



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 12:54 pm BST

PDB ID : 9SMX / pdb_00009smx
EMDB ID : EMD-55043
Title : CM1-activated gTuRC in complex with nascent alpha-E254D mutant microtubules
Authors : Llorca, O.; Serna, M.; Lopez-Perrote, A.
Deposited on : 2025-09-09
Resolution : 3.67 Å (reported)
Based on initial models : 6X0U, 7AS4

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:

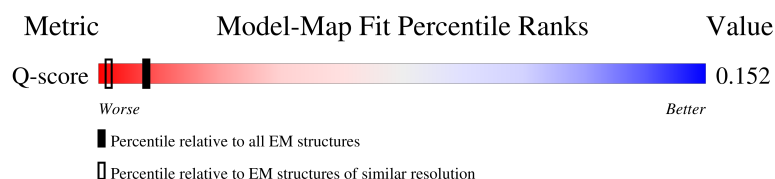
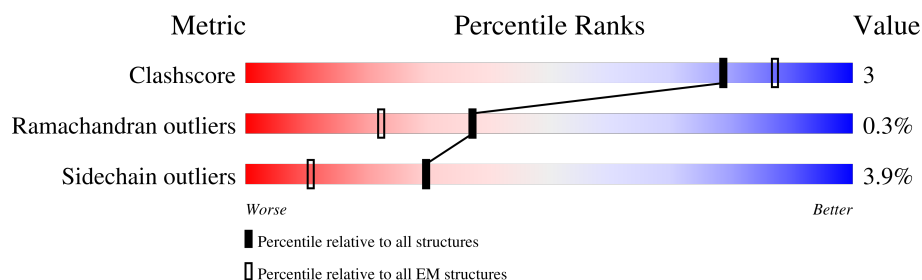
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.67 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	11424 (3.17 - 4.17)

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	3	907	 10% . 89%
1	B	907	 8% 59% 10% 30%
1	D	907	 9% 58% 9% 33%
1	F	907	 5% 55% 9% . 36%

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Mol	Chain	Length	Quality of chain
1	H	907	
1	N	907	
2	4	82	
2	6	82	
2	Y	82	
3	5	1819	
3	L	1819	
4	7	374	
5	A	902	
5	C	902	
5	CN	902	
5	E	902	
5	EN	902	
5	G	902	
5	GN	902	
5	M	902	
6	AC	229	
6	CC	229	
6	Cc	229	
6	EC	229	
6	Ec	229	
6	GC	229	
6	Gc	229	
6	MC	229	
6	Mc	229	

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Mol	Chain	Length	Quality of chain
7	BA	451	
7	CA	451	
7	DA	451	
7	EA	451	
7	FA	451	
7	GA	451	
7	HA	451	
7	IA	451	
7	JA	451	
7	KA	451	
7	LA	451	
8	BB	451	
8	CB	451	
8	DB	451	
8	EB	451	
8	FB	451	
8	GB	451	
8	HB	451	
8	IB	451	
8	JB	451	
8	KB	451	
8	LB	451	
9	CM	158	
9	EM	158	
9	GM	158	

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Mol	Chain	Length	Quality of chain
9	MM	158	
10	I	667	
10	K	667	
11	J	1024	
11	Z	1024	
12	a	451	
12	b	451	
12	c	451	
12	d	451	
12	e	451	
12	f	451	
12	g	451	
12	h	451	
12	i	451	
12	j	451	
12	k	451	
12	l	451	
12	m	451	
12	n	451	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 405906 atoms, of which 200969 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 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	3	102	Total	C	H	N	O	S	0	0
			1693	525	861	156	149	2		
1	B	635	Total	C	H	N	O	S	0	0
			10402	3319	5183	917	957	26		
1	D	610	Total	C	H	N	O	S	0	0
			10017	3196	5000	885	911	25		
1	F	581	Total	C	H	N	O	S	0	0
			9576	3061	4780	842	868	25		
1	H	581	Total	C	H	N	O	S	0	0
			9576	3061	4780	842	868	25		
1	N	635	Total	C	H	N	O	S	0	0
			10368	3313	5161	911	957	26		

- Molecule 2 is a protein called Mitotic-spindle organizing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	4	60	Total	C	H	N	O	S	0	0
			926	278	474	79	91	4		
2	6	61	Total	C	H	N	O	S	0	0
			936	281	479	80	92	4		
2	Y	56	Total	C	H	N	O	S	0	0
			877	263	451	75	84	4		

- Molecule 3 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	5	46	Total	C	H	N	O	S	0	0
			737	229	382	58	67	1		
3	L	616	Total	C	H	N	O	S	0	0
			9873	3211	4954	826	856	26		

- Molecule 4 is a protein called Actin, cytoplasmic 2, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	364	Total	C	H	N	O	0	0
			2764	1103	932	364	365		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	2	ASP	GLU	conflict	UNP P63261
7	5	VAL	ILE	conflict	UNP P63261
7	10	VAL	ILE	conflict	UNP P63261
7	153	LEU	MET	conflict	UNP P63261
7	160	SER	THR	conflict	UNP P63261
7	204	GLU	ALA	conflict	UNP P63261
7	243	LYS	PRO	conflict	UNP P63261
7	271	ALA	SER	conflict	UNP P63261
7	279	TYR	PHE	conflict	UNP P63261

- Molecule 5 is a protein called Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	697	Total 11240	C 3604	H 5617	N 948	O 1036	S 35	0	0
5	C	697	Total 11258	C 3607	H 5629	N 951	O 1036	S 35	0	0
5	CN	111	Total 1803	C 565	H 907	N 156	O 174	S 1	0	0
5	E	654	Total 10667	C 3427	H 5347	N 894	O 966	S 33	0	0
5	EN	111	Total 1803	C 565	H 907	N 156	O 174	S 1	0	0
5	G	654	Total 10666	C 3427	H 5346	N 894	O 966	S 33	0	0
5	GN	111	Total 1803	C 565	H 907	N 156	O 174	S 1	0	0
5	M	846	Total 13534	C 4320	H 6768	N 1141	O 1268	S 37	0	0

- Molecule 6 is a protein called Ubiquitin-like protein SMT3,CDK5 regulatory subunit-associated protein 2, Microtubule-associated protein RP/EB family member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
6	AC	35	Total	C	H	N	O	S	0	0
			631	197	318	58	56	2		

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Mol	Chain	Residues	Atoms						AltConf	Trace
6	CC	35	Total 631	C 197	H 318	N 58	O 56	S 2	0	0
6	Cc	35	Total 632	C 202	H 315	N 55	O 58	S 2	0	0
6	EC	33	Total 597	C 188	H 300	N 53	O 54	S 2	0	0
6	Ec	29	Total 520	C 167	H 259	N 44	O 49	S 1	0	0
6	GC	34	Total 607	C 191	H 305	N 54	O 55	S 2	0	0
6	Gc	31	Total 556	C 178	H 277	N 47	O 53	S 1	0	0
6	MC	32	Total 573	C 182	H 287	N 49	O 53	S 2	0	0
6	Mc	32	Total 574	C 183	H 287	N 48	O 54	S 2	0	0

There are 189 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	-68	MET	-	initiating methionine	UNP Q12306
AC	-67	GLY	-	expression tag	UNP Q12306
AC	-66	SER	-	expression tag	UNP Q12306
AC	-65	SER	-	expression tag	UNP Q12306
AC	-64	HIS	-	expression tag	UNP Q12306
AC	-63	HIS	-	expression tag	UNP Q12306
AC	-62	HIS	-	expression tag	UNP Q12306
AC	-61	HIS	-	expression tag	UNP Q12306
AC	-60	HIS	-	expression tag	UNP Q12306
AC	-59	HIS	-	expression tag	UNP Q12306
AC	-58	GLY	-	expression tag	UNP Q12306
AC	41	TRP	-	linker	UNP Q12306
AC	42	SER	-	linker	UNP Q12306
AC	43	HIS	-	linker	UNP Q12306
AC	44	PRO	-	linker	UNP Q12306
AC	45	GLN	-	linker	UNP Q12306
AC	46	PHE	-	linker	UNP Q12306
AC	47	GLU	-	linker	UNP Q12306
AC	48	LYS	-	linker	UNP Q12306
AC	49	SER	-	linker	UNP Q12306
AC	50	ALA	-	linker	UNP Q12306
CC	-68	MET	-	initiating methionine	UNP Q12306
CC	-67	GLY	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
CC	-66	SER	-	expression tag	UNP Q12306
CC	-65	SER	-	expression tag	UNP Q12306
CC	-64	HIS	-	expression tag	UNP Q12306
CC	-63	HIS	-	expression tag	UNP Q12306
CC	-62	HIS	-	expression tag	UNP Q12306
CC	-61	HIS	-	expression tag	UNP Q12306
CC	-60	HIS	-	expression tag	UNP Q12306
CC	-59	HIS	-	expression tag	UNP Q12306
CC	-58	GLY	-	expression tag	UNP Q12306
CC	41	TRP	-	linker	UNP Q12306
CC	42	SER	-	linker	UNP Q12306
CC	43	HIS	-	linker	UNP Q12306
CC	44	PRO	-	linker	UNP Q12306
CC	45	GLN	-	linker	UNP Q12306
CC	46	PHE	-	linker	UNP Q12306
CC	47	GLU	-	linker	UNP Q12306
CC	48	LYS	-	linker	UNP Q12306
CC	49	SER	-	linker	UNP Q12306
CC	50	ALA	-	linker	UNP Q12306
Cc	-68	MET	-	initiating methionine	UNP Q12306
Cc	-67	GLY	-	expression tag	UNP Q12306
Cc	-66	SER	-	expression tag	UNP Q12306
Cc	-65	SER	-	expression tag	UNP Q12306
Cc	-64	HIS	-	expression tag	UNP Q12306
Cc	-63	HIS	-	expression tag	UNP Q12306
Cc	-62	HIS	-	expression tag	UNP Q12306
Cc	-61	HIS	-	expression tag	UNP Q12306
Cc	-60	HIS	-	expression tag	UNP Q12306
Cc	-59	HIS	-	expression tag	UNP Q12306
Cc	-58	GLY	-	expression tag	UNP Q12306
Cc	41	TRP	-	linker	UNP Q12306
Cc	42	SER	-	linker	UNP Q12306
Cc	43	HIS	-	linker	UNP Q12306
Cc	44	PRO	-	linker	UNP Q12306
Cc	45	GLN	-	linker	UNP Q12306
Cc	46	PHE	-	linker	UNP Q12306
Cc	47	GLU	-	linker	UNP Q12306
Cc	48	LYS	-	linker	UNP Q12306
Cc	49	SER	-	linker	UNP Q12306
Cc	50	ALA	-	linker	UNP Q12306
EC	-68	MET	-	initiating methionine	UNP Q12306
EC	-67	GLY	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
EC	-66	SER	-	expression tag	UNP Q12306
EC	-65	SER	-	expression tag	UNP Q12306
EC	-64	HIS	-	expression tag	UNP Q12306
EC	-63	HIS	-	expression tag	UNP Q12306
EC	-62	HIS	-	expression tag	UNP Q12306
EC	-61	HIS	-	expression tag	UNP Q12306
EC	-60	HIS	-	expression tag	UNP Q12306
EC	-59	HIS	-	expression tag	UNP Q12306
EC	-58	GLY	-	expression tag	UNP Q12306
EC	41	TRP	-	linker	UNP Q12306
EC	42	SER	-	linker	UNP Q12306
EC	43	HIS	-	linker	UNP Q12306
EC	44	PRO	-	linker	UNP Q12306
EC	45	GLN	-	linker	UNP Q12306
EC	46	PHE	-	linker	UNP Q12306
EC	47	GLU	-	linker	UNP Q12306
EC	48	LYS	-	linker	UNP Q12306
EC	49	SER	-	linker	UNP Q12306
EC	50	ALA	-	linker	UNP Q12306
Ec	-68	MET	-	initiating methionine	UNP Q12306
Ec	-67	GLY	-	expression tag	UNP Q12306
Ec	-66	SER	-	expression tag	UNP Q12306
Ec	-65	SER	-	expression tag	UNP Q12306
Ec	-64	HIS	-	expression tag	UNP Q12306
Ec	-63	HIS	-	expression tag	UNP Q12306
Ec	-62	HIS	-	expression tag	UNP Q12306
Ec	-61	HIS	-	expression tag	UNP Q12306
Ec	-60	HIS	-	expression tag	UNP Q12306
Ec	-59	HIS	-	expression tag	UNP Q12306
Ec	-58	GLY	-	expression tag	UNP Q12306
Ec	41	TRP	-	linker	UNP Q12306
Ec	42	SER	-	linker	UNP Q12306
Ec	43	HIS	-	linker	UNP Q12306
Ec	44	PRO	-	linker	UNP Q12306
Ec	45	GLN	-	linker	UNP Q12306
Ec	46	PHE	-	linker	UNP Q12306
Ec	47	GLU	-	linker	UNP Q12306
Ec	48	LYS	-	linker	UNP Q12306
Ec	49	SER	-	linker	UNP Q12306
Ec	50	ALA	-	linker	UNP Q12306
GC	-68	MET	-	initiating methionine	UNP Q12306
GC	-67	GLY	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
GC	-66	SER	-	expression tag	UNP Q12306
GC	-65	SER	-	expression tag	UNP Q12306
GC	-64	HIS	-	expression tag	UNP Q12306
GC	-63	HIS	-	expression tag	UNP Q12306
GC	-62	HIS	-	expression tag	UNP Q12306
GC	-61	HIS	-	expression tag	UNP Q12306
GC	-60	HIS	-	expression tag	UNP Q12306
GC	-59	HIS	-	expression tag	UNP Q12306
GC	-58	GLY	-	expression tag	UNP Q12306
GC	41	TRP	-	linker	UNP Q12306
GC	42	SER	-	linker	UNP Q12306
GC	43	HIS	-	linker	UNP Q12306
GC	44	PRO	-	linker	UNP Q12306
GC	45	GLN	-	linker	UNP Q12306
GC	46	PHE	-	linker	UNP Q12306
GC	47	GLU	-	linker	UNP Q12306
GC	48	LYS	-	linker	UNP Q12306
GC	49	SER	-	linker	UNP Q12306
GC	50	ALA	-	linker	UNP Q12306
Gc	-68	MET	-	initiating methionine	UNP Q12306
Gc	-67	GLY	-	expression tag	UNP Q12306
Gc	-66	SER	-	expression tag	UNP Q12306
Gc	-65	SER	-	expression tag	UNP Q12306
Gc	-64	HIS	-	expression tag	UNP Q12306
Gc	-63	HIS	-	expression tag	UNP Q12306
Gc	-62	HIS	-	expression tag	UNP Q12306
Gc	-61	HIS	-	expression tag	UNP Q12306
Gc	-60	HIS	-	expression tag	UNP Q12306
Gc	-59	HIS	-	expression tag	UNP Q12306
Gc	-58	GLY	-	expression tag	UNP Q12306
Gc	41	TRP	-	linker	UNP Q12306
Gc	42	SER	-	linker	UNP Q12306
Gc	43	HIS	-	linker	UNP Q12306
Gc	44	PRO	-	linker	UNP Q12306
Gc	45	GLN	-	linker	UNP Q12306
Gc	46	PHE	-	linker	UNP Q12306
Gc	47	GLU	-	linker	UNP Q12306
Gc	48	LYS	-	linker	UNP Q12306
Gc	49	SER	-	linker	UNP Q12306
Gc	50	ALA	-	linker	UNP Q12306
MC	-68	MET	-	initiating methionine	UNP Q12306
MC	-67	GLY	-	expression tag	UNP Q12306

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Chain	Residue	Modelled	Actual	Comment	Reference
MC	-66	SER	-	expression tag	UNP Q12306
MC	-65	SER	-	expression tag	UNP Q12306
MC	-64	HIS	-	expression tag	UNP Q12306
MC	-63	HIS	-	expression tag	UNP Q12306
MC	-62	HIS	-	expression tag	UNP Q12306
MC	-61	HIS	-	expression tag	UNP Q12306
MC	-60	HIS	-	expression tag	UNP Q12306
MC	-59	HIS	-	expression tag	UNP Q12306
MC	-58	GLY	-	expression tag	UNP Q12306
MC	41	TRP	-	linker	UNP Q12306
MC	42	SER	-	linker	UNP Q12306
MC	43	HIS	-	linker	UNP Q12306
MC	44	PRO	-	linker	UNP Q12306
MC	45	GLN	-	linker	UNP Q12306
MC	46	PHE	-	linker	UNP Q12306
MC	47	GLU	-	linker	UNP Q12306
MC	48	LYS	-	linker	UNP Q12306
MC	49	SER	-	linker	UNP Q12306
MC	50	ALA	-	linker	UNP Q12306
Mc	-68	MET	-	initiating methionine	UNP Q12306
Mc	-67	GLY	-	expression tag	UNP Q12306
Mc	-66	SER	-	expression tag	UNP Q12306
Mc	-65	SER	-	expression tag	UNP Q12306
Mc	-64	HIS	-	expression tag	UNP Q12306
Mc	-63	HIS	-	expression tag	UNP Q12306
Mc	-62	HIS	-	expression tag	UNP Q12306
Mc	-61	HIS	-	expression tag	UNP Q12306
Mc	-60	HIS	-	expression tag	UNP Q12306
Mc	-59	HIS	-	expression tag	UNP Q12306
Mc	-58	GLY	-	expression tag	UNP Q12306
Mc	41	TRP	-	linker	UNP Q12306
Mc	42	SER	-	linker	UNP Q12306
Mc	43	HIS	-	linker	UNP Q12306
Mc	44	PRO	-	linker	UNP Q12306
Mc	45	GLN	-	linker	UNP Q12306
Mc	46	PHE	-	linker	UNP Q12306
Mc	47	GLU	-	linker	UNP Q12306
Mc	48	LYS	-	linker	UNP Q12306
Mc	49	SER	-	linker	UNP Q12306
Mc	50	ALA	-	linker	UNP Q12306

- Molecule 7 is a protein called Isoform 1 of Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	BA	438	Total	C	H	N	O	S	0	0
			6675	2148	3275	577	654	21		
7	CA	428	Total	C	H	N	O	S	0	0
			6552	2104	3230	566	631	21		
7	DA	428	Total	C	H	N	O	S	0	0
			6552	2104	3230	566	631	21		
7	EA	428	Total	C	H	N	O	S	0	0
			6553	2104	3231	566	631	21		
7	FA	428	Total	C	H	N	O	S	0	0
			6552	2104	3230	566	631	21		
7	GA	428	Total	C	H	N	O	S	0	0
			6544	2104	3222	566	631	21		
7	HA	428	Total	C	H	N	O	S	0	0
			6552	2104	3230	566	631	21		
7	IA	428	Total	C	H	N	O	S	0	0
			6553	2104	3231	566	631	21		
7	JA	428	Total	C	H	N	O	S	0	0
			6551	2104	3229	566	631	21		
7	KA	428	Total	C	H	N	O	S	0	0
			6553	2104	3231	566	631	21		
7	LA	428	Total	C	H	N	O	S	0	0
			6552	2104	3230	566	631	21		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	254	ASP	GLU	engineered mutation	UNP P68363
CA	254	ASP	GLU	engineered mutation	UNP P68363
DA	254	ASP	GLU	engineered mutation	UNP P68363
EA	254	ASP	GLU	engineered mutation	UNP P68363
FA	254	ASP	GLU	engineered mutation	UNP P68363
GA	254	ASP	GLU	engineered mutation	UNP P68363
HA	254	ASP	GLU	engineered mutation	UNP P68363
IA	254	ASP	GLU	engineered mutation	UNP P68363
JA	254	ASP	GLU	engineered mutation	UNP P68363
KA	254	ASP	GLU	engineered mutation	UNP P68363
LA	254	ASP	GLU	engineered mutation	UNP P68363

- Molecule 8 is a protein called Tubulin beta-3 chain.

Mol	Chain	Residues	Atoms							AltConf	Trace
8	BB	426	Total	C	H	N	O	P	S	0	0
			6525	2094	3189	563	652	2	25		

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Mol	Chain	Residues	Atoms							AltConf	Trace
8	CB	426	Total	C	H	N	O	P	S	0	0
			6576	2103	3222	572	652	2	25		
8	DB	426	Total	C	H	N	O	P	S	0	0
			6559	2100	3211	569	652	2	25		
8	EB	426	Total	C	H	N	O	P	S	0	0
			6577	2103	3223	572	652	2	25		
8	FB	426	Total	C	H	N	O	P	S	0	0
			6576	2103	3222	572	652	2	25		
8	GB	426	Total	C	H	N	O	P	S	0	0
			6576	2103	3222	572	652	2	25		
8	HB	426	Total	C	H	N	O	P	S	0	0
			6577	2103	3223	572	652	2	25		
8	IB	426	Total	C	H	N	O	P	S	0	0
			6577	2103	3223	572	652	2	25		
8	JB	426	Total	C	H	N	O	P	S	0	0
			6577	2103	3223	572	652	2	25		
8	KB	426	Total	C	H	N	O	P	S	0	0
			6576	2103	3222	572	652	2	25		
8	LB	426	Total	C	H	N	O	P	S	0	0
			6576	2103	3222	572	652	2	25		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	501	GDP	-	expression tag	UNP Q13509
CB	501	GDP	-	expression tag	UNP Q13509
DB	501	GDP	-	expression tag	UNP Q13509
EB	501	GDP	-	expression tag	UNP Q13509
FB	501	GDP	-	expression tag	UNP Q13509
GB	501	GDP	-	expression tag	UNP Q13509
HB	501	GDP	-	expression tag	UNP Q13509
IB	501	GDP	-	expression tag	UNP Q13509
JB	501	GDP	-	expression tag	UNP Q13509
KB	501	GDP	-	expression tag	UNP Q13509
LB	501	GDP	-	expression tag	UNP Q13509

- Molecule 9 is a protein called Mitotic-spindle organizing protein 2A.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	CM	54	Total	C	H	N	O	S	0	0
			837	263	429	65	76	4		
9	EM	54	Total	C	H	N	O	S	0	0
			837	263	429	65	76	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
9	GM	53	Total	C	H	N	O	S	0	0
			813	257	416	61	75	4		
9	MM	53	Total	C	H	N	O	S	0	0
			813	257	416	61	75	4		

- Molecule 10 is a protein called Gamma-tubulin complex component 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	521	Total	C	H	N	O	S	0	0
			8477	2734	4255	720	750	18		
10	K	553	Total	C	H	N	O	S	0	0
			9006	2915	4509	765	800	17		

- Molecule 11 is a protein called Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	594	Total	C	H	N	O	S	0	0
			9521	3086	4748	798	863	26		
11	Z	124	Total	C	H	N	O	S	0	0
			1988	642	982	175	188	1		

- Molecule 12 is a protein called Tubulin gamma-1 chain.

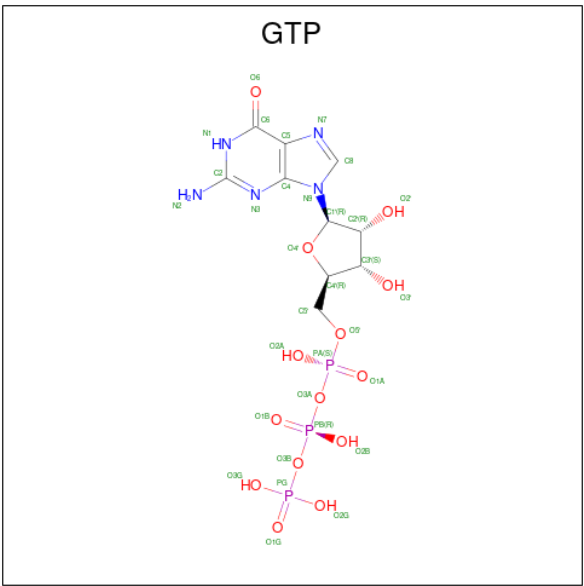
Mol	Chain	Residues	Atoms						AltConf	Trace
12	a	412	Total	C	H	N	O	S	0	0
			6595	2100	3282	576	622	15		
12	b	412	Total	C	H	N	O	S	0	0
			6595	2100	3282	576	622	15		
12	c	412	Total	C	H	N	O	S	0	0
			6596	2100	3283	576	622	15		
12	d	419	Total	C	H	N	O	S	0	0
			6697	2132	3328	585	637	15		
12	e	419	Total	C	H	N	O	S	0	0
			6680	2129	3317	582	637	15		
12	f	412	Total	C	H	N	O	S	0	0
			6595	2100	3282	576	622	15		
12	g	419	Total	C	H	N	O	S	0	0
			6646	2123	3295	576	637	15		
12	h	412	Total	C	H	N	O	S	0	0
			6578	2097	3271	573	622	15		
12	i	419	Total	C	H	N	O	S	0	0
			6697	2132	3328	585	637	15		

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Mol	Chain	Residues	Atoms						AltConf	Trace
12	j	419	Total	C	H	N	O	S	0	0
			6680	2129	3317	582	637	15		
12	k	412	Total	C	H	N	O	S	0	0
			6588	2099	3277	576	621	15		
12	l	419	Total	C	H	N	O	S	0	0
			6691	2131	3324	585	636	15		
12	m	412	Total	C	H	N	O	S	0	0
			6596	2100	3283	576	622	15		
12	n	412	Total	C	H	N	O	S	0	0
			6595	2100	3282	576	622	15		

- Molecule 13 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



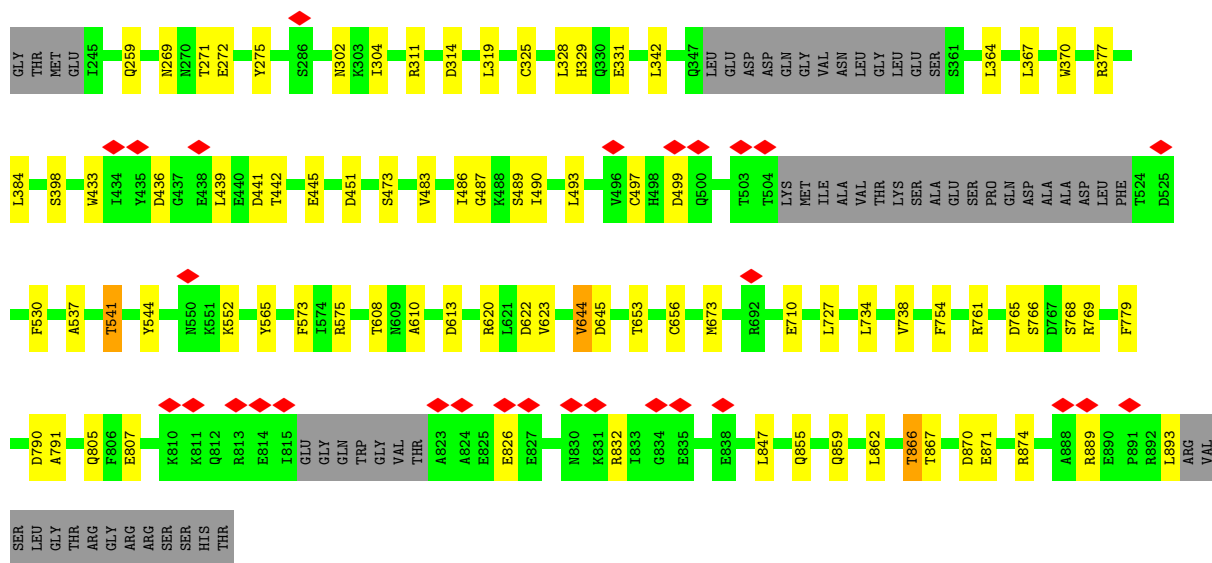
Mol	Chain	Residues	Atoms						AltConf
13	BA	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
13	CA	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
13	DA	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
13	EA	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
13	FA	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
13	GA	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

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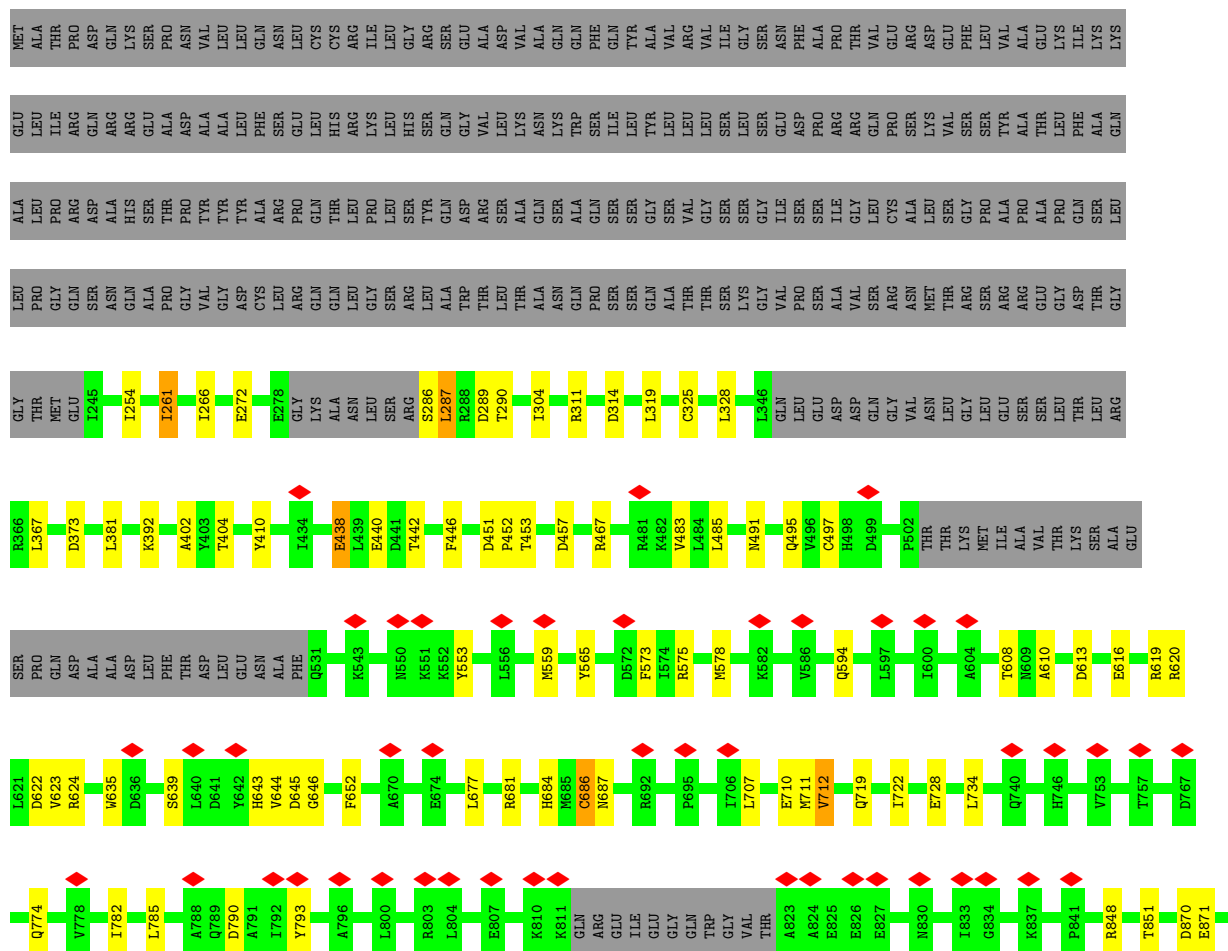
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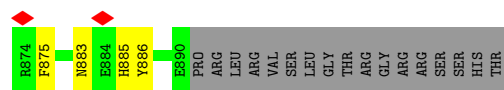
Mol	Chain	Residues	Atoms						AltConf
13	HA	1	Total 44	C 10	H 12	N 5	O 14	P 3	0
13	IA	1	Total 44	C 10	H 12	N 5	O 14	P 3	0
13	JA	1	Total 44	C 10	H 12	N 5	O 14	P 3	0
13	KA	1	Total 44	C 10	H 12	N 5	O 14	P 3	0
13	LA	1	Total 44	C 10	H 12	N 5	O 14	P 3	0



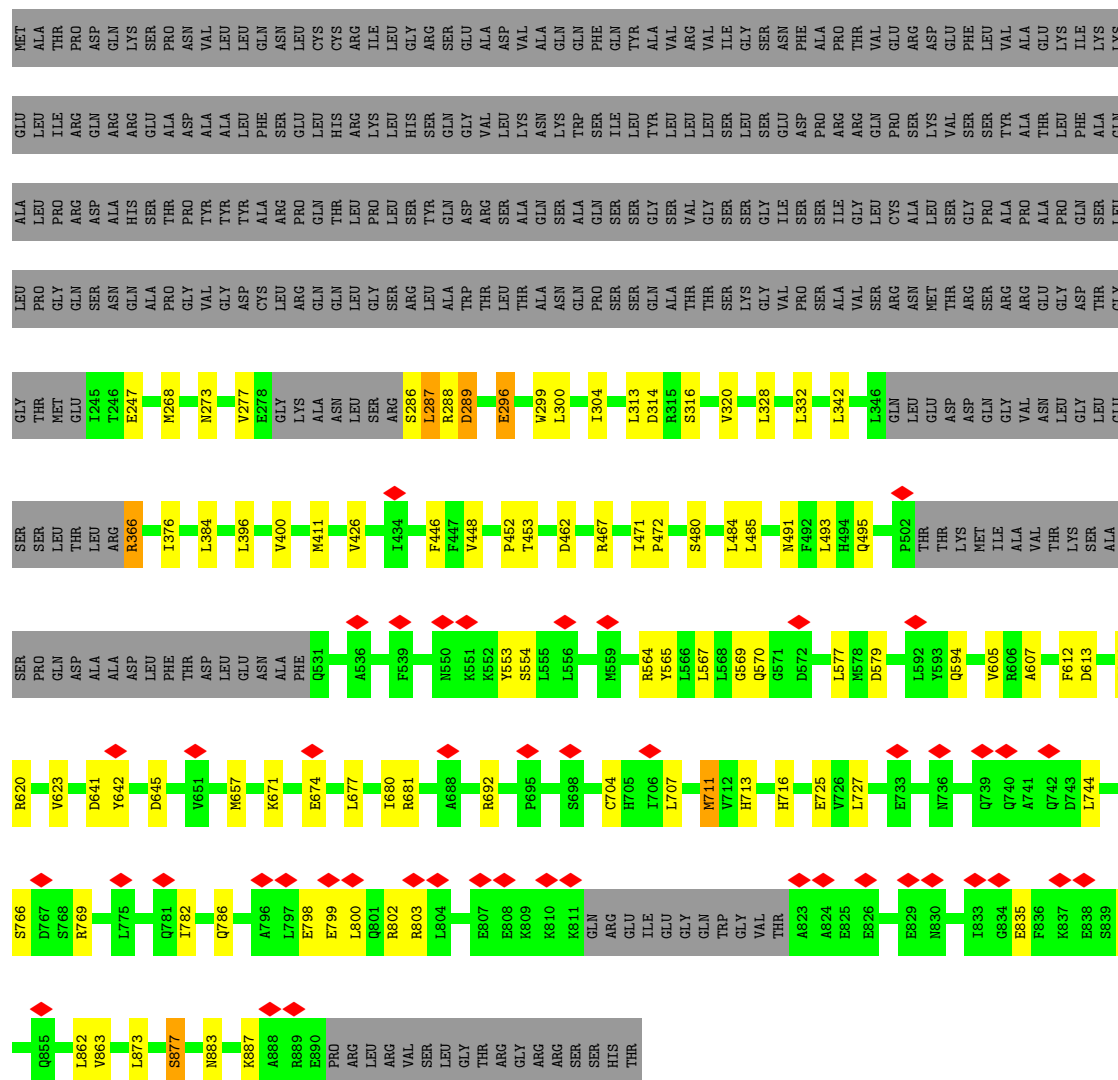


• Molecule 1: Gamma-tubulin complex component 3

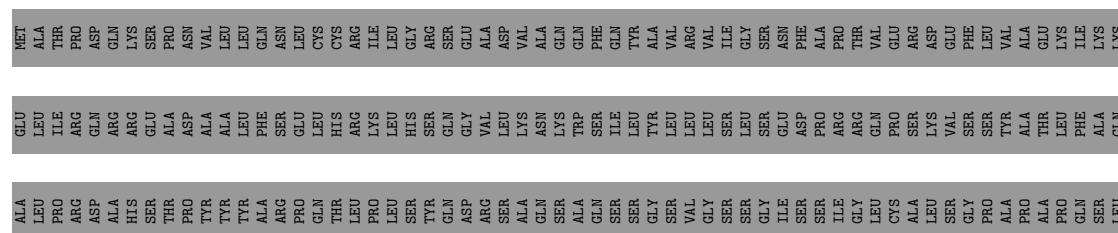


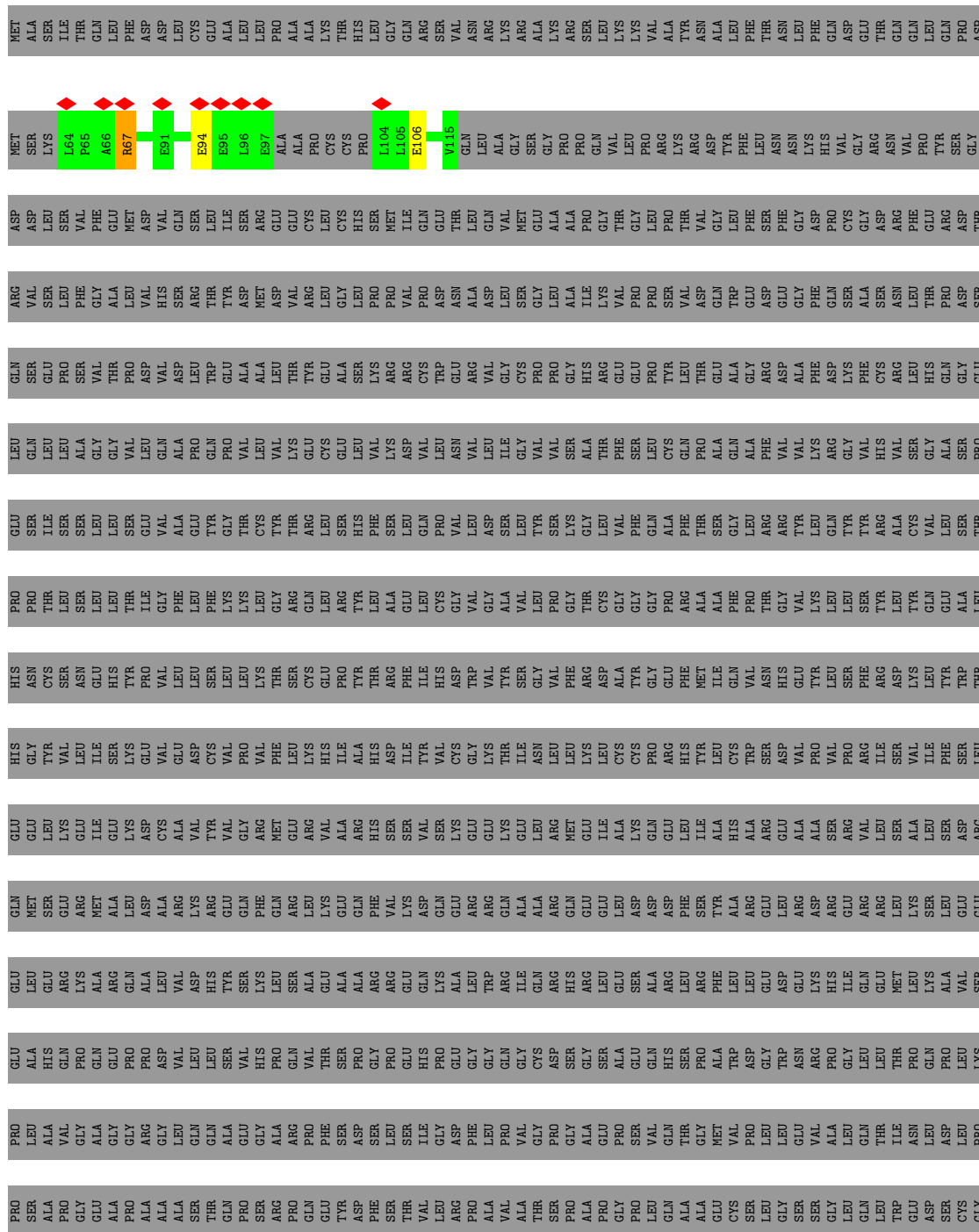


• Molecule 1: Gamma-tubulin complex component 3

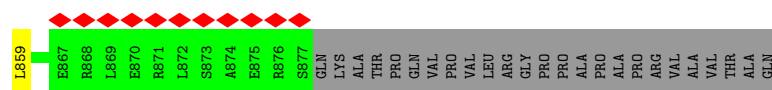


• Molecule 1: Gamma-tubulin complex component 3

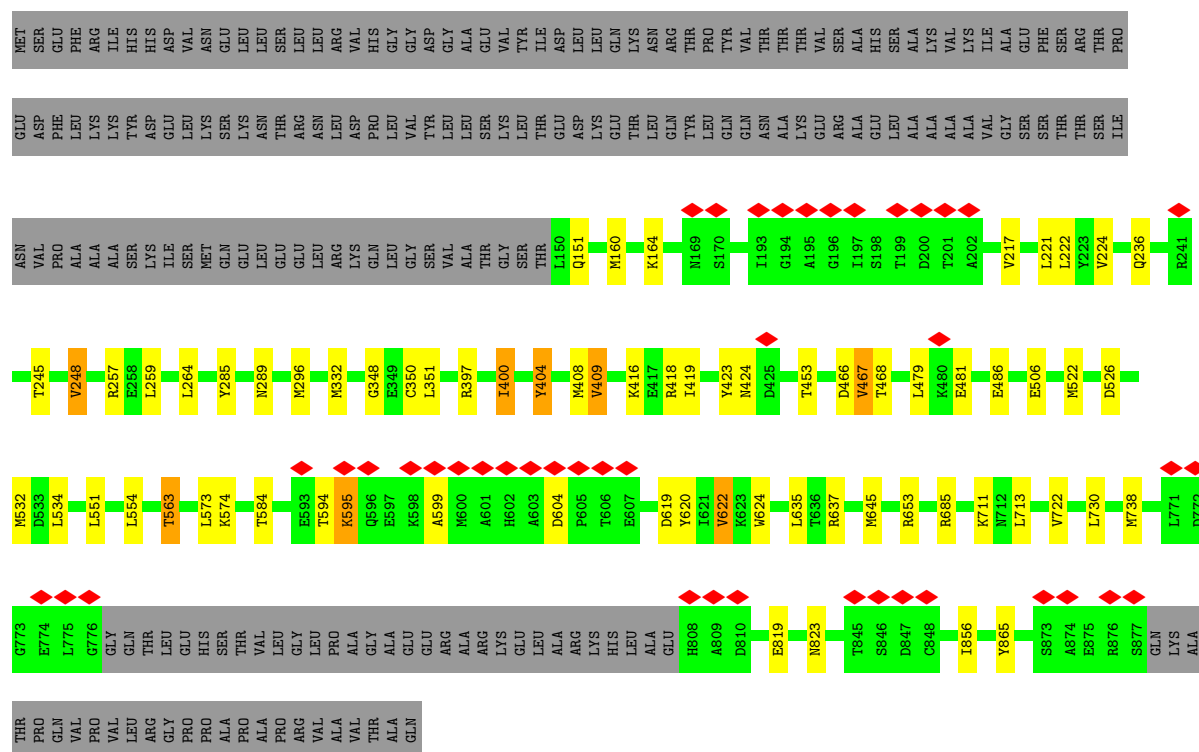




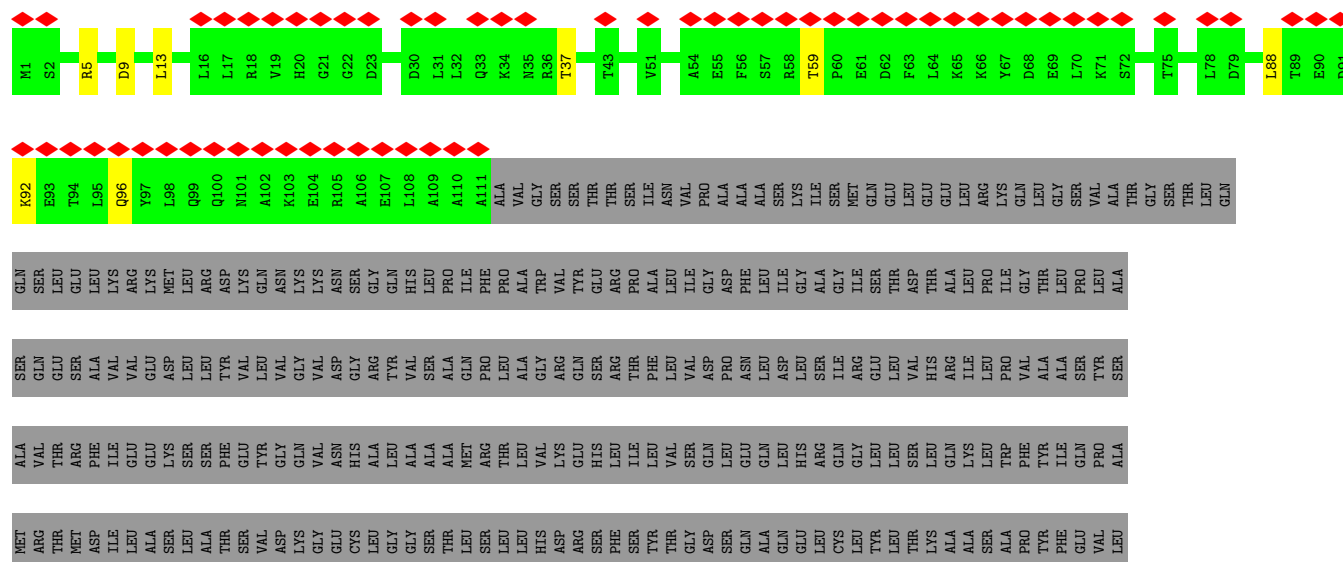




• Molecule 5: Gamma-tubulin complex component 2



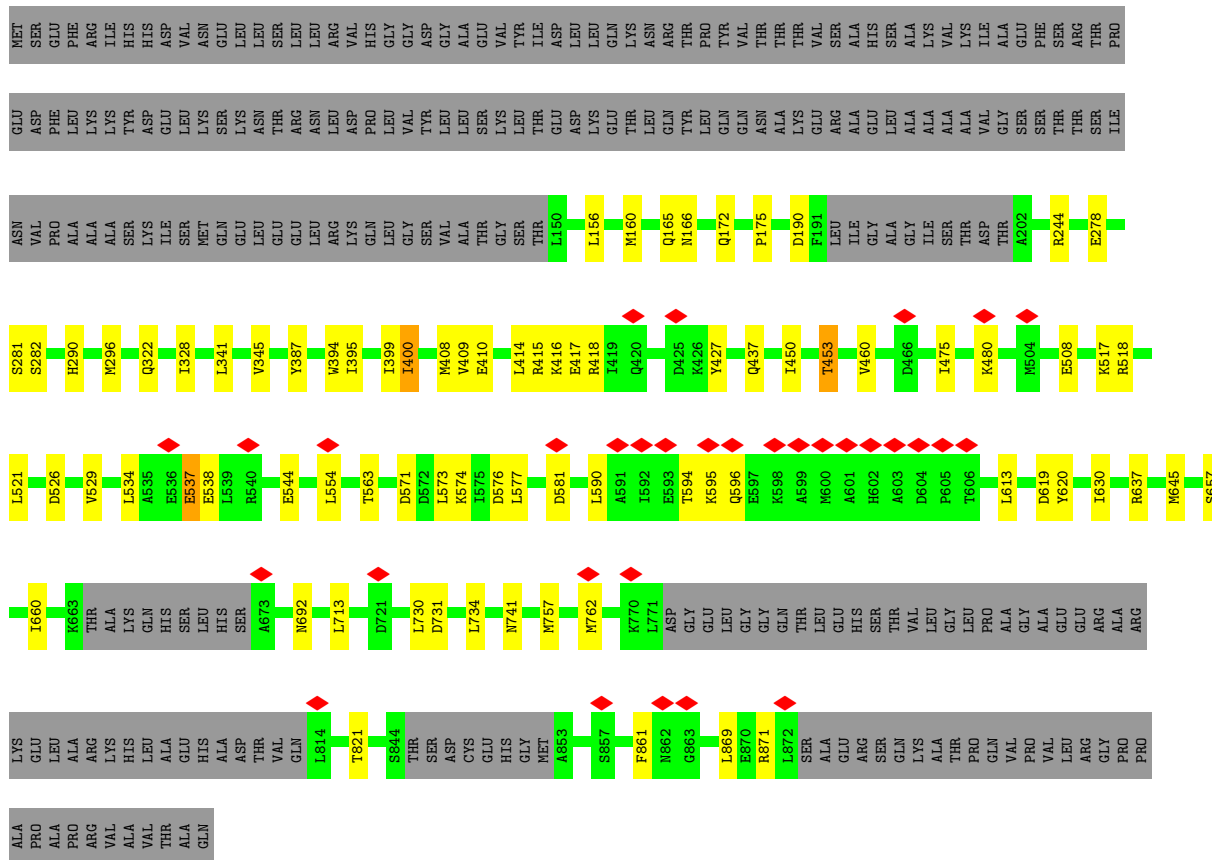
• Molecule 5: Gamma-tubulin complex component 2



[illegible]

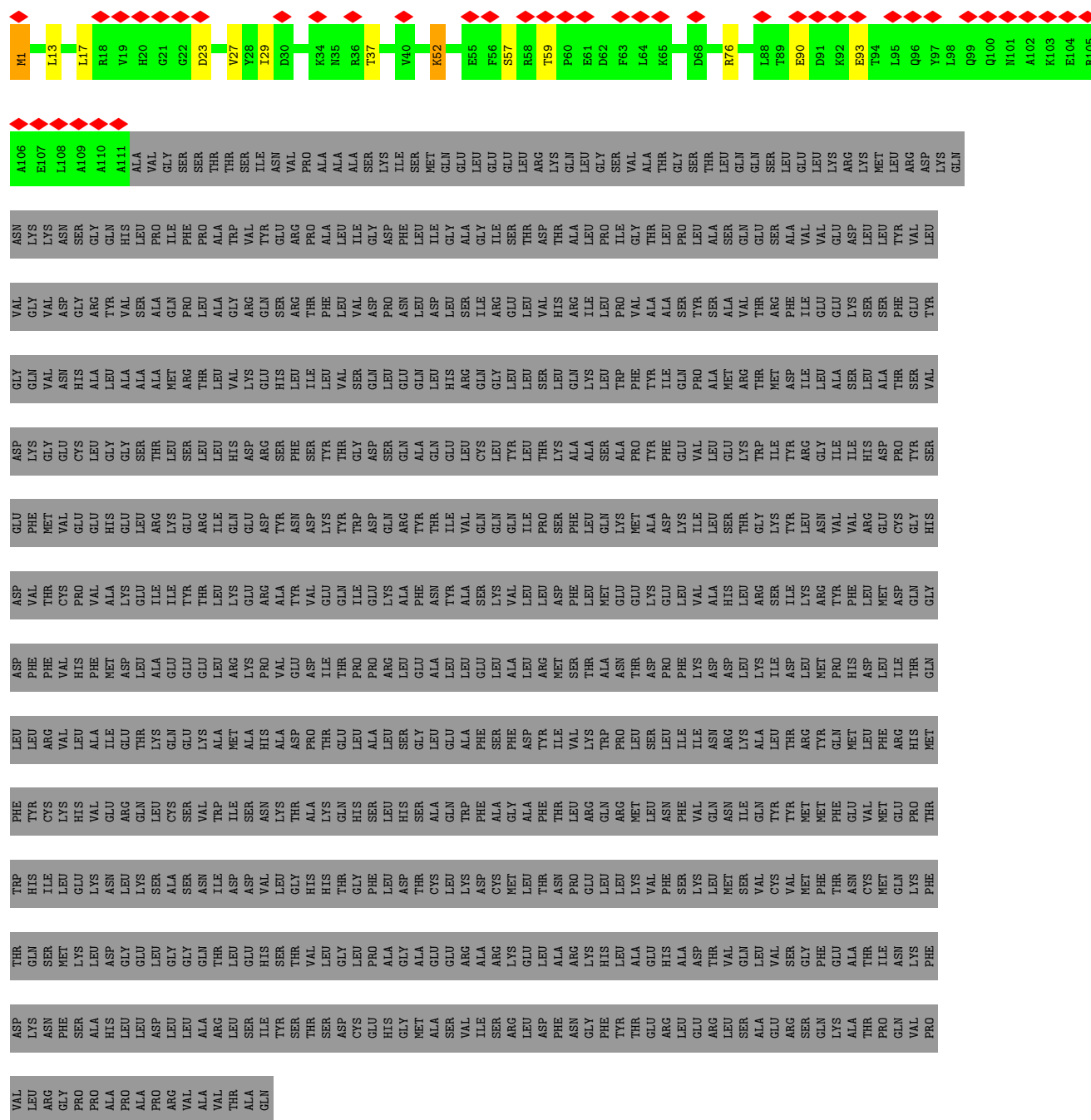
- Molecule 5: Gamma-tubulin complex component 2

Chain E: 64% 8% 27%



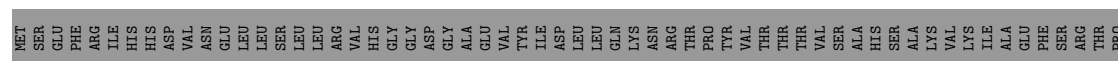
- Molecule 5: Gamma-tubulin complex component 2

Chain EN:  5% 11% 88%



- Molecule 5: Gamma-tubulin complex component 2

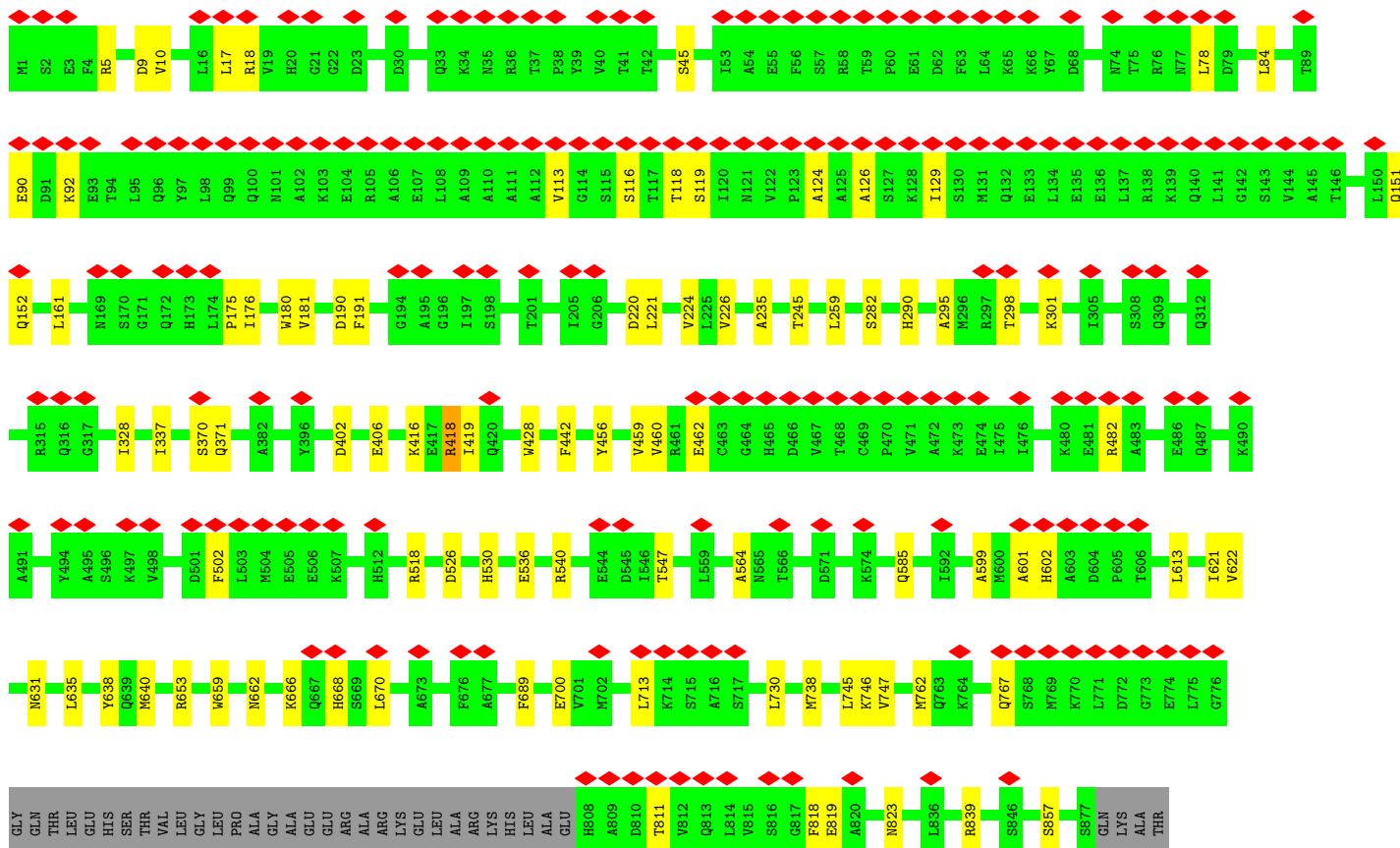
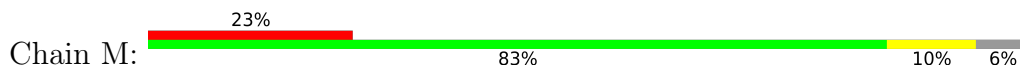
Chain G:  5% 63% 9% 27%





[illegible]

- Molecule 5: Gamma-tubulin complex component 2



Chain Gc:  13% 86%

GLU	LEU	ILE	CYS	GLN	GLY	ASN	GLY	GLU	GLY	ASP	ASN	PRO	VAL	LEU	GLN	ARG	ILE	VAL	ASP	ILE	ILE	TYR	THR	ALA	ALA	GLU	PHE	VAL	ILE																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
VAL	SER	PRO	THR	ARG	ALA	ARG	ASN	MET	K61	E67	E73	K79	L84	Q89	Q90	E91	PHE	HIS	GLY	ASP	GLY	ASP	GLU	ALA	ALA	GLU	LEU	MET	GLN	VAL	ASN	GLN	ASP	ILE	ARG	GLN	THR	PRO	GLU	GLY	GLY	ILE	ASP	GLU	GLY	ASP	LEU	THR	ALA	THR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					

- Molecule 6: Ubiquitin-like protein SMT3,CDK5 regulatory subunit-associated protein 2, Microtubule-associated protein RP/EB family member 1

Chain MC:  11% 86%


ILE	CYS	GLN	GLU	ASN	GLU	GLY	GLU	GLY	N59	M60	K61	K72	E73	L84	M88	Q89	Q90	GLU	PHE	HIS	GLY	ASP	ASP	GLU	ALA	ALA	GLU	GLU	LEU	MET	GLN	GLN	VAL	ASN	ASN	VAL	LEU	LYS	LEU	LYS	THR	VAL	GLU	GLU	LEU	LEU	GLY	LYS	GLY	THR	ARG	ASP	PHE	TYR	PHE	GLY	LYS	LEU	ASN	ILE	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
MET	GLY	SER	ALA	SER	THR	LYS	ARG	HIS	HIS	HIS	HIS	HIS	HIS	HIS	ASP	SER	ASP	SER	LEU	ARG	ARG	PHE	TYR	ASN	GLN	GLY	ALA	VAL	LYS	PRO	GLU	THR	ILE	ASN	ASN	LEU	ASP	ASP	ILE	LYS	ILE	GLY	ALA	HIS	SER	SER	GLU	ILE	PHE	GLY	LYS	LYS	THR	THR	PRO	GLN	PHE	GLY	LYS	ARG	LEU	ARG	LEU	MET	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
VAL	SER	PRO	THR	ARG	ALA	ALA	ARG	GLY	ARG	N59	M60	K61	K72	E73	L84	M88	Q89	Q90	GLU	PHE	HIS	GLY	ASP	ASP	GLU	ALA	ALA	GLU	GLU	LEU	MET	GLN	GLN	VAL	ASN	ASN	VAL	LEU	LYS	LEU	LYS	THR	VAL	GLU	GLU	LEU	LEU	GLY	LYS	GLY	THR	ARG	ASP	PHE	TYR	PHE	GLY	LYS	LEU	ASN	ILE	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
ILE	CYS	GLN	GLU	ASN	GLU	GLY	GLU	GLY	GLY	ASP	ASN	PRO	VAL	LEU	GLN	VAL	VAL	ASP	ASP	ILE	LEU	TYR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						

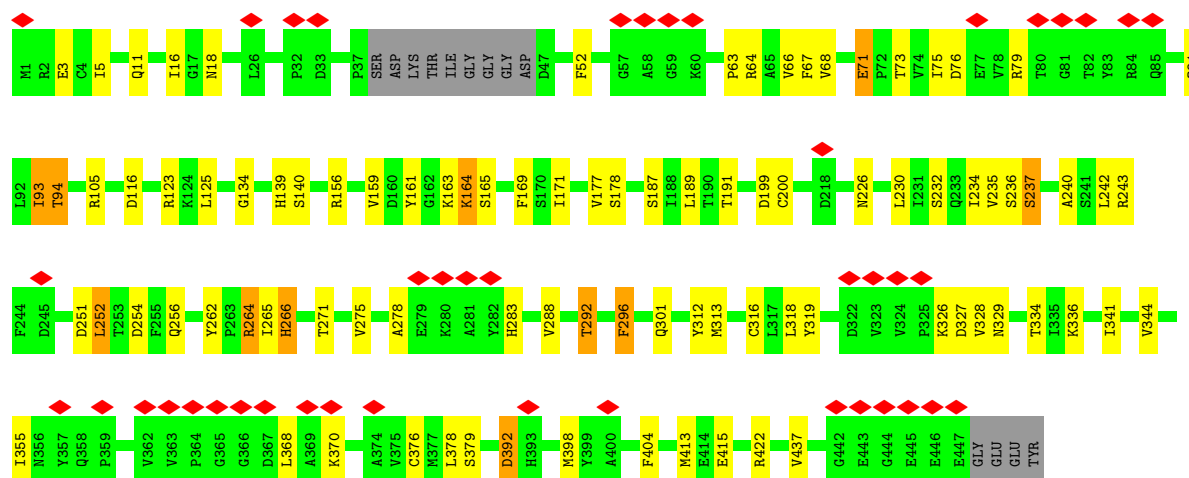
- Molecule 6: Ubiquitin-like protein SMT3,CDK5 regulatory subunit-associated protein 2, Microtubule-associated protein RP/EB family member 1

Chain Mc:  6% 13% 86%

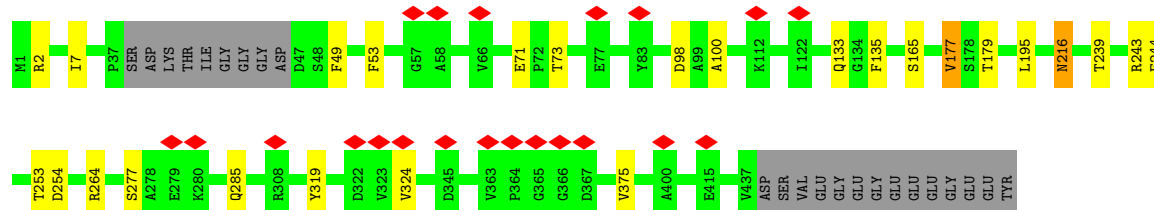
THR	PHE	GLY	LYS	LEU	ARG	ASN	ILE	GLU	LEU	GLY	GLY	GLY	ASN	ASP	PRO	VAL	LEU	GLN	ARG	ILE	VAL	ASP	ILE	LEU	TYR	ALA	THR	THR	ASP	GLY	GLY	PHE	VAL	ILE																														
VAL	SER	PRO	THR	ARG	ALA	ARG	ASN	M60	K61	D62	F63	E64	N65	T68	E69	L70	K71	K72	E73	F74	F75	N76	L77	M88	Q89	Q90	E91	PHE	HIS	HIS	GLY	ASP	ASP	GLU	GLU	ALA	ALA	GLY	LEU	MET	GLN	GLN	GLY	GLY	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLY	LYS	LYS	THR	PRO	GLY	ARG	LEU	ARG	LEU	MET	GLU	
MET	GLY	SER	ALA	SER	HIS	HIS	HIS	HIS	HIS	HIS	GLY	ASP	SER	GLY	ASP	GLU	VAL	ASN	GLN	GLY	ASN	TYR	ASP	GLY	ILE	ALA	ARG	LYS	PRO	GLU	VAL	LYS	PRO	GLU	GLN	ASP	ALA	VAL	LYS	PRO	GLU	THR	HIS	ILE	ASN	LEU	SER	SER	GLY	GLU	ILE	PHE	PHE	LYS	ILE	GLY	GLU	VAL	ASN	GLY	LYS	GLY	ALA	THR

- Molecule 7: Isoform 1 of Tubulin alpha-1B chain

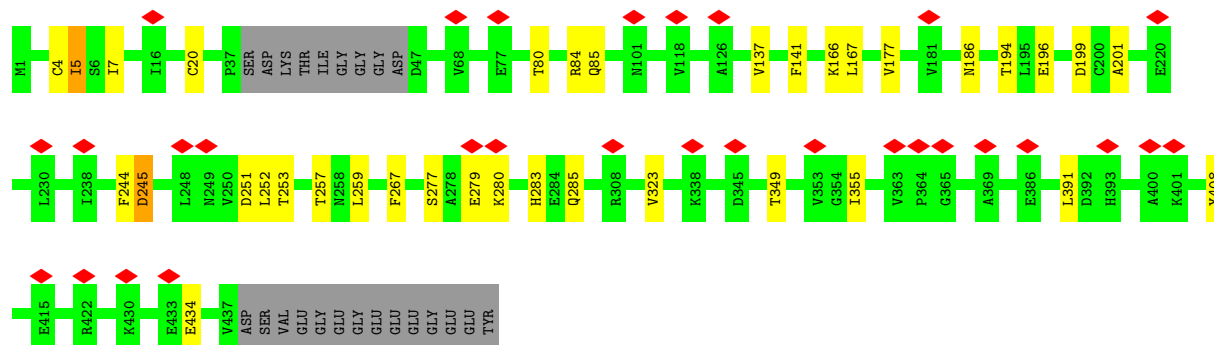
Chain BA:  10% 76% 18%



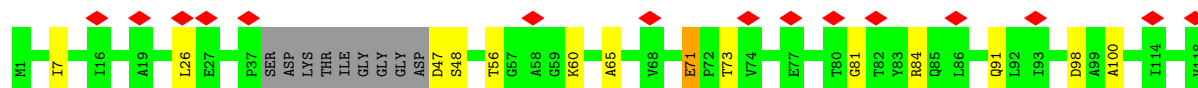
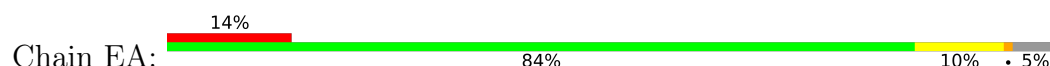
• Molecule 7: Isoform 1 of Tubulin alpha-1B chain

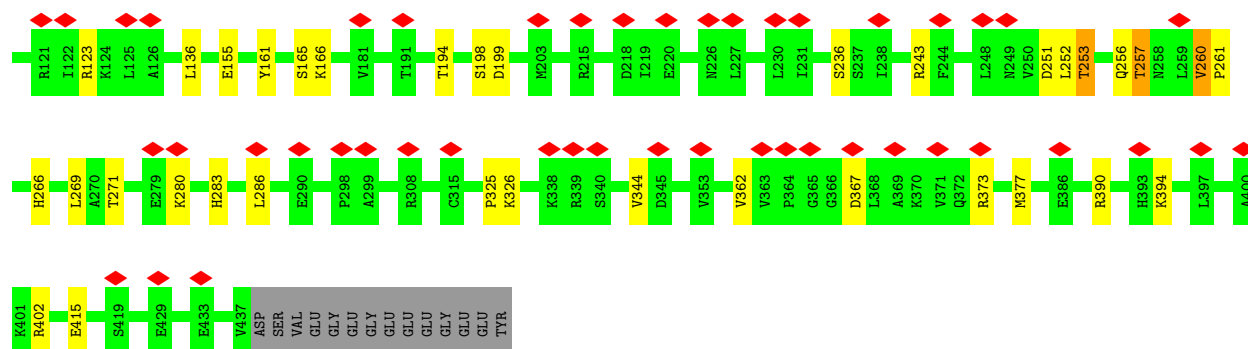


• Molecule 7: Isoform 1 of Tubulin alpha-1B chain

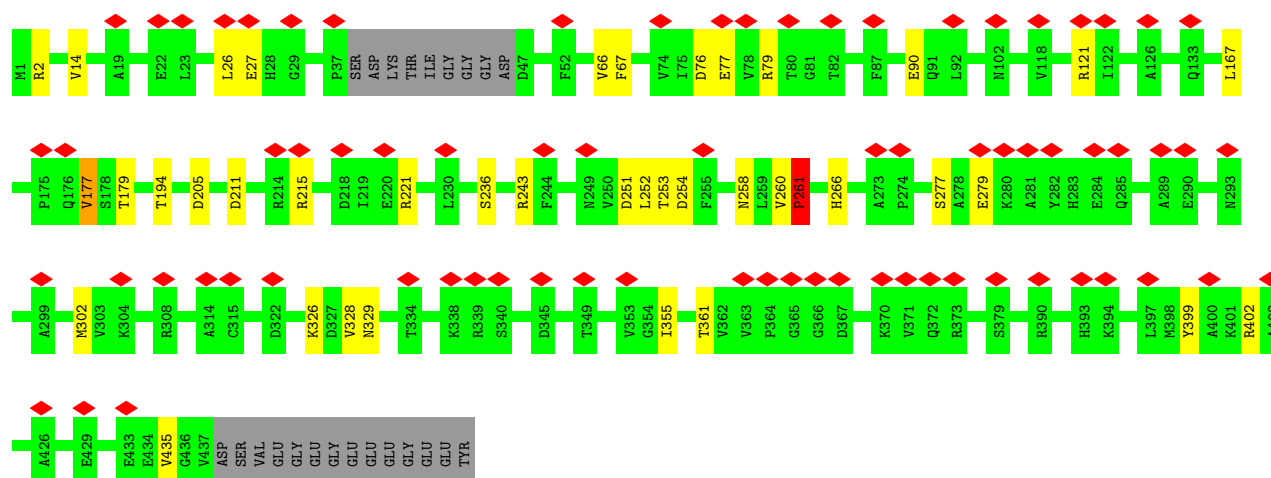


• Molecule 7: Isoform 1 of Tubulin alpha-1B chain

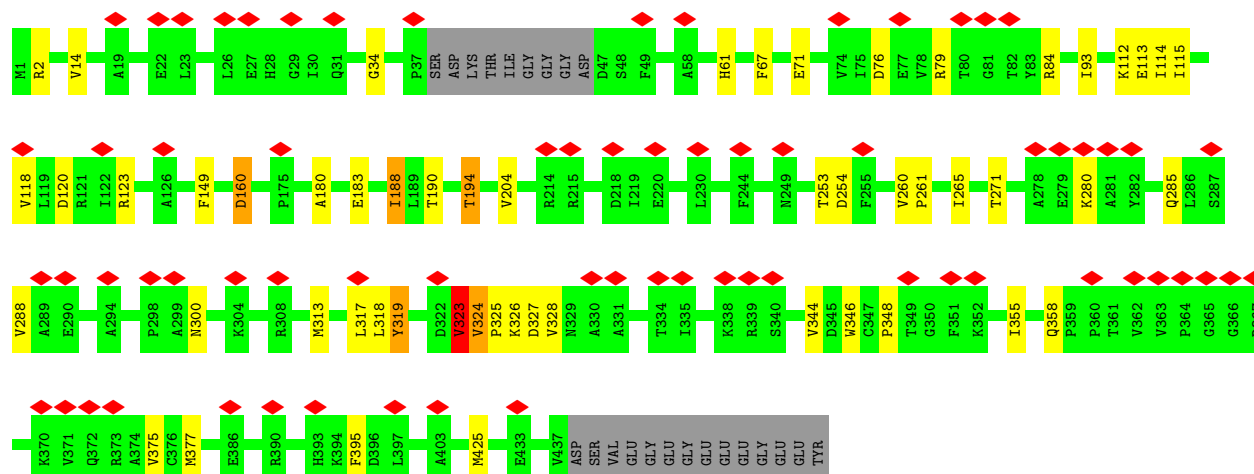
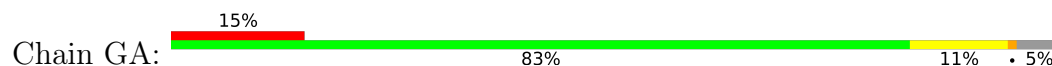





• Molecule 7: Isoform 1 of Tubulin alpha-1B chain

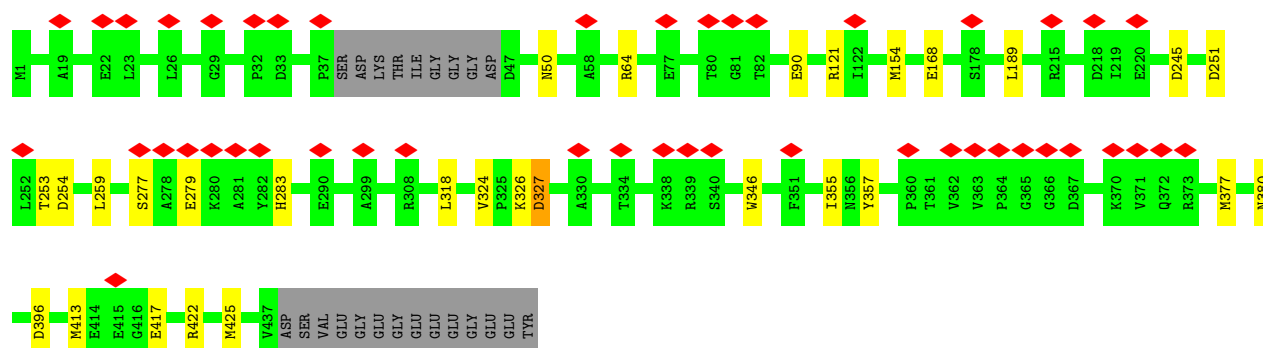


• Molecule 7: Isoform 1 of Tubulin alpha-1B chain




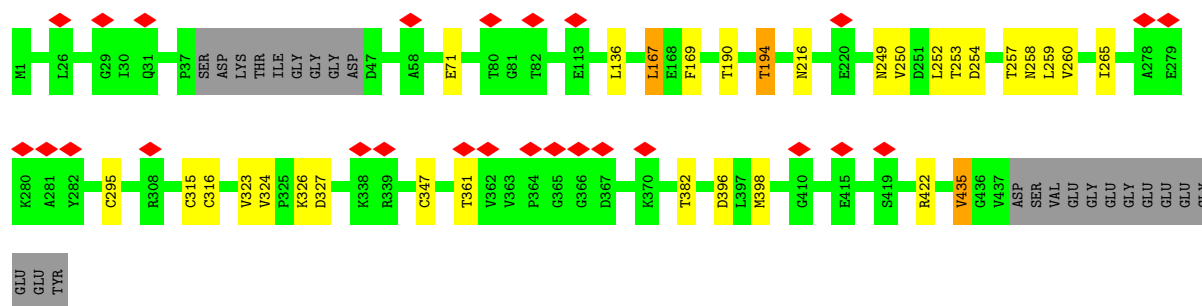
• Molecule 7: Isoform 1 of Tubulin alpha-1B chain

Chain HA: 




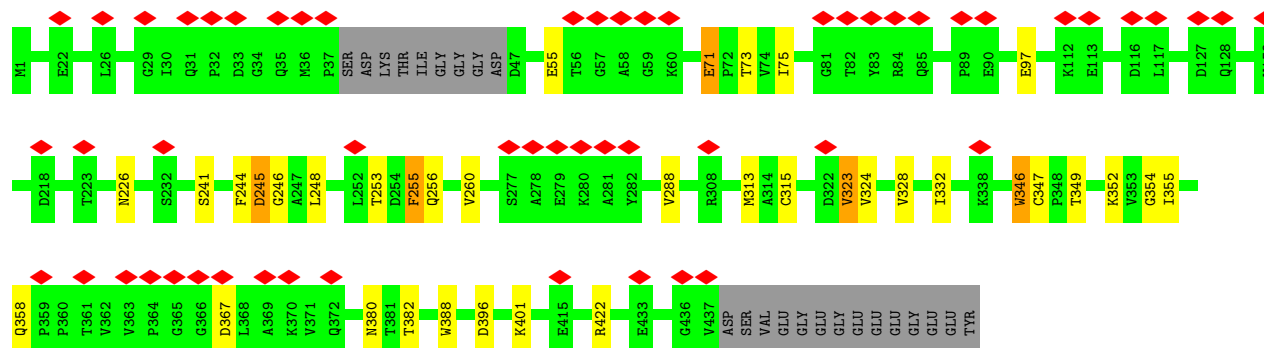
• Molecule 7: Isoform 1 of Tubulin alpha-1B chain

Chain IA: 




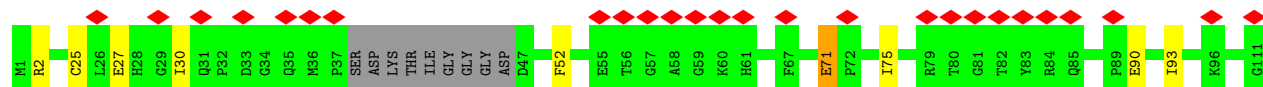
• Molecule 7: Isoform 1 of Tubulin alpha-1B chain

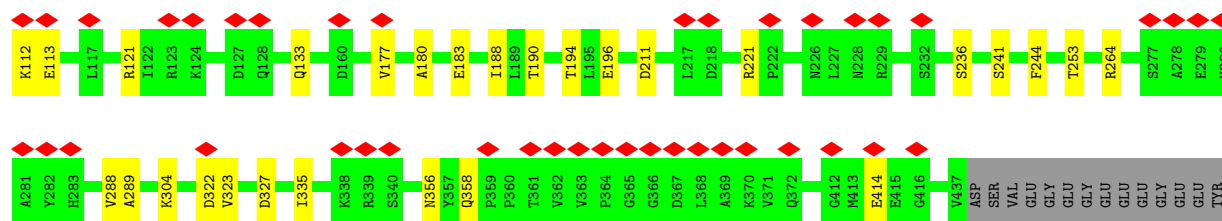
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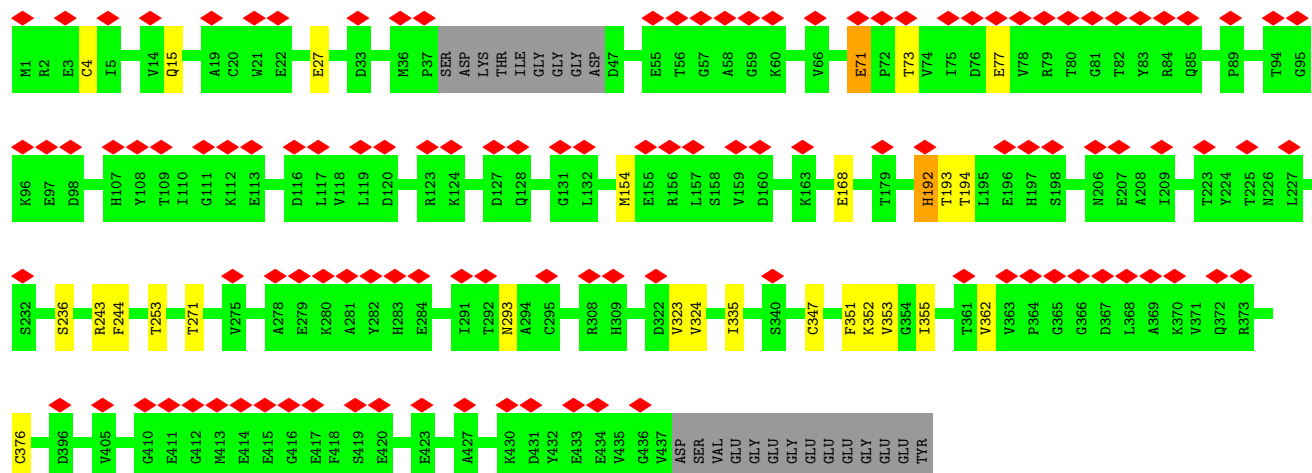
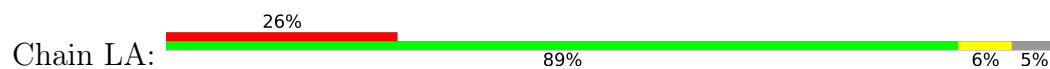
• Molecule 7: Isoform 1 of Tubulin alpha-1B chain

Chain KA: 

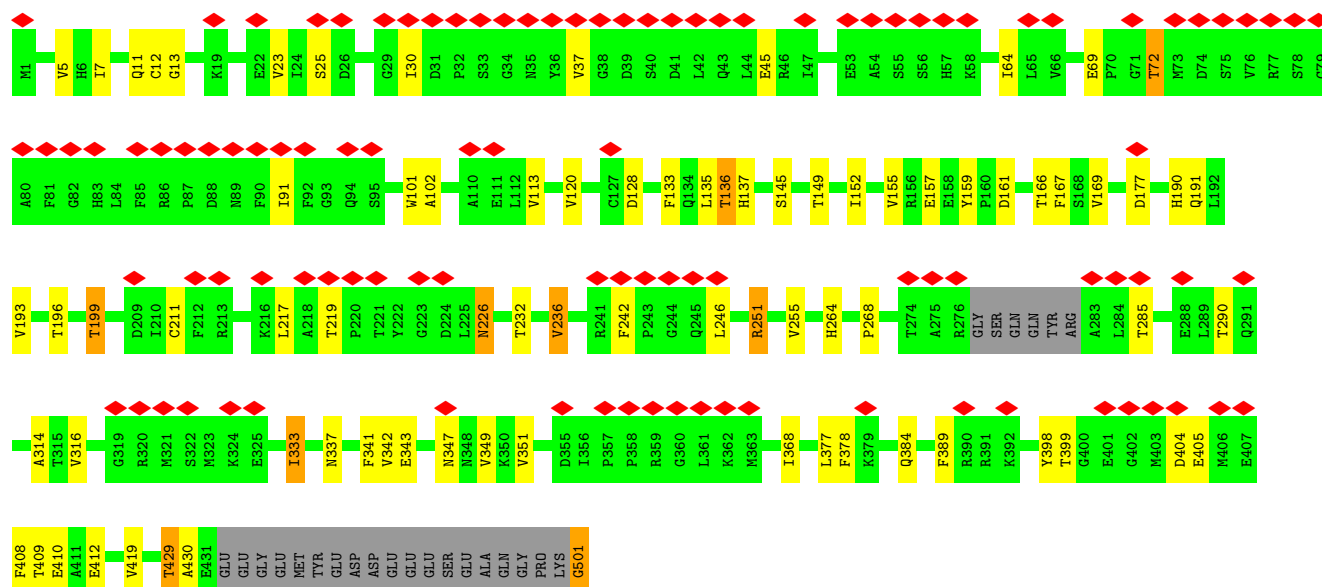
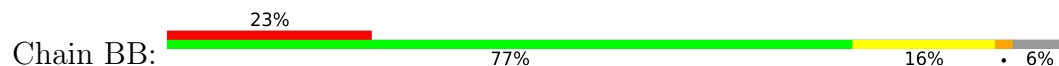




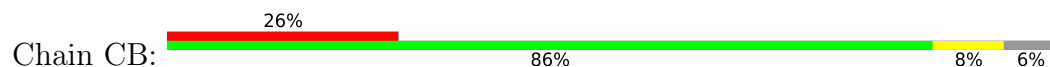
• Molecule 7: Isoform 1 of Tubulin alpha-1B chain

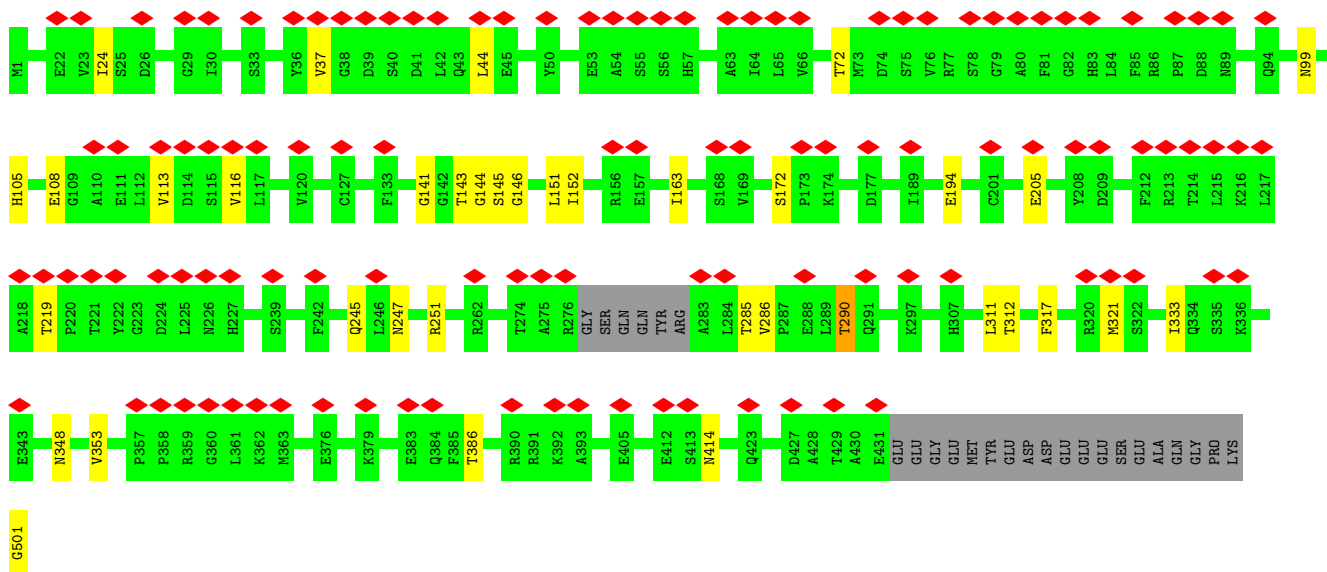


• Molecule 8: Tubulin beta-3 chain

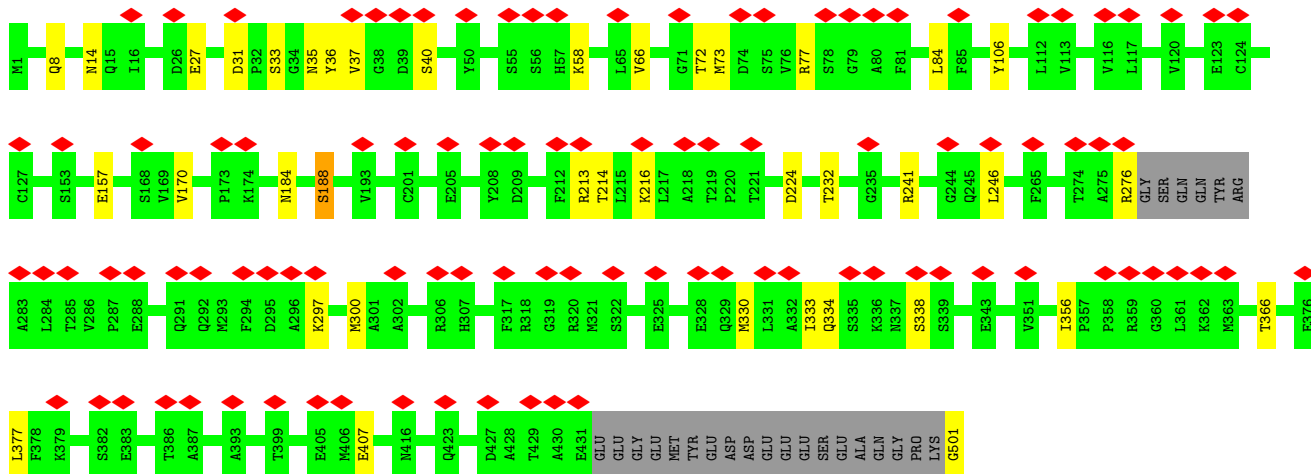


• Molecule 8: Tubulin beta-3 chain

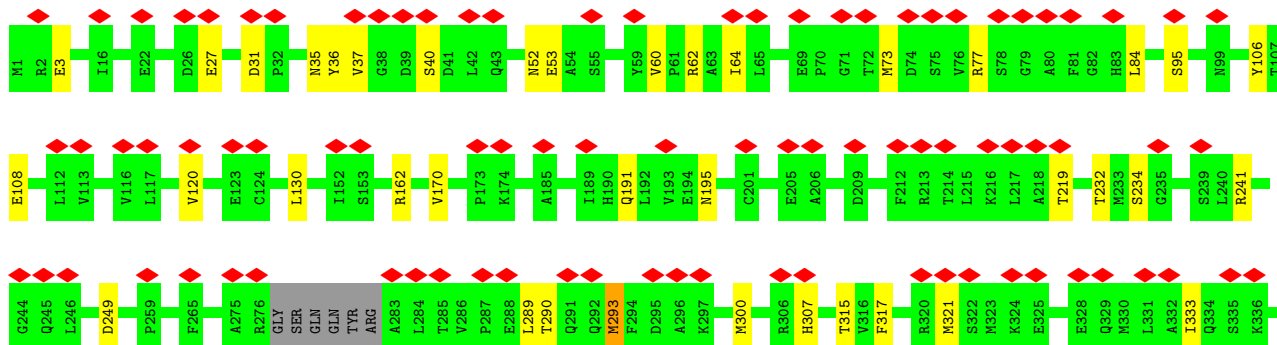
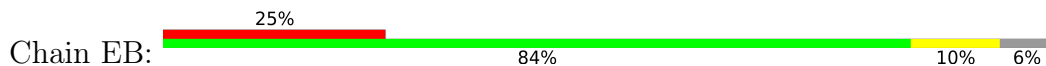


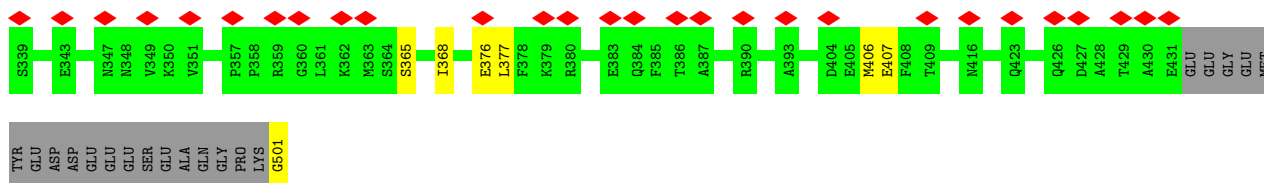


• Molecule 8: Tubulin beta-3 chain

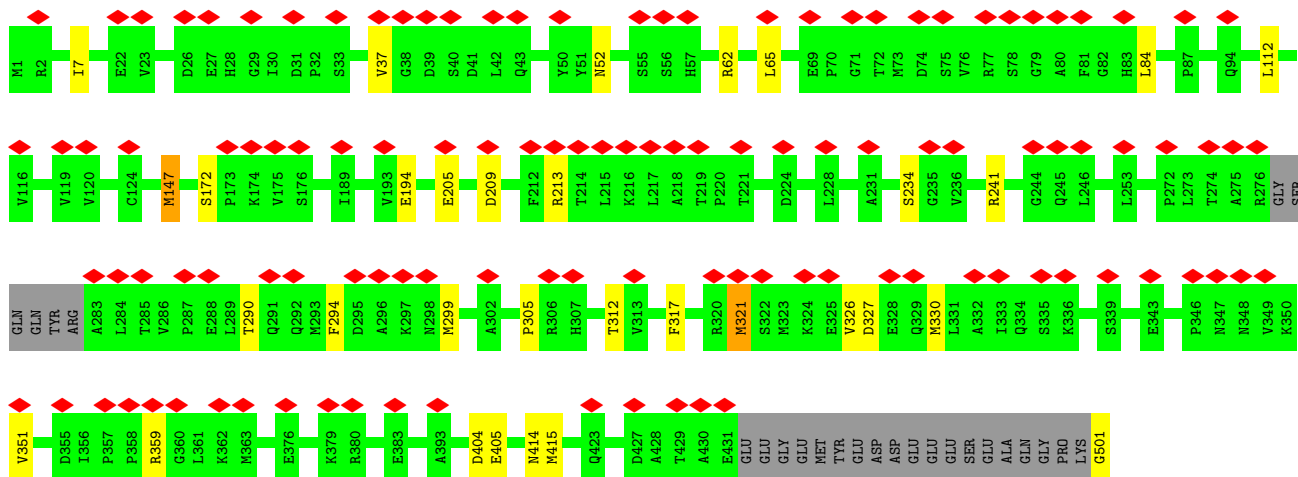
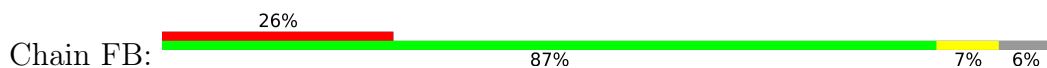


• Molecule 8: Tubulin beta-3 chain

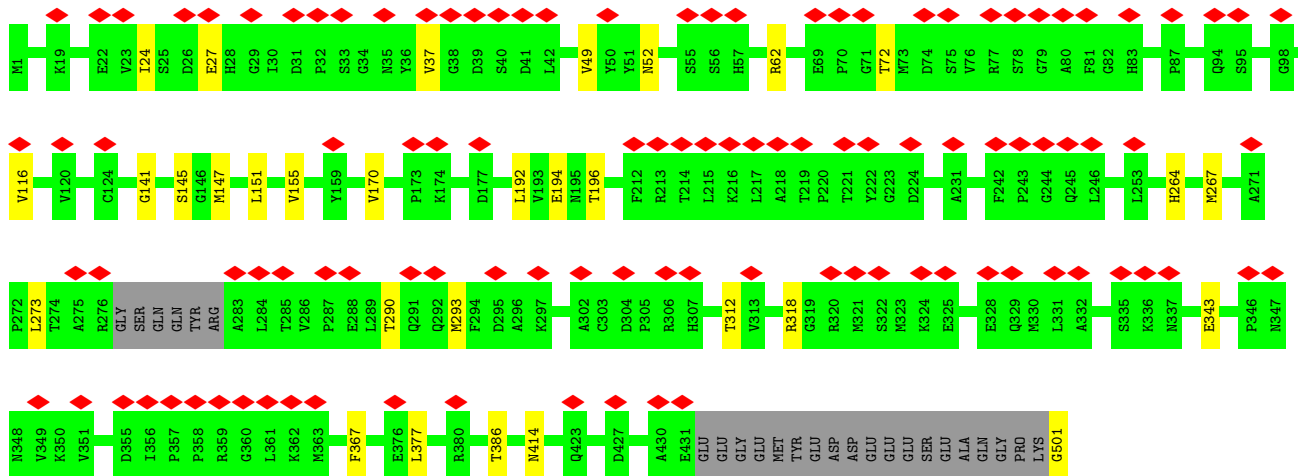
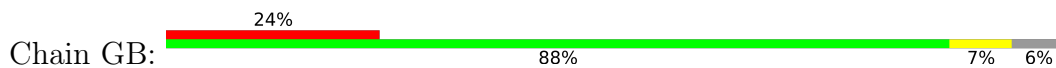




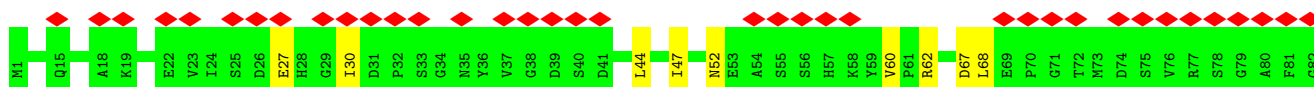
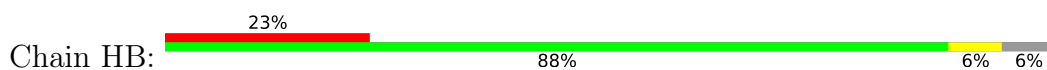
• Molecule 8: Tubulin beta-3 chain

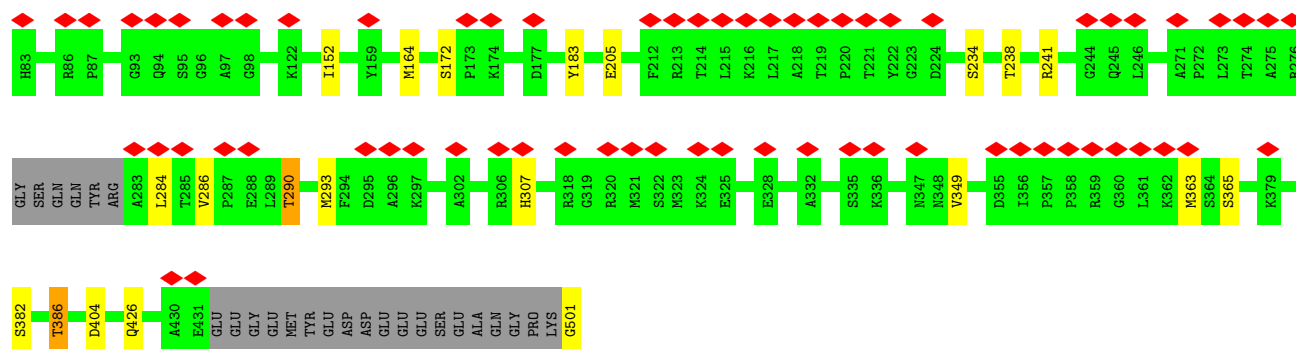


• Molecule 8: Tubulin beta-3 chain

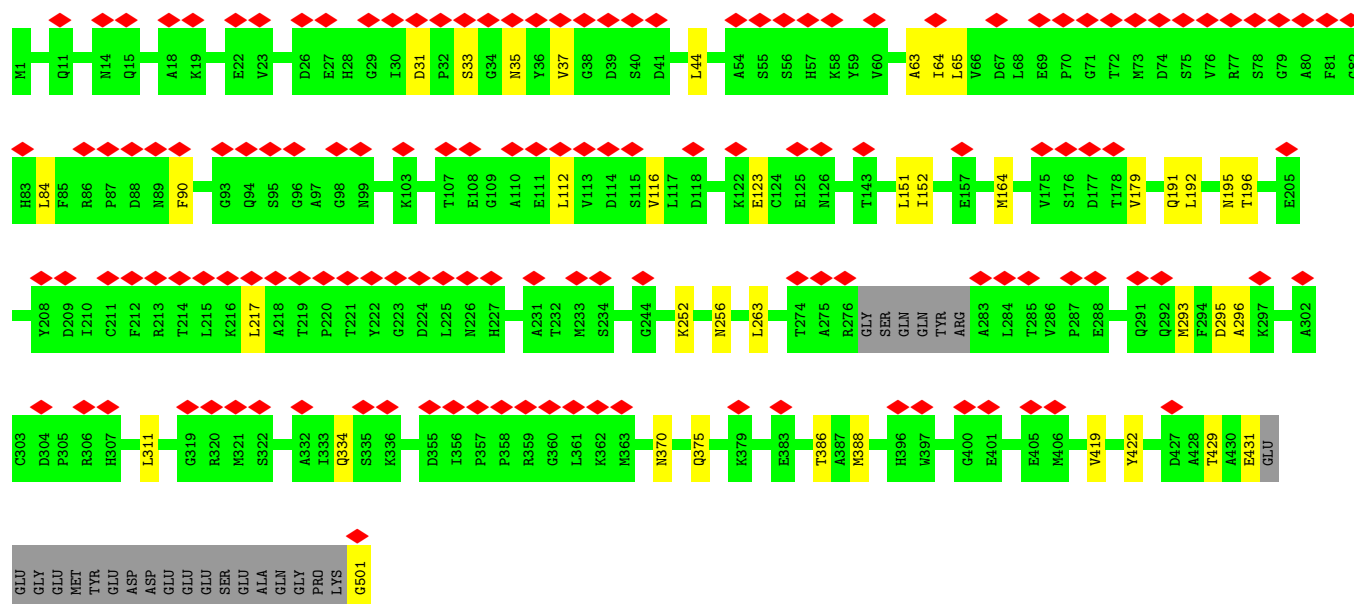
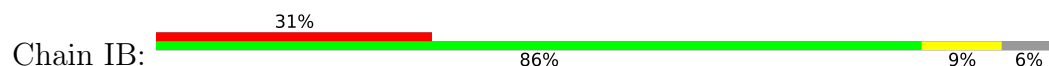


• Molecule 8: Tubulin beta-3 chain

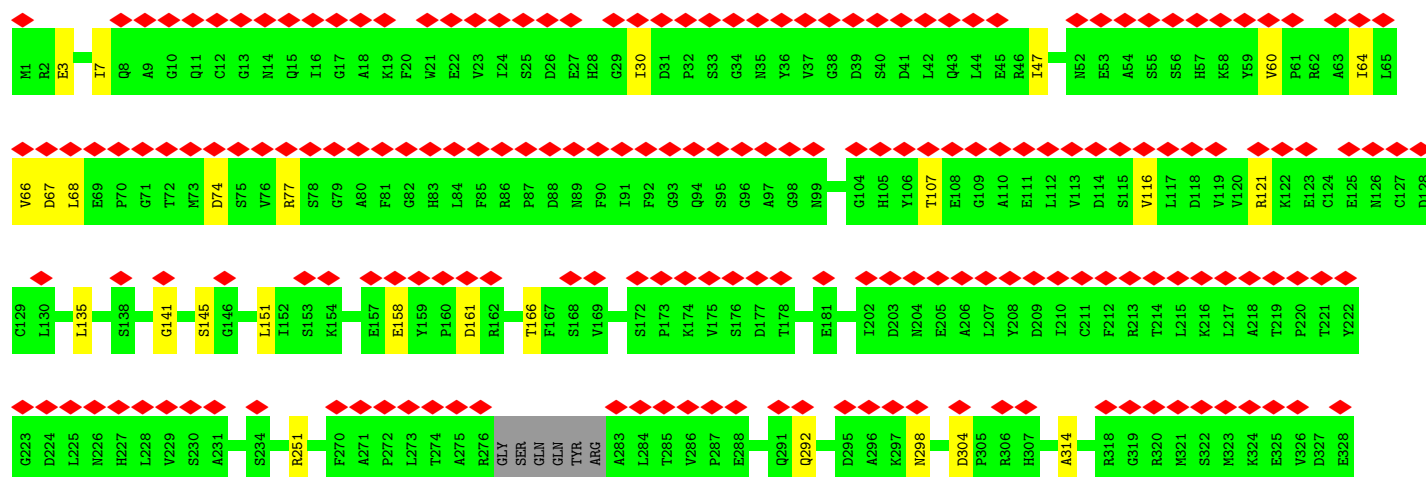
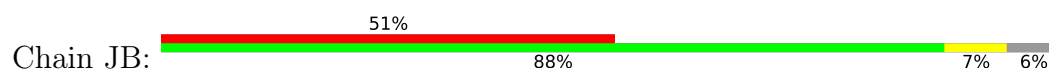


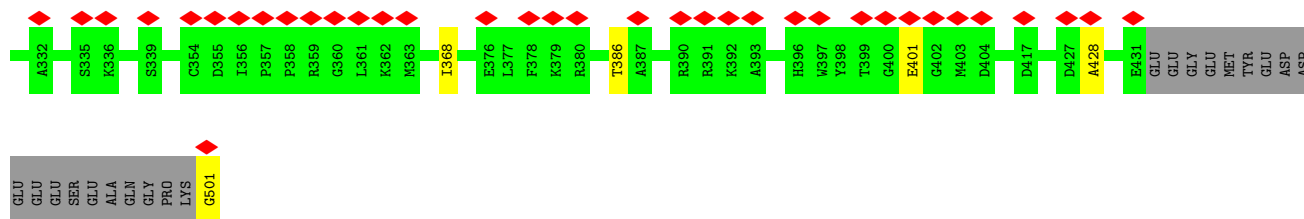


• Molecule 8: Tubulin beta-3 chain

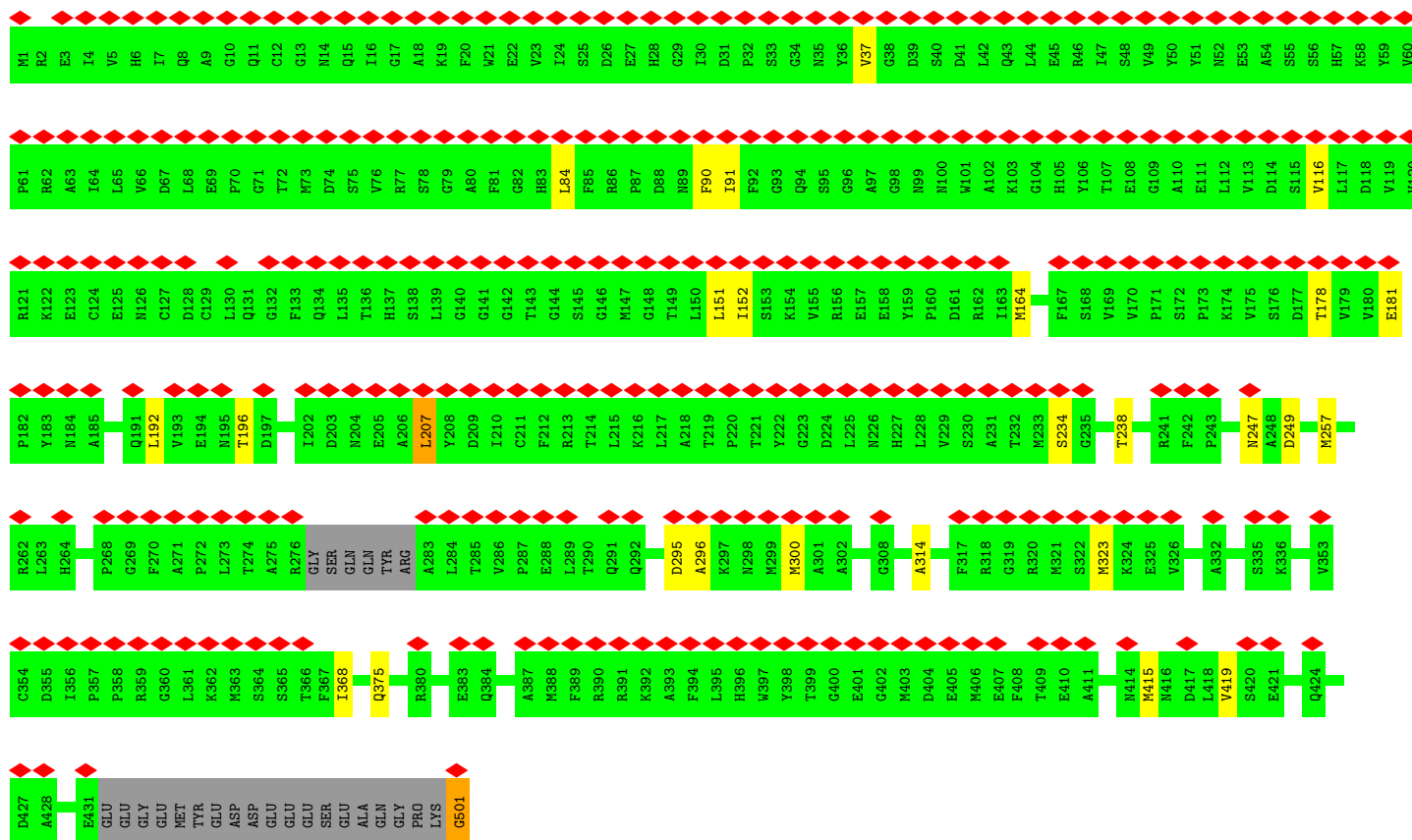
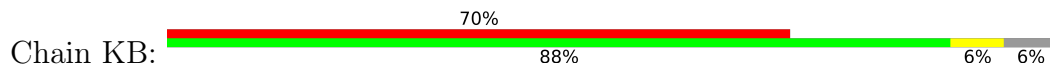


• Molecule 8: Tubulin beta-3 chain

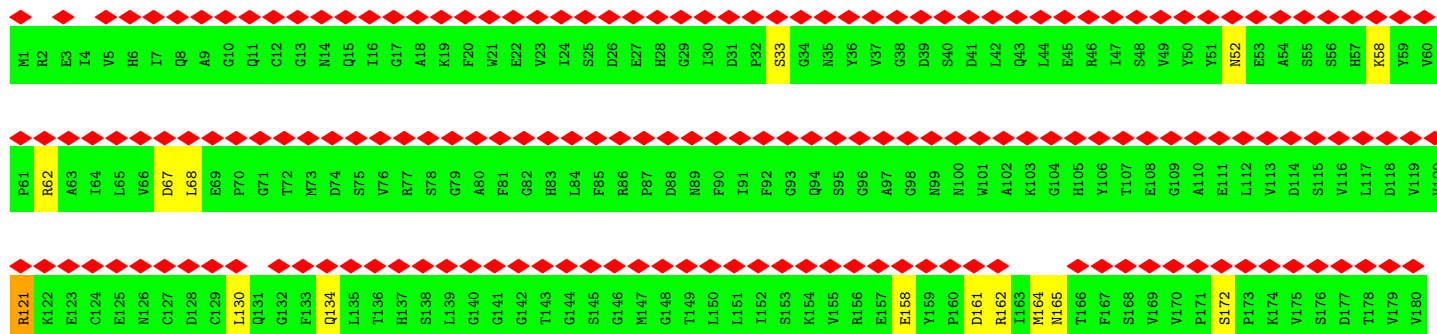
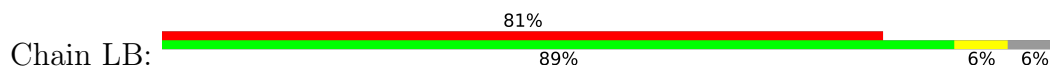


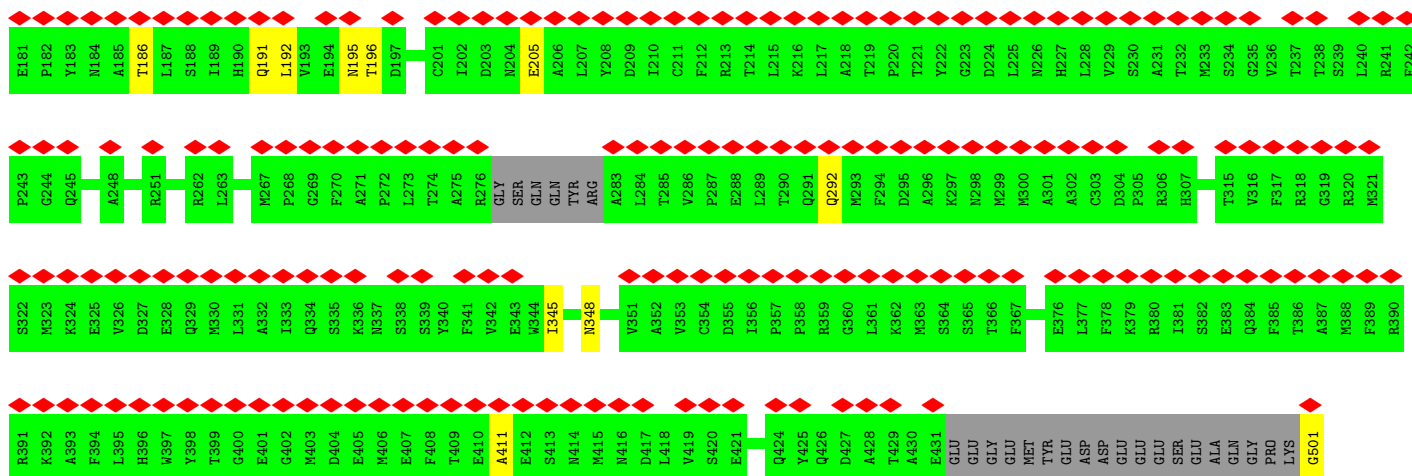


• Molecule 8: Tubulin beta-3 chain

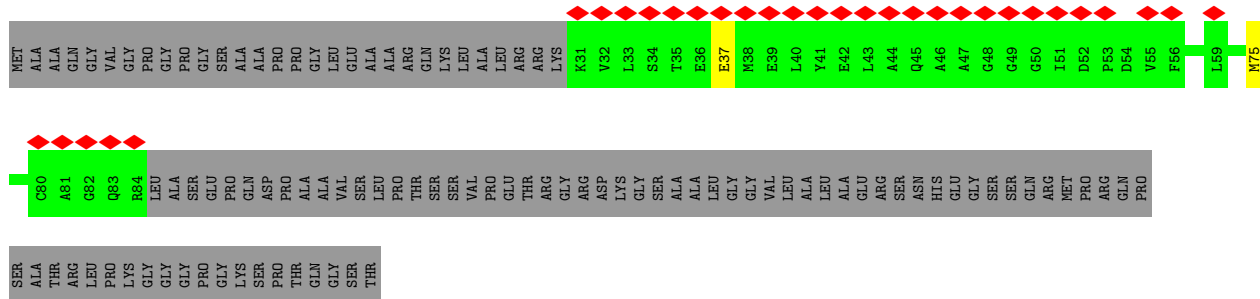


• Molecule 8: Tubulin beta-3 chain

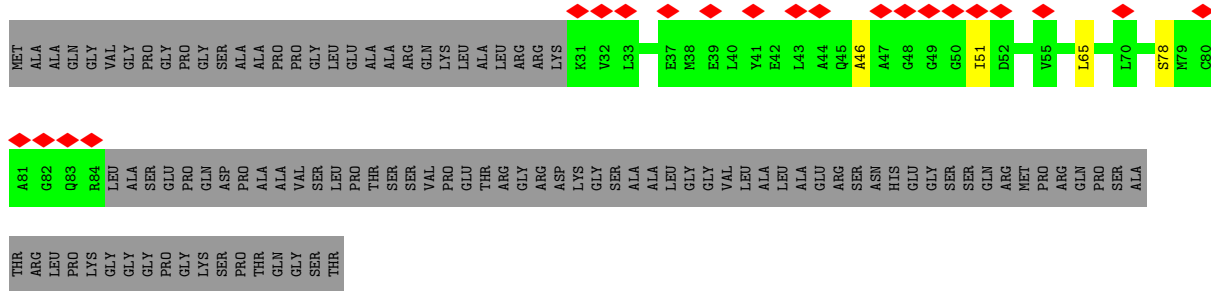




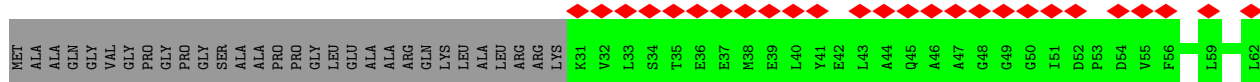
- Molecule 9: Mitotic-spindle organizing protein 2A

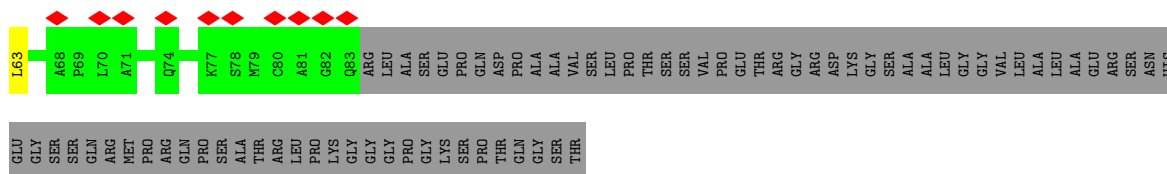


- Molecule 9: Mitotic-spindle organizing protein 2A

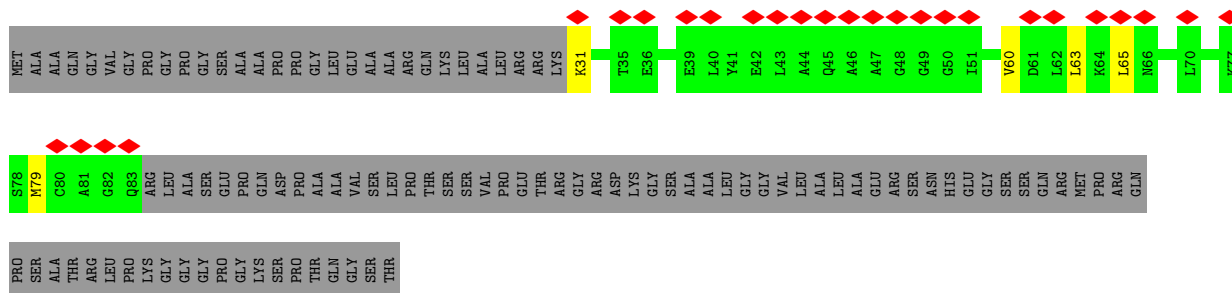


- Molecule 9: Mitotic-spindle organizing protein 2A

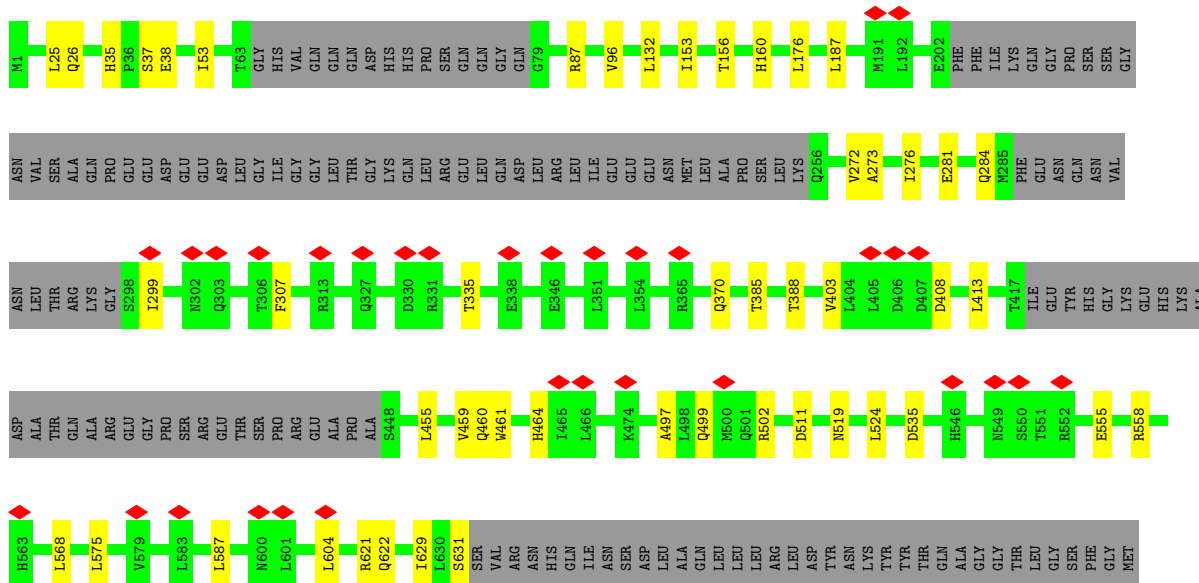




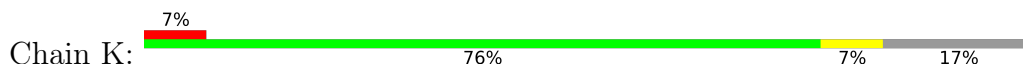
- Molecule 9: Mitotic-spindle organizing protein 2A



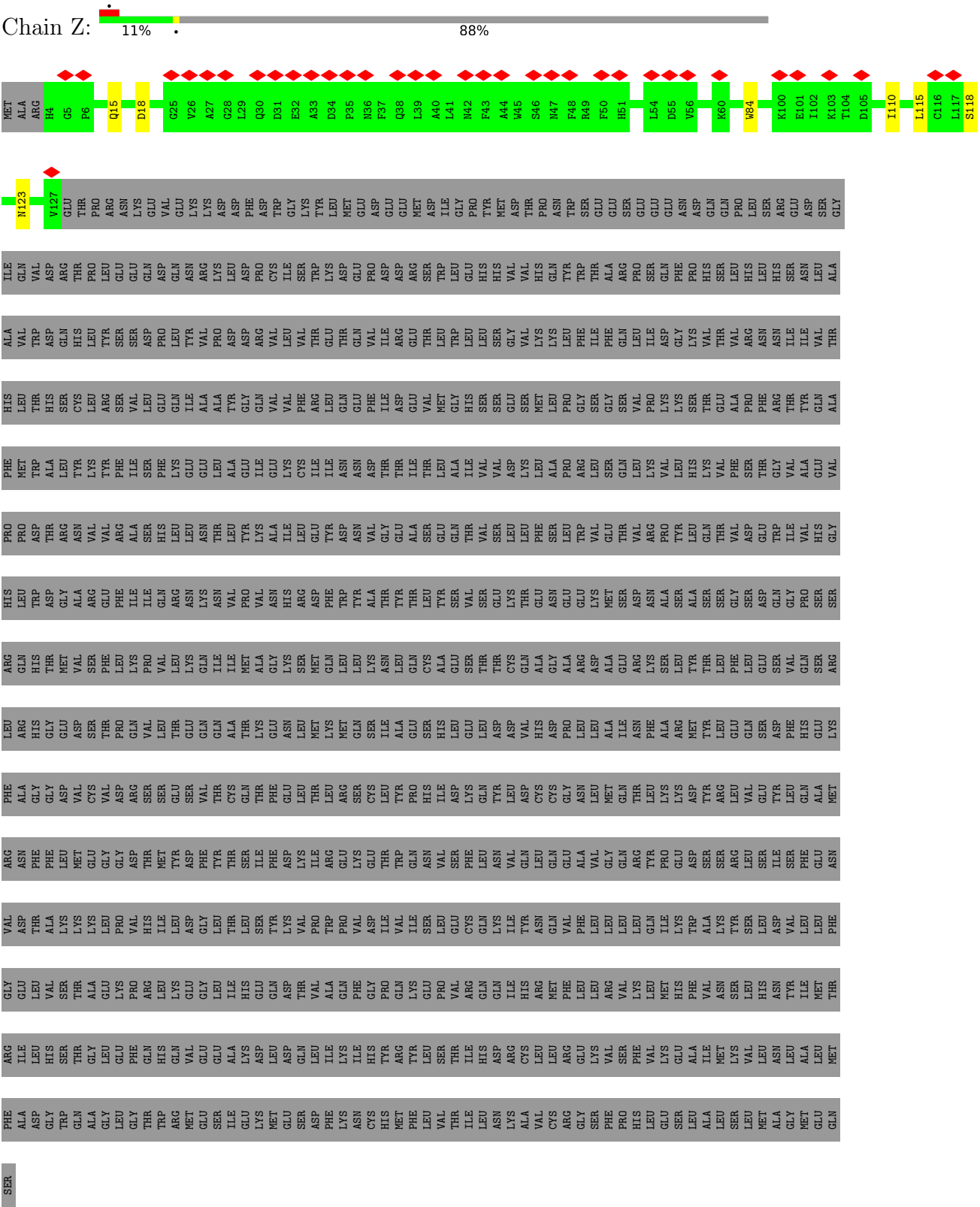
- Molecule 10: Gamma-tubulin complex component 4



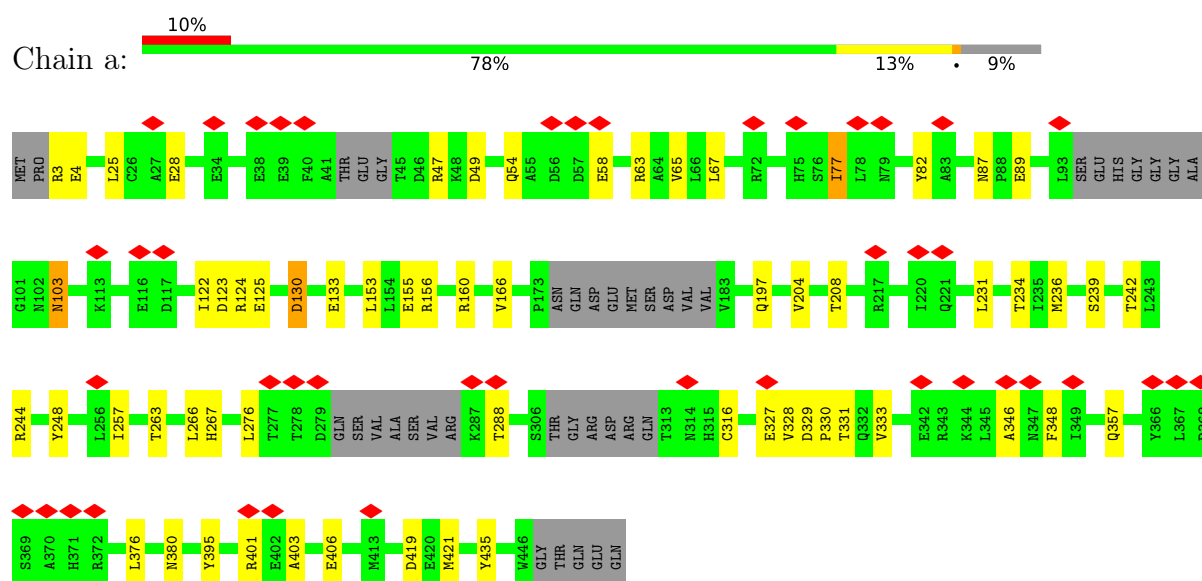
- Molecule 10: Gamma-tubulin complex component 4



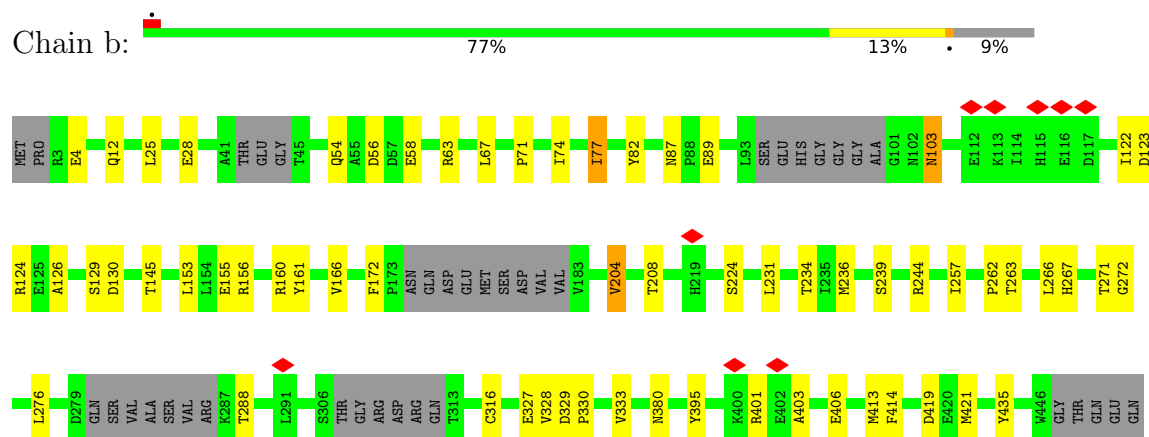
● Molecule 11: Gamma-tubulin complex component 5



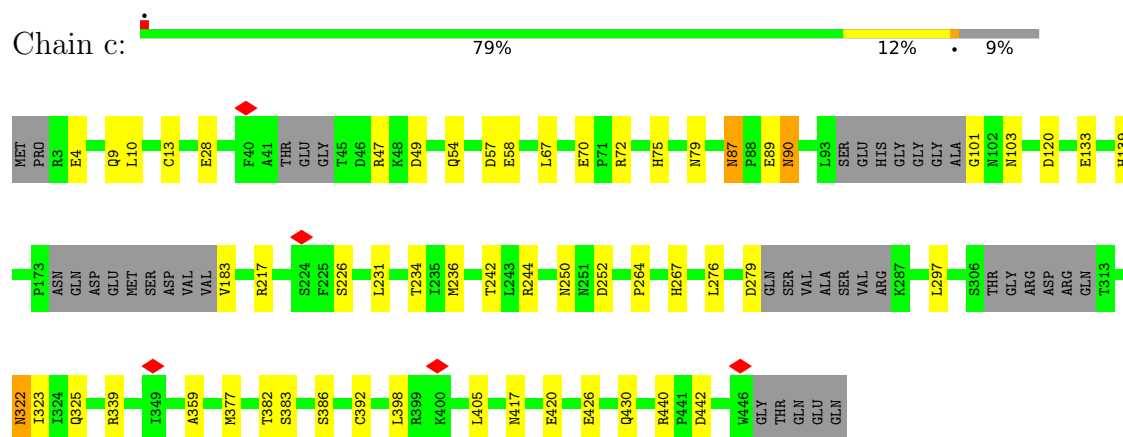
● Molecule 12: Tubulin gamma-1 chain



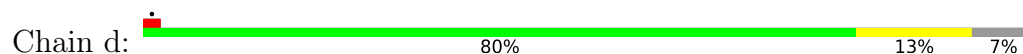
• Molecule 12: Tubulin gamma-1 chain

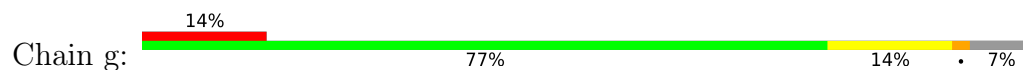


• Molecule 12: Tubulin gamma-1 chain

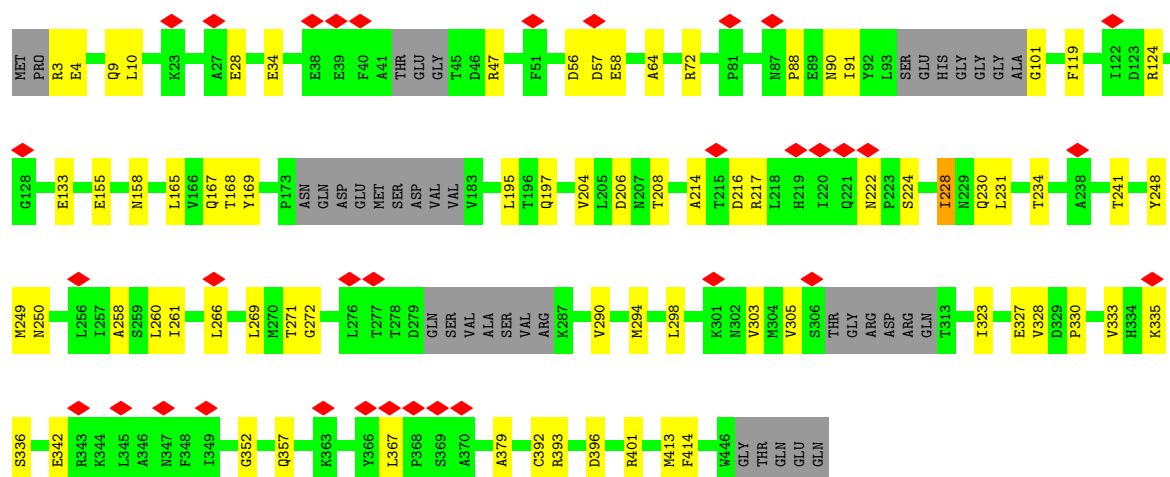
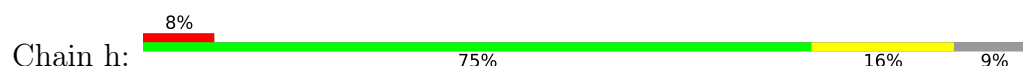


• Molecule 12: Tubulin gamma-1 chain

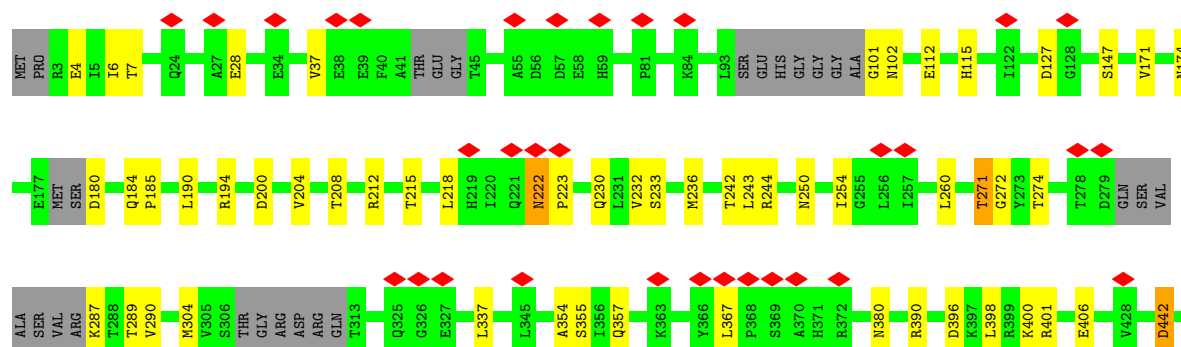




- Molecule 12: Tubulin gamma-1 chain




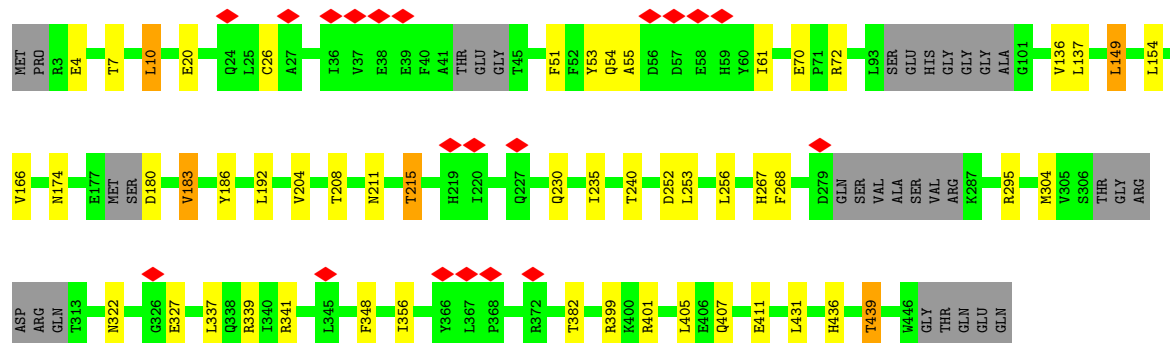
- Molecule 12: Tubulin gamma-1 chain






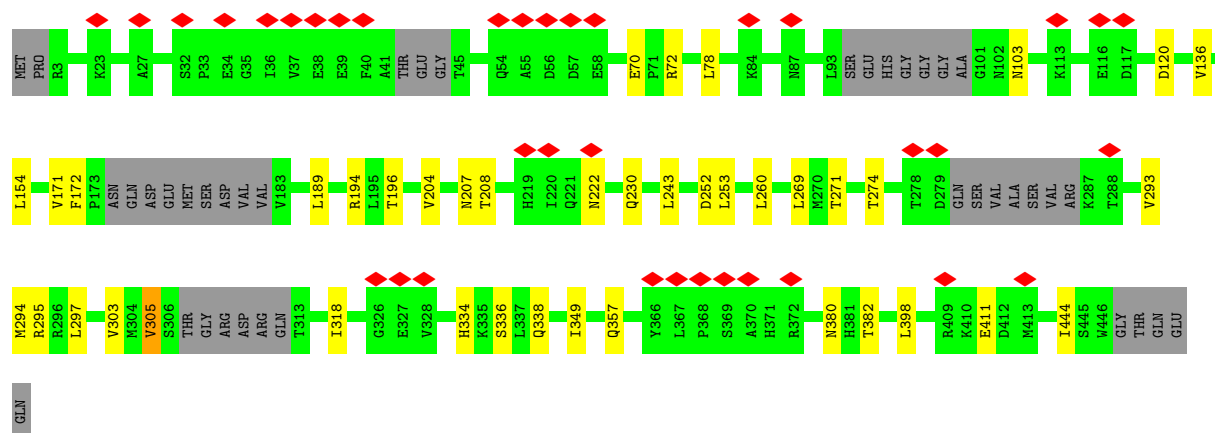
• Molecule 12: Tubulin gamma-1 chain

Chain j:  81% 10% 7%




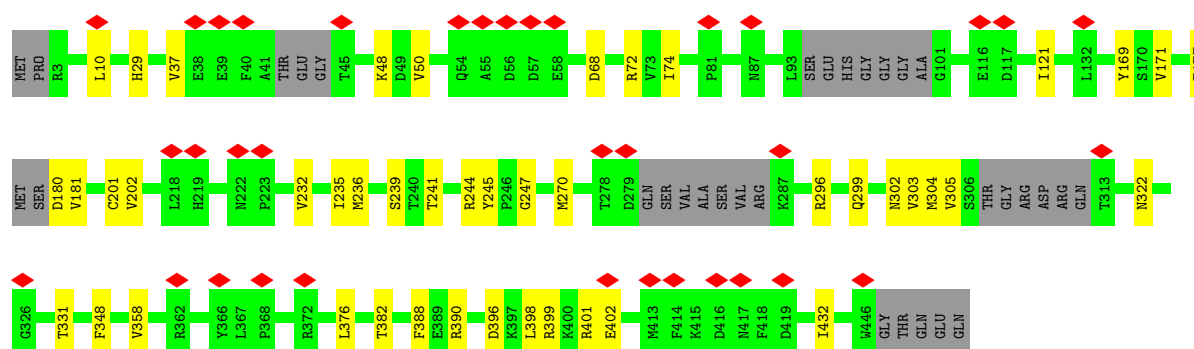
• Molecule 12: Tubulin gamma-1 chain

Chain k:  8% 82% 9% 9%

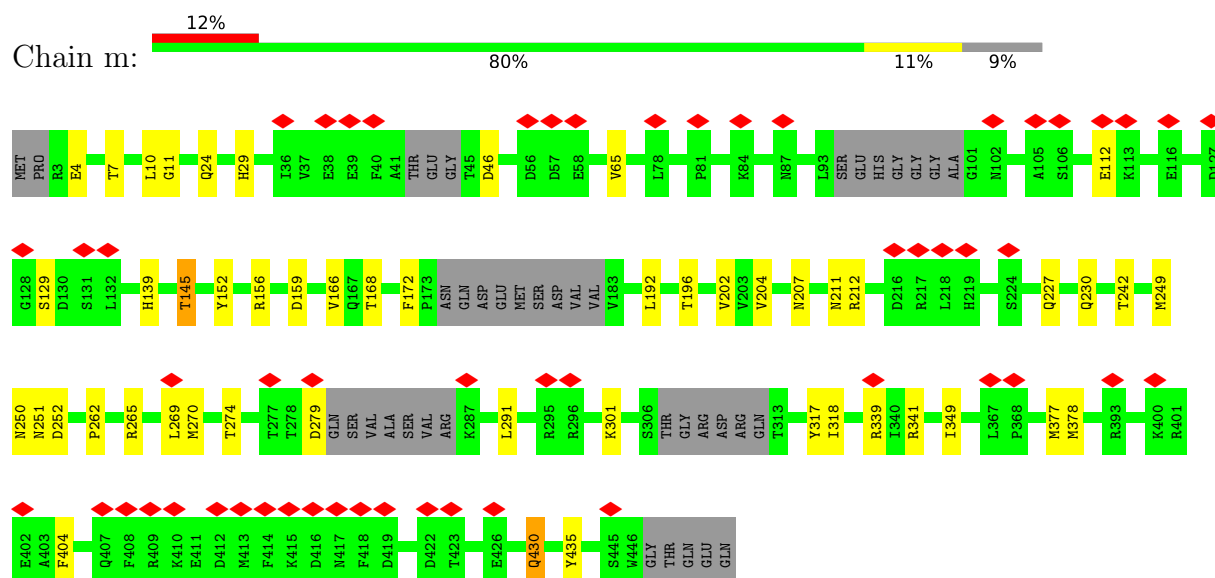


• Molecule 12: Tubulin gamma-1 chain

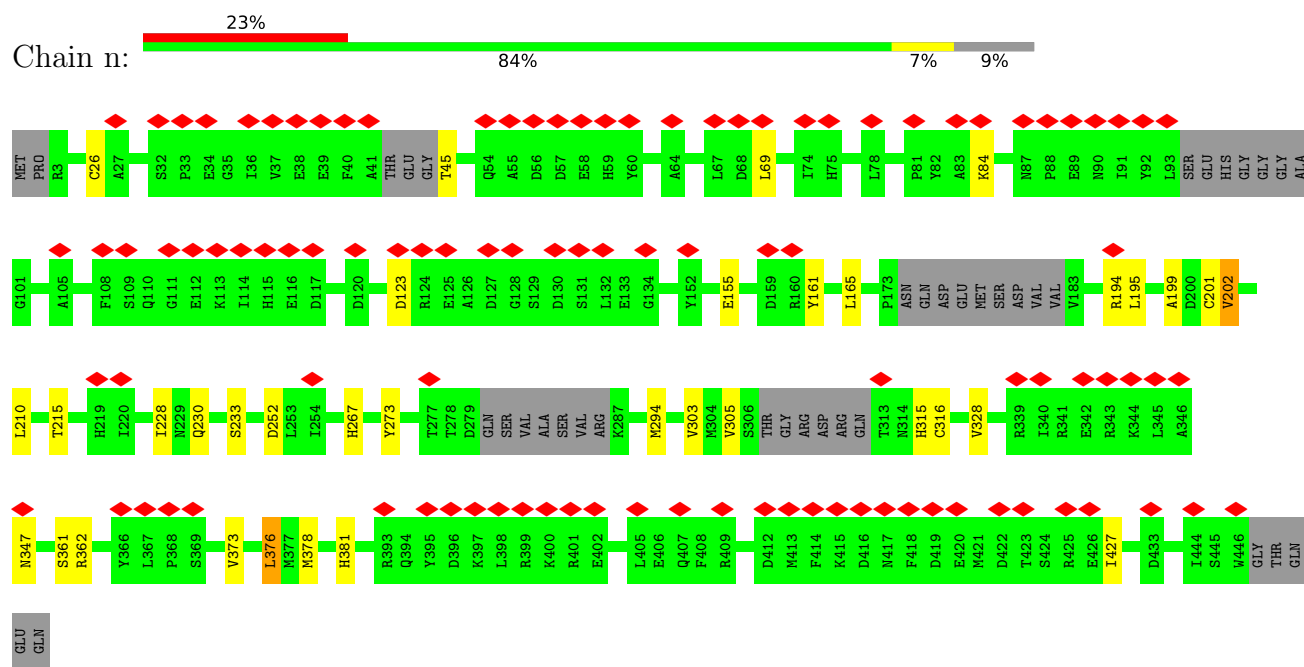
Chain l:  8% 83% 10% 7%



- Molecule 12: Tubulin gamma-1 chain



- Molecule 12: 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	652699	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.01	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.018	Depositor
Minimum map value	-0.005	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0035	Depositor
Map size (Å)	576.63995, 576.63995, 576.63995	wwPDB
Map dimensions	544, 544, 544	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	3	0.29	0/844	0.55	0/1134
1	B	0.30	0/5328	0.56	0/7197
1	D	0.31	0/5121	0.53	0/6915
1	F	0.32	0/4897	0.55	0/6610
1	H	0.31	0/4897	0.52	0/6610
1	N	0.30	0/5316	0.49	0/7183
2	4	0.24	0/452	0.47	0/610
2	6	0.24	0/457	0.47	0/617
2	Y	0.31	0/426	0.58	0/574
3	5	0.25	0/356	0.46	0/478
3	L	0.37	1/5052 (0.0%)	0.55	0/6862
4	7	0.15	0/1848	0.33	0/2582
5	A	0.31	0/5742	0.55	0/7761
5	C	0.30	0/5748	0.53	0/7768
5	CN	0.23	0/910	0.48	0/1228
5	E	0.34	0/5432	0.56	0/7336
5	EN	0.26	0/910	0.55	0/1228
5	G	0.33	0/5432	0.56	0/7336
5	GN	0.24	0/910	0.49	0/1228
5	M	0.28	0/6901	0.54	0/9331
6	AC	0.28	0/316	0.48	0/417
6	CC	0.30	0/316	0.52	0/417
6	Cc	0.26	0/321	0.46	0/424
6	EC	0.29	0/300	0.50	0/396
6	Ec	0.27	0/264	0.46	0/350
6	GC	0.36	0/305	0.62	0/403
6	Gc	0.35	0/282	0.64	0/373
6	MC	0.31	0/289	0.48	0/382
6	Mc	0.34	0/290	0.53	0/383
7	BA	0.39	0/3473	0.71	0/4715
7	CA	0.28	1/3395 (0.0%)	0.48	0/4612
7	DA	0.28	0/3395	0.51	0/4612

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	EA	0.29	0/3395	0.51	0/4612
7	FA	0.32	0/3395	0.55	0/4612
7	GA	0.33	0/3395	0.58	0/4612
7	HA	0.28	0/3395	0.52	0/4612
7	IA	0.29	1/3395 (0.0%)	0.55	0/4612
7	JA	0.28	0/3395	0.49	0/4612
7	KA	0.23	0/3395	0.44	0/4612
7	LA	0.24	0/3395	0.44	0/4612
8	BB	0.34	0/3381	0.64	0/4584
8	CB	0.23	0/3399	0.46	0/4605
8	DB	0.24	0/3393	0.45	0/4598
8	EB	0.26	0/3399	0.46	0/4605
8	FB	0.25	0/3399	0.45	0/4605
8	GB	0.24	0/3399	0.46	0/4605
8	HB	0.24	0/3399	0.46	0/4605
8	IB	0.23	0/3399	0.43	0/4605
8	JB	0.25	0/3399	0.44	0/4605
8	KB	0.25	0/3399	0.46	0/4605
8	LB	0.24	0/3399	0.44	0/4605
9	CM	0.23	0/412	0.44	0/554
9	EM	0.24	0/412	0.48	0/554
9	GM	0.25	0/401	0.43	0/540
9	MM	0.26	0/401	0.47	0/540
10	I	0.29	0/4319	0.52	0/5849
10	K	0.26	0/4600	0.49	0/6227
11	J	0.37	2/4875 (0.0%)	0.56	0/6609
11	Z	0.26	0/1032	0.45	0/1399
12	a	0.36	0/3381	0.60	0/4579
12	b	0.28	0/3381	0.55	0/4579
12	c	0.32	0/3381	0.55	0/4579
12	d	0.32	0/3437	0.56	0/4656
12	e	0.34	0/3431	0.62	0/4649
12	f	0.35	0/3381	0.58	0/4579
12	g	0.38	0/3419	0.63	0/4635
12	h	0.36	0/3375	0.60	0/4572
12	i	0.30	0/3437	0.56	0/4656
12	j	0.29	0/3431	0.54	0/4649
12	k	0.27	0/3379	0.50	0/4576
12	l	0.26	0/3435	0.52	0/4653
12	m	0.29	0/3381	0.54	0/4579
12	n	0.26	0/3381	0.50	0/4579
All	All	0.30	5/208532 (0.0%)	0.53	0/282387

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	1767	HIS	C-N	14.38	1.45	1.33
11	J	470	ARG	C-N	12.18	1.44	1.33
11	J	489	ALA	C-N	-7.00	1.23	1.33
7	IA	323	VAL	C-N	-5.64	1.28	1.33
7	CA	324	VAL	C-N	5.06	1.39	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	832	861	860	5	0
1	B	5219	5183	5181	39	0
1	D	5017	5000	4996	38	0
1	F	4796	4780	4775	43	0
1	H	4796	4780	4775	46	0
1	N	5207	5161	5159	16	0
2	4	452	474	473	2	0
2	6	457	479	478	2	0
2	Y	426	451	450	2	0
3	5	355	382	380	2	0
3	L	4919	4954	4951	26	0
4	7	1832	932	928	2	0
5	A	5623	5617	5631	17	0
5	C	5629	5629	5642	32	0
5	CN	896	907	907	2	0
5	E	5320	5347	5357	37	0
5	EN	896	907	907	5	0
5	G	5320	5346	5357	39	0
5	GN	896	907	907	3	0
5	M	6766	6768	6780	40	0
6	AC	313	318	317	0	0
6	CC	313	318	317	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Cc	317	315	314	2	0
6	EC	297	300	299	2	0
6	Ec	261	259	258	0	0
6	GC	302	305	304	1	0
6	Gc	279	277	277	1	0
6	MC	286	287	286	2	0
6	Mc	287	287	286	1	0
7	BA	3400	3275	3294	44	0
7	CA	3322	3230	3229	11	0
7	DA	3322	3230	3229	15	0
7	EA	3322	3231	3229	25	0
7	FA	3322	3230	3229	21	0
7	GA	3322	3222	3229	34	0
7	HA	3322	3230	3229	16	0
7	IA	3322	3231	3229	12	0
7	JA	3322	3229	3229	18	0
7	KA	3322	3231	3229	19	0
7	LA	3322	3230	3229	11	0
8	BB	3336	3189	3187	31	0
8	CB	3354	3222	3220	15	0
8	DB	3348	3211	3209	14	0
8	EB	3354	3223	3220	21	0
8	FB	3354	3222	3220	12	0
8	GB	3354	3222	3220	13	0
8	HB	3354	3223	3220	14	0
8	IB	3354	3223	3220	16	0
8	JB	3354	3223	3220	14	0
8	KB	3354	3222	3220	13	0
8	LB	3354	3222	3220	13	0
9	CM	408	429	428	0	0
9	EM	408	429	428	3	0
9	GM	397	416	415	0	0
9	MM	397	416	415	4	0
10	I	4222	4255	4250	15	0
10	K	4497	4509	4507	18	0
11	J	4773	4748	4742	19	0
11	Z	1006	982	981	4	0
12	a	3313	3282	3276	27	0
12	b	3313	3282	3276	28	0
12	c	3313	3283	3276	27	0
12	d	3369	3328	3322	23	0
12	e	3363	3317	3311	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	f	3313	3282	3276	36	0
12	g	3351	3295	3289	43	0
12	h	3307	3271	3265	37	0
12	i	3369	3328	3322	30	0
12	j	3363	3317	3311	22	0
12	k	3311	3277	3271	21	0
12	l	3367	3324	3317	24	0
12	m	3313	3283	3276	21	0
12	n	3313	3282	3276	12	0
13	BA	32	12	12	0	0
13	CA	32	12	12	0	0
13	DA	32	12	12	0	0
13	EA	32	12	12	0	0
13	FA	32	12	12	0	0
13	GA	32	12	12	0	0
13	HA	32	12	12	0	0
13	IA	32	12	12	0	0
13	JA	32	12	12	0	0
13	KA	32	12	12	0	0
13	LA	32	12	12	0	0
All	All	204937	200969	200874	1132	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 3.

All (1132) 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)
5:G:696:TYR:HH	5:G:853:ALA:N	1.78	0.80
12:e:383:SER:O	12:e:386:SER:OG	2.01	0.78
1:F:681:ARG:NH1	12:f:261:ILE:O	2.17	0.78
12:h:56:ASP:OD1	12:i:287:LYS:N	2.17	0.77
12:d:415:LYS:NZ	12:d:419:ASP:OD1	2.15	0.77
1:H:681:ARG:NH1	12:h:261:ILE:O	2.18	0.76
7:FA:254:ASP:OD1	7:FA:258:ASN:ND2	2.19	0.76
12:d:396:ASP:OD1	12:d:425:ARG:NH1	2.19	0.76
7:GA:254:ASP:OD1	12:g:101:GLY:N	2.20	0.75
1:D:710:GLU:OE1	1:D:855:GLN:NE2	2.19	0.75
5:G:184:ARG:NH2	1:H:273:ASN:O	2.19	0.75
7:HA:326:LYS:NZ	12:h:224:SER:OG	2.21	0.74
5:E:762:MET:SD	5:E:821:THR:OG1	2.44	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BA:63:PRO:O	7:BA:91:GLN:NE2	2.21	0.73
1:H:799:GLU:OE2	1:H:803:ARG:NH2	2.20	0.73
10:I:87:ARG:NH2	11:J:446:GLU:OE2	2.22	0.73
5:C:400:ILE:HD12	5:C:409:VAL:HG13	1.69	0.73
7:LA:347:CYS:O	12:l:396:ASP:N	2.22	0.73
8:IB:192:LEU:O	8:IB:196:THR:OG1	2.06	0.73
12:d:56:ASP:OD2	12:e:287:LYS:N	2.21	0.73
1:H:620:ARG:NH1	1:H:645:ASP:OD1	2.23	0.72
7:JA:226:ASN:ND2	7:JA:367:ASP:OD2	2.23	0.72
12:a:89:GLU:O	12:a:124:ARG:NH2	2.22	0.72
12:b:89:GLU:O	12:b:124:ARG:NH2	2.23	0.71
11:J:905:ILE:O	11:J:909:THR:OG1	2.07	0.71
1:D:497:CYS:SG	1:D:552:LYS:NZ	2.62	0.71
8:EB:95:SER:OG	8:EB:108:GLU:OE2	2.08	0.71
8:HB:293:MET:SD	8:HB:365:SER:OG	2.45	0.70
5:E:637:ARG:NH1	6:EC:76:ASN:OD1	2.24	0.70
5:G:497:LYS:NZ	5:G:501:ASP:OD2	2.24	0.70
12:i:242:THR:OG1	12:i:250:ASN:O	2.09	0.70
1:F:684:HIS:HD1	1:F:793:TYR:HH	1.38	0.70
1:D:311:ARG:NH2	1:D:314:ASP:OD2	2.24	0.70
8:DB:106:TYR:OH	8:DB:407:GLU:OE1	2.10	0.70
5:M:301:LYS:NZ	1:N:369:VAL:O	2.25	0.70
12:f:64:ALA:O	12:f:90:ASN:ND2	2.25	0.69
7:CA:254:ASP:OD1	12:c:101:GLY:N	2.25	0.69
1:H:883:ASN:ND2	12:h:352:GLY:O	2.25	0.69
7:IA:315:CYS:SG	7:IA:316:CYS:N	2.65	0.69
8:CB:172:SER:OG	8:CB:205:GLU:OE1	2.11	0.69
12:g:231:LEU:O	12:g:234:THR:OG1	2.11	0.69
5:A:858:ARG:NH2	12:a:357:GLN:OE1	2.27	0.68
12:d:206:ASP:OD2	12:d:306:SER:OG	2.06	0.68
12:a:4:GLU:OE1	12:a:63:ARG:NH2	2.27	0.68
1:H:286:SER:OG	1:H:288:ARG:NH1	2.26	0.68
12:m:172:PHE:O	12:m:207:ASN:ND2	2.27	0.67
7:BA:165:SER:HB2	7:BA:252:LEU:HB3	1.77	0.67
1:H:707:LEU:HD13	1:H:851:THR:HG22	1.75	0.67
12:e:133:GLU:OE2	12:e:254:ILE:N	2.27	0.67
12:c:231:LEU:O	12:c:234:THR:OG1	2.12	0.67
12:l:399:ARG:NH1	12:l:401:ARG:O	2.28	0.67
12:i:127:ASP:O	12:j:339:ARG:NH1	2.26	0.67
12:i:180:ASP:OD1	12:i:184:GLN:NE2	2.28	0.67
5:M:662:ASN:ND2	5:M:762:MET:SD	2.68	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:EA:280:LYS:O	7:EA:283:HIS:NE2	2.27	0.66
8:HB:27:GLU:OE2	8:HB:234:SER:OG	2.14	0.66
12:m:196:THR:O	12:m:265:ARG:NH1	2.28	0.66
8:BB:7:ILE:HG23	8:BB:135:LEU:HD13	1.77	0.66
7:FA:236:SER:O	7:FA:243:ARG:NH2	2.29	0.66
3:L:477:CYS:SG	3:L:478:GLY:N	2.68	0.66
5:G:434:ILE:HG13	5:G:451:LEU:HD13	1.78	0.66
1:B:246:THR:OG1	1:B:247:GLU:OE1	2.06	0.65
7:HA:251:ASP:OD2	12:h:101:GLY:N	2.28	0.65
7:BA:178:SER:OG	8:BB:349:VAL:O	2.14	0.65
5:C:573:LEU:O	5:C:574:LYS:NZ	2.27	0.65
1:D:734:LEU:HD22	1:D:754:PHE:CG	2.31	0.65
7:FA:76:ASP:OD1	7:FA:79:ARG:NH1	2.29	0.65
5:M:180:TRP:NE1	1:N:386:ASP:OD2	2.30	0.65
7:HA:254:ASP:OD1	12:h:101:GLY:N	2.30	0.65
5:M:402:ASP:OD2	5:M:406:GLU:N	2.29	0.65
7:BA:161:TYR:CE1	7:BA:163:LYS:HD2	2.32	0.65
12:c:264:PRO:O	12:c:267:HIS:ND1	2.29	0.65
1:B:257:VAL:O	1:B:301:HIS:ND1	2.30	0.64
8:CB:317:PHE:HB3	8:CB:321:MET:HE1	1.78	0.64
1:H:579:ASP:OD2	12:h:3:ARG:NH2	2.29	0.64
7:GA:190:THR:O	7:GA:194:THR:OG1	2.09	0.64
12:e:361:SER:OG	12:e:362:ARG:N	2.29	0.64
1:F:438:GLU:N	1:F:438:GLU:OE1	2.31	0.64
12:d:11:GLY:O	12:d:15:ASN:ND2	2.30	0.64
1:B:388:CYS:HA	1:B:396:LEU:HD22	1.80	0.64
5:M:118:THR:HG1	9:MM:31:LYS:N	1.96	0.64
7:CA:71:GLU:OE1	7:CA:73:THR:OG1	2.10	0.64
8:DB:27:GLU:OE1	8:DB:241:ARG:NH2	2.31	0.64
3:L:369:SER:OG	3:L:376:ALA:O	2.16	0.63
12:g:156:ARG:NH2	12:g:159:ASP:OD2	2.30	0.63
12:n:378:MET:SD	12:n:378:MET:N	2.71	0.63
5:E:415:ARG:NH2	5:E:417:GLU:OE1	2.32	0.63
1:N:406:THR:O	1:N:412:ARG:NH2	2.31	0.63
7:DA:277:SER:OG	7:DA:279:GLU:OE1	2.15	0.63
12:l:236:MET:O	12:l:239:SER:OG	2.14	0.63
12:i:127:ASP:OD2	12:j:295:ARG:NE	2.31	0.63
8:CB:141:GLY:O	8:CB:145:SER:OG	2.15	0.63
7:DA:80:THR:O	7:DA:84:ARG:NH2	2.31	0.63
7:JA:71:GLU:OE1	7:JA:73:THR:OG1	2.13	0.63
8:DB:184:ASN:O	8:DB:188:SER:OG	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:GA:112:LYS:NZ	7:GA:113:GLU:OE2	2.31	0.63
5:E:387:TYR:OH	5:E:408:MET:HE3	1.99	0.63
5:G:684:GLN:NE2	12:g:261:ILE:O	2.32	0.62
12:f:13:CYS:O	12:f:17:ILE:HD13	2.00	0.62
12:h:167:GLN:OE1	12:h:169:TYR:OH	2.05	0.62
5:C:248:VAL:O	5:C:257:ARG:NH2	2.32	0.62
7:LA:27:GLU:OE2	7:LA:236:SER:OG	2.16	0.62
5:E:508:GLU:N	5:E:508:GLU:OE1	2.31	0.62
12:n:195:LEU:HA	12:n:199:ALA:HB3	1.82	0.62
1:D:565:TYR:OH	1:D:613:ASP:OD2	2.16	0.62
12:b:123:ASP:OD2	12:b:160:ARG:NH2	2.32	0.62
11:J:285:PHE:O	11:J:297:ARG:NH2	2.33	0.62
10:K:488:VAL:HG22	10:K:591:HIS:HE1	1.65	0.62
12:l:322:ASN:ND2	12:l:376:LEU:O	2.32	0.62
12:g:382:THR:HG23	12:g:435:TYR:HD1	1.64	0.61
1:B:622:ASP:OD2	1:B:643:HIS:NE2	2.33	0.61
3:L:460:GLY:O	3:L:464:LYS:NZ	2.32	0.61
12:a:329:ASP:OD2	12:a:331:THR:OG1	2.16	0.61
5:C:423:TYR:O	5:C:424:ASN:ND2	2.33	0.61
5:G:713:LEU:HD11	5:G:722:VAL:HG13	1.81	0.61
7:KA:196:GLU:OE2	7:KA:264:ARG:NH1	2.32	0.61
12:b:103:ASN:OD1	12:b:103:ASN:N	2.33	0.61
7:HA:396:ASP:OD1	7:HA:422:ARG:NH2	2.33	0.61
7:KA:27:GLU:OE2	7:KA:236:SER:OG	2.16	0.61
7:KA:241:SER:O	12:k:72:ARG:NH2	2.33	0.61
12:i:355:SER:O	12:i:357:GLN:NE2	2.34	0.61
5:A:666:LYS:O	12:a:197:GLN:NE2	2.32	0.61
12:m:242:THR:OG1	12:m:250:ASN:O	2.14	0.61
5:A:352:GLY:O	5:A:355:THR:OG1	2.16	0.61
5:C:506:GLU:N	5:C:506:GLU:OE1	2.33	0.61
5:G:399:ILE:HG23	5:G:461:ARG:HE	1.66	0.61
8:HB:30:ILE:HD11	8:HB:47:ILE:HD11	1.83	0.61
1:B:332:LEU:HD12	1:B:336:TYR:CE2	2.36	0.61
8:LB:52:ASN:OD1	8:LB:62:ARG:NH2	2.34	0.61
7:LA:15:GLN:NE2	7:LA:77:GLU:OE1	2.33	0.60
8:EB:36:TYR:OH	8:EB:40:SER:O	2.18	0.60
5:G:297:ARG:HE	1:H:376:ILE:HD13	1.66	0.60
1:D:673:MET:HE3	1:D:779:PHE:HB3	1.83	0.60
1:N:244:GLU:OE1	1:N:282:ASN:ND2	2.34	0.60
12:d:66:LEU:HB3	12:d:74:ILE:HD13	1.84	0.60
12:k:260:LEU:HD12	12:k:269:LEU:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:54:GLN:NE2	12:d:58:GLU:OE1	2.35	0.60
12:g:238:ALA:HB3	12:g:376:LEU:HD22	1.84	0.60
8:DB:224:ASP:OD1	8:DB:276:ARG:NH1	2.34	0.60
7:EA:260:VAL:HG13	7:EA:266:HIS:HB3	1.83	0.60
7:JA:313:MET:N	7:JA:380:ASN:O	2.34	0.60
1:B:591:THR:O	6:Cc:58:ARG:NH2	2.34	0.60
8:FB:234:SER:O	8:FB:241:ARG:NH2	2.35	0.60
12:a:123:ASP:OD2	12:a:160:ARG:NH2	2.35	0.60
5:E:534:LEU:HB3	5:E:554:LEU:HD22	1.82	0.59
12:f:426:GLU:OE2	12:f:430:GLN:NE2	2.35	0.59
7:HA:90:GLU:O	7:HA:121:ARG:NH1	2.34	0.59
7:CA:244:PHE:O	12:c:72:ARG:NH1	2.36	0.59
7:IA:265:ILE:HG13	7:IA:435:VAL:HG21	1.83	0.59
2:Y:53:GLN:NE2	11:Z:18:ASP:OD2	2.35	0.59
12:b:54:GLN:NE2	12:b:58:GLU:OE1	2.36	0.59
11:J:477:ASP:OD2	11:J:637:GLU:N	2.34	0.59
12:d:24:GLN:NE2	12:d:233:SER:OG	2.35	0.59
7:CA:253:THR:HG1	12:c:101:GLY:N	2.01	0.59
8:EB:290:THR:HG22	8:EB:333:ILE:HD11	1.83	0.59
1:F:304:ILE:HD11	1:F:328:LEU:HG	1.83	0.59
7:JA:241:SER:O	12:j:72:ARG:NE	2.35	0.59
7:HA:259:LEU:O	7:HA:380:ASN:ND2	2.34	0.59
12:c:420:GLU:OE1	12:c:420:GLU:N	2.35	0.59
12:f:52:PHE:O	12:f:63:ARG:NH1	2.34	0.59
3:L:1814:ASN:ND2	12:l:348:PHE:O	2.36	0.59
12:e:323:ILE:HG22	12:e:359:ALA:HB3	1.84	0.59
7:BA:165:SER:CB	7:BA:252:LEU:HB3	2.32	0.59
1:D:765:ASP:OD1	1:D:768:SER:OG	2.21	0.59
3:L:557:ASN:O	3:L:571:HIS:ND1	2.36	0.59
6:CC:77:LEU:HD23	6:Cc:77:LEU:HB3	1.84	0.59
7:FA:90:GLU:O	7:FA:121:ARG:NH1	2.36	0.59
12:f:54:GLN:O	12:g:287:LYS:NZ	2.35	0.59
7:LA:244:PHE:O	12:l:72:ARG:NH1	2.35	0.58
1:H:247:GLU:OE2	1:H:366:ARG:NH1	2.35	0.58
12:d:136:VAL:HG12	12:d:167:GLN:HB2	1.84	0.58
1:B:531:GLN:NE2	1:B:535:ASP:OD2	2.37	0.58
8:EB:232:THR:OG1	8:EB:300:MET:SD	2.53	0.58
10:I:281:GLU:OE1	10:I:284:GLN:NE2	2.37	0.58
8:HB:234:SER:O	8:HB:238:THR:OG1	2.20	0.58
8:HB:286:VAL:O	8:HB:290:THR:OG1	2.21	0.58
7:DA:283:HIS:O	7:DA:285:GLN:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:DB:31:ASP:OD2	8:DB:33:SER:OG	2.14	0.58
8:EB:317:PHE:HB3	8:EB:321:MET:HE1	1.86	0.58
11:J:277:LEU:HD22	11:J:287:PHE:CG	2.38	0.58
5:E:416:LYS:HE3	5:E:418:ARG:HB2	1.85	0.58
7:EA:123:ARG:NE	7:EA:161:TYR:OH	2.35	0.58
5:G:350:CYS:O	5:G:355:THR:OG1	2.15	0.58
12:g:116:GLU:N	12:g:116:GLU:OE1	2.36	0.58
10:I:555:GLU:OE1	10:I:558:ARG:NH2	2.36	0.58
1:H:594:GLN:NE2	1:H:623:VAL:O	2.37	0.58
12:a:54:GLN:NE2	12:a:58:GLU:OE1	2.36	0.58
1:B:681:ARG:NH1	12:b:262:PRO:O	2.36	0.57
5:CN:92:LYS:NZ	5:CN:96:GLN:OE1	2.31	0.57
3:L:548:ALA:O	5:M:45:SER:OG	2.22	0.57
12:l:296:ARG:O	12:l:302:ASN:ND2	2.37	0.57
8:JB:30:ILE:HD11	8:JB:47:ILE:HD11	1.87	0.57
7:KA:112:LYS:NZ	7:KA:113:GLU:OE2	2.37	0.57
8:CB:116:VAL:HG11	8:CB:151:LEU:HD22	1.86	0.57
5:G:184:ARG:NH1	1:H:296:GLU:OE2	2.37	0.57
1:H:384:LEU:HD11	1:H:400:VAL:HG12	1.86	0.57
12:d:321:LEU:HD12	12:d:357:GLN:HG3	1.87	0.57
12:e:169:TYR:CD1	12:e:236:MET:HE2	2.39	0.57
8:BB:101:TRP:NE1	8:BB:145:SER:OG	2.37	0.57
8:DB:213:ARG:NH2	8:DB:297:LYS:O	2.37	0.57
5:E:692:ASN:OD1	12:e:357:GLN:NE2	2.38	0.57
1:H:692:ARG:NH2	12:h:197:GLN:O	2.37	0.57
8:JB:135:LEU:HB3	8:JB:166:THR:HG22	1.86	0.57
5:M:418:ARG:HD3	5:M:622:VAL:O	2.04	0.57
12:c:242:THR:OG1	12:c:250:ASN:O	2.21	0.57
1:D:275:TYR:OH	1:D:302:ASN:OD1	2.19	0.57
5:M:161:LEU:HD13	5:M:176:ILE:HD13	1.87	0.57
5:A:397:ARG:HH11	5:A:467:VAL:HG13	1.70	0.57
12:n:155:GLU:OE2	12:n:194:ARG:NE	2.38	0.57
1:B:707:LEU:HD13	1:B:851:THR:HG22	1.87	0.57
12:d:388:PHE:HB2	12:d:432:ILE:HD11	1.87	0.57
12:f:139:HIS:CE1	12:f:141:ILE:HD13	2.40	0.57
1:H:299:TRP:HE3	1:H:300:LEU:HD12	1.70	0.57
10:K:488:VAL:HG21	10:K:587:LEU:HD22	1.86	0.57
12:i:28:GLU:HA	12:i:367:LEU:HD21	1.85	0.57
12:a:28:GLU:OE2	12:a:244:ARG:NH2	2.36	0.56
12:c:383:SER:O	12:c:386:SER:OG	2.09	0.56
12:f:395:TYR:OH	12:f:399:ARG:NH1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:j:20:GLU:OE2	12:j:230:GLN:NE2	2.38	0.56
7:BA:76:ASP:OD1	7:BA:79:ARG:NH1	2.38	0.56
5:G:763:GLN:O	5:G:766:THR:N	2.38	0.56
1:H:641:ASP:OD1	1:H:642:TYR:N	2.38	0.56
12:m:242:THR:O	12:m:251:ASN:ND2	2.37	0.56
5:E:156:LEU:HG	5:E:160:MET:HE2	1.87	0.56
7:EA:251:ASP:OD1	7:EA:252:LEU:N	2.39	0.56
7:GA:76:ASP:OD1	7:GA:79:ARG:NH1	2.38	0.56
8:GB:170:VAL:HG21	8:GB:377:LEU:HD21	1.87	0.56
12:e:137:LEU:HD23	12:e:139:HIS:HB2	1.88	0.56
12:n:294:MET:SD	12:n:294:MET:N	2.78	0.56
5:G:574:LYS:N	5:G:619:ASP:O	2.38	0.56
8:DB:31:ASP:OD1	8:DB:35:ASN:N	2.38	0.56
7:JA:288:VAL:HG11	7:JA:328:VAL:HG22	1.88	0.56
12:g:4:GLU:N	12:g:4:GLU:OE1	2.38	0.56
1:D:537:ALA:O	1:D:541:THR:OG1	2.24	0.56
5:E:537:GLU:OE1	5:E:538:GLU:N	2.38	0.56
7:IA:190:THR:O	7:IA:194:THR:OG1	2.15	0.56
12:e:9:GLN:O	12:e:15:ASN:ND2	2.38	0.56
12:g:411:GLU:N	12:g:411:GLU:OE1	2.38	0.56
8:CB:311:LEU:O	8:CB:348:ASN:ND2	2.39	0.56
1:F:622:ASP:OD1	1:F:623:VAL:N	2.39	0.56
1:H:766:SER:O	1:H:769:ARG:NE	2.33	0.56
8:LB:192:LEU:O	8:LB:196:THR:OG1	2.24	0.56
12:f:346:ALA:HB1	12:f:348:PHE:HE1	1.70	0.56
5:A:508:GLU:OE1	5:A:508:GLU:N	2.39	0.56
10:K:358:LYS:HA	10:K:362:LEU:HD12	1.87	0.56
12:d:103:ASN:ND2	12:d:411:GLU:OE2	2.39	0.56
7:BA:189:LEU:HD13	7:BA:413:MET:HE1	1.88	0.56
5:G:351:LEU:O	5:G:354:SER:OG	2.23	0.56
1:H:873:LEU:O	1:H:877:SER:OG	2.24	0.56
8:LB:345:ILE:HG22	8:LB:348:ASN:HB3	1.87	0.56
1:B:296:GLU:OE1	1:B:297:LEU:N	2.39	0.56
7:CA:239:THR:HG23	7:CA:243:ARG:HE	1.70	0.56
8:DB:214:THR:O	8:DB:216:LYS:NZ	2.39	0.56
7:HA:189:LEU:HD22	7:HA:413:MET:HE1	1.87	0.56
10:K:652:ASN:O	10:K:656:THR:OG1	2.24	0.56
12:b:122:ILE:HD12	12:b:153:LEU:HD13	1.87	0.56
12:g:133:GLU:OE2	12:g:254:ILE:N	2.39	0.56
12:h:88:PRO:O	12:h:124:ARG:NH2	2.40	0.56
12:i:4:GLU:OE1	12:i:4:GLU:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:i:242:THR:HG23	12:i:243:LEU:HD22	1.88	0.55
10:I:524:LEU:HD13	12:i:354:ALA:HA	1.88	0.55
10:K:488:VAL:HG22	10:K:591:HIS:CE1	2.39	0.55
3:L:354:LYS:O	3:L:358:ASN:ND2	2.39	0.55
3:L:1538:LEU:HD23	3:L:1561:VAL:HG12	1.87	0.55
12:a:122:ILE:HD12	12:a:153:LEU:HD13	1.89	0.55
12:d:218:LEU:O	12:d:220:ILE:HD12	2.06	0.55
7:BA:288:VAL:O	7:BA:292:THR:OG1	2.23	0.55
8:BB:314:ALA:HB3	8:BB:368:ILE:HB	1.89	0.55
11:Z:115:LEU:O	11:Z:118:SER:OG	2.20	0.55
12:b:155:GLU:OE1	12:b:156:ARG:NH1	2.40	0.55
7:BA:237:SER:N	7:BA:376:CYS:SG	2.80	0.55
12:m:265:ARG:NH2	12:m:430:GLN:OE1	2.39	0.55
1:B:868:SER:OG	1:B:874:ARG:NH1	2.40	0.55
7:BA:68:VAL:HG22	7:BA:93:ILE:HB	1.88	0.55
5:E:619:ASP:OD1	5:E:620:TYR:N	2.39	0.55
1:F:885:HIS:NE2	12:f:351:TRP:O	2.39	0.55
7:JA:248:LEU:HD22	7:JA:354:GLY:HA3	1.88	0.55
5:M:116:SER:OG	5:M:119:SER:O	2.18	0.55
12:d:64:ALA:O	12:d:90:ASN:ND2	2.40	0.55
12:k:103:ASN:ND2	12:k:411:GLU:OE1	2.37	0.55
12:g:168:THR:HG1	12:g:170:SER:HG	1.51	0.55
5:C:534:LEU:HB3	5:C:554:LEU:HD12	1.88	0.55
1:D:826:GLU:OE1	1:D:826:GLU:N	2.39	0.55
11:J:437:LEU:HD22	11:J:469:VAL:HG12	1.89	0.55
7:JA:352:LYS:O	12:j:180:ASP:N	2.39	0.55
1:B:367:LEU:O	1:B:371:THR:HG23	2.07	0.55
7:BA:66:VAL:O	7:BA:68:VAL:HG23	2.07	0.55
5:E:278:GLU:O	5:E:281:SER:OG	2.25	0.55
5:E:517:LYS:HG2	5:E:521:LEU:HD12	1.89	0.55
1:H:448:VAL:HG22	1:H:484:LEU:HD12	1.88	0.55
7:HA:346:TRP:CD1	12:h:401:ARG:CB	2.89	0.55
7:IA:326:LYS:HD3	12:i:208:THR:HG22	1.89	0.54
5:G:450:ILE:O	5:G:453:THR:OG1	2.24	0.54
12:i:271:THR:OG1	12:i:272:GLY:N	2.39	0.54
7:FA:277:SER:OG	7:FA:279:GLU:OE1	2.25	0.54
7:GA:271:THR:HG23	7:GA:300:ASN:O	2.07	0.54
10:I:499:GLN:NE2	12:i:200:ASP:OD1	2.39	0.54
3:L:381:ARG:HE	3:L:383:VAL:HG12	1.72	0.54
12:h:216:ASP:OD1	12:h:217:ARG:N	2.40	0.54
5:A:244:ARG:NH1	5:A:271:SER:OG	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BB:236:VAL:HG12	8:BB:368:ILE:HD13	1.90	0.54
1:F:711:MET:SD	1:F:782:ILE:HG22	2.46	0.54
8:FB:194:GLU:OE2	8:FB:414:ASN:ND2	2.40	0.54
10:K:555:GLU:OE1	10:K:558:ARG:NH1	2.41	0.54
3:L:1673:MET:HE3	3:L:1777:TYR:CE1	2.43	0.54
5:M:416:LYS:HG3	5:M:418:ARG:HG2	1.89	0.54
12:m:4:GLU:OE1	12:m:129:SER:OG	2.23	0.54
8:JB:314:ALA:HB3	8:JB:368:ILE:HB	1.90	0.54
5:C:418:ARG:NH2	5:C:620:TYR:O	2.39	0.54
5:C:418:ARG:HH21	5:C:622:VAL:HG22	1.72	0.54
10:I:25:LEU:HD11	10:I:53:ILE:HD12	1.90	0.54
12:a:103:ASN:OD1	12:a:103:ASN:N	2.38	0.54
12:n:315:HIS:O	12:n:347:ASN:ND2	2.39	0.54
5:G:738:MET:HB3	5:G:745:LEU:HD12	1.89	0.54
12:b:231:LEU:O	12:b:234:THR:OG1	2.24	0.54
12:h:392:CYS:SG	12:h:393:ARG:NH2	2.81	0.54
12:j:7:THR:HG22	12:j:136:VAL:HG23	1.89	0.54
5:A:837:LEU:HD22	5:A:859:LEU:HD21	1.89	0.54
8:FB:172:SER:OG	8:FB:205:GLU:OE1	2.25	0.54
7:KA:133:GLN:NE2	12:k:70:GLU:OE1	2.40	0.54
3:L:616:TRP:O	5:M:482:ARG:NH2	2.40	0.54
5:A:460:VAL:HG12	5:A:464:GLY:HA2	1.89	0.54
7:JA:313:MET:C	7:JA:380:ASN:O	2.51	0.54
12:e:139:HIS:CE1	12:e:141:ILE:HD13	2.43	0.54
4:7:243:LYS:O	5:C:711:LYS:NZ	2.41	0.53
5:C:619:ASP:OD1	5:C:620:TYR:N	2.41	0.53
12:h:4:GLU:O	12:h:133:GLU:N	2.42	0.53
1:F:677:LEU:HD12	1:F:712:VAL:HG23	1.90	0.53
12:l:303:VAL:HG12	12:l:305:VAL:H	1.73	0.53
8:BB:135:LEU:HG	8:BB:166:THR:HG23	1.90	0.53
1:D:304:ILE:HD11	1:D:328:LEU:HG	1.89	0.53
5:M:9:ASP:OD1	5:M:10:VAL:N	2.40	0.53
12:h:271:THR:OG1	12:h:272:GLY:N	2.41	0.53
12:n:273:TYR:HD1	12:n:376:LEU:HD12	1.74	0.53
1:B:252:ARG:NH1	1:B:350:ASP:OD1	2.41	0.53
7:BA:232:SER:HA	7:BA:235:VAL:HG12	1.91	0.53
7:DA:201:ALA:HB3	7:DA:267:PHE:HD1	1.73	0.53
8:DB:170:VAL:HG11	8:DB:377:LEU:HD11	1.89	0.53
7:EA:271:THR:HB	7:EA:377:MET:HE3	1.91	0.53
8:FB:299:MET:HE3	8:FB:305:PRO:HG3	1.89	0.53
8:JB:116:VAL:HG11	8:JB:151:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:GB:194:GLU:OE2	8:GB:414:ASN:ND2	2.42	0.53
3:L:621:VAL:O	3:L:623:ARG:N	2.41	0.53
12:i:190:LEU:O	12:i:194:ARG:NH1	2.40	0.53
8:IB:31:ASP:OD1	8:IB:35:ASN:N	2.42	0.53
1:N:252:ARG:O	1:N:252:ARG:NH1	2.42	0.53
12:l:232:VAL:HA	12:l:235:ILE:HD12	1.91	0.53
5:A:765:PHE:HB3	5:A:814:LEU:HD21	1.91	0.53
10:I:629:ILE:HG23	10:I:631:SER:H	1.74	0.53
12:d:68:ASP:N	12:d:68:ASP:OD1	2.42	0.53
12:e:318:ILE:N	12:e:380:ASN:O	2.40	0.53
5:E:175:PRO:HG3	1:F:402:ALA:HB1	1.89	0.53
1:F:261:ILE:HD11	5:G:255:SER:O	2.08	0.53
1:H:681:ARG:NH1	12:h:258:ALA:O	2.41	0.53
5:M:190:ASP:O	1:N:293:ARG:NH2	2.42	0.53
12:a:266:LEU:O	12:a:380:ASN:ND2	2.40	0.53
5:M:747:VAL:HG21	5:M:839:ARG:HD2	1.91	0.53
7:BA:163:LYS:O	7:BA:164:LYS:C	2.51	0.52
7:EA:71:GLU:OE1	7:EA:73:THR:OG1	2.20	0.52
12:m:29:HIS:ND1	12:m:46:ASP:OD2	2.42	0.52
7:BA:199:ASP:OD1	7:BA:256:GLN:NE2	2.42	0.52
5:C:637:ARG:NH2	6:CC:76:ASN:OD1	2.43	0.52
12:g:252:ASP:OD1	12:g:252:ASP:N	2.42	0.52
12:h:231:LEU:O	12:h:234:THR:OG1	2.26	0.52
7:BA:264:ARG:O	7:BA:264:ARG:NE	2.41	0.52
1:F:620:ARG:NH1	1:F:643:HIS:O	2.41	0.52
1:H:798:GLU:OE1	1:H:802:ARG:NH1	2.41	0.52
10:I:307:PHE:HZ	10:I:335:THR:HG21	1.74	0.52
12:m:172:PHE:CG	12:m:204:VAL:HG13	2.45	0.52
7:BA:161:TYR:CD1	7:BA:163:LYS:HG3	2.44	0.52
1:N:446:PHE:O	1:N:467:ARG:NH1	2.43	0.52
8:BB:161:ASP:O	8:BB:251:ARG:NH2	2.42	0.52
8:CB:163:ILE:HD11	8:CB:251:ARG:HG3	1.92	0.52
1:F:373:ASP:OD1	1:F:410:TYR:OH	2.27	0.52
11:J:1015:LEU:O	12:j:341:ARG:NH1	2.43	0.52
12:b:329:ASP:OD1	12:b:329:ASP:N	2.41	0.52
1:B:456:THR:OG1	1:B:457:ASP:N	2.43	0.52
12:h:413:MET:SD	12:h:414:PHE:N	2.83	0.52
12:n:210:LEU:HB3	12:n:228:ILE:HD12	1.91	0.52
5:M:540:ARG:HA	5:M:613:LEU:HD23	1.91	0.52
7:BA:236:SER:O	7:BA:240:ALA:N	2.43	0.52
7:BA:319:TYR:CD2	7:BA:327:ASP:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:282:SER:O	5:E:290:HIS:NE2	2.40	0.52
7:EA:325:PRO:O	12:e:220:ILE:HD12	2.10	0.52
8:KB:90:PHE:C	8:KB:91:ILE:HD12	2.35	0.52
3:L:1480:LEU:HD23	3:L:1484:MET:HG3	1.92	0.52
7:BA:3:GLU:OE1	7:BA:64:ARG:NE	2.38	0.51
8:DB:36:TYR:OH	8:DB:40:SER:O	2.27	0.51
7:EA:165:SER:OG	7:EA:256:GLN:NE2	2.40	0.51
5:G:637:ARG:NH2	5:G:727:THR:OG1	2.43	0.51
1:H:471:ILE:HD12	1:H:472:PRO:HD2	1.92	0.51
8:KB:314:ALA:HB3	8:KB:368:ILE:HB	1.91	0.51
3:L:1766:GLU:O	3:L:1767:HIS:C	2.52	0.51
12:e:206:ASP:HB2	12:e:209:ALA:HB3	1.92	0.51
12:f:236:MET:O	12:f:239:SER:OG	2.23	0.51
12:g:382:THR:HG23	12:g:435:TYR:CD1	2.45	0.51
1:B:325:CYS:SG	1:B:326:ALA:N	2.84	0.51
1:B:575:ARG:NH1	1:B:579:ASP:OD2	2.42	0.51
1:D:364:LEU:HD12	1:D:370:TRP:HE1	1.74	0.51
5:M:175:PRO:HB3	1:N:402:ALA:HB1	1.93	0.51
12:b:4:GLU:OE1	12:b:63:ARG:NH2	2.43	0.51
12:d:261:ILE:HD12	12:d:267:HIS:HA	1.93	0.51
1:D:622:ASP:OD1	1:D:623:VAL:N	2.44	0.51
7:LA:293:ASN:HA	7:LA:335:ILE:HD13	1.92	0.51
12:h:64:ALA:O	12:h:90:ASN:ND2	2.42	0.51
1:B:641:ASP:OD1	1:B:642:TYR:N	2.43	0.51
5:E:450:ILE:O	5:E:453:THR:OG1	2.27	0.51
8:FB:294:PHE:HZ	8:FB:330:MET:HE1	1.75	0.51
10:K:202:GLU:OE1	10:K:260:ARG:NE	2.44	0.51
8:JB:67:ASP:OD1	8:JB:68:LEU:N	2.42	0.51
1:D:608:THR:HG23	1:D:610:ALA:H	1.76	0.51
9:EM:78:SER:OG	5:EN:23:ASP:OD2	2.26	0.51
1:H:716:HIS:ND1	12:h:357:GLN:OE1	2.42	0.51
12:c:323:ILE:HD12	12:c:359:ALA:HB3	1.92	0.51
12:g:130:ASP:OD1	12:h:335:LYS:NZ	2.43	0.51
12:j:174:ASN:O	12:j:208:THR:OG1	2.23	0.51
7:BA:392:ASP:OD1	7:BA:422:ARG:NH1	2.44	0.51
8:EB:191:GLN:OE1	8:EB:195:ASN:ND2	2.44	0.51
12:j:235:ILE:HD11	12:j:304:MET:HE3	1.93	0.51
12:k:295:ARG:NH2	12:k:336:SER:OG	2.43	0.51
7:HA:245:ASP:OD1	12:h:72:ARG:NH1	2.44	0.51
12:a:330:PRO:HA	12:a:333:VAL:HG12	1.92	0.51
8:BB:166:THR:HG22	8:BB:167:PHE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:EB:170:VAL:HG11	8:EB:377:LEU:HD11	1.93	0.51
1:H:847:LEU:O	1:H:851:THR:HG23	2.11	0.51
7:EA:81:GLY:O	7:EA:84:ARG:NE	2.44	0.51
8:HB:164:MET:SD	8:HB:164:MET:N	2.85	0.51
10:I:35:HIS:ND1	10:I:37:SER:OG	2.38	0.51
11:J:888:VAL:HA	11:J:891:MET:HE3	1.93	0.51
1:B:594:GLN:OE1	1:B:598:THR:OG1	2.16	0.50
1:B:620:ARG:NH1	1:B:645:ASP:O	2.41	0.50
1:F:491:ASN:ND2	1:F:495:GLN:OE1	2.44	0.50
5:G:288:VAL:HG21	5:G:352:GLY:HA2	1.93	0.50
3:L:1485:LYS:HD2	3:L:1488:ILE:HD12	1.93	0.50
1:D:761:ARG:NH1	1:D:870:ASP:OD2	2.44	0.50
7:GA:323:VAL:CB	12:g:223:PRO:HG3	2.41	0.50
8:HB:27:GLU:OE1	8:HB:241:ARG:NH2	2.43	0.50
5:M:221:LEU:HA	5:M:224:VAL:HG22	1.94	0.50
1:B:559:MET:SD	1:B:751:HIS:NE2	2.85	0.50
1:F:286:SER:OG	1:F:287:LEU:N	2.45	0.50
7:JA:97:GLU:N	7:JA:97:GLU:OE1	2.44	0.50
7:KA:322:ASP:OD2	12:k:222:ASN:ND2	2.44	0.50
12:c:322:ASN:OD1	12:c:322:ASN:N	2.43	0.50
12:d:181:VAL:O	12:d:184:GLN:N	2.42	0.50
12:h:214:ALA:HB2	12:h:228:ILE:HD13	1.94	0.50
12:i:442:ASP:O	12:i:445:SER:OG	2.24	0.50
12:m:156:ARG:NH1	12:m:159:ASP:OD2	2.44	0.50
7:GA:325:PRO:HB3	12:g:220:ILE:HG23	1.93	0.50
8:GB:196:THR:HG1	8:GB:264:HIS:HE2	1.59	0.50
8:KB:207:LEU:HD21	8:KB:300:MET:HE2	1.93	0.50
1:B:332:LEU:HD12	1:B:336:TYR:CZ	2.47	0.50
7:EA:236:SER:O	7:EA:243:ARG:NH2	2.44	0.50
1:F:644:VAL:HG21	1:F:652:PHE:HD2	1.76	0.50
1:F:681:ARG:NH1	12:f:258:ALA:O	2.44	0.50
5:G:456:TYR:OH	5:G:718:ASN:OD1	2.18	0.50
3:L:559:GLU:HB3	3:L:567:LEU:HD23	1.93	0.50
12:b:77:ILE:HD13	12:b:82:TYR:HB2	1.93	0.50
1:F:286:SER:N	1:F:289:ASP:OD1	2.45	0.50
3:L:1791:VAL:HG21	3:L:1806:PHE:HD2	1.76	0.50
7:LA:71:GLU:OE1	7:LA:73:THR:OG1	2.18	0.50
12:f:240:THR:OG1	12:f:244:ARG:NH1	2.44	0.50
7:EA:198:SER:OG	7:EA:199:ASP:N	2.44	0.50
7:FA:251:ASP:OD1	7:FA:252:LEU:N	2.45	0.50
11:J:723:MET:HE2	11:J:821:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:h:303:VAL:HG12	12:h:305:VAL:H	1.77	0.50
7:BA:265:ILE:HG23	7:BA:266:HIS:H	1.75	0.50
1:D:342:LEU:HD22	1:D:367:LEU:HD22	1.94	0.50
7:DA:196:GLU:OE1	7:DA:196:GLU:N	2.42	0.50
7:DA:201:ALA:HB3	7:DA:267:PHE:CD1	2.45	0.50
8:IB:375:GLN:HB2	8:IB:419:VAL:HG13	1.93	0.50
10:K:47:ARG:NH1	10:K:130:GLN:OE1	2.45	0.50
7:CA:135:PHE:N	7:CA:165:SER:O	2.45	0.49
5:G:333:ARG:NH2	5:G:369:ASP:OD2	2.46	0.49
1:H:314:ASP:OD1	1:H:316:SER:OG	2.27	0.49
1:N:274:CYS:SG	1:N:275:TYR:N	2.85	0.49
12:a:155:GLU:OE1	12:a:156:ARG:NH1	2.43	0.49
12:f:271:THR:OG1	12:f:272:GLY:N	2.44	0.49
12:f:297:LEU:HD13	12:f:377:MET:HB3	1.93	0.49
1:D:451:ASP:N	1:D:451:ASP:OD1	2.43	0.49
5:E:861:PHE:HE1	12:e:337:LEU:HD12	1.76	0.49
1:H:286:SER:OG	1:H:287:LEU:N	2.45	0.49
1:H:304:ILE:HD11	1:H:328:LEU:HG	1.93	0.49
8:IB:31:ASP:OD2	8:IB:33:SER:OG	2.28	0.49
5:M:585:GLN:NE2	5:M:640:MET:SD	2.84	0.49
8:GB:141:GLY:O	8:GB:145:SER:OG	2.26	0.49
7:LA:192:HIS:CD2	7:LA:193:THR:HG23	2.47	0.49
12:i:28:GLU:OE1	12:i:244:ARG:NH1	2.44	0.49
1:3:65:GLN:NE2	1:3:103:ASP:OD2	2.45	0.49
1:D:398:SER:OG	1:D:473:SER:N	2.43	0.49
8:EB:53:GLU:OE1	8:EB:53:GLU:N	2.44	0.49
8:EB:234:SER:O	8:EB:241:ARG:NH2	2.41	0.49
5:GN:69:GLU:O	5:GN:72:SER:OG	2.24	0.49
8:HB:284:LEU:HB2	8:HB:363:MET:HB3	1.93	0.49
8:LB:134:GLN:NE2	8:LB:165:ASN:OD1	2.44	0.49
12:i:396:ASP:O	12:i:400:LYS:NZ	2.45	0.49
5:E:165:GLN:NE2	5:E:172:GLN:OE1	2.45	0.49
5:G:508:GLU:N	5:G:508:GLU:OE1	2.40	0.49
7:IA:167:LEU:HD22	7:IA:252:LEU:HD22	1.93	0.49
8:KB:295:ASP:OD1	8:KB:296:ALA:N	2.45	0.49
8:LB:161:ASP:OD2	8:LB:162:ARG:NH2	2.44	0.49
8:BB:404:ASP:OD1	8:BB:405:GLU:N	2.46	0.49
8:GB:293:MET:HE3	8:GB:293:MET:HA	1.94	0.49
12:b:330:PRO:HA	12:b:333:VAL:HG12	1.94	0.49
12:g:213:ILE:HD13	12:g:304:MET:HE2	1.93	0.49
8:BB:378:PHE:HB2	8:BB:419:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BB:429:THR:OG1	8:BB:430:ALA:N	2.44	0.49
8:GB:116:VAL:HG11	8:GB:151:LEU:HD22	1.94	0.49
12:b:12:GLN:OE1	12:b:145:THR:OG1	2.21	0.49
12:e:120:ASP:OD1	12:f:295:ARG:NH2	2.43	0.49
12:m:24:GLN:OE1	12:m:230:GLN:NE2	2.45	0.49
3:5:67:ARG:NH2	3:5:94:GLU:OE2	2.45	0.49
8:BB:135:LEU:HD11	8:BB:137:HIS:HD2	1.78	0.49
8:FB:52:ASN:OD1	8:FB:62:ARG:NH2	2.45	0.49
7:GA:180:ALA:HB3	7:GA:183:GLU:HG3	1.94	0.49
8:IB:64:ILE:HD11	8:IB:123:GLU:HG3	1.94	0.49
3:L:1506:TYR:HD2	3:L:1511:LEU:HD23	1.77	0.49
5:M:738:MET:HB3	5:M:745:LEU:HD12	1.95	0.49
5:A:227:GLY:O	1:B:293:ARG:NH2	2.45	0.49
7:GA:115:ILE:HA	7:GA:118:VAL:HG22	1.95	0.49
8:IB:164:MET:SD	8:IB:164:MET:N	2.85	0.49
8:BB:398:TYR:HB3	8:BB:408:PHE:CZ	2.48	0.49
7:HA:327:ASP:HB3	12:h:222:ASN:HA	1.95	0.49
8:IB:63:ALA:O	8:IB:64:ILE:HD13	2.13	0.49
12:k:334:HIS:O	12:k:338:GLN:NE2	2.43	0.49
1:B:608:THR:HG23	1:B:610:ALA:H	1.78	0.48
5:G:594:THR:OG1	5:G:595:LYS:N	2.44	0.48
1:N:632:ASP:OD1	11:Z:123:ASN:ND2	2.46	0.48
5:GN:16:LEU:O	5:GN:105:ARG:NH2	2.42	0.48
7:KA:71:GLU:OE2	8:KB:247:ASN:ND2	2.43	0.48
3:L:530:GLU:OE1	3:L:534:ARG:NH2	2.46	0.48
5:M:191:PHE:HD2	5:M:235:ALA:HB2	1.78	0.48
12:n:230:GLN:O	12:n:233:SER:OG	2.22	0.48
1:F:848:ARG:O	1:F:851:THR:OG1	2.29	0.48
5:CN:5:ARG:NH1	5:CN:9:ASP:OD1	2.44	0.48
1:F:616:GLU:OE1	1:F:619:ARG:NE	2.40	0.48
1:H:616:GLU:OE2	1:H:619:ARG:NH2	2.45	0.48
7:BA:71:GLU:OE2	7:BA:73:THR:OG1	2.30	0.48
12:e:57:ASP:OD2	12:e:59:HIS:ND1	2.47	0.48
12:f:317:TYR:CD1	12:f:320:ILE:HD11	2.49	0.48
12:k:357:GLN:OE1	12:k:357:GLN:N	2.46	0.48
5:M:418:ARG:HD2	5:M:419:ILE:HG12	1.95	0.48
12:a:47:ARG:NE	12:a:49:ASP:OD1	2.46	0.48
7:BA:5:ILE:HD12	7:BA:125:LEU:HD13	1.95	0.48
1:H:564:ARG:O	1:H:569:GLY:N	2.46	0.48
1:H:725:GLU:O	1:H:761:ARG:NH2	2.44	0.48
7:HA:324:VAL:HG22	7:HA:357:TYR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:IB:263:LEU:HD22	8:IB:422:TYR:CZ	2.48	0.48
12:m:112:GLU:OE1	12:m:152:TYR:OH	2.23	0.48
7:BA:251:ASP:O	7:BA:254:ASP:HB2	2.14	0.48
8:BB:190:HIS:O	8:BB:193:VAL:HG12	2.14	0.48
1:F:608:THR:HG23	1:F:610:ALA:H	1.78	0.48
1:B:829:GLU:OE1	1:B:832:ARG:NE	2.43	0.48
1:F:573:PHE:HB2	1:F:608:THR:HG21	1.96	0.48
1:N:245:ILE:HB	1:N:283:LEU:HD13	1.96	0.48
12:b:236:MET:O	12:b:239:SER:OG	2.24	0.48
5:A:461:ARG:O	5:A:463:CYS:N	2.47	0.48
7:FA:254:ASP:O	7:FA:258:ASN:ND2	2.43	0.48
7:FA:279:GLU:OE1	7:FA:279:GLU:N	2.47	0.48
7:IA:258:ASN:O	7:IA:260:VAL:N	2.46	0.48
8:IB:429:THR:HG23	8:IB:431:GLU:HG3	1.96	0.48
7:KA:289:ALA:N	7:KA:327:ASP:OD2	2.47	0.48
12:b:28:GLU:OE2	12:b:244:ARG:NH2	2.41	0.48
12:j:10:LEU:HD13	12:j:149:LEU:HB3	1.94	0.48
8:EB:130:LEU:HD23	8:EB:162:ARG:HG2	1.94	0.47
1:H:452:PRO:O	1:H:453:THR:OG1	2.28	0.47
1:H:607:ALA:O	12:h:47:ARG:NH2	2.47	0.47
12:k:172:PHE:CD1	12:k:204:VAL:HG23	2.49	0.47
12:a:329:ASP:OD1	12:a:329:ASP:N	2.46	0.47
12:e:231:LEU:O	12:e:234:THR:OG1	2.27	0.47
12:j:322:ASN:CG	12:j:356:ILE:HD11	2.38	0.47
7:EA:260:VAL:O	7:EA:260:VAL:HG12	2.14	0.47
8:EB:52:ASN:OD1	8:EB:62:ARG:NE	2.44	0.47
7:GA:323:VAL:HB	12:g:223:PRO:HG3	1.96	0.47
10:K:607:ARG:O	10:K:611:GLN:NE2	2.47	0.47
12:a:3:ARG:NH1	12:a:133:GLU:OE1	2.47	0.47
12:l:177:GLU:OE1	12:l:390:ARG:NH1	2.45	0.47
5:C:164:LYS:NZ	5:C:404:TYR:O	2.41	0.47
1:D:790:ASP:OD1	1:D:791:ALA:N	2.46	0.47
8:JB:74:ASP:OD1	8:JB:77:ARG:NH2	2.45	0.47
7:LA:27:GLU:OE1	7:LA:243:ARG:NH1	2.47	0.47
12:k:243:LEU:HD21	12:k:253:LEU:HB2	1.97	0.47
5:C:486:GLU:OE1	5:C:486:GLU:N	2.45	0.47
5:E:394:TRP:CZ2	5:E:409:VAL:HG21	2.49	0.47
8:EB:289:LEU:O	8:EB:293:MET:HE3	2.15	0.47
5:G:402:ASP:OD1	5:G:405:SER:N	2.47	0.47
1:H:289:ASP:N	1:H:289:ASP:OD1	2.47	0.47
7:HA:50:ASN:OD1	7:HA:64:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:HB:307:HIS:O	8:HB:426:GLN:NE2	2.46	0.47
5:A:734:LEU:O	5:A:740:THR:OG1	2.31	0.47
5:C:221:LEU:HA	5:C:224:VAL:HG22	1.96	0.47
5:E:594:THR:O	5:E:596:GLN:N	2.47	0.47
5:E:657:SER:HA	5:E:660:ILE:HG22	1.95	0.47
7:FA:221:ARG:NH1	8:FB:327:ASP:OD2	2.47	0.47
8:HB:67:ASP:OD1	8:HB:68:LEU:N	2.48	0.47
7:JA:244:PHE:O	7:JA:246:GLY:N	2.48	0.47
5:M:295:ALA:O	5:M:298:THR:OG1	2.32	0.47
12:g:420:GLU:N	12:g:420:GLU:OE1	2.47	0.47
12:k:294:MET:SD	12:k:294:MET:N	2.88	0.47
5:C:466:ASP:OD2	5:C:468:THR:OG1	2.31	0.47
8:CB:113:VAL:HG23	8:CB:151:LEU:HD23	1.96	0.47
1:D:870:ASP:OD1	1:D:871:GLU:N	2.47	0.47
8:EB:307:HIS:ND1	8:EB:376:GLU:OE2	2.45	0.47
1:F:624:ARG:O	1:F:639:SER:N	2.47	0.47
7:GA:118:VAL:HG21	7:GA:149:PHE:HZ	1.80	0.47
8:JB:292:GLN:NE2	8:JB:298:ASN:OD1	2.46	0.47
5:M:456:TYR:O	5:M:459:VAL:HG22	2.15	0.47
5:M:638:TYR:CE2	5:M:730:LEU:HD11	2.50	0.47
12:a:77:ILE:HD13	12:a:82:TYR:HB2	1.97	0.47
12:b:266:LEU:O	12:b:380:ASN:ND2	2.48	0.47
12:b:401:ARG:O	12:b:403:ALA:N	2.47	0.47
7:BA:134:GLY:HA3	7:BA:252:LEU:HD12	1.95	0.47
7:FA:260:VAL:N	7:FA:261:PRO:CD	2.77	0.47
8:IB:179:VAL:HB	8:IB:388:MET:HE1	1.97	0.47
3:L:1673:MET:HE1	3:L:1780:PHE:HD2	1.80	0.47
12:e:237:SER:O	12:e:244:ARG:NH2	2.42	0.47
7:GA:317:LEU:HB3	7:GA:319:TYR:HE1	1.80	0.47
8:KB:116:VAL:HG11	8:KB:151:LEU:HD22	1.97	0.47
5:M:526:ASP:OD1	5:M:530:HIS:NE2	2.48	0.47
2:Y:55:ILE:HD11	11:Z:15:GLN:CD	2.40	0.47
12:c:217:ARG:NH1	12:c:279:ASP:OD1	2.44	0.47
1:D:871:GLU:OE1	1:D:874:ARG:NH1	2.48	0.47
7:DA:166:LYS:N	7:DA:199:ASP:OD2	2.48	0.47
7:DA:245:ASP:OD1	7:DA:245:ASP:N	2.46	0.47
8:EB:64:ILE:HD13	8:EB:120:VAL:HG12	1.95	0.47
1:F:575:ARG:NE	12:f:252:ASP:OD2	2.48	0.47
10:I:460:GLN:O	10:I:464:HIS:N	2.47	0.47
7:LA:154:MET:HE3	7:LA:168:GLU:HG2	1.96	0.47
12:c:297:LEU:HD13	12:c:377:MET:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BB:69:GLU:O	8:BB:72:THR:OG1	2.29	0.46
7:DA:280:LYS:O	7:DA:283:HIS:NE2	2.44	0.46
7:EA:260:VAL:N	7:EA:261:PRO:CD	2.78	0.46
12:g:420:GLU:HA	12:g:423:THR:HG22	1.96	0.46
1:3:20:ILE:HG21	2:4:67:LEU:HB3	1.97	0.46
12:h:155:GLU:O	12:h:158:ASN:ND2	2.48	0.46
12:i:222:ASN:CB	12:i:223:PRO:CD	2.93	0.46
12:k:260:LEU:O	12:k:380:ASN:ND2	2.46	0.46
7:DA:186:ASN:OD1	7:DA:408:TYR:OH	2.28	0.46
9:EM:65:LEU:HD21	5:EN:1:MET:HE1	1.97	0.46
7:FA:205:ASP:N	7:FA:302:MET:O	2.47	0.46
7:GA:344:VAL:HG21	7:GA:346:TRP:CZ2	2.50	0.46
8:GB:293:MET:HE2	8:GB:367:PHE:HB3	1.96	0.46
7:HA:324:VAL:O	7:HA:355:ILE:HG21	2.16	0.46
7:KA:288:VAL:HG11	7:KA:323:VAL:HG13	1.96	0.46
12:a:242:THR:O	12:a:242:THR:OG1	2.34	0.46
12:e:271:THR:OG1	12:e:272:GLY:N	2.48	0.46
12:g:67:LEU:HD23	12:g:118:ILE:HD12	1.96	0.46
12:g:238:ALA:CB	12:g:376:LEU:HD22	2.44	0.46
5:E:394:TRP:CE2	5:E:409:VAL:HG11	2.50	0.46
8:FB:404:ASP:OD1	8:FB:405:GLU:N	2.48	0.46
11:J:734:THR:OG1	11:J:735:MET:N	2.47	0.46
7:BA:326:LYS:CB	7:BA:327:ASP:HA	2.46	0.46
1:D:575:ARG:NH1	12:d:251:ASN:O	2.47	0.46
3:L:1673:MET:HE1	3:L:1780:PHE:CD2	2.51	0.46
5:M:653:ARG:NH2	12:m:252:ASP:OD2	2.46	0.46
7:CA:133:GLN:NE2	12:c:70:GLU:OE2	2.49	0.46
8:CB:143:THR:OG1	8:CB:144:GLY:N	2.49	0.46
7:EA:7:ILE:N	7:EA:136:LEU:O	2.48	0.46
8:FB:321:MET:HE3	8:FB:326:VAL:HG21	1.96	0.46
7:GA:260:VAL:N	7:GA:261:PRO:CD	2.78	0.46
8:KB:192:LEU:O	8:KB:196:THR:OG1	2.29	0.46
3:L:1548:THR:O	3:L:1550:GLY:N	2.48	0.46
8:CB:286:VAL:O	8:CB:290:THR:OG1	2.29	0.46
1:D:331:GLU:OE2	1:D:377:ARG:NH1	2.47	0.46
12:a:395:TYR:HE1	12:a:421:MET:HE2	1.79	0.46
5:E:637:ARG:HB3	5:E:730:LEU:HD12	1.98	0.46
1:N:440:GLU:OE1	1:N:440:GLU:N	2.49	0.46
12:a:395:TYR:CE1	12:a:421:MET:HE2	2.51	0.46
1:B:660:TYR:OH	1:B:758:ILE:HG21	2.16	0.46
1:D:734:LEU:O	1:D:738:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:DA:167:LEU:HD13	7:DA:252:LEU:HD22	1.98	0.46
5:E:190:ASP:OD2	5:E:244:ARG:NH1	2.49	0.46
1:F:594:GLN:OE1	1:F:594:GLN:N	2.49	0.46
12:f:204:VAL:HG13	12:f:305:VAL:HG21	1.98	0.46
12:i:232:VAL:HG12	12:i:236:MET:HE2	1.98	0.46
12:l:245:TYR:O	12:l:247:GLY:N	2.47	0.46
1:D:441:ASP:OD1	1:D:442:THR:N	2.49	0.46
5:E:571:ASP:OD1	5:E:571:ASP:N	2.47	0.46
7:FA:326:LYS:HG2	12:f:228:ILE:HD12	1.98	0.46
5:G:572:ASP:N	5:G:572:ASP:OD1	2.48	0.46
12:e:304:MET:SD	12:e:304:MET:N	2.88	0.46
12:h:269:LEU:HD13	12:h:379:ALA:C	2.41	0.46
7:CA:195:LEU:HD21	7:CA:264:ARG:HH12	1.81	0.45
5:E:576:ASP:OD1	5:E:577:LEU:N	2.49	0.45
7:FA:399:TYR:O	7:FA:402:ARG:NH1	2.45	0.45
11:J:403:ALA:HB3	11:J:404:PRO:HD3	1.98	0.45
8:LB:130:LEU:O	8:LB:162:ARG:NH1	2.46	0.45
12:k:172:PHE:O	12:k:207:ASN:ND2	2.44	0.45
12:n:361:SER:OG	12:n:362:ARG:N	2.49	0.45
5:A:390:VAL:O	5:A:394:TRP:N	2.48	0.45
5:C:160:MET:HE3	5:C:351:LEU:HD11	1.97	0.45
8:DB:232:THR:OG1	8:DB:300:MET:SD	2.61	0.45
1:F:272:GLU:N	1:F:272:GLU:OE1	2.50	0.45
7:GA:84:ARG:O	7:GA:84:ARG:NH1	2.45	0.45
8:HB:172:SER:OG	8:HB:205:GLU:OE1	2.33	0.45
10:I:497:ALA:HB3	10:I:502:ARG:HH21	1.81	0.45
1:3:29:ALA:HB1	3:5:67:ARG:HH11	1.80	0.45
1:B:763:LEU:HD11	1:B:771:LEU:HB3	1.98	0.45
8:BB:149:THR:HG23	8:BB:191:GLN:HG3	1.97	0.45
1:D:269:ASN:ND2	1:D:271:THR:OG1	2.48	0.45
7:EA:98:ASP:OD1	7:EA:100:ALA:N	2.44	0.45
12:i:174:ASN:OD1	12:i:390:ARG:NH2	2.46	0.45
12:i:212:ARG:O	12:i:215:THR:OG1	2.24	0.45
12:j:268:PHE:HE2	12:j:431:LEU:HD11	1.81	0.45
1:B:462:ASP:OD1	1:B:462:ASP:N	2.50	0.45
1:D:487:GLY:HA2	1:D:490:ILE:HG22	1.98	0.45
7:FA:211:ASP:OD2	7:FA:215:ARG:NH1	2.46	0.45
7:IA:254:ASP:OD2	12:i:101:GLY:N	2.50	0.45
12:h:269:LEU:HD13	12:h:379:ALA:O	2.17	0.45
5:E:581:ASP:OD1	5:E:581:ASP:N	2.47	0.45
7:IA:347:CYS:O	12:i:401:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:944:ARG:O	11:J:946:LYS:N	2.49	0.45
7:KA:180:ALA:HB3	7:KA:183:GLU:HG3	1.99	0.45
7:KA:244:PHE:O	7:KA:356:ASN:ND2	2.45	0.45
8:LB:191:GLN:OE1	8:LB:195:ASN:ND2	2.49	0.45
1:N:497:CYS:SG	1:N:552:LYS:NZ	2.90	0.45
12:f:34:GLU:OE1	12:f:34:GLU:N	2.46	0.45
5:C:594:THR:OG1	5:C:595:LYS:N	2.50	0.45
5:E:861:PHE:CE1	12:e:337:LEU:HD12	2.52	0.45
1:F:620:ARG:NH1	1:F:645:ASP:OD1	2.49	0.45
1:H:707:LEU:CD1	1:H:711:MET:HE1	2.47	0.45
8:JB:161:ASP:O	8:JB:251:ARG:NH2	2.48	0.45
5:M:819:GLU:OE2	5:M:823:ASN:ND2	2.50	0.45
12:a:236:MET:O	12:a:239:SER:OG	2.28	0.45
1:B:848:ARG:O	1:B:851:THR:OG1	2.31	0.45
1:D:573:PHE:HB2	1:D:608:THR:HG21	1.99	0.45
1:D:862:LEU:O	1:D:866:THR:OG1	2.33	0.45
8:EB:3:GLU:OE1	8:EB:3:GLU:N	2.47	0.45
5:G:399:ILE:HG23	5:G:461:ARG:NE	2.32	0.45
7:GA:326:LYS:O	12:g:222:ASN:HA	2.17	0.45
8:GB:27:GLU:OE2	8:GB:318:ARG:NH2	2.50	0.45
1:H:680:ILE:HD11	1:H:786:GLN:HG2	1.99	0.45
8:LB:67:ASP:OD1	8:LB:68:LEU:N	2.49	0.45
1:N:729:CYS:SG	1:N:730:SER:N	2.89	0.45
7:BA:319:TYR:CE2	7:BA:327:ASP:O	2.70	0.45
8:EB:27:GLU:OE1	8:EB:241:ARG:NH1	2.50	0.45
5:G:594:THR:O	5:G:596:GLN:N	2.50	0.45
8:JB:7:ILE:HG12	8:JB:64:ILE:HD12	1.99	0.45
10:K:157:VAL:HG23	10:K:172:LEU:HD12	1.98	0.45
12:c:57:ASP:OD1	12:c:57:ASP:N	2.49	0.45
12:c:426:GLU:OE1	12:c:430:GLN:NE2	2.50	0.45
12:l:388:PHE:HB2	12:l:432:ILE:HD11	1.98	0.45
12:m:270:MET:HE1	12:m:317:TYR:HE1	1.82	0.45
2:6:13:ALA:O	2:6:17:ASN:ND2	2.50	0.45
1:B:447:PHE:O	1:B:467:ARG:N	2.49	0.45
1:B:711:MET:HE1	1:B:854:TYR:CE1	2.52	0.45
7:BA:16:ILE:HD13	7:BA:171:ILE:HD12	1.99	0.45
1:D:889:ARG:H	1:D:893:LEU:HD11	1.80	0.45
7:DA:4:CYS:SG	7:DA:5:ILE:N	2.90	0.45
8:IB:65:LEU:HD22	8:IB:90:PHE:HE1	1.82	0.45
11:J:271:ILE:O	11:J:274:THR:OG1	2.28	0.45
10:K:114:ASP:OD1	10:K:114:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:241:THR:OG1	12:l:244:ARG:NH2	2.44	0.45
5:G:516:ILE:HD12	5:G:620:TYR:CD2	2.52	0.45
5:G:614:GLU:O	5:G:643:ARG:NH2	2.50	0.45
8:IB:252:LYS:O	8:IB:256:ASN:ND2	2.50	0.45
11:J:880:ILE:HG22	11:J:975:TRP:HE1	1.80	0.45
10:K:532:LEU:HD11	10:K:640:SER:HB3	1.98	0.45
12:l:402:GLU:OE1	12:l:402:GLU:N	2.50	0.45
7:DA:434:GLU:O	12:d:401:ARG:NH2	2.50	0.44
7:GA:261:PRO:HB2	12:g:404:PHE:CD1	2.52	0.44
10:I:26:GLN:OE1	10:I:26:GLN:N	2.47	0.44
7:KA:358:GLN:N	7:KA:358:GLN:OE1	2.50	0.44
5:M:84:LEU:HD13	9:MM:63:LEU:HD11	1.98	0.44
5:M:631:ASN:O	5:M:635:LEU:N	2.40	0.44
5:M:767:GLN:OE1	5:M:767:GLN:N	2.49	0.44
12:b:395:TYR:CE1	12:b:421:MET:HE2	2.52	0.44
12:f:124:ARG:NH2	12:f:125:GLU:OE2	2.49	0.44
7:EA:367:ASP:OD1	7:EA:367:ASP:N	2.50	0.44
1:F:446:PHE:O	1:F:467:ARG:NH1	2.50	0.44
5:G:518:ARG:NH1	5:G:567:ASP:OD2	2.50	0.44
6:MC:73:GLU:OE1	6:Mc:74:ASN:ND2	2.47	0.44
12:h:58:GLU:OE2	12:i:287:LYS:NZ	2.27	0.44
1:B:794:ARG:NH1	1:B:798:GLU:OE1	2.49	0.44
8:BB:11:GLN:N	8:BB:501:GDP:O2A	2.50	0.44
10:K:340:LEU:HD23	10:K:554:PHE:CG	2.52	0.44
12:c:54:GLN:NE2	12:c:58:GLU:OE1	2.51	0.44
12:i:260:LEU:O	12:i:380:ASN:ND2	2.49	0.44
12:n:201:CYS:SG	12:n:202:VAL:N	2.91	0.44
7:GA:260:VAL:N	7:GA:261:PRO:HD3	2.33	0.44
8:KB:234:SER:O	8:KB:238:THR:OG1	2.35	0.44
3:L:540:VAL:O	3:L:1495:HIS:NE2	2.50	0.44
5:M:518:ARG:HD3	5:M:564:ALA:HB1	1.99	0.44
12:e:324:ILE:HD12	12:e:328:VAL:HG11	1.99	0.44
12:h:260:LEU:HG	12:h:269:LEU:HD11	1.99	0.44
12:m:11:GLY:HA2	12:m:145:THR:HG22	1.98	0.44
1:3:93:ILE:HD12	2:4:28:LEU:HD21	1.99	0.44
7:BA:67:PHE:HB3	7:BA:75:ILE:HD13	2.00	0.44
8:BB:136:THR:HG23	8:BB:167:PHE:HB2	1.99	0.44
5:C:408:MET:HE2	5:C:408:MET:N	2.33	0.44
1:D:272:GLU:N	1:D:272:GLU:OE1	2.49	0.44
5:E:418:ARG:O	5:E:418:ARG:HG2	2.18	0.44
7:EA:402:ARG:NE	7:EA:415:GLU:OE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:710:GLU:OE1	1:F:886:TYR:OH	2.30	0.44
7:FA:260:VAL:O	7:FA:261:PRO:C	2.61	0.44
7:FA:435:VAL:O	12:f:401:ARG:NH1	2.50	0.44
8:JB:107:THR:OG1	8:JB:401:GLU:OE1	2.20	0.44
5:M:599:ALA:O	5:M:601:ALA:N	2.48	0.44
12:h:57:ASP:OD1	12:h:57:ASP:N	2.48	0.44
12:i:289:THR:OG1	12:i:290:VAL:N	2.44	0.44
5:A:450:ILE:HD11	5:A:488:ILE:HD12	2.00	0.44
5:G:214:GLU:OE2	5:G:320:SER:OG	2.29	0.44
7:IA:396:ASP:OD1	7:IA:422:ARG:NE	2.49	0.44
8:LB:164:MET:SD	8:LB:164:MET:N	2.88	0.44
12:b:395:TYR:HE1	12:b:421:MET:HE2	1.82	0.44
7:BA:161:TYR:CD2	7:BA:163:LYS:HE3	2.53	0.44
8:BB:102:ALA:HB3	8:BB:398:TYR:CD1	2.52	0.44
5:C:236:GLN:HB2	5:C:245:THR:HG23	1.98	0.44
5:EN:52:LYS:NZ	5:EN:90:GLU:OE1	2.50	0.44
1:F:578:MET:HE2	1:F:635:TRP:HZ3	1.83	0.44
5:G:188:ILE:HG22	5:G:278:GLU:HG2	2.00	0.44
7:IA:249:ASN:OD1	7:IA:258:ASN:ND2	2.50	0.44
12:c:90:ASN:OD1	12:c:90:ASN:N	2.49	0.44
7:BA:116:ASP:OD1	7:BA:156:ARG:NH2	2.51	0.44
1:H:564:ARG:NE	1:H:570:GLN:OE1	2.51	0.44
1:H:727:LEU:HD23	1:H:758:ILE:HD12	1.98	0.44
11:J:423:VAL:HG22	11:J:426:ASP:H	1.83	0.44
8:LB:172:SER:OG	8:LB:205:GLU:OE1	2.34	0.44
12:g:229:ASN:HA	12:g:232:VAL:HG22	2.00	0.44
12:h:206:ASP:OD1	12:h:208:THR:HG22	2.18	0.44
8:BB:290:THR:HG23	8:BB:333:ILE:HD11	1.98	0.44
7:EA:65:ALA:O	7:EA:91:GLN:NE2	2.45	0.44
7:HA:154:MET:HE3	7:HA:168:GLU:OE2	2.17	0.44
8:HB:52:ASN:OD1	8:HB:62:ARG:NH2	2.51	0.44
12:c:87:ASN:O	12:c:89:GLU:N	2.46	0.44
12:d:176:ASP:OD2	12:d:390:ARG:NH1	2.49	0.44
12:k:252:ASP:OD1	12:k:252:ASP:N	2.50	0.44
1:3:51:GLU:OE1	1:3:51:GLU:N	2.50	0.43
1:D:653:THR:HG1	1:D:656:CYS:HG	1.59	0.43
7:EA:47:ASP:OD1	7:EA:48:SER:N	2.48	0.43
1:F:311:ARG:NH1	1:F:314:ASP:OD2	2.51	0.43
7:FA:177:VAL:O	7:FA:179:THR:N	2.50	0.43
1:H:491:ASN:ND2	1:H:495:GLN:OE1	2.50	0.43
1:H:671:LYS:NZ	1:H:674:GLU:OE1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:IB:191:GLN:OE1	8:IB:195:ASN:ND2	2.49	0.43
7:JA:346:TRP:HB2	12:j:399:ARG:CB	2.48	0.43
5:M:118:THR:OG1	9:MM:31:LYS:N	2.51	0.43
12:k:154:LEU:HD23	12:k:194:ARG:HB3	2.00	0.43
1:B:662:ARG:NH2	1:B:762:CYS:SG	2.91	0.43
5:C:522:MET:HE2	5:C:645:MET:HB3	2.00	0.43
8:CB:290:THR:HG22	8:CB:333:ILE:HD12	2.00	0.43
7:EA:326:LYS:N	12:e:223:PRO:O	2.51	0.43
7:GA:34:GLY:O	7:GA:61:HIS:ND1	2.47	0.43
10:I:621:ARG:NH2	10:I:622:GLN:OE1	2.51	0.43
8:IB:116:VAL:HG11	8:IB:151:LEU:HD22	2.00	0.43
8:IB:295:ASP:OD1	8:IB:296:ALA:N	2.50	0.43
12:d:274:THR:HG21	12:d:293:VAL:HG22	2.00	0.43
12:f:68:ASP:HB2	12:f:74:ILE:HD11	1.99	0.43
12:g:297:LEU:HD13	12:g:377:MET:HB2	2.00	0.43
12:h:294:MET:SD	12:h:336:SER:OG	2.75	0.43
12:l:29:HIS:O	12:l:48:LYS:NZ	2.38	0.43
1:F:707:LEU:HD13	1:F:851:THR:HG22	2.01	0.43
7:JA:323:VAL:HG23	7:JA:355:ILE:HG23	2.00	0.43
12:c:440:ARG:NH1	12:c:442:ASP:OD1	2.50	0.43
12:k:318:ILE:HD11	12:k:382:THR:HG23	2.01	0.43
1:B:862:LEU:HD21	1:B:880:LEU:HB3	1.99	0.43
1:B:869:SER:OG	1:B:871:GLU:OE1	2.31	0.43
8:DB:8:GLN:NE2	8:DB:14:ASN:OD1	2.52	0.43
8:IB:311:LEU:N	8:IB:370:ASN:O	2.46	0.43
7:JA:382:THR:HG21	12:j:401:ARG:HE	1.83	0.43
7:LA:352:LYS:N	12:l:180:ASP:OD1	2.51	0.43
12:a:67:LEU:HD21	12:a:122:ILE:HD11	1.99	0.43
12:a:401:ARG:O	12:a:403:ALA:N	2.50	0.43
8:BB:166:THR:HB	8:BB:199:THR:HG23	1.99	0.43
8:BB:232:THR:HG22	8:BB:268:PRO:HB2	2.00	0.43
1:F:565:TYR:OH	1:F:613:ASP:OD2	2.29	0.43
7:HA:277:SER:OG	7:HA:279:GLU:OE1	2.34	0.43
11:J:757:PHE:O	11:J:761:GLN:NE2	2.51	0.43
10:K:589:LEU:HD11	10:K:619:PHE:HD1	1.82	0.43
12:a:231:LEU:O	12:a:234:THR:OG1	2.31	0.43
12:c:47:ARG:NH1	12:c:49:ASP:OD2	2.52	0.43
12:n:123:ASP:OD1	12:n:161:TYR:OH	2.34	0.43
1:D:433:TRP:NE1	1:D:483:VAL:O	2.52	0.43
1:N:622:ASP:OD2	1:N:643:HIS:NE2	2.51	0.43
12:c:325:GLN:N	12:c:325:GLN:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BB:347:ASN:O	8:BB:349:VAL:N	2.50	0.43
7:CA:216:ASN:N	7:CA:216:ASN:OD1	2.51	0.43
7:GA:160:ASP:OD1	7:GA:160:ASP:N	2.50	0.43
12:b:129:SER:O	12:c:339:ARG:NH2	2.52	0.43
12:f:120:ASP:OD1	12:g:295:ARG:NH2	2.49	0.43
12:g:382:THR:HG21	12:g:439:THR:HG22	2.00	0.43
12:i:112:GLU:O	12:i:115:HIS:ND1	2.50	0.43
12:k:303:VAL:HG12	12:k:305:VAL:H	1.82	0.43
12:l:50:VAL:HG11	12:l:244:ARG:HG2	1.99	0.43
4:7:238:LYS:O	4:7:251:GLY:N	2.52	0.43
5:C:526:ASP:OD2	5:C:563:THR:OG1	2.36	0.43
5:C:685:ARG:NH2	5:C:865:TYR:OH	2.52	0.43
5:E:437:GLN:OE1	5:EN:76:ARG:NH2	2.52	0.43
1:F:457:ASP:OD2	1:F:646:GLY:N	2.47	0.43
5:G:475:ILE:HD11	5:G:484:TYR:HD1	1.84	0.43
7:GA:325:PRO:CB	12:g:220:ILE:HG23	2.49	0.43
7:JA:55:GLU:OE1	7:JA:55:GLU:N	2.52	0.43
7:KA:93:ILE:HD11	7:KA:121:ARG:HD3	2.00	0.43
7:KA:190:THR:O	7:KA:194:THR:OG1	2.23	0.43
12:e:417:ASN:OD1	12:e:417:ASN:N	2.51	0.43
12:j:211:ASN:O	12:j:215:THR:OG1	2.36	0.43
5:A:578:MET:HE3	5:A:643:ARG:HH22	1.84	0.43
7:EA:56:THR:OG1	7:EA:60:LYS:O	2.22	0.43
7:EA:253:THR:O	7:EA:257:THR:OG1	2.37	0.43
8:FB:112:LEU:HB3	8:FB:147:MET:HE1	2.01	0.43
7:GA:358:GLN:N	7:GA:358:GLN:OE1	2.51	0.43
12:c:28:GLU:OE1	12:c:244:ARG:NH1	2.52	0.43
12:f:346:ALA:HB1	12:f:348:PHE:CE1	2.51	0.43
12:f:405:LEU:O	12:f:407:GLN:N	2.52	0.43
7:BA:319:TYR:CG	7:BA:327:ASP:HB3	2.54	0.43
1:H:462:ASP:N	1:H:462:ASP:OD1	2.49	0.43
8:KB:249:ASP:OD1	8:KB:249:ASP:N	2.51	0.43
12:f:303:VAL:HG12	12:f:305:VAL:H	1.84	0.43
7:BA:79:ARG:NH2	7:BA:94:THR:OG1	2.48	0.42
7:BA:328:VAL:HG13	12:b:224:SER:H	1.84	0.42
8:CB:245:GLN:O	8:CB:247:ASN:ND2	2.51	0.42
1:D:620:ARG:NH1	1:D:645:ASP:O	2.47	0.42
7:DA:7:ILE:HD11	7:DA:137:VAL:HG22	2.01	0.42
5:E:400:ILE:HD12	5:E:409:VAL:HG13	2.00	0.42
1:F:719:GLN:HA	1:F:722:ILE:HG22	2.00	0.42
7:FA:14:VAL:HG22	7:FA:67:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:GA:326:LYS:HD3	12:g:211:ASN:HA	2.01	0.42
8:GB:52:ASN:OD1	8:GB:62:ARG:NH2	2.50	0.42
5:M:17:LEU:HD13	9:MM:79:MET:HE2	2.01	0.42
12:b:126:ALA:HB1	12:b:161:TYR:HE2	1.84	0.42
7:IA:136:LEU:HD22	7:IA:169:PHE:HE2	1.84	0.42
7:JA:245:ASP:OD2	7:JA:358:GLN:NE2	2.52	0.42
8:JB:3:GLU:OE1	8:JB:3:GLU:N	2.50	0.42
12:j:252:ASP:OD1	12:j:252:ASP:N	2.49	0.42
8:CB:194:GLU:OE2	8:CB:414:ASN:ND2	2.49	0.42
1:D:734:LEU:HD22	1:D:754:PHE:CD2	2.54	0.42
7:FA:260:VAL:HG13	7:FA:266:HIS:HB3	2.01	0.42
7:GA:260:VAL:O	7:GA:261:PRO:C	2.62	0.42
7:JA:401:LYS:HE2	8:JB:428:ALA:HB1	2.02	0.42
8:JB:141:GLY:O	8:JB:145:SER:OG	2.35	0.42
7:KA:221:ARG:HE	8:KB:323:MET:HE2	1.84	0.42
7:KA:414:GLU:OE1	7:KA:414:GLU:N	2.49	0.42
3:L:540:VAL:HG13	3:L:541:TYR:H	1.85	0.42
12:k:172:PHE:CG	12:k:204:VAL:HG23	2.54	0.42
5:C:819:GLU:OE2	5:C:823:ASN:ND2	2.50	0.42
8:GB:170:VAL:HG11	8:GB:377:LEU:HD11	2.00	0.42
8:GB:343:GLU:OE1	8:GB:343:GLU:N	2.49	0.42
8:LB:33:SER:O	8:LB:58:LYS:NZ	2.52	0.42
12:f:323:ILE:HG22	12:f:359:ALA:HB3	2.01	0.42
12:h:168:THR:HG21	12:h:195:LEU:HD21	2.01	0.42
12:l:37:VAL:HG23	12:l:48:LYS:HE3	2.01	0.42
7:CA:98:ASP:OD1	7:CA:100:ALA:N	2.51	0.42
7:EA:286:LEU:O	7:EA:373:ARG:NH1	2.47	0.42
8:FB:290:THR:HG23	8:FB:317:PHE:HZ	1.84	0.42
7:GA:265:ILE:HG21	7:GA:313:MET:HE1	2.02	0.42
7:JA:396:ASP:OD1	7:JA:422:ARG:NE	2.53	0.42
8:JB:121:ARG:NE	8:JB:158:GLU:OE2	2.52	0.42
12:b:67:LEU:HD21	12:b:122:ILE:HD11	2.01	0.42
12:c:75:HIS:O	12:c:79:ASN:ND2	2.50	0.42
1:B:301:HIS:HA	1:B:304:ILE:HG22	2.01	0.42
7:BA:75:ILE:HD12	7:BA:94:THR:HG23	2.01	0.42
5:C:713:LEU:HD22	5:C:722:VAL:HG13	2.00	0.42
8:GB:49:VAL:O	8:GB:62:ARG:NH1	2.53	0.42
12:d:417:ASN:N	12:d:417:ASN:OD1	2.52	0.42
12:k:120:ASP:OD1	12:l:299:GLN:NE2	2.50	0.42
2:6:52:GLU:OE1	2:6:52:GLU:N	2.45	0.42
8:BB:389:PHE:CE1	8:BB:408:PHE:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:397:ARG:NH1	5:C:467:VAL:O	2.47	0.42
8:DB:73:MET:HE3	8:DB:77:ARG:HD2	2.01	0.42
8:EB:31:ASP:OD1	8:EB:35:ASN:N	2.49	0.42
5:G:657:SER:O	5:G:661:SER:OG	2.35	0.42
1:H:268:MET:HE1	1:H:299:TRP:HD1	1.84	0.42
10:K:385:THR:OG1	10:K:386:ALA:N	2.52	0.42
12:e:420:GLU:OE1	12:e:420:GLU:N	2.52	0.42
12:m:279:ASP:OD1	12:m:279:ASP:N	2.50	0.42
5:A:424:ASN:HD22	5:A:631:ASN:HB2	1.85	0.42
8:DB:334:GLN:O	8:DB:338:SER:OG	2.35	0.42
8:GB:192:LEU:O	8:GB:196:THR:OG1	2.37	0.42
7:KA:211:ASP:OD2	7:KA:304:LYS:NZ	2.44	0.42
12:j:436:HIS:O	12:j:439:THR:OG1	2.35	0.42
12:m:377:MET:SD	12:m:378:MET:N	2.92	0.42
7:BA:271:THR:HG23	7:BA:301:GLN:HA	2.02	0.42
1:D:499:ASP:OD2	1:D:544:TYR:OH	2.29	0.42
7:JA:256:GLN:O	7:JA:260:VAL:HG22	2.19	0.42
8:KB:181:GLU:OE2	8:KB:501:GDP:O3'	2.37	0.42
8:KB:375:GLN:HB2	8:KB:419:VAL:HG13	2.01	0.42
7:LA:323:VAL:HG23	7:LA:355:ILE:HG23	2.02	0.42
5:M:668:HIS:HB3	5:M:670:LEU:HD22	2.01	0.42
12:m:211:ASN:OD1	12:m:211:ASN:N	2.50	0.42
5:C:348:GLY:O	5:C:350:CYS:N	2.53	0.42
1:F:451:ASP:OD1	1:F:451:ASP:N	2.52	0.42
1:F:452:PRO:O	1:F:453:THR:OG1	2.26	0.42
6:GC:84:LEU:HD22	6:Gc:84:LEU:HB3	2.02	0.42
12:b:56:ASP:OD1	12:b:56:ASP:N	2.52	0.42
12:i:230:GLN:O	12:i:233:SER:OG	2.38	0.42
12:l:68:ASP:N	12:l:68:ASP:OD1	2.52	0.42
7:BA:156:ARG:O	7:BA:159:VAL:HG12	2.20	0.41
8:BB:337:ASN:O	8:BB:341:PHE:N	2.47	0.41
5:C:532:MET:HE3	5:C:653:ARG:HH21	1.85	0.41
8:CB:105:HIS:ND1	8:CB:146:GLY:O	2.46	0.41
8:EB:249:ASP:N	8:EB:249:ASP:OD1	2.51	0.41
5:G:623:LYS:O	5:G:627:SER:N	2.53	0.41
7:GA:14:VAL:HG22	7:GA:67:PHE:HD2	1.85	0.41
7:GA:323:VAL:HG12	12:g:223:PRO:HG3	2.01	0.41
1:H:707:LEU:O	1:H:711:MET:HE3	2.19	0.41
8:HB:382:SER:O	8:HB:386:THR:OG1	2.37	0.41
11:J:506:ASP:OD1	11:J:807:TRP:NE1	2.49	0.41
8:KB:152:ILE:HG23	8:KB:164:MET:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:e:419:ASP:OD1	12:e:420:GLU:N	2.53	0.41
12:f:114:ILE:O	12:f:114:ILE:HG22	2.20	0.41
12:g:216:ASP:OD2	12:g:217:ARG:NH2	2.51	0.41
12:j:53:TYR:N	12:j:61:ILE:O	2.52	0.41
12:l:235:ILE:HD13	12:l:304:MET:HE3	2.01	0.41
1:B:300:LEU:HD13	1:B:374:PRO:HB2	2.01	0.41
1:B:636:ASP:OD1	1:B:669:ARG:NH1	2.53	0.41
5:E:395:ILE:HD11	5:E:475:ILE:HD11	2.02	0.41
5:E:869:LEU:O	5:E:871:ARG:NH1	2.53	0.41
1:F:707:LEU:HD23	1:F:785:LEU:HD13	2.01	0.41
7:GA:254:ASP:OD1	12:g:102:ASN:N	2.53	0.41
1:H:565:TYR:OH	1:H:613:ASP:OD2	2.35	0.41
12:a:346:ALA:HB3	12:a:348:PHE:CD2	2.56	0.41
12:l:169:TYR:HB3	12:l:236:MET:HE2	2.02	0.41
12:m:202:VAL:O	12:m:269:LEU:N	2.52	0.41
8:BB:152:ILE:HG21	8:BB:191:GLN:HB3	2.03	0.41
8:BB:226:ASN:OD1	8:BB:226:ASN:N	2.52	0.41
8:BB:409:THR:HA	8:BB:412:GLU:HG2	2.02	0.41
5:C:416:LYS:HE3	5:C:418:ARG:HG2	2.02	0.41
5:E:414:LEU:HD13	5:E:427:TYR:HA	2.02	0.41
7:FA:27:GLU:HG3	7:FA:361:THR:HG22	2.03	0.41
8:FB:209:ASP:OD2	8:FB:213:ARG:NH1	2.46	0.41
5:G:221:LEU:HA	5:G:224:VAL:HG22	2.03	0.41
5:G:741:ASN:O	5:G:744:LEU:N	2.49	0.41
7:GA:120:ASP:OD1	7:GA:123:ARG:NH1	2.53	0.41
5:GN:42:THR:HG23	5:GN:80:PRO:HG3	2.01	0.41
12:f:268:PHE:HE2	12:f:431:LEU:HD11	1.85	0.41
12:g:216:ASP:OD1	12:g:216:ASP:N	2.54	0.41
12:j:137:LEU:HD13	12:j:166:VAL:HG13	2.02	0.41
7:DA:323:VAL:HG23	7:DA:355:ILE:HG23	2.02	0.41
8:EB:52:ASN:O	8:EB:60:VAL:N	2.50	0.41
5:M:282:SER:O	5:M:290:HIS:NE2	2.53	0.41
12:h:249:MET:SD	12:h:250:ASN:N	2.87	0.41
7:BA:187:SER:O	7:BA:191:THR:OG1	2.35	0.41
7:FA:167:LEU:HD22	7:FA:252:LEU:HD22	2.02	0.41
7:GA:93:ILE:HG22	7:GA:114:ILE:HD11	2.01	0.41
11:J:465:TRP:O	11:J:469:VAL:HG22	2.20	0.41
3:L:577:SER:O	3:L:579:GLU:N	2.54	0.41
12:a:65:VAL:HG21	12:a:125:GLU:HG3	2.03	0.41
12:c:417:ASN:N	12:c:417:ASN:OD1	2.53	0.41
12:f:330:PRO:HA	12:f:333:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:10:LEU:HD11	12:m:139:HIS:CD2	2.55	0.41
5:A:279:GLU:OE2	5:A:285:TYR:OH	2.23	0.41
7:BA:262:TYR:O	7:BA:265:ILE:HG22	2.20	0.41
5:C:285:TYR:O	5:C:289:ASN:ND2	2.48	0.41
1:F:440:GLU:O	1:F:442:THR:N	2.54	0.41
7:GA:348:PRO:HD3	12:g:398:LEU:HD13	2.02	0.41
1:H:446:PHE:O	1:H:467:ARG:NH1	2.53	0.41
10:I:156:THR:O	10:I:160:HIS:ND1	2.54	0.41
12:d:348:PHE:O	12:d:349:ILE:HD13	2.21	0.41
12:e:136:VAL:HG13	12:e:169:TYR:HE1	1.86	0.41
12:j:4:GLU:N	12:j:4:GLU:OE1	2.53	0.41
12:j:54:GLN:NE2	12:j:55:ALA:O	2.53	0.41
12:k:274:THR:OG1	12:k:297:LEU:HD22	2.21	0.41
5:E:731:ASP:OD2	6:EC:76:ASN:ND2	2.52	0.41
7:EA:166:LYS:N	7:EA:199:ASP:OD2	2.48	0.41
10:K:517:LEU:HD12	12:k:444:ILE:HG13	2.03	0.41
7:KA:90:GLU:O	7:KA:121:ARG:NE	2.53	0.41
12:c:4:GLU:O	12:c:133:GLU:N	2.52	0.41
12:f:50:VAL:HG13	12:f:51:PHE:HD1	1.86	0.41
12:f:412:ASP:OD1	12:f:412:ASP:N	2.53	0.41
12:l:201:CYS:SG	12:l:202:VAL:N	2.93	0.41
12:l:270:MET:HE2	12:l:303:VAL:HG11	2.01	0.41
7:BA:234:ILE:O	7:BA:234:ILE:CG2	2.68	0.41
8:BB:120:VAL:O	8:BB:159:TYR:OH	2.39	0.41
7:CA:49:PHE:O	7:CA:53:PHE:N	2.54	0.41
12:g:93:LEU:HD23	12:g:93:LEU:O	2.21	0.41
8:BB:211:CYS:O	8:BB:217:LEU:N	2.54	0.41
5:C:418:ARG:O	5:C:419:ILE:HG23	2.21	0.41
8:CB:99:ASN:O	8:CB:99:ASN:ND2	2.54	0.41
1:F:644:VAL:HG21	1:F:652:PHE:CD2	2.56	0.41
7:GA:348:PRO:CD	12:g:398:LEU:HD13	2.51	0.41
7:IA:216:ASN:OD1	7:IA:216:ASN:N	2.54	0.41
10:K:362:LEU:HD13	10:K:537:LEU:HD13	2.02	0.41
1:N:762:CYS:C	1:N:763:LEU:HD22	2.46	0.41
12:b:172:PHE:CD1	12:b:204:VAL:HG23	2.56	0.41
12:f:216:ASP:OD1	12:f:217:ARG:N	2.54	0.41
12:g:303:VAL:HG12	12:g:305:VAL:H	1.85	0.41
7:BA:161:TYR:CD1	7:BA:163:LYS:CG	3.04	0.41
9:EM:46:ALA:O	5:EN:57:SER:OG	2.34	0.41
1:F:287:LEU:O	1:F:290:THR:OG1	2.36	0.41
1:F:686:CYS:SG	1:F:687:ASN:N	2.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LB:121:ARG:NE	8:LB:158:GLU:OE2	2.51	0.41
8:LB:186:THR:HG22	8:LB:411:ALA:HB1	2.03	0.41
6:MC:59:ASN:O	6:MC:61:LYS:N	2.54	0.41
12:b:413:MET:SD	12:b:414:PHE:N	2.94	0.41
12:i:102:ASN:O	12:i:147:SER:OG	2.38	0.41
12:n:303:VAL:HG12	12:n:305:VAL:H	1.85	0.41
1:B:743:ASP:OD1	1:B:744:LEU:N	2.54	0.40
7:BA:278:ALA:HB1	7:BA:370:LYS:HG2	2.03	0.40
5:E:574:LYS:N	5:E:619:ASP:O	2.53	0.40
1:F:261:ILE:HD12	5:G:258:GLU:HB3	2.03	0.40
7:GA:188:ILE:HD13	7:GA:395:PHE:HB2	2.03	0.40
1:H:268:MET:HE1	1:H:299:TRP:CD1	2.55	0.40
7:HA:413:MET:HE2	7:HA:417:GLU:HB3	2.02	0.40
8:HB:404:ASP:OD1	8:HB:404:ASP:N	2.55	0.40
10:I:273:ALA:HA	10:I:276:ILE:HD12	2.03	0.40
5:M:418:ARG:HH12	5:M:621:ILE:HB	1.86	0.40
12:g:70:GLU:O	12:g:72:ARG:N	2.54	0.40
12:g:271:THR:OG1	12:g:272:GLY:N	2.54	0.40
7:BA:296:PHE:O	7:BA:312:TYR:OH	2.38	0.40
8:CB:321:MET:HE3	8:CB:353:VAL:HG13	2.03	0.40
7:EA:390:ARG:O	7:EA:394:LYS:NZ	2.52	0.40
8:EB:73:MET:HE2	8:EB:77:ARG:HE	1.86	0.40
8:EB:406:MET:SD	8:EB:407:GLU:N	2.94	0.40
5:G:271:SER:OG	5:G:275:ARG:NH2	2.54	0.40
1:H:320:VAL:HG12	1:H:396:LEU:HD23	2.03	0.40
8:BB:25:SER:HB3	8:BB:30:ILE:HB	2.03	0.40
1:F:304:ILE:HD12	1:F:381:LEU:HB3	2.03	0.40
7:GA:324:VAL:HG12	12:g:225:PHE:O	2.21	0.40
11:J:331:ILE:HD11	11:J:368:LEU:HB3	2.03	0.40
5:M:124:ALA:O	5:M:126:ALA:N	2.54	0.40
12:c:252:ASP:OD1	12:c:252:ASP:N	2.54	0.40
12:e:200:ASP:OD1	12:e:200:ASP:N	2.53	0.40
12:h:330:PRO:HA	12:h:333:VAL:HG12	2.03	0.40
7:BA:139:HIS:ND1	7:BA:140:SER:O	2.52	0.40
5:C:151:GLN:OE1	5:C:151:GLN:N	2.53	0.40
5:C:479:LEU:O	5:C:481:GLU:N	2.54	0.40
1:D:766:SER:OG	1:D:769:ARG:NH2	2.53	0.40
5:G:684:GLN:NE2	12:g:258:ALA:O	2.48	0.40
3:L:1753:SER:OG	3:L:1754:GLN:NE2	2.51	0.40
5:M:460:VAL:HG23	5:M:502:PHE:CE1	2.57	0.40
5:M:662:ASN:OD1	5:M:662:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:b:71:PRO:HB2	12:b:74:ILE:HG23	2.03	0.40
12:f:317:TYR:CG	12:f:320:ILE:HD11	2.57	0.40
12:i:185:PRO:HG2	12:i:398:LEU:HD22	2.03	0.40
1:B:726:VAL:HG22	1:B:761:ARG:HH11	1.86	0.40
1:D:259:GLN:NE2	5:E:322:GLN:OE1	2.55	0.40
10:K:305:ASP:OD1	10:K:306:THR:N	2.55	0.40
7:KA:25:CYS:O	7:KA:30:ILE:N	2.54	0.40
12:a:130:ASP:OD1	12:a:130:ASP:N	2.51	0.40
12:b:271:THR:OG1	12:b:272:GLY:N	2.53	0.40
12:j:268:PHE:CE2	12:j:431:LEU:HD11	2.56	0.40
12:m:212:ARG:NH2	12:m:301:LYS:O	2.52	0.40
12:m:262:PRO:HG3	12:m:318:ILE:HG21	2.03	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	3	100/907 (11%)	94 (94%)	6 (6%)	0	100	100
1	B	631/907 (70%)	585 (93%)	46 (7%)	0	100	100
1	D	602/907 (66%)	572 (95%)	29 (5%)	1 (0%)	43	71
1	F	571/907 (63%)	544 (95%)	25 (4%)	2 (0%)	30	60
1	H	571/907 (63%)	550 (96%)	20 (4%)	1 (0%)	43	71
1	N	631/907 (70%)	604 (96%)	26 (4%)	1 (0%)	43	71
2	4	58/82 (71%)	57 (98%)	1 (2%)	0	100	100
2	6	59/82 (72%)	59 (100%)	0	0	100	100
2	Y	54/82 (66%)	52 (96%)	2 (4%)	0	100	100
3	5	42/1819 (2%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	610/1819 (34%)	567 (93%)	43 (7%)	0	100	100
4	7	360/374 (96%)	357 (99%)	3 (1%)	0	100	100
5	A	693/902 (77%)	645 (93%)	42 (6%)	6 (1%)	14	45
5	C	693/902 (77%)	646 (93%)	44 (6%)	3 (0%)	30	60
5	CN	109/902 (12%)	103 (94%)	6 (6%)	0	100	100
5	E	644/902 (71%)	591 (92%)	52 (8%)	1 (0%)	43	71
5	EN	109/902 (12%)	104 (95%)	5 (5%)	0	100	100
5	G	644/902 (71%)	598 (93%)	44 (7%)	2 (0%)	36	65
5	GN	109/902 (12%)	103 (94%)	5 (5%)	1 (1%)	14	45
5	M	842/902 (93%)	793 (94%)	46 (6%)	3 (0%)	30	60
6	AC	33/229 (14%)	33 (100%)	0	0	100	100
6	CC	33/229 (14%)	33 (100%)	0	0	100	100
6	Cc	33/229 (14%)	32 (97%)	1 (3%)	0	100	100
6	EC	31/229 (14%)	30 (97%)	1 (3%)	0	100	100
6	Ec	27/229 (12%)	27 (100%)	0	0	100	100
6	GC	32/229 (14%)	32 (100%)	0	0	100	100
6	Gc	29/229 (13%)	29 (100%)	0	0	100	100
6	MC	30/229 (13%)	29 (97%)	0	1 (3%)	3	24
6	Mc	30/229 (13%)	30 (100%)	0	0	100	100
7	BA	434/451 (96%)	375 (86%)	54 (12%)	5 (1%)	10	39
7	CA	424/451 (94%)	408 (96%)	14 (3%)	2 (0%)	24	56
7	DA	424/451 (94%)	405 (96%)	18 (4%)	1 (0%)	43	71
7	EA	424/451 (94%)	408 (96%)	15 (4%)	1 (0%)	43	71
7	FA	424/451 (94%)	398 (94%)	23 (5%)	3 (1%)	18	50
7	GA	424/451 (94%)	401 (95%)	18 (4%)	5 (1%)	10	39
7	HA	424/451 (94%)	404 (95%)	19 (4%)	1 (0%)	43	71
7	IA	424/451 (94%)	408 (96%)	15 (4%)	1 (0%)	43	71
7	JA	424/451 (94%)	396 (93%)	25 (6%)	3 (1%)	18	50
7	KA	424/451 (94%)	412 (97%)	10 (2%)	2 (0%)	24	56
7	LA	424/451 (94%)	412 (97%)	12 (3%)	0	100	100
8	BB	421/451 (93%)	382 (91%)	36 (9%)	3 (1%)	18	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CB	421/451 (93%)	410 (97%)	11 (3%)	0	100	100
8	DB	421/451 (93%)	412 (98%)	9 (2%)	0	100	100
8	EB	421/451 (93%)	407 (97%)	14 (3%)	0	100	100
8	FB	421/451 (93%)	413 (98%)	8 (2%)	0	100	100
8	GB	421/451 (93%)	416 (99%)	5 (1%)	0	100	100
8	HB	421/451 (93%)	408 (97%)	13 (3%)	0	100	100
8	IB	421/451 (93%)	415 (99%)	6 (1%)	0	100	100
8	JB	421/451 (93%)	410 (97%)	11 (3%)	0	100	100
8	KB	421/451 (93%)	409 (97%)	12 (3%)	0	100	100
8	LB	421/451 (93%)	414 (98%)	7 (2%)	0	100	100
9	CM	52/158 (33%)	51 (98%)	1 (2%)	0	100	100
9	EM	52/158 (33%)	50 (96%)	2 (4%)	0	100	100
9	GM	51/158 (32%)	50 (98%)	1 (2%)	0	100	100
9	MM	51/158 (32%)	49 (96%)	2 (4%)	0	100	100
10	I	511/667 (77%)	480 (94%)	29 (6%)	2 (0%)	30	60
10	K	539/667 (81%)	518 (96%)	19 (4%)	2 (0%)	30	60
11	J	580/1024 (57%)	546 (94%)	30 (5%)	4 (1%)	18	50
11	Z	122/1024 (12%)	119 (98%)	3 (2%)	0	100	100
12	a	400/451 (89%)	359 (90%)	41 (10%)	0	100	100
12	b	400/451 (89%)	354 (88%)	46 (12%)	0	100	100
12	c	400/451 (89%)	380 (95%)	18 (4%)	2 (0%)	24	56
12	d	407/451 (90%)	380 (93%)	26 (6%)	1 (0%)	43	71
12	e	407/451 (90%)	376 (92%)	29 (7%)	2 (0%)	24	56
12	f	400/451 (89%)	380 (95%)	19 (5%)	1 (0%)	36	65
12	g	407/451 (90%)	374 (92%)	30 (7%)	3 (1%)	18	50
12	h	400/451 (89%)	374 (94%)	26 (6%)	0	100	100
12	i	407/451 (90%)	380 (93%)	25 (6%)	2 (0%)	24	56
12	j	407/451 (90%)	370 (91%)	36 (9%)	1 (0%)	43	71
12	k	400/451 (89%)	372 (93%)	27 (7%)	1 (0%)	36	65
12	l	407/451 (90%)	377 (93%)	29 (7%)	1 (0%)	43	71
12	m	400/451 (89%)	368 (92%)	30 (8%)	2 (0%)	24	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	n	400/451 (89%)	381 (95%)	19 (5%)	0	100	100
All	All	25315/39227 (64%)	23952 (95%)	1290 (5%)	73 (0%)	37	65

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	604	ASP
5	A	858	ARG
7	BA	52	PHE
7	BA	164	LYS
7	BA	177	VAL
7	BA	329	ASN
8	BB	410	GLU
5	C	604	ASP
7	CA	177	VAL
7	DA	177	VAL
7	FA	177	VAL
7	GA	327	ASP
7	GA	328	VAL
7	JA	245	ASP
7	JA	255	PHE
5	M	370	SER
12	e	222	ASN
12	g	223	PRO
12	i	222	ASN
12	j	183	VAL
5	A	523	ASP
5	A	595	LYS
7	BA	296	PHE
5	G	424	ASN
5	GN	13	LEU
10	I	385	THR
7	IA	259	LEU
11	J	491	GLU
10	K	639	ASN
5	M	462	GLU
12	c	87	ASN
12	c	226	SER
12	d	223	PRO
12	f	406	GLU
12	k	349	ILE
12	m	227	GLN

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Mol	Chain	Res	Type
5	A	197	ILE
5	A	462	GLU
8	BB	242	PHE
1	F	870	ASP
5	G	595	LYS
11	J	490	ARG
11	J	945	GLU
12	g	371	HIS
12	i	406	GLU
12	m	274	THR
7	CA	2	ARG
7	GA	2	ARG
7	GA	324	VAL
1	H	887	LYS
10	K	404	LEU
7	KA	2	ARG
5	M	602	HIS
1	N	762	CYS
1	D	644	VAL
5	E	595	LYS
1	F	871	GLU
7	FA	2	ARG
10	I	511	ASP
7	JA	346	TRP
5	C	595	LYS
5	C	599	ALA
7	HA	327	ASP
6	MC	60	MET
8	BB	13	GLY
12	e	223	PRO
7	GA	323	VAL
7	EA	260	VAL
7	FA	261	PRO
12	l	181	VAL
7	KA	177	VAL
12	g	222	ASN
11	J	795	ILE

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	91/798 (11%)	87 (96%)	4 (4%)	25	49
1	B	570/798 (71%)	539 (95%)	31 (5%)	20	46
1	D	548/798 (69%)	527 (96%)	21 (4%)	29	52
1	F	525/798 (66%)	502 (96%)	23 (4%)	25	49
1	H	525/798 (66%)	493 (94%)	32 (6%)	17	43
1	N	568/798 (71%)	545 (96%)	23 (4%)	28	52
2	4	51/62 (82%)	49 (96%)	2 (4%)	28	52
2	6	51/62 (82%)	50 (98%)	1 (2%)	48	64
2	Y	49/62 (79%)	38 (78%)	11 (22%)	1	6
3	5	40/1546 (3%)	38 (95%)	2 (5%)	22	47
3	L	539/1546 (35%)	521 (97%)	18 (3%)	33	55
4	7	18/317 (6%)	18 (100%)	0	100	100
5	A	618/791 (78%)	600 (97%)	18 (3%)	37	57
5	C	619/791 (78%)	598 (97%)	21 (3%)	32	54
5	CN	99/791 (12%)	95 (96%)	4 (4%)	28	52
5	E	585/791 (74%)	559 (96%)	26 (4%)	25	49
5	EN	99/791 (12%)	90 (91%)	9 (9%)	9	32
5	G	585/791 (74%)	564 (96%)	21 (4%)	31	54
5	GN	99/791 (12%)	95 (96%)	4 (4%)	28	52
5	M	744/791 (94%)	713 (96%)	31 (4%)	26	50
6	AC	34/207 (16%)	33 (97%)	1 (3%)	37	57
6	CC	34/207 (16%)	33 (97%)	1 (3%)	37	57
6	Cc	35/207 (17%)	35 (100%)	0	100	100
6	EC	33/207 (16%)	30 (91%)	3 (9%)	9	32
6	Ec	29/207 (14%)	27 (93%)	2 (7%)	14	41
6	GC	33/207 (16%)	31 (94%)	2 (6%)	17	43
6	Gc	31/207 (15%)	30 (97%)	1 (3%)	34	55
6	MC	32/207 (16%)	30 (94%)	2 (6%)	16	43
6	Mc	32/207 (16%)	30 (94%)	2 (6%)	16	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	BA	364/379 (96%)	328 (90%)	36 (10%)	7	30
7	CA	355/379 (94%)	347 (98%)	8 (2%)	44	62
7	DA	355/379 (94%)	342 (96%)	13 (4%)	30	53
7	EA	355/379 (94%)	346 (98%)	9 (2%)	42	60
7	FA	355/379 (94%)	346 (98%)	9 (2%)	42	60
7	GA	355/379 (94%)	339 (96%)	16 (4%)	24	49
7	HA	355/379 (94%)	350 (99%)	5 (1%)	59	70
7	IA	355/379 (94%)	342 (96%)	13 (4%)	30	53
7	JA	355/379 (94%)	344 (97%)	11 (3%)	35	56
7	KA	355/379 (94%)	349 (98%)	6 (2%)	53	67
7	LA	355/379 (94%)	344 (97%)	11 (3%)	35	56
8	BB	360/386 (93%)	325 (90%)	35 (10%)	8	30
8	CB	363/386 (94%)	352 (97%)	11 (3%)	36	57
8	DB	362/386 (94%)	350 (97%)	12 (3%)	33	55
8	EB	363/386 (94%)	355 (98%)	8 (2%)	45	62
8	FB	363/386 (94%)	353 (97%)	10 (3%)	38	58
8	GB	363/386 (94%)	353 (97%)	10 (3%)	38	58
8	HB	363/386 (94%)	356 (98%)	7 (2%)	50	65
8	IB	363/386 (94%)	354 (98%)	9 (2%)	42	60
8	JB	363/386 (94%)	359 (99%)	4 (1%)	65	72
8	KB	363/386 (94%)	357 (98%)	6 (2%)	53	67
8	LB	363/386 (94%)	361 (99%)	2 (1%)	78	79
9	CM	44/118 (37%)	42 (96%)	2 (4%)	24	49
9	EM	44/118 (37%)	43 (98%)	1 (2%)	44	62
9	GM	43/118 (36%)	42 (98%)	1 (2%)	44	62
9	MM	43/118 (36%)	41 (95%)	2 (5%)	23	48
10	I	471/594 (79%)	449 (95%)	22 (5%)	23	48
10	K	499/594 (84%)	485 (97%)	14 (3%)	38	58
11	J	523/933 (56%)	507 (97%)	16 (3%)	35	56
11	Z	111/933 (12%)	109 (98%)	2 (2%)	51	66
12	a	369/400 (92%)	348 (94%)	21 (6%)	18	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	b	369/400 (92%)	350 (95%)	19 (5%)	21	47
12	c	369/400 (92%)	353 (96%)	16 (4%)	26	50
12	d	376/400 (94%)	360 (96%)	16 (4%)	26	50
12	e	375/400 (94%)	352 (94%)	23 (6%)	17	43
12	f	369/400 (92%)	354 (96%)	15 (4%)	27	51
12	g	373/400 (93%)	347 (93%)	26 (7%)	14	41
12	h	368/400 (92%)	347 (94%)	21 (6%)	18	45
12	i	376/400 (94%)	364 (97%)	12 (3%)	34	55
12	j	375/400 (94%)	352 (94%)	23 (6%)	17	43
12	k	368/400 (92%)	357 (97%)	11 (3%)	36	57
12	l	375/400 (94%)	367 (98%)	8 (2%)	47	63
12	m	369/400 (92%)	355 (96%)	14 (4%)	29	52
12	n	369/400 (92%)	354 (96%)	15 (4%)	27	51
All	All	22197/34115 (65%)	21330 (96%)	867 (4%)	30	52

All (867) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	28	VAL
1	3	51	GLU
1	3	86	VAL
1	3	87	LEU
2	4	26	ASP
2	4	68	ARG
3	5	67	ARG
3	5	106	GLU
2	6	28	LEU
5	A	169	ASN
5	A	218	VAL
5	A	226	VAL
5	A	252	LEU
5	A	296	MET
5	A	426	LYS
5	A	478	THR
5	A	563	THR
5	A	600	MET
5	A	674	GLN

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Mol	Chain	Res	Type
5	A	686	MET
5	A	690	VAL
5	A	698	MET
5	A	699	PHE
5	A	702	MET
5	A	734	LEU
5	A	739	LEU
5	A	745	LEU
6	AC	67	ILE
1	B	296	GLU
1	B	325	CYS
1	B	331	GLU
1	B	335	TYR
1	B	346	LEU
1	B	354	VAL
1	B	363	THR
1	B	368	LEU
1	B	373	ASP
1	B	378	LEU
1	B	384	LEU
1	B	400	VAL
1	B	411	MET
1	B	418	ILE
1	B	439	LEU
1	B	454	VAL
1	B	459	LEU
1	B	490	ILE
1	B	492	PHE
1	B	493	LEU
1	B	496	VAL
1	B	526	LEU
1	B	558	HIS
1	B	576	HIS
1	B	577	LEU
1	B	622	ASP
1	B	642	TYR
1	B	659	HIS
1	B	772	LEU
1	B	819	TRP
1	B	843	MET
7	BA	11	GLN
7	BA	18	ASN

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Mol	Chain	Res	Type
7	BA	71	GLU
7	BA	93	ILE
7	BA	94	THR
7	BA	105	ARG
7	BA	123	ARG
7	BA	169	PHE
7	BA	200	CYS
7	BA	226	ASN
7	BA	230	LEU
7	BA	237	SER
7	BA	242	LEU
7	BA	243	ARG
7	BA	252	LEU
7	BA	264	ARG
7	BA	266	HIS
7	BA	275	VAL
7	BA	283	HIS
7	BA	292	THR
7	BA	313	MET
7	BA	316	CYS
7	BA	318	LEU
7	BA	334	THR
7	BA	336	LYS
7	BA	341	ILE
7	BA	344	VAL
7	BA	355	ILE
7	BA	368	LEU
7	BA	378	LEU
7	BA	379	SER
7	BA	392	ASP
7	BA	398	MET
7	BA	404	PHE
7	BA	415	GLU
7	BA	437	VAL
8	BB	5	VAL
8	BB	12	CYS
8	BB	23	VAL
8	BB	37	VAL
8	BB	45	GLU
8	BB	64	ILE
8	BB	72	THR
8	BB	91	ILE

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Mol	Chain	Res	Type
8	BB	113	VAL
8	BB	128	ASP
8	BB	133	PHE
8	BB	136	THR
8	BB	155	VAL
8	BB	157	GLU
8	BB	169	VAL
8	BB	177	ASP
8	BB	196	THR
8	BB	199	THR
8	BB	219	THR
8	BB	226	ASN
8	BB	236	VAL
8	BB	246	LEU
8	BB	251	ARG
8	BB	255	VAL
8	BB	264	HIS
8	BB	285	THR
8	BB	316	VAL
8	BB	333	ILE
8	BB	342	VAL
8	BB	343	GLU
8	BB	351	VAL
8	BB	377	LEU
8	BB	384	GLN
8	BB	399	THR
8	BB	429	THR
5	C	217	VAL
5	C	222	LEU
5	C	248	VAL
5	C	259	LEU
5	C	264	LEU
5	C	296	MET
5	C	332	MET
5	C	400	ILE
5	C	404	TYR
5	C	409	VAL
5	C	453	THR
5	C	467	VAL
5	C	551	LEU
5	C	563	THR
5	C	584	THR

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Mol	Chain	Res	Type
5	C	622	VAL
5	C	624	TRP
5	C	635	LEU
5	C	730	LEU
5	C	738	MET
5	C	856	ILE
7	CA	7	ILE
7	CA	177	VAL
7	CA	179	THR
7	CA	216	ASN
7	CA	277	SER
7	CA	285	GLN
7	CA	319	TYR
7	CA	375	VAL
8	CB	24	ILE
8	CB	37	VAL
8	CB	44	LEU
8	CB	72	THR
8	CB	108	GLU
8	CB	152	ILE
8	CB	219	THR
8	CB	285	THR
8	CB	290	THR
8	CB	312	THR
8	CB	386	THR
6	CC	87	ARG
9	CM	37	GLU
9	CM	75	MET
5	CN	13	LEU
5	CN	37	THR
5	CN	59	THR
5	CN	88	LEU
1	D	319	LEU
1	D	325	CYS
1	D	329	HIS
1	D	384	LEU
1	D	436	ASP
1	D	439	LEU
1	D	445	GLU
1	D	486	ILE
1	D	489	SER
1	D	493	LEU

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Mol	Chain	Res	Type
1	D	530	PHE
1	D	541	THR
1	D	644	VAL
1	D	727	LEU
1	D	805	GLN
1	D	807	GLU
1	D	832	ARG
1	D	847	LEU
1	D	859	GLN
1	D	866	THR
1	D	867	THR
7	DA	5	ILE
7	DA	20	CYS
7	DA	85	GLN
7	DA	141	PHE
7	DA	194	THR
7	DA	244	PHE
7	DA	245	ASP
7	DA	251	ASP
7	DA	253	THR
7	DA	257	THR
7	DA	259	LEU
7	DA	349	THR
7	DA	391	LEU
8	DB	37	VAL
8	DB	58	LYS
8	DB	66	VAL
8	DB	72	THR
8	DB	84	LEU
8	DB	157	GLU
8	DB	188	SER
8	DB	246	LEU
8	DB	330	MET
8	DB	333	ILE
8	DB	356	ILE
8	DB	366	THR
5	E	166	ASN
5	E	296	MET
5	E	328	ILE
5	E	341	LEU
5	E	345	VAL
5	E	399	ILE

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Mol	Chain	Res	Type
5	E	400	ILE
5	E	410	GLU
5	E	453	THR
5	E	460	VAL
5	E	480	LYS
5	E	518	ARG
5	E	526	ASP
5	E	529	VAL
5	E	537	GLU
5	E	544	GLU
5	E	563	THR
5	E	573	LEU
5	E	590	LEU
5	E	613	LEU
5	E	630	ILE
5	E	645	MET
5	E	713	LEU
5	E	734	LEU
5	E	741	ASN
5	E	757	MET
7	EA	26	LEU
7	EA	71	GLU
7	EA	155	GLU
7	EA	194	THR
7	EA	253	THR
7	EA	257	THR
7	EA	269	LEU
7	EA	344	VAL
7	EA	362	VAL
8	EB	37	VAL
8	EB	84	LEU
8	EB	106	TYR
8	EB	219	THR
8	EB	293	MET
8	EB	315	THR
8	EB	365	SER
8	EB	368	ILE
6	EC	60	MET
6	EC	62	ASP
6	EC	81	ILE
9	EM	51	ILE
5	EN	1	MET

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Mol	Chain	Res	Type
5	EN	13	LEU
5	EN	17	LEU
5	EN	27	VAL
5	EN	29	ILE
5	EN	37	THR
5	EN	52	LYS
5	EN	59	THR
5	EN	93	GLU
6	Ec	73	GLU
6	Ec	78	LYS
1	F	254	ILE
1	F	261	ILE
1	F	266	ILE
1	F	287	LEU
1	F	319	LEU
1	F	325	CYS
1	F	367	LEU
1	F	392	LYS
1	F	404	THR
1	F	438	GLU
1	F	483	VAL
1	F	485	LEU
1	F	497	CYS
1	F	553	TYR
1	F	559	MET
1	F	686	CYS
1	F	712	VAL
1	F	728	GLU
1	F	734	LEU
1	F	774	GLN
1	F	790	ASP
1	F	875	PHE
1	F	883	ASN
7	FA	26	LEU
7	FA	66	VAL
7	FA	77	GLU
7	FA	194	THR
7	FA	253	THR
7	FA	261	PRO
7	FA	328	VAL
7	FA	329	ASN
7	FA	355	ILE

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Mol	Chain	Res	Type
8	FB	7	ILE
8	FB	37	VAL
8	FB	65	LEU
8	FB	84	LEU
8	FB	147	MET
8	FB	312	THR
8	FB	321	MET
8	FB	351	VAL
8	FB	359	ARG
8	FB	415	MET
5	G	159	LYS
5	G	233	VAL
5	G	273	VAL
5	G	321	LEU
5	G	355	THR
5	G	414	LEU
5	G	433	THR
5	G	462	GLU
5	G	512	HIS
5	G	530	HIS
5	G	557	LEU
5	G	563	THR
5	G	572	ASP
5	G	585	GLN
5	G	654	GLN
5	G	658	VAL
5	G	663	LYS
5	G	709	LEU
5	G	733	CYS
5	G	744	LEU
5	G	765	PHE
7	GA	71	GLU
7	GA	160	ASP
7	GA	188	ILE
7	GA	194	THR
7	GA	204	VAL
7	GA	253	THR
7	GA	280	LYS
7	GA	285	GLN
7	GA	288	VAL
7	GA	318	LEU
7	GA	319	TYR

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Mol	Chain	Res	Type
7	GA	323	VAL
7	GA	355	ILE
7	GA	375	VAL
7	GA	377	MET
7	GA	425	MET
8	GB	24	ILE
8	GB	37	VAL
8	GB	72	THR
8	GB	147	MET
8	GB	155	VAL
8	GB	267	MET
8	GB	273	LEU
8	GB	290	THR
8	GB	312	THR
8	GB	386	THR
6	GC	72	LYS
6	GC	84	LEU
9	GM	63	LEU
5	GN	42	THR
5	GN	43	THR
5	GN	59	THR
5	GN	81	LEU
6	Gc	73	GLU
1	H	277	VAL
1	H	287	LEU
1	H	289	ASP
1	H	296	GLU
1	H	313	LEU
1	H	332	LEU
1	H	342	LEU
1	H	366	ARG
1	H	411	MET
1	H	426	VAL
1	H	480	SER
1	H	485	LEU
1	H	493	LEU
1	H	553	TYR
1	H	554	SER
1	H	567	LEU
1	H	577	LEU
1	H	605	VAL
1	H	612	PHE

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Mol	Chain	Res	Type
1	H	657	MET
1	H	677	LEU
1	H	704	CYS
1	H	711	MET
1	H	713	HIS
1	H	744	LEU
1	H	782	ILE
1	H	800	LEU
1	H	835	GLU
1	H	840	ILE
1	H	862	LEU
1	H	863	VAL
1	H	877	SER
7	HA	253	THR
7	HA	283	HIS
7	HA	318	LEU
7	HA	377	MET
7	HA	425	MET
8	HB	44	LEU
8	HB	60	VAL
8	HB	152	ILE
8	HB	183	TYR
8	HB	290	THR
8	HB	349	VAL
8	HB	386	THR
10	I	38	GLU
10	I	96	VAL
10	I	132	LEU
10	I	153	ILE
10	I	176	LEU
10	I	187	LEU
10	I	272	VAL
10	I	299	ILE
10	I	370	GLN
10	I	388	THR
10	I	403	VAL
10	I	408	ASP
10	I	413	LEU
10	I	455	LEU
10	I	459	VAL
10	I	461	TRP
10	I	519	ASN

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Mol	Chain	Res	Type
10	I	535	ASP
10	I	568	LEU
10	I	575	LEU
10	I	587	LEU
10	I	604	LEU
7	IA	71	GLU
7	IA	167	LEU
7	IA	194	THR
7	IA	250	VAL
7	IA	253	THR
7	IA	257	THR
7	IA	295	CYS
7	IA	324	VAL
7	IA	327	ASP
7	IA	361	THR
7	IA	382	THR
7	IA	398	MET
7	IA	435	VAL
8	IB	37	VAL
8	IB	44	LEU
8	IB	84	LEU
8	IB	112	LEU
8	IB	152	ILE
8	IB	217	LEU
8	IB	293	MET
8	IB	334	GLN
8	IB	386	THR
11	J	258	VAL
11	J	263	VAL
11	J	409	LEU
11	J	423	VAL
11	J	450	VAL
11	J	473	LEU
11	J	495	GLN
11	J	682	THR
11	J	717	VAL
11	J	734	THR
11	J	803	TYR
11	J	821	TYR
11	J	826	LEU
11	J	947	VAL
11	J	995	VAL

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Mol	Chain	Res	Type
11	J	998	LEU
7	JA	71	GLU
7	JA	75	ILE
7	JA	253	THR
7	JA	255	PHE
7	JA	315	CYS
7	JA	323	VAL
7	JA	324	VAL
7	JA	332	ILE
7	JA	347	CYS
7	JA	349	THR
7	JA	388	TRP
8	JB	60	VAL
8	JB	66	VAL
8	JB	304	ASP
8	JB	386	THR
10	K	5	LEU
10	K	112	LEU
10	K	127	ASP
10	K	153	ILE
10	K	192	LEU
10	K	263	ILE
10	K	279	VAL
10	K	312	HIS
10	K	410	LEU
10	K	455	LEU
10	K	468	THR
10	K	563	HIS
10	K	569	LEU
10	K	612	LEU
7	KA	52	PHE
7	KA	71	GLU
7	KA	75	ILE
7	KA	188	ILE
7	KA	253	THR
7	KA	335	ILE
8	KB	37	VAL
8	KB	84	LEU
8	KB	178	THR
8	KB	207	LEU
8	KB	257	MET
8	KB	415	MET

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Mol	Chain	Res	Type
3	L	359	VAL
3	L	369	SER
3	L	378	VAL
3	L	418	VAL
3	L	573	TYR
3	L	1548	THR
3	L	1551	GLU
3	L	1557	VAL
3	L	1587	LEU
3	L	1589	GLU
3	L	1598	VAL
3	L	1599	LEU
3	L	1608	VAL
3	L	1617	THR
3	L	1661	VAL
3	L	1666	LEU
3	L	1740	ILE
3	L	1807	LEU
7	LA	4	CYS
7	LA	71	GLU
7	LA	192	HIS
7	LA	194	THR
7	LA	253	THR
7	LA	271	THR
7	LA	324	VAL
7	LA	351	PHE
7	LA	353	VAL
7	LA	362	VAL
7	LA	376	CYS
8	LB	121	ARG
8	LB	292	GLN
5	M	5	ARG
5	M	18	ARG
5	M	78	LEU
5	M	90	GLU
5	M	92	LYS
5	M	113	VAL
5	M	129	ILE
5	M	151	GLN
5	M	152	GLN
5	M	181	VAL
5	M	220	ASP

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Mol	Chain	Res	Type
5	M	226	VAL
5	M	245	THR
5	M	259	LEU
5	M	328	ILE
5	M	337	ILE
5	M	371	GLN
5	M	418	ARG
5	M	428	TRP
5	M	442	PHE
5	M	536	GLU
5	M	547	THR
5	M	659	TRP
5	M	666	LYS
5	M	689	PHE
5	M	700	GLU
5	M	713	LEU
5	M	746	LYS
5	M	811	THR
5	M	818	PHE
5	M	857	SER
6	MC	72	LYS
6	MC	84	LEU
9	MM	60	VAL
9	MM	65	LEU
6	Mc	60	MET
6	Mc	71	LYS
1	N	254	ILE
1	N	268	MET
1	N	459	LEU
1	N	490	ILE
1	N	497	CYS
1	N	524	THR
1	N	526	LEU
1	N	530	PHE
1	N	549	LEU
1	N	562	MET
1	N	566	LEU
1	N	591	THR
1	N	598	THR
1	N	603	THR
1	N	617	ILE
1	N	622	ASP

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Mol	Chain	Res	Type
1	N	627	GLU
1	N	656	CYS
1	N	673	MET
1	N	721	TYR
1	N	722	ILE
1	N	819	TRP
1	N	857	ILE
2	Y	23	GLU
2	Y	25	MET
2	Y	27	VAL
2	Y	28	LEU
2	Y	29	LEU
2	Y	31	ILE
2	Y	32	SER
2	Y	43	THR
2	Y	44	LEU
2	Y	46	ILE
2	Y	58	GLU
11	Z	84	TRP
11	Z	110	ILE
12	a	25	LEU
12	a	77	ILE
12	a	87	ASN
12	a	103	ASN
12	a	130	ASP
12	a	166	VAL
12	a	204	VAL
12	a	208	THR
12	a	248	TYR
12	a	257	ILE
12	a	263	THR
12	a	267	HIS
12	a	276	LEU
12	a	288	THR
12	a	316	CYS
12	a	327	GLU
12	a	328	VAL
12	a	376	LEU
12	a	406	GLU
12	a	419	ASP
12	a	435	TYR
12	b	25	LEU

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Mol	Chain	Res	Type
12	b	77	ILE
12	b	87	ASN
12	b	103	ASN
12	b	130	ASP
12	b	166	VAL
12	b	204	VAL
12	b	208	THR
12	b	257	ILE
12	b	263	THR
12	b	267	HIS
12	b	276	LEU
12	b	288	THR
12	b	316	CYS
12	b	327	GLU
12	b	328	VAL
12	b	406	GLU
12	b	419	ASP
12	b	435	TYR
12	c	9	GLN
12	c	10	LEU
12	c	13	CYS
12	c	67	LEU
12	c	90	ASN
12	c	103	ASN
12	c	120	ASP
12	c	139	HIS
12	c	183	VAL
12	c	236	MET
12	c	276	LEU
12	c	322	ASN
12	c	382	THR
12	c	392	CYS
12	c	398	LEU
12	c	405	LEU
12	d	78	LEU
12	d	93	LEU
12	d	120	ASP
12	d	171	VAL
12	d	183	VAL
12	d	192	LEU
12	d	195	LEU
12	d	205	LEU

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Mol	Chain	Res	Type
12	d	222	ASN
12	d	243	LEU
12	d	263	THR
12	d	271	THR
12	d	316	CYS
12	d	376	LEU
12	d	398	LEU
12	d	402	GLU
12	e	5	ILE
12	e	20	GLU
12	e	25	LEU
12	e	66	LEU
12	e	67	LEU
12	e	120	ASP
12	e	137	LEU
12	e	154	LEU
12	e	171	VAL
12	e	190	LEU
12	e	200	ASP
12	e	212	ARG
12	e	220	ILE
12	e	223	PRO
12	e	263	THR
12	e	267	HIS
12	e	322	ASN
12	e	328	VAL
12	e	337	LEU
12	e	374	SER
12	e	378	MET
12	e	382	THR
12	e	392	CYS
12	f	46	ASP
12	f	67	LEU
12	f	93	LEU
12	f	166	VAL
12	f	171	VAL
12	f	189	LEU
12	f	190	LEU
12	f	260	LEU
12	f	266	LEU
12	f	269	LEU
12	f	321	LEU

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Mol	Chain	Res	Type
12	f	323	ILE
12	f	328	VAL
12	f	376	LEU
12	f	378	MET
12	g	10	LEU
12	g	13	CYS
12	g	25	LEU
12	g	37	VAL
12	g	56	ASP
12	g	65	VAL
12	g	67	LEU
12	g	78	LEU
12	g	133	GLU
12	g	154	LEU
12	g	168	THR
12	g	171	VAL
12	g	190	LEU
12	g	216	ASP
12	g	217	ARG
12	g	221	GLN
12	g	222	ASN
12	g	226	SER
12	g	260	LEU
12	g	263	THR
12	g	277	THR
12	g	304	MET
12	g	323	ILE
12	g	325	GLN
12	g	328	VAL
12	g	349	ILE
12	h	9	GLN
12	h	10	LEU
12	h	28	GLU
12	h	34	GLU
12	h	91	ILE
12	h	119	PHE
12	h	165	LEU
12	h	204	VAL
12	h	228	ILE
12	h	230	GLN
12	h	241	THR
12	h	248	TYR

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Mol	Chain	Res	Type
12	h	266	LEU
12	h	290	VAL
12	h	298	LEU
12	h	323	ILE
12	h	327	GLU
12	h	328	VAL
12	h	342	GLU
12	h	367	LEU
12	h	396	ASP
12	i	6	ILE
12	i	7	THR
12	i	37	VAL
12	i	171	VAL
12	i	204	VAL
12	i	218	LEU
12	i	254	ILE
12	i	271	THR
12	i	274	THR
12	i	304	MET
12	i	337	LEU
12	i	442	ASP
12	j	10	LEU
12	j	26	CYS
12	j	51	PHE
12	j	70	GLU
12	j	149	LEU
12	j	154	LEU
12	j	183	VAL
12	j	186	TYR
12	j	192	LEU
12	j	204	VAL
12	j	215	THR
12	j	240	THR
12	j	253	LEU
12	j	256	LEU
12	j	267	HIS
12	j	327	GLU
12	j	337	LEU
12	j	348	PHE
12	j	382	THR
12	j	405	LEU
12	j	407	GLN

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Mol	Chain	Res	Type
12	j	411	GLU
12	j	439	THR
12	k	78	LEU
12	k	136	VAL
12	k	171	VAL
12	k	189	LEU
12	k	196	THR
12	k	208	THR
12	k	230	GLN
12	k	271	THR
12	k	293	VAL
12	k	305	VAL
12	k	398	LEU
12	l	10	LEU
12	l	74	ILE
12	l	121	ILE
12	l	171	VAL
12	l	331	THR
12	l	358	VAL
12	l	382	THR
12	l	398	LEU
12	m	7	THR
12	m	65	VAL
12	m	145	THR
12	m	166	VAL
12	m	168	THR
12	m	192	LEU
12	m	249	MET
12	m	291	LEU
12	m	339	ARG
12	m	341	ARG
12	m	349	ILE
12	m	404	PHE
12	m	430	GLN
12	m	435	TYR
12	n	26	CYS
12	n	45	THR
12	n	69	LEU
12	n	84	LYS
12	n	165	LEU
12	n	202	VAL
12	n	215	THR

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Mol	Chain	Res	Type
12	n	252	ASP
12	n	267	HIS
12	n	316	CYS
12	n	328	VAL
12	n	373	VAL
12	n	376	LEU
12	n	381	HIS
12	n	427	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (190) such sidechains are listed below:

Mol	Chain	Res	Type
2	4	19	ASN
5	A	684	GLN
5	A	725	HIS
6	AC	59	ASN
6	AC	65	ASN
1	B	329	HIS
1	B	461	HIS
1	B	560	GLN
1	B	595	HIS
1	B	596	ASN
1	B	702	HIS
1	B	719	GLN
1	B	774	GLN
1	B	781	GLN
1	B	860	GLN
7	BA	18	ASN
7	BA	133	GLN
7	BA	206	ASN
8	BB	137	HIS
8	BB	204	ASN
8	BB	347	ASN
8	BB	396	HIS
5	C	251	ASN
5	C	261	HIS
5	C	424	ASN
5	C	862	ASN
7	CA	31	GLN
7	CA	283	HIS
7	CA	329	ASN
8	CB	190	HIS

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Mol	Chain	Res	Type
8	CB	298	ASN
6	Cc	59	ASN
1	D	424	HIS
1	D	461	HIS
1	D	491	ASN
7	DA	176	GLN
7	DA	216	ASN
7	DA	258	ASN
8	DB	83	HIS
5	E	401	HIS
5	E	524	GLN
5	E	688	ASN
5	E	725	HIS
7	EA	192	HIS
7	EA	233	GLN
8	EB	8	GLN
8	EB	195	ASN
8	EB	329	GLN
6	Ec	66	GLN
1	F	570	GLN
1	F	687	ASN
1	F	740	GLN
7	FA	216	ASN
7	FA	283	HIS
8	FB	43	GLN
8	FB	291	GLN
8	FB	347	ASN
5	G	166	ASN
5	G	493	ASN
5	G	644	HIS
7	GA	18	ASN
8	GB	89	ASN
8	GB	134	GLN
8	GB	307	HIS
8	GB	334	GLN
8	GB	375	GLN
8	GB	426	GLN
9	GM	74	GLN
5	GN	20	HIS
5	GN	77	ASN
5	GN	99	GLN
1	H	387	HIS

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Mol	Chain	Res	Type
1	H	416	GLN
1	H	558	HIS
1	H	855	GLN
7	HA	35	GLN
7	HA	216	ASN
8	HB	6	HIS
8	HB	15	GLN
8	HB	89	ASN
8	HB	190	HIS
8	HB	347	ASN
10	I	61	GLN
10	I	123	ASN
10	I	152	GLN
10	I	186	GLN
10	I	397	GLN
10	I	499	GLN
10	I	529	GLN
7	IA	11	GLN
7	IA	35	GLN
7	IA	249	ASN
7	IA	256	GLN
7	IA	258	ASN
7	IA	329	ASN
8	IB	89	ASN
11	J	438	ASN
11	J	753	GLN
11	J	759	ASN
11	J	763	GLN
11	J	892	HIS
11	J	899	ASN
11	J	930	HIS
7	JA	226	ASN
7	JA	233	GLN
8	JB	43	GLN
10	K	193	HIS
10	K	312	HIS
10	K	415	HIS
10	K	499	GLN
10	K	600	ASN
10	K	622	GLN
7	KA	101	ASN
7	KA	216	ASN

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Mol	Chain	Res	Type
8	KB	14	ASN
8	KB	43	GLN
8	KB	375	GLN
3	L	430	GLN
3	L	593	HIS
3	L	1547	GLN
3	L	1686	ASN
3	L	1754	GLN
7	LA	18	ASN
7	LA	61	HIS
7	LA	226	ASN
7	LA	301	GLN
7	LA	356	ASN
8	LB	43	GLN
8	LB	195	ASN
5	M	132	GLN
5	M	152	GLN
5	M	169	ASN
5	M	694	GLN
5	M	763	GLN
5	M	823	ASN
5	M	862	ASN
6	MC	66	GLN
1	N	717	GLN
12	a	222	ASN
12	a	299	GLN
12	b	198	ASN
12	b	211	ASN
12	b	219	HIS
12	b	222	ASN
12	b	299	GLN
12	b	429	GLN
12	c	9	GLN
12	c	54	GLN
12	c	158	ASN
12	c	198	ASN
12	c	207	ASN
12	c	211	ASN
12	c	332	GLN
12	c	347	ASN
12	c	429	GLN
12	d	12	GLN

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Mol	Chain	Res	Type
12	d	79	ASN
12	d	197	GLN
12	d	227	GLN
12	e	197	GLN
12	e	250	ASN
12	f	16	GLN
12	f	207	ASN
12	f	338	GLN
12	g	227	GLN
12	g	315	HIS
12	g	322	ASN
12	g	332	GLN
12	g	371	HIS
12	h	207	ASN
12	h	229	ASN
12	i	110	GLN
12	i	158	ASN
12	i	315	HIS
12	i	436	HIS
12	j	54	GLN
12	j	158	ASN
12	j	299	GLN
12	j	315	HIS
12	k	9	GLN
12	k	158	ASN
12	k	315	HIS
12	l	16	GLN
12	l	115	HIS
12	m	9	GLN
12	m	347	ASN
12	m	357	GLN
12	n	12	GLN
12	n	24	GLN
12	n	250	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues 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
8	GDP	DB	501	-	28,30,30	3.36	13 (46%)	44,47,47	1.75	10 (22%)
8	GDP	FB	501	-	28,30,30	3.37	13 (46%)	44,47,47	1.81	11 (25%)
8	GDP	JB	501	-	28,30,30	3.35	13 (46%)	44,47,47	1.77	11 (25%)
8	GDP	CB	501	-	28,30,30	3.34	13 (46%)	44,47,47	1.74	10 (22%)
8	GDP	HB	501	-	28,30,30	3.37	13 (46%)	44,47,47	1.76	10 (22%)
8	GDP	IB	501	-	28,30,30	3.36	13 (46%)	44,47,47	1.80	11 (25%)
8	GDP	LB	501	-	28,30,30	3.36	13 (46%)	44,47,47	1.78	11 (25%)
8	GDP	EB	501	-	28,30,30	3.36	13 (46%)	44,47,47	1.79	11 (25%)
8	GDP	BB	501	-	28,30,30	3.30	14 (50%)	44,47,47	1.63	10 (22%)
8	GDP	GB	501	-	28,30,30	3.37	13 (46%)	44,47,47	1.86	12 (27%)
8	GDP	KB	501	-	28,30,30	3.35	13 (46%)	44,47,47	1.79	11 (25%)

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
8	GDP	DB	501	-	-	2/16/32/32	0/3/3/3
8	GDP	FB	501	-	-	0/16/32/32	0/3/3/3
8	GDP	JB	501	-	-	4/16/32/32	0/3/3/3
8	GDP	CB	501	-	-	4/16/32/32	0/3/3/3
8	GDP	HB	501	-	-	5/16/32/32	0/3/3/3
8	GDP	IB	501	-	-	2/16/32/32	0/3/3/3
8	GDP	LB	501	-	-	3/16/32/32	0/3/3/3
8	GDP	EB	501	-	-	1/16/32/32	0/3/3/3
8	GDP	BB	501	-	-	5/16/32/32	0/3/3/3
8	GDP	GB	501	-	-	3/16/32/32	0/3/3/3
8	GDP	KB	501	-	-	2/16/32/32	0/3/3/3

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	LB	501	GDP	C3'-C4'	-8.87	1.30	1.53
8	HB	501	GDP	C3'-C4'	-8.85	1.30	1.53
8	GB	501	GDP	C3'-C4'	-8.82	1.30	1.53
8	IB	501	GDP	C3'-C4'	-8.79	1.30	1.53
8	FB	501	GDP	C3'-C4'	-8.78	1.30	1.53
8	KB	501	GDP	C3'-C4'	-8.76	1.30	1.53
8	CB	501	GDP	C3'-C4'	-8.69	1.30	1.53
8	JB	501	GDP	C3'-C4'	-8.68	1.30	1.53
8	DB	501	GDP	C3'-C4'	-8.67	1.30	1.53
8	EB	501	GDP	C3'-C4'	-8.61	1.31	1.53
8	BB	501	GDP	C3'-C4'	-8.36	1.31	1.53
8	EB	501	GDP	O4'-C4'	7.79	1.62	1.45
8	GB	501	GDP	O4'-C4'	7.78	1.62	1.45
8	HB	501	GDP	O4'-C4'	7.77	1.62	1.45
8	BB	501	GDP	O4'-C4'	7.75	1.62	1.45
8	FB	501	GDP	O4'-C4'	7.72	1.62	1.45
8	DB	501	GDP	O4'-C4'	7.72	1.62	1.45
8	JB	501	GDP	O4'-C4'	7.70	1.62	1.45
8	KB	501	GDP	O4'-C4'	7.69	1.62	1.45
8	LB	501	GDP	O4'-C4'	7.67	1.62	1.45
8	IB	501	GDP	O4'-C4'	7.67	1.62	1.45
8	CB	501	GDP	O4'-C4'	7.65	1.62	1.45
8	DB	501	GDP	C4-N3	6.58	1.49	1.34
8	EB	501	GDP	C4-N3	6.55	1.49	1.34
8	JB	501	GDP	C4-N3	6.55	1.49	1.34
8	CB	501	GDP	C4-N3	6.53	1.49	1.34
8	FB	501	GDP	C4-N3	6.52	1.49	1.34
8	HB	501	GDP	C4-N3	6.51	1.49	1.34
8	IB	501	GDP	C4-N3	6.49	1.49	1.34
8	LB	501	GDP	C4-N3	6.48	1.49	1.34
8	GB	501	GDP	C4-N3	6.47	1.49	1.34
8	KB	501	GDP	C4-N3	6.43	1.49	1.34
8	BB	501	GDP	C4-N3	6.41	1.49	1.34
8	HB	501	GDP	C2-N3	5.69	1.46	1.33
8	FB	501	GDP	C2-N3	5.62	1.46	1.33
8	JB	501	GDP	C2-N3	5.61	1.46	1.33
8	EB	501	GDP	C2-N3	5.61	1.46	1.33
8	DB	501	GDP	C2-N3	5.61	1.46	1.33
8	IB	501	GDP	C2-N3	5.60	1.46	1.33
8	GB	501	GDP	C2-N3	5.59	1.46	1.33
8	CB	501	GDP	C2-N3	5.58	1.46	1.33
8	KB	501	GDP	C2-N3	5.54	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	BB	501	GDP	C2-N3	5.43	1.46	1.33
8	LB	501	GDP	C2-N3	5.43	1.46	1.33
8	FB	501	GDP	C2-N2	4.82	1.45	1.34
8	DB	501	GDP	C2-N2	4.82	1.45	1.34
8	EB	501	GDP	C2-N2	4.82	1.45	1.34
8	HB	501	GDP	C2-N2	4.81	1.45	1.34
8	JB	501	GDP	C2-N2	4.81	1.45	1.34
8	IB	501	GDP	C2-N2	4.79	1.45	1.34
8	CB	501	GDP	C2-N2	4.79	1.45	1.34
8	GB	501	GDP	C2-N2	4.78	1.45	1.34
8	LB	501	GDP	C2-N2	4.76	1.45	1.34
8	KB	501	GDP	C2-N2	4.72	1.45	1.34
8	BB	501	GDP	C2-N2	4.50	1.44	1.34
8	LB	501	GDP	O4'-C1'	-4.49	1.31	1.42
8	KB	501	GDP	O4'-C1'	-4.47	1.31	1.42
8	IB	501	GDP	O4'-C1'	-4.47	1.31	1.42
8	DB	501	GDP	O4'-C1'	-4.47	1.31	1.42
8	BB	501	GDP	O4'-C1'	-4.47	1.31	1.42
8	GB	501	GDP	O4'-C1'	-4.45	1.31	1.42
8	HB	501	GDP	O4'-C1'	-4.43	1.31	1.42
8	JB	501	GDP	O4'-C1'	-4.43	1.31	1.42
8	CB	501	GDP	O4'-C1'	-4.40	1.31	1.42
8	FB	501	GDP	O4'-C1'	-4.38	1.31	1.42
8	EB	501	GDP	O4'-C1'	-4.37	1.31	1.42
8	BB	501	GDP	O3'-C3'	3.04	1.50	1.43
8	HB	501	GDP	C5-N7	-3.02	1.33	1.39
8	EB	501	GDP	O3'-C3'	3.00	1.50	1.43
8	JB	501	GDP	O2'-C2'	-2.96	1.36	1.43
8	IB	501	GDP	O2'-C2'	-2.95	1.36	1.43
8	KB	501	GDP	O2'-C2'	-2.95	1.36	1.43
8	LB	501	GDP	O2'-C2'	-2.93	1.36	1.43
8	JB	501	GDP	C5-N7	-2.93	1.33	1.39
8	BB	501	GDP	O2'-C2'	-2.93	1.36	1.43
8	EB	501	GDP	O2'-C2'	-2.92	1.36	1.43
8	GB	501	GDP	O3'-C3'	2.92	1.49	1.43
8	HB	501	GDP	O2'-C2'	-2.90	1.36	1.43
8	GB	501	GDP	O2'-C2'	-2.90	1.36	1.43
8	DB	501	GDP	O2'-C2'	-2.90	1.36	1.43
8	CB	501	GDP	O2'-C2'	-2.90	1.36	1.43
8	FB	501	GDP	O2'-C2'	-2.89	1.36	1.43
8	IB	501	GDP	O3'-C3'	2.89	1.49	1.43
8	LB	501	GDP	C5-N7	-2.87	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	FB	501	GDP	C5-N7	-2.86	1.33	1.39
8	DB	501	GDP	O3'-C3'	2.86	1.49	1.43
8	BB	501	GDP	C5-N7	-2.86	1.33	1.39
8	KB	501	GDP	C5-N7	-2.85	1.33	1.39
8	KB	501	GDP	O3'-C3'	2.84	1.49	1.43
8	IB	501	GDP	C5-N7	-2.83	1.33	1.39
8	CB	501	GDP	C5-N7	-2.82	1.33	1.39
8	LB	501	GDP	O3'-C3'	2.82	1.49	1.43
8	DB	501	GDP	C5-N7	-2.81	1.33	1.39
8	EB	501	GDP	C5-N7	-2.81	1.33	1.39
8	EB	501	GDP	C2-N1	2.80	1.44	1.37
8	CB	501	GDP	O3'-C3'	2.80	1.49	1.43
8	JB	501	GDP	O3'-C3'	2.79	1.49	1.43
8	KB	501	GDP	C2-N1	2.79	1.44	1.37
8	GB	501	GDP	C5-N7	-2.78	1.33	1.39
8	FB	501	GDP	O3'-C3'	2.77	1.49	1.43
8	HB	501	GDP	C2-N1	2.74	1.44	1.37
8	CB	501	GDP	C2-N1	2.72	1.44	1.37
8	FB	501	GDP	C2-N1	2.72	1.44	1.37
8	DB	501	GDP	C2-N1	2.72	1.44	1.37
8	IB	501	GDP	C2-N1	2.70	1.44	1.37
8	GB	501	GDP	C2-N1	2.69	1.44	1.37
8	LB	501	GDP	C2-N1	2.67	1.44	1.37
8	BB	501	GDP	C2-N1	2.66	1.44	1.37
8	HB	501	GDP	O3'-C3'	2.65	1.49	1.43
8	EB	501	GDP	C6-N1	2.65	1.43	1.38
8	JB	501	GDP	C2-N1	2.64	1.44	1.37
8	CB	501	GDP	C6-N1	2.60	1.43	1.38
8	GB	501	GDP	C6-N1	2.60	1.43	1.38
8	LB	501	GDP	C6-N1	2.59	1.43	1.38
8	KB	501	GDP	C5-C6	2.59	1.54	1.44
8	LB	501	GDP	C5-C6	2.59	1.54	1.44
8	GB	501	GDP	C5-C6	2.58	1.54	1.44
8	FB	501	GDP	O6-C6	-2.57	1.18	1.23
8	IB	501	GDP	C5-C6	2.57	1.53	1.44
8	DB	501	GDP	C5-C6	2.57	1.53	1.44
8	DB	501	GDP	C6-N1	2.57	1.43	1.38
8	FB	501	GDP	C5-C6	2.56	1.53	1.44
8	EB	501	GDP	C5-C6	2.56	1.53	1.44
8	IB	501	GDP	C6-N1	2.54	1.43	1.38
8	CB	501	GDP	C5-C6	2.52	1.53	1.44
8	JB	501	GDP	C5-C6	2.51	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	JB	501	GDP	O6-C6	-2.51	1.18	1.23
8	DB	501	GDP	O6-C6	-2.50	1.18	1.23
8	JB	501	GDP	C6-N1	2.50	1.43	1.38
8	IB	501	GDP	O6-C6	-2.49	1.18	1.23
8	LB	501	GDP	O6-C6	-2.48	1.18	1.23
8	HB	501	GDP	C5-C6	2.48	1.53	1.44
8	KB	501	GDP	C6-N1	2.48	1.43	1.38
8	CB	501	GDP	O6-C6	-2.48	1.18	1.23
8	BB	501	GDP	O6-C6	-2.47	1.18	1.23
8	KB	501	GDP	O6-C6	-2.47	1.18	1.23
8	FB	501	GDP	C6-N1	2.46	1.43	1.38
8	GB	501	GDP	O6-C6	-2.45	1.18	1.23
8	BB	501	GDP	C5-C6	2.44	1.53	1.44
8	HB	501	GDP	O6-C6	-2.43	1.19	1.23
8	BB	501	GDP	C6-N1	2.40	1.43	1.38
8	HB	501	GDP	C6-N1	2.40	1.43	1.38
8	EB	501	GDP	O6-C6	-2.39	1.19	1.23
8	BB	501	GDP	C4-N9	-2.10	1.32	1.38

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	HB	501	GDP	C5-C4-N3	-5.37	119.75	128.46
8	GB	501	GDP	C5-C4-N3	-5.20	120.03	128.46
8	EB	501	GDP	C5-C4-N3	-5.11	120.16	128.46
8	IB	501	GDP	C5-C4-N3	-5.11	120.17	128.46
8	KB	501	GDP	C5-C4-N3	-5.10	120.19	128.46
8	JB	501	GDP	C5-C4-N3	-5.09	120.21	128.46
8	CB	501	GDP	C5-C4-N3	-5.08	120.22	128.46
8	FB	501	GDP	C5-C4-N3	-5.04	120.29	128.46
8	LB	501	GDP	C5-C4-N3	-5.01	120.34	128.46
8	DB	501	GDP	C5-C4-N3	-5.01	120.34	128.46
8	GB	501	GDP	C2-N3-C4	4.66	120.60	112.30
8	BB	501	GDP	C5-C4-N3	-4.65	120.92	128.46
8	EB	501	GDP	C2-N3-C4	4.52	120.35	112.30
8	LB	501	GDP	C2-N3-C4	4.50	120.32	112.30
8	DB	501	GDP	C2-N3-C4	4.47	120.26	112.30
8	CB	501	GDP	C2-N3-C4	4.40	120.14	112.30
8	KB	501	GDP	C2-N3-C4	4.39	120.12	112.30
8	FB	501	GDP	C2-N3-C4	4.39	120.12	112.30
8	IB	501	GDP	C2-N3-C4	4.38	120.11	112.30
8	JB	501	GDP	C2-N3-C4	4.37	120.09	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	HB	501	GDP	C2-N3-C4	4.33	120.01	112.30
8	BB	501	GDP	C2-N3-C4	3.84	119.14	112.30
8	HB	501	GDP	N9-C4-N3	3.59	133.14	125.94
8	BB	501	GDP	N9-C8-N7	-3.42	106.95	113.39
8	JB	501	GDP	N9-C4-N3	3.31	132.59	125.94
8	CB	501	GDP	N9-C4-N3	3.25	132.46	125.94
8	IB	501	GDP	N9-C4-N3	3.23	132.43	125.94
8	DB	501	GDP	N9-C4-N3	3.21	132.39	125.94
8	GB	501	GDP	N9-C4-N3	3.21	132.38	125.94
8	BB	501	GDP	N9-C4-N3	3.18	132.33	125.94
8	EB	501	GDP	N9-C4-N3	3.18	132.31	125.94
8	GB	501	GDP	N9-C8-N7	-3.17	107.41	113.39
8	FB	501	GDP	N9-C4-N3	3.17	132.31	125.94
8	IB	501	GDP	N9-C8-N7	-3.16	107.44	113.39
8	CB	501	GDP	N9-C8-N7	-3.14	107.48	113.39
8	JB	501	GDP	N9-C8-N7	-3.12	107.51	113.39
8	LB	501	GDP	N9-C4-N3	3.12	132.20	125.94
8	FB	501	GDP	N9-C8-N7	-3.11	107.54	113.39
8	LB	501	GDP	N9-C8-N7	-3.10	107.55	113.39
8	KB	501	GDP	N9-C4-N3	3.08	132.13	125.94
8	DB	501	GDP	N9-C8-N7	-3.07	107.62	113.39
8	LB	501	GDP	PA-O3A-PB	-3.06	122.31	132.83
8	KB	501	GDP	N9-C8-N7	-3.05	107.64	113.39
8	GB	501	GDP	C2-N1-C6	-3.05	119.53	125.10
8	JB	501	GDP	PA-O3A-PB	-3.05	122.36	132.83
8	IB	501	GDP	C2-N1-C6	-3.04	119.56	125.10
8	HB	501	GDP	C2-N1-C6	-3.04	119.56	125.10
8	KB	501	GDP	C2-N1-C6	-3.02	119.60	125.10
8	EB	501	GDP	N9-C8-N7	-2.99	107.77	113.39
8	FB	501	GDP	C2-N1-C6	-2.96	119.71	125.10
8	JB	501	GDP	C2-N1-C6	-2.95	119.72	125.10
8	HB	501	GDP	N9-C8-N7	-2.95	107.84	113.39
8	FB	501	GDP	C1'-N9-C4	-2.92	117.82	126.50
8	EB	501	GDP	C2-N1-C6	-2.88	119.84	125.10
8	KB	501	GDP	C1'-N9-C4	-2.88	117.94	126.50
8	IB	501	GDP	C1'-N9-C4	-2.88	117.95	126.50
8	CB	501	GDP	C2-N1-C6	-2.86	119.89	125.10
8	LB	501	GDP	C2-N1-C6	-2.86	119.89	125.10
8	GB	501	GDP	C5-C6-N1	2.83	120.37	113.19
8	BB	501	GDP	C2-N1-C6	-2.83	119.95	125.10
8	FB	501	GDP	PA-O3A-PB	-2.79	123.25	132.83
8	DB	501	GDP	C2-N1-C6	-2.77	120.04	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	FB	501	GDP	C5-C6-N1	2.75	120.18	113.19
8	JB	501	GDP	C5-C6-N1	2.75	120.17	113.19
8	IB	501	GDP	C5-C6-N1	2.72	120.11	113.19
8	KB	501	GDP	PA-O3A-PB	-2.71	123.54	132.83
8	DB	501	GDP	C5-C6-N1	2.70	120.05	113.19
8	KB	501	GDP	C5-C6-N1	2.70	120.04	113.19
8	LB	501	GDP	C5-C6-N1	2.70	120.04	113.19
8	EB	501	GDP	C5-C6-N1	2.70	120.04	113.19
8	GB	501	GDP	C1'-N9-C4	-2.69	118.51	126.50
8	HB	501	GDP	PA-O3A-PB	-2.69	123.59	132.83
8	EB	501	GDP	C1'-N9-C4	-2.69	118.51	126.50
8	GB	501	GDP	O6-C6-C5	-2.65	119.57	126.60
8	EB	501	GDP	O6-C6-C5	-2.65	119.58	126.60
8	HB	501	GDP	C5-C6-N1	2.65	119.91	113.19
8	CB	501	GDP	C5-C6-N1	2.64	119.88	113.19
8	LB	501	GDP	C1'-N9-C4	-2.63	118.70	126.50
8	JB	501	GDP	C1'-N9-C4	-2.61	118.74	126.50
8	HB	501	GDP	O6-C6-C5	-2.61	119.69	126.60
8	CB	501	GDP	O6-C6-C5	-2.60	119.70	126.60
8	DB	501	GDP	PA-O3A-PB	-2.59	123.94	132.83
8	FB	501	GDP	O6-C6-C5	-2.56	119.81	126.60
8	JB	501	GDP	O6-C6-C5	-2.55	119.84	126.60
8	DB	501	GDP	C1'-N9-C4	-2.54	118.97	126.50
8	CB	501	GDP	C1'-N9-C4	-2.53	118.99	126.50
8	BB	501	GDP	C5-C6-N1	2.51	119.56	113.19
8	KB	501	GDP	O6-C6-C5	-2.51	119.95	126.60
8	BB	501	GDP	PA-O3A-PB	-2.50	124.25	132.83
8	IB	501	GDP	O6-C6-C5	-2.49	119.99	126.60
8	DB	501	GDP	O6-C6-C5	-2.49	119.99	126.60
8	LB	501	GDP	O6-C6-C5	-2.48	120.02	126.60
8	BB	501	GDP	O6-C6-C5	-2.45	120.11	126.60
8	KB	501	GDP	C1'-N9-C8	2.40	133.52	126.70
8	GB	501	GDP	PA-O3A-PB	-2.37	124.70	132.83
8	FB	501	GDP	C1'-N9-C8	2.36	133.43	126.70
8	CB	501	GDP	PA-O3A-PB	-2.33	124.81	132.83
8	IB	501	GDP	PA-O3A-PB	-2.31	124.91	132.83
8	IB	501	GDP	C1'-N9-C8	2.29	133.22	126.70
8	HB	501	GDP	C1'-N9-C4	-2.29	119.71	126.50
8	GB	501	GDP	C8-N7-C5	2.27	108.35	104.24
8	EB	501	GDP	PA-O3A-PB	-2.26	125.07	132.83
8	GB	501	GDP	C3'-C2'-C1'	2.23	105.67	101.43
8	IB	501	GDP	C8-N7-C5	2.23	108.28	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	EB	501	GDP	C1'-N9-C8	2.20	132.97	126.70
8	KB	501	GDP	C8-N7-C5	2.20	108.22	104.24
8	CB	501	GDP	C8-N7-C5	2.19	108.20	104.24
8	BB	501	GDP	C8-N7-C5	2.18	108.19	104.24
8	LB	501	GDP	C8-N7-C5	2.17	108.17	104.24
8	DB	501	GDP	C8-N7-C5	2.14	108.11	104.24
8	FB	501	GDP	C8-N7-C5	2.14	108.11	104.24
8	JB	501	GDP	C8-N7-C5	2.13	108.10	104.24
8	EB	501	GDP	C8-N7-C5	2.12	108.08	104.24
8	GB	501	GDP	C1'-N9-C8	2.12	132.73	126.70
8	HB	501	GDP	C8-N7-C5	2.11	108.06	104.24
8	BB	501	GDP	C1'-N9-C4	-2.10	120.27	126.50
8	LB	501	GDP	C1'-N9-C8	2.06	132.55	126.70
8	JB	501	GDP	C1'-N9-C8	2.01	132.42	126.70

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	BB	501	GDP	PA-O3A-PB-O3B
8	BB	501	GDP	C5'-O5'-PA-O3A
8	BB	501	GDP	C5'-O5'-PA-O1A
8	BB	501	GDP	C5'-O5'-PA-O2A
8	CB	501	GDP	C5'-O5'-PA-O3A
8	CB	501	GDP	C5'-O5'-PA-O1A
8	CB	501	GDP	O4'-C4'-C5'-O5'
8	CB	501	GDP	C3'-C4'-C5'-O5'
8	EB	501	GDP	C5'-O5'-PA-O1A
8	JB	501	GDP	O4'-C4'-C5'-O5'
8	JB	501	GDP	C3'-C4'-C5'-O5'
8	HB	501	GDP	C3'-C4'-C5'-O5'
8	IB	501	GDP	C3'-C4'-C5'-O5'
8	KB	501	GDP	C3'-C4'-C5'-O5'
8	HB	501	GDP	O4'-C4'-C5'-O5'
8	IB	501	GDP	O4'-C4'-C5'-O5'
8	KB	501	GDP	O4'-C4'-C5'-O5'
8	LB	501	GDP	C3'-C4'-C5'-O5'
8	GB	501	GDP	PB-O3A-PA-O2A
8	HB	501	GDP	PB-O3A-PA-O2A
8	JB	501	GDP	PB-O3A-PA-O2A
8	DB	501	GDP	C3'-C4'-C5'-O5'
8	LB	501	GDP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
8	BB	501	GDP	PA-O3A-PB-O2B
8	GB	501	GDP	PB-O3A-PA-O1A
8	HB	501	GDP	PB-O3A-PA-O1A
8	JB	501	GDP	PB-O3A-PA-O1A
8	LB	501	GDP	PB-O3A-PA-O2A
8	GB	501	GDP	C5'-O5'-PA-O1A
8	HB	501	GDP	C5'-O5'-PA-O1A
8	DB	501	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	BB	501	GDP	1	0
8	KB	501	GDP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	GTP	BA	501	-	30,34,34	0.55	0	46,54,54	0.54	0
13	GTP	IA	501	-	30,34,34	0.55	0	46,54,54	0.58	0
13	GTP	FA	501	-	30,34,34	0.54	0	46,54,54	0.55	0
13	GTP	JA	501	-	30,34,34	0.54	0	46,54,54	0.58	0
13	GTP	CA	501	-	30,34,34	0.55	0	46,54,54	0.64	0
13	GTP	EA	501	-	30,34,34	0.58	0	46,54,54	0.59	0
13	GTP	DA	501	-	30,34,34	0.57	0	46,54,54	0.64	0
13	GTP	HA	501	-	30,34,34	0.55	0	46,54,54	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	GTP	GA	501	-	30,34,34	0.54	0	46,54,54	0.49	0
13	GTP	KA	501	-	30,34,34	0.54	0	46,54,54	0.54	0
13	GTP	LA	501	-	30,34,34	0.54	0	46,54,54	0.54	0

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	GTP	BA	501	-	-	0/22/38/38	0/3/3/3
13	GTP	IA	501	-	-	3/22/38/38	0/3/3/3
13	GTP	FA	501	-	-	2/22/38/38	0/3/3/3
13	GTP	JA	501	-	-	4/22/38/38	0/3/3/3
13	GTP	CA	501	-	-	1/22/38/38	0/3/3/3
13	GTP	EA	501	-	-	3/22/38/38	0/3/3/3
13	GTP	DA	501	-	-	0/22/38/38	0/3/3/3
13	GTP	HA	501	-	-	4/22/38/38	0/3/3/3
13	GTP	GA	501	-	-	2/22/38/38	0/3/3/3
13	GTP	KA	501	-	-	2/22/38/38	0/3/3/3
13	GTP	LA	501	-	-	2/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	FA	501	GTP	O4'-C4'-C5'-O5'
13	FA	501	GTP	C3'-C4'-C5'-O5'
13	GA	501	GTP	O4'-C4'-C5'-O5'
13	GA	501	GTP	C3'-C4'-C5'-O5'
13	HA	501	GTP	C5'-O5'-PA-O1A
13	JA	501	GTP	O4'-C4'-C5'-O5'
13	JA	501	GTP	C3'-C4'-C5'-O5'
13	LA	501	GTP	C5'-O5'-PA-O3A
13	LA	501	GTP	C5'-O5'-PA-O2A
13	IA	501	GTP	C3'-C4'-C5'-O5'
13	IA	501	GTP	C4'-C5'-O5'-PA

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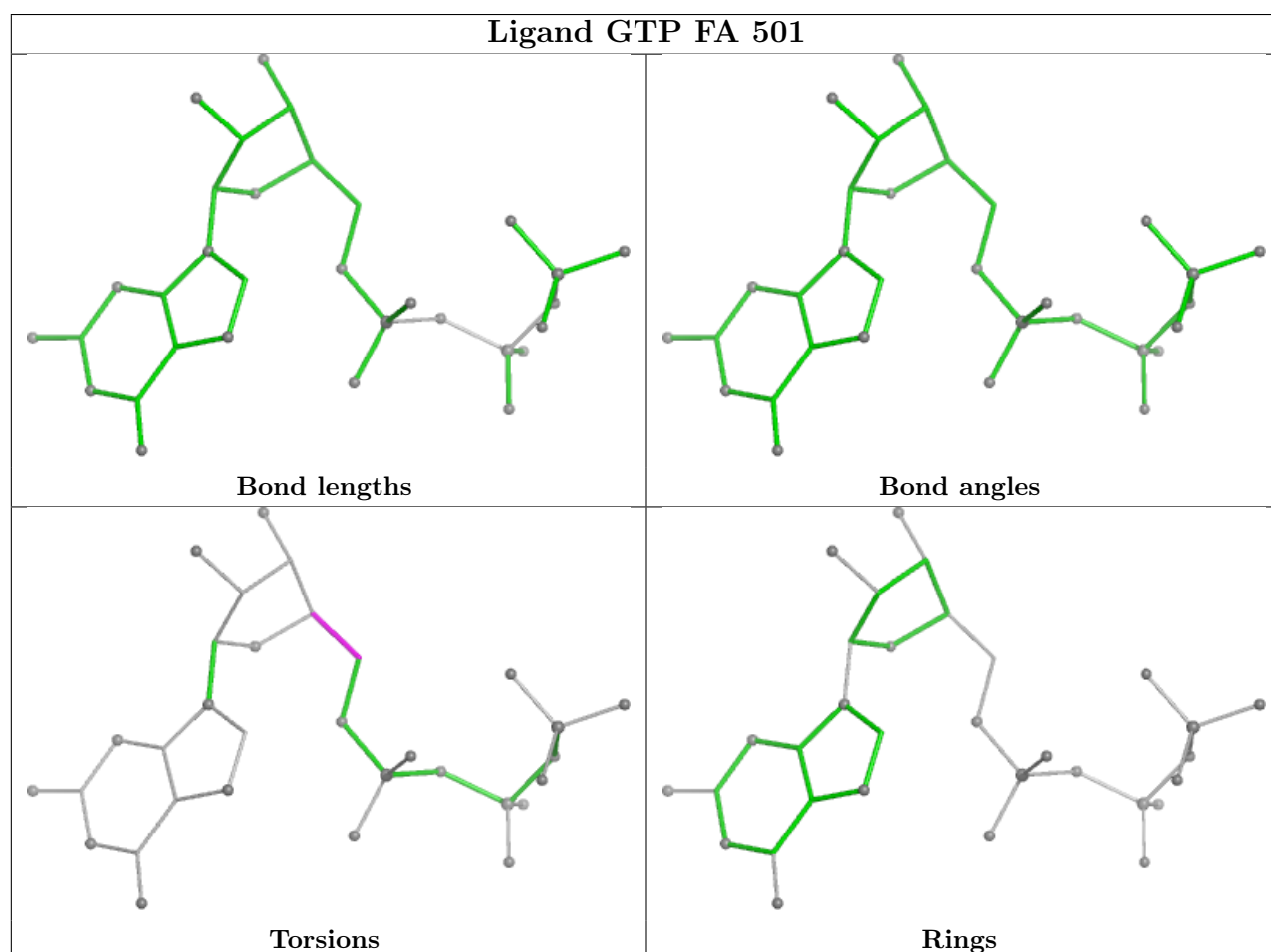
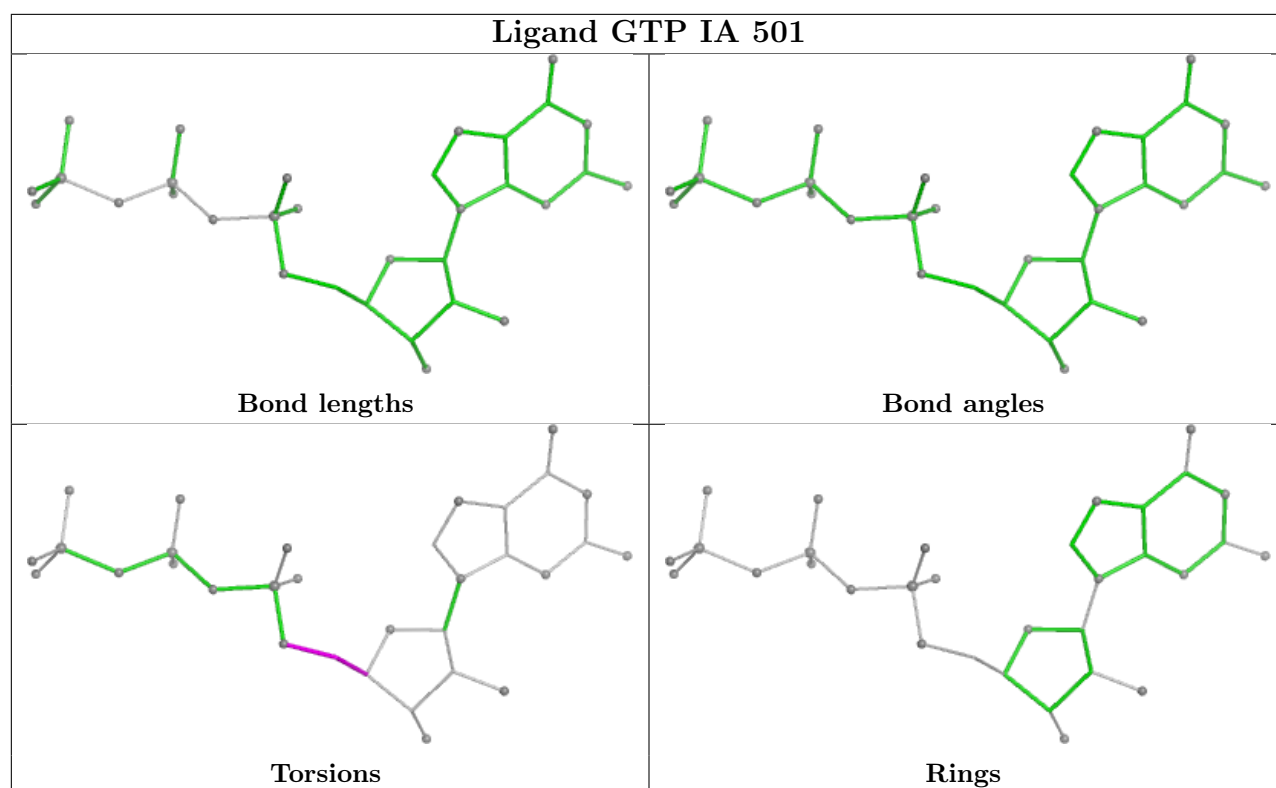
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Mol	Chain	Res	Type	Atoms
13	EA	501	GTP	C4'-C5'-O5'-PA
13	HA	501	GTP	C4'-C5'-O5'-PA
13	KA	501	GTP	C4'-C5'-O5'-PA
13	EA	501	GTP	PB-O3A-PA-O5'
13	IA	501	GTP	O4'-C4'-C5'-O5'
13	HA	501	GTP	C3'-C4'-C5'-O5'
13	CA	501	GTP	C4'-C5'-O5'-PA
13	EA	501	GTP	PB-O3B-PG-O3G
13	HA	501	GTP	C5'-O5'-PA-O3A
13	KA	501	GTP	C5'-O5'-PA-O3A
13	JA	501	GTP	PB-O3A-PA-O1A
13	JA	501	GTP	PB-O3A-PA-O2A

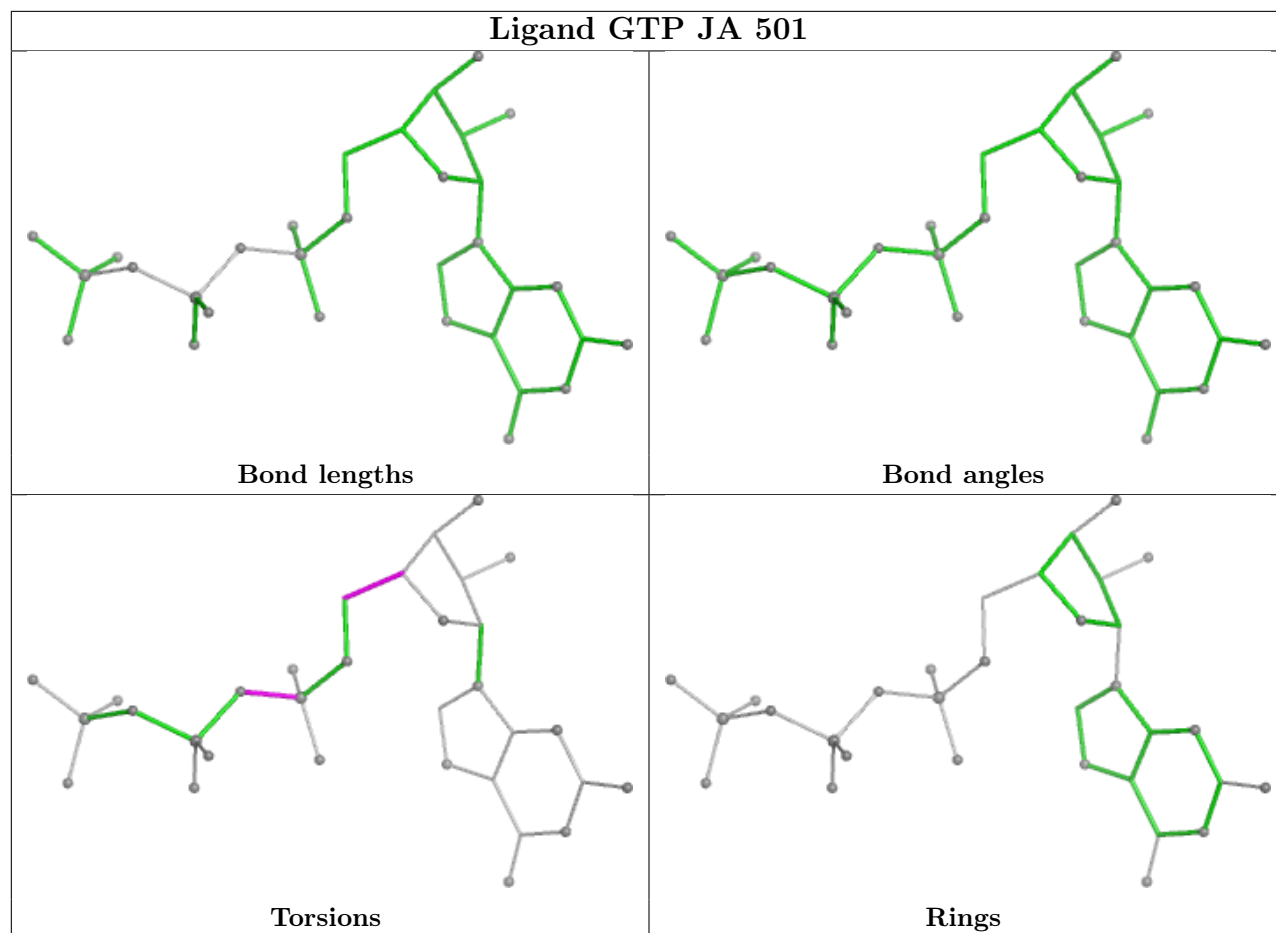
There are no ring outliers.

No monomer is involved in short contacts.

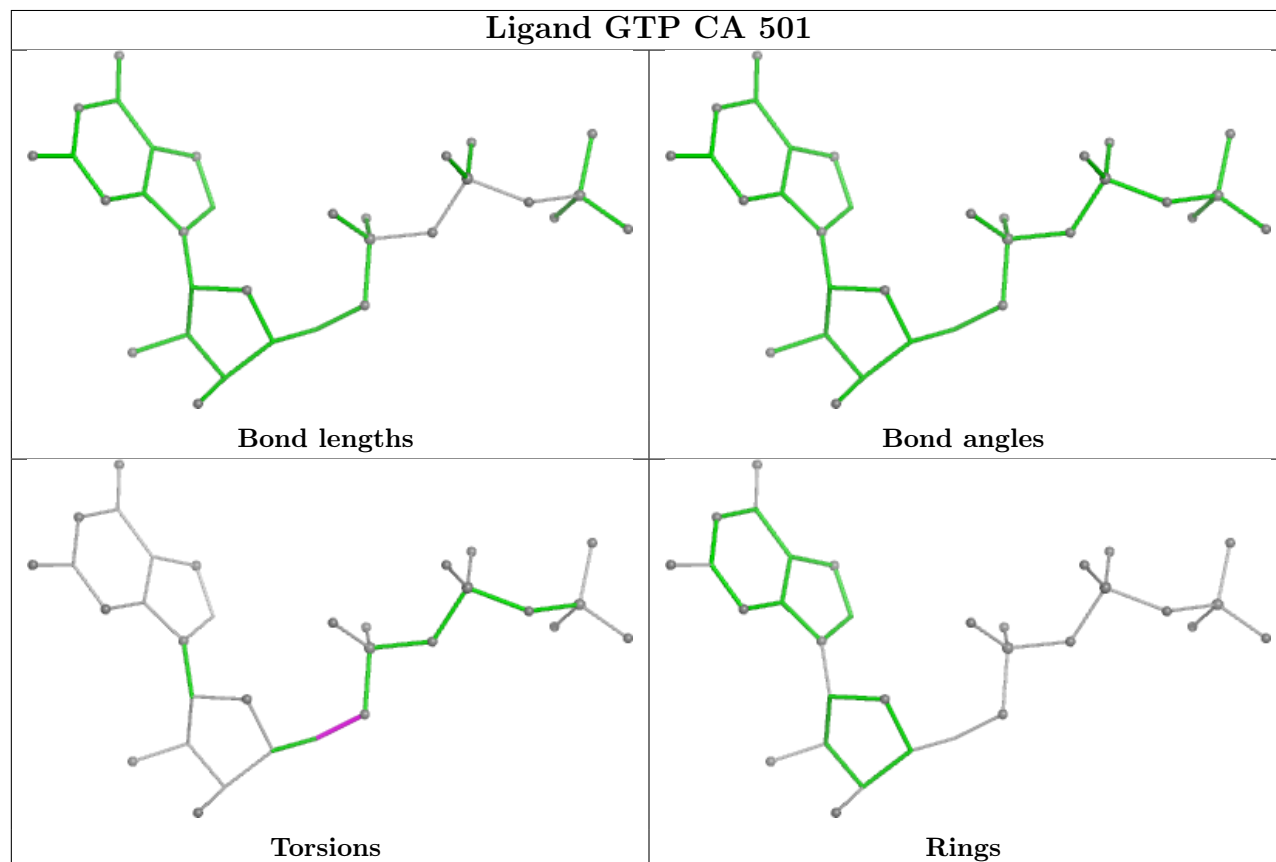
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

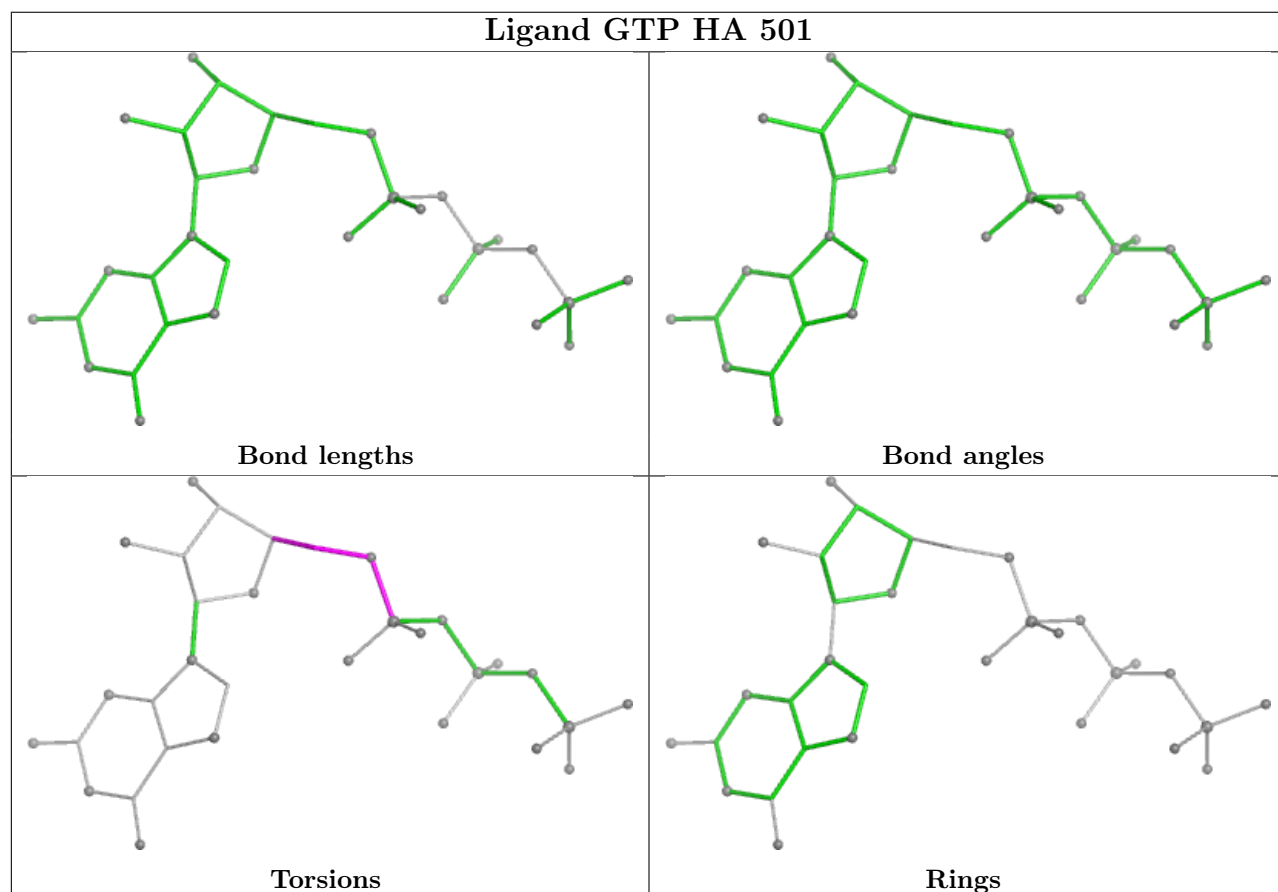
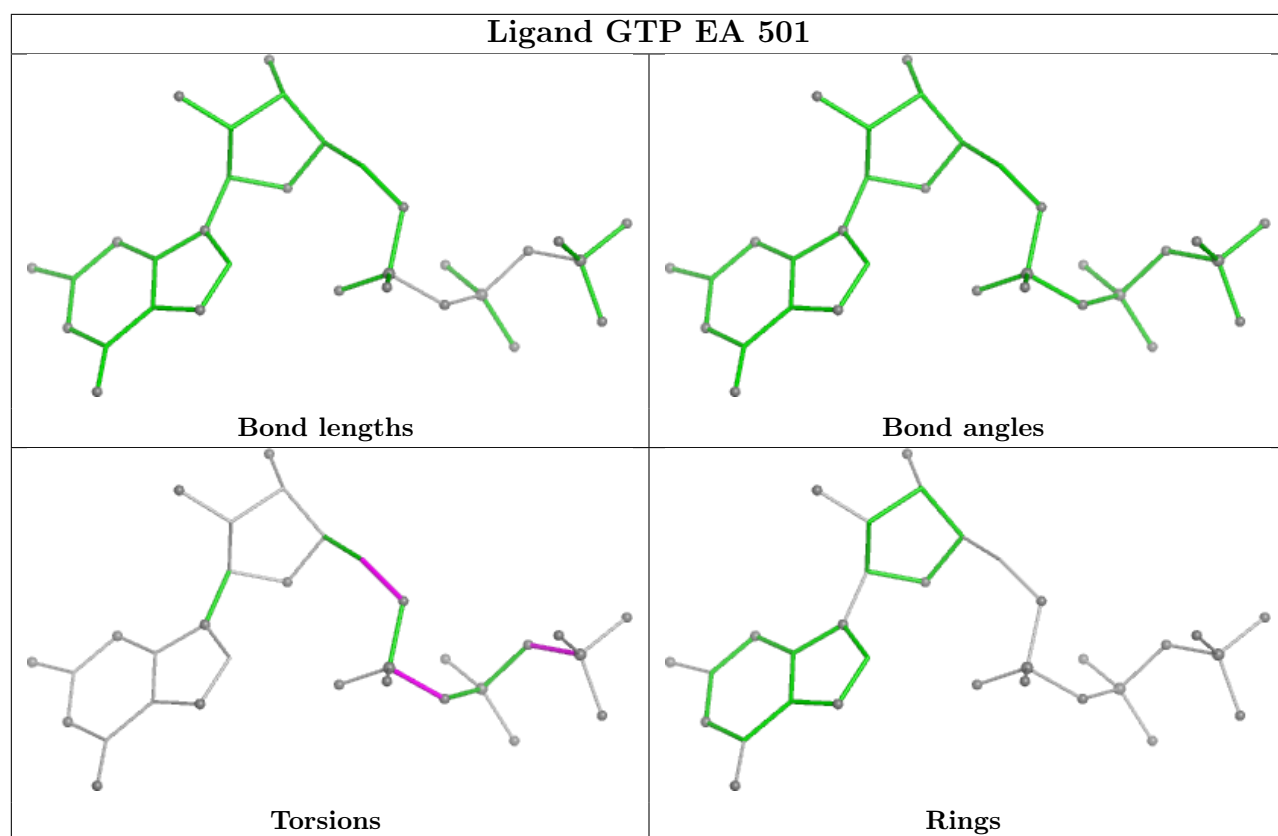


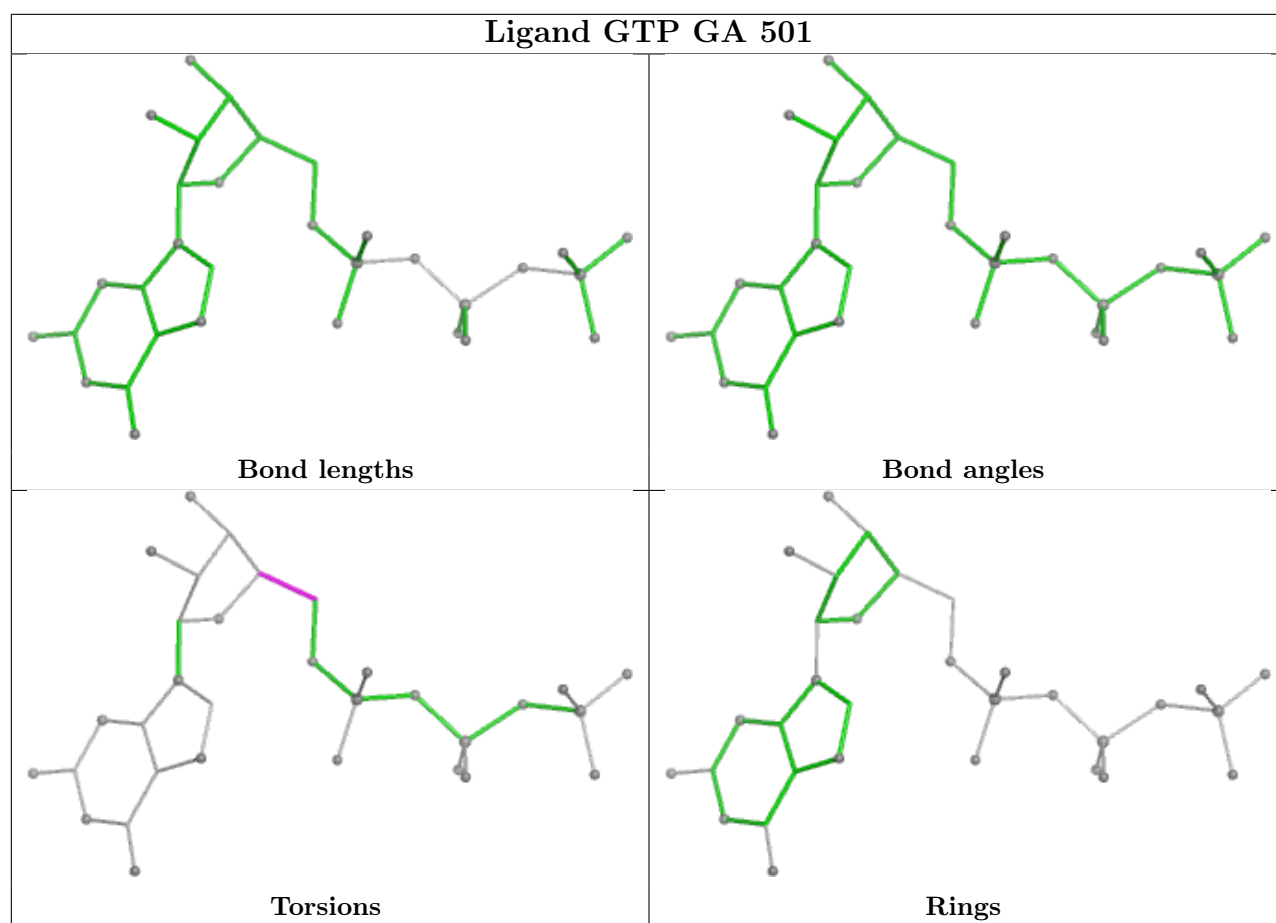
Ligand GTP JA 501



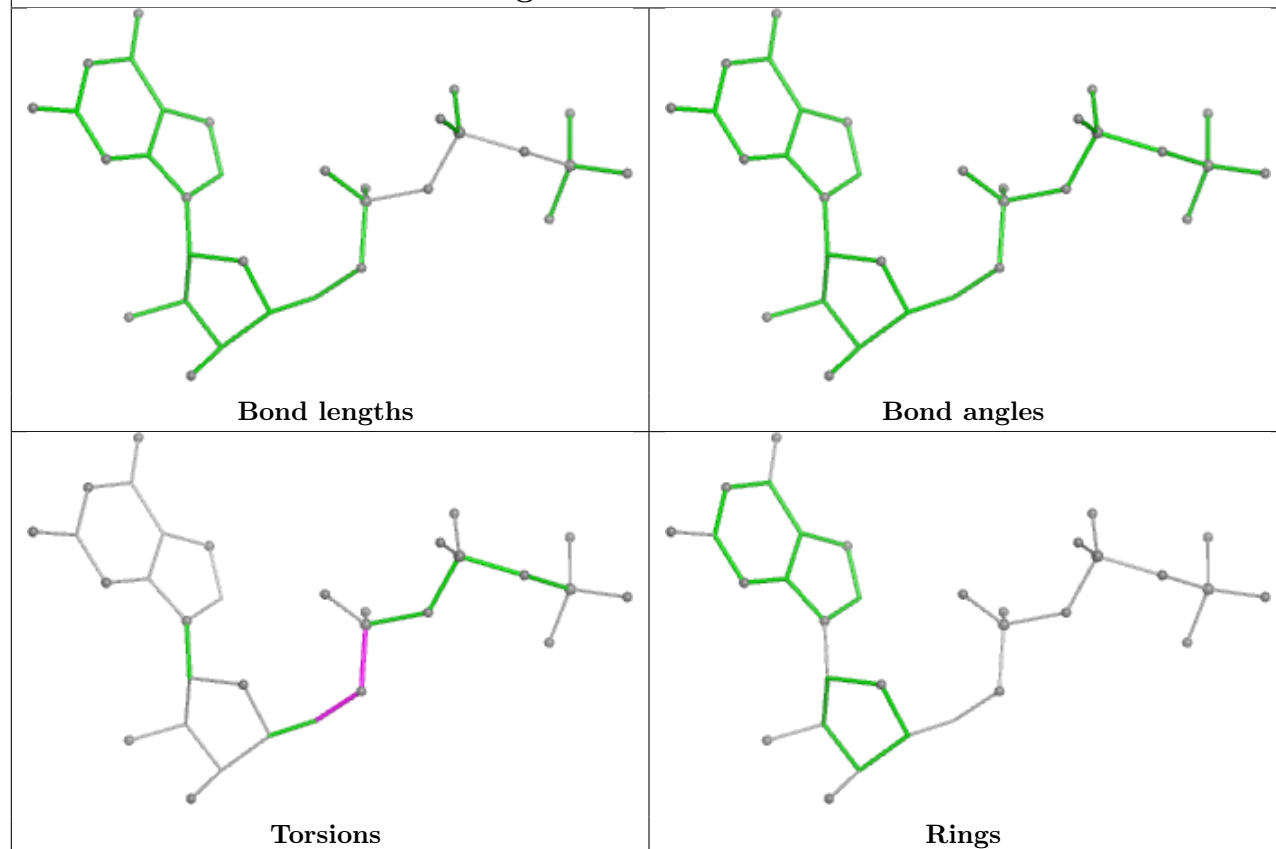
Ligand GTP CA 501



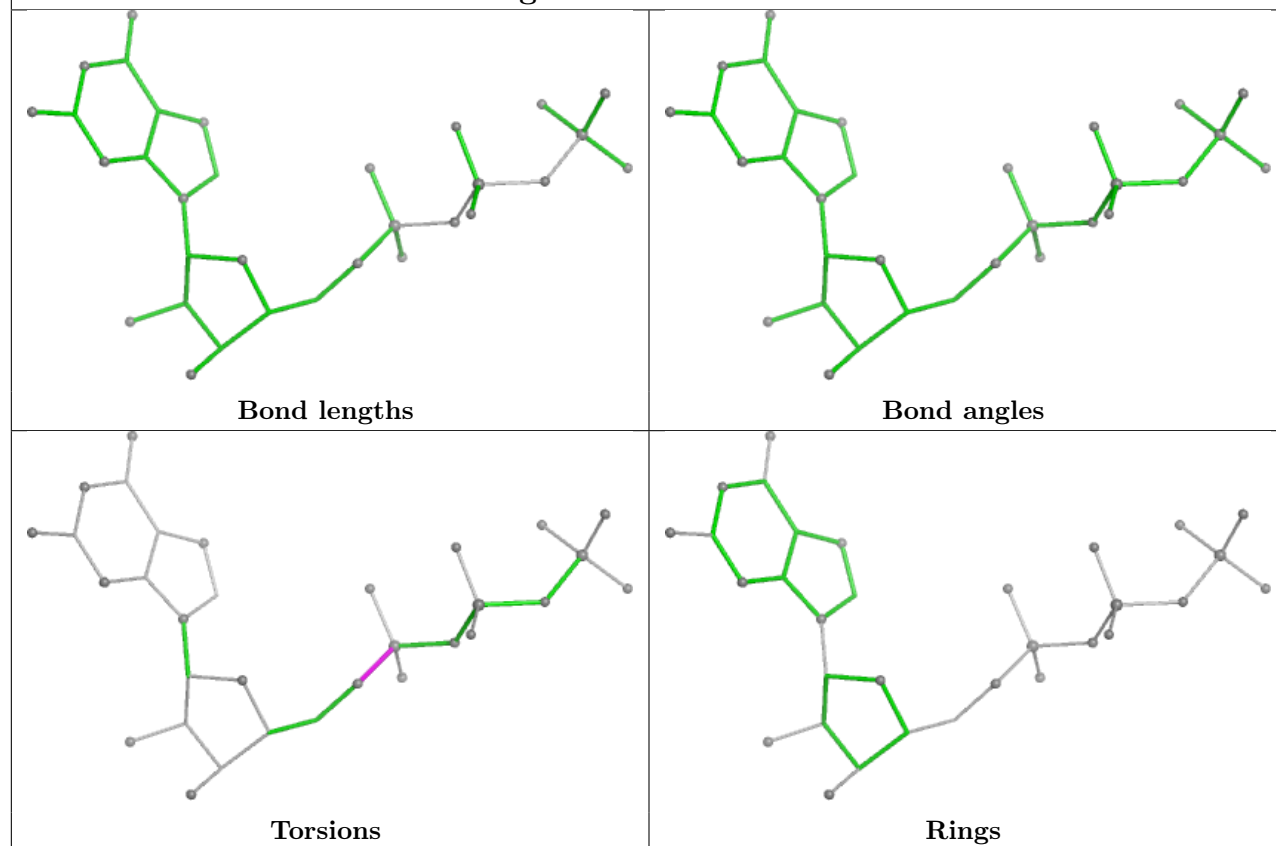




Ligand GTP KA 501



Ligand GTP LA 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

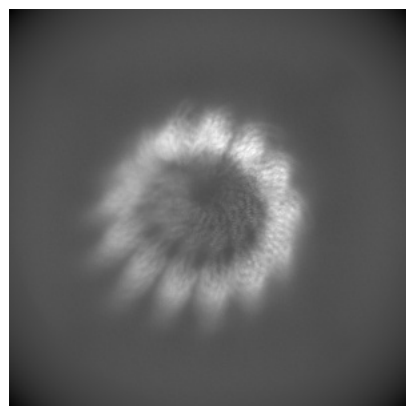
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55043. These allow visual inspection of the internal detail of the map and identification of artifacts.

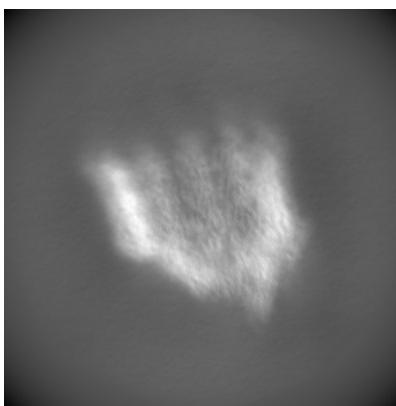
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

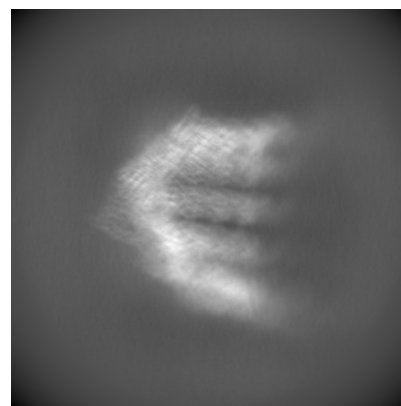
6.1.1 Primary map



X

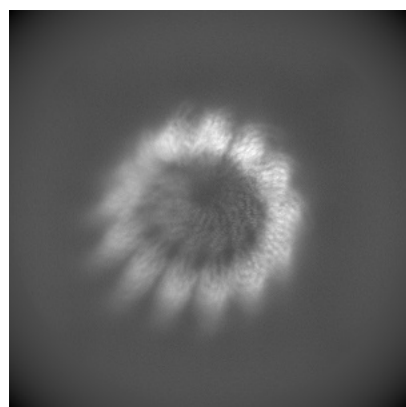


Y

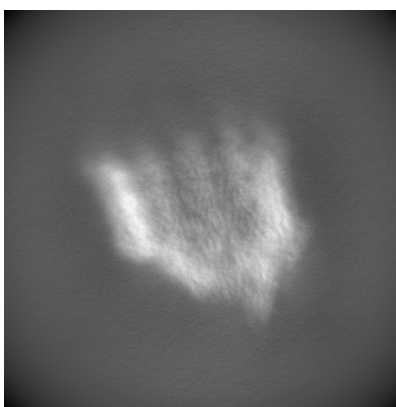


Z

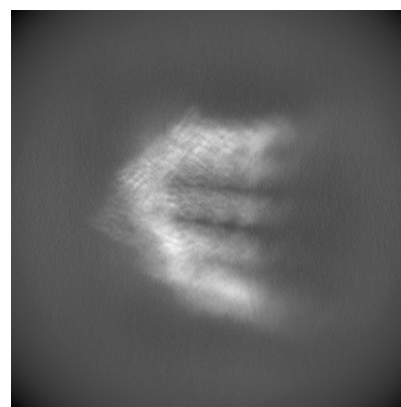
6.1.2 Raw map



X



Y

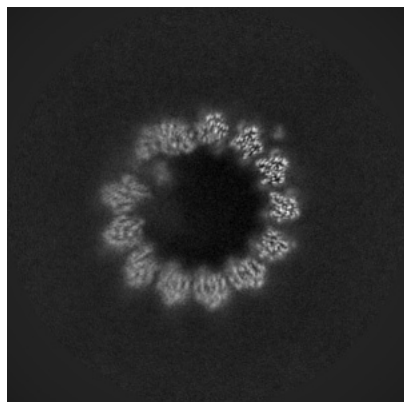


Z

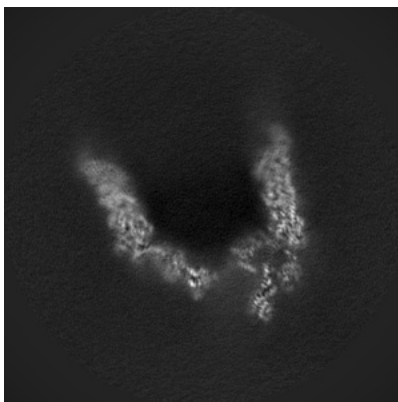
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

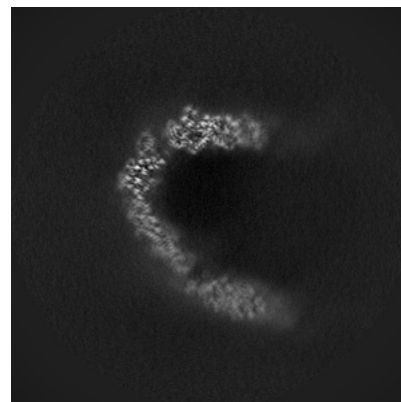
6.2.1 Primary map



X Index: 272

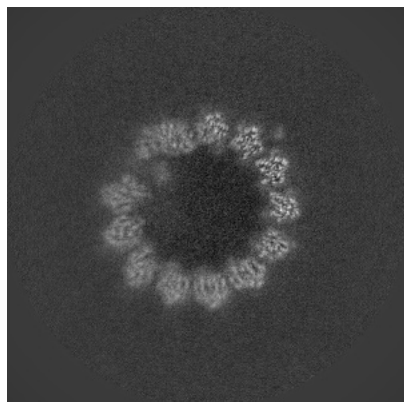


Y Index: 272

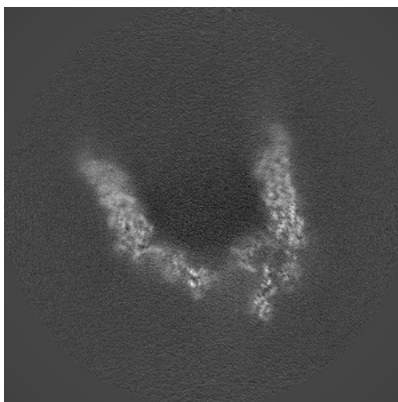


Z Index: 272

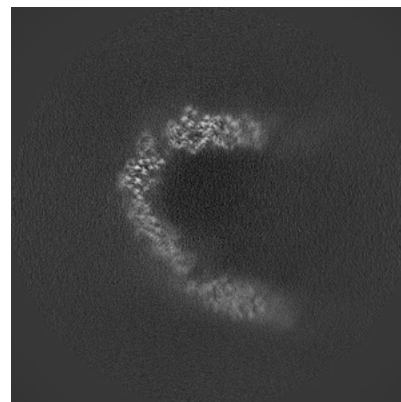
6.2.2 Raw map



X Index: 272



Y Index: 272

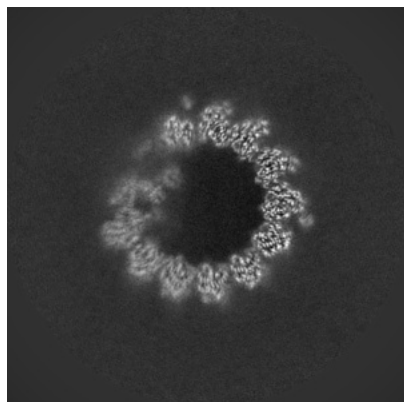


Z Index: 272

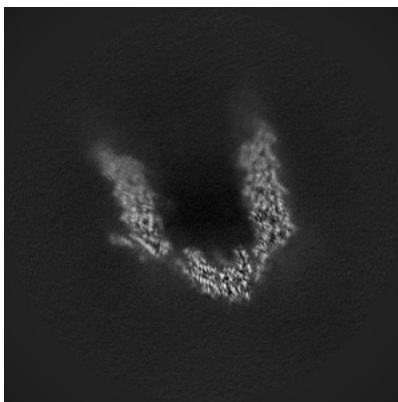
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

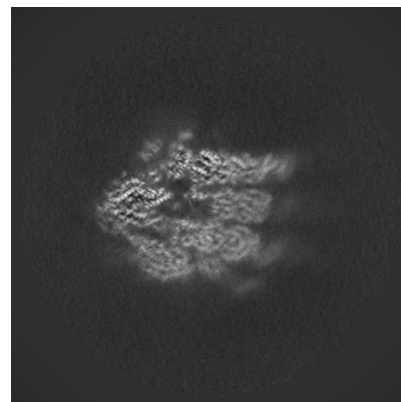
6.3.1 Primary map



X Index: 251

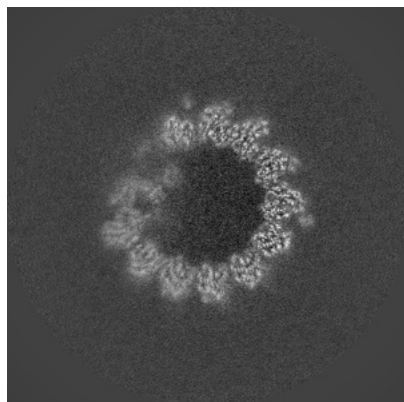


Y Index: 326

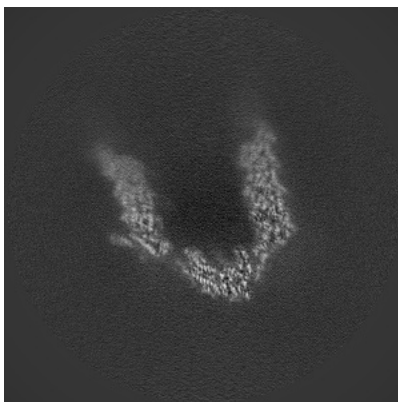


Z Index: 358

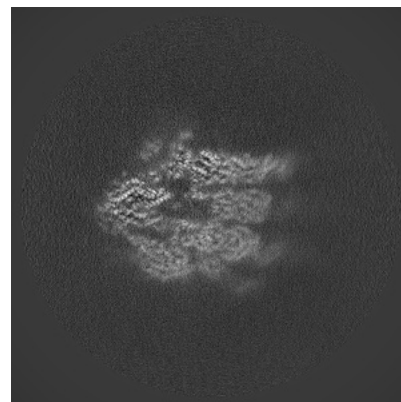
6.3.2 Raw map



X Index: 251



Y Index: 326

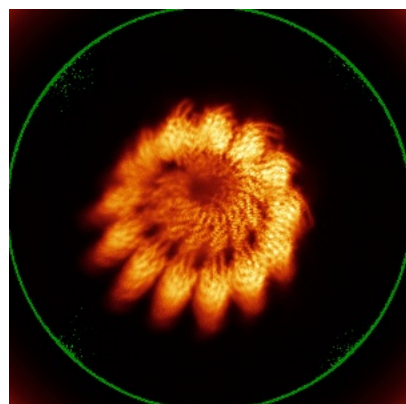


Z Index: 358

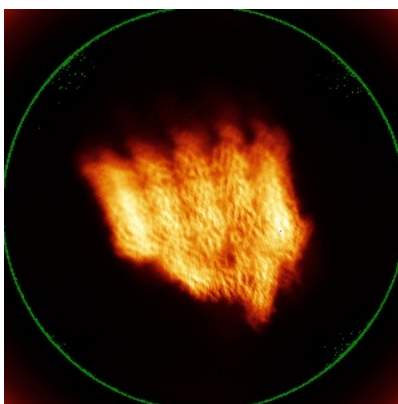
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

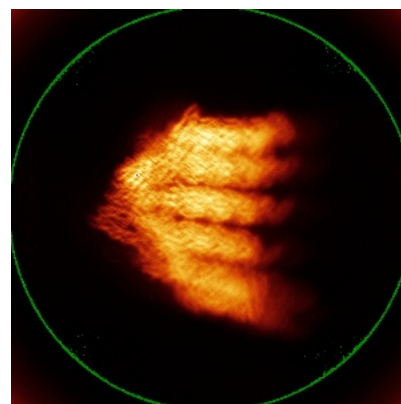
6.4.1 Primary map



X

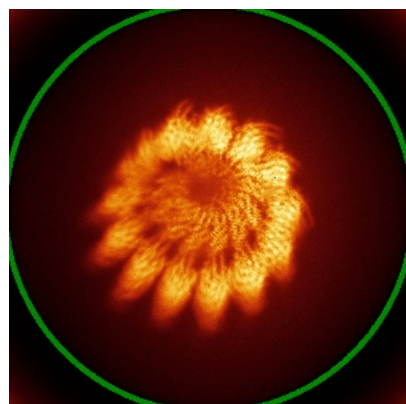


Y

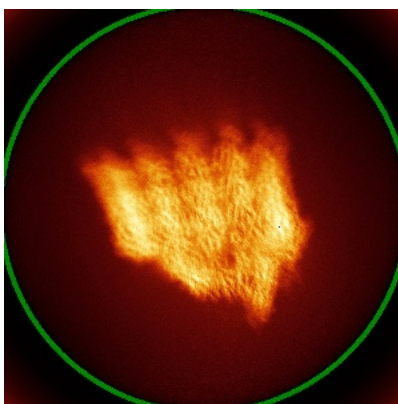


Z

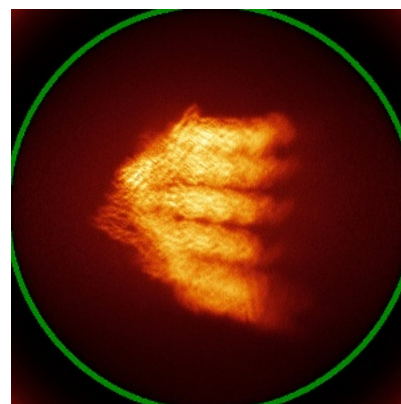
6.4.2 Raw map



X



Y

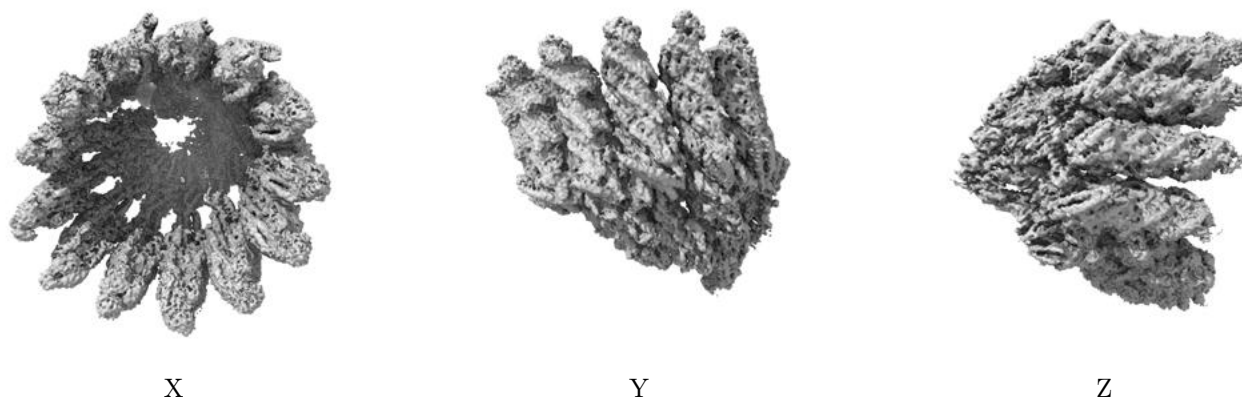


Z

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.

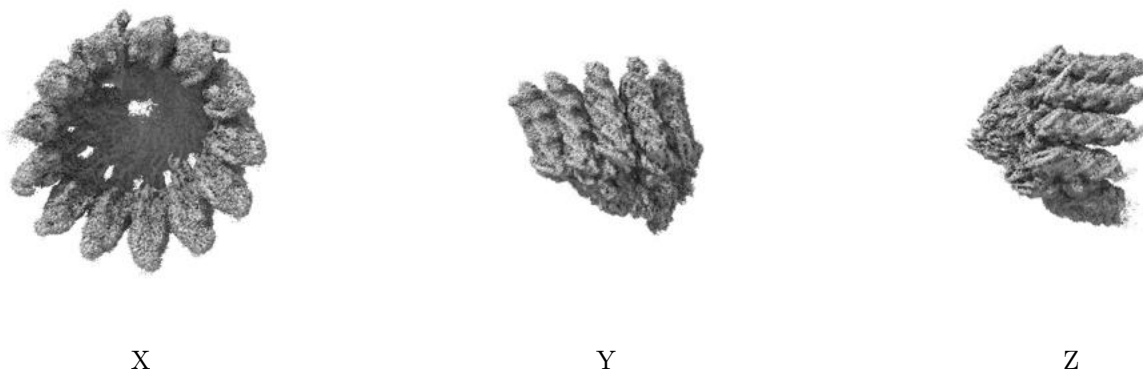
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

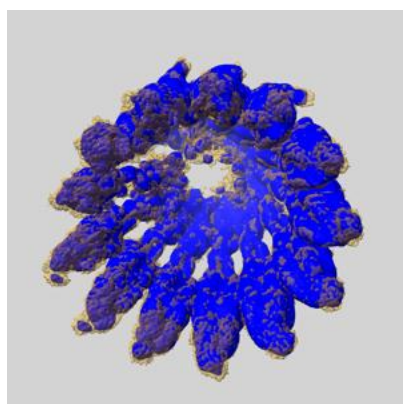
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

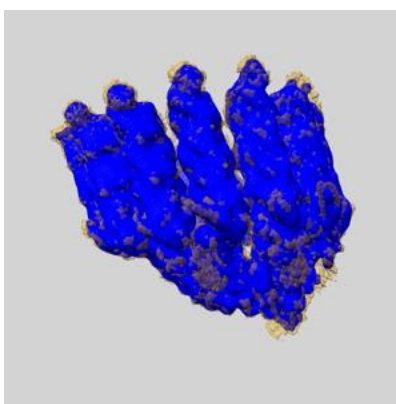
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

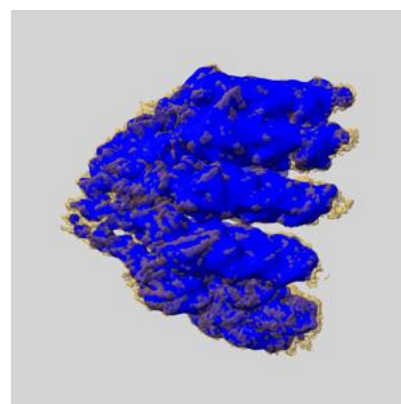
6.6.1 emd_55043_msk_1.map [i](#)



X



Y

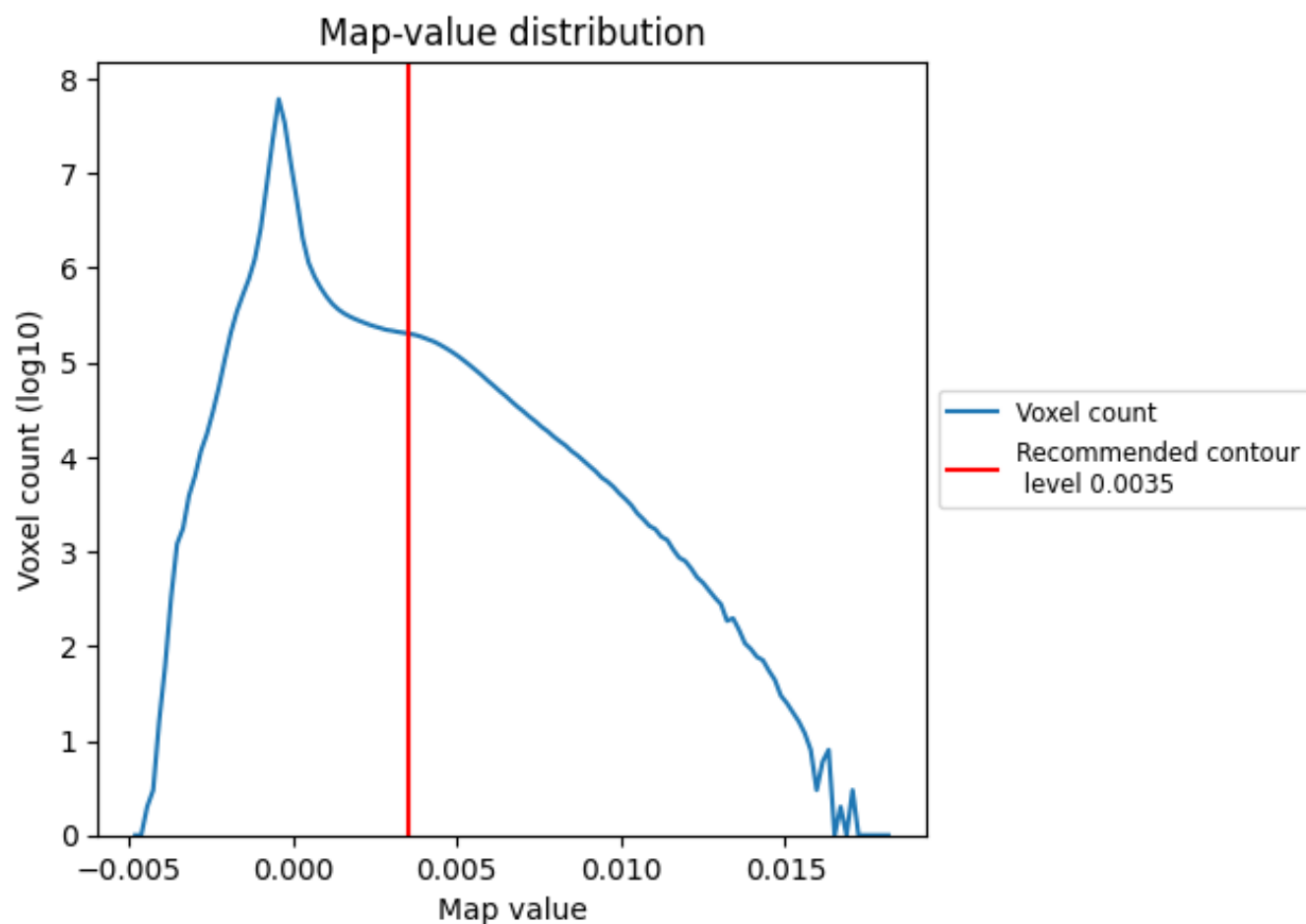


Z

7 Map analysis [i](#)

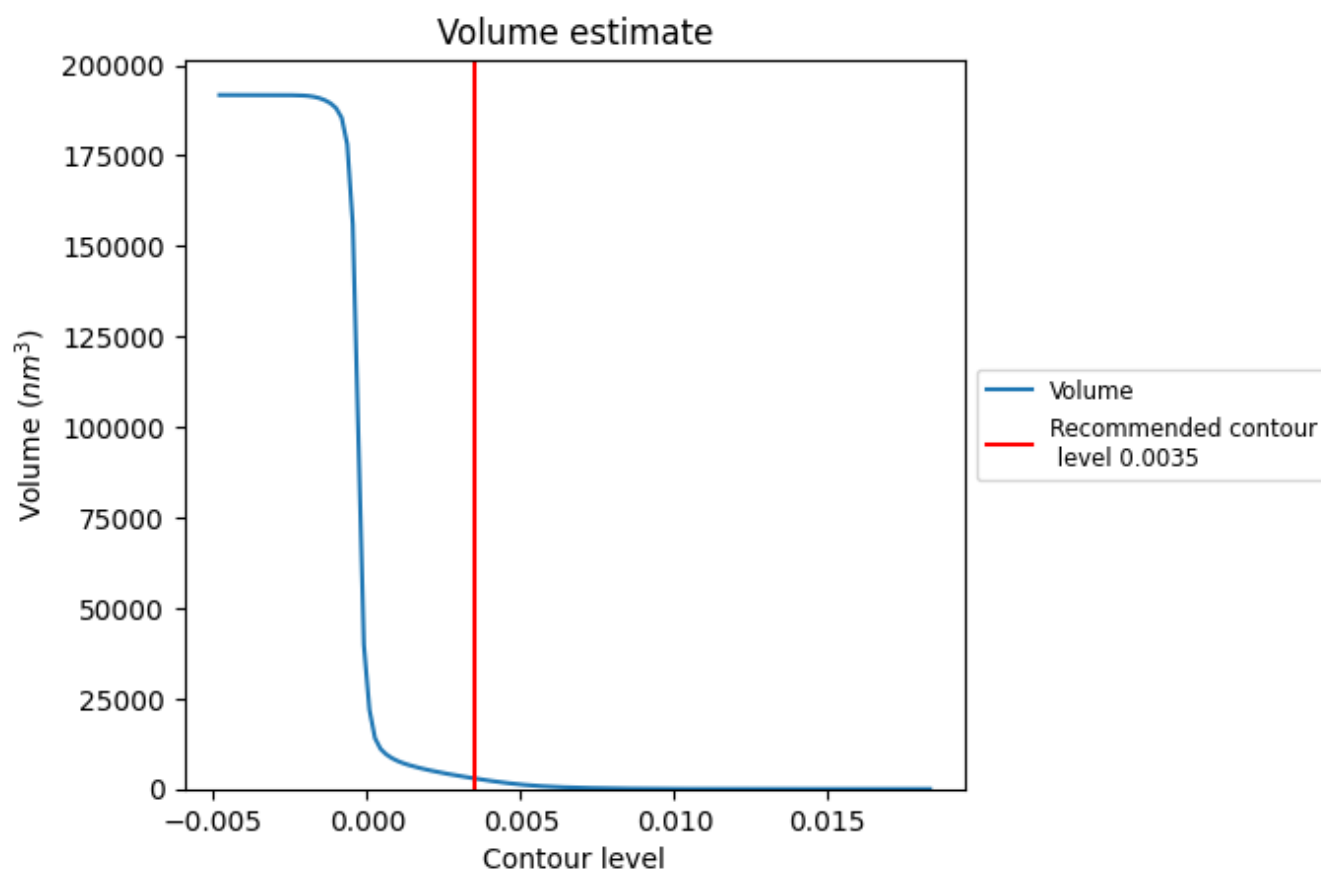
This section contains the results of statistical analysis of the map.

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.

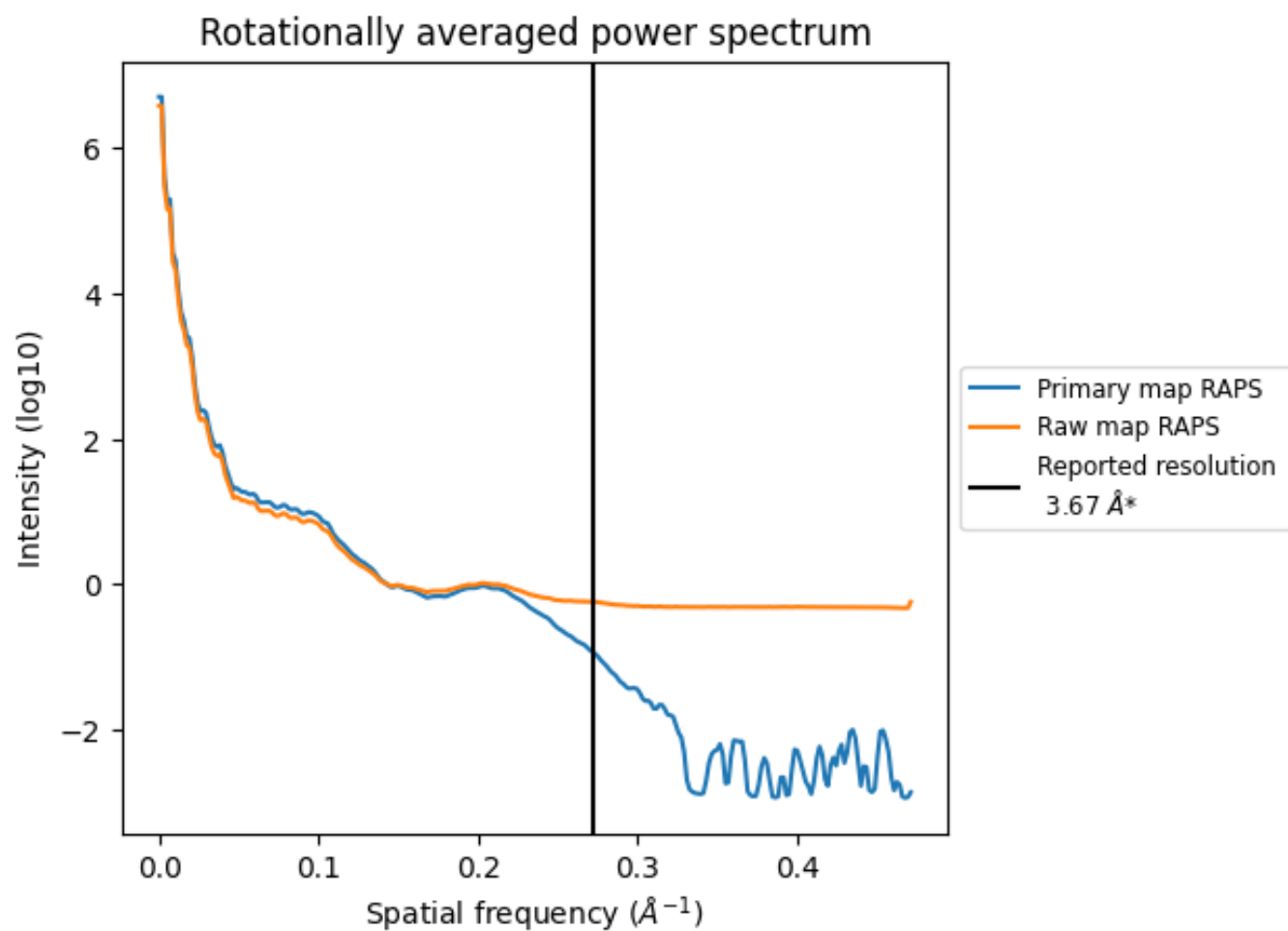
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2908 nm^3 ; this corresponds to an approximate mass of 2627 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 ⓘ

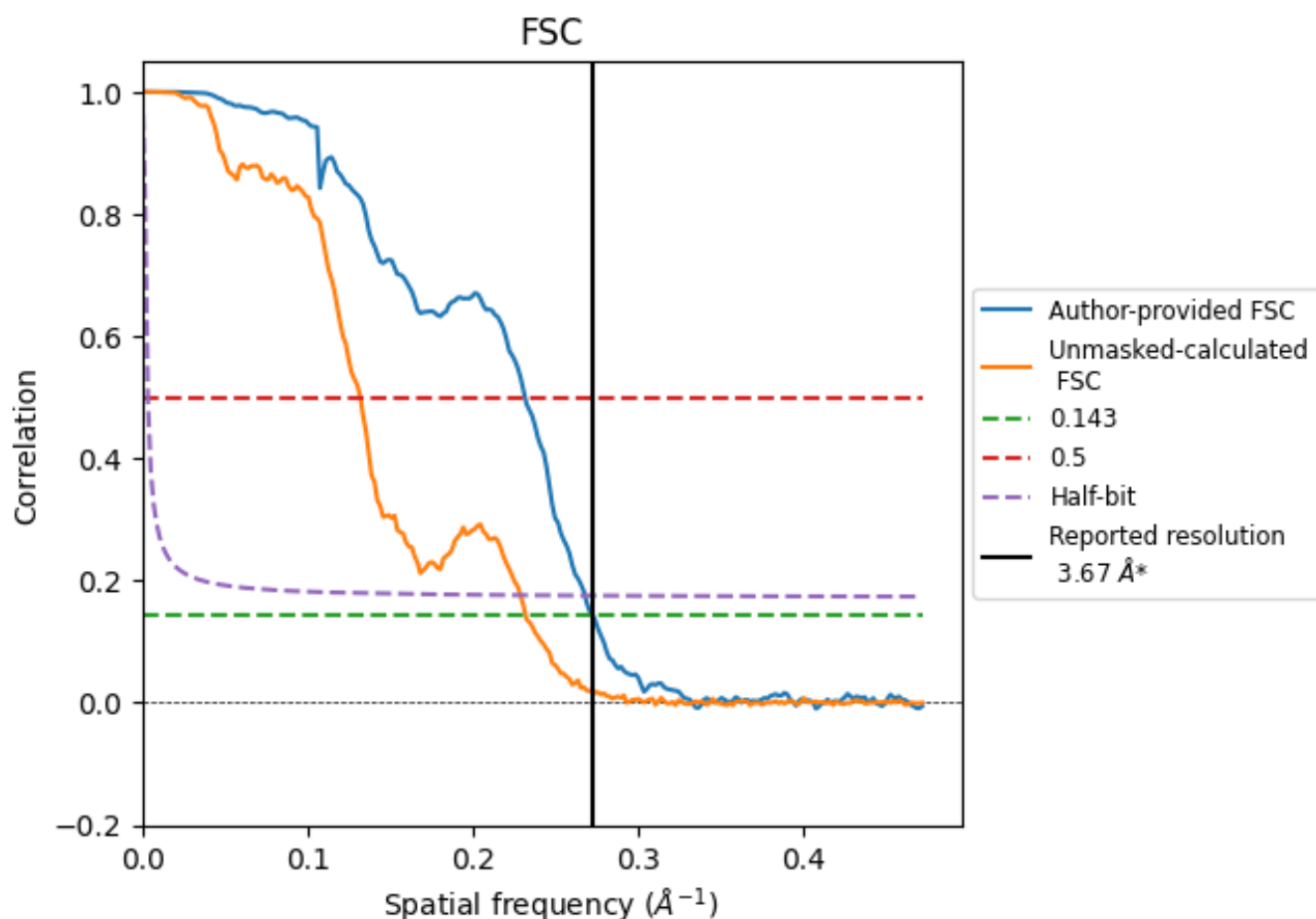


*Reported resolution corresponds to spatial frequency of 0.272 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.272 \AA^{-1}

8.2 Resolution estimates [i](#)

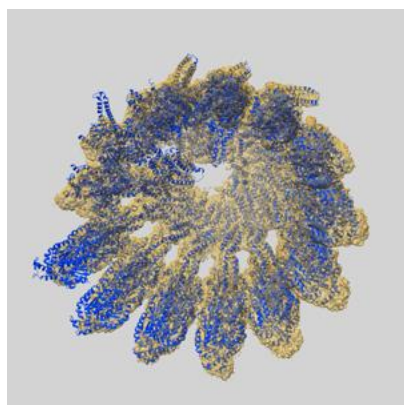
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.67	-	-
Author-provided FSC curve	3.67	4.32	3.74
Unmasked-calculated*	4.31	7.58	4.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.31 differs from the reported value 3.67 by more than 10 %

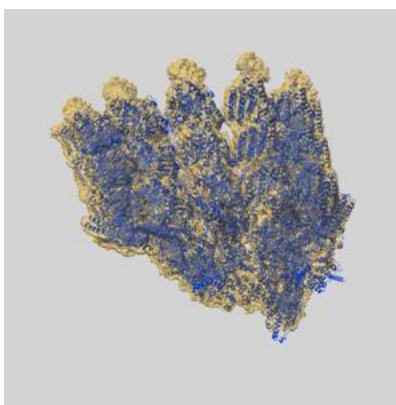
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55043 and PDB model 9SMX. Per-residue inclusion information can be found in section [3](#) on page [18](#).

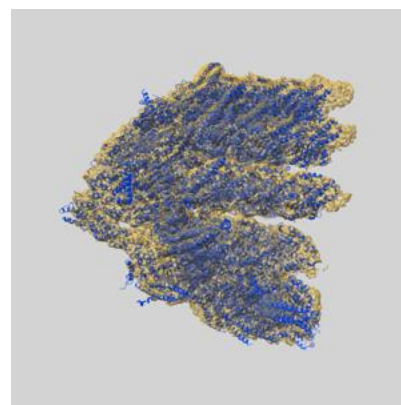
9.1 Map-model overlay [i](#)



X



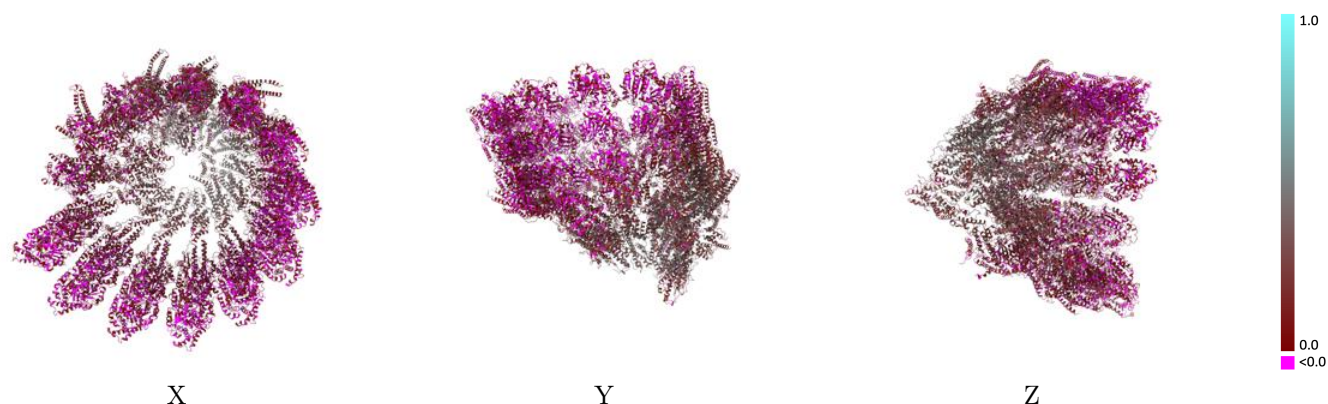
Y



Z

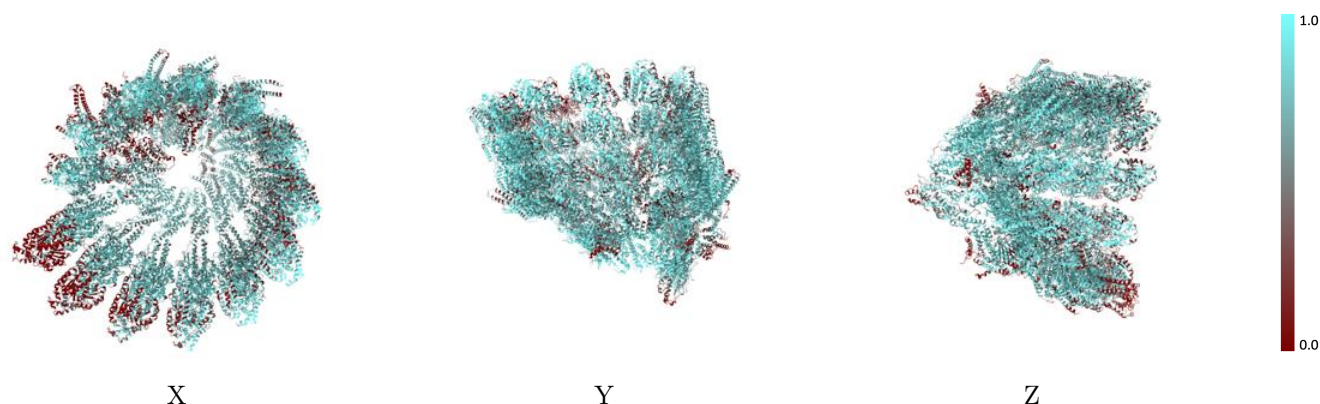
The images above show the 3D surface view of the map at the recommended contour level 0.0035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



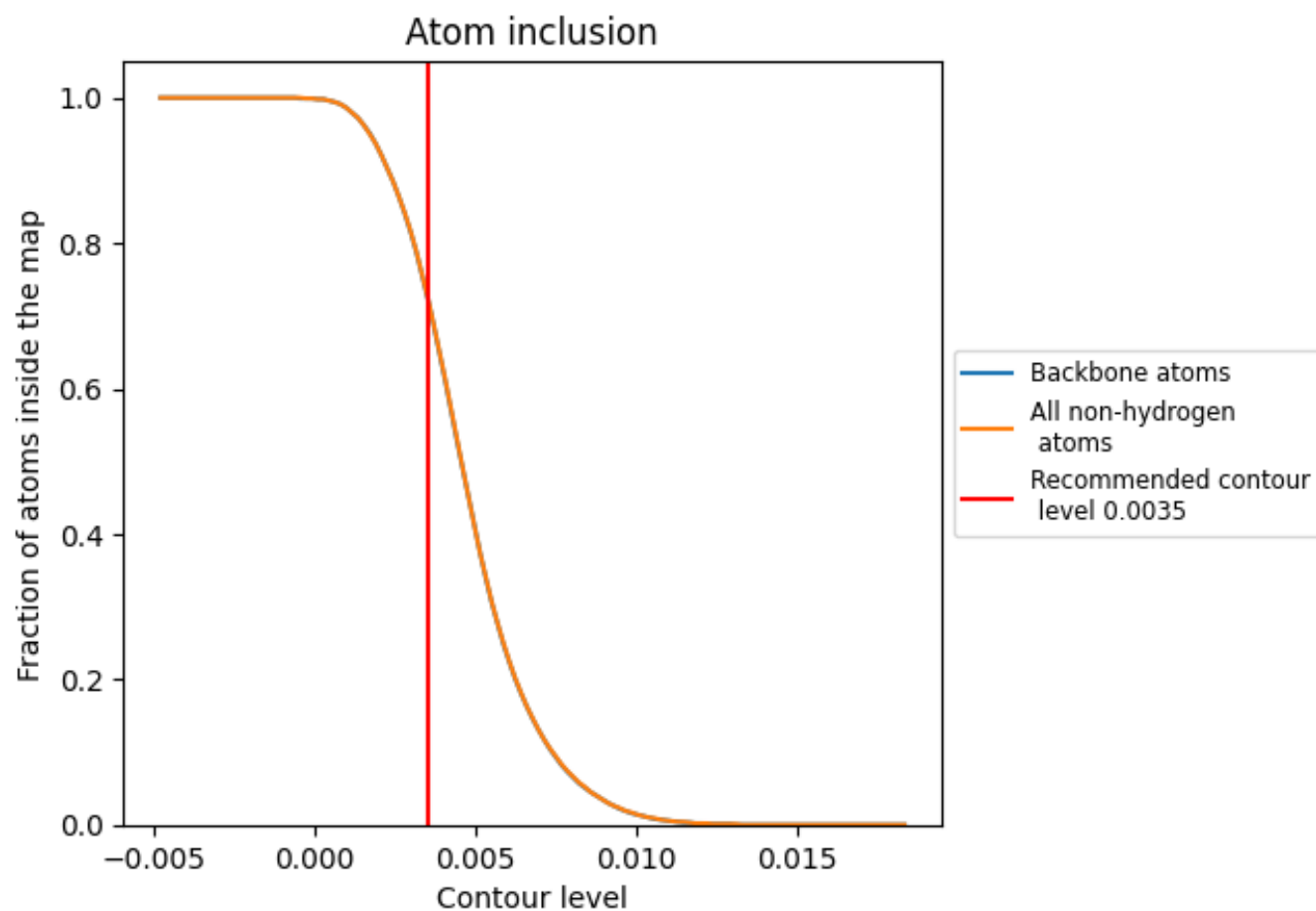
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 73% 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 (0.0035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7260	 0.1520
3	 0.6120	 0.2970
4	 0.6010	 0.3120
5	 0.6360	 0.3160
6	 0.5880	 0.2700
7	 0.5500	 0.3170
A	 0.6130	 0.2200
AC	 0.1350	 0.1170
B	 0.7470	 0.2800
BA	 0.8240	 0.1520
BB	 0.6900	 0.0940
C	 0.8470	 0.3500
CA	 0.8520	 0.1770
CB	 0.6320	 0.0890
CC	 0.7860	 0.3540
CM	 0.3140	 0.2820
CN	 0.3770	 0.2960
Cc	 0.6580	 0.2840
D	 0.8530	 0.3070
DA	 0.8090	 0.1050
DB	 0.6730	 0.0540
E	 0.8440	 0.3060
EA	 0.7400	 0.0250
EB	 0.6760	 0.0280
EC	 0.7970	 0.2830
EM	 0.5040	 0.2450
EN	 0.5150	 0.2460
Ec	 0.7190	 0.2440
F	 0.8050	 0.2250
FA	 0.7370	 0.0080
FB	 0.6850	 0.0250
G	 0.7990	 0.2080
GA	 0.7680	 0.0220
GB	 0.6920	 0.0550
GC	 0.5760	 -0.0220



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
GM	 0.3330	 0.1790
GN	 0.4490	 0.1740
Gc	 0.6530	 0.0270
H	 0.8090	 0.1930
HA	 0.8500	 0.0560
HB	 0.7060	 0.0320
I	 0.8350	 0.1960
IA	 0.9030	 0.0890
IB	 0.6010	 0.0440
J	 0.8710	 0.1980
JA	 0.8360	 0.0790
JB	 0.4190	 0.0430
K	 0.8450	 0.2030
KA	 0.7770	 0.0820
KB	 0.2310	 0.0460
L	 0.8150	 0.1690
LA	 0.6590	 0.0870
LB	 0.1320	 0.0520
M	 0.6680	 0.1690
MC	 0.7900	 0.1880
MM	 0.4600	 0.1280
Mc	 0.4860	 0.1430
N	 0.4480	 0.1520
Y	 0.6870	 0.1490
Z	 0.6420	 0.1230
a	 0.8050	 0.1550
b	 0.9140	 0.2940
c	 0.9030	 0.3170
d	 0.8570	 0.2520
e	 0.8100	 0.1670
f	 0.7440	 0.0590
g	 0.7410	 0.0580
h	 0.7920	 0.0810
i	 0.8250	 0.1060
j	 0.8860	 0.1370
k	 0.8430	 0.1400
l	 0.8340	 0.1560
m	 0.7720	 0.1230
n	 0.6630	 0.0980