11:e:130:ASP:OD1	11:f:343:ARG:NH1	2.40	0.54
11:g:170:SER:HB2	11:g:202:LEU:HD21	1.90	0.54
11:i:355:SER:OG	11:i:356:ILE:N	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:m:170:SER:HB2	11:m:202:LEU:HD21	1.90	0.54
2:B:689:LYS:NZ	11:b:198:ASN:O	2.40	0.54
1:C:298:TYR:HE1	1:C:328:VAL:HG13	1.72	0.54
4:J:262:ARG:HA	4:J:299:ASN:HB3	1.88	0.54
4:J:487:ASP:OD1	4:J:488:GLY:N	2.40	0.54
4:J:754:ASN:OD1	4:J:757:PHE:N	2.31	0.54
1:M:368:SER:O	1:M:371:THR:HG23	2.08	0.54
11:b:171:VAL:HG11	13:b:501:GDP:HN22	1.72	0.54
11:g:47:ARG:HE	11:g:50:VAL:HG23	1.72	0.54
11:i:322:ASN:N	11:i:357:GLN:O	2.40	0.54
11:k:123:ASP:OD1	11:k:161:TYR:OH	2.24	0.54
11:k:231:LEU:O	11:k:234:THR:OG1	2.23	0.54
2:D:432:ARG:NE	1:E:508:LYS:HZ2	2.00	0.54
2:D:484:LEU:HD23	2:D:484:LEU:C	2.32	0.54
2:D:603:THR:HG21	11:e:343:ARG:HH11	1.72	0.54
2:F:689:LYS:NZ	11:f:198:ASN:O	2.40	0.54
2:F:799:GLU:OE2	2:F:803:ARG:NH1	2.35	0.54
1:G:298:TYR:HE1	1:G:328:VAL:HG13	1.72	0.54
1:G:327:LEU:HD12	1:G:366:LEU:HD11	1.87	0.54
1:M:537:LEU:O	1:M:541:LEU:HG	2.07	0.54
1:A:890:ASN:HD21	11:a:354:ALA:HB3	1.72	0.54
1:C:468:PRO:HG2	1:C:471:LEU:HD12	1.90	0.54
2:F:387:HIS:CD2	2:F:403:TYR:HE1	2.26	0.54
4:J:946:LYS:HA	4:J:949:PHE:HD2	1.72	0.54
3:K:492:GLN:HE22	11:k:255:GLY:HA2	1.73	0.54
11:c:170:SER:HB2	11:c:202:LEU:HD21	1.90	0.54
11:e:247:GLY:O	11:e:251:ASN:ND2	2.40	0.54
4:J:684:GLU:H	4:J:687:LEU:HB3	1.72	0.54
3:K:552:ASP:OD1	3:K:553:PHE:N	2.40	0.54
1:M:673:MET:CE	1:M:730:MET:HE1	2.38	0.54
11:c:374:SER:OG	11:c:375:GLY:N	2.40	0.54
2:B:572:ASP:HB2	11:b:246:PRO:HB3	1.90	0.54
3:I:618:PHE:O	3:I:622:SER:N	2.40	0.54
4:J:364:PHE:HA	4:J:468:THR:HG22	1.89	0.54
11:j:39:GLU:HG2	11:j:40:PHE:H	1.72	0.54
11:k:263:THR:HG23	11:k:266:LEU:H	1.73	0.54
3:I:588:LEU:HD21	3:I:618:PHE:HB2	1.89	0.54
4:J:324:VAL:HG23	4:J:372:PHE:HE2	1.73	0.54
1:C:581:ALA:HB1	11:d:339:ARG:HG3	1.90	0.54
2:H:484:LEU:HD23	2:H:484:LEU:C	2.33	0.54
4:J:278:LEU:CB	4:J:379:LEU:CD2	2.85	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:374:SER:OG	11:d:375:GLY:N	2.40	0.54
2:D:805:GLN:HA	2:D:808:GLU:HG2	1.88	0.54
3:I:51:ASP:O	3:I:55:PHE:HD2	1.92	0.54
3:I:150:GLY:HA2	3:I:202:GLU:OE1	2.08	0.54
5:L:1671:VAL:HA	11:l:357:GLN:HE22	1.73	0.54
11:a:130:ASP:OD1	11:b:343:ARG:NH1	2.40	0.54
11:e:327:GLU:OE1	11:e:327:GLU:N	2.41	0.54
11:k:20:GLU:HA	11:k:23:LYS:HG2	1.89	0.54
3:I:380:LEU:HD23	3:I:449:TRP:CD2	2.43	0.53
3:I:473:LYS:HB2	3:I:564:LEU:HD21	1.90	0.53
1:M:468:PRO:HG2	1:M:471:LEU:HD12	1.90	0.53
10:X:1317:UNK:HA	10:X:1401:UNK:CB	2.37	0.53
11:a:327:GLU:OE1	11:a:327:GLU:N	2.41	0.53
11:e:5:ILE:CD1	11:e:253:LEU:HD22	2.38	0.53
11:g:6:ILE:HG21	11:g:135:PHE:CE2	2.43	0.53
11:k:172:PHE:HE1	11:k:204:VAL:HG23	1.59	0.53
1:C:320:LEU:HD13	1:C:387:LEU:HD11	1.89	0.53
2:F:546:LEU:HD11	2:F:742:GLN:HA	1.91	0.53
1:G:256:VAL:CG2	2:H:289:ASP:CB	2.86	0.53
3:I:302:ASN:OD1	3:I:303:GLN:NE2	2.41	0.53
11:a:115:HIS:ND1	11:a:119:PHE:CD2	2.76	0.53
11:g:23:LYS:HG3	11:g:82:TYR:CZ	2.44	0.53
11:g:290:VAL:HG13	11:g:328:VAL:HG21	1.88	0.53
1:A:722:GLN:CB	11:a:249:MET:SD	2.96	0.53
2:F:484:LEU:HD23	2:F:484:LEU:C	2.33	0.53
3:K:498:GLN:HE21	3:K:515:ARG:HG3	1.73	0.53
11:h:171:VAL:HG11	13:h:501:GDP:HN22	1.73	0.53
1:A:373:VAL:HG22	1:A:386:LEU:HD23	1.91	0.53
2:B:799:GLU:OE2	2:B:803:ARG:NH1	2.35	0.53
1:C:339:GLU:OE2	2:D:365:ARG:CG	2.56	0.53
1:E:550:MET:HE3	1:E:556:PHE:CE1	2.43	0.53
2:H:689:LYS:NZ	11:h:198:ASN:O	2.40	0.53
11:a:374:SER:OG	11:a:375:GLY:N	2.41	0.53
11:f:374:SER:OG	11:f:375:GLY:N	2.40	0.53
2:B:484:LEU:HD23	2:B:484:LEU:C	2.32	0.53
2:D:546:LEU:HD11	2:D:742:GLN:HA	1.91	0.53
1:E:373:VAL:HG22	1:E:386:LEU:HD23	1.91	0.53
2:F:572:ASP:HB2	11:f:246:PRO:HB3	1.90	0.53
2:H:319:LEU:N	2:H:445:GLU:OE2	2.40	0.53
4:J:922:ASP:OD1	4:J:923:LEU:N	2.41	0.53
5:L:1500:PHE:HE1	5:L:1505:LEU:HD23	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:201:CYS:SG	11:a:202:LEU:N	2.81	0.53
11:c:4:GLU:OE1	11:c:63:ARG:NE	2.42	0.53
11:g:54:GLN:NE2	11:g:60:TYR:HE2	2.05	0.53
3:K:409:ASN:O	3:K:410:LEU:HG	2.08	0.53
11:a:252:ASP:N	11:a:252:ASP:OD1	2.42	0.53
11:e:201:CYS:SG	11:e:202:LEU:N	2.81	0.53
11:l:229:ASN:ND2	13:l:501:GDP:O6	2.37	0.53
2:B:546:LEU:HD11	2:B:742:GLN:HA	1.91	0.53
1:E:311:PHE:CE2	2:F:406:THR:HB	2.44	0.53
1:G:342:HIS:C	1:G:344:GLN:H	2.16	0.53
3:I:107:LEU:HD21	3:I:125:PHE:CD2	2.44	0.53
3:I:578:VAL:HG22	3:I:582:LEU:HD23	1.90	0.53
11:l:214:ALA:HA	11:l:218:LEU:HD13	1.90	0.53
1:E:554:ASP:OD2	1:E:591:THR:HG22	2.08	0.53
1:E:682:GLN:HE22	1:E:784:VAL:HG23	1.74	0.53
2:F:251:VAL:HG12	2:F:346:LEU:HD12	1.91	0.53
3:I:409:ASN:O	3:I:410:LEU:HG	2.09	0.53
5:L:1547:PRO:HB3	8:V:3:UNK:CB	2.39	0.53
11:e:124:ARG:HH22	11:f:301:LYS:HD3	1.74	0.53
11:m:4:GLU:OE1	11:m:63:ARG:NE	2.42	0.53
3:K:16:ILE:HG23	3:K:31:PHE:CZ	2.43	0.53
3:K:35:HIS:HB3	3:K:38:GLU:HB2	1.89	0.53
11:a:115:HIS:HD1	11:a:119:PHE:HE2	1.56	0.53
11:g:54:GLN:CD	11:g:60:TYR:HE2	2.17	0.53
11:i:296:ARG:O	11:i:302:ASN:ND2	2.42	0.53
2:F:297:LEU:HD22	2:F:297:LEU:N	2.24	0.53
4:J:283:LYS:O	3:K:37:SER:CB	2.57	0.53
11:a:5:ILE:CD1	11:a:253:LEU:HD22	2.39	0.53
11:c:195:LEU:HD13	11:c:202:LEU:HD11	1.91	0.53
11:d:355:SER:OG	11:d:356:ILE:N	2.42	0.53
11:i:321:LEU:HA	11:i:357:GLN:HB2	1.90	0.53
11:j:114:ILE:HB	11:j:117:ASP:HB3	1.90	0.53
2:D:799:GLU:OE2	2:D:803:ARG:NH1	2.35	0.52
1:E:277:ASP:HB3	1:E:280:LEU:HB2	1.91	0.52
11:l:395:TYR:OH	11:l:399:ARG:NH1	2.41	0.52
1:G:247:GLU:O	1:G:251:TYR:HD2	1.87	0.52
10:X:1317:UNK:CA	10:X:1401:UNK:CB	2.87	0.52
11:a:250:ASN:HB3	11:a:256:LEU:CD1	2.39	0.52
11:d:291:LEU:HB2	11:d:339:ARG:NH2	2.24	0.52
11:e:374:SER:OG	11:e:375:GLY:N	2.41	0.52
1:E:723:TYR:CD2	11:e:249:MET:CE	2.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:337:ARG:HB2	3:I:124:TYR:CE1	2.44	0.52
4:J:951:LYS:HE2	4:J:955:MET:HG2	1.90	0.52
11:g:73:VAL:O	11:g:76:SER:OG	2.20	0.52
11:k:141:ILE:HD13	11:k:141:ILE:H	1.75	0.52
2:H:546:LEU:HD11	2:H:742:GLN:HA	1.91	0.52
3:I:531:LEU:HD22	3:I:643:GLN:HB2	1.92	0.52
4:J:335:MET:SD	3:K:131:LEU:HD22	2.49	0.52
1:M:731:GLU:HA	1:M:731:GLU:OE2	2.08	0.52
11:d:291:LEU:HB2	11:d:339:ARG:HH21	1.74	0.52
11:e:340:ILE:HD13	11:e:345:LEU:HD13	1.92	0.52
1:E:311:PHE:HA	1:E:318:HIS:CE1	2.45	0.52
2:H:319:LEU:N	2:H:319:LEU:CD1	2.73	0.52
3:I:131:LEU:HG	3:I:131:LEU:O	2.09	0.52
11:g:52:PHE:CE2	11:g:62:PRO:HG3	2.43	0.52
11:g:195:LEU:HD13	11:g:202:LEU:HD11	1.91	0.52
11:h:355:SER:OG	11:h:356:ILE:N	2.42	0.52
11:j:341:ARG:HA	11:j:341:ARG:NH1	2.25	0.52
11:l:193:LYS:HD3	11:l:194:ARG:HD2	1.92	0.52
11:l:355:SER:OG	11:l:356:ILE:N	2.42	0.52
2:F:304:ILE:HG12	2:F:304:ILE:O	2.09	0.52
2:H:572:ASP:HB2	11:h:246:PRO:HB3	1.90	0.52
3:I:191:MET:HE3	3:I:279:VAL:HG21	1.92	0.52
11:e:363:LYS:NZ	11:e:372:ARG:HB3	2.25	0.52
11:i:4:GLU:OE1	11:i:63:ARG:NE	2.43	0.52
11:k:17:ILE:HD11	11:k:138:CYS:HB3	1.92	0.52
2:B:384:LEU:HD11	2:B:400:VAL:HG23	1.92	0.52
2:B:575:ARG:NH2	11:b:252:ASP:OD2	2.40	0.52
1:C:583:LEU:CD2	1:C:603:ILE:CD1	2.70	0.52
2:D:365:ARG:HD2	2:D:365:ARG:N	2.25	0.52
2:D:572:ASP:HB2	11:d:246:PRO:HB3	1.90	0.52
2:H:384:LEU:HD11	2:H:400:VAL:HG23	1.92	0.52
3:I:551:ARG:HA	3:I:551:ARG:HH11	1.73	0.52
4:J:716:LEU:HD23	4:J:716:LEU:O	2.10	0.52
2:T:885:HIS:CB	11:t:353:PRO:CB	2.87	0.52
11:i:52:PHE:O	11:i:63:ARG:NH2	2.43	0.52
1:A:552:GLN:HE22	1:A:591:THR:HG23	1.75	0.52
1:E:724:TYR:O	1:E:728:GLU:HB3	2.10	0.52
3:I:107:LEU:HD21	3:I:125:PHE:CB	2.40	0.52
11:b:355:SER:OG	11:b:356:ILE:N	2.42	0.52
11:e:113:LYS:HB2	11:e:113:LYS:HZ1	1.74	0.52
11:i:361:SER:OG	11:i:362:ARG:N	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:i:424:SER:HA	11:i:427:ILE:HG22	1.91	0.52
2:D:319:LEU:HD22	2:D:429:PHE:HZ	1.75	0.52
2:D:384:LEU:HD11	2:D:400:VAL:HG23	1.92	0.52
11:c:291:LEU:HD21	11:c:339:ARG:HD2	1.92	0.52
11:i:144:GLY:O	11:i:147:SER:OG	2.22	0.52
11:j:297:LEU:HD23	11:j:377:MET:HB2	1.91	0.52
1:A:724:TYR:O	1:A:728:GLU:HB3	2.10	0.52
1:C:537:LEU:O	1:C:541:LEU:HG	2.10	0.52
1:C:731:GLU:HB3	1:C:732:PRO:CD	2.36	0.52
4:J:715:ARG:HG3	4:J:718:GLU:HB3	1.90	0.52
3:K:581:CYS:SG	3:K:582:LEU:N	2.83	0.52
11:e:113:LYS:NZ	11:e:113:LYS:CB	2.73	0.52
11:j:229:ASN:ND2	13:j:501:GDP:O6	2.35	0.52
11:l:201:CYS:SG	11:l:202:LEU:N	2.83	0.52
1:C:251:TYR:HE1	2:D:365:ARG:NE	2.06	0.51
4:J:814:SER:OG	4:J:815:LEU:N	2.42	0.51
11:c:123:ASP:OD1	11:c:161:TYR:OH	2.27	0.51
11:e:119:PHE:CE2	11:e:160:ARG:CD	2.75	0.51
1:C:547:TYR:CG	1:C:601:LEU:HD11	2.45	0.51
2:F:464:TYR:CD2	2:F:488:LYS:HE2	2.46	0.51
2:F:575:ARG:NH2	11:f:252:ASP:OD2	2.40	0.51
11:g:22:TRP:CD1	11:g:86:TYR:OH	2.52	0.51
11:i:374:SER:OG	11:i:375:GLY:N	2.43	0.51
11:m:291:LEU:HD21	11:m:339:ARG:HD2	1.92	0.51
1:C:547:TYR:CD1	1:C:601:LEU:HD11	2.45	0.51
1:C:549:LEU:N	1:C:549:LEU:CD1	2.73	0.51
1:E:289:HIS:CD2	1:E:292:LEU:CD1	2.93	0.51
2:F:245:ILE:N	2:F:245:ILE:CD1	2.73	0.51
11:a:340:ILE:HD13	11:a:345:LEU:HD13	1.92	0.51
11:m:195:LEU:HD13	11:m:202:LEU:HD11	1.91	0.51
2:D:433:TRP:CZ3	2:D:439:LEU:HD22	2.46	0.51
1:E:682:GLN:O	1:E:685:SER:N	2.42	0.51
3:K:279:VAL:HG13	3:K:336:VAL:HG11	1.91	0.51
11:g:397:LYS:HD3	11:g:398:LEU:HD22	1.92	0.51
11:j:130:ASP:N	11:j:130:ASP:OD1	2.43	0.51
2:B:245:ILE:N	2:B:245:ILE:CD1	2.73	0.51
1:E:289:HIS:HA	1:E:292:LEU:CD1	2.40	0.51
4:J:716:LEU:CD1	4:J:809:VAL:HG13	2.40	0.51
4:J:723:MET:SD	4:J:723:MET:C	2.94	0.51
4:J:904:ARG:HH12	11:j:331:THR:HA	1.74	0.51
11:k:46:ASP:OD1	11:k:46:ASP:N	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:l:442:ASP:OD1	11:l:442:ASP:N	2.43	0.51
1:E:354:PHE:O	1:E:357:GLN:HG2	2.11	0.51
1:E:555:PHE:O	1:E:559:PHE:N	2.43	0.51
2:F:367:LEU:O	2:F:371:THR:HG22	2.11	0.51
3:I:166:PRO:HD2	3:I:167:PRO:HD2	1.91	0.51
3:K:515:ARG:HA	3:K:518:ASN:HB3	1.93	0.51
11:d:137:LEU:HB2	11:d:168:THR:HG22	1.93	0.51
11:g:291:LEU:HD21	11:g:339:ARG:HD2	1.92	0.51
11:i:195:LEU:HD23	11:i:202:LEU:HD11	1.92	0.51
11:i:394:GLN:O	11:i:398:LEU:HG	2.11	0.51
1:C:351:LYS:HE2	1:C:355:TYR:CE2	2.46	0.51
2:D:575:ARG:NH2	11:d:252:ASP:OD2	2.40	0.51
2:H:365:ARG:N	2:H:365:ARG:CD	2.73	0.51
4:J:370:LYS:O	4:J:373:ILE:HG23	2.11	0.51
1:M:748:ASP:N	1:M:748:ASP:OD1	2.43	0.51
2:B:251:VAL:HG12	2:B:346:LEU:HD12	1.91	0.51
1:C:748:ASP:OD1	1:C:748:ASP:N	2.43	0.51
2:D:553:TYR:CZ	2:D:647:PRO:HG2	2.46	0.51
1:G:351:LYS:HE2	1:G:355:TYR:CE2	2.46	0.51
1:G:604:ASP:HB2	1:G:647:ASP:HB2	1.93	0.51
2:H:464:TYR:CD2	2:H:488:LYS:HE2	2.46	0.51
11:f:333:VAL:HG21	11:f:360:LEU:HD11	1.93	0.51
11:h:137:LEU:HB2	11:h:168:THR:HG22	1.93	0.51
11:j:123:ASP:OD2	11:j:160:ARG:NH1	2.35	0.51
11:k:232:VAL:HG12	11:k:236:MET:HE2	1.93	0.51
11:l:306:SER:OG	11:l:390:ARG:NH1	2.43	0.51
2:B:553:TYR:CZ	2:B:647:PRO:HG2	2.46	0.51
3:K:32:PRO:HD2	3:K:33:PHE:CE1	2.46	0.51
5:L:393:ILE:O	5:L:397:LEU:N	2.41	0.51
11:b:4:GLU:OE1	11:b:63:ARG:NE	2.44	0.51
11:b:333:VAL:HG21	11:b:360:LEU:HD11	1.93	0.51
11:d:333:VAL:HG21	11:d:360:LEU:HD11	1.93	0.51
2:D:367:LEU:O	2:D:371:THR:HG22	2.11	0.51
5:L:1534:LYS:HG2	5:L:1544:LEU:HD13	1.93	0.51
11:b:137:LEU:HB2	11:b:168:THR:HG22	1.93	0.51
11:d:291:LEU:HG	11:d:295:ARG:HH12	1.76	0.51
11:g:6:ILE:HG23	11:g:6:ILE:O	2.11	0.51
11:g:54:GLN:CD	11:g:60:TYR:CE2	2.88	0.51
11:h:4:GLU:OE1	11:h:63:ARG:NE	2.44	0.51
2:B:464:TYR:CD2	2:B:488:LYS:HE2	2.46	0.50
2:F:553:TYR:CZ	2:F:647:PRO:HG2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:748:ASP:N	1:G:748:ASP:OD1	2.43	0.50
1:M:549:LEU:N	1:M:549:LEU:CD1	2.73	0.50
11:f:4:GLU:OE1	11:f:63:ARG:NE	2.44	0.50
4:J:278:LEU:HB2	4:J:379:LEU:HD23	1.93	0.50
11:d:4:GLU:OE1	11:d:63:ARG:NE	2.44	0.50
11:l:381:HIS:CE1	11:l:383:SER:HG	2.29	0.50
2:F:606:ARG:HE	11:g:339:ARG:HH21	1.60	0.50
2:H:581:LEU:HD23	2:H:585:LEU:HD11	1.93	0.50
3:I:349:ASP:OD1	3:I:349:ASP:N	2.43	0.50
4:J:324:VAL:HG23	4:J:372:PHE:CE2	2.47	0.50
1:M:550:MET:HA	1:M:556:PHE:CE2	2.46	0.50
11:i:298:LEU:HD12	11:i:345:LEU:HD22	1.92	0.50
1:M:351:LYS:HE2	1:M:355:TYR:CE2	2.46	0.50
11:j:46:ASP:OD1	11:j:46:ASP:N	2.43	0.50
11:l:275:PRO:HG3	11:l:374:SER:HA	1.93	0.50
2:H:553:TYR:CZ	2:H:647:PRO:HG2	2.46	0.50
1:M:604:ASP:HB2	1:M:647:ASP:HB2	1.93	0.50
11:c:397:LYS:HD3	11:c:398:LEU:HD22	1.92	0.50
2:D:364:LEU:HB2	2:D:365:ARG:HH11	1.77	0.50
2:F:573:PHE:HB2	2:F:608:THR:HG21	1.94	0.50
2:H:247:GLU:O	2:H:251:VAL:HG23	2.12	0.50
3:K:304:GLU:OE1	3:K:304:GLU:N	2.45	0.50
11:c:229:ASN:OD1	13:c:501:GDP:N1	2.42	0.50
11:m:397:LYS:HD3	11:m:398:LEU:HD22	1.92	0.50
2:B:367:LEU:O	2:B:371:THR:HG22	2.11	0.50
1:C:604:ASP:HB2	1:C:647:ASP:HB2	1.93	0.50
4:J:723:MET:HE1	4:J:821:TYR:CE1	2.47	0.50
3:K:480:TYR:O	3:K:483:SER:OG	2.26	0.50
5:L:1614:SER:O	5:L:1617:SER:OG	2.27	0.50
11:k:376:LEU:HD12	11:k:377:MET:H	1.77	0.50
2:B:865:LEU:HD21	2:B:876:LEU:HD23	1.94	0.50
2:D:307:TYR:CE2	2:D:324:PHE:CE2	3.00	0.50
3:K:38:GLU:HA	3:K:38:GLU:OE2	2.12	0.50
5:L:535:PHE:CZ	5:L:551:GLU:OE2	2.64	0.50
11:i:326:GLY:HA3	11:i:373:VAL:HG22	1.93	0.50
1:G:342:HIS:C	1:G:344:GLN:N	2.69	0.50
1:G:585:LEU:CD2	11:h:343:ARG:CB	2.88	0.50
5:L:1513:ARG:HE	5:L:1519:GLU:HG3	1.77	0.50
5:L:1633:LEU:HD21	5:L:1666:GLN:HB2	1.94	0.50
11:b:444:ILE:O	11:b:445:SER:OG	2.27	0.50
11:h:333:VAL:HG21	11:h:360:LEU:HD11	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:317:PHE:CD1	2:H:321:GLY:HA3	2.47	0.49
2:H:799:GLU:OE2	2:H:803:ARG:NH1	2.35	0.49
2:F:401:HIS:CE1	2:F:474:PHE:HB3	2.47	0.49
1:G:536:GLU:CG	1:G:539:ALA:HB3	2.43	0.49
3:K:25:LEU:HD21	3:K:53:ILE:HD12	1.94	0.49
3:K:34:LEU:C	3:K:34:LEU:CD1	2.85	0.49
11:c:291:LEU:HG	11:c:295:ARG:HH12	1.77	0.49
11:e:329:ASP:OD1	11:e:331:THR:HG22	2.12	0.49
1:C:590:SER:C	1:C:592:ALA:N	2.70	0.49
1:C:726:MET:SD	11:c:248:TYR:HB3	2.52	0.49
1:G:535:LYS:HG3	1:G:654:LEU:HD21	1.93	0.49
4:J:477:ASP:OD2	4:J:637:GLU:N	2.45	0.49
11:a:329:ASP:OD1	11:a:331:THR:HG22	2.12	0.49
11:g:13:CYS:O	11:g:17:ILE:HG12	2.12	0.49
11:h:6:ILE:HG13	11:h:132:LEU:HD11	1.95	0.49
11:i:322:ASN:HB2	11:i:358:VAL:HA	1.95	0.49
1:E:554:ASP:OD2	1:E:591:THR:HG21	2.11	0.49
2:H:865:LEU:HD21	2:H:876:LEU:HD23	1.94	0.49
3:I:623:SER:OG	3:I:656:GLN:OE1	2.25	0.49
4:J:261:ASP:OD1	4:J:262:ARG:N	2.45	0.49
4:J:375:PHE:CE1	4:J:405:ARG:HB3	2.37	0.49
4:J:806:PRO:HB2	4:J:808:PRO:HD2	1.94	0.49
11:b:39:GLU:H	11:b:39:GLU:CD	2.21	0.49
11:f:6:ILE:HG13	11:f:132:LEU:HD11	1.95	0.49
11:g:207:ASN:OD1	13:g:501:GDP:N2	2.45	0.49
11:h:293:VAL:HG11	11:h:324:ILE:CD1	2.43	0.49
11:i:185:PRO:HG2	11:i:398:LEU:HD11	1.95	0.49
11:l:266:LEU:HG	11:l:435:TYR:CE1	2.48	0.49
1:A:682:GLN:O	1:A:685:SER:N	2.40	0.49
1:E:397:ASP:C	1:E:399:GLN:H	2.19	0.49
1:G:299:SER:O	1:G:299:SER:OG	2.28	0.49
2:H:324:PHE:HB2	2:H:422:VAL:HG22	1.95	0.49
2:H:601:LEU:HD22	2:H:623:VAL:HG23	1.94	0.49
3:I:198:ASP:OD1	3:I:199:GLN:N	2.45	0.49
1:M:690:ASN:OD1	1:M:691:LYS:N	2.46	0.49
11:b:235:ILE:HG23	11:b:376:LEU:HD11	1.95	0.49
11:c:252:ASP:OD1	11:c:252:ASP:N	2.45	0.49
11:e:40:PHE:HB2	11:e:366:TYR:HE1	1.77	0.49
11:l:263:THR:HG23	11:l:266:LEU:H	1.77	0.49
2:B:581:LEU:HD23	2:B:585:LEU:HD11	1.94	0.49
1:E:311:PHE:HA	1:E:318:HIS:HE1	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:b:17:ILE:HD11	11:b:138:CYS:HB3	1.95	0.49
11:c:361:SER:OG	11:c:362:ARG:N	2.45	0.49
11:e:320:ILE:HB	11:e:356:ILE:HG13	1.95	0.49
11:f:137:LEU:HB2	11:f:168:THR:HG22	1.93	0.49
1:C:690:ASN:OD1	1:C:691:LYS:N	2.46	0.49
2:D:255:LEU:HD12	2:D:346:LEU:HD12	1.93	0.49
2:D:332:LEU:HB3	2:D:336:TYR:HE2	1.77	0.49
2:F:581:LEU:HD23	2:F:585:LEU:HD11	1.93	0.49
4:J:302:VAL:HG23	4:J:310:LEU:HD22	1.94	0.49
4:J:715:ARG:HG3	4:J:715:ARG:O	2.13	0.49
4:J:736:TYR:OH	11:j:3:ARG:NH2	2.45	0.49
11:c:290:VAL:CG1	11:c:328:VAL:HG11	2.43	0.49
2:D:464:TYR:CD2	2:D:488:LYS:HE2	2.48	0.49
2:D:790:ASP:N	2:D:790:ASP:OD1	2.45	0.49
1:E:287:LEU:C	1:E:287:LEU:CD2	2.86	0.49
1:G:690:ASN:OD1	1:G:691:LYS:N	2.46	0.49
3:K:136:VAL:HG23	3:K:172:LEU:HD21	1.95	0.49
11:f:355:SER:OG	11:f:356:ILE:N	2.42	0.49
11:g:361:SER:OG	11:g:362:ARG:N	2.45	0.49
11:h:39:GLU:H	11:h:39:GLU:CD	2.21	0.49
11:h:218:LEU:CD2	11:h:218:LEU:N	2.76	0.49
11:k:10:LEU:HD11	11:k:153:LEU:HD12	1.94	0.49
11:l:139:HIS:HE1	11:l:141:ILE:CG2	2.26	0.49
3:I:524:VAL:O	3:I:528:GLN:HB2	2.13	0.49
3:I:648:LEU:O	11:i:341:ARG:NH2	2.46	0.49
11:c:217:ARG:HH22	11:c:301:LYS:HB3	1.78	0.49
11:h:288:THR:HG21	11:h:296:ARG:NH2	2.28	0.49
11:l:62:PRO:HG2	11:l:85:LEU:HG	1.95	0.49
1:A:571:VAL:HG13	1:A:572:GLU:OE1	2.13	0.49
2:D:323:SER:OG	1:E:396:GLY:HA3	2.13	0.49
1:G:726:MET:SD	11:g:248:TYR:HB3	2.53	0.49
2:H:573:PHE:HB2	2:H:608:THR:HG21	1.94	0.49
11:b:6:ILE:HG13	11:b:132:LEU:HD11	1.95	0.49
11:g:217:ARG:HH22	11:g:301:LYS:HB3	1.78	0.49
11:m:217:ARG:HH22	11:m:301:LYS:HB3	1.78	0.49
11:m:351:TRP:CD1	11:m:351:TRP:H	2.31	0.49
2:F:790:ASP:OD1	2:F:790:ASP:N	2.45	0.48
1:G:341:LEU:HD23	1:G:341:LEU:O	2.13	0.48
3:I:55:PHE:HZ	3:I:136:VAL:HG13	1.78	0.48
3:I:532:GLN:HA	3:I:535:VAL:HG12	1.95	0.48
5:L:1574:LEU:HD21	5:L:1594:LEU:HD21	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:d:235:ILE:HG23	11:d:376:LEU:HD11	1.95	0.48
11:f:39:GLU:CD	11:f:39:GLU:H	2.21	0.48
1:C:244:ALA:HA	1:C:247:GLU:CD	2.37	0.48
1:C:555:PHE:HE1	1:C:587:LEU:CD2	2.14	0.48
2:D:581:LEU:HD23	2:D:585:LEU:HD11	1.93	0.48
3:I:188:SER:HB2	3:I:311:LEU:HG	1.95	0.48
3:I:515:ARG:HA	3:I:518:ASN:HB3	1.95	0.48
4:J:902:MET:HA	4:J:906:LEU:HB2	1.95	0.48
11:g:123:ASP:OD1	11:g:161:TYR:OH	2.27	0.48
11:m:291:LEU:HG	11:m:295:ARG:HH12	1.77	0.48
1:C:578:ARG:O	1:C:582:LEU:HG	2.13	0.48
1:C:774:LYS:O	1:C:777:SER:OG	2.29	0.48
2:D:346:LEU:C	2:D:346:LEU:CD2	2.85	0.48
2:D:468:LYS:HD2	2:D:477:MET:HE1	1.96	0.48
1:G:585:LEU:CD2	11:h:343:ARG:CD	2.71	0.48
4:J:358:PHE:HE1	4:J:429:ASN:HB2	1.78	0.48
4:J:828:LEU:O	4:J:832:LYS:HG2	2.14	0.48
3:K:15:SER:OG	5:L:391:GLU:OE2	2.24	0.48
5:L:545:PHE:CE2	5:L:547:ASP:HB2	2.49	0.48
1:M:304:PHE:CE2	1:M:308:LYS:HG3	2.49	0.48
1:M:733:THR:HG21	1:M:757:PHE:CD1	2.46	0.48
11:e:253:LEU:O	11:e:257:ILE:HG12	2.13	0.48
11:j:377:MET:SD	11:j:379:ALA:HB2	2.53	0.48
11:k:289:THR:OG1	11:k:332:GLN:NE2	2.46	0.48
11:l:39:GLU:HG2	11:l:40:PHE:H	1.77	0.48
11:m:13:CYS:O	11:m:17:ILE:HG12	2.12	0.48
11:m:207:ASN:OD1	13:m:501:GDP:N2	2.45	0.48
1:A:723:TYR:CD1	11:a:249:MET:CE	2.96	0.48
2:B:573:PHE:HB2	2:B:608:THR:HG21	1.94	0.48
2:B:606:ARG:HE	11:c:339:ARG:HH21	1.60	0.48
2:H:319:LEU:HD12	2:H:319:LEU:H	1.77	0.48
5:L:1741:SER:OG	5:L:1742:GLN:OE1	2.29	0.48
1:M:550:MET:HA	1:M:556:PHE:HE2	1.78	0.48
11:g:206:ASP:OD2	11:g:208:THR:OG1	2.31	0.48
11:l:12:GLN:CB	13:l:501:GDP:O1A	2.54	0.48
1:C:355:TYR:CD1	8:Y:56:UNK:O	2.67	0.48
2:D:336:TYR:CD1	1:E:353:TRP:NE1	2.79	0.48
3:K:38:GLU:OE1	3:K:41:VAL:HG11	2.12	0.48
1:M:726:MET:SD	11:m:248:TYR:HB3	2.53	0.48
11:a:118:ILE:HD11	11:a:153:LEU:HD21	1.95	0.48
11:c:13:CYS:O	11:c:17:ILE:HG12	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:e:110:GLN:HA	11:e:113:LYS:CD	2.43	0.48
2:B:717:GLN:OE1	11:b:357:GLN:NE2	2.44	0.48
1:C:248:ASP:CG	1:C:259:ARG:H	2.21	0.48
1:C:304:PHE:CE2	1:C:308:LYS:HG3	2.49	0.48
1:C:578:ARG:NH1	11:d:344:LYS:HE2	2.28	0.48
1:E:462:ILE:HD11	1:E:479:LEU:HB2	1.96	0.48
2:F:865:LEU:HD21	2:F:876:LEU:HD23	1.94	0.48
3:I:203:PHE:HE2	3:I:205:ILE:HD12	1.79	0.48
5:L:1699:GLU:OE1	5:L:1702:GLN:NE2	2.47	0.48
1:M:556:PHE:HB3	1:M:560:MET:HE3	1.95	0.48
11:e:229:ASN:HA	11:e:232:VAL:HG12	1.95	0.48
11:g:60:TYR:N	11:g:60:TYR:CD1	2.81	0.48
11:g:291:LEU:HG	11:g:295:ARG:HH12	1.77	0.48
11:i:32:SER:OG	11:i:34:GLU:HG2	2.13	0.48
11:l:320:ILE:HD12	11:l:356:ILE:HD12	1.95	0.48
1:C:581:ALA:HB1	11:d:339:ARG:HA	1.96	0.48
1:E:888:ASP:OD1	1:E:889:PHE:N	2.47	0.48
3:K:359:ASP:O	3:K:364:GLY:N	2.47	0.48
3:K:470:VAL:HG21	3:K:560:HIS:HE1	1.79	0.48
11:g:252:ASP:N	11:g:252:ASP:OD1	2.45	0.48
11:h:17:ILE:HD11	11:h:138:CYS:HB3	1.95	0.48
11:i:336:SER:O	11:i:340:ILE:HG12	2.13	0.48
2:D:255:LEU:HD12	2:D:346:LEU:CD1	2.43	0.48
2:F:468:LYS:HD2	2:F:477:MET:HE1	1.95	0.48
2:H:324:PHE:HB2	2:H:422:VAL:CG2	2.43	0.48
3:I:114:ASP:OD1	3:I:115:PRO:CD	2.60	0.48
3:I:353:GLN:HG3	3:I:462:LEU:HD11	1.93	0.48
4:J:716:LEU:HA	4:J:809:VAL:HG21	1.95	0.48
11:a:320:ILE:HB	11:a:356:ILE:HG13	1.95	0.48
11:e:163:LYS:HE2	11:e:163:LYS:HB3	1.57	0.48
11:e:274:THR:OG1	11:e:275:PRO:HD3	2.14	0.48
1:C:726:MET:HB3	11:c:248:TYR:CD1	2.49	0.48
2:D:305:ARG:HG2	2:D:305:ARG:NH1	2.11	0.48
2:D:401:HIS:CD2	2:D:473:SER:HB3	2.46	0.48
2:D:717:GLN:OE1	11:d:357:GLN:NE2	2.44	0.48
2:D:865:LEU:HD21	2:D:876:LEU:HD23	1.94	0.48
1:E:272:ARG:NH2	1:E:299:SER:OG	2.47	0.48
1:E:571:VAL:HG13	1:E:572:GLU:OE1	2.13	0.48
1:G:556:PHE:HB3	1:G:560:MET:HE3	1.95	0.48
2:H:468:LYS:HD2	2:H:477:MET:HE1	1.96	0.48
3:I:2:ILE:HG21	3:I:111:PHE:CD2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:266:THR:HG23	4:J:269:GLN:HB2	1.95	0.48
5:L:1589:ASP:OD1	5:L:1590:VAL:N	2.41	0.48
11:b:202:LEU:HD13	11:b:268:PHE:CE2	2.49	0.48
11:c:206:ASP:OD2	11:c:208:THR:OG1	2.31	0.48
11:f:195:LEU:HD13	11:f:202:LEU:HD11	1.96	0.48
11:h:335:LYS:O	11:h:339:ARG:CD	2.62	0.48
11:k:304:MET:N	11:k:304:MET:SD	2.87	0.48
1:C:339:GLU:CD	2:D:365:ARG:CB	2.87	0.48
11:e:262:PRO:HG3	11:e:318:ILE:HG21	1.96	0.48
11:f:202:LEU:HD13	11:f:268:PHE:CE2	2.49	0.48
11:f:235:ILE:HG23	11:f:376:LEU:HD11	1.95	0.48
11:i:184:GLN:N	11:i:185:PRO:CD	2.77	0.48
11:m:206:ASP:OD2	11:m:208:THR:OG1	2.31	0.48
11:m:361:SER:OG	11:m:362:ARG:N	2.45	0.48
1:A:888:ASP:OD1	1:A:889:PHE:N	2.47	0.47
2:D:333:ARG:HG2	1:E:357:GLN:HG3	1.95	0.47
1:E:556:PHE:HB3	1:E:560:MET:HE3	1.96	0.47
1:E:774:LYS:O	1:E:777:SER:OG	2.32	0.47
1:G:310:SER:HB3	1:G:312:GLU:OE1	2.14	0.47
2:H:288:ARG:O	2:H:292:VAL:HG23	2.13	0.47
11:a:421:MET:O	11:a:424:SER:OG	2.28	0.47
11:d:6:ILE:HG13	11:d:132:LEU:HD11	1.95	0.47
11:f:17:ILE:HD11	11:f:138:CYS:HB3	1.95	0.47
11:g:84:LYS:HA	11:h:219:HIS:CD2	2.49	0.47
11:h:339:ARG:HD3	11:h:339:ARG:N	2.29	0.47
1:C:556:PHE:HB3	1:C:560:MET:HE3	1.95	0.47
3:I:530:TYR:C	3:I:532:GLN:H	2.23	0.47
1:M:456:TRP:CE3	1:M:483:LYS:HD3	2.50	0.47
11:d:17:ILE:HD11	11:d:138:CYS:HB3	1.95	0.47
11:d:39:GLU:CD	11:d:39:GLU:H	2.21	0.47
11:d:195:LEU:HD13	11:d:202:LEU:HD11	1.96	0.47
11:l:322:ASN:HD21	11:l:377:MET:HG2	1.79	0.47
2:B:882:PHE:HE2	11:b:348:PHE:HE2	1.63	0.47
1:C:456:TRP:CE3	1:C:483:LYS:HD3	2.49	0.47
1:C:555:PHE:HA	1:C:590:SER:HB3	1.96	0.47
1:G:246:VAL:O	1:G:250:LEU:HB2	2.14	0.47
1:G:456:TRP:CE3	1:G:483:LYS:HD3	2.50	0.47
1:G:890:ASN:OD1	11:g:348:PHE:HB2	2.15	0.47
2:H:564:ARG:NH2	2:H:613:ASP:OD1	2.47	0.47
2:H:717:GLN:OE1	11:h:357:GLN:NE2	2.44	0.47
3:K:604:ASP:OD1	3:K:605:GLU:N	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:547:TYR:CG	1:M:601:LEU:HD11	2.49	0.47
11:b:195:LEU:HD13	11:b:202:LEU:HD11	1.96	0.47
11:c:351:TRP:CD1	11:c:351:TRP:H	2.31	0.47
1:A:272:ARG:NH2	1:A:299:SER:OG	2.46	0.47
1:C:728:GLU:HG2	11:c:334:HIS:HB3	1.97	0.47
2:D:564:ARG:NH2	2:D:613:ASP:OD1	2.47	0.47
2:F:374:PRO:O	2:F:378:LEU:CD2	2.50	0.47
2:F:882:PHE:HE2	11:f:348:PHE:HE2	1.62	0.47
1:G:595:ASP:O	1:G:598:LYS:HG2	2.13	0.47
4:J:326:ARG:HH12	4:J:413:HIS:HE1	1.62	0.47
5:L:539:TRP:HH2	5:L:554:ILE:HG21	1.80	0.47
5:L:1668:PHE:CE2	5:L:1732:ILE:HG21	2.50	0.47
1:M:372:SER:HA	9:W:203:UNK:CB	2.44	0.47
11:c:207:ASN:OD1	13:c:501:GDP:N2	2.45	0.47
11:g:395:TYR:CE2	11:g:425:ARG:HD3	2.50	0.47
11:h:202:LEU:HD13	11:h:268:PHE:CE2	2.49	0.47
11:j:186:TYR:HE2	11:j:398:LEU:HD23	1.78	0.47
11:j:315:HIS:CE1	11:j:383:SER:HA	2.49	0.47
11:k:202:LEU:HD23	11:k:203:VAL:N	2.28	0.47
2:B:468:LYS:HD2	2:B:477:MET:HE1	1.96	0.47
2:B:790:ASP:N	2:B:790:ASP:OD1	2.45	0.47
1:C:299:SER:O	1:C:299:SER:OG	2.28	0.47
2:D:670:ALA:O	2:D:719:GLN:NE2	2.47	0.47
1:E:242:GLU:OE2	1:E:349:LEU:N	2.48	0.47
1:E:317:ASN:ND2	1:E:383:THR:HG21	2.28	0.47
3:I:607:GLY:O	3:I:611:LEU:N	2.47	0.47
3:K:117:LEU:HD21	3:K:121:HIS:CD2	2.50	0.47
3:K:190:TRP:CH2	3:K:280:GLY:HA3	2.49	0.47
11:a:274:THR:OG1	11:a:275:PRO:HD3	2.14	0.47
11:d:202:LEU:HD13	11:d:268:PHE:CE2	2.49	0.47
11:i:241:THR:HA	11:i:244:ARG:HH21	1.79	0.47
1:A:467:ILE:HG22	1:A:469:SER:H	1.80	0.47
2:B:564:ARG:NH2	2:B:613:ASP:OD1	2.48	0.47
1:E:467:ILE:HG22	1:E:469:SER:H	1.80	0.47
2:H:401:HIS:CD2	2:H:473:SER:HB3	2.46	0.47
4:J:906:LEU:HD13	4:J:937:ILE:HD11	1.97	0.47
11:j:207:ASN:O	11:j:211:ASN:N	2.44	0.47
11:k:241:THR:HA	11:k:244:ARG:HH21	1.79	0.47
2:D:573:PHE:CB	2:D:608:THR:HG21	2.44	0.47
2:F:296:GLU:CD	6:Q:34:UNK:CB	2.87	0.47
2:F:564:ARG:NH2	2:F:613:ASP:OD1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:890:ASN:OD1	11:m:348:PHE:HB2	2.15	0.47
11:a:229:ASN:HA	11:a:232:VAL:HG12	1.95	0.47
11:e:40:PHE:CB	11:e:366:TYR:HE1	2.28	0.47
11:h:195:LEU:HD13	11:h:202:LEU:HD11	1.96	0.47
11:i:103:ASN:O	11:i:106:SER:OG	2.28	0.47
11:k:232:VAL:HA	11:k:235:ILE:HD12	1.97	0.47
11:m:395:TYR:CE2	11:m:425:ARG:HD3	2.50	0.47
1:G:312:GLU:N	1:G:312:GLU:CD	2.73	0.47
3:I:158:TYR:O	3:I:161:SER:OG	2.30	0.47
2:D:319:LEU:HD22	2:D:429:PHE:CZ	2.50	0.47
2:F:559:MET:HE2	2:F:751:HIS:CD2	2.50	0.47
4:J:552:LEU:HD23	4:J:552:LEU:H	1.80	0.47
11:g:351:TRP:H	11:g:351:TRP:CD1	2.31	0.47
1:A:318:HIS:ND1	2:B:406:THR:O	2.48	0.47
2:F:599:GLY:O	2:F:603:THR:OG1	2.32	0.47
2:F:601:LEU:O	2:F:605:VAL:HG23	2.15	0.47
1:G:341:LEU:CD2	1:G:346:LEU:HB3	2.28	0.47
2:H:559:MET:HE2	2:H:751:HIS:CD2	2.50	0.47
11:a:5:ILE:HD11	11:a:253:LEU:HD22	1.97	0.47
2:F:378:LEU:N	2:F:378:LEU:CD2	2.78	0.46
1:G:304:PHE:CE2	1:G:308:LYS:HG3	2.49	0.46
1:G:528:LEU:O	1:G:532:MET:HG2	2.15	0.46
3:I:108:GLU:CD	3:I:112:LEU:HD21	2.38	0.46
3:K:111:PHE:CE2	3:K:117:LEU:HB3	2.50	0.46
1:M:414:PRO:O	1:M:417:GLU:HG2	2.15	0.46
11:k:66:LEU:HD11	11:k:86:TYR:CZ	2.50	0.46
11:l:202:LEU:HD23	11:l:268:PHE:CE2	2.50	0.46
11:l:272:GLY:N	11:l:377:MET:O	2.48	0.46
1:A:462:ILE:HD11	1:A:479:LEU:HB2	1.96	0.46
2:B:559:MET:HE2	2:B:751:HIS:CD2	2.50	0.46
1:E:553:GLY:HA3	11:e:251:ASN:ND2	2.30	0.46
2:F:479:GLN:NE2	2:F:531:GLN:OE1	2.44	0.46
1:G:728:GLU:HG2	11:g:334:HIS:HB3	1.97	0.46
3:K:353:GLN:HG3	3:K:462:LEU:CD1	2.44	0.46
11:i:293:VAL:O	11:i:297:LEU:HG	2.15	0.46
11:j:3:ARG:HB3	11:j:133:GLU:HB2	1.96	0.46
1:A:320:LEU:HD13	1:A:387:LEU:HD11	1.98	0.46
1:C:414:PRO:O	1:C:417:GLU:HG2	2.15	0.46
1:E:330:GLU:OE1	1:E:333:ILE:CD1	2.60	0.46
4:J:324:VAL:CG2	4:J:372:PHE:HE2	2.28	0.46
4:J:945:GLU:HG3	4:J:946:LYS:H	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:727:PHE:CE1	11:m:248:TYR:CD2	3.04	0.46
11:a:262:PRO:HG3	11:a:318:ILE:HG21	1.96	0.46
11:a:272:GLY:HA3	11:a:377:MET:HE3	1.98	0.46
11:c:144:GLY:N	13:c:501:GDP:O3A	2.49	0.46
11:l:32:SER:OG	11:l:36:ILE:O	2.29	0.46
11:m:123:ASP:OD1	11:m:161:TYR:OH	2.26	0.46
1:A:724:TYR:OH	1:A:764:ASP:OD1	2.27	0.46
1:C:890:ASN:OD1	11:c:348:PHE:HB2	2.15	0.46
3:I:23:SER:HG	3:I:26:GLN:NE2	2.12	0.46
3:K:35:HIS:HB3	3:K:38:GLU:CB	2.45	0.46
11:a:115:HIS:ND1	11:a:119:PHE:CE2	2.84	0.46
11:h:248:TYR:HD1	11:h:249:MET:HG3	1.80	0.46
11:i:274:THR:HG21	11:i:293:VAL:HG13	1.98	0.46
11:l:103:ASN:OD1	11:l:104:TRP:N	2.48	0.46
11:l:361:SER:OG	11:l:362:ARG:N	2.49	0.46
2:B:601:LEU:O	2:B:605:VAL:HG23	2.15	0.46
2:D:259:GLN:HE21	2:D:339:LEU:HD13	1.80	0.46
2:D:319:LEU:N	2:D:319:LEU:CD1	2.77	0.46
1:E:397:ASP:OD2	1:E:400:ALA:CB	2.60	0.46
2:H:308:THR:OG1	2:H:325:CYS:SG	2.50	0.46
2:H:670:ALA:O	2:H:719:GLN:NE2	2.47	0.46
4:J:764:GLU:HG3	11:k:342:GLU:CD	2.40	0.46
4:J:892:HIS:CE1	11:j:355:SER:HB3	2.50	0.46
5:L:427:LEU:HD23	5:L:535:PHE:CZ	2.49	0.46
1:M:728:GLU:HG2	11:m:334:HIS:HB3	1.97	0.46
11:e:225:PHE:HD1	11:e:228:ILE:HD11	1.80	0.46
11:k:349:ILE:HB	11:k:351:TRP:CD1	2.50	0.46
11:l:272:GLY:HA3	11:l:377:MET:HE3	1.98	0.46
11:l:291:LEU:O	11:l:295:ARG:NH1	2.48	0.46
1:A:291:ILE:O	1:A:294:VAL:HG12	2.16	0.46
2:B:387:HIS:CG	2:B:403:TYR:HE1	2.32	0.46
2:D:677:LEU:HD23	2:D:677:LEU:HA	1.80	0.46
1:G:414:PRO:O	1:G:417:GLU:HG2	2.15	0.46
2:H:392:LYS:O	2:H:470:MET:HE1	2.16	0.46
3:I:14:GLY:HA3	4:J:309:CYS:SG	2.56	0.46
4:J:723:MET:HE1	4:J:821:TYR:CZ	2.51	0.46
3:K:29:GLN:O	3:K:31:PHE:CE1	2.68	0.46
2:T:411:MET:C	2:T:413:SER:H	2.23	0.46
11:b:248:TYR:HD1	11:b:249:MET:HG3	1.81	0.46
11:g:22:TRP:HA	11:g:22:TRP:CE3	2.50	0.46
11:g:62:PRO:CD	11:g:85:LEU:HD11	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:i:17:ILE:O	11:i:21:PHE:N	2.42	0.46
2:D:255:LEU:HD11	2:D:346:LEU:HD12	1.97	0.46
2:D:479:GLN:NE2	2:D:531:GLN:OE1	2.44	0.46
2:D:559:MET:HE2	2:D:751:HIS:CD2	2.50	0.46
2:D:882:PHE:HE2	11:d:348:PHE:HE2	1.63	0.46
3:I:131:LEU:C	3:I:131:LEU:CD2	2.86	0.46
4:J:716:LEU:CB	4:J:809:VAL:HG22	2.46	0.46
5:L:1630:MET:SD	5:L:1673:GLN:NE2	2.89	0.46
11:a:40:PHE:HB2	11:a:366:TYR:CD1	2.48	0.46
11:g:144:GLY:N	13:g:501:GDP:O3A	2.49	0.46
11:i:291:LEU:HD22	11:i:339:ARG:HD2	1.98	0.46
11:l:241:THR:HG21	11:l:325:GLN:HG2	1.97	0.46
11:l:274:THR:HG21	11:l:293:VAL:HG13	1.97	0.46
2:F:387:HIS:CG	2:F:403:TYR:HE1	2.34	0.46
1:G:544:ILE:CD1	1:G:658:ILE:CD1	2.94	0.46
3:I:581:CYS:SG	3:I:582:LEU:N	2.89	0.46
4:J:293:LYS:HA	4:J:322:GLN:HE22	1.80	0.46
11:c:395:TYR:CE2	11:c:425:ARG:HD3	2.50	0.46
11:e:351:TRP:CD1	11:e:351:TRP:H	2.34	0.46
11:i:377:MET:HE3	11:i:377:MET:HB3	1.85	0.46
2:D:245:ILE:N	2:D:245:ILE:CD1	2.73	0.46
2:H:319:LEU:CD1	2:H:319:LEU:H	2.28	0.46
2:H:329:HIS:ND1	3:I:131:LEU:HD12	2.30	0.46
3:K:530:TYR:C	3:K:532:GLN:H	2.24	0.46
11:a:235:ILE:HG23	11:a:376:LEU:HD11	1.98	0.46
11:d:162:PRO:HG2	11:d:163:LYS:HG2	1.98	0.46
11:f:248:TYR:HD1	11:f:249:MET:HG3	1.81	0.46
11:k:266:LEU:HD21	11:k:318:ILE:HG13	1.98	0.46
11:k:326:GLY:HA3	11:k:373:VAL:HG22	1.98	0.46
11:t:102:ASN:HA	11:t:144:GLY:HA2	1.97	0.46
1:A:583:LEU:HD22	1:A:603:ILE:HD11	1.98	0.46
1:C:280:LEU:HD23	1:C:285:ARG:HG2	1.98	0.46
1:C:555:PHE:CZ	1:C:587:LEU:CD2	2.78	0.46
2:D:882:PHE:HE2	11:d:348:PHE:CE2	2.34	0.46
3:I:588:LEU:O	3:I:591:SER:OG	2.30	0.46
4:J:913:PHE:HE1	4:J:930:HIS:HA	1.81	0.46
3:K:353:GLN:HG3	3:K:462:LEU:HD11	1.96	0.46
5:L:1797:ASP:OD1	11:l:334:HIS:HB2	2.16	0.46
11:a:351:TRP:CD1	11:a:351:TRP:H	2.34	0.46
11:b:162:PRO:HG2	11:b:163:LYS:HG2	1.98	0.46
11:c:290:VAL:HG12	11:c:328:VAL:HG11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:m:229:ASN:OD1	13:m:501:GDP:N1	2.42	0.46
1:A:262:SER:OG	1:A:263:ALA:N	2.48	0.45
1:E:602:LYS:O	1:E:647:ASP:N	2.49	0.45
1:E:724:TYR:OH	1:E:764:ASP:OD1	2.27	0.45
2:F:882:PHE:HE2	11:f:348:PHE:CE2	2.34	0.45
2:H:463:LYS:O	2:H:463:LYS:HG2	2.17	0.45
2:H:595:HIS:CE1	3:I:648:LEU:HD23	2.36	0.45
1:M:311:PHE:CE2	2:T:406:THR:HA	2.51	0.45
11:c:73:VAL:O	11:c:76:SER:OG	2.20	0.45
11:d:216:ASP:OD2	11:d:217:ARG:HG3	2.16	0.45
11:i:6:ILE:HG22	11:i:63:ARG:HB3	1.98	0.45
11:i:29:HIS:ND1	11:i:46:ASP:OD2	2.49	0.45
11:i:225:PHE:HB3	13:i:501:GDP:O6	2.16	0.45
2:B:441:ASP:OD1	2:B:441:ASP:N	2.49	0.45
1:E:310:SER:HB2	1:E:313:TYR:CD1	2.51	0.45
1:E:536:GLU:OE1	1:E:536:GLU:N	2.34	0.45
1:E:550:MET:HE3	1:E:556:PHE:CZ	2.51	0.45
2:F:374:PRO:C	2:F:378:LEU:HD23	2.37	0.45
1:G:280:LEU:HD23	1:G:285:ARG:HG2	1.99	0.45
4:J:739:TYR:HA	4:J:742:ILE:HD12	1.98	0.45
1:M:280:LEU:HD23	1:M:285:ARG:HG2	1.99	0.45
11:a:225:PHE:HD1	11:a:228:ILE:HD11	1.80	0.45
11:f:162:PRO:HG2	11:f:163:LYS:HG2	1.98	0.45
11:h:193:LYS:HD3	11:h:194:ARG:HD2	1.98	0.45
11:m:252:ASP:OD1	11:m:252:ASP:N	2.45	0.45
2:D:602:GLU:OE1	2:D:602:GLU:HA	2.15	0.45
1:G:544:ILE:HD11	1:G:658:ILE:HD12	1.99	0.45
3:I:97:LEU:HD13	3:I:97:LEU:HA	1.76	0.45
3:I:587:ASP:N	3:I:587:ASP:OD1	2.49	0.45
4:J:841:LEU:HD23	4:J:841:LEU:H	1.81	0.45
4:J:990:CYS:HA	4:J:993:PHE:HB2	1.98	0.45
5:L:450:THR:O	5:L:452:PRO:HD3	2.16	0.45
7:U:14:SER:HA	7:U:71:ILE:O	2.16	0.45
11:e:4:GLU:OE1	11:e:63:ARG:NE	2.49	0.45
11:f:193:LYS:HD3	11:f:194:ARG:HD2	1.98	0.45
11:h:444:ILE:O	11:h:445:SER:OG	2.27	0.45
11:i:184:GLN:CD	11:i:184:GLN:N	2.73	0.45
11:j:236:MET:O	11:j:239:SER:OG	2.29	0.45
11:l:225:PHE:O	11:l:229:ASN:ND2	2.49	0.45
1:C:248:ASP:OD1	1:C:258:GLY:HA3	2.16	0.45
2:H:311:ARG:HB3	2:H:317:PHE:HD2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:790:ASP:OD1	2:H:790:ASP:N	2.46	0.45
2:H:882:PHE:HE2	11:h:348:PHE:CE2	2.34	0.45
4:J:263:VAL:HG12	4:J:299:ASN:O	2.16	0.45
1:M:276:VAL:HG23	1:M:277:ASP:N	2.31	0.45
1:M:669:LEU:CD1	1:M:730:MET:CE	2.60	0.45
11:b:193:LYS:HD3	11:b:194:ARG:HD2	1.98	0.45
11:d:248:TYR:HD1	11:d:249:MET:HG3	1.81	0.45
11:i:184:GLN:N	11:i:184:GLN:OE1	2.31	0.45
11:k:141:ILE:HG22	11:k:191:THR:CG2	2.46	0.45
11:l:242:THR:HG21	11:l:256:LEU:HD11	1.99	0.45
2:D:441:ASP:N	2:D:441:ASP:OD1	2.49	0.45
1:E:262:SER:OG	1:E:263:ALA:N	2.48	0.45
3:I:650:TYR:CE2	11:i:354:ALA:HB3	2.51	0.45
4:J:707:MET:HE3	4:J:707:MET:HB3	1.81	0.45
11:k:52:PHE:O	11:k:63:ARG:NH2	2.49	0.45
2:B:463:LYS:HG2	2:B:463:LYS:O	2.17	0.45
2:B:479:GLN:NE2	2:B:531:GLN:OE1	2.44	0.45
2:B:882:PHE:HE2	11:b:348:PHE:CE2	2.34	0.45
1:C:552:GLN:NE2	1:C:591:THR:HG23	2.32	0.45
2:D:418:ILE:O	2:D:422:VAL:HG23	2.15	0.45
2:F:606:ARG:HH12	11:g:342:GLU:HG3	1.81	0.45
1:G:539:ALA:HA	1:G:542:ARG:HD2	1.97	0.45
4:J:444:ILE:HG21	4:J:684:GLU:OE1	2.17	0.45
4:J:645:LEU:HD11	4:J:690:CYS:HB3	1.97	0.45
11:a:4:GLU:OE1	11:a:63:ARG:NE	2.49	0.45
11:e:4:GLU:OE2	11:e:63:ARG:NH2	2.50	0.45
11:e:245:TYR:OH	11:e:364:SER:HB2	2.17	0.45
11:e:362:ARG:HB2	11:e:362:ARG:NH2	2.32	0.45
11:i:329:ASP:OD1	11:i:331:THR:HG23	2.17	0.45
11:l:296:ARG:O	11:l:302:ASN:ND2	2.49	0.45
11:t:172:PHE:N	11:t:205:LEU:O	2.40	0.45
2:B:401:HIS:CD2	2:B:473:SER:HB3	2.46	0.45
1:C:250:LEU:HD12	1:C:335:VAL:HG13	1.98	0.45
2:D:433:TRP:CG	2:D:433:TRP:O	2.70	0.45
2:F:441:ASP:N	2:F:441:ASP:OD1	2.49	0.45
1:G:474:MET:HE3	1:G:474:MET:HB2	1.86	0.45
1:G:547:TYR:OH	1:G:595:ASP:CG	2.60	0.45
1:G:585:LEU:HD22	11:h:343:ARG:HB2	1.95	0.45
2:H:315:ARG:CG	2:H:315:ARG:NH2	2.72	0.45
4:J:335:MET:HE3	4:J:365:MET:HE3	1.99	0.45
4:J:716:LEU:C	4:J:716:LEU:CD2	2.86	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:b:216:ASP:OD2	11:b:217:ARG:HG3	2.16	0.45
11:d:39:GLU:HG2	11:d:40:PHE:N	2.31	0.45
11:e:39:GLU:HG2	11:e:40:PHE:H	1.82	0.45
11:m:144:GLY:N	13:m:501:GDP:O3A	2.49	0.45
2:B:433:TRP:CZ3	2:B:439:LEU:HD22	2.52	0.45
2:B:677:LEU:HD23	2:B:677:LEU:HA	1.80	0.45
1:E:583:LEU:HD22	1:E:603:ILE:HD11	1.98	0.45
2:F:463:LYS:O	2:F:463:LYS:HG2	2.17	0.45
4:J:934:LEU:HA	4:J:937:ILE:HG22	1.98	0.45
5:L:432:PHE:HE1	5:L:524:LEU:HD13	1.81	0.45
5:L:1640:LEU:HD11	5:L:1655:PHE:HE1	1.82	0.45
1:M:774:LYS:O	1:M:777:SER:OG	2.29	0.45
11:a:4:GLU:OE2	11:a:63:ARG:NH2	2.50	0.45
11:a:115:HIS:ND1	11:a:119:PHE:HD2	2.15	0.45
11:e:250:ASN:HD22	11:e:250:ASN:N	2.15	0.45
11:j:121:ILE:HD13	11:j:124:ARG:HD3	1.98	0.45
11:m:265:ARG:O	11:m:267:HIS:ND1	2.50	0.45
1:A:433:SER:O	1:A:433:SER:OG	2.32	0.45
1:G:578:ARG:O	1:G:582:LEU:HG	2.17	0.45
2:H:315:ARG:HG3	2:H:315:ARG:NH2	2.13	0.45
5:L:1482:ALA:HB3	5:L:1483:PRO:HD3	1.99	0.45
5:L:1601:ASP:OD1	5:L:1603:PRO:HD2	2.17	0.45
11:d:193:LYS:HD3	11:d:194:ARG:HD2	1.98	0.45
11:e:5:ILE:HD11	11:e:253:LEU:HD22	1.98	0.45
11:e:110:GLN:HA	11:e:113:LYS:HD3	1.99	0.45
11:g:392:CYS:HB3	11:g:425:ARG:HH12	1.82	0.45
11:h:274:THR:N	11:h:275:PRO:CD	2.80	0.45
11:h:295:ARG:CB	11:h:295:ARG:NH1	2.73	0.45
11:k:261:ILE:HG12	11:k:267:HIS:HA	1.99	0.45
1:A:602:LYS:O	1:A:647:ASP:N	2.49	0.45
2:B:592:LEU:HD23	2:B:592:LEU:HA	1.84	0.45
1:G:297:SER:HB3	1:G:363:MET:O	2.17	0.45
1:G:540:HIS:CE1	1:G:650:VAL:HG12	2.49	0.45
2:H:882:PHE:HE2	11:h:348:PHE:HE2	1.63	0.45
4:J:907:HIS:CD2	11:j:330:PRO:HG3	2.51	0.45
3:K:406:ASP:HB3	11:l:339:ARG:HH22	1.82	0.45
2:B:606:ARG:HH12	11:c:342:GLU:HG3	1.81	0.44
1:C:297:SER:HB3	1:C:363:MET:O	2.17	0.44
1:E:723:TYR:CE2	11:e:249:MET:CE	3.00	0.44
11:a:115:HIS:CE1	11:a:119:PHE:CD2	3.05	0.44
11:c:274:THR:HB	11:c:297:LEU:HD23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:f:216:ASP:OD2	11:f:217:ARG:HG3	2.16	0.44
11:g:274:THR:HB	11:g:297:LEU:HD23	1.99	0.44
11:i:184:GLN:HB2	11:i:185:PRO:HD3	1.98	0.44
11:l:247:GLY:O	11:l:251:ASN:ND2	2.32	0.44
11:m:392:CYS:HB3	11:m:425:ARG:HH12	1.82	0.44
2:H:599:GLY:CA	11:i:338:GLN:HE21	2.20	0.44
3:I:530:TYR:O	3:I:531:LEU:HB3	2.17	0.44
5:L:427:LEU:HB3	5:L:551:GLU:CD	2.42	0.44
5:L:1667:HIS:HE1	11:l:355:SER:HB3	1.82	0.44
11:c:202:LEU:HD13	11:c:268:PHE:CE2	2.53	0.44
11:e:272:GLY:HA3	11:e:377:MET:HE3	1.98	0.44
11:h:162:PRO:HG2	11:h:163:LYS:HG2	1.98	0.44
11:h:218:LEU:N	11:h:218:LEU:HD22	2.31	0.44
1:A:555:PHE:HZ	1:A:646:PHE:CZ	2.35	0.44
1:C:248:ASP:HA	1:C:251:TYR:HD2	1.80	0.44
2:D:283:LEU:HD13	2:D:287:LEU:HB2	1.99	0.44
2:F:433:TRP:O	2:F:433:TRP:CG	2.70	0.44
2:F:717:GLN:OE1	11:f:357:GLN:NE2	2.44	0.44
4:J:889:LYS:HG2	4:J:987:PHE:HE2	1.82	0.44
4:J:904:ARG:HH12	11:j:331:THR:CA	2.30	0.44
11:a:294:MET:SD	11:a:336:SER:OG	2.67	0.44
11:d:320:ILE:HB	11:d:356:ILE:HG13	1.99	0.44
11:e:235:ILE:HG23	11:e:376:LEU:HD11	1.98	0.44
11:g:53:TYR:CD2	11:g:53:TYR:O	2.70	0.44
11:g:202:LEU:HD13	11:g:268:PHE:CE2	2.53	0.44
1:A:414:PRO:O	1:A:417:GLU:HG2	2.17	0.44
2:B:670:ALA:O	2:B:719:GLN:NE2	2.47	0.44
3:I:56:THR:HA	3:I:59:ILE:HD12	1.99	0.44
3:I:190:TRP:CH2	3:I:280:GLY:HA3	2.52	0.44
4:J:326:ARG:HE	4:J:416:PHE:HE2	1.64	0.44
3:K:397:GLN:HE22	3:K:411:LEU:HG	1.82	0.44
3:K:650:TYR:CD2	11:k:354:ALA:HB3	2.53	0.44
11:c:392:CYS:HB3	11:c:425:ARG:HH12	1.82	0.44
1:A:647:ASP:OD1	1:A:648:TYR:N	2.51	0.44
2:D:463:LYS:HG2	2:D:463:LYS:O	2.17	0.44
1:E:343:ARG:NH2	1:E:343:ARG:HA	2.32	0.44
2:F:297:LEU:N	2:F:297:LEU:CD2	2.81	0.44
2:H:441:ASP:OD1	2:H:441:ASP:N	2.49	0.44
3:I:190:TRP:CZ3	3:I:280:GLY:HA3	2.53	0.44
4:J:548:MET:HE2	4:J:548:MET:HB3	1.84	0.44
4:J:938:HIS:CD2	4:J:944:ARG:HB3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:173:GLU:OE1	3:K:319:LEU:HD13	2.16	0.44
11:f:39:GLU:HG2	11:f:40:PHE:N	2.32	0.44
11:g:60:TYR:N	11:g:60:TYR:HD1	2.16	0.44
1:C:474:MET:HE3	1:C:474:MET:HB2	1.86	0.44
1:E:292:LEU:N	1:E:293:PRO:CD	2.81	0.44
1:E:312:GLU:CD	1:E:312:GLU:N	2.73	0.44
1:E:552:GLN:HE22	1:E:591:THR:CG2	2.14	0.44
3:K:401:HIS:CD2	11:l:339:ARG:HH21	2.27	0.44
3:K:529:TYR:HE2	11:k:249:MET:HB3	1.82	0.44
1:M:297:SER:HB3	1:M:363:MET:O	2.17	0.44
1:M:758:LEU:HD23	1:M:758:LEU:HA	1.83	0.44
11:b:39:GLU:HG2	11:b:40:PHE:N	2.32	0.44
11:b:320:ILE:HB	11:b:356:ILE:HG13	1.99	0.44
11:h:320:ILE:HB	11:h:356:ILE:HG13	1.99	0.44
11:i:229:ASN:ND2	13:i:501:GDP:O6	2.28	0.44
11:j:144:GLY:O	11:j:147:SER:OG	2.34	0.44
2:B:322:GLN:O	2:B:326:ALA:N	2.47	0.44
2:B:433:TRP:CG	2:B:433:TRP:O	2.70	0.44
2:D:562:MET:SD	2:D:660:TYR:HE2	2.41	0.44
2:F:670:ALA:O	2:F:719:GLN:NE2	2.47	0.44
1:G:723:TYR:HB3	1:G:886:ARG:NH1	2.33	0.44
4:J:266:THR:OG1	4:J:267:GLU:N	2.51	0.44
4:J:327:LEU:HD22	4:J:368:LEU:HD21	1.99	0.44
3:K:196:LEU:HD23	3:K:196:LEU:H	1.83	0.44
5:L:1574:LEU:HD23	5:L:1574:LEU:C	2.42	0.44
11:i:190:LEU:HD21	11:i:421:MET:HG2	2.00	0.44
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.90	0.44
1:A:684:CYS:SG	11:a:254:ILE:HG12	2.58	0.44
1:C:387:LEU:O	1:C:408:THR:OG1	2.35	0.44
2:H:433:TRP:O	2:H:433:TRP:CG	2.70	0.44
4:J:375:PHE:CD1	4:J:405:ARG:HD2	2.53	0.44
1:M:314:GLY:HA2	1:M:432:TYR:CD2	2.53	0.44
1:M:474:MET:HE3	1:M:474:MET:HB2	1.86	0.44
11:h:39:GLU:HG2	11:h:40:PHE:N	2.32	0.44
11:j:21:PHE:CE1	11:j:236:MET:HG2	2.52	0.44
11:j:24:GLN:HG3	11:j:28:GLU:OE1	2.18	0.44
11:j:420:GLU:HB3	11:j:421:MET:HE2	2.00	0.44
11:k:225:PHE:HD1	11:k:228:ILE:HD11	1.82	0.44
11:m:202:LEU:HD13	11:m:268:PHE:CE2	2.52	0.44
1:G:387:LEU:O	1:G:408:THR:OG1	2.35	0.44
3:I:38:GLU:C	3:I:40:SER:H	2.25	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:380:LEU:HD12	3:I:380:LEU:HA	1.85	0.44
1:M:544:ILE:HG23	1:M:548:PHE:CD1	2.53	0.44
1:M:547:TYR:CE1	1:M:587:LEU:HD21	2.53	0.44
11:e:32:SER:OG	11:e:34:GLU:HG2	2.18	0.44
11:f:320:ILE:HB	11:f:356:ILE:HG13	1.99	0.44
11:j:66:LEU:HD11	11:j:86:TYR:CZ	2.53	0.44
1:E:414:PRO:O	1:E:417:GLU:HG2	2.17	0.43
3:K:259:LEU:HB2	3:K:277:LEU:HD22	1.99	0.43
11:c:107:GLY:HA3	11:c:148:GLY:HA3	2.00	0.43
11:j:142:ALA:HB3	13:j:501:GDP:H4'	2.00	0.43
11:k:397:LYS:HD3	11:k:398:LEU:HD23	2.00	0.43
11:m:274:THR:HB	11:m:297:LEU:HD23	1.99	0.43
1:A:547:TYR:CG	1:A:601:LEU:HD11	2.54	0.43
2:B:778:VAL:HG22	2:B:857:ILE:HG23	2.01	0.43
1:C:673:MET:CE	1:C:730:MET:SD	3.05	0.43
1:E:306:GLU:OE1	6:Q:36:UNK:HA	2.18	0.43
3:I:29:GLN:O	3:I:31:PHE:CD1	2.71	0.43
3:I:133:PHE:HB2	3:I:134:PRO:HD3	1.98	0.43
3:I:305:ASP:OD1	3:I:306:THR:N	2.50	0.43
3:I:539:GLN:NE2	3:I:566:ASN:HD22	2.16	0.43
1:M:311:PHE:HE2	2:T:406:THR:HA	1.83	0.43
1:M:368:SER:O	1:M:371:THR:HG22	2.15	0.43
11:a:32:SER:OG	11:a:34:GLU:HG2	2.18	0.43
11:b:242:THR:HG21	11:b:256:LEU:HD11	2.00	0.43
11:e:321:LEU:N	11:e:378:MET:O	2.40	0.43
11:g:61:ILE:N	11:g:61:ILE:CD1	2.81	0.43
11:i:252:ASP:OD1	11:i:254:ILE:HG22	2.18	0.43
11:k:240:THR:HG23	11:k:243:LEU:HD12	2.01	0.43
1:C:339:GLU:OE2	2:D:365:ARG:CB	2.65	0.43
2:H:562:MET:SD	2:H:660:TYR:HE2	2.41	0.43
3:I:31:PHE:HB3	3:I:33:PHE:HE1	1.70	0.43
3:I:133:PHE:HA	3:I:136:VAL:HG12	2.00	0.43
3:K:547:ILE:HG23	3:K:556:ILE:HD11	2.00	0.43
5:L:430:GLN:O	5:L:434:SER:N	2.46	0.43
5:L:1535:LEU:HD23	5:L:1535:LEU:H	1.82	0.43
5:L:1616:TYR:CE1	5:L:1709:LEU:HD12	2.53	0.43
5:L:1671:VAL:HA	11:l:357:GLN:NE2	2.32	0.43
2:T:411:MET:C	2:T:413:SER:N	2.73	0.43
11:e:270:MET:HE2	11:e:270:MET:HB3	1.91	0.43
2:B:251:VAL:HG12	2:B:346:LEU:CD1	2.49	0.43
2:B:562:MET:SD	2:B:660:TYR:HE2	2.41	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ASP:OD2	1:C:260:TYR:N	2.40	0.43
1:C:723:TYR:HB3	1:C:886:ARG:NH1	2.33	0.43
1:G:731:GLU:HB3	1:G:732:PRO:CD	2.44	0.43
3:I:599:ASN:ND2	3:I:601:GLY:O	2.51	0.43
5:L:569:TRP:CD1	5:L:1606:ILE:HD11	2.53	0.43
1:M:535:LYS:NZ	1:M:653:PRO:HG2	2.33	0.43
11:d:214:ALA:O	11:d:219:HIS:N	2.52	0.43
11:g:46:ASP:OD1	11:g:46:ASP:N	2.49	0.43
11:l:395:TYR:O	11:l:399:ARG:N	2.50	0.43
1:A:343:ARG:HA	1:A:343:ARG:NH2	2.33	0.43
1:A:774:LYS:O	1:A:777:SER:OG	2.32	0.43
2:B:840:ILE:HA	2:B:843:MET:HE2	2.01	0.43
1:C:535:LYS:NZ	1:C:653:PRO:HG2	2.33	0.43
2:D:427:LEU:HD22	2:D:427:LEU:HA	1.76	0.43
2:D:743:ASP:C	2:D:745:ASP:H	2.27	0.43
1:E:281:ASP:HB2	1:E:284:ILE:HG13	2.01	0.43
1:E:535:LYS:HE2	1:E:535:LYS:HB3	1.82	0.43
2:F:677:LEU:HD23	2:F:677:LEU:HA	1.80	0.43
2:F:778:VAL:HG22	2:F:857:ILE:HG23	2.00	0.43
2:F:840:ILE:HA	2:F:843:MET:HE2	2.01	0.43
1:G:549:LEU:N	1:G:549:LEU:CD1	2.81	0.43
3:K:387:VAL:HA	5:L:1788:ASN:HD21	1.83	0.43
7:U:218:TYR:O	7:U:255:PHE:HA	2.19	0.43
11:c:160:ARG:O	11:c:162:PRO:HD3	2.19	0.43
11:j:52:PHE:HE1	11:j:62:PRO:HG3	1.82	0.43
11:j:260:LEU:HD21	11:j:321:LEU:HB2	2.00	0.43
1:A:582:LEU:HD23	1:A:582:LEU:HA	1.86	0.43
1:C:252:VAL:HG21	1:C:261:VAL:HG11	2.00	0.43
1:E:566:GLU:OE2	1:E:578:ARG:NE	2.51	0.43
1:G:276:VAL:HG23	1:G:277:ASP:N	2.31	0.43
2:H:256:TYR:CE2	3:I:37:SER:OG	2.71	0.43
2:H:294:LEU:HD23	2:H:294:LEU:HA	1.88	0.43
2:H:840:ILE:HA	2:H:843:MET:HE2	2.01	0.43
3:I:35:HIS:CG	3:I:36:PRO:CD	2.95	0.43
4:J:470:ARG:N	4:J:471:PRO:HD2	2.34	0.43
4:J:904:ARG:HA	4:J:904:ARG:HD2	1.78	0.43
3:K:124:TYR:O	3:K:124:TYR:CD1	2.70	0.43
3:K:582:LEU:HA	3:K:585:ILE:HG13	2.00	0.43
5:L:441:GLN:O	5:L:445:ALA:N	2.51	0.43
5:L:1554:LEU:HD13	5:L:1574:LEU:HB2	2.00	0.43
5:L:1623:LEU:HD12	5:L:1623:LEU:HA	1.90	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:40:PHE:CB	11:a:366:TYR:HD1	2.29	0.43
11:a:372:ARG:HD2	11:a:372:ARG:HA	1.91	0.43
11:c:128:GLY:O	11:d:299:GLN:OE1	2.36	0.43
11:d:242:THR:HG21	11:d:256:LEU:HD11	2.00	0.43
11:e:124:ARG:NH2	11:f:301:LYS:HD3	2.33	0.43
11:h:298:LEU:N	11:h:298:LEU:CD2	2.81	0.43
2:B:606:ARG:HE	11:c:339:ARG:HE	1.65	0.43
1:C:422:TRP:CG	1:C:422:TRP:O	2.70	0.43
2:D:592:LEU:HD23	2:D:592:LEU:HA	1.84	0.43
2:H:743:ASP:C	2:H:745:ASP:H	2.27	0.43
3:I:46:CYS:C	3:I:48:LEU:N	2.76	0.43
4:J:288:GLN:NE2	4:J:297:ARG:HG3	2.33	0.43
4:J:297:ARG:HG2	4:J:298:ASN:H	1.84	0.43
4:J:905:ILE:HD13	4:J:940:ARG:HB3	2.00	0.43
3:K:530:TYR:O	3:K:531:LEU:HB3	2.19	0.43
1:M:673:MET:CE	1:M:730:MET:CE	2.96	0.43
1:M:723:TYR:HB3	1:M:886:ARG:NH1	2.33	0.43
11:f:242:THR:HG21	11:f:256:LEU:HD11	2.00	0.43
11:i:392:CYS:HB3	11:i:425:ARG:NH1	2.34	0.43
11:j:186:TYR:CE2	11:j:398:LEU:HD23	2.54	0.43
11:j:318:ILE:HB	11:j:380:ASN:HB3	2.00	0.43
11:m:127:ASP:OD1	11:m:127:ASP:N	2.51	0.43
2:H:260:GLY:HA3	2:H:302:ASN:OD1	2.18	0.43
3:I:38:GLU:C	3:I:40:SER:N	2.76	0.43
3:I:622:SER:OG	3:I:623:SER:N	2.52	0.43
3:K:527:LEU:HD12	3:K:646:LEU:HB3	2.01	0.43
5:L:1515:PHE:HE2	5:L:1569:ALA:HA	1.84	0.43
1:M:683:LEU:O	1:M:686:VAL:HG12	2.19	0.43
11:d:444:ILE:O	11:d:445:SER:OG	2.27	0.43
11:i:6:ILE:HD11	11:i:135:PHE:CE2	2.53	0.43
11:i:186:TYR:OH	11:i:398:LEU:CB	2.67	0.43
11:j:104:TRP:CE3	11:j:190:LEU:HD13	2.54	0.43
11:m:160:ARG:O	11:m:162:PRO:HD3	2.19	0.43
1:E:788:ASN:O	1:E:791:GLN:HB2	2.19	0.43
3:K:579:PHE:O	3:K:583:ASN:HB2	2.19	0.43
11:b:132:LEU:HA	11:b:132:LEU:HD12	1.87	0.43
11:j:160:ARG:O	11:j:162:PRO:HD3	2.18	0.43
11:j:272:GLY:N	11:j:377:MET:O	2.51	0.43
1:A:535:LYS:HB3	1:A:535:LYS:HE2	1.82	0.43
2:B:319:LEU:N	2:B:445:GLU:OE2	2.42	0.43
2:B:599:GLY:O	2:B:603:THR:OG1	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:684:CYS:SG	11:e:254:ILE:HG12	2.58	0.43
11:a:231:LEU:HD12	11:a:231:LEU:HA	1.87	0.43
11:c:127:ASP:N	11:c:127:ASP:OD1	2.51	0.43
11:f:214:ALA:O	11:f:219:HIS:N	2.52	0.43
11:h:376:LEU:C	11:h:376:LEU:CD2	2.92	0.43
11:i:225:PHE:HA	11:i:228:ILE:HG12	2.00	0.43
11:k:115:HIS:CE1	11:k:119:PHE:HE2	2.37	0.43
1:C:723:TYR:CG	11:c:249:MET:HE1	2.54	0.42
1:E:647:ASP:OD1	1:E:648:TYR:N	2.51	0.42
2:F:251:VAL:HG12	2:F:346:LEU:CD1	2.49	0.42
2:F:257:VAL:HG11	2:F:295:SER:HB2	2.00	0.42
2:F:501:THR:O	2:F:501:THR:OG1	2.30	0.42
2:F:653:THR:C	2:F:655:GLU:H	2.27	0.42
2:H:398:SER:OG	2:H:473:SER:HB2	2.19	0.42
3:K:406:ASP:OD1	3:K:406:ASP:N	2.51	0.42
5:L:1562:LEU:HD13	11:l:47:ARG:HG3	2.00	0.42
11:a:39:GLU:HG2	11:a:40:PHE:H	1.82	0.42
11:c:77:ILE:O	11:c:80:SER:OG	2.33	0.42
11:j:291:LEU:HD22	11:j:339:ARG:HD2	2.00	0.42
1:A:741:LEU:HD22	1:A:750:VAL:HG22	2.00	0.42
2:B:299:TRP:O	2:B:302:ASN:HB2	2.19	0.42
2:D:653:THR:C	2:D:655:GLU:H	2.27	0.42
2:D:778:VAL:HG22	2:D:857:ILE:HG23	2.01	0.42
2:D:840:ILE:HA	2:D:843:MET:HE2	2.01	0.42
1:E:547:TYR:CG	1:E:601:LEU:HD11	2.53	0.42
2:F:476:THR:HG23	2:F:479:GLN:H	1.84	0.42
2:F:662:ARG:NH2	2:F:764:LEU:O	2.53	0.42
2:H:476:THR:HG23	2:H:479:GLN:H	1.84	0.42
11:a:115:HIS:CE1	11:a:119:PHE:HD2	2.37	0.42
11:e:245:TYR:CE1	11:e:362:ARG:O	2.73	0.42
11:g:392:CYS:CA	11:g:425:ARG:HH12	2.32	0.42
11:h:376:LEU:HD23	11:h:377:MET:N	2.34	0.42
11:j:188:SER:O	11:j:192:LEU:HG	2.19	0.42
11:j:294:MET:HE1	11:j:337:LEU:HD23	2.01	0.42
1:A:312:GLU:N	1:A:312:GLU:CD	2.76	0.42
2:B:255:LEU:HA	2:B:255:LEU:HD23	1.86	0.42
1:C:257:ASP:HB2	2:D:289:ASP:OD2	2.18	0.42
2:D:398:SER:OG	2:D:473:SER:HB2	2.19	0.42
2:F:322:GLN:O	2:F:326:ALA:N	2.47	0.42
2:F:562:MET:SD	2:F:660:TYR:HE2	2.41	0.42
2:F:606:ARG:HE	11:g:339:ARG:HE	1.65	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:333:ILE:CG1	2:H:369:VAL:HG23	2.48	0.42
1:G:683:LEU:O	1:G:686:VAL:HG12	2.19	0.42
4:J:477:ASP:O	4:J:481:VAL:HG22	2.19	0.42
3:K:111:PHE:CE1	3:K:117:LEU:HD23	2.55	0.42
3:K:524:VAL:HG23	3:K:647:ARG:HH22	1.84	0.42
3:K:650:TYR:CD2	11:k:348:PHE:HB3	2.55	0.42
5:L:535:PHE:HB3	5:L:552:PHE:CE1	2.54	0.42
11:d:184:GLN:OE1	11:d:184:GLN:N	2.47	0.42
11:e:190:LEU:HD23	11:e:190:LEU:HA	1.93	0.42
11:e:247:GLY:O	11:e:251:ASN:OD1	2.37	0.42
11:j:297:LEU:CD2	11:j:377:MET:HB2	2.49	0.42
11:m:139:HIS:O	11:m:170:SER:HA	2.20	0.42
11:m:293:VAL:O	11:m:297:LEU:HG	2.20	0.42
1:A:474:MET:HE1	1:A:513:VAL:HA	2.01	0.42
1:A:566:GLU:OE2	1:A:578:ARG:NE	2.51	0.42
2:B:398:SER:OG	2:B:473:SER:HB2	2.19	0.42
2:B:401:HIS:ND1	2:B:401:HIS:O	2.53	0.42
2:B:501:THR:O	2:B:501:THR:OG1	2.30	0.42
2:B:662:ARG:NH2	2:B:764:LEU:O	2.53	0.42
1:E:334:LEU:O	1:E:338:LEU:HD13	2.20	0.42
1:G:716:ASN:OD1	1:G:720:ASN:ND2	2.52	0.42
2:H:717:GLN:HG3	2:H:879:ARG:HB3	2.02	0.42
3:I:190:TRP:HD1	3:I:195:LEU:C	2.27	0.42
1:M:723:TYR:CG	11:m:249:MET:HE1	2.54	0.42
11:c:265:ARG:O	11:c:267:HIS:ND1	2.50	0.42
11:g:107:GLY:HA3	11:g:148:GLY:HA3	2.00	0.42
11:h:392:CYS:HB3	11:h:425:ARG:HH12	1.84	0.42
2:B:476:THR:HG23	2:B:479:GLN:H	1.84	0.42
1:C:683:LEU:O	1:C:686:VAL:HG12	2.19	0.42
1:C:716:ASN:ND2	11:c:353:PRO:O	2.52	0.42
2:F:459:LEU:HG	2:F:459:LEU:O	2.20	0.42
2:F:741:ALA:HB1	2:F:746:HIS:HB2	2.02	0.42
2:H:252:ARG:HD3	3:I:35:HIS:NE2	2.34	0.42
11:a:5:ILE:HD13	11:a:253:LEU:HD22	2.01	0.42
11:b:214:ALA:O	11:b:219:HIS:N	2.52	0.42
11:d:192:LEU:HD23	11:d:192:LEU:HA	1.86	0.42
11:g:160:ARG:O	11:g:162:PRO:HD3	2.19	0.42
11:g:265:ARG:O	11:g:267:HIS:ND1	2.50	0.42
11:h:242:THR:HG21	11:h:256:LEU:HD11	2.01	0.42
11:m:392:CYS:CA	11:m:425:ARG:HH12	2.32	0.42
1:A:334:LEU:O	1:A:338:LEU:HD13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:553:TYR:CE2	2:B:647:PRO:HG2	2.55	0.42
2:D:553:TYR:CE2	2:D:647:PRO:HG2	2.55	0.42
2:F:553:TYR:CE2	2:F:647:PRO:HG2	2.55	0.42
2:H:662:ARG:NH2	2:H:764:LEU:O	2.53	0.42
2:H:778:VAL:HG22	2:H:857:ILE:HG23	2.01	0.42
3:K:42:LEU:HD21	3:K:119:ILE:HG21	2.02	0.42
5:L:546:ARG:NE	1:M:395:THR:HG23	2.29	0.42
5:L:1678:ASN:O	5:L:1683:VAL:HG22	2.20	0.42
1:M:716:ASN:OD1	1:M:720:ASN:ND2	2.52	0.42
11:c:392:CYS:CA	11:c:425:ARG:HH12	2.32	0.42
11:d:392:CYS:HB3	11:d:425:ARG:HH12	1.84	0.42
11:e:294:MET:SD	11:e:336:SER:OG	2.67	0.42
11:j:172:PHE:O	11:j:207:ASN:ND2	2.53	0.42
11:k:171:VAL:HG23	11:k:171:VAL:O	2.19	0.42
2:B:449:ALA:HB2	2:B:467:ARG:HD2	2.02	0.42
1:C:716:ASN:OD1	1:C:720:ASN:ND2	2.52	0.42
2:D:459:LEU:O	2:D:459:LEU:HG	2.20	0.42
2:D:476:THR:HG23	2:D:479:GLN:H	1.84	0.42
2:F:833:ILE:O	2:F:837:LYS:HG2	2.20	0.42
1:G:547:TYR:CD2	1:G:601:LEU:HD11	2.54	0.42
2:H:401:HIS:ND1	2:H:401:HIS:O	2.53	0.42
2:H:459:LEU:HG	2:H:459:LEU:O	2.19	0.42
2:H:553:TYR:CE2	2:H:647:PRO:HG2	2.55	0.42
3:I:35:HIS:HD1	3:I:36:PRO:CD	2.23	0.42
3:K:31:PHE:HD1	3:K:34:LEU:HD21	1.84	0.42
3:K:385:THR:HG23	3:K:387:VAL:HG12	2.02	0.42
3:K:587:ASP:HA	3:K:590:HIS:CD2	2.53	0.42
3:K:605:GLU:O	3:K:606:ARG:HG2	2.18	0.42
2:T:653:THR:C	2:T:655:GLU:H	2.28	0.42
11:c:139:HIS:O	11:c:170:SER:HA	2.20	0.42
11:e:422:ASP:HA	11:e:425:ARG:HB3	2.02	0.42
11:i:395:TYR:CE2	11:i:425:ARG:HD3	2.55	0.42
11:k:12:GLN:HE21	11:k:16:GLN:HE22	1.66	0.42
11:m:107:GLY:HA3	11:m:148:GLY:HA3	2.00	0.42
1:E:281:ASP:HB2	1:E:284:ILE:CG1	2.50	0.42
1:E:474:MET:HE1	1:E:513:VAL:HA	2.01	0.42
1:G:716:ASN:ND2	11:g:353:PRO:O	2.52	0.42
2:H:653:THR:C	2:H:655:GLU:H	2.27	0.42
3:I:51:ASP:O	3:I:55:PHE:CD2	2.72	0.42
3:K:3:HIS:O	3:K:7:LEU:HG	2.20	0.42
2:T:743:ASP:C	2:T:745:ASP:H	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:321:LEU:N	11:a:378:MET:O	2.40	0.42
11:e:119:PHE:HD2	11:e:160:ARG:HH11	1.68	0.42
11:e:355:SER:OG	11:e:356:ILE:N	2.53	0.42
11:g:51:PHE:HD2	11:g:244:ARG:HG2	1.85	0.42
11:j:270:MET:HE2	11:j:305:VAL:HG21	2.01	0.42
2:F:387:HIS:CG	2:F:403:TYR:CE1	3.08	0.42
2:F:743:ASP:C	2:F:745:ASP:H	2.27	0.42
1:G:262:SER:OG	1:G:263:ALA:N	2.53	0.42
1:G:548:PHE:CZ	1:G:648:TYR:HB2	2.55	0.42
1:G:550:MET:CG	1:G:556:PHE:CZ	2.95	0.42
1:G:669:LEU:HD13	1:G:730:MET:CE	2.50	0.42
1:G:723:TYR:CG	11:g:249:MET:HE1	2.54	0.42
2:H:833:ILE:O	2:H:837:LYS:HG2	2.20	0.42
3:I:1:MET:HE3	3:I:1:MET:HB3	1.84	0.42
3:I:97:LEU:HD12	3:I:100:TYR:HB3	2.02	0.42
4:J:641:VAL:C	4:J:644:PRO:HD2	2.45	0.42
5:L:1515:PHE:CD2	5:L:1572:LEU:HD11	2.55	0.42
11:a:270:MET:HE2	11:a:305:VAL:HG21	2.01	0.42
11:d:388:PHE:HB2	11:d:432:ILE:HD11	2.02	0.42
11:e:270:MET:HE2	11:e:305:VAL:HG21	2.01	0.42
11:h:184:GLN:OE1	11:h:184:GLN:N	2.47	0.42
11:l:317:TYR:HD2	11:l:320:ILE:HD11	1.85	0.42
11:m:392:CYS:HA	11:m:425:ARG:HH12	1.85	0.42
1:A:514:GLU:OE2	1:A:518:LYS:NZ	2.53	0.42
2:B:373:ASP:C	2:B:375:LYS:H	2.27	0.42
2:B:459:LEU:HG	2:B:459:LEU:O	2.20	0.42
2:B:618:LEU:HD23	2:B:618:LEU:HA	1.91	0.42
2:B:743:ASP:C	2:B:745:ASP:H	2.27	0.42
1:C:430:ASP:OD1	1:C:434:GLU:HG2	2.20	0.42
1:C:583:LEU:O	1:C:587:LEU:HG	2.20	0.42
1:E:741:LEU:HD22	1:E:750:VAL:HG22	2.00	0.42
2:F:290:THR:O	2:F:294:LEU:N	2.53	0.42
1:G:679:VAL:HG21	1:G:780:MET:CE	2.50	0.42
3:I:527:LEU:HD11	11:i:355:SER:HB3	2.02	0.42
4:J:302:VAL:HG12	4:J:303:THR:N	2.35	0.42
3:K:652:LYS:HD2	11:k:353:PRO:HB3	2.01	0.42
1:M:262:SER:OG	1:M:263:ALA:N	2.53	0.42
1:M:723:TYR:CD2	11:m:249:MET:HE1	2.55	0.42
11:c:137:LEU:HG	11:c:139:HIS:HD2	1.85	0.42
11:f:392:CYS:HB3	11:f:425:ARG:HH12	1.84	0.42
11:g:62:PRO:HD3	11:g:85:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:g:332:GLN:O	11:g:335:LYS:HB3	2.20	0.42
11:i:321:LEU:HD12	11:i:322:ASN:H	1.85	0.42
11:j:209:ALA:HA	11:j:212:ARG:HD2	2.01	0.42
11:j:275:PRO:HG3	11:j:375:GLY:H	1.85	0.42
1:A:484:TYR:OH	1:A:748:ASP:OD2	2.33	0.41
1:A:788:ASN:O	1:A:791:GLN:HB2	2.19	0.41
2:D:662:ARG:NH2	2:D:764:LEU:O	2.53	0.41
1:E:514:GLU:OE2	1:E:518:LYS:NZ	2.53	0.41
1:E:685:SER:O	1:E:688:ILE:HG22	2.20	0.41
2:F:332:LEU:HD23	2:F:332:LEU:HA	1.92	0.41
2:H:402:ALA:O	6:R:23:UNK:CB	2.68	0.41
3:I:402:LYS:HE3	3:I:402:LYS:HB2	1.82	0.41
3:I:533:VAL:O	3:I:537:GLU:HB2	2.20	0.41
4:J:942:LEU:C	4:J:943:LEU:HD12	2.45	0.41
5:L:502:LEU:HD11	5:L:529:CYS:HB3	2.01	0.41
1:M:673:MET:HE1	1:M:730:MET:SD	2.60	0.41
1:M:679:VAL:HG21	1:M:780:MET:CE	2.50	0.41
11:b:392:CYS:HB3	11:b:425:ARG:HH12	1.84	0.41
11:g:127:ASP:OD1	11:g:127:ASP:N	2.51	0.41
11:g:139:HIS:O	11:g:170:SER:HA	2.20	0.41
11:i:46:ASP:OD1	11:i:46:ASP:N	2.42	0.41
11:j:4:GLU:HG2	11:j:50:VAL:HA	2.02	0.41
11:j:301:LYS:HD3	11:j:301:LYS:HA	1.86	0.41
11:k:322:ASN:HB2	11:k:358:VAL:HA	2.02	0.41
11:l:143:GLY:HA2	11:l:187:ASN:CB	2.50	0.41
11:l:351:TRP:CD1	11:l:351:TRP:H	2.37	0.41
1:A:685:SER:O	1:A:688:ILE:HG22	2.20	0.41
2:B:833:ILE:O	2:B:837:LYS:HG2	2.20	0.41
1:C:262:SER:OG	1:C:263:ALA:N	2.53	0.41
2:D:741:ALA:HB1	2:D:746:HIS:HB2	2.02	0.41
1:E:297:SER:HB3	1:E:363:MET:O	2.20	0.41
1:G:595:ASP:HB3	1:G:598:LYS:HB3	2.01	0.41
1:G:610:LEU:HD12	1:G:610:LEU:HA	1.90	0.41
3:K:33:PHE:CD1	3:K:33:PHE:N	2.88	0.41
3:K:484:VAL:HA	3:K:487:VAL:HG12	2.02	0.41
5:L:1806:ASN:OD1	5:L:1807:TYR:N	2.46	0.41
11:c:392:CYS:HA	11:c:425:ARG:HH12	1.85	0.41
11:e:193:LYS:HG3	11:e:427:ILE:HG21	2.02	0.41
11:f:171:VAL:HG11	13:f:501:GDP:N2	2.35	0.41
11:g:84:LYS:HA	11:h:219:HIS:NE2	2.35	0.41
11:i:36:ILE:HD12	11:i:36:ILE:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:m:137:LEU:HG	11:m:139:HIS:HD2	1.85	0.41
1:C:550:MET:HA	1:C:556:PHE:CE2	2.56	0.41
1:C:723:TYR:CD2	11:c:249:MET:HE1	2.55	0.41
2:D:401:HIS:ND1	2:D:401:HIS:O	2.53	0.41
1:E:272:ARG:HD3	1:E:272:ARG:HA	1.94	0.41
2:H:324:PHE:CA	2:H:422:VAL:HG22	2.50	0.41
2:H:412:ARG:O	2:H:416:GLN:HB2	2.20	0.41
2:H:711:MET:HE3	2:H:711:MET:HB2	1.96	0.41
3:K:38:GLU:O	3:K:41:VAL:HG12	2.20	0.41
3:K:133:PHE:HA	3:K:136:VAL:HG12	2.01	0.41
1:M:430:ASP:OD1	1:M:434:GLU:HG2	2.20	0.41
11:a:124:ARG:HH22	11:b:301:LYS:CD	2.24	0.41
11:a:355:SER:OG	11:a:356:ILE:N	2.53	0.41
11:c:293:VAL:O	11:c:297:LEU:HG	2.20	0.41
11:f:297:LEU:HD13	11:f:377:MET:HB2	2.02	0.41
1:C:276:VAL:HG23	1:C:277:ASP:N	2.31	0.41
2:D:252:ARG:HG3	1:E:238:LEU:HD21	2.03	0.41
2:D:833:ILE:O	2:D:837:LYS:HG2	2.20	0.41
2:D:864:LEU:HD23	2:D:864:LEU:HA	1.93	0.41
1:E:555:PHE:HZ	1:E:583:LEU:HD13	1.80	0.41
2:H:305:ARG:HA	2:H:305:ARG:HD2	1.76	0.41
2:H:741:ALA:HB1	2:H:746:HIS:HB2	2.02	0.41
2:H:882:PHE:CE1	11:h:341:ARG:HB2	2.56	0.41
3:I:470:VAL:HG21	3:I:560:HIS:HE1	1.85	0.41
11:e:231:LEU:HD12	11:e:231:LEU:HA	1.87	0.41
11:e:392:CYS:SG	11:e:425:ARG:NH1	2.93	0.41
11:h:217:ARG:NH1	11:h:276:LEU:HB2	2.31	0.41
11:i:238:ALA:HA	11:i:325:GLN:HE22	1.86	0.41
11:k:374:SER:OG	11:k:375:GLY:N	2.53	0.41
11:l:429:GLN:HA	11:l:432:ILE:HG22	2.03	0.41
11:m:338:GLN:O	11:m:342:GLU:HG2	2.21	0.41
1:A:556:PHE:HB3	1:A:560:MET:HE3	2.02	0.41
2:B:753:VAL:O	2:B:757:THR:HG23	2.20	0.41
1:C:610:LEU:HD12	1:C:610:LEU:HA	1.90	0.41
2:D:449:ALA:HB2	2:D:467:ARG:HD2	2.01	0.41
2:F:882:PHE:CE1	11:f:341:ARG:HB2	2.56	0.41
1:G:256:VAL:HG21	2:H:289:ASP:CB	2.49	0.41
1:G:673:MET:CE	1:G:730:MET:SD	3.05	0.41
2:H:315:ARG:HG2	2:H:315:ARG:O	2.21	0.41
2:H:479:GLN:NE2	2:H:531:GLN:OE1	2.44	0.41
3:I:107:LEU:O	3:I:111:PHE:HD1	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:408:GLN:NE2	4:J:456:GLN:HG2	2.35	0.41
4:J:469:VAL:HG22	4:J:473:LEU:HD23	2.02	0.41
4:J:550:SER:HA	4:J:553:LYS:HB2	2.02	0.41
4:J:637:GLU:O	4:J:641:VAL:HG23	2.21	0.41
3:K:158:TYR:O	3:K:161:SER:OG	2.30	0.41
5:L:433:THR:HG22	5:L:437:ARG:HH12	1.85	0.41
5:L:1545:LEU:HD23	5:L:1545:LEU:HA	1.90	0.41
5:L:1779:LEU:O	5:L:1783:VAL:HG12	2.21	0.41
5:L:1804:PHE:HE2	11:l:348:PHE:CE1	2.39	0.41
1:M:314:GLY:N	1:M:318:HIS:NE2	2.67	0.41
11:a:193:LYS:HG3	11:a:427:ILE:HG21	2.02	0.41
11:b:192:LEU:HD23	11:b:192:LEU:HA	1.86	0.41
11:b:297:LEU:HD13	11:b:377:MET:HB2	2.02	0.41
11:f:132:LEU:HD12	11:f:132:LEU:HA	1.87	0.41
11:f:396:ASP:OD2	11:f:425:ARG:NH2	2.53	0.41
2:B:883:ASN:OD1	2:B:883:ASN:C	2.64	0.41
1:C:550:MET:HA	1:C:556:PHE:HE2	1.85	0.41
2:D:883:ASN:OD1	2:D:883:ASN:C	2.64	0.41
1:G:723:TYR:CD2	11:g:249:MET:HE1	2.55	0.41
2:H:326:ALA:HB2	3:I:165:LEU:HD22	2.03	0.41
2:H:677:LEU:HD23	2:H:677:LEU:HA	1.80	0.41
3:I:394:VAL:O	3:I:398:GLN:HG2	2.20	0.41
4:J:361:TYR:HE1	4:J:436:LEU:HD22	1.85	0.41
3:K:321:SER:OG	3:K:324:ASP:HB2	2.21	0.41
5:L:359:VAL:HG21	5:L:368:PHE:CZ	2.56	0.41
5:L:513:CYS:HG	5:L:514:SER:N	2.18	0.41
5:L:1578:TYR:HB3	5:L:1593:CYS:SG	2.61	0.41
11:a:39:GLU:CD	11:a:39:GLU:H	2.29	0.41
11:a:422:ASP:HA	11:a:425:ARG:HB3	2.02	0.41
11:d:274:THR:CG2	11:d:275:PRO:HD3	2.50	0.41
11:i:241:THR:HA	11:i:244:ARG:NH2	2.36	0.41
11:k:264:PRO:O	11:k:267:HIS:ND1	2.47	0.41
11:k:376:LEU:HD12	11:k:377:MET:N	2.35	0.41
11:l:165:LEU:HD12	11:l:166:VAL:H	1.85	0.41
1:A:272:ARG:HD3	1:A:272:ARG:HA	1.94	0.41
1:A:297:SER:HB3	1:A:363:MET:O	2.20	0.41
2:B:653:THR:C	2:B:655:GLU:H	2.27	0.41
2:F:412:ARG:O	2:F:416:GLN:HB2	2.20	0.41
1:G:531:LEU:HD12	1:G:747:ILE:HD11	2.03	0.41
3:I:359:ASP:HA	3:I:364:GLY:HA3	2.01	0.41
1:M:673:MET:HE1	1:M:730:MET:HE1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:726:MET:SD	11:m:249:MET:HE2	2.60	0.41
11:b:396:ASP:OD2	11:b:425:ARG:NH2	2.53	0.41
11:c:50:VAL:O	11:c:63:ARG:NH1	2.54	0.41
11:g:338:GLN:O	11:g:342:GLU:HG2	2.21	0.41
11:m:192:LEU:HD23	11:m:192:LEU:HA	1.94	0.41
2:B:603:THR:HA	2:B:606:ARG:HH11	1.85	0.41
2:B:741:ALA:HB1	2:B:746:HIS:HB2	2.02	0.41
1:C:248:ASP:OD1	1:C:259:ARG:N	2.50	0.41
4:J:273:GLU:HA	4:J:276:TRP:HE3	1.85	0.41
1:M:248:ASP:OD2	1:M:260:TYR:N	2.33	0.41
11:a:392:CYS:SG	11:a:425:ARG:NH1	2.93	0.41
11:g:137:LEU:HG	11:g:139:HIS:HD2	1.85	0.41
11:g:293:VAL:O	11:g:297:LEU:HG	2.20	0.41
11:k:169:TYR:CD2	11:k:236:MET:HG2	2.55	0.41
11:l:165:LEU:HD23	11:l:253:LEU:HD23	2.03	0.41
11:l:206:ASP:OD1	11:l:206:ASP:N	2.44	0.41
11:l:268:PHE:CE2	11:l:388:PHE:HZ	2.39	0.41
11:l:321:LEU:HD23	11:l:321:LEU:HA	1.79	0.41
1:A:604:ASP:HB2	1:A:647:ASP:HB2	2.03	0.41
1:A:751:LEU:HD23	1:A:751:LEU:HA	1.96	0.41
2:B:246:THR:HG23	2:B:249:ALA:H	1.86	0.41
2:B:849:ILE:HD12	2:B:849:ILE:HA	1.92	0.41
2:B:882:PHE:CE1	11:b:341:ARG:HB2	2.56	0.41
1:C:252:VAL:HG21	1:C:261:VAL:HB	2.01	0.41
2:D:433:TRP:CE2	2:D:448:VAL:HG11	2.56	0.41
2:D:717:GLN:HG3	2:D:879:ARG:HB3	2.02	0.41
2:D:882:PHE:CE1	11:d:341:ARG:HB2	2.56	0.41
1:E:318:HIS:CG	2:F:406:THR:O	2.73	0.41
2:F:603:THR:HA	2:F:606:ARG:HH11	1.85	0.41
2:F:711:MET:HE3	2:F:711:MET:HB2	1.96	0.41
2:H:578:MET:HE2	2:H:578:MET:HB3	1.98	0.41
3:K:12:TYR:CD2	5:L:396:LEU:HD12	2.56	0.41
3:K:203:PHE:HE2	3:K:205:ILE:HD12	1.85	0.41
3:K:359:ASP:OD2	3:K:365:ARG:NH2	2.54	0.41
3:K:533:VAL:O	3:K:537:GLU:HB2	2.21	0.41
5:L:533:THR:O	5:L:537:HIS:N	2.54	0.41
5:L:1654:GLN:HG2	5:L:1759:HIS:CG	2.56	0.41
5:L:1794:HIS:CG	5:L:1795:LEU:N	2.89	0.41
1:M:583:LEU:HD22	1:M:603:ILE:HD11	2.03	0.41
1:M:659:ASN:OD1	1:M:659:ASN:N	2.54	0.41
1:M:716:ASN:ND2	11:m:353:PRO:O	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:747:ILE:HD13	1:M:747:ILE:HA	1.90	0.41
11:b:157:LEU:HD23	11:b:157:LEU:HA	1.91	0.41
11:d:396:ASP:OD2	11:d:425:ARG:NH2	2.53	0.41
11:e:5:ILE:HD13	11:e:253:LEU:HD22	2.02	0.41
11:e:119:PHE:O	11:e:122:ILE:N	2.54	0.41
11:f:388:PHE:HB2	11:f:432:ILE:HD11	2.02	0.41
11:h:132:LEU:HA	11:h:132:LEU:HD12	1.87	0.41
11:h:388:PHE:HB2	11:h:432:ILE:HD11	2.02	0.41
11:i:344:LYS:O	11:i:344:LYS:HG2	2.20	0.41
11:j:291:LEU:HG	11:j:295:ARG:NH1	2.36	0.41
11:j:347:ASN:OD1	11:j:347:ASN:N	2.54	0.41
11:k:214:ALA:O	11:k:219:HIS:N	2.54	0.41
11:l:146:GLY:CA	11:l:149:LEU:HB2	2.47	0.41
11:l:170:SER:HB3	11:l:202:LEU:HD11	2.02	0.41
11:l:374:SER:OG	11:l:375:GLY:N	2.53	0.41
11:l:424:SER:O	11:l:428:VAL:HG22	2.21	0.41
1:A:277:ASP:HB3	1:A:280:LEU:HB2	2.02	0.41
2:B:412:ARG:O	2:B:416:GLN:HB2	2.20	0.41
1:C:535:LYS:HB3	1:C:535:LYS:HE2	1.84	0.41
1:C:589:MET:O	1:C:589:MET:SD	2.79	0.41
2:D:412:ARG:O	2:D:416:GLN:HB2	2.20	0.41
1:E:604:ASP:HB2	1:E:647:ASP:HB2	2.03	0.41
2:F:293:ARG:NH2	6:Q:37:UNK:O	2.54	0.41
2:F:883:ASN:OD1	2:F:883:ASN:C	2.64	0.41
1:G:545:LYS:HG3	1:G:549:LEU:HB2	2.03	0.41
3:I:110:GLU:OE1	3:I:110:GLU:N	2.54	0.41
4:J:375:PHE:HD1	4:J:405:ARG:HD2	1.85	0.41
1:M:316:VAL:C	1:M:318:HIS:H	2.29	0.41
11:c:338:GLN:O	11:c:342:GLU:HG2	2.21	0.41
11:f:274:THR:CG2	11:f:275:PRO:HD3	2.50	0.41
11:h:396:ASP:OD2	11:h:425:ARG:NH2	2.53	0.41
11:k:154:LEU:CD1	11:k:195:LEU:HD23	2.51	0.41
2:B:717:GLN:HG3	2:B:879:ARG:HB3	2.02	0.40
1:C:324:MET:HE3	1:C:324:MET:HB2	1.96	0.40
1:C:339:GLU:CD	2:D:365:ARG:HB2	2.47	0.40
1:E:304:PHE:CD2	1:E:304:PHE:C	2.99	0.40
1:E:541:LEU:HB3	1:E:734:TRP:HH2	1.86	0.40
1:G:387:LEU:HB3	1:G:408:THR:OG1	2.21	0.40
1:G:566:GLU:OE2	1:G:578:ARG:NE	2.55	0.40
3:I:373:ILE:HD11	3:I:482:LEU:HD11	2.02	0.40
4:J:724:ARG:HH11	4:J:914:GLN:NE2	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:40:PHE:CG	11:a:366:TYR:HD1	2.34	0.40
11:b:388:PHE:HB2	11:b:432:ILE:HD11	2.02	0.40
11:i:377:MET:SD	11:i:379:ALA:HB2	2.61	0.40
11:i:436:HIS:O	11:i:439:THR:HG22	2.20	0.40
1:A:541:LEU:HB3	1:A:734:TRP:HH2	1.87	0.40
2:F:717:GLN:HG3	2:F:879:ARG:HB3	2.02	0.40
1:G:430:ASP:OD1	1:G:434:GLU:HG2	2.20	0.40
3:I:333:ARG:HD3	3:I:554:GLU:CD	2.46	0.40
3:I:605:GLU:O	3:I:606:ARG:HG2	2.22	0.40
3:K:31:PHE:O	3:K:34:LEU:HG	2.21	0.40
3:K:61:GLN:O	3:K:63:THR:HG23	2.22	0.40
1:M:368:SER:HA	1:M:371:THR:HG21	2.01	0.40
1:M:387:LEU:HB3	1:M:408:THR:OG1	2.21	0.40
1:M:550:MET:HG2	1:M:556:PHE:CE2	2.56	0.40
1:M:566:GLU:OE2	1:M:578:ARG:NE	2.55	0.40
11:a:253:LEU:O	11:a:257:ILE:HG12	2.21	0.40
11:d:297:LEU:HD13	11:d:377:MET:HB2	2.02	0.40
11:f:184:GLN:OE1	11:f:184:GLN:N	2.47	0.40
11:l:46:ASP:OD1	11:l:46:ASP:N	2.46	0.40
11:l:48:LYS:HD2	11:l:60:TYR:CZ	2.57	0.40
11:l:120:ASP:OD2	11:m:301:LYS:HE3	2.21	0.40
11:l:320:ILE:HB	11:l:356:ILE:HG13	2.03	0.40
11:l:376:LEU:HD23	11:l:377:MET:N	2.37	0.40
11:m:50:VAL:O	11:m:63:ARG:NH1	2.54	0.40
1:A:274:PHE:HE2	1:A:296:ALA:HB2	1.86	0.40
2:B:711:MET:HE3	2:B:711:MET:HB2	1.96	0.40
1:C:387:LEU:HB3	1:C:408:THR:OG1	2.21	0.40
2:D:332:LEU:C	2:D:336:TYR:HD2	2.25	0.40
1:G:544:ILE:HG12	1:G:648:TYR:CD2	2.57	0.40
2:H:601:LEU:CD2	2:H:623:VAL:HG23	2.50	0.40
3:I:31:PHE:HA	3:I:32:PRO:HD3	1.98	0.40
4:J:360:THR:O	4:J:364:PHE:N	2.54	0.40
3:K:143:ILE:HG12	3:K:148:ILE:HD12	2.04	0.40
5:L:406:CYS:HA	5:L:409:ARG:HB2	2.03	0.40
5:L:469:GLN:HG3	5:L:517:HIS:CE1	2.56	0.40
1:M:332:LEU:HD23	1:M:332:LEU:HA	1.87	0.40
11:b:202:LEU:HD23	11:b:203:VAL:N	2.37	0.40
11:g:392:CYS:HA	11:g:425:ARG:HH12	1.85	0.40
11:k:266:LEU:HD21	11:k:318:ILE:HG21	2.02	0.40
1:A:733:THR:HG22	1:A:757:PHE:HD1	1.87	0.40
1:C:679:VAL:HG21	1:C:780:MET:CE	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:790:MET:HE3	1:C:790:MET:HB3	1.92	0.40
1:E:582:LEU:HD23	1:E:582:LEU:HA	1.86	0.40
2:F:319:LEU:N	2:F:445:GLU:OE2	2.42	0.40
2:F:449:ALA:HB2	2:F:467:ARG:HD2	2.02	0.40
2:H:601:LEU:HD12	2:H:601:LEU:O	2.21	0.40
2:H:618:LEU:HD23	2:H:618:LEU:HA	1.91	0.40
2:H:753:VAL:O	2:H:757:THR:HG23	2.20	0.40
3:I:45:LEU:HD21	3:I:123:ASN:HA	2.03	0.40
3:I:304:GLU:N	3:I:304:GLU:OE1	2.55	0.40
3:K:359:ASP:HA	3:K:364:GLY:HA3	2.02	0.40
1:M:314:GLY:CA	1:M:318:HIS:CE1	3.04	0.40
1:M:733:THR:HG22	1:M:757:PHE:CE1	2.45	0.40
11:e:39:GLU:H	11:e:39:GLU:CD	2.28	0.40
11:e:184:GLN:CD	11:e:184:GLN:H	2.30	0.40
2:B:433:TRP:CE2	2:B:448:VAL:HG11	2.56	0.40
1:C:566:GLU:OE2	1:C:578:ARG:NE	2.55	0.40
2:D:319:LEU:N	2:D:445:GLU:OE2	2.42	0.40
2:D:753:VAL:O	2:D:757:THR:HG23	2.21	0.40
1:E:274:PHE:HE2	1:E:296:ALA:HB2	1.86	0.40
1:E:289:HIS:O	1:E:293:PRO:HD3	2.22	0.40
1:E:741:LEU:HD23	1:E:741:LEU:HA	1.93	0.40
2:F:753:VAL:O	2:F:757:THR:HG23	2.20	0.40
1:G:250:LEU:O	1:G:250:LEU:HG	2.21	0.40
2:H:449:ALA:HB2	2:H:467:ARG:HD2	2.02	0.40
4:J:331:ILE:HG21	4:J:369:TYR:HD1	1.86	0.40
1:M:387:LEU:O	1:M:408:THR:OG1	2.35	0.40
11:c:3:ARG:HB3	11:c:133:GLU:HB2	2.04	0.40
11:g:132:LEU:HD21	11:g:135:PHE:HE1	1.86	0.40
11:i:25:LEU:HD12	11:i:25:LEU:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	521/930 (56%)	483 (93%)	37 (7%)	1 (0%)	43	77
1	C	521/930 (56%)	488 (94%)	32 (6%)	1 (0%)	43	77
1	E	521/930 (56%)	483 (93%)	36 (7%)	2 (0%)	30	66
1	G	521/930 (56%)	487 (94%)	34 (6%)	0	100	100
1	M	521/930 (56%)	485 (93%)	35 (7%)	1 (0%)	43	77
2	B	552/907 (61%)	530 (96%)	22 (4%)	0	100	100
2	D	552/907 (61%)	532 (96%)	20 (4%)	0	100	100
2	F	552/907 (61%)	531 (96%)	21 (4%)	0	100	100
2	H	552/907 (61%)	532 (96%)	20 (4%)	0	100	100
2	T	552/907 (61%)	531 (96%)	21 (4%)	0	100	100
3	I	531/667 (80%)	497 (94%)	32 (6%)	2 (0%)	30	66
3	K	531/667 (80%)	508 (96%)	22 (4%)	1 (0%)	43	77
4	J	456/1024 (44%)	435 (95%)	20 (4%)	1 (0%)	43	77
5	L	471/1819 (26%)	438 (93%)	33 (7%)	0	100	100
7	U	360/374 (96%)	352 (98%)	8 (2%)	0	100	100
11	a	345/451 (76%)	328 (95%)	17 (5%)	0	100	100
11	b	345/451 (76%)	327 (95%)	18 (5%)	0	100	100
11	c	345/451 (76%)	332 (96%)	13 (4%)	0	100	100
11	d	345/451 (76%)	327 (95%)	18 (5%)	0	100	100
11	e	345/451 (76%)	326 (94%)	18 (5%)	1 (0%)	36	71
11	f	345/451 (76%)	327 (95%)	18 (5%)	0	100	100
11	g	345/451 (76%)	330 (96%)	15 (4%)	0	100	100
11	h	345/451 (76%)	325 (94%)	19 (6%)	1 (0%)	36	71
11	i	345/451 (76%)	330 (96%)	15 (4%)	0	100	100
11	j	345/451 (76%)	329 (95%)	16 (5%)	0	100	100
11	k	348/451 (77%)	329 (94%)	19 (6%)	0	100	100
11	l	348/451 (77%)	329 (94%)	19 (6%)	0	100	100
11	m	345/451 (76%)	332 (96%)	13 (4%)	0	100	100
11	t	348/451 (77%)	332 (95%)	16 (5%)	0	100	100
All	All	12553/20050 (63%)	11915 (95%)	627 (5%)	11 (0%)	49	83

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	127	ASP
4	J	715	ARG
1	A	312	GLU
1	M	315	GLN
1	C	591	THR
1	E	313	TYR
11	e	160	ARG
3	K	349	ASP
1	E	398	SER
3	I	39	THR
11	h	275	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	481/816 (59%)	479 (100%)	2 (0%)	84	82
1	C	481/816 (59%)	477 (99%)	4 (1%)	73	77
1	E	481/816 (59%)	479 (100%)	2 (0%)	84	82
1	G	481/816 (59%)	475 (99%)	6 (1%)	63	73
1	M	481/816 (59%)	479 (100%)	2 (0%)	84	82
2	B	519/798 (65%)	518 (100%)	1 (0%)	87	85
2	D	519/798 (65%)	513 (99%)	6 (1%)	63	73
2	F	519/798 (65%)	515 (99%)	4 (1%)	73	77
2	H	519/798 (65%)	518 (100%)	1 (0%)	87	85
3	I	474/594 (80%)	462 (98%)	12 (2%)	42	62
3	K	474/594 (80%)	470 (99%)	4 (1%)	73	77
4	J	445/933 (48%)	443 (100%)	2 (0%)	84	82
5	L	436/1546 (28%)	436 (100%)	0	100	100
11	a	328/400 (82%)	325 (99%)	3 (1%)	70	76
11	b	328/400 (82%)	328 (100%)	0	100	100
11	c	328/400 (82%)	327 (100%)	1 (0%)	86	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	d	328/400 (82%)	328 (100%)	0	100	100
11	e	328/400 (82%)	317 (97%)	11 (3%)	32	54
11	f	328/400 (82%)	328 (100%)	0	100	100
11	g	328/400 (82%)	326 (99%)	2 (1%)	78	80
11	h	328/400 (82%)	326 (99%)	2 (1%)	78	80
11	i	328/400 (82%)	328 (100%)	0	100	100
11	j	328/400 (82%)	328 (100%)	0	100	100
11	k	328/400 (82%)	327 (100%)	1 (0%)	86	84
11	l	328/400 (82%)	328 (100%)	0	100	100
11	m	328/400 (82%)	328 (100%)	0	100	100
All	All	10574/16139 (66%)	10508 (99%)	66 (1%)	76	80

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	551	ASP
1	A	555	PHE
2	B	245	ILE
1	C	427	ILE
1	C	502	GLU
1	C	515	GLN
1	C	589	MET
2	D	245	ILE
2	D	305	ARG
2	D	323	SER
2	D	426	VAL
2	D	427	LEU
2	D	428	SER
1	E	284	ILE
1	E	318	HIS
2	F	245	ILE
2	F	293	ARG
2	F	294	LEU
2	F	413	SER
1	G	427	ILE
1	G	536	GLU
1	G	538	VAL
1	G	550	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	551	ASP
1	G	731	GLU
2	H	323	SER
3	I	33	PHE
3	I	48	LEU
3	I	97	LEU
3	I	110	GLU
3	I	112	LEU
3	I	117	LEU
3	I	130	GLN
3	I	131	LEU
3	I	132	LEU
3	I	135	SER
3	I	136	VAL
3	I	165	LEU
4	J	373	ILE
4	J	717	VAL
3	K	33	PHE
3	K	39	THR
3	K	472[A]	GLU
3	K	472[B]	GLU
1	M	427	ILE
1	M	731	GLU
11	a	28	GLU
11	a	125	GLU
11	a	361	SER
11	c	328	VAL
11	e	113	LYS
11	e	114	ILE
11	e	116	GLU
11	e	117	ASP
11	e	118	ILE
11	e	119	PHE
11	e	156	ARG
11	e	157	LEU
11	e	161	TYR
11	e	163	LYS
11	e	361	SER
11	g	60	TYR
11	g	61	ILE
11	h	295	ARG
11	h	298	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	k	141	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (263) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	401	GLN
1	A	429	HIS
1	A	486	ASN
1	A	552	GLN
1	A	608	HIS
1	A	682	GLN
1	A	851	ASN
1	A	890	ASN
2	B	345	GLN
2	B	387	HIS
2	B	401	HIS
2	B	491	ASN
2	B	570	GLN
2	B	576	HIS
2	B	643	HIS
2	B	773	ASN
2	B	846	GLN
2	B	860	GLN
1	C	264	GLN
1	C	486	ASN
1	C	540	HIS
1	C	682	GLN
1	C	851	ASN
2	D	259	GLN
2	D	345	GLN
2	D	401	HIS
2	D	417	HIS
2	D	491	ASN
2	D	570	GLN
2	D	576	HIS
2	D	643	HIS
2	D	773	ASN
2	D	846	GLN
2	D	860	GLN
1	E	289	HIS
1	E	317	ASN
1	E	318	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	337	GLN
1	E	401	GLN
1	E	429	HIS
1	E	486	ASN
1	E	552	GLN
1	E	608	HIS
1	E	682	GLN
1	E	851	ASN
1	E	890	ASN
2	F	345	GLN
2	F	387	HIS
2	F	570	GLN
2	F	576	HIS
2	F	643	HIS
2	F	773	ASN
2	F	846	GLN
2	F	860	GLN
1	G	264	GLN
1	G	486	ASN
1	G	540	HIS
1	G	558	HIS
1	G	682	GLN
1	G	851	ASN
2	H	345	GLN
2	H	387	HIS
2	H	389	GLN
2	H	401	HIS
2	H	417	HIS
2	H	570	GLN
2	H	576	HIS
2	H	595	HIS
2	H	643	HIS
2	H	773	ASN
2	H	846	GLN
2	H	860	GLN
3	I	26	GLN
3	I	123	ASN
3	I	130	GLN
3	I	149	HIS
3	I	200	HIS
3	I	303	GLN
3	I	390	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	393	ASN
3	I	397	GLN
3	I	415	HIS
3	I	498	GLN
3	I	518	ASN
3	I	539	GLN
3	I	542	GLN
3	I	560	HIS
4	J	269	GLN
4	J	328	GLN
4	J	362	GLN
4	J	408	GLN
4	J	413	HIS
4	J	474	GLN
4	J	642	HIS
4	J	698	GLN
4	J	705	ASN
4	J	818	GLN
4	J	822	ASN
4	J	830	GLN
4	J	898	HIS
4	J	907	HIS
4	J	925	GLN
4	J	938	HIS
3	K	29	GLN
3	K	82	HIS
3	K	98	GLN
3	K	123	ASN
3	K	316	GLN
3	K	377	GLN
3	K	397	GLN
3	K	401	HIS
3	K	488	GLN
3	K	492	GLN
3	K	498	GLN
3	K	528	GLN
3	K	539	GLN
3	K	542	GLN
3	K	560	HIS
3	K	566	ASN
3	K	590	HIS
3	K	610	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	441	GLN
5	L	469	GLN
5	L	512	ASN
5	L	517	HIS
5	L	1492	ASN
5	L	1508	HIS
5	L	1559	GLN
5	L	1568	HIS
5	L	1667	HIS
5	L	1678	ASN
5	L	1679	GLN
5	L	1702	GLN
5	L	1705	HIS
5	L	1777	HIS
5	L	1788	ASN
5	L	1805	ASN
1	M	264	GLN
1	M	464	GLN
1	M	486	ASN
1	M	540	HIS
1	M	678	HIS
1	M	682	GLN
1	M	851	ASN
11	a	24	GLN
11	a	75	HIS
11	a	139	HIS
11	a	250	ASN
11	a	325	GLN
11	a	430	GLN
11	a	436	HIS
11	b	24	GLN
11	b	250	ASN
11	b	251	ASN
11	b	314	ASN
11	b	381	HIS
11	b	394	GLN
11	b	417	ASN
11	b	430	GLN
11	c	12	GLN
11	c	54	GLN
11	c	115	HIS
11	c	139	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	c	227	GLN
11	c	250	ASN
11	c	315	HIS
11	c	322	ASN
11	c	325	GLN
11	c	334	HIS
11	c	381	HIS
11	c	430	GLN
11	d	24	GLN
11	d	75	HIS
11	d	250	ASN
11	d	251	ASN
11	d	314	ASN
11	d	381	HIS
11	d	394	GLN
11	d	417	ASN
11	d	430	GLN
11	e	24	GLN
11	e	115	HIS
11	e	139	HIS
11	e	250	ASN
11	e	325	GLN
11	e	430	GLN
11	e	436	HIS
11	f	24	GLN
11	f	167	GLN
11	f	250	ASN
11	f	251	ASN
11	f	314	ASN
11	f	381	HIS
11	f	394	GLN
11	f	430	GLN
11	g	16	GLN
11	g	54	GLN
11	g	115	HIS
11	g	139	HIS
11	g	227	GLN
11	g	250	ASN
11	g	251	ASN
11	g	315	HIS
11	g	322	ASN
11	g	325	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	g	381	HIS
11	g	430	GLN
11	h	24	GLN
11	h	211	ASN
11	h	250	ASN
11	h	251	ASN
11	h	314	ASN
11	h	381	HIS
11	h	394	GLN
11	h	417	ASN
11	h	430	GLN
11	i	12	GLN
11	i	75	HIS
11	i	250	ASN
11	i	325	GLN
11	i	338	GLN
11	i	430	GLN
11	j	16	GLN
11	j	54	GLN
11	j	299	GLN
11	j	315	HIS
11	j	322	ASN
11	j	325	GLN
11	j	357	GLN
11	j	381	HIS
11	j	417	ASN
11	j	430	GLN
11	k	12	GLN
11	k	15	ASN
11	k	54	GLN
11	k	139	HIS
11	k	219	HIS
11	k	322	ASN
11	k	332	GLN
11	k	429	GLN
11	k	430	GLN
11	l	139	HIS
11	l	167	GLN
11	l	211	ASN
11	l	322	ASN
11	l	357	GLN
11	l	417	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	l	430	GLN
11	l	436	HIS
11	m	12	GLN
11	m	54	GLN
11	m	115	HIS
11	m	139	HIS
11	m	227	GLN
11	m	250	ASN
11	m	251	ASN
11	m	315	HIS
11	m	322	ASN
11	m	325	GLN
11	m	332	GLN
11	m	334	HIS
11	m	381	HIS
11	m	430	GLN

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](#)

15 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	GDP	l	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)
13	GDP	i	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
13	GDP	f	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.79	7 (15%)
13	GDP	a	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	7 (15%)
13	GDP	t	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
13	GDP	b	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)
13	GDP	e	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
13	GDP	g	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
13	GDP	h	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.80	7 (15%)
13	GDP	c	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
13	GDP	d	501	-	29,30,30	1.15	2 (6%)	45,47,47	1.78	7 (15%)
13	GDP	m	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.77	7 (15%)
12	ADP	U	800	-	28,29,29	0.48	0	43,45,45	0.55	1 (2%)
13	GDP	j	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.75	7 (15%)
13	GDP	k	501	-	29,30,30	1.17	3 (10%)	45,47,47	1.79	7 (15%)

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	GDP	l	501	-	-	1/16/32/32	0/3/3/3
13	GDP	i	501	-	-	1/16/32/32	0/3/3/3
13	GDP	f	501	-	-	1/16/32/32	0/3/3/3
13	GDP	a	501	-	-	1/16/32/32	0/3/3/3
13	GDP	t	501	-	-	1/16/32/32	0/3/3/3
13	GDP	b	501	-	-	1/16/32/32	0/3/3/3
13	GDP	e	501	-	-	0/16/32/32	0/3/3/3
13	GDP	g	501	-	-	1/16/32/32	0/3/3/3
13	GDP	h	501	-	-	1/16/32/32	0/3/3/3
13	GDP	c	501	-	-	1/16/32/32	0/3/3/3
13	GDP	d	501	-	-	1/16/32/32	0/3/3/3
13	GDP	m	501	-	-	1/16/32/32	0/3/3/3
12	ADP	U	800	-	-	0/16/32/32	0/3/3/3
13	GDP	j	501	-	-	1/16/32/32	0/3/3/3
13	GDP	k	501	-	-	1/16/32/32	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	h	501	GDP	C5-C4	3.18	1.47	1.38
13	f	501	GDP	C5-C4	3.18	1.47	1.38
13	k	501	GDP	C5-C4	3.18	1.47	1.38
13	l	501	GDP	C5-C4	3.18	1.47	1.38
13	b	501	GDP	C5-C4	3.17	1.47	1.38
13	d	501	GDP	C5-C4	3.15	1.47	1.38
13	t	501	GDP	C5-C4	3.14	1.47	1.38
13	j	501	GDP	C5-C4	3.13	1.47	1.38
13	c	501	GDP	C5-C4	3.02	1.47	1.38
13	m	501	GDP	C5-C4	3.01	1.47	1.38
13	a	501	GDP	C5-C4	3.01	1.47	1.38
13	i	501	GDP	C5-C4	3.00	1.47	1.38
13	e	501	GDP	C5-C4	3.00	1.47	1.38
13	g	501	GDP	C5-C4	3.00	1.47	1.38
13	e	501	GDP	C6-N1	-2.66	1.33	1.38
13	a	501	GDP	C6-N1	-2.63	1.33	1.38
13	g	501	GDP	C6-N1	-2.61	1.34	1.38
13	m	501	GDP	C6-N1	-2.60	1.34	1.38
13	c	501	GDP	C6-N1	-2.60	1.34	1.38
13	i	501	GDP	C6-N1	-2.60	1.34	1.38
13	t	501	GDP	C6-N1	-2.50	1.34	1.38
13	j	501	GDP	C6-N1	-2.49	1.34	1.38
13	b	501	GDP	C6-N1	-2.43	1.34	1.38
13	f	501	GDP	C6-N1	-2.41	1.34	1.38
13	k	501	GDP	C6-N1	-2.40	1.34	1.38
13	l	501	GDP	C6-N1	-2.40	1.34	1.38
13	d	501	GDP	C6-N1	-2.39	1.34	1.38
13	h	501	GDP	C6-N1	-2.38	1.34	1.38
13	g	501	GDP	C5-N7	-2.21	1.34	1.39
13	m	501	GDP	C5-N7	-2.20	1.34	1.39
13	c	501	GDP	C5-N7	-2.18	1.34	1.39
13	e	501	GDP	C5-N7	-2.18	1.34	1.39
13	a	501	GDP	C5-N7	-2.17	1.34	1.39
13	t	501	GDP	C5-N7	-2.14	1.34	1.39
13	i	501	GDP	C5-N7	-2.12	1.34	1.39
13	f	501	GDP	C5-N7	-2.09	1.34	1.39
13	j	501	GDP	C5-N7	-2.08	1.34	1.39
13	b	501	GDP	C5-N7	-2.05	1.35	1.39
13	h	501	GDP	C5-N7	-2.03	1.35	1.39
13	k	501	GDP	C5-N7	-2.03	1.35	1.39
13	l	501	GDP	C5-N7	-2.02	1.35	1.39

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	h	501	GDP	C5-C4-N3	-6.20	118.53	128.39
13	f	501	GDP	C5-C4-N3	-6.18	118.56	128.39
13	l	501	GDP	C5-C4-N3	-6.18	118.56	128.39
13	k	501	GDP	C5-C4-N3	-6.17	118.56	128.39
13	b	501	GDP	C5-C4-N3	-6.17	118.58	128.39
13	d	501	GDP	C5-C4-N3	-6.13	118.64	128.39
13	t	501	GDP	C5-C4-N3	-6.12	118.65	128.39
13	m	501	GDP	C5-C4-N3	-6.11	118.67	128.39
13	c	501	GDP	C5-C4-N3	-6.09	118.69	128.39
13	g	501	GDP	C5-C4-N3	-6.09	118.70	128.39
13	e	501	GDP	C5-C4-N3	-6.07	118.74	128.39
13	a	501	GDP	C5-C4-N3	-6.05	118.76	128.39
13	j	501	GDP	C5-C4-N3	-6.02	118.80	128.39
13	i	501	GDP	C5-C4-N3	-6.00	118.84	128.39
13	h	501	GDP	C2-N3-C4	5.06	121.02	112.30
13	l	501	GDP	C2-N3-C4	5.06	121.01	112.30
13	f	501	GDP	C2-N3-C4	5.06	121.01	112.30
13	j	501	GDP	C2-N3-C4	5.03	120.96	112.30
13	k	501	GDP	C2-N3-C4	5.03	120.96	112.30
13	b	501	GDP	C2-N3-C4	5.03	120.96	112.30
13	m	501	GDP	C2-N3-C4	5.03	120.95	112.30
13	d	501	GDP	C2-N3-C4	5.01	120.93	112.30
13	t	501	GDP	C2-N3-C4	5.01	120.92	112.30
13	c	501	GDP	C2-N3-C4	5.01	120.92	112.30
13	g	501	GDP	C2-N3-C4	4.99	120.90	112.30
13	e	501	GDP	C2-N3-C4	4.93	120.79	112.30
13	i	501	GDP	C2-N3-C4	4.93	120.79	112.30
13	a	501	GDP	C2-N3-C4	4.92	120.78	112.30
13	h	501	GDP	N9-C4-N3	4.61	135.17	125.95
13	k	501	GDP	N9-C4-N3	4.60	135.14	125.95
13	f	501	GDP	N9-C4-N3	4.59	135.13	125.95
13	t	501	GDP	N9-C4-N3	4.58	135.12	125.95
13	l	501	GDP	N9-C4-N3	4.57	135.09	125.95
13	b	501	GDP	N9-C4-N3	4.57	135.08	125.95
13	m	501	GDP	N9-C4-N3	4.55	135.05	125.95
13	c	501	GDP	N9-C4-N3	4.53	135.00	125.95
13	g	501	GDP	N9-C4-N3	4.51	134.98	125.95
13	d	501	GDP	N9-C4-N3	4.51	134.96	125.95
13	i	501	GDP	N9-C4-N3	4.47	134.89	125.95
13	e	501	GDP	N9-C4-N3	4.44	134.84	125.95
13	j	501	GDP	N9-C4-N3	4.43	134.82	125.95
13	a	501	GDP	N9-C4-N3	4.43	134.81	125.95
13	j	501	GDP	C6-C5-N7	3.26	136.22	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	i	501	GDP	C6-C5-N7	3.22	136.16	130.29
13	m	501	GDP	C6-C5-N7	3.22	136.15	130.29
13	c	501	GDP	C6-C5-N7	3.22	136.15	130.29
13	l	501	GDP	C6-C5-N7	3.21	136.14	130.29
13	a	501	GDP	C6-C5-N7	3.20	136.12	130.29
13	d	501	GDP	C6-C5-N7	3.20	136.12	130.29
13	b	501	GDP	C6-C5-N7	3.20	136.12	130.29
13	t	501	GDP	C6-C5-N7	3.20	136.12	130.29
13	g	501	GDP	C6-C5-N7	3.19	136.10	130.29
13	e	501	GDP	C6-C5-N7	3.19	136.10	130.29
13	h	501	GDP	C6-C5-N7	3.19	136.10	130.29
13	k	501	GDP	C6-C5-N7	3.18	136.09	130.29
13	f	501	GDP	C6-C5-N7	3.18	136.08	130.29
13	l	501	GDP	C4-C5-N7	-2.58	106.58	110.67
13	b	501	GDP	C4-C5-N7	-2.57	106.60	110.67
13	h	501	GDP	C4-C5-N7	-2.56	106.61	110.67
13	d	501	GDP	C4-C5-N7	-2.56	106.61	110.67
13	k	501	GDP	C4-C5-N7	-2.56	106.62	110.67
13	j	501	GDP	C4-C5-N7	-2.55	106.63	110.67
13	t	501	GDP	C4-C5-N7	-2.55	106.63	110.67
13	e	501	GDP	C4-C5-N7	-2.54	106.65	110.67
13	a	501	GDP	C4-C5-N7	-2.54	106.65	110.67
13	f	501	GDP	C4-C5-N7	-2.54	106.65	110.67
13	i	501	GDP	C4-C5-N7	-2.51	106.69	110.67
13	c	501	GDP	C4-C5-N7	-2.50	106.71	110.67
13	m	501	GDP	C4-C5-N7	-2.50	106.72	110.67
13	g	501	GDP	C4-C5-N7	-2.47	106.75	110.67
13	f	501	GDP	C3'-C2'-C1'	2.32	105.86	101.46
13	k	501	GDP	C3'-C2'-C1'	2.32	105.86	101.46
13	h	501	GDP	C3'-C2'-C1'	2.32	105.85	101.46
13	t	501	GDP	C3'-C2'-C1'	2.32	105.85	101.46
13	d	501	GDP	C3'-C2'-C1'	2.31	105.83	101.46
13	m	501	GDP	C3'-C2'-C1'	2.31	105.83	101.46
13	c	501	GDP	C3'-C2'-C1'	2.30	105.81	101.46
13	b	501	GDP	C3'-C2'-C1'	2.30	105.81	101.46
13	l	501	GDP	C3'-C2'-C1'	2.28	105.78	101.46
13	g	501	GDP	C3'-C2'-C1'	2.28	105.77	101.46
13	e	501	GDP	O6-C6-C5	-2.20	120.73	126.53
13	a	501	GDP	O6-C6-C5	-2.20	120.73	126.53
13	m	501	GDP	O6-C6-C5	-2.15	120.86	126.53
13	i	501	GDP	O6-C6-C5	-2.15	120.86	126.53
13	c	501	GDP	O6-C6-C5	-2.13	120.92	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	g	501	GDP	O6-C6-C5	-2.12	120.93	126.53
13	j	501	GDP	C3'-C2'-C1'	2.12	105.47	101.46
13	t	501	GDP	O6-C6-C5	-2.12	120.94	126.53
13	k	501	GDP	O6-C6-C5	-2.11	120.96	126.53
13	b	501	GDP	O6-C6-C5	-2.11	120.96	126.53
12	U	800	ADP	O2B-PB-O1B	2.10	119.03	110.83
13	f	501	GDP	O6-C6-C5	-2.10	121.00	126.53
13	l	501	GDP	O6-C6-C5	-2.09	121.01	126.53
13	j	501	GDP	O6-C6-C5	-2.09	121.01	126.53
13	h	501	GDP	O6-C6-C5	-2.09	121.01	126.53
13	d	501	GDP	O6-C6-C5	-2.07	121.06	126.53
13	a	501	GDP	C3'-C2'-C1'	2.07	105.39	101.46
13	e	501	GDP	C3'-C2'-C1'	2.07	105.39	101.46
13	i	501	GDP	C3'-C2'-C1'	2.06	105.35	101.46

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	b	501	GDP	C5'-O5'-PA-O1A
13	d	501	GDP	C5'-O5'-PA-O1A
13	f	501	GDP	C5'-O5'-PA-O1A
13	h	501	GDP	C5'-O5'-PA-O1A
13	k	501	GDP	C5'-O5'-PA-O1A
13	l	501	GDP	C5'-O5'-PA-O1A
13	t	501	GDP	C5'-O5'-PA-O1A
13	a	501	GDP	C5'-O5'-PA-O1A
13	c	501	GDP	C5'-O5'-PA-O1A
13	g	501	GDP	C5'-O5'-PA-O1A
13	i	501	GDP	C5'-O5'-PA-O1A
13	j	501	GDP	C5'-O5'-PA-O1A
13	m	501	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

10 monomers are involved in 24 short contacts:

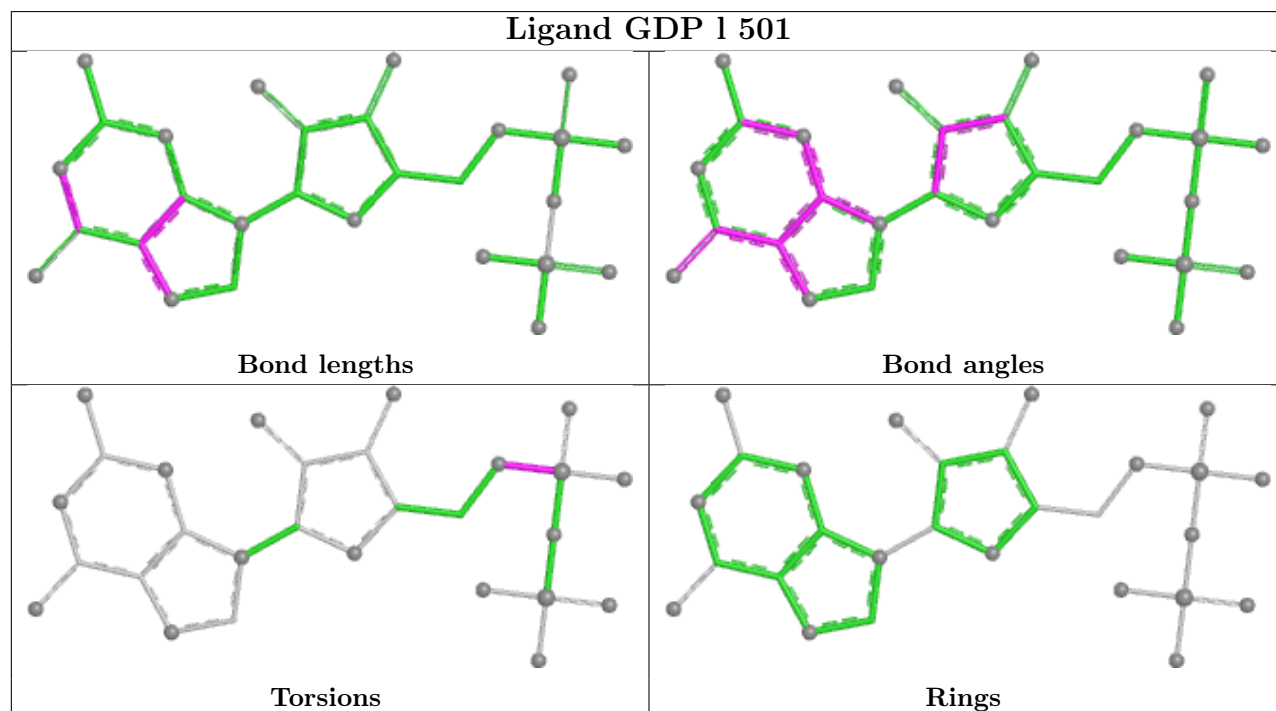
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	l	501	GDP	4	0
13	i	501	GDP	2	0
13	f	501	GDP	2	0
13	b	501	GDP	1	0

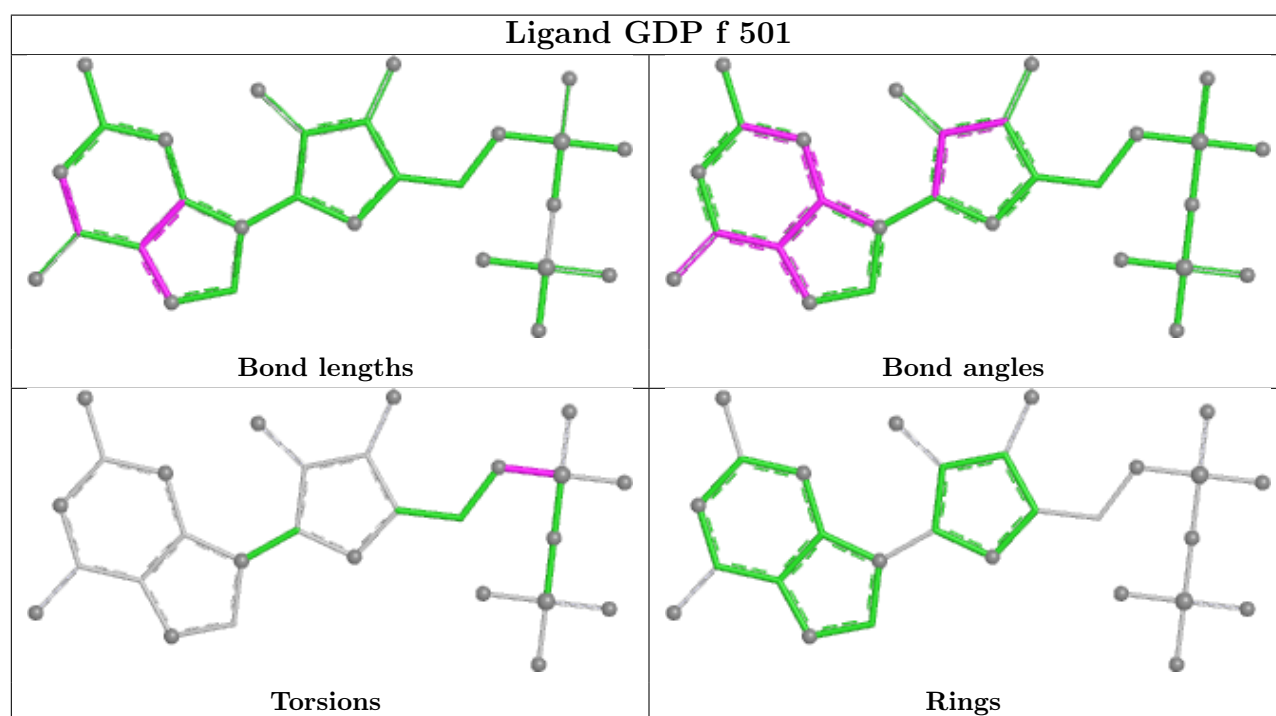
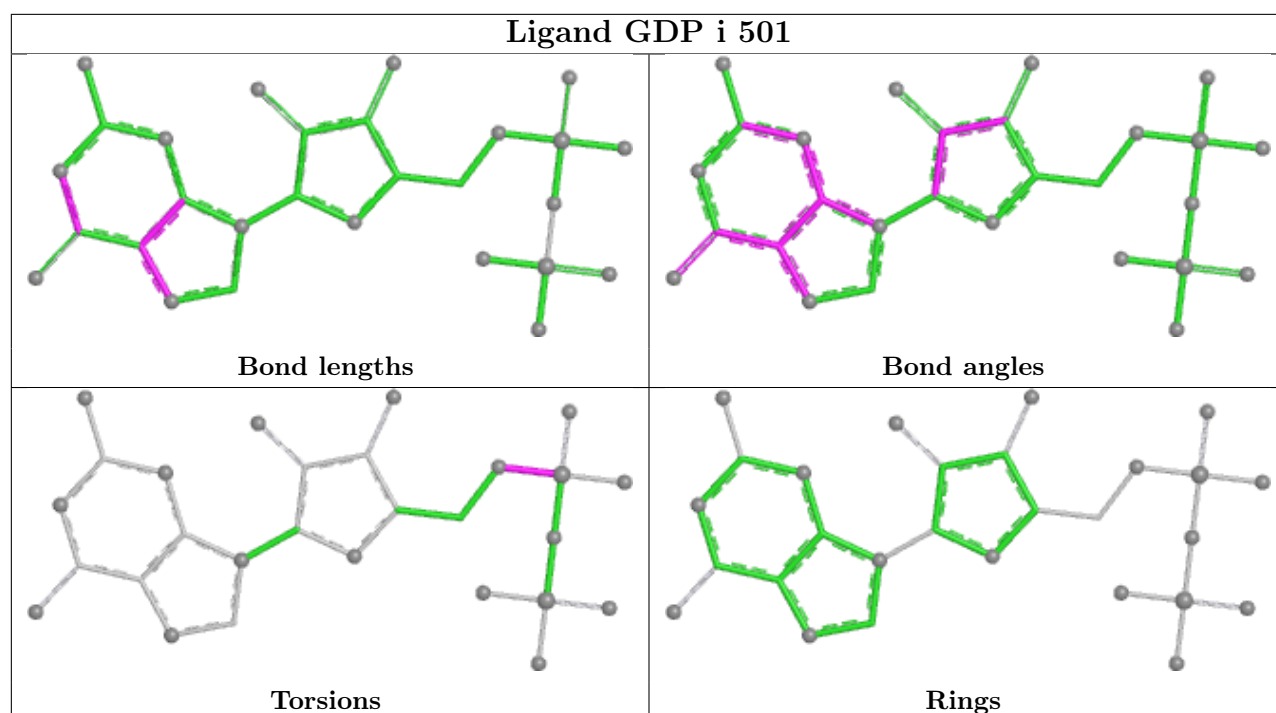
Continued on next page...

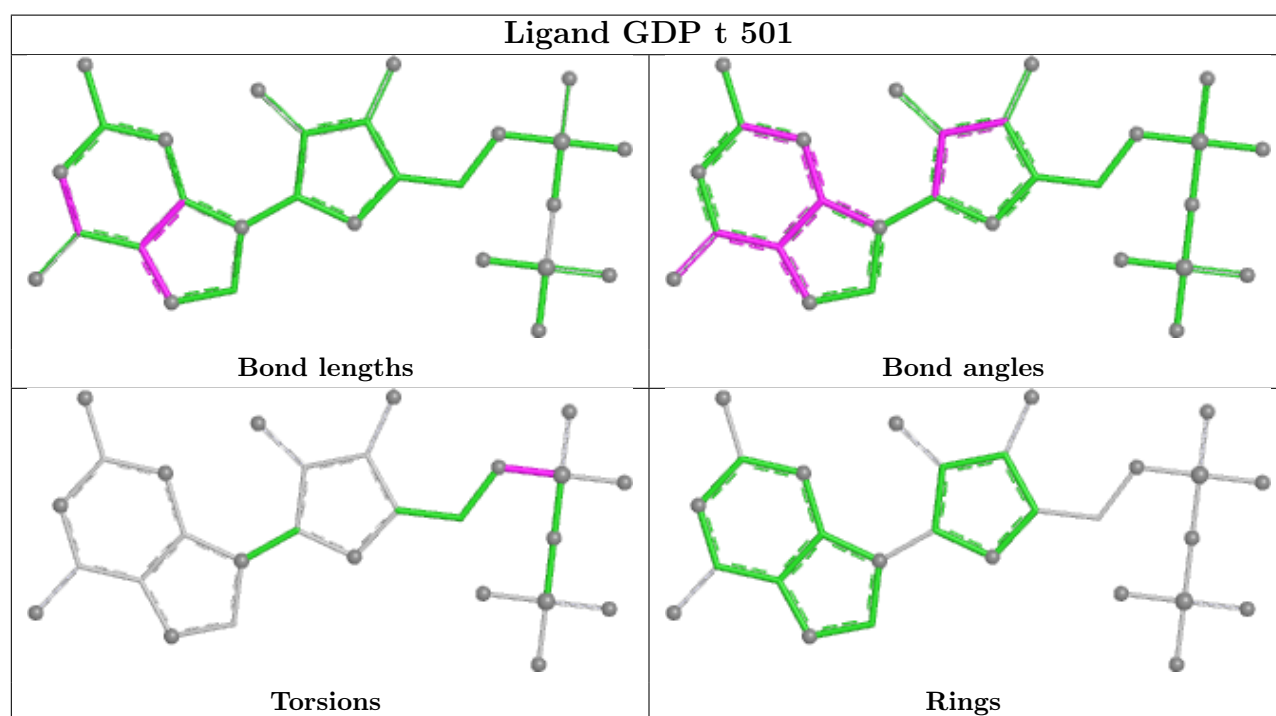
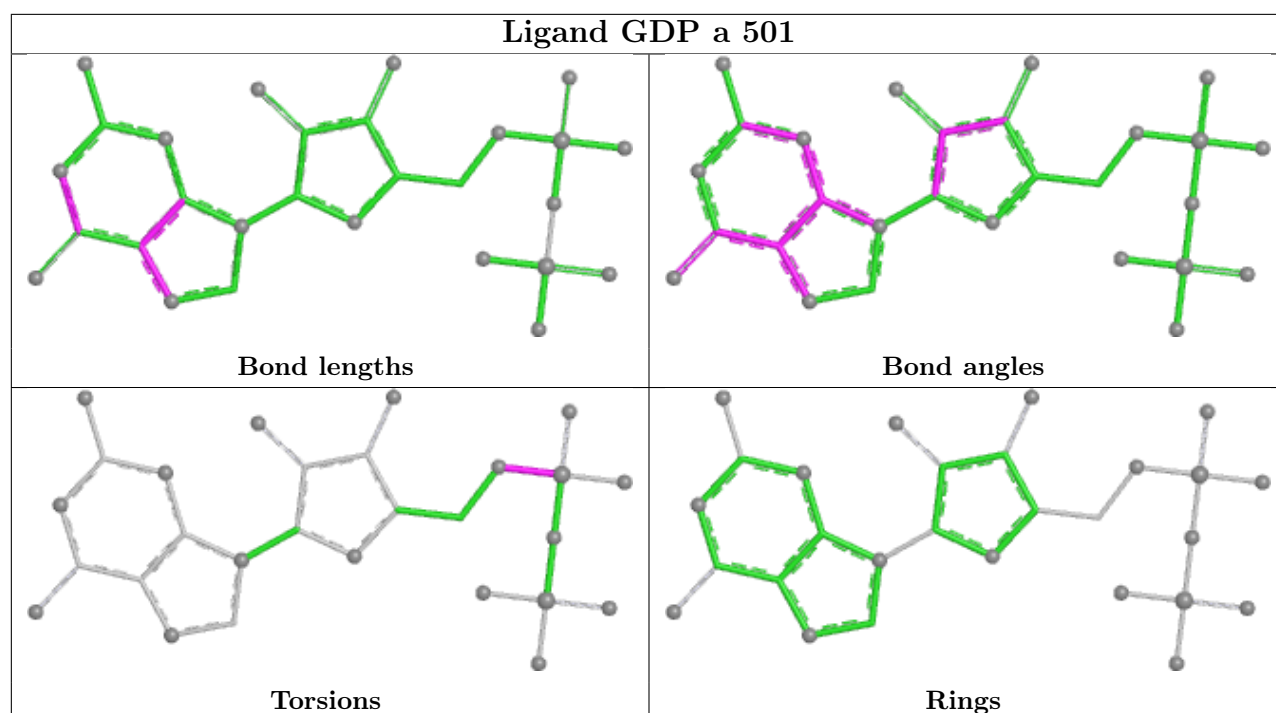
Continued from previous page...

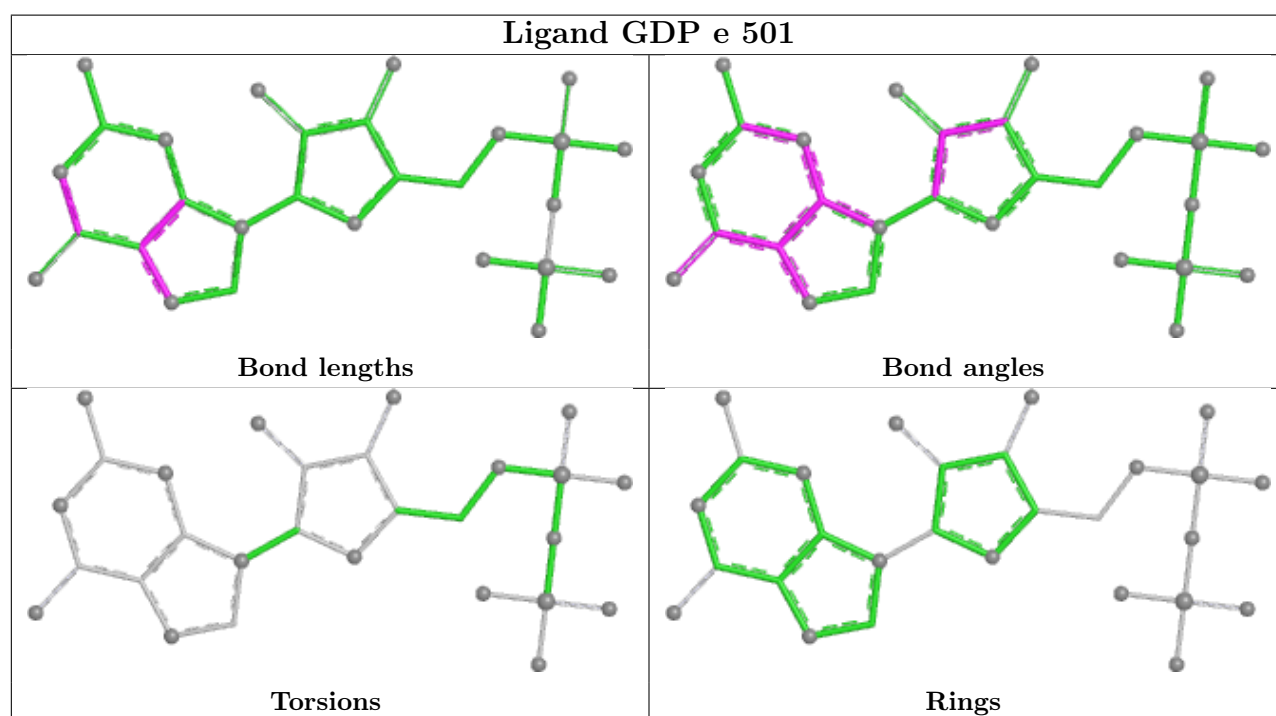
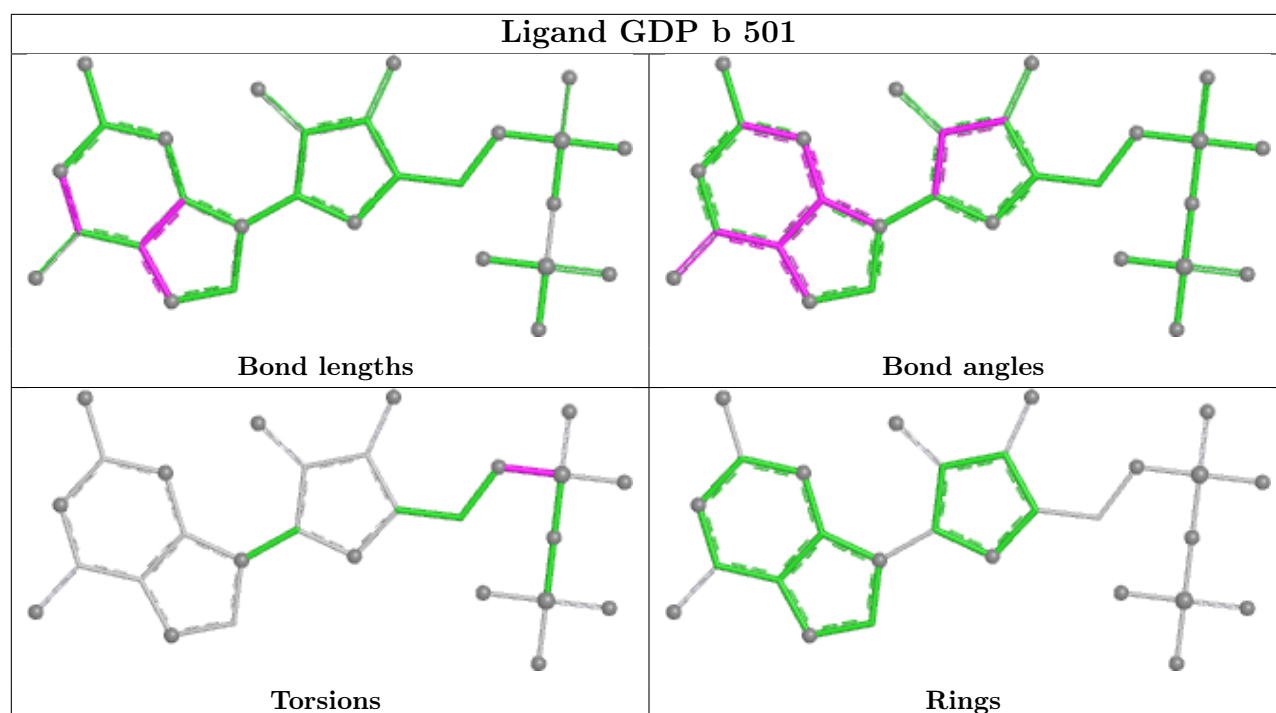
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	g	501	GDP	3	0
13	h	501	GDP	1	0
13	c	501	GDP	4	0
13	d	501	GDP	1	0
13	m	501	GDP	4	0
13	j	501	GDP	2	0

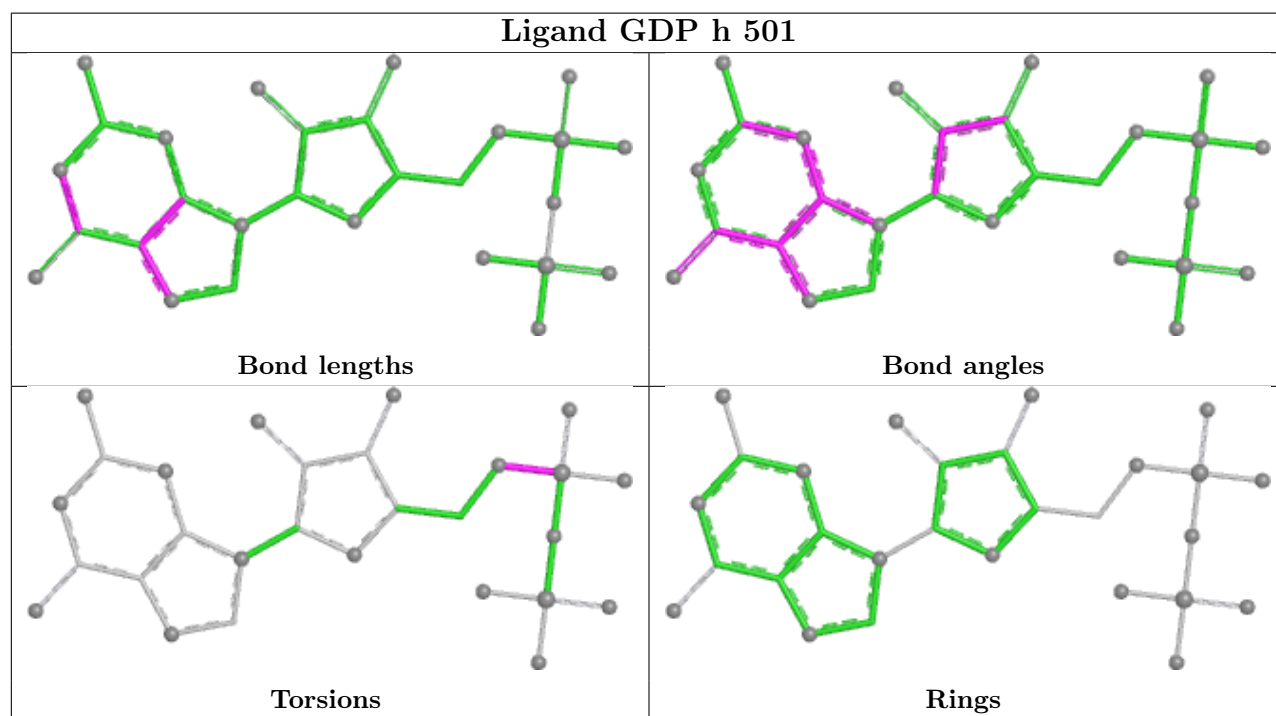
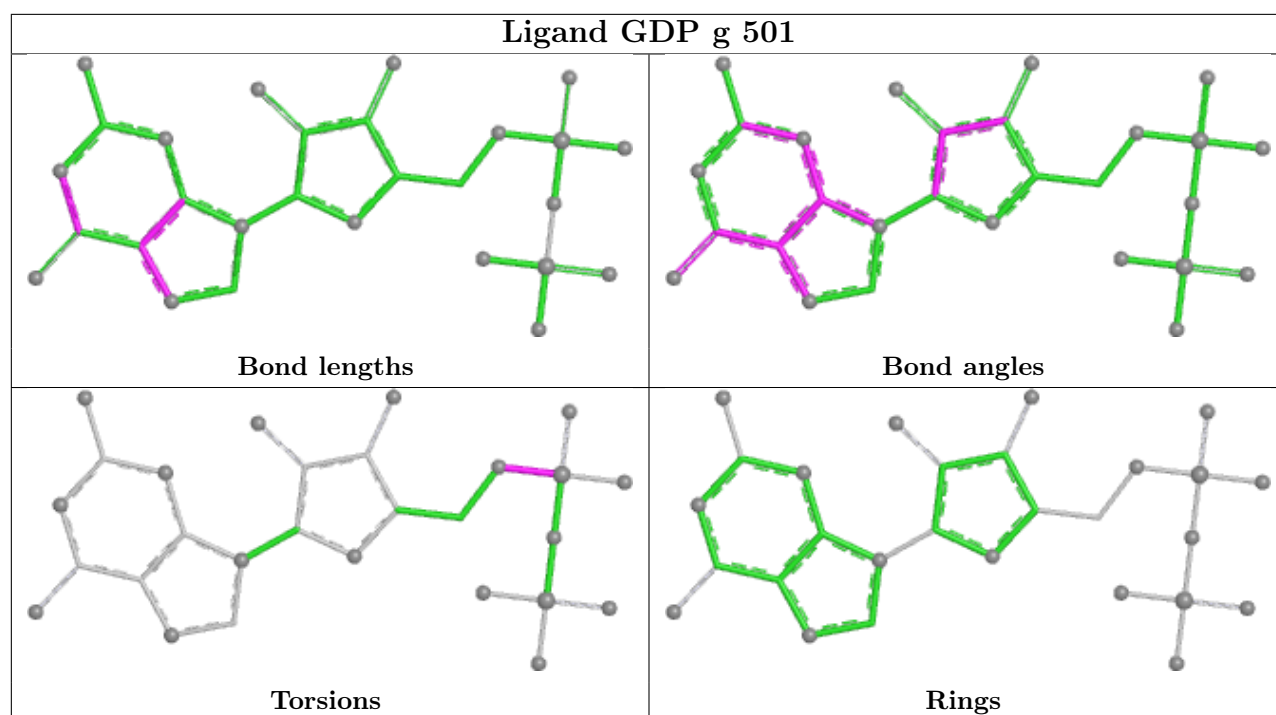
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

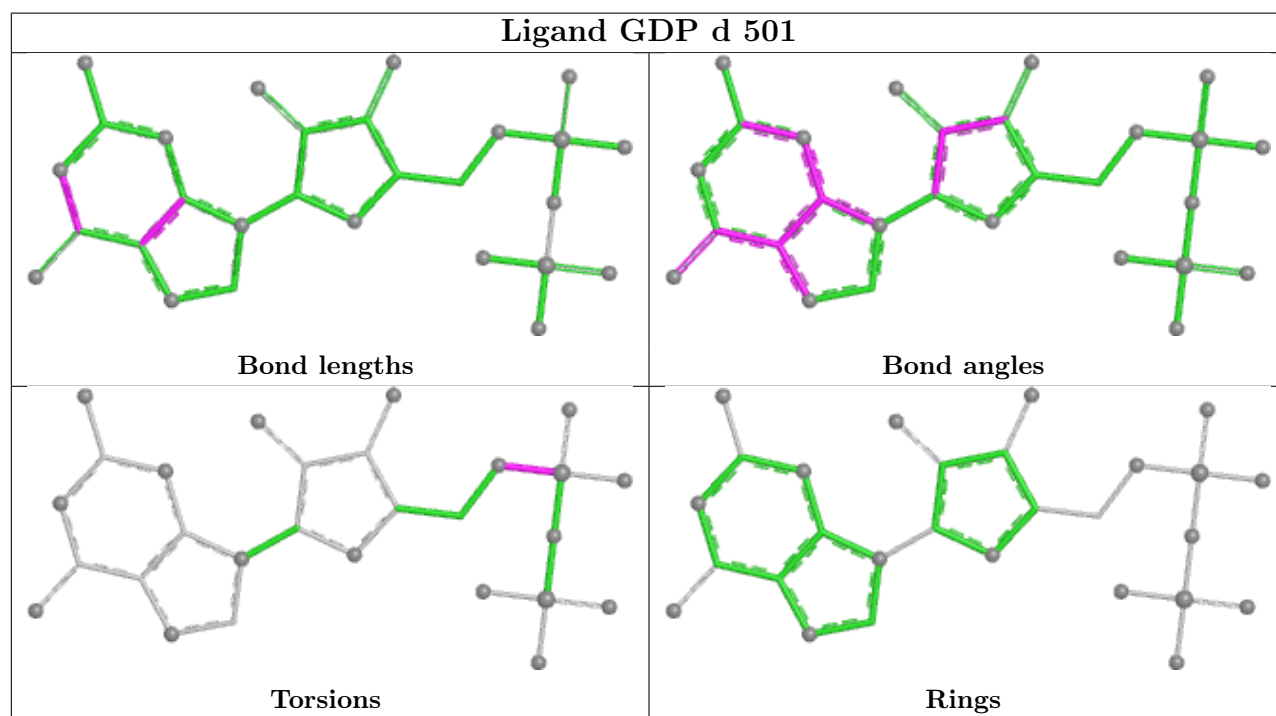
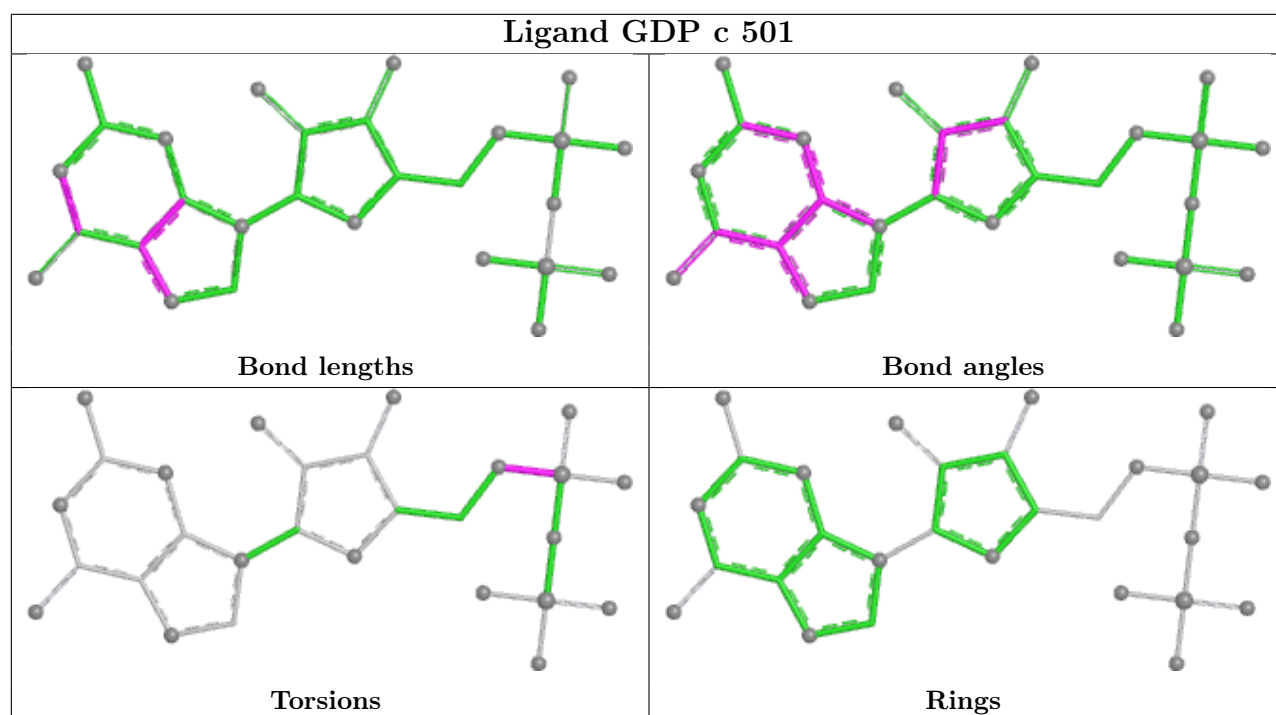


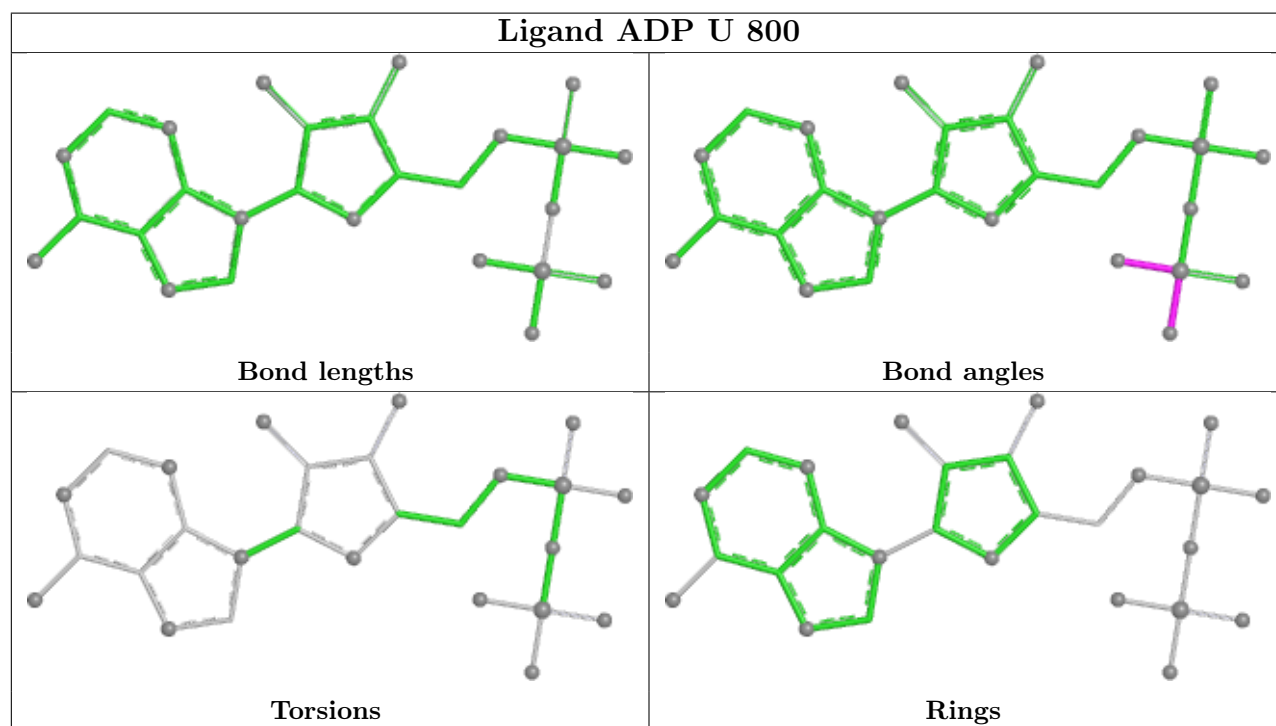
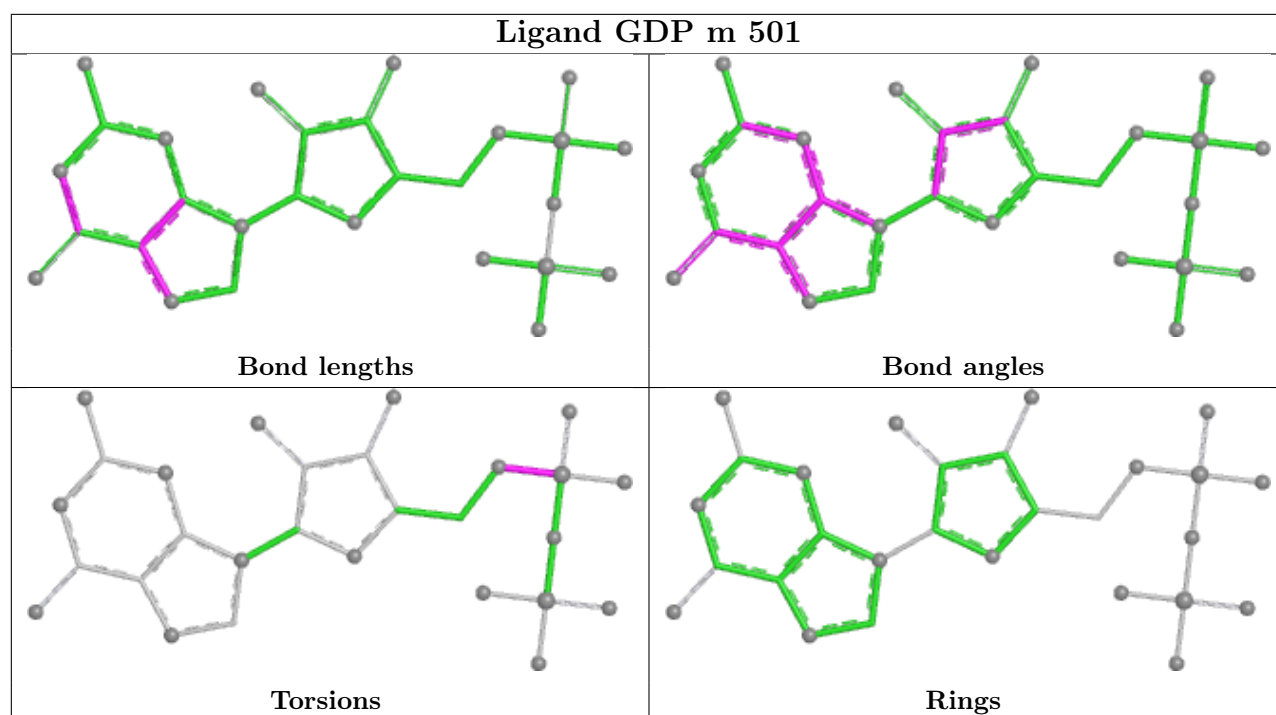


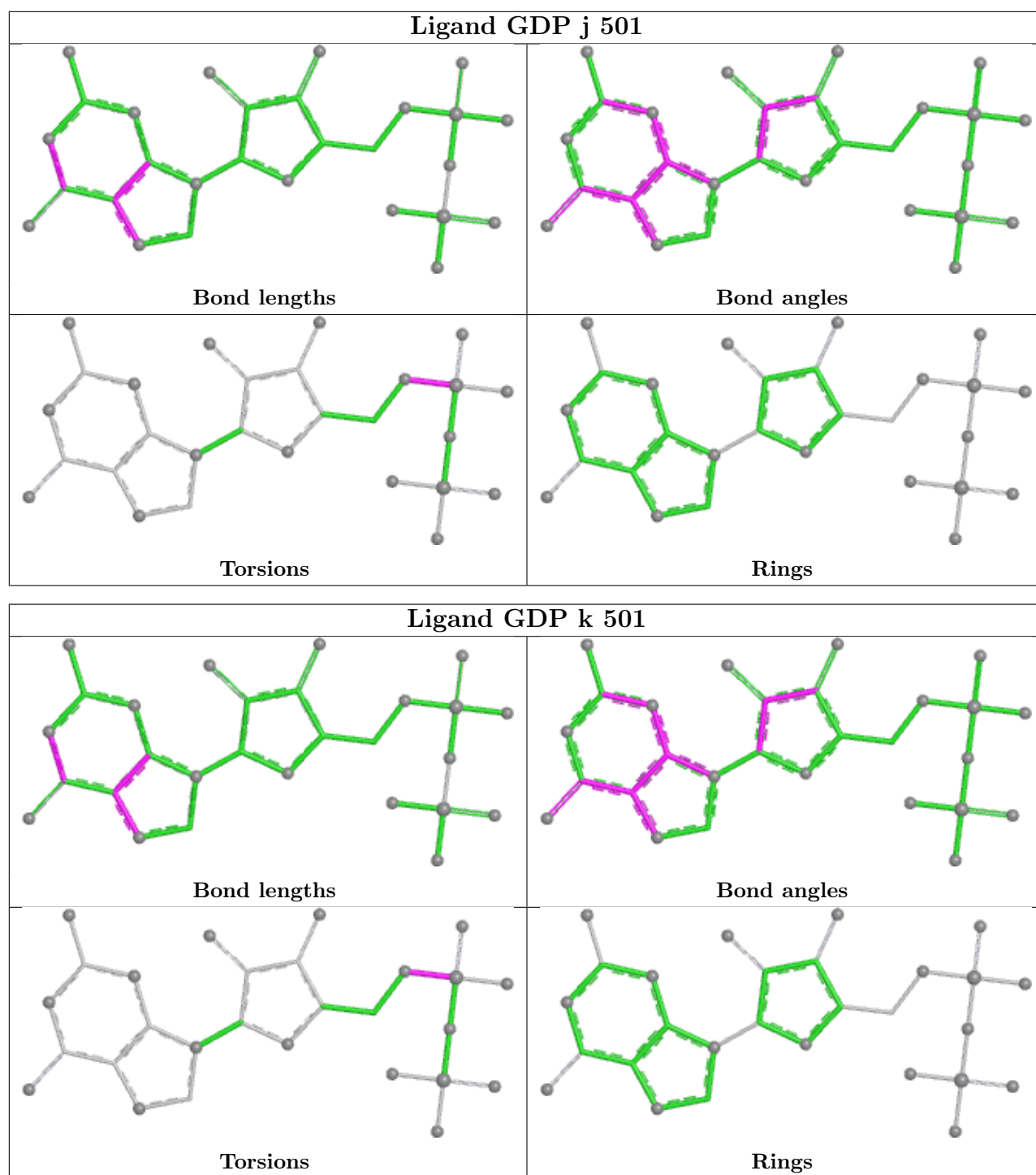












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	X	15
9	W	8
8	V	1
6	R	1
6	N	1
6	Q	1
6	O	1
6	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	31:UNK	C	101:UNK	N	47.63
1	X	1115:UNK	C	1201:UNK	N	30.30
1	W	220:UNK	C	301:UNK	N	29.84
1	W	315:UNK	C	401:UNK	N	27.18
1	X	715:UNK	C	801:UNK	N	25.87
1	X	114:UNK	C	201:UNK	N	25.19
1	X	914:UNK	C	1001:UNK	N	24.31
1	X	1225:UNK	C	1301:UNK	N	23.86
1	X	20:UNK	C	101:UNK	N	23.09
1	X	412:UNK	C	501:UNK	N	22.33
1	W	717:UNK	C	801:UNK	N	21.58
1	W	421:UNK	C	501:UNK	N	20.54
1	W	113:UNK	C	201:UNK	N	18.14
1	X	814:UNK	C	901:UNK	N	17.97
1	X	1017:UNK	C	1101:UNK	N	17.65
1	X	217:UNK	C	301:UNK	N	17.47
1	W	516:UNK	C	601:UNK	N	14.36
1	X	513:UNK	C	601:UNK	N	13.75
1	X	616:UNK	C	701:UNK	N	13.56
1	X	1418:UNK	C	1501:UNK	N	13.24
1	W	621:UNK	C	701:UNK	N	12.28
1	W	19:UNK	C	101:UNK	N	12.19
1	X	314:UNK	C	401:UNK	N	10.51
1	R	17:UNK	C	20:UNK	N	9.90
1	N	15:UNK	C	19:UNK	N	9.55
1	Q	18:UNK	C	21:UNK	N	8.78
1	O	19:UNK	C	21:UNK	N	7.27
1	S	19:UNK	C	21:UNK	N	6.55
1	X	1317:UNK	C	1401:UNK	N	6.32

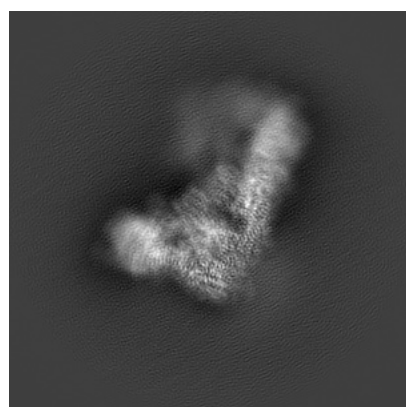
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21073. These allow visual inspection of the internal detail of the map and identification of artifacts.

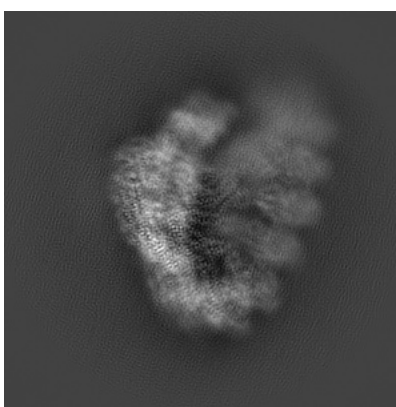
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

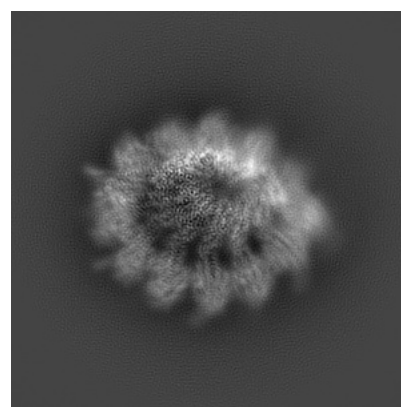
6.1.1 Primary map



X



Y



Z

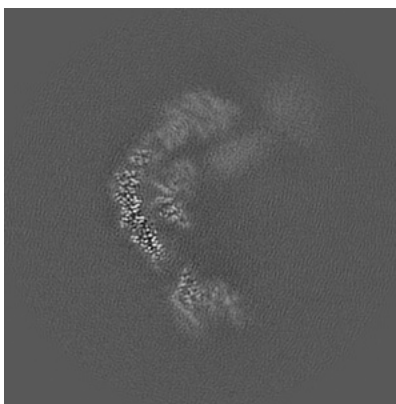
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

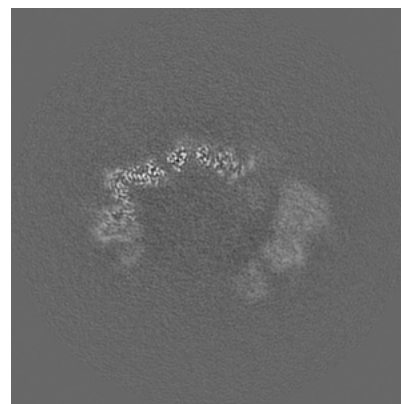
6.2.1 Primary map



X Index: 184



Y Index: 184

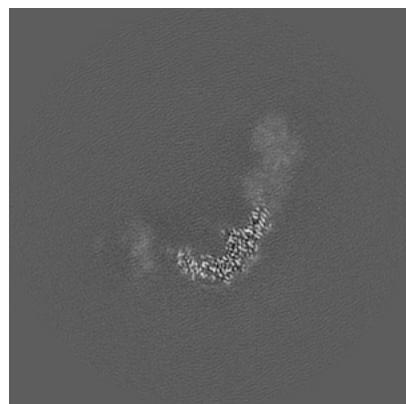


Z Index: 184

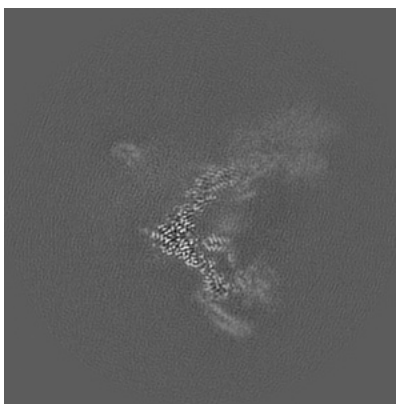
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

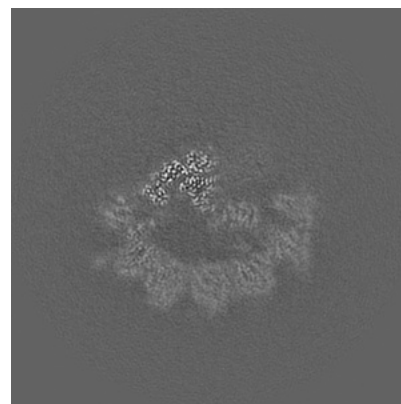
6.3.1 Primary map



X Index: 162



Y Index: 220

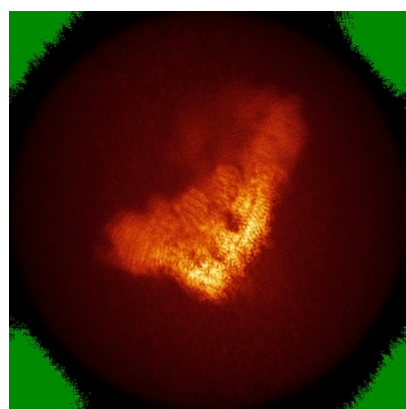


Z Index: 159

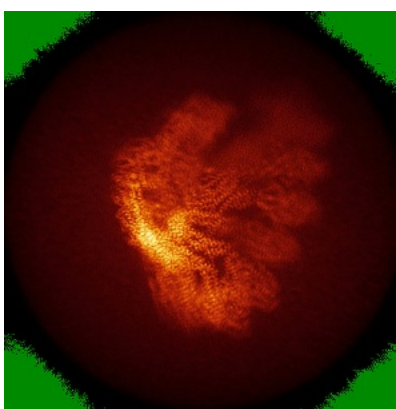
The images above show the largest variance slices of the map in three orthogonal directions.

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

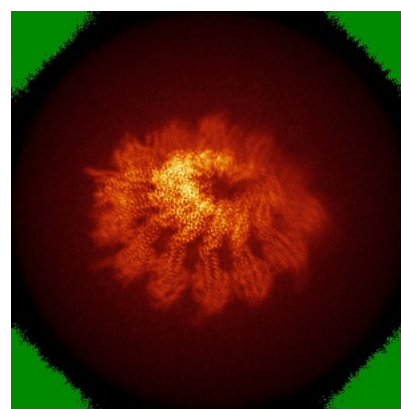
6.4.1 Primary map



X



Y

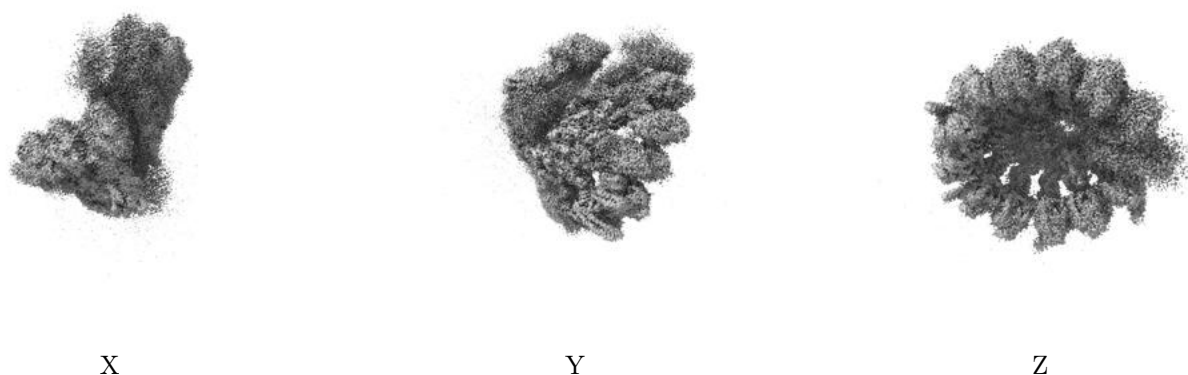


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

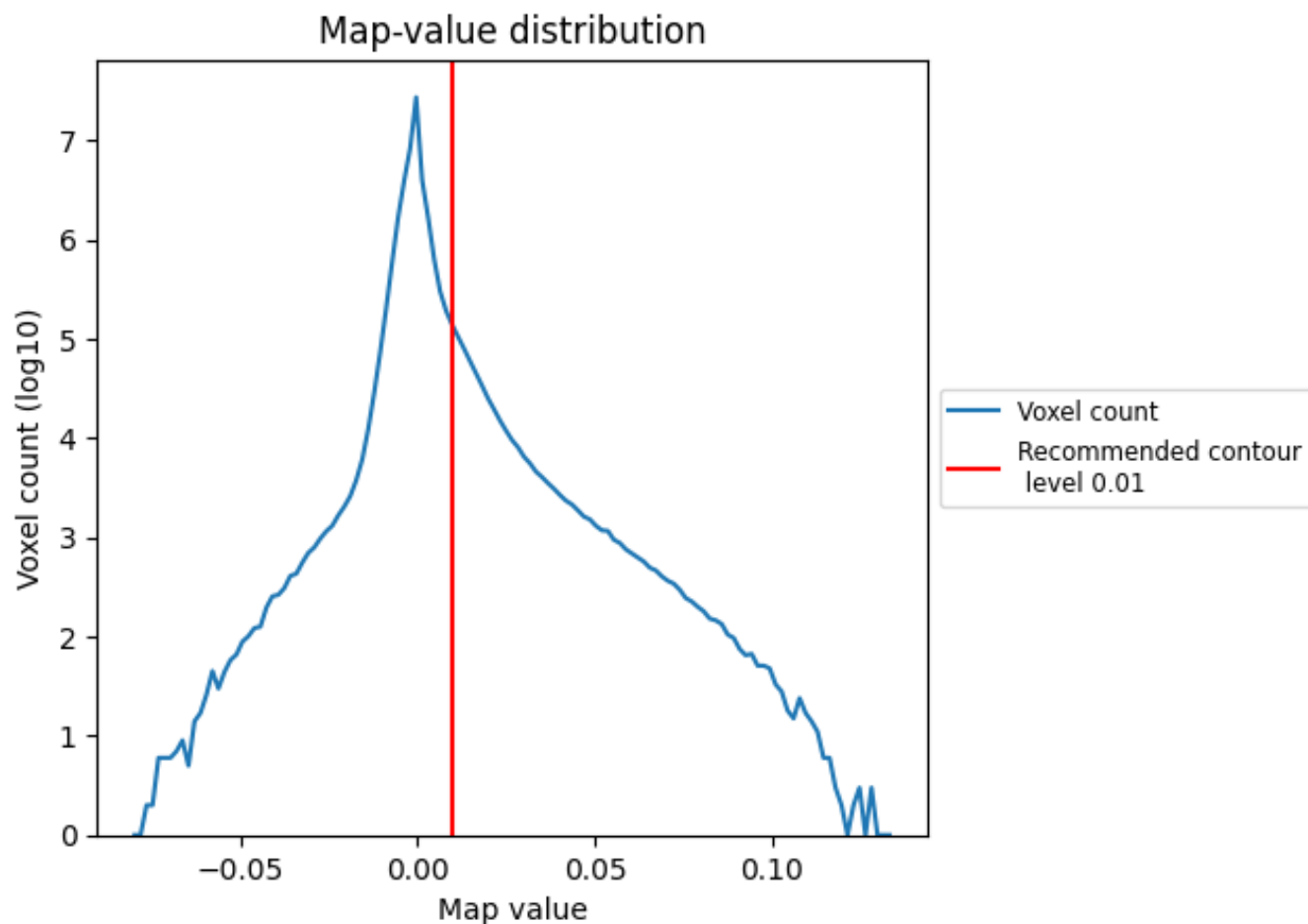
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

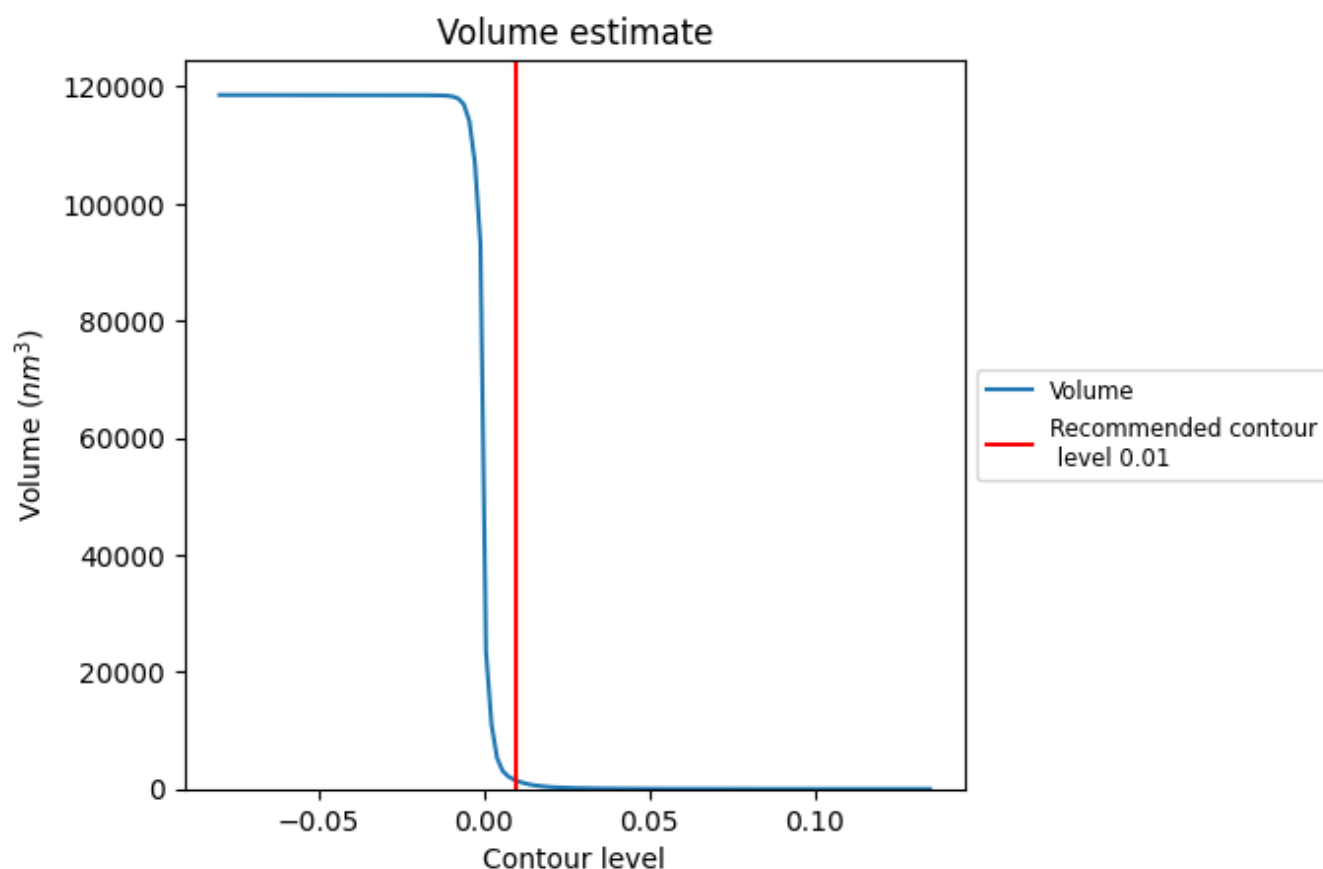
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

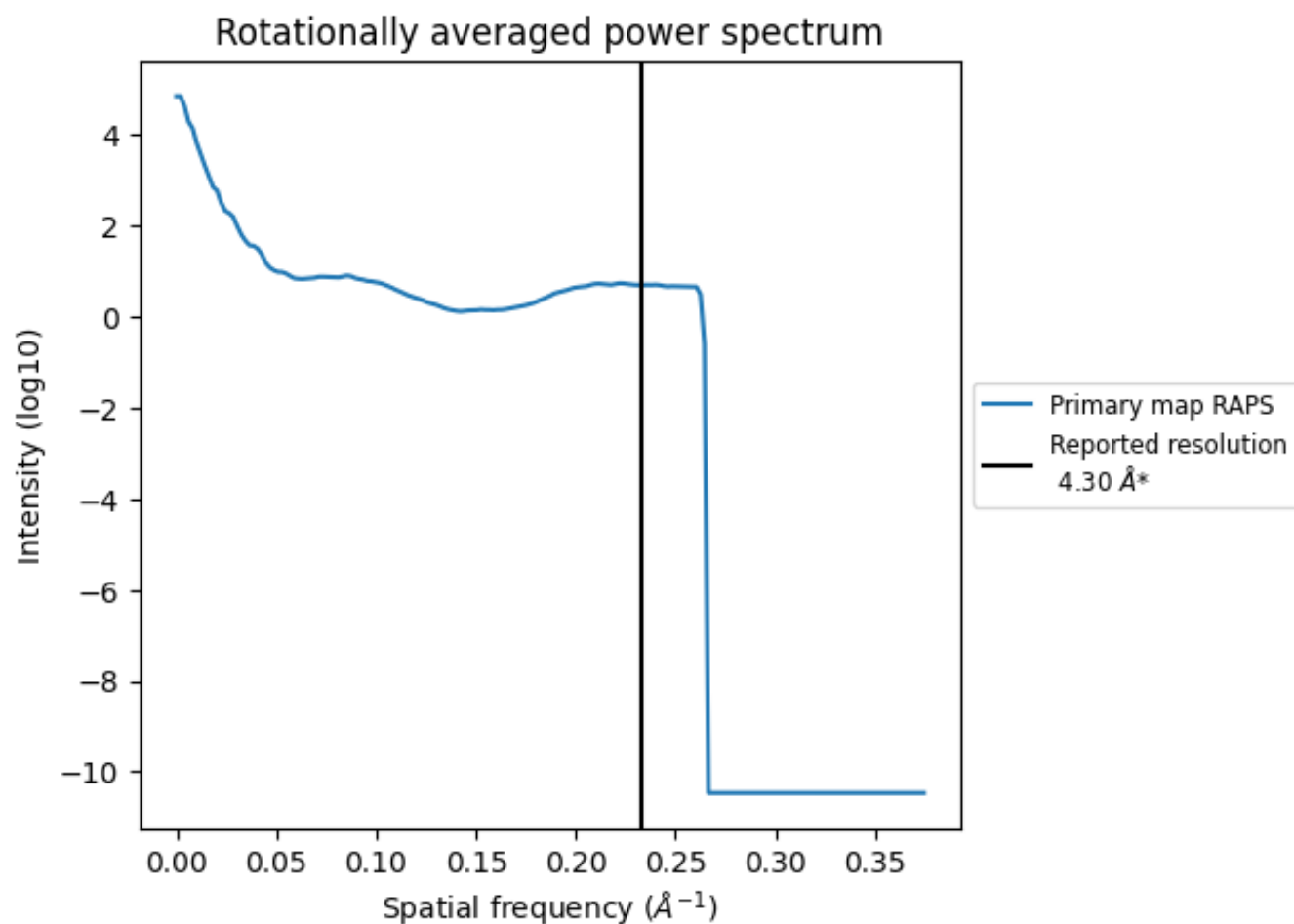
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1413 nm³; this corresponds to an approximate mass of 1276 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 0.233 Å⁻¹

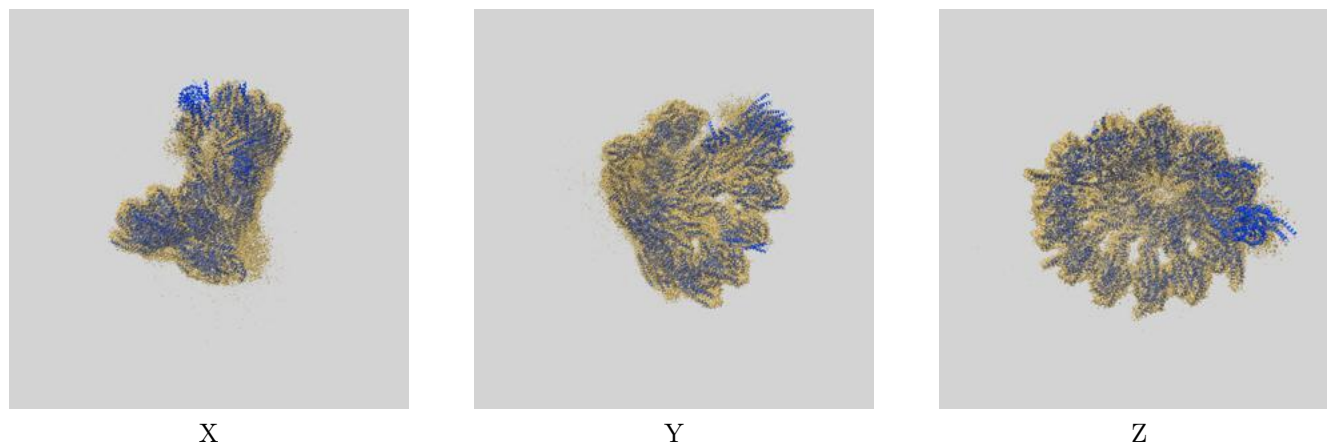
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

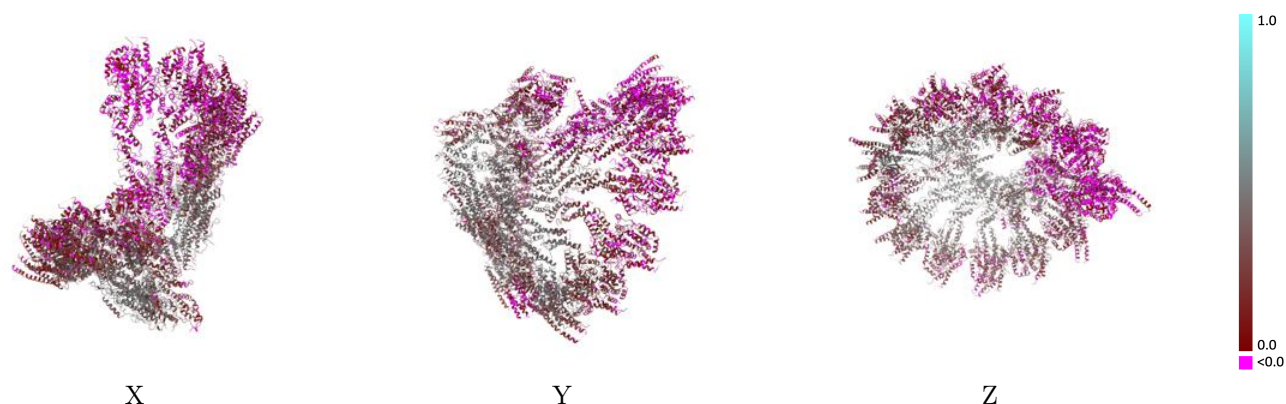
This section contains information regarding the fit between EMDB map EMD-21073 and PDB model 6V6S. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



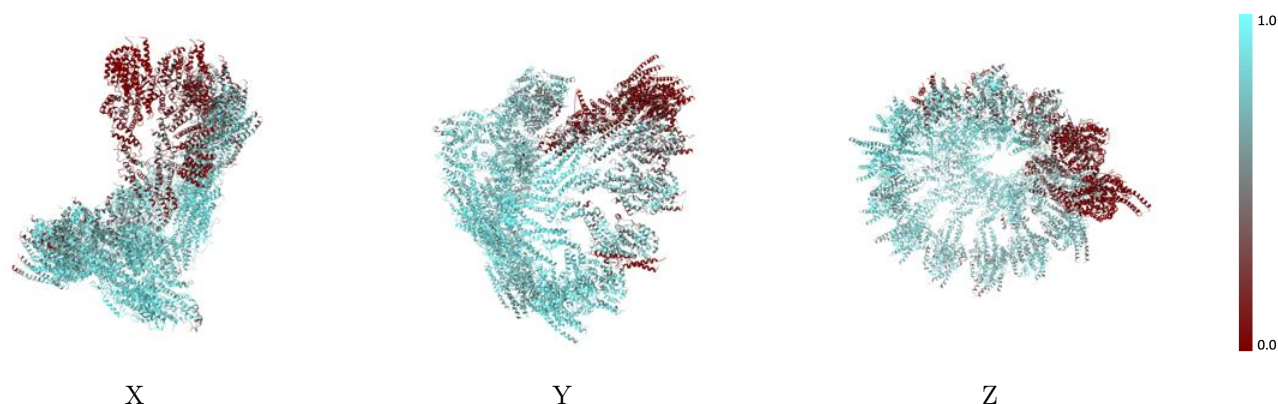
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



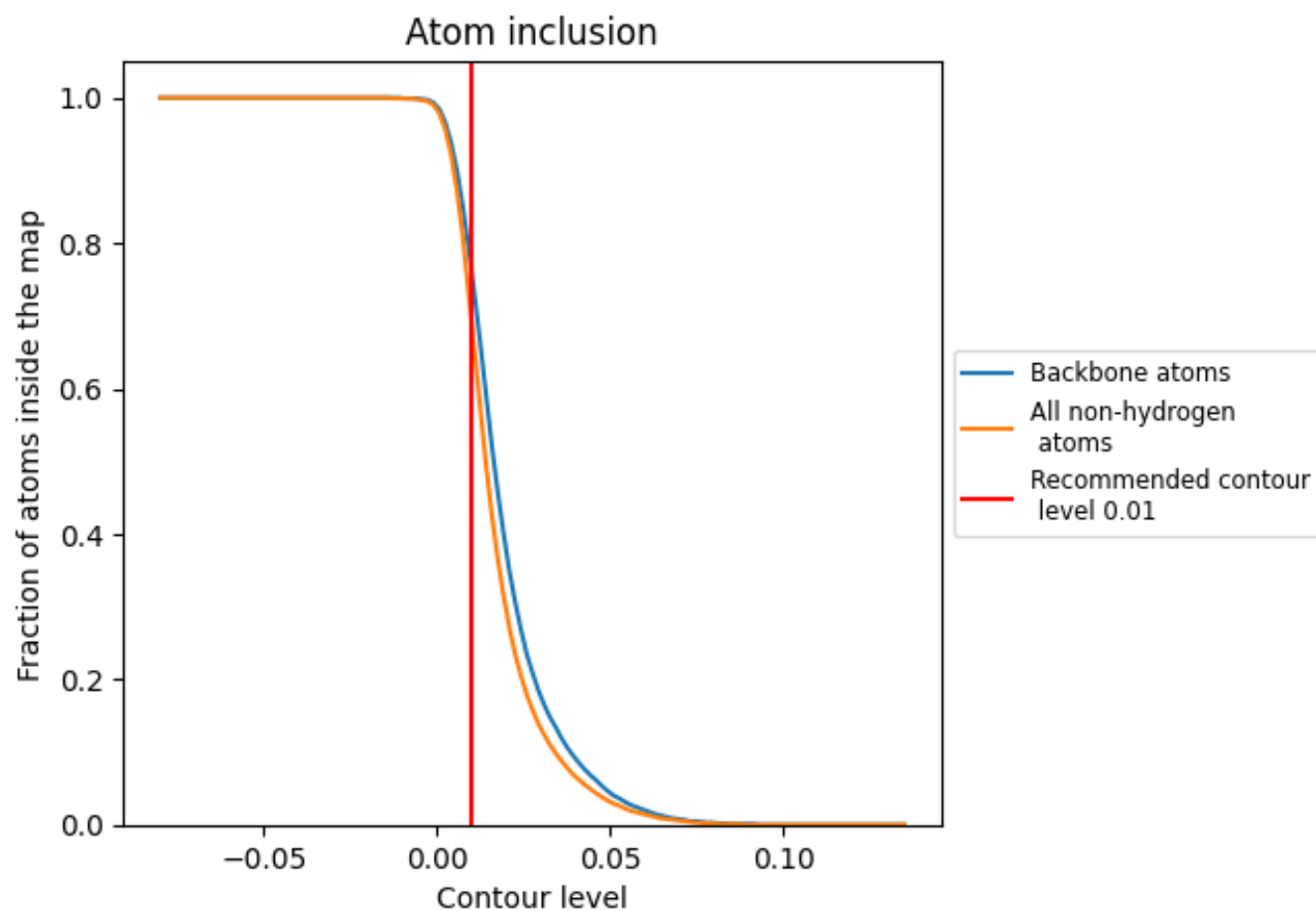
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 69% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6910	 0.2180
A	 0.7330	 0.2010
B	 0.8130	 0.2940
C	 0.8840	 0.3780
D	 0.8310	 0.3150
E	 0.8550	 0.3490
F	 0.8900	 0.3850
G	 0.7350	 0.1760
H	 0.9040	 0.4000
I	 0.8830	 0.3550
J	 0.7250	 0.2400
K	 0.7610	 0.2210
L	 0.6610	 0.1540
M	 0.2410	 0.0130
N	 0.8060	 0.2690
O	 0.9450	 0.4140
Q	 0.9580	 0.4000
R	 0.9540	 0.4030
S	 0.2950	 0.0020
T	 0.1440	 0.0100
U	 0.7620	 0.2370
V	 0.1420	 0.0480
W	 0.1060	 0.0520
X	 0.9580	 0.4270
Y	 0.8950	 0.3840
a	 0.6070	 0.0740
b	 0.7220	 0.1710
c	 0.7480	 0.2060
d	 0.7100	 0.1730
e	 0.7360	 0.1750
f	 0.8340	 0.2890
g	 0.7770	 0.1980
h	 0.8910	 0.3610
i	 0.8120	 0.2160
j	 0.5390	 0.0810



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.5930	 0.0630
l	 0.4250	 0.0450
m	 0.1050	 0.0110
t	 0.0100	 -0.0200