Full wwPDB EM Validation Report ⓘ

Dec 9, 2021 – 03:33 pm GMT

PDB ID	:	7PQP
EMDB ID	:	EMD-7522
Title	:	tau-microtubule structural ensemble based on CryoEM data
Authors	:	Brotzakis, Z.F.; Vendruscolo, M.
Deposited on	:	2021-09-18
Resolution	:	4.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

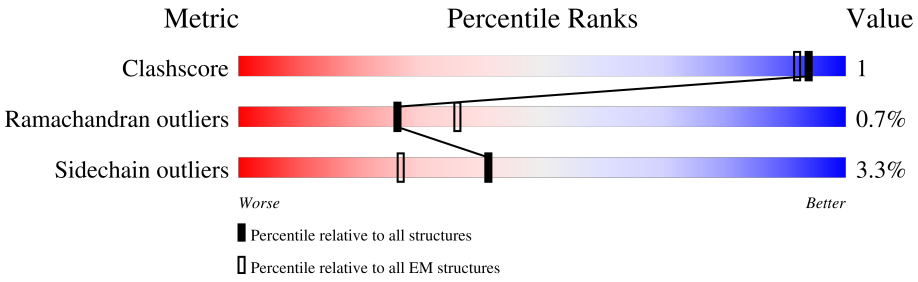
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	445	6% 82% 16% ·
1	C	445	5% 82% 16% ·
1	E	445	5% 86% 13% ·
1	G	445	6% 87% 12% ·
1	I	445	5% 85% 13% ·
1	K	445	5% 82% 16% ·
1	M	445	5% 82% 17% ·
2	B	451	8% 82% 17% ·

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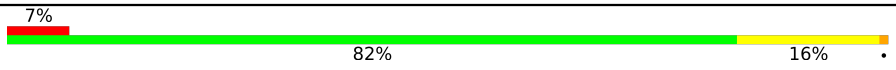
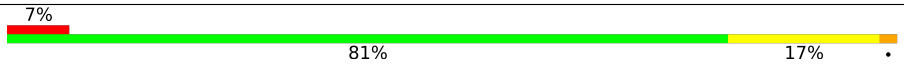
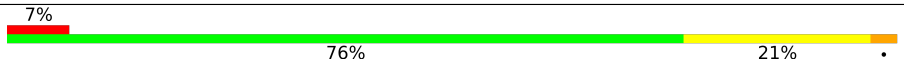
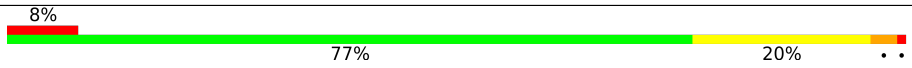
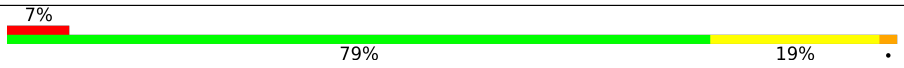
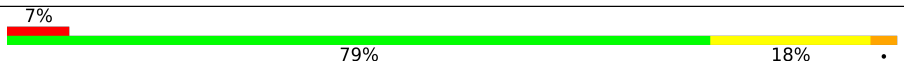
Mol	Chain	Length	Quality of chain
2	D	451	
2	F	451	
2	H	451	
2	J	451	
2	L	451	
2	N	451	
3	O	194	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 51036 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		
1	C	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		
1	E	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		
1	G	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		
1	I	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		
1	K	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		
1	M	445	Total	C	N	O	S	0	0
			3498	2189	595	688	26		

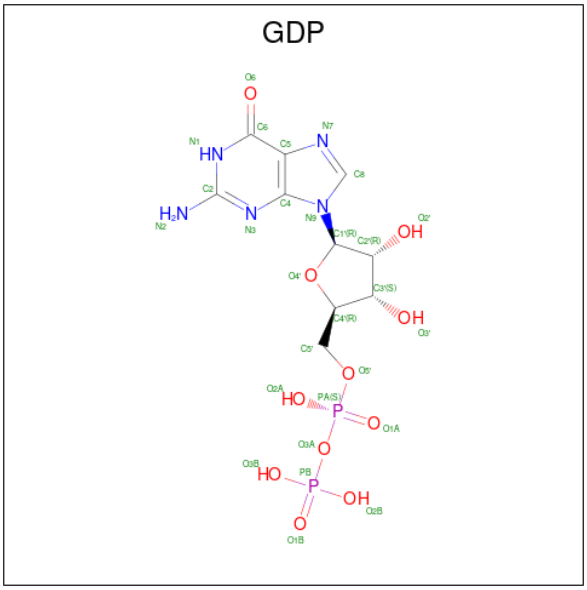
- Molecule 2 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		
2	D	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		
2	F	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		
2	H	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		
2	J	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		
2	L	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		
2	N	451	Total	C	N	O	S	0	0
			3524	2225	595	682	22		

- Molecule 3 is a protein called Isoform Tau-F of Microtubule-associated protein tau.

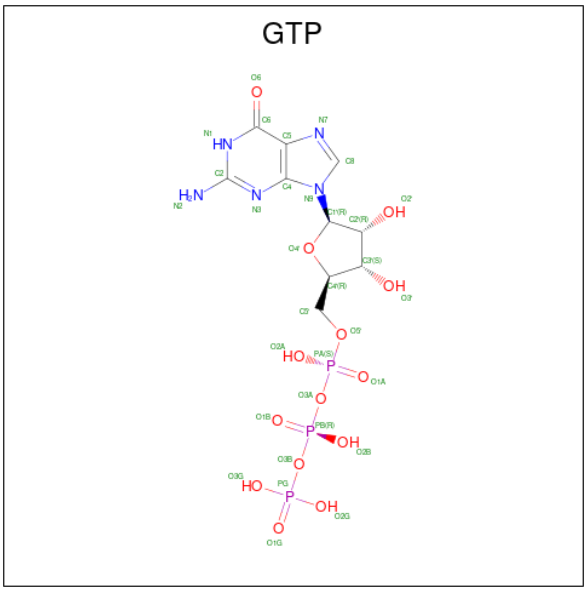
Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	194	Total	C	N	O	S	0	0
			1455	904	273	275	3		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	C	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	E	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	G	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	I	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	K	1	Total	C	N	O	P	0
			28	10	5	11	2	
4	M	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	F	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	H	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	J	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	L	1	Total	C	N	O	P	0
			32	10	5	14	3	
5	N	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	
6	D	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	
6	H	1	Total	Mg	0
			1	1	

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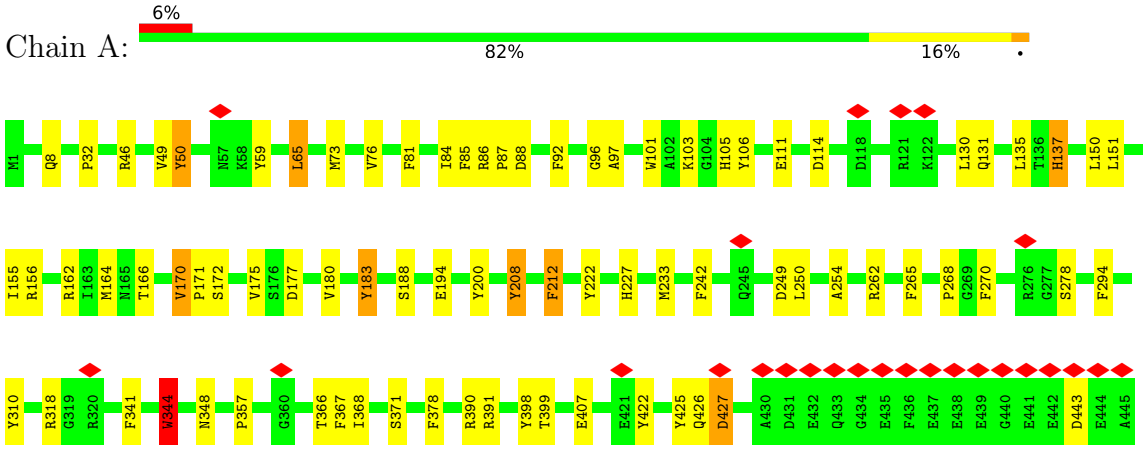
Mol	Chain	Residues	Atoms	AltConf
6	J	1	Total Mg 1 1	0
6	L	1	Total Mg 1 1	0
6	N	1	Total Mg 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

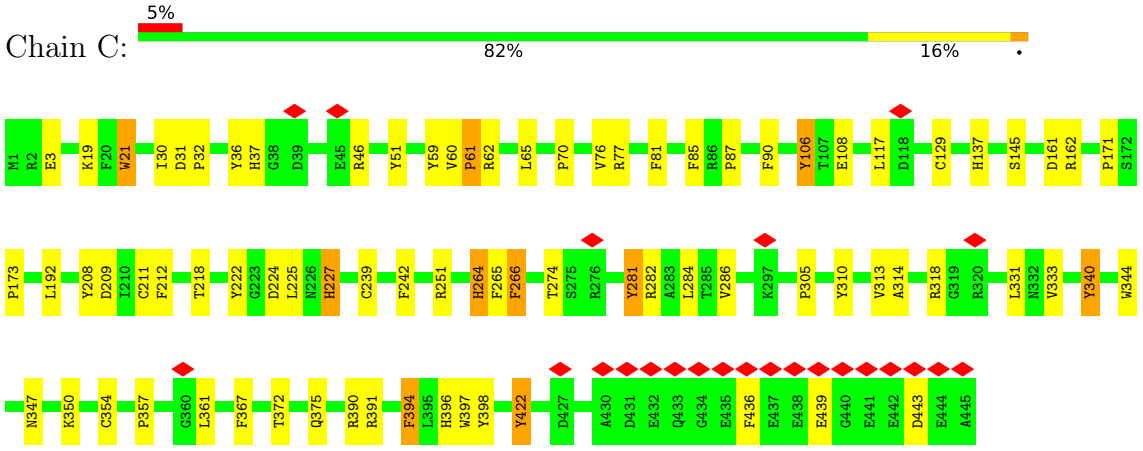
• Molecule 1: Tubulin beta chain

Chain A:



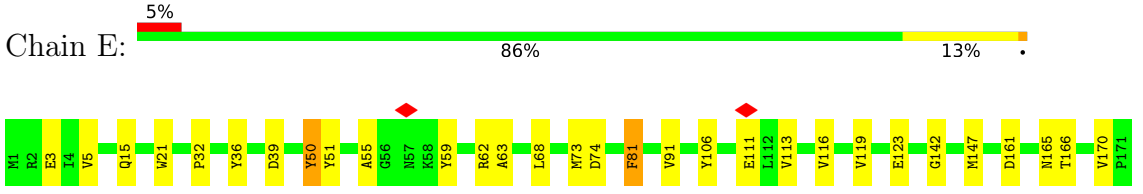
• Molecule 1: Tubulin beta chain

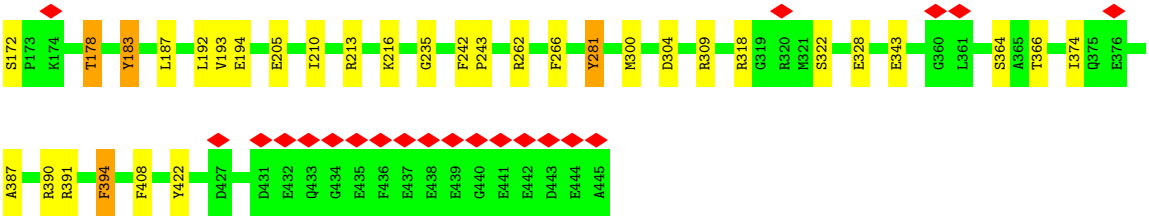
Chain C:



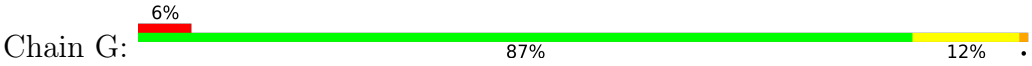
• Molecule 1: Tubulin beta chain

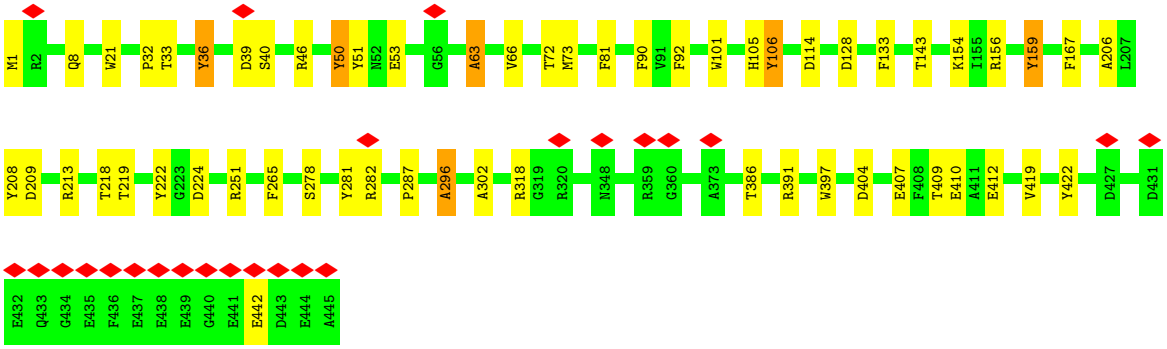
Chain E:



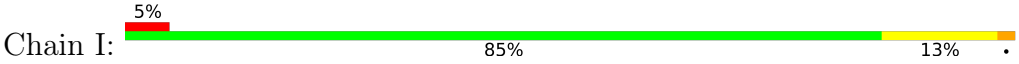


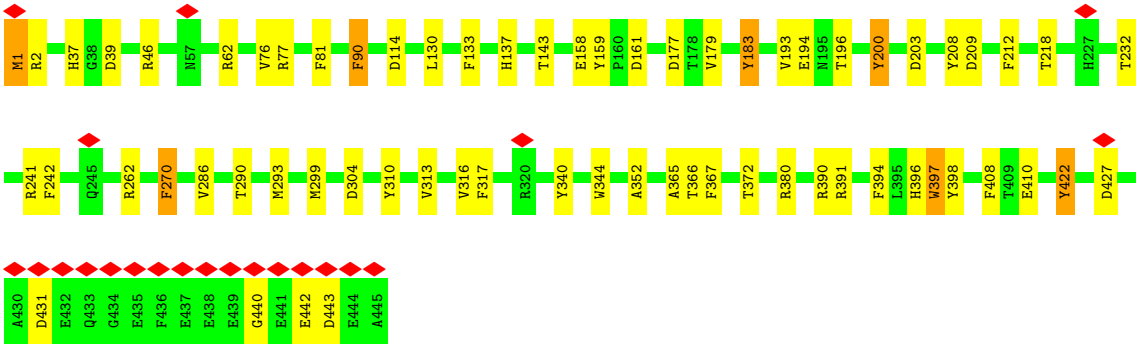
• Molecule 1: Tubulin beta chain



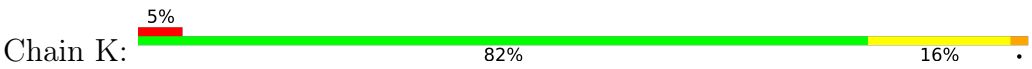


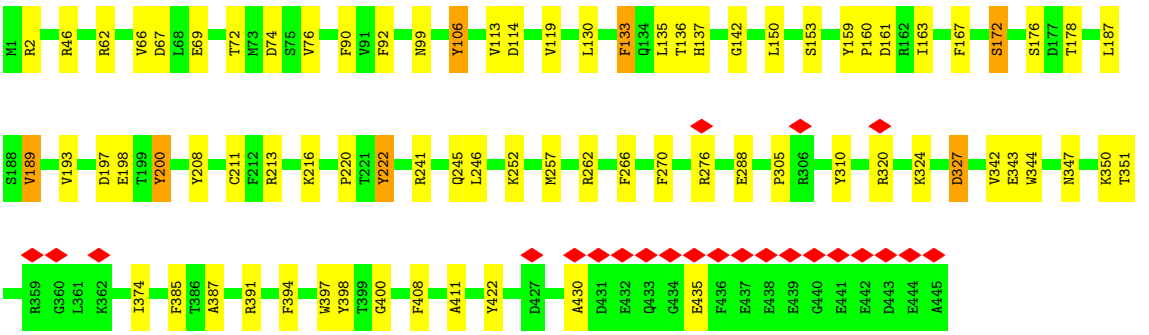
• Molecule 1: Tubulin beta chain





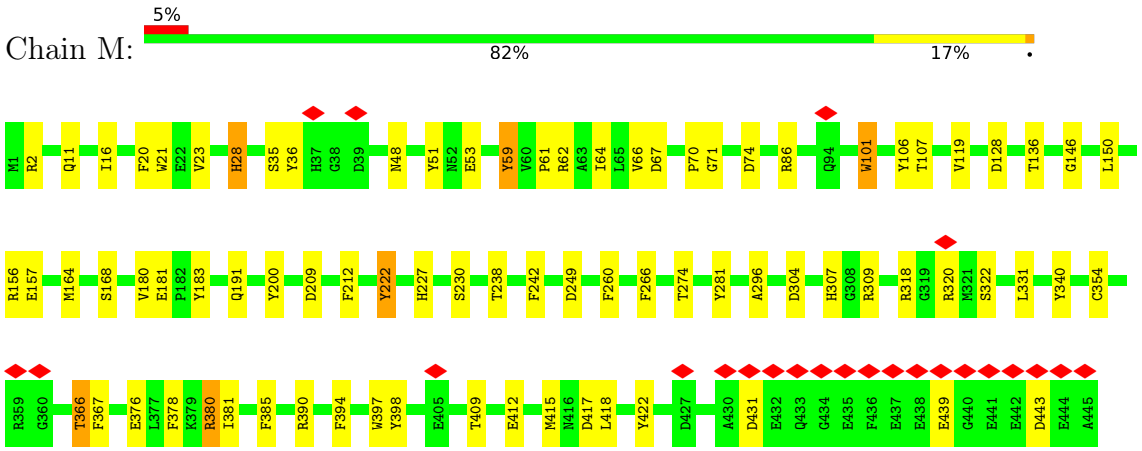
• Molecule 1: Tubulin beta chain





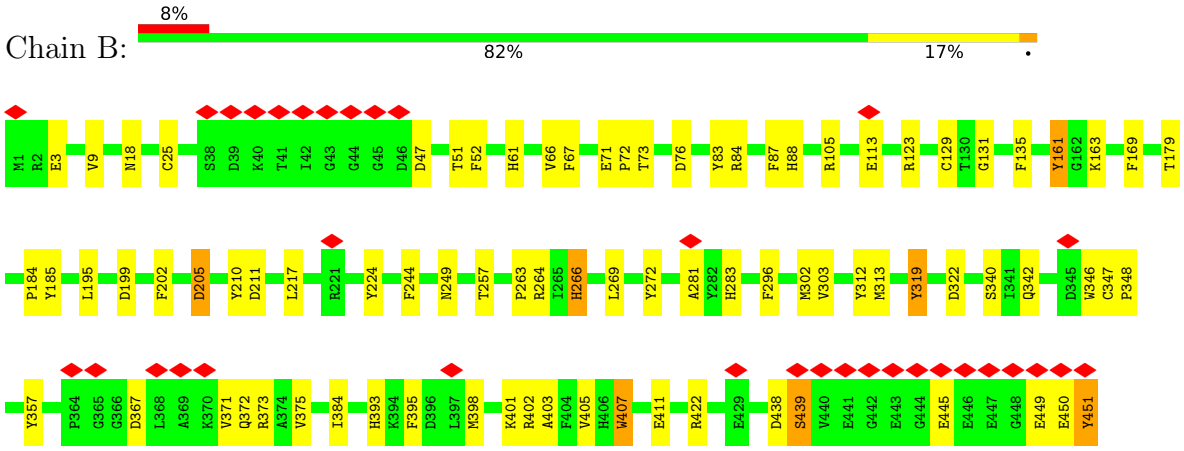
• Molecule 1: Tubulin beta chain

Chain M:



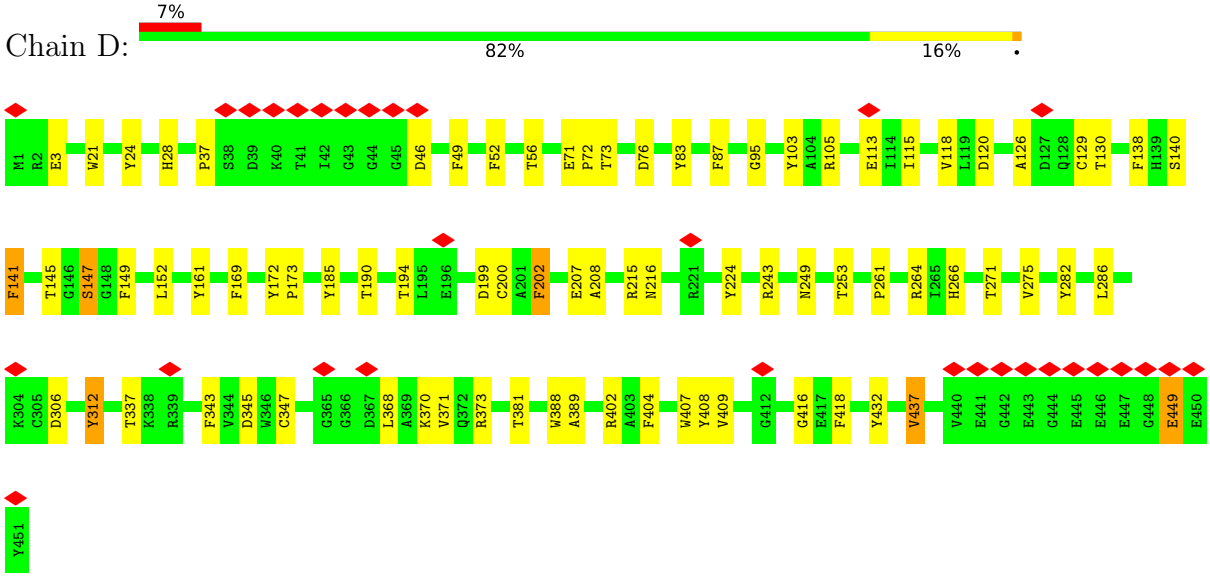
• Molecule 2: Tubulin alpha-1B chain

Chain B:



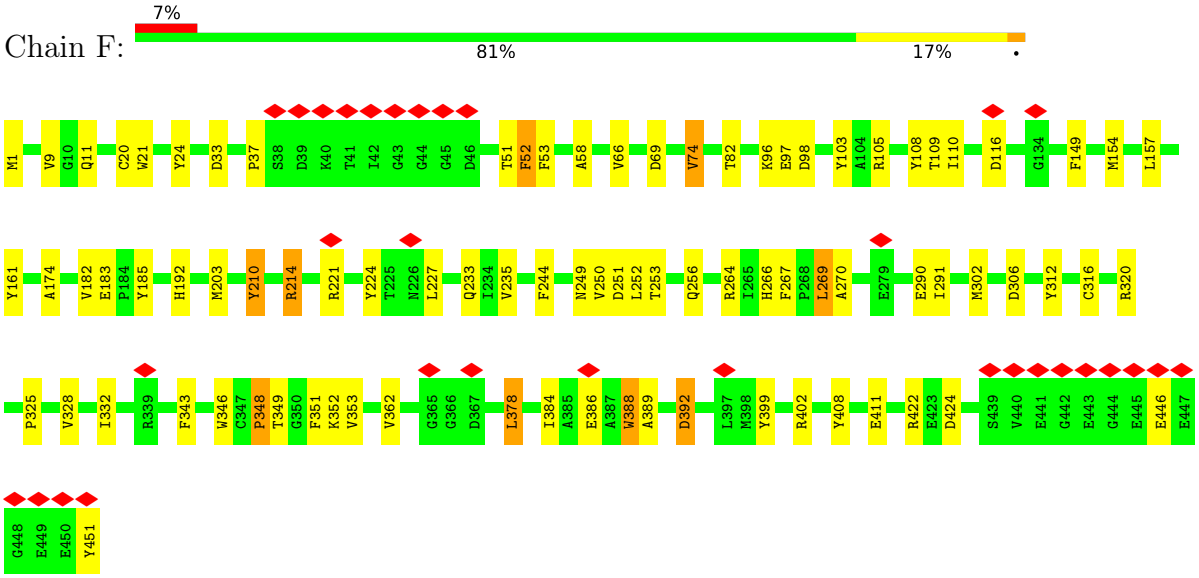
• Molecule 2: Tubulin alpha-1B chain

Chain D:



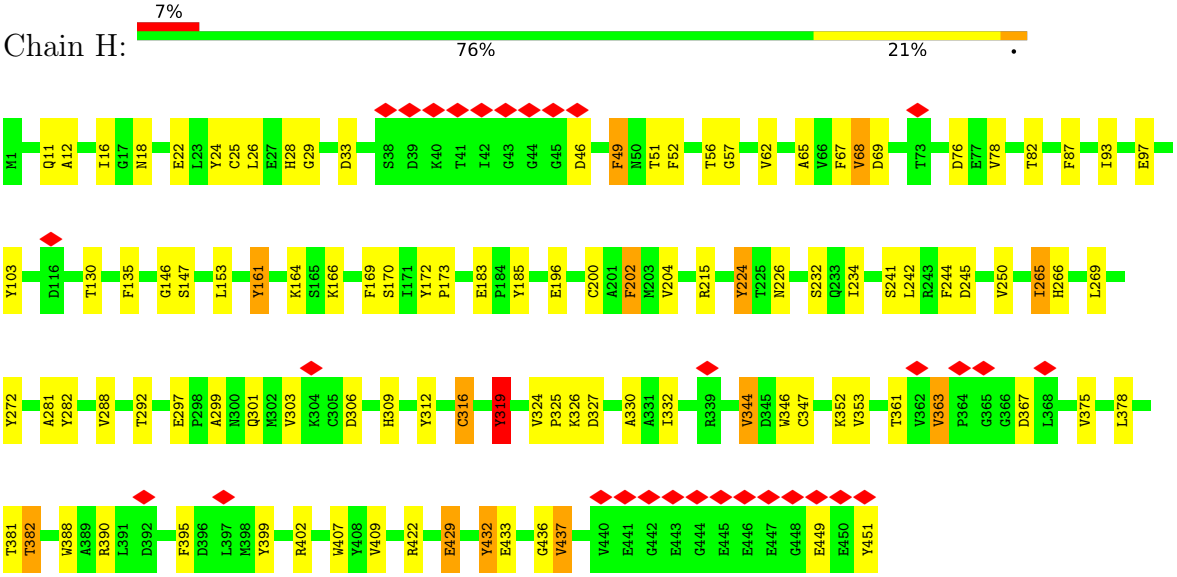
• Molecule 2: Tubulin alpha-1B chain

Chain F:



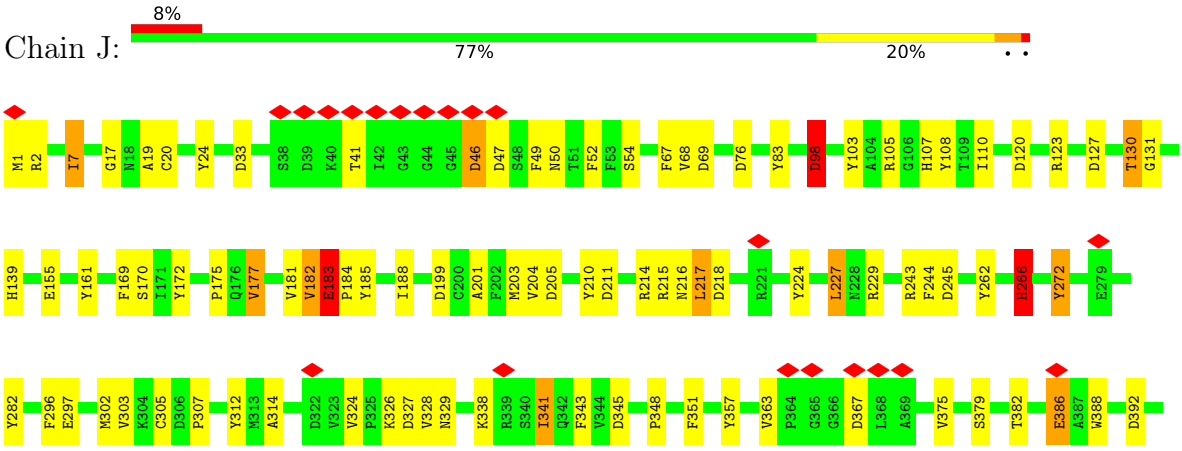
• Molecule 2: Tubulin alpha-1B chain

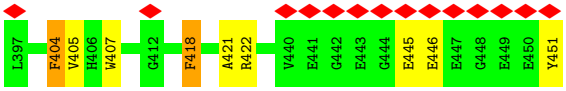
Chain H:



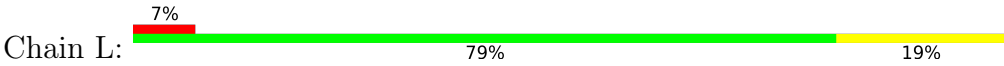
• Molecule 2: Tubulin alpha-1B chain

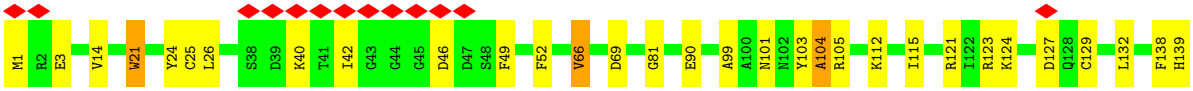
Chain J:

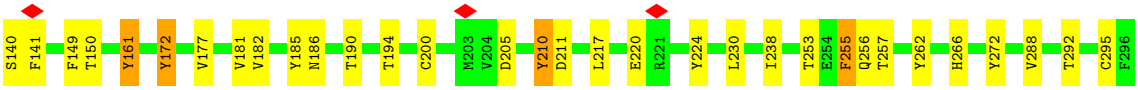


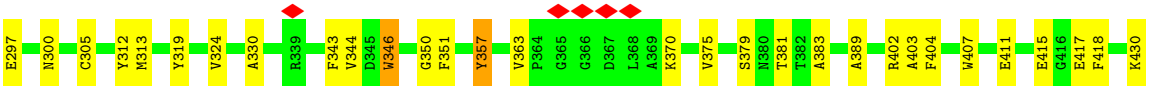


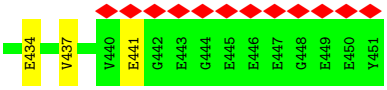
• Molecule 2: Tubulin alpha-1B chain



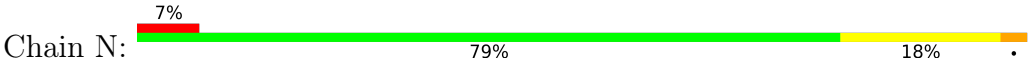


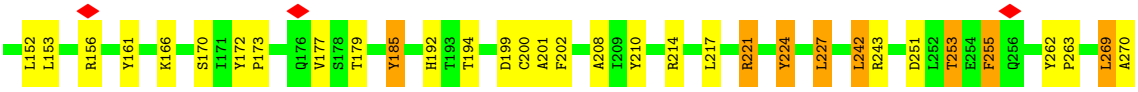


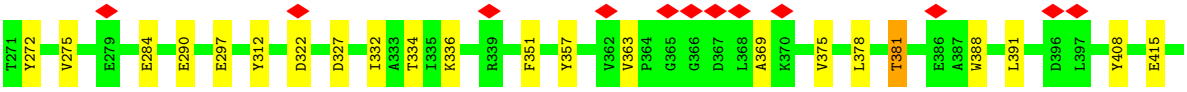


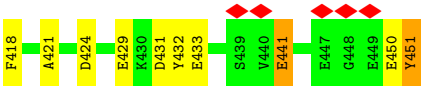


• Molecule 2: Tubulin alpha-1B chain

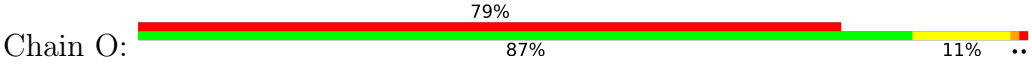


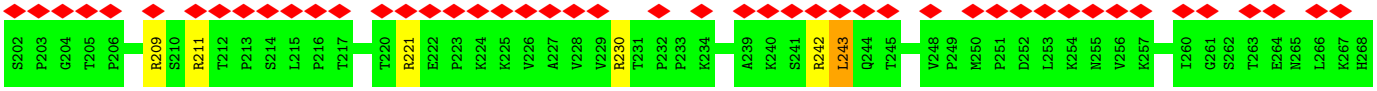


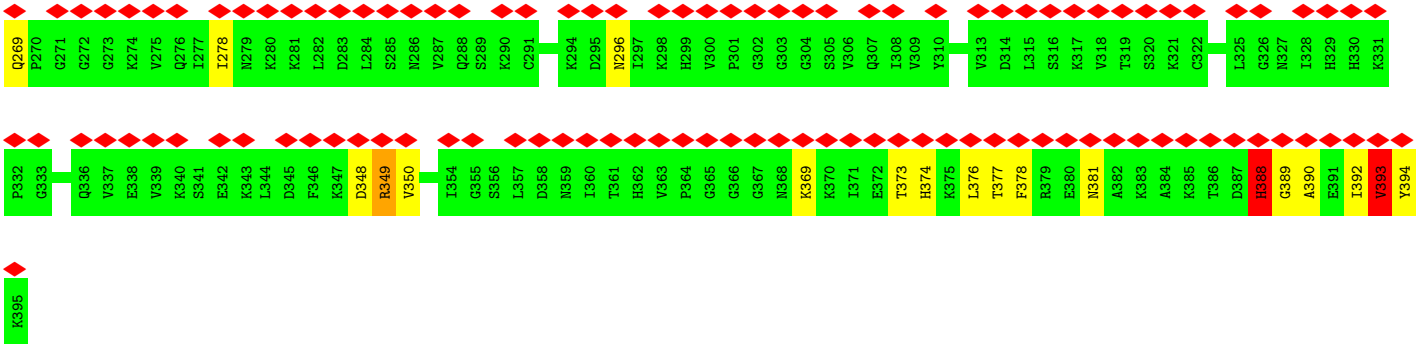




• Molecule 3: Isoform Tau-F of Microtubule-associated protein tau






Q269 P270 G271 G272 G273 K274 V275 Q276 I277 I278 N279 K280 K281 L282 D283 L284 S285 N286 V287 Q288 S289 K290 C291 K294 D295 N296 I297 K298 H299 V300 P301 G302 G303 G304 S305 V306 Q307 I308 V309 Y310 V313 D314 L315 S316 K317 V318 T319 S320 K321 C322 L325 G326 N327 I328 H329 H330 K331
P332 G333 Q336 V337 E338 V339 K340 S341 E342 K343 L344 D345 F346 K347 D348 R349 V350 I354 G355 S356 L357 D358 N359 I360 T361 H362 V363 P364 G365 G366 G367 N368 K369 K370 I371 E372 T373 H374 K375 L376 T377 F378 R379 E380 N381 A382 K383 A384 K385 T386 D387 H388 G389 A390 E391 I392 V393 Y394
K395

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25963	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Images were drift-corrected using UCSF motioncorr software . CTFFIND4 was used to estimate CTFs for the drift-corrected images	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.789	Depositor
Minimum map value	-4.020	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.413	Depositor
Recommended contour level	1.26	Depositor
Map size (Å)	675.84, 675.84, 675.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.60	1/3574 (0.0%)	1.78	59/4839 (1.2%)
1	C	0.64	4/3574 (0.1%)	1.75	68/4839 (1.4%)
1	E	0.63	2/3574 (0.1%)	1.64	46/4839 (1.0%)
1	G	0.61	0/3574	1.64	51/4839 (1.1%)
1	I	0.63	1/3574 (0.0%)	1.59	60/4839 (1.2%)
1	K	0.62	1/3574 (0.0%)	1.78	71/4839 (1.5%)
1	M	0.60	1/3574 (0.0%)	1.77	64/4839 (1.3%)
2	B	0.60	0/3603	1.73	69/4889 (1.4%)
2	D	0.61	1/3603 (0.0%)	1.76	66/4889 (1.3%)
2	F	0.57	0/3603	1.80	76/4889 (1.6%)
2	H	0.59	0/3603	1.84	84/4889 (1.7%)
2	J	0.57	0/3603	1.85	87/4889 (1.8%)
2	L	0.57	0/3603	1.84	81/4889 (1.7%)
2	N	0.58	2/3603 (0.1%)	1.88	79/4889 (1.6%)
3	O	0.67	0/1483	1.21	15/1996 (0.8%)
All	All	0.60	13/51722 (0.0%)	1.75	976/70092 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	C	0	10
1	E	0	7
1	G	0	5
1	I	0	6
1	K	0	4
1	M	0	9
2	B	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	8
2	F	0	11
2	H	0	8
2	J	0	11
2	L	0	12
2	N	0	12
All	All	0	122

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	TRP	CZ3-CH2	9.41	1.55	1.40
1	K	397	TRP	CZ3-CH2	7.37	1.51	1.40
1	E	343	GLU	CD-OE2	-7.24	1.17	1.25
1	C	3	GLU	CD-OE2	-7.05	1.17	1.25
2	D	21	TRP	CZ3-CH2	6.68	1.50	1.40
1	I	344	TRP	CZ3-CH2	-6.61	1.29	1.40
1	C	21	TRP	CZ3-CH2	6.54	1.50	1.40
2	N	388	TRP	CZ3-CH2	6.21	1.50	1.40
1	C	129	CYS	C-O	-6.09	1.11	1.23
2	N	21	TRP	CZ3-CH2	5.91	1.49	1.40
1	C	3	GLU	CD-OE1	-5.67	1.19	1.25
1	M	397	TRP	CZ3-CH2	5.57	1.49	1.40
1	E	343	GLU	CD-OE1	-5.23	1.19	1.25

All (976) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	422	TYR	CB-CG-CD2	-15.72	111.57	121.00
2	N	172	TYR	CB-CG-CD2	-15.33	111.80	121.00
2	H	185	TYR	CB-CG-CD2	-15.17	111.90	121.00
2	J	69	ASP	CB-CG-OD2	15.00	131.80	118.30
1	A	183	TYR	CB-CG-CD2	-14.71	112.17	121.00
1	C	340	TYR	CB-CG-CD2	-14.03	112.58	121.00
2	D	224	TYR	CB-CG-CD2	-12.56	113.46	121.00
1	G	106	TYR	CB-CG-CD1	-12.56	113.47	121.00
2	D	172	TYR	CB-CG-CD1	-12.04	113.77	121.00
2	D	24	TYR	CB-CG-CD2	-11.99	113.81	121.00
2	D	282	TYR	CB-CG-CD1	-11.84	113.90	121.00
2	D	141	PHE	CB-CG-CD1	-11.76	112.57	120.80
1	E	106	TYR	CB-CG-CD2	-11.73	113.96	121.00
2	N	202	PHE	CB-CG-CD1	-11.71	112.61	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	149	PHE	CB-CG-CD1	-11.38	112.83	120.80
1	G	422	TYR	CB-CG-CD1	-11.36	114.19	121.00
2	B	161	TYR	CG-CD1-CE1	-11.35	112.22	121.30
2	J	67	PHE	CB-CG-CD2	-11.02	113.08	120.80
2	D	264	ARG	NE-CZ-NH1	11.01	125.80	120.30
1	G	50	TYR	CB-CG-CD2	-10.87	114.48	121.00
1	K	422	TYR	CB-CG-CD1	10.62	127.37	121.00
1	E	281	TYR	CB-CG-CD2	-10.54	114.68	121.00
2	L	346	TRP	CD1-NE1-CE2	10.43	118.39	109.00
2	B	244	PHE	CB-CG-CD1	-10.39	113.53	120.80
1	M	385	PHE	CB-CG-CD2	10.29	128.00	120.80
1	M	200	TYR	CB-CG-CD2	-10.20	114.88	121.00
2	J	296	PHE	CB-CG-CD1	-10.14	113.70	120.80
2	J	24	TYR	CB-CG-CD1	10.10	127.06	121.00
1	A	294	PHE	CB-CG-CD1	-10.04	113.77	120.80
2	H	183	GLU	OE1-CD-OE2	-10.04	111.25	123.30
1	K	90	PHE	CB-CG-CD1	-10.02	113.79	120.80
1	M	378	PHE	CB-CG-CD1	-10.01	113.80	120.80
1	K	270	PHE	CB-CG-CD2	-9.96	113.83	120.80
2	J	69	ASP	OD1-CG-OD2	-9.94	104.41	123.30
1	M	443	ASP	CB-CG-OD2	9.89	127.20	118.30
2	H	69	ASP	CB-CG-OD2	9.85	127.17	118.30
1	A	222	TYR	CB-CG-CD1	-9.84	115.10	121.00
1	K	320	ARG	CD-NE-CZ	9.80	137.32	123.60
1	C	51	TYR	CB-CG-CD1	-9.80	115.12	121.00
2	J	451	TYR	CB-CG-CD1	-9.76	115.15	121.00
2	F	348	PRO	N-CA-CB	9.70	114.94	103.30
2	L	343	PHE	CB-CG-CD1	-9.60	114.08	120.80
3	O	230	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	M	394	PHE	CB-CG-CD2	-9.53	114.13	120.80
1	A	341	PHE	CB-CG-CD2	-9.41	114.21	120.80
2	J	103	TYR	CB-CG-CD1	-9.38	115.37	121.00
2	F	267	PHE	CB-CG-CD2	-9.32	114.27	120.80
1	K	106	TYR	CG-CD1-CE1	-9.28	113.87	121.30
2	L	210	TYR	CB-CG-CD2	-9.19	115.48	121.00
2	N	415	GLU	OE1-CD-OE2	-9.19	112.28	123.30
2	L	52	PHE	CB-CG-CD1	-9.14	114.40	120.80
2	L	418	PHE	CB-CG-CD1	-9.09	114.43	120.80
1	E	213	ARG	CD-NE-CZ	9.09	136.33	123.60
2	B	357	TYR	CB-CG-CD1	-9.08	115.55	121.00
1	C	90	PHE	CB-CG-CD2	-9.04	114.47	120.80
2	N	2	ARG	CD-NE-CZ	9.03	136.25	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	208	TYR	CB-CG-CD1	-9.02	115.59	121.00
1	K	270	PHE	CB-CG-CD1	8.95	127.07	120.80
2	L	312	TYR	CB-CG-CD2	-8.92	115.65	121.00
2	J	367	ASP	CB-CG-OD2	8.85	126.26	118.30
2	F	103	TYR	CB-CG-CD1	-8.84	115.69	121.00
3	O	243	LEU	CB-CG-CD1	8.74	125.85	111.00
1	E	39	ASP	CB-CG-OD1	8.73	126.16	118.30
1	M	266	PHE	CB-CG-CD1	-8.73	114.69	120.80
1	E	106	TYR	CB-CG-CD1	8.70	126.22	121.00
2	L	141	PHE	CB-CG-CD2	-8.69	114.72	120.80
1	A	443	ASP	CB-CG-OD2	8.67	126.11	118.30
1	I	203	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	M	366	THR	CA-CB-CG2	8.60	124.43	112.40
2	B	83	TYR	CB-CG-CD1	-8.58	115.85	121.00
2	B	161	TYR	CB-CG-CD1	-8.57	115.86	121.00
2	B	47	ASP	CB-CG-OD1	8.50	125.95	118.30
1	A	183	TYR	CB-CG-CD1	8.49	126.10	121.00
2	F	24	TYR	CB-CG-CD2	-8.46	115.93	121.00
2	F	52	PHE	CB-CG-CD1	-8.42	114.90	120.80
1	G	222	TYR	CG-CD2-CE2	-8.40	114.58	121.30
1	C	398	TYR	CB-CG-CD2	-8.40	115.96	121.00
1	G	265	PHE	CB-CG-CD1	8.37	126.66	120.80
1	A	341	PHE	CB-CG-CD1	8.37	126.66	120.80
1	C	340	TYR	CD1-CG-CD2	8.36	127.10	117.90
1	I	317	PHE	CB-CG-CD1	-8.36	114.95	120.80
1	K	46	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	C	281	TYR	CB-CG-CD1	-8.35	115.99	121.00
1	M	222	TYR	CB-CG-CD1	-8.34	115.99	121.00
1	A	398	TYR	CB-CG-CD1	-8.32	116.01	121.00
2	H	33	ASP	CB-CG-OD1	8.29	125.76	118.30
2	D	202	PHE	CB-CG-CD1	8.29	126.60	120.80
2	F	210	TYR	CB-CG-CD2	-8.28	116.03	121.00
2	B	224	TYR	CB-CG-CD1	8.18	125.91	121.00
1	M	417	ASP	CB-CG-OD2	-8.17	110.94	118.30
2	B	407	TRP	CE2-CD2-CG	8.16	113.83	107.30
1	C	224	ASP	CB-CG-OD2	8.16	125.64	118.30
2	H	87	PHE	CB-CG-CD2	-8.12	115.11	120.80
2	B	105	ARG	NE-CZ-NH1	8.12	124.36	120.30
2	N	52	PHE	CB-CG-CD2	8.10	126.47	120.80
1	A	81	PHE	CB-CG-CD1	8.09	126.46	120.80
2	F	98	ASP	CB-CG-OD1	8.08	125.57	118.30
1	C	208	TYR	CB-CG-CD1	-8.07	116.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	ASP	CB-CG-OD1	8.06	125.56	118.30
2	L	14	VAL	CA-CB-CG1	8.06	122.99	110.90
2	J	127	ASP	CB-CG-OD2	8.05	125.55	118.30
2	L	255	PHE	CB-CG-CD2	-8.04	115.17	120.80
2	L	434	GLU	OE1-CD-OE2	-8.02	113.67	123.30
2	H	422	ARG	NE-CZ-NH1	8.02	124.31	120.30
2	N	351	PHE	CB-CG-CD1	-8.02	115.19	120.80
1	E	178	THR	CA-CB-CG2	8.00	123.59	112.40
1	G	404	ASP	CB-CG-OD1	-7.99	111.11	118.30
2	N	69	ASP	CB-CG-OD2	7.97	125.47	118.30
2	J	272	TYR	CB-CG-CD1	-7.94	116.23	121.00
2	D	224	TYR	CB-CG-CD1	7.92	125.75	121.00
2	J	33	ASP	CB-CG-OD1	7.91	125.42	118.30
1	M	318	ARG	NE-CZ-NH1	7.91	124.25	120.30
2	D	408	TYR	CB-CG-CD1	-7.90	116.26	121.00
2	H	272	TYR	CB-CG-CD2	-7.90	116.26	121.00
2	F	21	TRP	CD1-CG-CD2	-7.85	100.02	106.30
2	N	172	TYR	CG-CD2-CE2	-7.85	115.02	121.30
2	N	172	TYR	CD1-CG-CD2	7.85	126.53	117.90
2	F	267	PHE	CB-CG-CD1	7.83	126.28	120.80
2	B	407	TRP	CD1-CG-CD2	-7.83	100.04	106.30
2	J	199	ASP	CB-CG-OD2	7.83	125.35	118.30
2	J	404	PHE	CB-CG-CD1	-7.82	115.33	120.80
1	A	81	PHE	CB-CG-CD2	-7.79	115.35	120.80
2	L	346	TRP	CG-CD1-NE1	-7.79	102.31	110.10
2	N	322	ASP	CB-CG-OD1	7.77	125.29	118.30
1	M	23	VAL	CA-CB-CG1	7.75	122.53	110.90
2	F	52	PHE	CB-CG-CD2	7.73	126.21	120.80
1	C	62	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	C	340	TYR	CG-CD2-CE2	-7.71	115.13	121.30
2	J	451	TYR	CB-CG-CD2	7.71	125.62	121.00
2	H	76	ASP	CB-CG-OD1	7.70	125.23	118.30
1	K	72	THR	CA-CB-CG2	7.68	123.16	112.40
2	H	312	TYR	CB-CG-CD1	7.68	125.61	121.00
2	N	102	ASN	N-CA-CB	-7.68	96.78	110.60
2	N	77	GLU	OE1-CD-OE2	-7.67	114.09	123.30
2	J	205	ASP	CB-CG-OD1	7.66	125.19	118.30
1	I	212	PHE	CB-CG-CD2	-7.64	115.45	120.80
2	J	98	ASP	CB-CG-OD2	7.64	125.18	118.30
1	A	151	LEU	CB-CG-CD2	-7.64	98.02	111.00
1	K	74	ASP	CB-CG-OD2	7.64	125.17	118.30
1	K	2	ARG	NE-CZ-NH1	7.63	124.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	408	PHE	CB-CG-CD1	-7.63	115.46	120.80
1	K	288	GLU	OE1-CD-OE2	-7.62	114.16	123.30
2	H	451	TYR	CB-CG-CD2	-7.61	116.44	121.00
1	E	74	ASP	CB-CG-OD2	7.59	125.14	118.30
2	H	312	TYR	CB-CG-CD2	-7.52	116.49	121.00
2	L	104	ALA	CB-CA-C	7.51	121.37	110.10
2	H	433	GLU	OE1-CD-OE2	-7.49	114.31	123.30
1	M	398	TYR	CB-CG-CD2	-7.49	116.51	121.00
2	L	161	TYR	CB-CG-CD1	-7.47	116.52	121.00
1	M	74	ASP	CB-CG-OD1	7.47	125.02	118.30
2	J	303	VAL	CA-CB-CG1	-7.46	99.70	110.90
1	M	209	ASP	CB-CG-OD1	-7.46	111.58	118.30
2	F	424	ASP	CB-CG-OD1	7.46	125.01	118.30
2	H	388	TRP	CA-CB-CG	7.45	127.85	113.70
2	H	363	VAL	CG1-CB-CG2	-7.42	99.03	110.90
2	F	402	ARG	NE-CZ-NH1	7.42	124.01	120.30
3	O	209	ARG	NE-CZ-NH1	7.41	124.01	120.30
2	D	52	PHE	CB-CG-CD2	7.41	125.99	120.80
1	K	161	ASP	CB-CG-OD2	7.41	124.97	118.30
2	H	135	PHE	CB-CG-CD2	-7.41	115.62	120.80
1	K	69	GLU	OE1-CD-OE2	-7.41	114.41	123.30
2	J	312	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	M	394	PHE	CB-CG-CD1	7.40	125.98	120.80
2	J	245	ASP	CB-CG-OD2	7.39	124.95	118.30
2	F	392	ASP	CB-CG-OD2	7.39	124.95	118.30
2	N	152	LEU	CB-CG-CD1	7.39	123.56	111.00
1	E	242	PHE	CB-CG-CD2	-7.34	115.67	120.80
2	L	69	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	344	TRP	NE1-CE2-CZ2	7.32	138.46	130.40
2	N	432	TYR	CB-CG-CD2	-7.32	116.61	121.00
2	B	161	TYR	CD1-CE1-CZ	7.32	126.39	119.80
2	D	103	TYR	CG-CD2-CE2	-7.32	115.45	121.30
2	H	407	TRP	CD1-NE1-CE2	7.31	115.58	109.00
1	I	286	VAL	CA-CB-CG1	7.31	121.86	110.90
1	A	294	PHE	CB-CG-CD2	7.29	125.90	120.80
2	N	408	TYR	CB-CG-CD1	-7.28	116.63	121.00
2	D	141	PHE	CB-CG-CD2	7.28	125.89	120.80
1	I	443	ASP	CB-CG-OD2	7.27	124.84	118.30
1	M	101	TRP	CE3-CZ3-CH2	-7.26	113.22	121.20
1	G	287	PRO	N-CA-CB	7.25	112.00	103.30
2	D	172	TYR	CB-CG-CD2	7.23	125.34	121.00
2	J	98	ASP	OD1-CG-OD2	-7.23	109.57	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	19	ALA	CB-CA-C	7.22	120.93	110.10
2	F	69	ASP	CB-CG-OD2	7.21	124.79	118.30
2	B	224	TYR	CB-CG-CD2	-7.21	116.67	121.00
2	D	243	ARG	NE-CZ-NH1	7.18	123.89	120.30
2	D	46	ASP	CB-CG-OD1	7.18	124.76	118.30
2	D	46	ASP	CB-CG-OD2	-7.15	111.86	118.30
2	N	272	TYR	CB-CG-CD2	-7.15	116.71	121.00
1	E	309	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	170	VAL	CA-CB-CG2	7.13	121.60	110.90
2	L	181	VAL	CA-CB-CG2	7.13	121.59	110.90
2	L	69	ASP	CB-CG-OD2	7.12	124.71	118.30
1	C	436	PHE	CB-CG-CD1	-7.10	115.83	120.80
2	J	367	ASP	CB-CG-OD1	-7.10	111.91	118.30
1	K	276	ARG	CD-NE-CZ	7.09	133.53	123.60
1	K	310	TYR	CB-CG-CD1	-7.09	116.75	121.00
1	C	443	ASP	CB-CG-OD2	7.07	124.67	118.30
1	E	262	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	G	208	TYR	CB-CG-CD2	7.07	125.24	121.00
2	D	130	THR	CA-CB-CG2	7.06	122.29	112.40
2	N	388	TRP	CD1-NE1-CE2	7.05	115.35	109.00
2	H	169	PHE	CB-CG-CD2	-7.05	115.87	120.80
1	I	177	ASP	CB-CG-OD2	7.04	124.64	118.30
1	M	431	ASP	CB-CG-OD1	7.02	124.62	118.30
2	J	224	TYR	CB-CG-CD2	-7.01	116.79	121.00
2	D	306	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	250	LEU	CB-CG-CD1	7.01	122.92	111.00
2	J	229	ARG	CD-NE-CZ	7.01	133.42	123.60
2	F	424	ASP	CB-CG-OD2	-7.01	111.99	118.30
2	H	52	PHE	CB-CG-CD1	-7.00	115.90	120.80
1	A	86	ARG	CD-NE-CZ	7.00	133.40	123.60
2	H	62	VAL	CA-CB-CG2	7.00	121.40	110.90
2	H	361	THR	CA-CB-CG2	7.00	122.19	112.40
2	N	388	TRP	NE1-CE2-CD2	-6.99	100.31	107.30
2	N	78	VAL	CA-CB-CG2	6.98	121.37	110.90
1	G	36	TYR	CB-CG-CD2	-6.98	116.81	121.00
2	D	418	PHE	CB-CG-CD1	-6.96	115.93	120.80
1	G	222	TYR	CB-CG-CD2	-6.96	116.83	121.00
2	J	357	TYR	CB-CG-CD2	-6.96	116.83	121.00
2	J	343	PHE	CB-CG-CD1	6.96	125.67	120.80
1	I	114	ASP	CB-CG-OD2	-6.95	112.04	118.30
2	N	297	GLU	OE1-CD-OE2	-6.95	114.96	123.30
1	K	241	ARG	NE-CZ-NH1	6.94	123.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	141	PHE	CB-CG-CD1	-6.94	115.94	120.80
2	L	346	TRP	NE1-CE2-CD2	-6.93	100.37	107.30
2	D	37	PRO	N-CA-CB	6.93	111.62	103.30
2	L	25	CYS	CA-CB-SG	-6.92	101.54	114.00
2	B	199	ASP	CB-CG-OD1	6.92	124.53	118.30
2	H	69	ASP	OD1-CG-OD2	-6.92	110.15	123.30
1	C	76	VAL	CA-CB-CG1	6.92	121.28	110.90
1	M	309	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	M	222	TYR	CG-CD1-CE1	-6.91	115.77	121.30
2	B	113	GLU	OE1-CD-OE2	-6.90	115.02	123.30
2	D	52	PHE	CB-CG-CD1	-6.89	115.98	120.80
1	E	318	ARG	NE-CZ-NH1	6.89	123.74	120.30
2	N	381	THR	CA-CB-CG2	6.88	122.04	112.40
2	B	348	PRO	N-CA-CB	6.88	111.56	103.30
2	F	203	MET	CG-SD-CE	-6.88	89.19	100.20
2	N	431	ASP	CB-CG-OD2	6.88	124.49	118.30
2	H	242	LEU	CB-CG-CD1	6.88	122.69	111.00
1	E	192	LEU	CB-CG-CD2	-6.87	99.32	111.00
2	H	97	GLU	OE1-CD-OE2	-6.87	115.06	123.30
2	B	445	GLU	OE1-CD-OE2	-6.87	115.06	123.30
2	D	282	TYR	CG-CD2-CE2	-6.86	115.81	121.30
2	N	202	PHE	CB-CG-CD2	6.84	125.59	120.80
2	D	24	TYR	CG-CD2-CE2	-6.84	115.83	121.30
1	E	281	TYR	CB-CG-CD1	6.84	125.10	121.00
1	A	422	TYR	O-C-N	-6.83	111.77	122.70
2	L	69	ASP	OD1-CG-OD2	-6.83	110.33	123.30
1	I	270	PHE	CB-CG-CD1	-6.81	116.03	120.80
2	H	172	TYR	CD1-CE1-CZ	-6.80	113.67	119.80
1	A	378	PHE	CB-CG-CD1	-6.80	116.04	120.80
2	N	255	PHE	CG-CD2-CE2	-6.79	113.33	120.80
1	A	92	PHE	CB-CG-CD1	-6.79	116.05	120.80
1	A	101	TRP	CZ3-CH2-CZ2	-6.78	113.46	121.60
1	C	108	GLU	OE1-CD-OE2	-6.78	115.17	123.30
2	D	87	PHE	CB-CG-CD1	-6.77	116.06	120.80
1	E	328	GLU	OE1-CD-OE2	-6.77	115.18	123.30
2	B	312	TYR	CB-CG-CD2	-6.77	116.94	121.00
2	B	264	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	E	390	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	I	209	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	C	397	TRP	NE1-CE2-CZ2	6.73	137.81	130.40
3	O	211	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	G	114	ASP	CB-CG-OD2	-6.73	112.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	21	TRP	CE3-CZ3-CH2	-6.72	113.80	121.20
2	D	76	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	I	367	PHE	CB-CG-CD1	-6.70	116.11	120.80
2	L	346	TRP	NE1-CE2-CZ2	6.70	137.77	130.40
1	E	266	PHE	CB-CG-CD1	6.69	125.48	120.80
1	K	113	VAL	CA-CB-CG1	6.69	120.94	110.90
1	G	209	ASP	CB-CG-OD1	-6.69	112.28	118.30
2	F	24	TYR	CD1-CG-CD2	6.67	125.23	117.90
2	F	328	VAL	CA-CB-CG2	6.67	120.90	110.90
1	A	73	MET	CG-SD-CE	-6.67	89.54	100.20
2	F	210	TYR	CG-CD2-CE2	-6.66	115.98	121.30
2	N	69	ASP	OD1-CG-OD2	-6.65	110.66	123.30
1	A	65	LEU	CB-CG-CD2	-6.65	99.70	111.00
1	M	36	TYR	CB-CG-CD1	-6.64	117.02	121.00
1	A	101	TRP	CD1-CG-CD2	-6.63	100.99	106.30
2	F	306	ASP	CB-CG-OD2	-6.63	112.33	118.30
2	L	330	ALA	N-CA-CB	-6.63	100.81	110.10
2	D	73	THR	O-C-N	-6.63	112.09	122.70
2	F	411	GLU	OE1-CD-OE2	-6.63	115.35	123.30
2	B	439	SER	N-CA-CB	6.62	120.42	110.50
1	K	161	ASP	CB-CG-OD1	-6.61	112.35	118.30
2	J	123	ARG	CD-NE-CZ	6.61	132.85	123.60
2	J	182	VAL	CG1-CB-CG2	-6.60	100.33	110.90
2	B	405	VAL	CG1-CB-CG2	-6.60	100.34	110.90
2	H	185	TYR	CG-CD2-CE2	-6.60	116.02	121.30
2	J	46	ASP	CB-CG-OD1	6.58	124.22	118.30
2	H	93	ILE	O-C-N	-6.57	112.18	122.70
1	K	344	TRP	NE1-CE2-CD2	-6.57	100.73	107.30
1	G	106	TYR	CB-CG-CD2	6.57	124.94	121.00
2	N	322	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	E	21	TRP	CZ3-CH2-CZ2	-6.57	113.72	121.60
2	D	368	LEU	CB-CA-C	6.56	122.67	110.20
2	F	269	LEU	CB-CG-CD2	6.56	122.15	111.00
2	F	353	VAL	CA-CB-CG2	6.56	120.74	110.90
2	J	312	TYR	CG-CD2-CE2	-6.56	116.05	121.30
2	J	314	ALA	CB-CA-C	6.55	119.92	110.10
1	A	262	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	L	357	TYR	CB-CG-CD2	-6.54	117.07	121.00
2	B	210	TYR	CG-CD1-CE1	-6.54	116.07	121.30
1	I	241	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	I	209	ASP	CB-CG-OD1	6.53	124.18	118.30
2	D	282	TYR	CD1-CG-CD2	6.53	125.09	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	46	ASP	C-N-CA	6.53	138.03	121.70
2	L	343	PHE	CB-CG-CD2	6.53	125.37	120.80
1	M	20	PHE	CB-CG-CD2	-6.53	116.23	120.80
1	C	390	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	D	138	PHE	CB-CG-CD1	6.52	125.36	120.80
2	D	312	TYR	CZ-CE2-CD2	-6.52	113.93	119.80
1	K	178	THR	CA-CB-CG2	6.51	121.52	112.40
2	L	262	TYR	CB-CG-CD2	-6.51	117.09	121.00
2	N	272	TYR	CG-CD1-CE1	-6.51	116.09	121.30
1	C	439	GLU	OE1-CD-OE2	-6.50	115.49	123.30
2	F	21	TRP	CE2-CD2-CG	6.50	112.50	107.30
2	J	103	TYR	CG-CD1-CE1	-6.50	116.10	121.30
2	F	362	VAL	CA-CB-CG2	6.50	120.64	110.90
2	J	328	VAL	CA-CB-CG2	-6.50	101.16	110.90
2	D	199	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	208	TYR	CG-CD1-CE1	6.49	126.49	121.30
2	J	297	GLU	OE1-CD-OE2	-6.49	115.52	123.30
2	H	327	ASP	CB-CG-OD1	-6.48	112.47	118.30
2	F	264	ARG	NE-CZ-NH1	6.48	123.54	120.30
2	H	325	PRO	N-CA-CB	6.47	111.07	103.30
1	K	62	ARG	NE-CZ-NH1	6.47	123.54	120.30
2	L	402	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	K	262	ARG	NE-CZ-NH1	6.46	123.53	120.30
2	B	319	TYR	CB-CG-CD1	-6.46	117.12	121.00
1	K	327	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	390	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	G	46	ARG	CD-NE-CZ	6.43	132.61	123.60
2	L	177	VAL	CG1-CB-CG2	-6.43	100.61	110.90
3	O	388	HIS	CA-C-N	6.43	129.06	116.20
1	K	90	PHE	CB-CG-CD2	6.42	125.30	120.80
1	G	422	TYR	CB-CG-CD2	6.42	124.85	121.00
2	F	408	TYR	CB-CG-CD2	-6.42	117.15	121.00
1	M	35	SER	N-CA-CB	-6.41	100.89	110.50
2	D	56	THR	CA-CB-CG2	6.38	121.33	112.40
2	H	437	VAL	CA-CB-CG1	6.37	120.45	110.90
2	L	1	MET	CB-CA-C	6.36	123.13	110.40
2	N	327	ASP	CB-CG-OD2	6.36	124.03	118.30
2	B	371	VAL	CA-CB-CG2	6.36	120.44	110.90
1	C	211	CYS	CA-CB-SG	-6.36	102.56	114.00
1	I	310	TYR	CB-CG-CD1	-6.36	117.19	121.00
2	J	46	ASP	O-C-N	-6.35	112.53	122.70
1	C	347	ASN	CB-CA-C	6.35	123.11	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	218	ASP	CB-CG-OD2	6.35	124.02	118.30
2	J	161	TYR	CB-CG-CD2	6.35	124.81	121.00
2	D	83	TYR	CD1-CE1-CZ	-6.34	114.09	119.80
2	H	292	THR	CA-CB-CG2	6.34	121.28	112.40
2	J	282	TYR	CG-CD1-CE1	-6.33	116.24	121.30
1	A	242	PHE	CG-CD1-CE1	-6.33	113.84	120.80
2	H	381	THR	CA-CB-CG2	6.32	121.25	112.40
1	I	344	TRP	NE1-CE2-CZ2	6.32	137.35	130.40
2	D	113	GLU	OE1-CD-OE2	-6.32	115.72	123.30
2	J	388	TRP	CG-CD2-CE3	6.32	139.58	133.90
2	J	405	VAL	CG1-CB-CG2	-6.31	100.81	110.90
2	J	422	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	162	ARG	NE-CZ-NH1	6.30	123.45	120.30
2	F	389	ALA	CB-CA-C	6.30	119.55	110.10
2	L	288	VAL	CG1-CB-CG2	-6.29	100.83	110.90
2	F	183	GLU	OE1-CD-OE2	-6.29	115.75	123.30
1	E	391	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	J	183	GLU	OE1-CD-OE2	-6.29	115.75	123.30
2	L	375	VAL	CA-CB-CG1	6.28	120.32	110.90
1	C	251	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	H	49	PHE	CB-CG-CD1	-6.28	116.41	120.80
2	L	182	VAL	CG1-CB-CG2	-6.27	100.87	110.90
1	G	222	TYR	CD1-CG-CD2	6.26	124.78	117.90
2	H	367	ASP	CB-CA-C	6.24	122.88	110.40
1	C	61	PRO	N-CA-CB	6.24	110.78	103.30
2	L	66	VAL	CA-CB-CG2	6.24	120.25	110.90
2	J	130	THR	CA-CB-CG2	6.23	121.13	112.40
1	G	90	PHE	CG-CD1-CE1	-6.23	113.94	120.80
2	H	24	TYR	CB-CG-CD1	6.23	124.74	121.00
2	B	296	PHE	CB-CG-CD2	-6.23	116.44	120.80
2	D	147	SER	N-CA-CB	-6.23	101.16	110.50
1	K	163	ILE	CB-CA-C	6.23	124.05	111.60
1	G	410	GLU	OE1-CD-OE2	-6.22	115.83	123.30
2	L	312	TYR	CG-CD1-CE1	-6.22	116.33	121.30
1	I	242	PHE	CG-CD2-CE2	-6.22	113.96	120.80
1	G	167	PHE	CB-CG-CD1	6.21	125.15	120.80
2	N	424	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	K	344	TRP	NE1-CE2-CZ2	6.20	137.22	130.40
2	F	9	VAL	CA-CB-CG2	6.20	120.20	110.90
1	C	397	TRP	CE3-CZ3-CH2	-6.20	114.39	121.20
2	B	422	ARG	NE-CZ-NH1	6.19	123.39	120.30
2	L	295	CYS	CA-CB-SG	-6.19	102.86	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	69	ASP	CB-CG-OD1	6.18	123.87	118.30
1	C	77	ARG	CD-NE-CZ	6.18	132.25	123.60
1	K	200	TYR	CG-CD2-CE2	-6.17	116.36	121.30
2	B	303	VAL	CA-CB-CG1	6.17	120.16	110.90
1	K	266	PHE	CB-CG-CD1	6.17	125.12	120.80
1	M	101	TRP	NE1-CE2-CZ2	6.17	137.18	130.40
2	F	96	LYS	N-CA-CB	-6.16	99.51	110.60
2	N	214	ARG	CA-CB-CG	6.16	126.95	113.40
1	C	209	ASP	CB-CG-OD1	6.16	123.84	118.30
1	M	274	THR	CA-CB-CG2	6.15	121.02	112.40
1	C	340	TYR	CG-CD1-CE1	-6.14	116.39	121.30
2	L	105	ARG	CD-NE-CZ	6.14	132.20	123.60
1	K	119	VAL	CG1-CB-CG2	-6.14	101.08	110.90
1	K	276	ARG	O-C-N	-6.14	112.76	123.20
2	L	24	TYR	CG-CD1-CE1	6.14	126.21	121.30
1	A	85	PHE	CB-CG-CD2	-6.13	116.51	120.80
1	C	106	TYR	CG-CD1-CE1	-6.13	116.39	121.30
1	I	380	ARG	CD-NE-CZ	6.13	132.18	123.60
2	N	357	TYR	CB-CG-CD2	-6.13	117.33	121.00
2	D	407	TRP	CG-CD2-CE3	6.12	139.41	133.90
1	G	218	THR	C-N-CA	6.12	137.00	121.70
1	A	76	VAL	CA-CB-CG2	6.12	120.08	110.90
2	F	343	PHE	CB-CG-CD2	-6.12	116.52	120.80
1	C	397	TRP	CE2-CD2-CG	6.12	112.19	107.30
1	A	399	THR	CA-CB-CG2	6.11	120.96	112.40
2	F	53	PHE	CB-CG-CD1	-6.11	116.52	120.80
2	J	343	PHE	CB-CG-CD2	-6.11	116.53	120.80
2	L	24	TYR	CB-CG-CD2	6.11	124.66	121.00
2	L	217	LEU	CB-CG-CD2	6.10	121.37	111.00
2	L	103	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	A	318	ARG	CD-NE-CZ	6.10	132.14	123.60
2	N	451	TYR	CB-CG-CD1	-6.10	117.34	121.00
1	I	365	ALA	O-C-N	-6.09	112.95	122.70
2	L	103	TYR	CB-CG-CD1	6.09	124.66	121.00
1	G	128	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	C	90	PHE	CZ-CE2-CD2	-6.09	112.80	120.10
1	I	194	GLU	N-CA-CB	-6.09	99.65	110.60
1	K	159	TYR	CB-CG-CD1	-6.09	117.35	121.00
1	A	194	GLU	OE1-CD-OE2	-6.08	116.00	123.30
1	I	398	TYR	CB-CG-CD1	-6.08	117.35	121.00
2	N	52	PHE	CB-CG-CD1	-6.07	116.55	120.80
2	L	407	TRP	CD1-NE1-CE2	6.05	114.45	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	262	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	C	333	VAL	CG1-CB-CG2	-6.04	101.23	110.90
2	D	202	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	M	318	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	H	332	ILE	CA-CB-CG1	6.04	122.48	111.00
1	I	200	TYR	CG-CD2-CE2	-6.04	116.47	121.30
2	N	357	TYR	CB-CG-CD1	6.04	124.62	121.00
2	B	357	TYR	CB-CG-CD2	6.03	124.62	121.00
1	A	265	PHE	CB-CG-CD2	6.02	125.02	120.80
2	L	383	ALA	CB-CA-C	6.02	119.13	110.10
3	O	242	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	N	68	VAL	CG1-CB-CG2	-6.02	101.27	110.90
1	I	391	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	E	183	TYR	CA-CB-CG	6.01	124.82	113.40
2	J	266	HIS	CA-CB-CG	6.00	123.80	113.60
1	M	304	ASP	CB-CG-OD1	6.00	123.70	118.30
1	I	46	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	I	81	PHE	CB-CG-CD2	6.00	125.00	120.80
2	N	451	TYR	CG-CD2-CE2	-5.99	116.51	121.30
2	H	429	GLU	CB-CA-C	5.98	122.36	110.40
1	C	372	THR	CA-CB-CG2	5.97	120.76	112.40
2	F	149	PHE	CB-CG-CD2	-5.97	116.62	120.80
2	J	69	ASP	CB-CG-OD1	5.97	123.67	118.30
1	K	246	LEU	CB-CG-CD1	-5.97	100.86	111.00
2	F	224	TYR	CA-CB-CG	5.96	124.73	113.40
1	G	167	PHE	CB-CG-CD2	-5.96	116.62	120.80
1	M	35	SER	CB-CA-C	5.96	121.43	110.10
2	B	199	ASP	CB-CG-OD2	-5.96	112.94	118.30
2	F	9	VAL	CG1-CB-CG2	-5.96	101.36	110.90
1	A	111	GLU	OE1-CD-OE2	-5.96	116.15	123.30
2	F	69	ASP	OD1-CG-OD2	-5.96	111.98	123.30
1	K	344	TRP	CD1-NE1-CE2	5.95	114.35	109.00
1	I	313	VAL	CA-CB-CG2	5.94	119.81	110.90
1	M	53	GLU	OE1-CD-OE2	-5.94	116.17	123.30
2	D	208	ALA	O-C-N	-5.94	113.20	122.70
1	K	197	ASP	CB-CG-OD1	5.92	123.63	118.30
2	H	172	TYR	CG-CD2-CE2	-5.92	116.57	121.30
2	B	87	PHE	CB-CG-CD1	-5.91	116.66	120.80
1	I	159	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	K	211	CYS	CA-CB-SG	-5.91	103.36	114.00
1	A	59	TYR	CB-CG-CD1	-5.90	117.46	121.00
2	D	408	TYR	CG-CD1-CE1	-5.90	116.58	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	320	ARG	CD-NE-CZ	5.90	131.86	123.60
2	L	224	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	C	192	LEU	CB-CA-C	5.89	121.40	110.20
2	N	381	THR	OG1-CB-CG2	-5.89	96.44	110.00
2	N	253	THR	CA-CB-CG2	5.89	120.65	112.40
2	B	51	THR	CA-CB-CG2	5.89	120.64	112.40
1	I	310	TYR	CG-CD2-CE2	-5.89	116.59	121.30
2	F	182	VAL	CA-CB-CG2	5.88	119.73	110.90
1	C	344	TRP	CE3-CZ3-CH2	-5.88	114.73	121.20
2	H	185	TYR	CD1-CG-CD2	5.88	124.37	117.90
1	I	366	THR	CA-CB-CG2	5.87	120.62	112.40
2	D	3	GLU	OE1-CD-OE2	-5.87	116.25	123.30
1	A	344	TRP	CD1-NE1-CE2	5.87	114.28	109.00
1	K	133	PHE	CB-CG-CD2	-5.87	116.69	120.80
2	D	161	TYR	CB-CG-CD2	-5.87	117.48	121.00
2	F	66	VAL	CG1-CB-CG2	-5.85	101.55	110.90
2	D	207	GLU	OE1-CD-OE2	-5.84	116.29	123.30
2	H	330	ALA	N-CA-CB	-5.84	101.92	110.10
2	F	244	PHE	CB-CG-CD1	5.84	124.89	120.80
2	J	120	ASP	CB-CG-OD1	5.83	123.55	118.30
1	K	160	PRO	N-CD-CG	5.83	111.95	103.20
1	K	189	VAL	CA-CB-CG1	5.82	119.62	110.90
2	J	210	TYR	CB-CG-CD2	-5.81	117.51	121.00
1	A	249	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	I	77	ARG	CB-CA-C	5.81	122.02	110.40
2	D	373	ARG	NE-CZ-NH1	5.81	123.20	120.30
2	H	429	GLU	N-CA-CB	-5.81	100.14	110.60
2	J	172	TYR	CB-CG-CD1	-5.81	117.52	121.00
1	K	397	TRP	NE1-CE2-CD2	-5.81	101.49	107.30
2	N	375	VAL	CB-CA-C	-5.81	100.37	111.40
2	D	118	VAL	CA-CB-CG1	5.80	119.61	110.90
2	J	83	TYR	CG-CD1-CE1	-5.80	116.66	121.30
1	M	340	TYR	CB-CG-CD2	-5.80	117.52	121.00
2	L	292	THR	CA-CB-CG2	5.80	120.52	112.40
3	O	369	LYS	C-N-CA	5.80	136.20	121.70
1	I	62	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	F	58	ALA	CB-CA-C	5.79	118.79	110.10
1	A	170	VAL	CG1-CB-CG2	-5.79	101.64	110.90
2	B	179	THR	CA-CB-CG2	-5.79	104.29	112.40
2	L	182	VAL	CA-CB-CG2	5.79	119.58	110.90
1	C	397	TRP	NE1-CE2-CD2	-5.78	101.52	107.30
2	N	4	CYS	CA-CB-SG	-5.78	103.60	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	177	VAL	CG1-CB-CG2	-5.78	101.65	110.90
2	B	205	ASP	CB-CG-OD2	5.78	123.50	118.30
1	G	296	ALA	C-N-CA	5.78	136.14	121.70
2	H	312	TYR	CD1-CE1-CZ	5.78	125.00	119.80
1	M	101	TRP	NE1-CE2-CD2	-5.78	101.53	107.30
2	B	135	PHE	CB-CG-CD1	-5.77	116.76	120.80
1	K	114	ASP	CB-CG-OD2	-5.77	113.11	118.30
2	L	363	VAL	CA-CB-CG1	5.76	119.55	110.90
1	C	422	TYR	CB-CG-CD2	-5.76	117.54	121.00
1	A	212	PHE	CB-CG-CD1	-5.76	116.77	120.80
2	B	367	ASP	CB-CG-OD2	5.76	123.48	118.30
3	O	392	ILE	C-N-CA	5.76	136.09	121.70
1	K	198	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	G	39	ASP	CB-CG-OD1	5.75	123.47	118.30
1	I	427	ASP	CB-CG-OD1	5.74	123.47	118.30
2	J	282	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	M	380	ARG	CB-CA-C	5.74	121.88	110.40
2	L	312	TYR	CD1-CG-CD2	5.74	124.21	117.90
1	K	135	LEU	CB-CG-CD1	5.74	120.75	111.00
2	B	185	TYR	CB-CG-CD1	5.73	124.44	121.00
1	C	106	TYR	CZ-CE2-CD2	-5.73	114.64	119.80
2	N	262	TYR	CB-CG-CD1	5.73	124.44	121.00
1	G	318	ARG	NE-CZ-NH1	5.73	123.17	120.30
2	H	103	TYR	CG-CD1-CE1	-5.73	116.72	121.30
1	M	20	PHE	CB-CG-CD1	5.73	124.81	120.80
1	C	209	ASP	CB-CG-OD2	-5.73	113.14	118.30
2	N	29	GLY	C-N-CA	5.73	136.02	121.70
2	B	398	MET	CG-SD-CE	5.72	109.36	100.20
2	D	138	PHE	CB-CG-CD2	-5.72	116.79	120.80
2	D	389	ALA	CB-CA-C	5.72	118.68	110.10
1	K	344	TRP	CE3-CZ3-CH2	-5.72	114.91	121.20
2	N	284	GLU	CB-CA-C	5.72	121.84	110.40
1	A	88	ASP	N-CA-CB	-5.71	100.32	110.60
2	N	136	LEU	CA-CB-CG	5.71	128.44	115.30
2	D	72	PRO	CA-N-CD	-5.71	103.51	111.50
1	E	194	GLU	OE1-CD-OE2	-5.71	116.45	123.30
2	L	14	VAL	CG1-CB-CG2	-5.71	101.77	110.90
1	A	130	LEU	CB-CG-CD2	-5.71	101.30	111.00
1	K	187	LEU	CB-CG-CD1	-5.71	101.30	111.00
2	B	66	VAL	CG1-CB-CG2	-5.70	101.78	110.90
2	D	249	ASN	OD1-CG-ND2	-5.70	108.79	121.90
1	K	90	PHE	CG-CD1-CE1	-5.70	114.53	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	288	VAL	CG1-CB-CG2	-5.70	101.79	110.90
2	H	382	THR	CA-CB-CG2	-5.70	104.43	112.40
1	K	398	TYR	CB-CG-CD1	-5.70	117.58	121.00
2	N	208	ALA	N-CA-CB	-5.69	102.13	110.10
1	C	106	TYR	CB-CG-CD1	-5.69	117.59	121.00
1	I	158	GLU	OE1-CD-OE2	-5.69	116.47	123.30
1	A	222	TYR	CB-CG-CD2	5.68	124.41	121.00
1	A	398	TYR	CB-CA-C	-5.68	99.03	110.40
2	N	153	LEU	CB-CG-CD1	5.68	120.65	111.00
3	O	388	HIS	CB-CA-C	5.68	121.75	110.40
1	M	107	THR	OG1-CB-CG2	-5.67	96.95	110.00
1	E	170	VAL	CA-CB-CG2	5.67	119.40	110.90
2	F	346	TRP	CD1-CG-CD2	-5.67	101.77	106.30
2	B	249	ASN	C-N-CA	5.66	135.85	121.70
2	L	21	TRP	CD1-NE1-CE2	5.66	114.09	109.00
2	D	409	VAL	CG1-CB-CG2	-5.65	101.86	110.90
2	H	402	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	B	67	PHE	CB-CG-CD2	-5.64	116.85	120.80
2	H	282	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	M	62	ARG	CD-NE-CZ	5.64	131.50	123.60
2	N	242	LEU	CB-CG-CD2	5.64	120.59	111.00
2	J	351	PHE	CG-CD2-CE2	5.64	127.00	120.80
1	K	67	ASP	CB-CG-OD1	5.64	123.38	118.30
1	M	59	TYR	CD1-CE1-CZ	-5.64	114.72	119.80
1	M	415	MET	O-C-N	-5.64	113.67	122.70
2	D	337	THR	CA-CB-CG2	5.64	120.29	112.40
1	K	106	TYR	CD1-CE1-CZ	5.64	124.87	119.80
1	M	281	TYR	CB-CG-CD2	-5.64	117.62	121.00
3	O	349	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	I	427	ASP	CB-CG-OD2	-5.63	113.24	118.30
2	H	24	TYR	CG-CD2-CE2	5.62	125.80	121.30
2	B	84	ARG	CD-NE-CZ	5.62	131.47	123.60
2	L	172	TYR	CB-CG-CD2	-5.62	117.63	121.00
2	L	138	PHE	CB-CG-CD1	-5.62	116.87	120.80
1	E	55	ALA	N-CA-CB	-5.61	102.24	110.10
1	G	224	ASP	CB-CG-OD2	5.61	123.35	118.30
2	J	177	VAL	CA-CB-CG1	5.61	119.31	110.90
2	L	418	PHE	CB-CG-CD2	5.61	124.73	120.80
1	K	276	ARG	CA-C-N	5.61	127.42	116.20
1	M	230	SER	O-C-N	5.61	131.67	122.70
1	I	196	THR	CA-CB-CG2	-5.61	104.55	112.40
1	M	157	GLU	OE1-CD-OE2	-5.61	116.57	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	345	ASP	CB-CG-OD1	5.60	123.34	118.30
1	G	281	TYR	CB-CG-CD2	5.60	124.36	121.00
1	G	287	PRO	CA-N-CD	-5.60	103.66	111.50
2	B	451	TYR	CB-CG-CD2	-5.60	117.64	121.00
2	J	363	VAL	CA-CB-CG1	5.59	119.29	110.90
1	K	374	ILE	CA-CB-CG1	5.59	121.63	111.00
2	H	146	GLY	C-N-CA	5.59	135.67	121.70
2	F	325	PRO	N-CA-CB	5.59	110.00	103.30
2	F	386	GLU	OE1-CD-OE2	-5.59	116.59	123.30
2	L	150	THR	CA-CB-CG2	5.58	120.22	112.40
2	L	324	VAL	CA-CB-CG1	5.58	119.28	110.90
2	L	403	ALA	C-N-CA	5.58	135.66	121.70
1	G	128	ASP	CB-CA-C	5.58	121.56	110.40
1	M	230	SER	CA-C-O	-5.58	108.38	120.10
1	M	180	VAL	CG1-CB-CG2	5.58	119.83	110.90
1	I	177	ASP	CB-CG-OD1	-5.58	113.28	118.30
2	J	227	LEU	CB-CA-C	5.58	120.80	110.20
2	J	386	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	M	418	LEU	CB-CG-CD2	5.58	120.48	111.00
1	C	305	PRO	N-CD-CG	5.57	111.56	103.20
1	I	410	GLU	OE1-CD-OE2	5.57	129.98	123.30
2	N	272	TYR	CD1-CG-CD2	5.57	124.02	117.90
2	N	201	ALA	N-CA-CB	-5.57	102.31	110.10
1	C	331	LEU	CB-CA-C	5.56	120.77	110.20
2	D	173	PRO	N-CA-CB	5.56	109.97	103.30
1	M	67	ASP	CB-CG-OD1	5.56	123.31	118.30
2	F	270	ALA	CB-CA-C	5.56	118.44	110.10
1	E	81	PHE	CB-CG-CD1	-5.55	116.91	120.80
2	F	384	ILE	CA-CB-CG1	5.55	121.54	111.00
1	E	119	VAL	CA-CB-CG1	5.55	119.22	110.90
2	J	407	TRP	CD1-NE1-CE2	5.54	113.99	109.00
1	M	119	VAL	CG1-CB-CG2	-5.54	102.03	110.90
2	B	184	PRO	N-CA-CB	5.54	109.95	103.30
1	C	31	ASP	CB-CG-OD1	-5.54	113.31	118.30
2	F	348	PRO	CA-N-CD	-5.54	103.74	111.50
2	H	169	PHE	CB-CG-CD1	5.54	124.68	120.80
1	E	243	PRO	N-CD-CG	5.54	111.51	103.20
2	B	264	ARG	CD-NE-CZ	5.54	131.35	123.60
1	G	92	PHE	CB-CG-CD1	-5.53	116.93	120.80
2	J	217	LEU	CB-CG-CD2	5.53	120.40	111.00
2	L	3	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	E	36	TYR	CZ-CE2-CD2	-5.52	114.83	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	294	PHE	N-CA-CB	-5.52	100.67	110.60
2	H	173	PRO	O-C-N	-5.52	113.87	122.70
2	B	72	PRO	N-CA-CB	5.52	109.92	103.30
2	L	90	GLU	OE1-CD-OE2	-5.52	116.68	123.30
2	N	270	ALA	N-CA-CB	-5.52	102.38	110.10
1	A	278	SER	O-C-N	-5.52	113.87	122.70
1	C	266	PHE	CB-CG-CD2	-5.52	116.94	120.80
2	F	349	THR	OG1-CB-CG2	-5.52	97.31	110.00
2	D	437	VAL	CG1-CB-CG2	-5.51	102.08	110.90
2	N	185	TYR	CA-CB-CG	5.51	123.88	113.40
2	H	16	ILE	O-C-N	-5.51	113.83	123.20
2	F	291	ILE	O-C-N	-5.51	113.89	122.70
1	E	116	VAL	O-C-N	-5.50	113.89	122.70
2	N	312	TYR	CG-CD1-CE1	-5.50	116.90	121.30
2	B	283	HIS	N-CA-CB	-5.50	100.69	110.60
2	B	313	MET	CA-CB-CG	-5.50	103.94	113.30
2	D	105	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	70	PRO	N-CD-CG	5.50	111.45	103.20
1	I	397	TRP	CD2-CE3-CZ3	5.50	125.95	118.80
1	K	245	GLN	CA-CB-CG	5.50	125.50	113.40
1	M	222	TYR	CD1-CE1-CZ	5.50	124.75	119.80
2	D	337	THR	OG1-CB-CG2	-5.50	97.36	110.00
2	B	312	TYR	CG-CD2-CE2	-5.49	116.91	121.30
2	J	155	GLU	OE1-CD-OE2	-5.49	116.72	123.30
1	K	344	TRP	CE2-CD2-CG	5.49	111.69	107.30
2	L	129	CYS	CA-CB-SG	-5.48	104.13	114.00
2	L	127	ASP	N-CA-CB	-5.48	100.73	110.60
1	E	322	SER	N-CA-CB	-5.48	102.28	110.50
2	L	81	GLY	O-C-N	-5.47	113.94	122.70
2	N	424	ASP	CB-CG-OD1	5.47	123.22	118.30
2	L	370	LYS	O-C-N	-5.47	113.95	122.70
2	L	149	PHE	CB-CG-CD2	5.47	124.63	120.80
1	C	398	TYR	CG-CD2-CE2	-5.47	116.93	121.30
2	J	272	TYR	CB-CG-CD2	5.47	124.28	121.00
2	L	123	ARG	O-C-N	-5.46	113.96	122.70
2	F	312	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	E	161	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	183	TYR	CB-CA-C	-5.46	99.49	110.40
2	H	306	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	I	1	MET	CG-SD-CE	5.46	108.93	100.20
1	K	200	TYR	CZ-CE2-CD2	5.46	124.71	119.80
2	N	262	TYR	CB-CG-CD2	-5.46	117.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	442	GLU	CB-CA-C	-5.45	99.49	110.40
2	D	103	TYR	CB-CG-CD1	-5.45	117.73	121.00
2	F	33	ASP	CB-CG-OD1	-5.45	113.39	118.30
2	N	224	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	C	171	PRO	O-C-N	-5.45	113.98	122.70
2	F	69	ASP	CB-CG-OD1	5.45	123.20	118.30
2	L	185	TYR	CB-CG-CD1	-5.45	117.73	121.00
2	L	415	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	G	282	ARG	CD-NE-CZ	5.45	131.22	123.60
1	I	340	TYR	CG-CD2-CE2	-5.45	116.94	121.30
2	B	340	SER	CB-CA-C	5.44	120.44	110.10
2	F	24	TYR	CG-CD1-CE1	-5.44	116.95	121.30
1	G	265	PHE	CB-CG-CD2	-5.44	117.00	120.80
1	K	387	ALA	N-CA-CB	-5.44	102.49	110.10
2	H	361	THR	O-C-N	-5.43	114.00	122.70
3	O	221	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	G	8	GLN	CA-CB-CG	5.43	125.34	113.40
2	D	449	GLU	O-C-N	-5.42	114.02	122.70
2	H	344	VAL	CA-CB-CG1	5.42	119.04	110.90
3	O	369	LYS	CB-CA-C	5.42	121.25	110.40
2	D	118	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	G	419	VAL	CG1-CB-CG2	-5.41	102.24	110.90
2	H	224	TYR	CA-CB-CG	5.41	123.68	113.40
2	H	25	CYS	CB-CA-C	5.41	121.22	110.40
1	K	222	TYR	CB-CG-CD1	-5.41	117.76	121.00
1	M	101	TRP	CD2-CE3-CZ3	5.41	125.83	118.80
2	N	227	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	I	232	THR	CA-CB-CG2	5.41	119.97	112.40
2	F	399	TYR	CB-CG-CD1	-5.40	117.76	121.00
2	L	319	TYR	CZ-CE2-CD2	5.40	124.66	119.80
2	B	272	TYR	CG-CD1-CE1	-5.40	116.98	121.30
1	E	5	VAL	N-CA-CB	-5.40	99.63	111.50
1	C	173	PRO	N-CA-CB	5.39	109.77	103.30
1	C	344	TRP	CD2-CE3-CZ3	5.39	125.81	118.80
1	E	304	ASP	CB-CG-OD2	5.39	123.15	118.30
2	H	281	ALA	CB-CA-C	5.39	118.19	110.10
2	J	382	THR	O-C-N	-5.39	114.07	122.70
1	E	68	LEU	CB-CA-C	5.39	120.44	110.20
2	N	429	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	A	310	TYR	CB-CG-CD1	-5.39	117.77	121.00
2	H	347	CYS	N-CA-CB	-5.38	100.91	110.60
1	K	397	TRP	CD1-CG-CD2	-5.38	102.00	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	348	PRO	CA-N-CD	-5.38	103.97	111.50
2	J	83	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	A	137	HIS	CA-CB-CG	5.38	122.74	113.60
1	E	73	MET	CA-CB-CG	-5.38	104.16	113.30
1	I	365	ALA	N-CA-CB	-5.38	102.57	110.10
2	B	244	PHE	CG-CD2-CE2	-5.37	114.89	120.80
2	H	147	SER	CB-CA-C	5.37	120.30	110.10
1	K	411	ALA	N-CA-CB	-5.37	102.59	110.10
1	E	63	ALA	N-CA-CB	-5.36	102.59	110.10
1	A	111	GLU	CG-CD-OE2	5.36	129.02	118.30
1	C	145	SER	N-CA-CB	-5.36	102.46	110.50
1	I	398	TYR	CB-CG-CD2	5.36	124.22	121.00
2	F	290	GLU	CB-CG-CD	-5.36	99.73	114.20
1	I	270	PHE	CB-CG-CD2	5.36	124.55	120.80
2	D	71	GLU	CA-CB-CG	5.36	125.19	113.40
2	D	120	ASP	CB-CG-OD2	-5.36	113.48	118.30
2	F	154	MET	N-CA-CB	5.36	120.24	110.60
1	A	97	ALA	CB-CA-C	5.35	118.13	110.10
2	H	161	TYR	CB-CG-CD2	-5.35	117.79	121.00
2	H	82	THR	O-C-N	-5.35	114.15	122.70
1	K	208	TYR	CB-CG-CD1	-5.35	117.79	121.00
2	H	232	SER	CB-CA-C	5.34	120.25	110.10
2	J	327	ASP	CB-CG-OD1	5.34	123.11	118.30
2	H	319	TYR	CB-CG-CD2	-5.34	117.80	121.00
2	D	343	PHE	CB-CG-CD1	-5.34	117.06	120.80
2	H	153	LEU	CB-CG-CD2	5.34	120.07	111.00
1	M	439	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	I	200	TYR	CD1-CE1-CZ	-5.33	115.00	119.80
1	I	90	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	K	133	PHE	CG-CD1-CE1	-5.33	114.94	120.80
1	G	206	ALA	CB-CA-C	-5.33	102.11	110.10
2	H	409	VAL	CG1-CB-CG2	-5.33	102.38	110.90
2	B	272	TYR	CZ-CE2-CD2	-5.33	115.01	119.80
1	I	179	VAL	CG1-CB-CG2	-5.33	102.38	110.90
2	B	211	ASP	CB-CG-OD2	5.32	123.09	118.30
1	M	70	PRO	N-CA-CB	5.32	109.68	103.30
1	C	313	VAL	C-N-CA	5.32	135.00	121.70
1	G	278	SER	CA-C-N	5.32	128.90	117.20
2	H	297	GLU	OE1-CD-OE2	-5.31	116.92	123.30
1	K	66	VAL	CA-CB-CG2	5.31	118.87	110.90
1	E	387	ALA	CB-CA-C	5.31	118.07	110.10
2	J	404	PHE	CZ-CE2-CD2	-5.31	113.72	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	255	PHE	CZ-CE2-CD2	5.31	126.47	120.10
1	I	193	VAL	CA-CB-CG1	5.31	118.87	110.90
2	F	51	THR	CA-CB-OG1	5.31	120.15	109.00
2	H	309	HIS	CA-CB-CG	5.31	122.62	113.60
2	J	76	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	310	TYR	CG-CD2-CE2	-5.30	117.06	121.30
1	C	340	TYR	CA-CB-CG	5.30	123.48	113.40
1	G	63	ALA	CB-CA-C	5.30	118.06	110.10
2	L	220	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	K	400	GLY	C-N-CA	5.30	134.95	121.70
2	J	24	TYR	CB-CG-CD2	-5.30	117.82	121.00
2	L	26	LEU	CB-CG-CD2	-5.30	102.00	111.00
1	M	150	LEU	CB-CA-C	5.30	120.26	110.20
2	H	303	VAL	O-C-N	-5.29	114.23	122.70
2	B	76	ASP	CB-CG-OD2	-5.29	113.54	118.30
2	J	307	PRO	N-CA-CB	5.29	109.65	103.30
2	N	214	ARG	CD-NE-CZ	5.29	131.01	123.60
1	K	430	ALA	CB-CA-C	5.29	118.03	110.10
2	L	46	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	357	PRO	N-CA-CB	5.29	109.64	103.30
1	A	391	ARG	CD-NE-CZ	5.29	131.00	123.60
2	N	68	VAL	CA-CB-CG2	5.28	118.82	110.90
2	J	407	TRP	CG-CD1-NE1	-5.28	104.82	110.10
2	N	388	TRP	CE2-CD2-CG	5.28	111.52	107.30
1	M	180	VAL	CA-CB-CG1	-5.28	102.98	110.90
1	M	422	TYR	CB-CG-CD2	5.28	124.17	121.00
2	N	104	ALA	CB-CA-C	5.28	118.02	110.10
1	C	265	PHE	CD1-CE1-CZ	5.28	126.43	120.10
2	F	214	ARG	CD-NE-CZ	5.28	130.99	123.60
2	B	403	ALA	N-CA-CB	-5.27	102.72	110.10
1	I	408	PHE	CB-CG-CD1	-5.27	117.11	120.80
1	E	142	GLY	O-C-N	-5.27	114.27	122.70
2	B	52	PHE	CD1-CE1-CZ	-5.27	113.78	120.10
2	J	54	SER	N-CA-CB	-5.26	102.60	110.50
2	D	402	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	J	296	PHE	CB-CG-CD2	5.26	124.48	120.80
2	N	369	ALA	N-CA-CB	-5.26	102.73	110.10
1	G	36	TYR	CB-CG-CD1	5.26	124.16	121.00
2	H	12	ALA	N-CA-CB	-5.26	102.74	110.10
2	B	264	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	J	224	TYR	CB-CG-CD1	5.26	124.16	121.00
1	C	394	PHE	CD1-CE1-CZ	5.26	126.41	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	264	HIS	CA-C-O	-5.25	109.07	120.10
1	G	133	PHE	CB-CG-CD2	-5.25	117.12	120.80
2	J	345	ASP	N-CA-CB	-5.25	101.14	110.60
1	E	266	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	I	313	VAL	CB-CA-C	5.25	121.38	111.40
2	J	446	GLU	OE1-CD-OE2	-5.25	117.00	123.30
2	N	221	ARG	CD-NE-CZ	5.25	130.95	123.60
2	B	371	VAL	CG1-CB-CG2	-5.25	102.51	110.90
2	H	56	THR	CA-CB-CG2	5.25	119.75	112.40
1	K	176	SER	CB-CA-C	5.24	120.06	110.10
2	B	407	TRP	NE1-CE2-CD2	-5.24	102.06	107.30
2	F	116	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	87	PRO	N-CD-CG	5.24	111.05	103.20
2	H	390	ARG	CD-NE-CZ	5.23	130.93	123.60
1	K	208	TYR	CG-CD1-CE1	-5.23	117.11	121.30
2	L	295	CYS	O-C-N	-5.23	114.33	122.70
1	A	177	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	E	62	ARG	N-CA-CB	-5.23	101.19	110.60
2	L	379	SER	N-CA-CB	5.23	118.34	110.50
2	N	210	TYR	CG-CD2-CE2	-5.23	117.12	121.30
2	F	174	ALA	N-CA-CB	-5.22	102.79	110.10
2	H	407	TRP	NE1-CE2-CD2	-5.22	102.08	107.30
1	A	156	ARG	N-CA-CB	-5.21	101.21	110.60
2	H	429	GLU	OE1-CD-OE2	-5.21	117.04	123.30
2	J	418	PHE	CB-CG-CD2	-5.21	117.15	120.80
1	I	208	TYR	O-C-N	-5.21	114.36	122.70
1	M	376	GLU	CA-CB-CG	5.21	124.86	113.40
2	N	251	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	B	161	TYR	CD1-CG-CD2	5.21	123.63	117.90
2	H	202	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	C	281	TYR	CB-CG-CD2	5.20	124.12	121.00
2	D	185	TYR	CA-CB-CG	5.20	123.28	113.40
1	A	426	GLN	CA-CB-CG	5.20	124.83	113.40
1	I	372	THR	N-CA-CB	5.19	120.17	110.30
1	A	270	PHE	CG-CD2-CE2	5.19	126.51	120.80
1	I	262	ARG	CD-NE-CZ	5.19	130.87	123.60
1	A	87	PRO	N-CD-CG	5.19	110.99	103.20
1	G	92	PHE	CG-CD2-CE2	-5.19	115.09	120.80
2	N	173	PRO	N-CA-CB	5.19	109.53	103.30
2	F	251	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	F	451	TYR	CB-CG-CD1	-5.19	117.89	121.00
1	I	242	PHE	CZ-CE2-CD2	5.18	126.32	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	115	ILE	O-C-N	-5.18	114.41	122.70
1	E	328	GLU	CA-CB-CG	5.18	124.79	113.40
1	G	213	ARG	CD-NE-CZ	5.17	130.84	123.60
2	H	22	GLU	OE1-CD-OE2	-5.17	117.09	123.30
2	J	312	TYR	CD1-CG-CD2	5.17	123.59	117.90
1	E	364	SER	N-CA-CB	-5.17	102.74	110.50
2	L	21	TRP	NE1-CE2-CD2	-5.17	102.13	107.30
2	N	156	ARG	CD-NE-CZ	5.17	130.84	123.60
3	O	393	VAL	CA-C-N	5.17	128.57	117.20
2	B	257	THR	CA-CB-CG2	5.17	119.63	112.40
2	J	2	ARG	CD-NE-CZ	5.17	130.83	123.60
2	H	234	ILE	CA-CB-CG1	5.17	120.81	111.00
1	C	397	TRP	CD2-CE3-CZ3	5.16	125.51	118.80
2	F	446	GLU	OE1-CD-OE2	-5.16	117.10	123.30
1	I	431	ASP	CB-CG-OD2	-5.16	113.65	118.30
2	L	262	TYR	CG-CD2-CE2	-5.16	117.17	121.30
1	C	60	VAL	CG1-CB-CG2	-5.16	102.64	110.90
1	M	66	VAL	CG1-CB-CG2	-5.16	102.65	110.90
2	N	433	GLU	OE1-CD-OE2	-5.16	117.11	123.30
2	D	388	TRP	NE1-CE2-CD2	-5.16	102.14	107.30
2	F	108	TYR	CG-CD1-CE1	-5.16	117.17	121.30
1	K	257	MET	CG-SD-CE	5.16	108.45	100.20
2	B	373	ARG	CB-CA-C	5.15	120.70	110.40
2	F	74	VAL	CA-CB-CG1	5.15	118.62	110.90
2	F	82	THR	OG1-CB-CG2	-5.15	98.16	110.00
1	I	422	TYR	CD1-CE1-CZ	-5.15	115.17	119.80
2	L	210	TYR	CB-CG-CD1	5.15	124.09	121.00
2	L	272	TYR	CD1-CE1-CZ	5.15	124.43	119.80
1	E	50	TYR	CG-CD1-CE1	-5.15	117.18	121.30
1	K	76	VAL	CA-CB-CG1	5.15	118.62	110.90
1	C	265	PHE	CG-CD1-CE1	-5.14	115.14	120.80
1	M	378	PHE	CD1-CG-CD2	5.14	124.99	118.30
2	J	181	VAL	CA-CB-CG2	5.14	118.61	110.90
2	H	265	ILE	CA-CB-CG1	5.14	120.76	111.00
2	N	14	VAL	CA-CB-CG2	5.14	118.61	110.90
2	B	217	LEU	C-N-CA	5.14	134.54	121.70
1	C	242	PHE	N-CA-CB	-5.13	101.36	110.60
2	H	130	THR	N-CA-CB	5.13	120.05	110.30
1	C	314	ALA	N-CA-CB	5.13	117.28	110.10
2	B	163	LYS	CB-CA-C	5.13	120.66	110.40
2	N	199	ASP	CB-CG-OD1	5.13	122.92	118.30
2	F	74	VAL	C-N-CA	5.12	134.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	64	ILE	CB-CA-C	5.12	121.83	111.60
2	H	68	VAL	O-C-N	-5.12	114.51	122.70
2	H	65	ALA	N-CA-CB	-5.11	102.94	110.10
1	K	172	SER	N-CA-CB	-5.11	102.83	110.50
2	F	422	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	M	183	TYR	CB-CG-CD2	-5.11	117.93	121.00
2	D	149	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	I	299	MET	N-CA-CB	-5.11	101.41	110.60
2	L	402	ARG	NE-CZ-NH2	-5.11	117.75	120.30
2	F	253	THR	CA-CB-CG2	-5.11	105.25	112.40
1	E	166	THR	CA-CB-CG2	5.10	119.55	112.40
1	M	378	PHE	CG-CD1-CE1	-5.10	115.19	120.80
2	F	244	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	G	206	ALA	O-C-N	-5.10	114.54	122.70
2	B	402	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	I	390	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	C	37	HIS	CA-CB-CG	5.09	122.25	113.60
2	F	362	VAL	CG1-CB-CG2	-5.09	102.75	110.90
2	N	242	LEU	CB-CG-CD1	-5.09	102.35	111.00
2	D	449	GLU	C-N-CA	5.09	134.42	121.70
1	C	32	PRO	N-CA-CB	5.08	109.40	103.30
1	G	159	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	G	302	ALA	CB-CA-C	-5.08	102.48	110.10
2	J	49	PHE	CB-CG-CD2	-5.08	117.25	120.80
1	E	123	GLU	OE1-CD-OE2	-5.08	117.21	123.30
2	F	221	ARG	CD-NE-CZ	5.08	130.71	123.60
1	G	73	MET	CG-SD-CE	-5.07	92.08	100.20
2	L	205	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	K	92	PHE	CB-CG-CD1	5.07	124.35	120.80
2	J	392	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	I	37	HIS	O-C-N	-5.07	114.58	123.20
2	B	340	SER	N-CA-CB	-5.07	102.90	110.50
1	M	11	GLN	OE1-CD-NE2	-5.07	110.25	121.90
1	K	408	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	M	222	TYR	CB-CG-CD2	5.06	124.04	121.00
3	O	377	THR	C-N-CA	5.06	134.35	121.70
2	F	378	LEU	CB-CG-CD2	-5.05	102.41	111.00
1	G	407	GLU	CB-CA-C	5.05	120.51	110.40
2	N	290	GLU	CG-CD-OE1	5.05	128.41	118.30
2	L	177	VAL	CA-CB-CG1	5.05	118.48	110.90
2	N	363	VAL	CA-CB-CG1	5.05	118.48	110.90
1	C	367	PHE	N-CA-CB	-5.05	101.51	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	154	LYS	CA-CB-CG	-5.05	102.30	113.40
1	I	397	TRP	CE3-CZ3-CH2	-5.05	115.65	121.20
2	L	238	ILE	CA-CB-CG2	5.05	121.00	110.90
1	E	59	TYR	CD1-CE1-CZ	-5.05	115.26	119.80
1	E	62	ARG	CB-CA-C	5.05	120.49	110.40
2	F	388	TRP	CB-CG-CD1	-5.04	120.44	127.00
2	N	21	TRP	CZ3-CH2-CZ2	-5.04	115.55	121.60
2	B	67	PHE	CD1-CG-CD2	5.04	124.86	118.30
2	J	41	THR	OG1-CB-CG2	-5.04	98.40	110.00
1	C	361	LEU	CB-CG-CD2	5.04	119.57	111.00
2	J	67	PHE	CG-CD2-CE2	-5.04	115.26	120.80
2	N	201	ALA	CB-CA-C	5.04	117.66	110.10
1	C	30	ILE	C-N-CA	5.04	134.30	121.70
2	J	185	TYR	CA-CB-CG	5.04	122.97	113.40
1	A	180	VAL	CG1-CB-CG2	-5.03	102.85	110.90
2	F	37	PRO	C-N-CA	5.03	134.28	121.70
2	J	216	ASN	OD1-CG-ND2	-5.03	110.32	121.90
1	M	181	GLU	CA-C-N	5.03	131.19	117.10
1	G	40	SER	N-CA-CB	-5.03	102.95	110.50
2	J	407	TRP	CD1-CG-CD2	5.03	110.32	106.30
2	B	3	GLU	OE1-CD-OE2	-5.03	117.27	123.30
2	B	129	CYS	CA-CB-SG	-5.03	104.95	114.00
1	G	251	ARG	CB-CG-CD	5.03	124.67	111.60
2	H	46	ASP	CB-CG-OD2	5.03	122.83	118.30
2	H	316	CYS	CA-CB-SG	-5.03	104.95	114.00
2	J	175	PRO	N-CD-CG	5.03	110.74	103.20
1	M	191	GLN	CB-CA-C	-5.03	100.34	110.40
1	I	183	TYR	CZ-CE2-CD2	-5.03	115.28	119.80
2	J	296	PHE	O-C-N	-5.03	114.66	122.70
2	L	305	CYS	CA-CB-SG	-5.03	104.95	114.00
2	H	324	VAL	CA-CB-CG1	5.02	118.43	110.90
1	M	28	HIS	CA-CB-CG	-5.02	105.07	113.60
1	M	101	TRP	CD1-NE1-CE2	5.02	113.52	109.00
3	O	376	LEU	N-CA-C	5.02	124.54	111.00
2	J	445	GLU	OE1-CD-OE2	-5.01	117.28	123.30
1	I	76	VAL	CA-CB-CG1	5.01	118.42	110.90
1	C	391	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	M	409	THR	OG1-CB-CG2	-5.00	98.49	110.00

There are no chirality outliers.

All (122) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	TYR	Sidechain
1	A	131	GLN	Peptide
1	A	175	VAL	Peptide
1	A	183	TYR	Sidechain
1	A	200	TYR	Sidechain
1	A	208	TYR	Sidechain
1	A	212	PHE	Sidechain
1	A	32	PRO	Peptide
1	A	344	TRP	Peptide
1	A	371	SER	Mainchain
1	A	425	TYR	Sidechain
1	A	50	TYR	Sidechain
2	B	161	TYR	Sidechain
2	B	302	MET	Peptide
2	B	347	CYS	Peptide
2	B	393	HIS	Sidechain
2	B	411	GLU	Peptide
2	B	61	HIS	Sidechain
2	B	88	HIS	Sidechain
1	C	106	TYR	Sidechain
1	C	222	TYR	Sidechain
1	C	227	HIS	Sidechain
1	C	264	HIS	Sidechain
1	C	281	TYR	Sidechain
1	C	36	TYR	Sidechain
1	C	375	GLN	Mainchain
1	C	422	TYR	Sidechain
1	C	59	TYR	Sidechain
1	C	85	PHE	Sidechain
2	D	202	PHE	Sidechain
2	D	215	ARG	Peptide
2	D	28	HIS	Sidechain
2	D	312	TYR	Sidechain
2	D	370	LYS	Mainchain
2	D	404	PHE	Sidechain
2	D	432	TYR	Sidechain
2	D	449	GLU	Mainchain
1	E	111	GLU	Mainchain
1	E	165	ASN	Sidechain
1	E	183	TYR	Sidechain
1	E	281	TYR	Sidechain
1	E	422	TYR	Sidechain
1	E	50	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	E	51	TYR	Sidechain
2	F	11	GLN	Mainchain
2	F	161	TYR	Sidechain
2	F	185	TYR	Sidechain
2	F	192	HIS	Sidechain
2	F	210	TYR	Sidechain
2	F	227	LEU	Mainchain
2	F	233	GLN	Mainchain
2	F	302	MET	Peptide
2	F	316	CYS	Mainchain
2	F	74	VAL	Mainchain
2	F	97	GLU	Mainchain
1	G	106	TYR	Sidechain
1	G	159	TYR	Sidechain
1	G	36	TYR	Sidechain
1	G	50	TYR	Sidechain
1	G	51	TYR	Sidechain
2	H	161	TYR	Sidechain
2	H	244	PHE	Sidechain
2	H	28	HIS	Sidechain
2	H	319	TYR	Sidechain
2	H	353	VAL	Peptide
2	H	429	GLU	Sidechain
2	H	67	PHE	Sidechain
2	H	68	VAL	Peptide
1	I	183	TYR	Sidechain
1	I	200	TYR	Sidechain
1	I	218	THR	Mainchain
1	I	270	PHE	Sidechain
1	I	422	TYR	Sidechain
1	I	90	PHE	Sidechain
2	J	169	PHE	Peptide
2	J	177	VAL	Peptide
2	J	183	GLU	Sidechain
2	J	244	PHE	Mainchain
2	J	262	TYR	Sidechain
2	J	266	HIS	Sidechain
2	J	272	TYR	Sidechain
2	J	302	MET	Peptide
2	J	341	ILE	Peptide
2	J	68	VAL	Peptide
2	J	98	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	K	106	TYR	Sidechain
1	K	222	TYR	Sidechain
1	K	385	PHE	Sidechain
1	K	391	ARG	Sidechain
2	L	139	HIS	Sidechain,Peptide
2	L	140	SER	Peptide
2	L	161	TYR	Sidechain
2	L	172	TYR	Sidechain
2	L	21	TRP	Mainchain
2	L	255	PHE	Sidechain
2	L	351	PHE	Sidechain
2	L	357	TYR	Sidechain
2	L	389	ALA	Mainchain
2	L	417	GLU	Peptide
2	L	99	ALA	Peptide
1	M	106	TYR	Sidechain
1	M	21	TRP	Peptide
1	M	222	TYR	Sidechain
1	M	227	HIS	Sidechain
1	M	260	PHE	Peptide
1	M	307	HIS	Sidechain
1	M	367	PHE	Sidechain
1	M	51	TYR	Sidechain
1	M	59	TYR	Sidechain
2	N	108	TYR	Sidechain
2	N	116	ASP	Peptide
2	N	149	PHE	Sidechain
2	N	161	TYR	Sidechain
2	N	170	SER	Peptide
2	N	185	TYR	Sidechain
2	N	194	THR	Mainchain
2	N	243	ARG	Mainchain
2	N	255	PHE	Sidechain
2	N	3	GLU	Peptide
2	N	451	TYR	Sidechain
2	N	68	VAL	Peptide

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	A	3498	0	3342	10	0
1	C	3498	0	3342	8	0
1	E	3498	0	3342	6	0
1	G	3498	0	3342	5	0
1	I	3498	0	3342	3	0
1	K	3498	0	3342	13	0
1	M	3498	0	3342	11	0
2	B	3524	0	3409	12	0
2	D	3524	0	3409	6	0
2	F	3524	0	3409	8	0
2	H	3524	0	3409	13	0
2	J	3524	0	3409	14	0
2	L	3524	0	3409	7	0
2	N	3524	0	3409	13	0
3	O	1455	0	1526	3	0
4	A	28	0	12	0	0
4	C	28	0	12	0	0
4	E	28	0	12	0	0
4	G	28	0	12	0	0
4	I	28	0	12	0	0
4	K	28	0	12	0	0
4	M	28	0	12	0	0
5	B	32	0	12	0	0
5	D	32	0	12	0	0
5	F	32	0	12	0	0
5	H	32	0	12	0	0
5	J	32	0	12	0	0
5	L	32	0	12	1	0
5	N	32	0	12	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	L	1	0	0	0	0
6	N	1	0	0	0	0
All	All	51036	0	48951	122	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 1.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2:ARG:NH2	1:M:249:ASP:HB3	2.03	0.74
2:H:382:THR:HG21	2:H:436:GLY:HA3	1.77	0.67
2:B:269:LEU:HD23	2:B:269:LEU:H	1.62	0.65
1:G:101:TRP:CH2	1:G:105:HIS:CG	2.86	0.64
2:B:123:ARG:HH11	2:B:123:ARG:HG3	1.61	0.64
2:H:202:PHE:CE1	2:H:378:LEU:HD13	2.38	0.59
2:F:256:GLN:HB3	1:G:397:TRP:CZ2	2.38	0.59
1:A:105:HIS:CE1	1:A:150:LEU:HD13	2.38	0.58
1:K:189:VAL:O	1:K:193:VAL:HG12	2.05	0.57
1:M:238:THR:HG22	1:M:354:CYS:SG	2.46	0.56
2:H:319:TYR:CD2	2:H:375:VAL:HG22	2.41	0.56
2:J:326:LYS:HD3	1:K:220:PRO:HG3	1.88	0.55
2:D:147:SER:HB2	2:D:190:THR:HG21	1.88	0.55
3:O:388:HIS:CG	3:O:389:GLY:HA2	2.42	0.54
1:K:324:LYS:HE2	2:L:210:TYR:HB3	1.89	0.53
1:M:2:ARG:HH11	2:N:97:GLU:HA	1.75	0.52
1:K:167:PHE:CE2	1:K:200:TYR:CE1	2.98	0.52
1:M:16:ILE:HG22	1:M:136:THR:HG21	1.91	0.52
2:J:105:ARG:NH2	2:J:110:ILE:HD11	2.25	0.51
1:A:170:VAL:HB	1:A:171:PRO:HD2	1.92	0.51
1:M:28:HIS:CE1	1:M:242:PHE:CZ	2.98	0.51
1:K:252:LYS:HE2	5:L:501:GTP:O1G	2.10	0.51
1:M:2:ARG:NH1	2:N:98:ASP:H	2.08	0.50
2:H:164:LYS:HE2	2:H:164:LYS:HA	1.94	0.50
2:J:211:ASP:CG	2:J:215:ARG:HH22	2.15	0.50
1:K:213:ARG:O	1:K:216:LYS:HE2	2.12	0.49
2:N:7:ILE:HG23	2:N:66:VAL:HG23	1.94	0.49
2:L:297:GLU:HB3	2:L:300:ASN:HD22	1.78	0.49
2:N:133:GLN:HE22	2:N:242:LEU:HD22	1.77	0.48
2:F:252:LEU:HD12	2:F:252:LEU:N	2.28	0.48
3:O:393:VAL:HB	3:O:394:TYR:HA	1.93	0.48
1:E:235:GLY:HA3	1:E:366:THR:HG21	1.96	0.48
2:J:52:PHE:CZ	2:J:243:ARG:HD3	2.49	0.48
1:C:212:PHE:CD1	1:C:218:THR:HA	2.48	0.48
1:G:101:TRP:CH2	1:G:105:HIS:CD2	3.02	0.48
1:M:156:ARG:HH11	1:M:164:MET:HB2	1.79	0.48
2:L:104:ALA:HB1	2:L:411:GLU:HB2	1.95	0.47
2:L:121:ARG:NH2	2:L:124:LYS:CB	2.78	0.47
1:I:396:HIS:CE1	1:I:397:TRP:CE2	3.03	0.47
2:J:17:GLY:HA2	2:J:20:CYS:SG	2.55	0.46
1:M:101:TRP:CD1	1:M:146:GLY:HA2	2.51	0.46
2:B:195:LEU:HD13	2:B:266:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:344:VAL:HG21	2:L:346:TRP:CZ2	2.51	0.46
1:E:210:ILE:CD1	1:E:300:MET:HG2	2.45	0.46
2:L:121:ARG:NH2	2:L:124:LYS:HB2	2.30	0.46
1:A:368:ILE:HD12	1:A:368:ILE:N	2.31	0.45
2:B:71:GLU:HG3	2:B:73:THR:H	1.81	0.45
2:J:1:MET:HA	2:J:130:THR:OG1	2.17	0.45
1:K:342:VAL:HG22	1:K:343:GLU:N	2.31	0.45
1:G:32:PRO:HB3	1:G:81:PHE:H	1.81	0.45
2:H:241:SER:CB	2:H:250:VAL:H	2.30	0.45
2:J:46:ASP:HA	2:J:47:ASP:HB2	1.97	0.45
1:M:2:ARG:NH2	1:M:249:ASP:CB	2.78	0.45
2:N:133:GLN:HE22	2:N:242:LEU:CD2	2.29	0.45
1:C:282:ARG:NH2	1:C:284:LEU:HD12	2.32	0.45
2:F:250:VAL:HG22	2:F:352:LYS:HE3	1.99	0.45
2:H:26:LEU:HD13	2:H:363:VAL:HG22	1.97	0.44
1:M:322:SER:CB	2:N:221:ARG:HB2	2.47	0.44
2:B:263:PRO:HD3	1:C:396:HIS:CG	2.52	0.44
2:F:20:CYS:SG	2:F:235:VAL:HG21	2.58	0.44
2:D:286:LEU:HD13	2:D:371:VAL:HG12	2.00	0.44
1:G:21:TRP:CZ2	1:G:63:ALA:HB2	2.53	0.44
2:B:438:ASP:CG	2:B:439:SER:H	2.21	0.44
2:J:107:HIS:HD2	2:J:108:TYR:CE2	2.35	0.44
2:B:319:TYR:CD2	2:B:375:VAL:HG22	2.53	0.43
2:F:332:ILE:CG2	2:F:351:PHE:CE1	3.02	0.43
2:N:269:LEU:HD12	2:N:269:LEU:O	2.18	0.43
2:B:169:PHE:CE2	2:B:202:PHE:CD2	3.07	0.43
2:B:342:GLN:HG2	2:B:451:TYR:CE2	2.53	0.43
1:E:32:PRO:HA	1:E:81:PHE:CE1	2.53	0.43
2:J:188:ILE:HG22	2:J:421:ALA:HB1	1.99	0.43
2:D:126:ALA:HA	2:D:129:CYS:SG	2.58	0.43
1:A:135:LEU:HB3	1:A:166:THR:HG23	2.01	0.43
1:M:380:ARG:NH1	1:M:381:ILE:HD11	2.34	0.43
1:C:21:TRP:CZ3	1:C:61:PRO:HB3	2.54	0.43
2:D:261:PRO:HA	1:E:394:PHE:CD1	2.54	0.42
2:H:215:ARG:NH2	2:H:299:ALA:HB1	2.34	0.42
2:H:344:VAL:HG21	2:H:346:TRP:CE2	2.54	0.42
2:N:269:LEU:HD12	2:N:269:LEU:C	2.38	0.42
1:I:290:THR:HA	1:I:293:MET:HG2	2.02	0.42
2:J:183:GLU:N	2:J:184:PRO:HD2	2.34	0.42
2:N:80:THR:HA	2:N:84:ARG:CZ	2.49	0.42
3:O:393:VAL:HB	3:O:394:TYR:CA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:O	1:A:49:VAL:HG23	2.19	0.42
2:F:105:ARG:NH2	2:F:110:ILE:HG13	2.34	0.42
2:F:157:LEU:HD23	2:F:157:LEU:HA	1.93	0.42
1:K:167:PHE:CD2	1:K:200:TYR:CD1	3.08	0.42
1:A:344:TRP:CE3	2:B:401:LYS:HG3	2.55	0.42
2:H:265:ILE:HG23	2:H:432:TYR:CZ	2.55	0.42
1:I:316:VAL:HG22	1:I:352:ALA:HB3	2.01	0.42
2:D:216:ASN:HB3	2:D:275:VAL:O	2.20	0.42
1:C:318:ARG:NH2	1:C:357:PRO:O	2.53	0.42
1:K:167:PHE:CE2	1:K:200:TYR:CD1	3.08	0.42
2:N:192:HIS:CD2	2:N:421:ALA:HA	2.54	0.42
2:H:18:ASN:HD21	2:H:78:VAL:HG22	1.86	0.41
2:H:319:TYR:CD2	2:H:375:VAL:CG2	3.03	0.41
2:H:316:CYS:HA	2:H:352:LYS:O	2.21	0.41
2:N:332:ILE:HG22	2:N:336:LYS:HE3	2.02	0.41
1:K:130:LEU:HD21	1:K:133:PHE:CZ	2.55	0.41
1:K:150:LEU:O	1:K:153:SER:HB2	2.21	0.41
2:N:42:ILE:HD12	2:N:43:GLY:N	2.36	0.41
1:A:155:ILE:HG22	1:A:164:MET:CE	2.51	0.41
2:B:449:GLU:HG2	2:B:451:TYR:O	2.21	0.41
1:C:19:LYS:HE3	1:C:227:HIS:CG	2.55	0.41
2:J:182:VAL:C	2:J:184:PRO:HD2	2.41	0.41
2:L:313:MET:HA	2:L:344:VAL:HG22	2.03	0.41
1:A:233:MET:HB3	1:A:233:MET:HE2	1.98	0.41
2:H:395:PHE:CZ	2:H:399:TYR:CD2	3.08	0.41
1:E:187:LEU:HD23	1:E:187:LEU:HA	1.87	0.41
2:J:201:ALA:HB1	2:J:203:MET:HE1	2.02	0.41
2:F:378:LEU:HA	2:F:378:LEU:HD23	1.91	0.40
2:J:7:ILE:HD13	2:J:7:ILE:HG21	1.94	0.40
2:J:139:HIS:CE1	2:J:170:SER:HB3	2.56	0.40
1:K:99:ASN:HA	1:K:142:GLY:HA3	2.03	0.40
1:K:167:PHE:CZ	1:K:200:TYR:CE1	3.10	0.40
1:A:254:ALA:HB1	2:B:407:TRP:CH2	2.57	0.40
1:C:19:LYS:CE	1:C:227:HIS:CG	3.05	0.40
1:C:239:CYS:SG	1:C:354:CYS:HB2	2.61	0.40
2:N:332:ILE:CG2	2:N:336:LYS:HE3	2.51	0.40
1:E:374:ILE:HD12	1:E:374:ILE:HA	2.01	0.40
1:A:96:GLY:O	1:A:103:LYS:HE2	2.21	0.40
2:D:115:ILE:HG12	2:D:152:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/445 (100%)	407 (92%)	33 (7%)	3 (1%)	22	60
1	C	443/445 (100%)	415 (94%)	26 (6%)	2 (0%)	29	67
1	E	443/445 (100%)	409 (92%)	32 (7%)	2 (0%)	29	67
1	G	443/445 (100%)	413 (93%)	29 (6%)	1 (0%)	47	80
1	I	443/445 (100%)	413 (93%)	27 (6%)	3 (1%)	22	60
1	K	443/445 (100%)	409 (92%)	32 (7%)	2 (0%)	29	67
1	M	443/445 (100%)	413 (93%)	26 (6%)	4 (1%)	17	54
2	B	449/451 (100%)	417 (93%)	29 (6%)	3 (1%)	22	60
2	D	449/451 (100%)	415 (92%)	31 (7%)	3 (1%)	22	60
2	F	449/451 (100%)	414 (92%)	34 (8%)	1 (0%)	47	80
2	H	449/451 (100%)	415 (92%)	32 (7%)	2 (0%)	34	71
2	J	449/451 (100%)	416 (93%)	28 (6%)	5 (1%)	14	50
2	L	449/451 (100%)	419 (93%)	25 (6%)	5 (1%)	14	50
2	N	449/451 (100%)	412 (92%)	36 (8%)	1 (0%)	47	80
3	O	192/194 (99%)	162 (84%)	23 (12%)	7 (4%)	3	28
All	All	6436/6466 (100%)	5949 (92%)	443 (7%)	44 (1%)	26	60

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	404	PHE
3	O	390	ALA
2	B	322	ASP
1	C	81	PHE
1	C	394	PHE
2	H	29	GLY
2	J	348	PRO
1	K	394	PHE

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Mol	Chain	Res	Type
2	L	132	LEU
2	L	350	GLY
2	L	404	PHE
3	O	350	VAL
3	O	388	HIS
2	B	281	ALA
1	E	394	PHE
2	H	57	GLY
1	I	394	PHE
1	M	48	ASN
3	O	278	ILE
3	O	393	VAL
1	A	348	ASN
2	D	416	GLY
1	G	296	ALA
2	J	338	LYS
2	L	186	ASN
1	M	296	ALA
1	A	268	PRO
1	E	216	LYS
2	L	112	LYS
1	M	128	ASP
2	N	441	GLU
3	O	269	GLN
1	A	427	ASP
2	D	437	VAL
1	I	304	ASP
2	J	341	ILE
1	K	305	PRO
3	O	349	ARG
1	M	71	GLY
2	D	95	GLY
2	B	131	GLY
2	F	348	PRO
2	J	131	GLY
1	I	440	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	381/381 (100%)	368 (97%)	13 (3%)	37	61
1	C	381/381 (100%)	370 (97%)	11 (3%)	42	64
1	E	381/381 (100%)	372 (98%)	9 (2%)	49	69
1	G	381/381 (100%)	369 (97%)	12 (3%)	40	63
1	I	381/381 (100%)	372 (98%)	9 (2%)	49	69
1	K	381/381 (100%)	373 (98%)	8 (2%)	53	72
1	M	381/381 (100%)	372 (98%)	9 (2%)	49	69
2	B	379/379 (100%)	369 (97%)	10 (3%)	46	67
2	D	379/379 (100%)	367 (97%)	12 (3%)	39	62
2	F	379/379 (100%)	370 (98%)	9 (2%)	49	69
2	H	379/379 (100%)	361 (95%)	18 (5%)	26	53
2	J	379/379 (100%)	364 (96%)	15 (4%)	31	57
2	L	379/379 (100%)	361 (95%)	18 (5%)	26	53
2	N	379/379 (100%)	359 (95%)	20 (5%)	22	51
3	O	168/168 (100%)	161 (96%)	7 (4%)	30	56
All	All	5488/5488 (100%)	5308 (97%)	180 (3%)	41	62

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	50	TYR
1	A	65	LEU
1	A	84	ILE
1	A	137	HIS
1	A	162	ARG
1	A	172	SER
1	A	188	SER
1	A	227	HIS
1	A	366	THR
1	A	367	PHE
1	A	407	GLU
1	A	427	ASP
2	B	9	VAL
2	B	18	ASN

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Mol	Chain	Res	Type
2	B	25	CYS
2	B	205	ASP
2	B	266	HIS
2	B	346	TRP
2	B	372	GLN
2	B	384	ILE
2	B	395	PHE
2	B	450	GLU
1	C	46	ARG
1	C	65	LEU
1	C	117	LEU
1	C	137	HIS
1	C	161	ASP
1	C	225	LEU
1	C	266	PHE
1	C	274	THR
1	C	286	VAL
1	C	340	TYR
1	C	350	LYS
2	D	49	PHE
2	D	140	SER
2	D	141	PHE
2	D	145	THR
2	D	169	PHE
2	D	194	THR
2	D	200	CYS
2	D	253	THR
2	D	266	HIS
2	D	271	THR
2	D	347	CYS
2	D	381	THR
1	E	3	GLU
1	E	15	GLN
1	E	91	VAL
1	E	113	VAL
1	E	147	MET
1	E	172	SER
1	E	178	THR
1	E	193	VAL
1	E	205	GLU
2	F	1	MET
2	F	52	PHE

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Mol	Chain	Res	Type
2	F	109	THR
2	F	214	ARG
2	F	249	ASN
2	F	266	HIS
2	F	269	LEU
2	F	388	TRP
2	F	392	ASP
1	G	1	MET
1	G	33	THR
1	G	53	GLU
1	G	66	VAL
1	G	72	THR
1	G	143	THR
1	G	156	ARG
1	G	219	THR
1	G	386	THR
1	G	391	ARG
1	G	409	THR
1	G	412	GLU
2	H	11	GLN
2	H	49	PHE
2	H	51	THR
2	H	166	LYS
2	H	170	SER
2	H	196	GLU
2	H	200	CYS
2	H	204	VAL
2	H	224	TYR
2	H	226	ASN
2	H	245	ASP
2	H	266	HIS
2	H	269	LEU
2	H	301	GLN
2	H	326	LYS
2	H	432	TYR
2	H	437	VAL
2	H	449	GLU
1	I	1	MET
1	I	2	ARG
1	I	39	ASP
1	I	130	LEU
1	I	133	PHE

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Mol	Chain	Res	Type
1	I	137	HIS
1	I	143	THR
1	I	161	ASP
1	I	442	GLU
2	J	7	ILE
2	J	50	ASN
2	J	98	ASP
2	J	204	VAL
2	J	214	ARG
2	J	217	LEU
2	J	227	LEU
2	J	266	HIS
2	J	305	CYS
2	J	324	VAL
2	J	329	ASN
2	J	375	VAL
2	J	379	SER
2	J	386	GLU
2	J	418	PHE
1	K	136	THR
1	K	137	HIS
1	K	172	SER
1	K	327	ASP
1	K	347	ASN
1	K	350	LYS
1	K	351	THR
1	K	435	GLU
2	L	40	LYS
2	L	42	ILE
2	L	49	PHE
2	L	66	VAL
2	L	101	ASN
2	L	190	THR
2	L	194	THR
2	L	200	CYS
2	L	211	ASP
2	L	230	LEU
2	L	253	THR
2	L	256	GLN
2	L	257	THR
2	L	266	HIS
2	L	381	THR

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Mol	Chain	Res	Type
2	L	430	LYS
2	L	437	VAL
2	L	441	GLU
1	M	61	PRO
1	M	86	ARG
1	M	168	SER
1	M	212	PHE
1	M	320	ARG
1	M	331	LEU
1	M	366	THR
1	M	390	ARG
1	M	412	GLU
2	N	42	ILE
2	N	94	THR
2	N	140	SER
2	N	166	LYS
2	N	179	THR
2	N	200	CYS
2	N	217	LEU
2	N	224	TYR
2	N	227	LEU
2	N	253	THR
2	N	263	PRO
2	N	269	LEU
2	N	275	VAL
2	N	334	THR
2	N	378	LEU
2	N	381	THR
2	N	391	LEU
2	N	418	PHE
2	N	441	GLU
2	N	450	GLU
3	O	243	LEU
3	O	296	ASN
3	O	348	ASP
3	O	373	THR
3	O	374	HIS
3	O	378	PHE
3	O	381	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	C	279	GLN
2	D	50	ASN
2	D	139	HIS
2	D	197	HIS
2	D	393	HIS
1	G	291	GLN
2	H	18	ASN
2	H	28	HIS
2	H	266	HIS
1	I	14	ASN
2	J	107	HIS
2	J	266	HIS
2	J	309	HIS
2	L	216	ASN
2	L	266	HIS
2	L	300	ASN
2	N	133	GLN
2	N	216	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 for Mogul analysis.

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	$\#\|Z\| > 2$
5	GTP	L	501	6	26,34,34	1.25	2 (7%)	33,54,54	2.34	11 (33%)
4	GDP	G	501	-	24,30,30	1.27	3 (12%)	31,47,47	2.43	11 (35%)
4	GDP	C	501	-	24,30,30	1.31	3 (12%)	31,47,47	3.18	18 (58%)
4	GDP	A	501	-	24,30,30	1.29	1 (4%)	31,47,47	2.31	13 (41%)
5	GTP	B	501	6	26,34,34	1.23	4 (15%)	33,54,54	2.25	7 (21%)
5	GTP	N	501	6	26,34,34	1.27	3 (11%)	33,54,54	2.07	6 (18%)
4	GDP	I	501	-	24,30,30	1.16	2 (8%)	31,47,47	2.06	6 (19%)
4	GDP	E	501	-	24,30,30	1.26	3 (12%)	31,47,47	1.91	8 (25%)
4	GDP	M	501	-	24,30,30	1.28	2 (8%)	31,47,47	2.17	10 (32%)
5	GTP	D	501	6	26,34,34	1.30	2 (7%)	33,54,54	2.32	10 (30%)
5	GTP	F	501	6	26,34,34	1.22	3 (11%)	33,54,54	2.05	6 (18%)
5	GTP	J	501	6	26,34,34	1.26	1 (3%)	33,54,54	2.20	6 (18%)
4	GDP	K	501	-	24,30,30	1.25	2 (8%)	31,47,47	2.19	9 (29%)
5	GTP	H	501	6	26,34,34	1.19	2 (7%)	33,54,54	2.06	6 (18%)

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
5	GTP	L	501	6	-	7/18/38/38	0/3/3/3
4	GDP	G	501	-	-	3/12/32/32	0/3/3/3
4	GDP	C	501	-	-	2/12/32/32	0/3/3/3
4	GDP	A	501	-	-	2/12/32/32	0/3/3/3
5	GTP	B	501	6	-	2/18/38/38	0/3/3/3
5	GTP	N	501	6	-	0/18/38/38	0/3/3/3
4	GDP	I	501	-	-	4/12/32/32	0/3/3/3
4	GDP	E	501	-	-	2/12/32/32	0/3/3/3
4	GDP	M	501	-	-	1/12/32/32	0/3/3/3
5	GTP	D	501	6	-	1/18/38/38	0/3/3/3
5	GTP	F	501	6	-	3/18/38/38	0/3/3/3
5	GTP	J	501	6	-	3/18/38/38	0/3/3/3
4	GDP	K	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	H	501	6	-	0/18/38/38	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	501	GTP	C6-N1	4.03	1.40	1.33
5	D	501	GTP	C6-N1	3.98	1.40	1.33
4	A	501	GDP	C6-N1	3.95	1.39	1.33
4	C	501	GDP	C6-N1	3.82	1.39	1.33
4	M	501	GDP	C6-N1	3.75	1.39	1.33
5	L	501	GTP	C6-N1	3.62	1.39	1.33
4	E	501	GDP	C6-N1	3.60	1.39	1.33
4	K	501	GDP	C6-N1	3.42	1.39	1.33
4	G	501	GDP	C6-N1	3.21	1.38	1.33
5	F	501	GTP	C6-N1	3.04	1.38	1.33
5	N	501	GTP	C6-N1	2.96	1.38	1.33
5	H	501	GTP	C6-N1	2.91	1.38	1.33
4	I	501	GDP	C6-N1	2.90	1.38	1.33
5	D	501	GTP	C8-N7	-2.58	1.30	1.34
4	G	501	GDP	C8-N7	-2.49	1.30	1.34
5	B	501	GTP	C6-N1	2.39	1.37	1.33
4	M	501	GDP	C8-N7	-2.35	1.30	1.34
4	C	501	GDP	C8-N7	-2.34	1.30	1.34
4	G	501	GDP	C2-N1	2.25	1.39	1.35
4	K	501	GDP	C8-N7	-2.21	1.30	1.34
5	N	501	GTP	PG-O3G	-2.18	1.46	1.54
5	B	501	GTP	PG-O2G	-2.18	1.46	1.54
4	E	501	GDP	C8-N7	-2.15	1.30	1.34
4	E	501	GDP	C2-N1	2.15	1.39	1.35
5	H	501	GTP	C8-N7	-2.14	1.30	1.34
5	N	501	GTP	PG-O2G	-2.13	1.46	1.54
5	B	501	GTP	PG-O3G	-2.12	1.46	1.54
5	F	501	GTP	C8-N7	-2.12	1.30	1.34
4	C	501	GDP	C2-N1	2.12	1.39	1.35
4	I	501	GDP	C8-N7	-2.09	1.31	1.34
5	F	501	GTP	C5-C6	2.09	1.45	1.41
5	B	501	GTP	C8-N7	-2.08	1.31	1.34
5	L	501	GTP	C2-N1	2.07	1.39	1.35

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	501	GTP	C5-C6-N1	-8.16	112.27	123.43
4	C	501	GDP	N3-C2-N1	-7.84	116.77	127.22
4	G	501	GDP	C5-C6-N1	-7.51	113.16	123.43
4	M	501	GDP	C5-C6-N1	-7.46	113.23	123.43
5	B	501	GTP	C5-C6-N1	-7.42	113.28	123.43
5	F	501	GTP	C5-C6-N1	-7.29	113.47	123.43
5	H	501	GTP	C5-C6-N1	-7.17	113.62	123.43
4	I	501	GDP	C5-C6-N1	-7.15	113.65	123.43
5	N	501	GTP	C5-C6-N1	-7.03	113.81	123.43
4	K	501	GDP	C4-C5-C6	-6.42	114.67	120.80
4	C	501	GDP	C5-C6-N1	-5.91	115.35	123.43
4	A	501	GDP	C5-C6-N1	-5.90	115.37	123.43
5	D	501	GTP	PB-O3B-PG	-5.86	112.73	132.83
5	L	501	GTP	C5-C6-N1	-5.81	115.49	123.43
5	B	501	GTP	C2-N1-C6	5.41	124.53	115.93
5	D	501	GTP	C4-C5-C6	-5.33	115.71	120.80
4	C	501	GDP	C2'-C3'-C4'	-5.30	92.34	102.64
4	E	501	GDP	C4-C5-C6	-5.29	115.75	120.80
4	C	501	GDP	C2-N1-C6	5.27	124.30	115.93
5	D	501	GTP	C5-C6-N1	-5.18	116.35	123.43
4	E	501	GDP	C5-C6-N1	-5.07	116.49	123.43
4	C	501	GDP	O4'-C1'-C2'	-4.98	99.65	106.93
5	J	501	GTP	N2-C2-N1	-4.96	109.54	117.25
4	I	501	GDP	C2-N1-C6	4.90	123.71	115.93
5	H	501	GTP	C2-N1-C6	4.82	123.58	115.93
4	C	501	GDP	O4'-C4'-C3'	4.80	114.62	105.11
4	G	501	GDP	C2-N1-C6	4.80	123.56	115.93
5	N	501	GTP	C2-N1-C6	4.69	123.38	115.93
4	C	501	GDP	C4-C5-C6	-4.66	116.35	120.80
4	A	501	GDP	C3'-C2'-C1'	-4.65	93.97	100.98
5	F	501	GTP	C2-N1-C6	4.65	123.32	115.93
5	L	501	GTP	N2-C2-N3	4.56	125.22	117.79
5	H	501	GTP	PB-O3B-PG	-4.55	117.21	132.83
5	D	501	GTP	PA-O3A-PB	4.39	147.89	132.83
5	B	501	GTP	PB-O3B-PG	-4.32	117.99	132.83
4	A	501	GDP	C4-C5-N7	4.32	113.90	109.40
4	G	501	GDP	C2-N3-C4	-4.30	110.44	115.36
4	M	501	GDP	C2-N1-C6	4.24	122.66	115.93
5	N	501	GTP	PB-O3B-PG	-4.22	118.33	132.83
5	L	501	GTP	PA-O3A-PB	-4.21	118.39	132.83
5	F	501	GTP	PA-O3A-PB	-4.08	118.83	132.83
4	K	501	GDP	PA-O3A-PB	-4.04	118.95	132.83
5	N	501	GTP	PA-O3A-PB	-3.89	119.47	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	GDP	O2'-C2'-C1'	3.85	125.07	110.85
5	F	501	GTP	PB-O3B-PG	-3.85	119.62	132.83
5	J	501	GTP	C2-N3-C4	-3.84	110.97	115.36
5	L	501	GTP	C2-N1-C6	3.84	122.03	115.93
4	I	501	GDP	PA-O3A-PB	-3.79	119.82	132.83
5	B	501	GTP	PA-O3A-PB	-3.78	119.85	132.83
5	L	501	GTP	N3-C2-N1	-3.69	122.30	127.22
4	E	501	GDP	C2-N1-C6	3.63	121.69	115.93
4	C	501	GDP	PA-O3A-PB	-3.62	120.42	132.83
4	G	501	GDP	C4-C5-C6	-3.60	117.36	120.80
5	L	501	GTP	C4-C5-C6	-3.55	117.40	120.80
4	K	501	GDP	C5-C6-N1	-3.50	118.65	123.43
5	J	501	GTP	C2-N1-C6	3.47	121.44	115.93
5	L	501	GTP	O4'-C1'-C2'	-3.46	101.87	106.93
5	D	501	GTP	C2-N1-C6	3.43	121.39	115.93
4	K	501	GDP	C1'-N9-C4	-3.41	120.65	126.64
5	J	501	GTP	N2-C2-N3	3.35	123.25	117.79
4	A	501	GDP	PA-O3A-PB	-3.32	121.44	132.83
4	C	501	GDP	C2-N3-C4	3.27	119.09	115.36
4	G	501	GDP	C4-C5-N7	3.26	112.80	109.40
5	L	501	GTP	N2-C2-N1	-3.20	112.27	117.25
4	C	501	GDP	C3'-C2'-C1'	3.16	105.74	100.98
4	A	501	GDP	C2-N3-C4	-3.13	111.78	115.36
5	H	501	GTP	PA-O3A-PB	-3.07	122.30	132.83
5	B	501	GTP	C4-C5-C6	-3.06	117.88	120.80
4	M	501	GDP	C4-C5-N7	3.00	112.53	109.40
4	M	501	GDP	N2-C2-N3	2.95	122.59	117.79
5	B	501	GTP	C2-N3-C4	-2.86	112.09	115.36
4	E	501	GDP	N3-C2-N1	-2.84	123.44	127.22
5	N	501	GTP	C4-C5-C6	-2.81	118.12	120.80
5	D	501	GTP	N2-C2-N1	2.77	121.57	117.25
5	H	501	GTP	C4-C5-C6	-2.72	118.20	120.80
4	E	501	GDP	O4'-C4'-C5'	2.71	118.30	109.37
4	M	501	GDP	N3-C2-N1	-2.71	123.61	127.22
4	K	501	GDP	N2-C2-N1	-2.66	113.11	117.25
5	L	501	GTP	O2G-PG-O3B	-2.65	95.74	104.64
4	K	501	GDP	C3'-C2'-C1'	-2.64	97.00	100.98
5	D	501	GTP	O5'-C5'-C4'	2.63	118.05	108.99
4	C	501	GDP	O2'-C2'-C1'	-2.60	101.24	110.85
4	I	501	GDP	O3B-PB-O2B	2.60	117.57	107.64
4	C	501	GDP	O3B-PB-O2B	2.56	117.43	107.64
4	I	501	GDP	C4-C5-C6	-2.55	118.36	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	501	GTP	N3-C2-N1	-2.54	123.84	127.22
4	C	501	GDP	N2-C2-N1	2.53	121.19	117.25
5	D	501	GTP	O2G-PG-O1G	2.51	120.50	110.68
4	M	501	GDP	PA-O3A-PB	2.50	141.40	132.83
4	M	501	GDP	N2-C2-N1	-2.47	113.40	117.25
4	A	501	GDP	O3'-C3'-C4'	2.47	118.18	111.05
4	G	501	GDP	O4'-C1'-C2'	2.45	110.50	106.93
4	G	501	GDP	O4'-C4'-C3'	2.44	109.95	105.11
4	A	501	GDP	O3B-PB-O2B	2.44	116.95	107.64
5	H	501	GTP	C2-N3-C4	-2.42	112.59	115.36
4	M	501	GDP	O3B-PB-O2B	2.41	116.85	107.64
4	A	501	GDP	C2-N1-C6	2.41	119.75	115.93
4	K	501	GDP	C4-C5-N7	2.41	111.91	109.40
4	M	501	GDP	O4'-C4'-C5'	2.37	117.18	109.37
4	C	501	GDP	N2-C2-N3	2.34	121.60	117.79
5	L	501	GTP	O4'-C4'-C5'	-2.32	101.75	109.37
5	F	501	GTP	C2-N3-C4	-2.31	112.72	115.36
4	G	501	GDP	O2'-C2'-C1'	-2.31	102.32	110.85
4	A	501	GDP	C4-C5-C6	-2.30	118.60	120.80
5	L	501	GTP	O2B-PB-O1B	2.29	123.54	112.24
4	I	501	GDP	C2-N3-C4	-2.28	112.75	115.36
4	K	501	GDP	O4'-C1'-C2'	-2.28	103.59	106.93
5	N	501	GTP	C2-N3-C4	-2.28	112.76	115.36
5	J	501	GTP	O3G-PG-O2G	2.26	116.29	107.64
4	A	501	GDP	N2-C2-N1	-2.25	113.76	117.25
5	D	501	GTP	C2-N3-C4	-2.22	112.82	115.36
4	G	501	GDP	N2-C2-N1	-2.19	113.84	117.25
4	A	501	GDP	O4'-C1'-C2'	-2.17	103.76	106.93
4	G	501	GDP	C3'-C2'-C1'	2.16	104.23	100.98
4	K	501	GDP	C2-N1-C6	2.15	119.34	115.93
5	B	501	GTP	N2-C2-N1	-2.15	113.92	117.25
4	E	501	GDP	C2-N3-C4	-2.14	112.91	115.36
5	F	501	GTP	C4-C5-C6	-2.14	118.76	120.80
4	E	501	GDP	C5'-C4'-C3'	-2.13	107.20	115.18
4	C	501	GDP	O3A-PB-O1B	-2.13	99.39	111.19
4	C	501	GDP	C5'-C4'-C3'	-2.10	107.32	115.18
4	C	501	GDP	O2A-PA-O1A	2.10	122.60	112.24
4	G	501	GDP	N2-C2-N3	2.08	121.18	117.79
4	C	501	GDP	O3'-C3'-C2'	2.04	118.44	111.82
4	A	501	GDP	C2'-C3'-C4'	2.02	106.57	102.64
4	M	501	GDP	O2'-C2'-C3'	2.01	118.33	111.82
4	E	501	GDP	O2A-PA-O1A	2.01	122.18	112.24

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GDP	PA-O3A-PB-O2B
4	C	501	GDP	PA-O3A-PB-O2B
4	G	501	GDP	C5'-O5'-PA-O3A
4	K	501	GDP	PA-O3A-PB-O2B
4	M	501	GDP	C5'-O5'-PA-O1A
5	J	501	GTP	PB-O3B-PG-O2G
5	L	501	GTP	PB-O3B-PG-O3G
5	L	501	GTP	C5'-O5'-PA-O1A
5	B	501	GTP	O4'-C4'-C5'-O5'
5	B	501	GTP	C3'-C4'-C5'-O5'
4	G	501	GDP	C3'-C4'-C5'-O5'
4	I	501	GDP	O4'-C4'-C5'-O5'
5	J	501	GTP	PA-O3A-PB-O1B
5	L	501	GTP	C5'-O5'-PA-O3A
5	L	501	GTP	PB-O3A-PA-O2A
4	G	501	GDP	C5'-O5'-PA-O2A
5	F	501	GTP	C5'-O5'-PA-O2A
5	L	501	GTP	C5'-O5'-PA-O2A
4	I	501	GDP	C3'-C4'-C5'-O5'
4	E	501	GDP	O4'-C4'-C5'-O5'
4	I	501	GDP	PB-O3A-PA-O2A
5	F	501	GTP	C4'-C5'-O5'-PA
4	K	501	GDP	PA-O3A-PB-O1B
4	E	501	GDP	C3'-C4'-C5'-O5'
4	C	501	GDP	PA-O3A-PB-O1B
4	A	501	GDP	PA-O3A-PB-O3B
5	J	501	GTP	PB-O3B-PG-O3G
5	L	501	GTP	PB-O3B-PG-O2G
5	F	501	GTP	C5'-O5'-PA-O3A
4	I	501	GDP	PB-O3A-PA-O1A
5	L	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

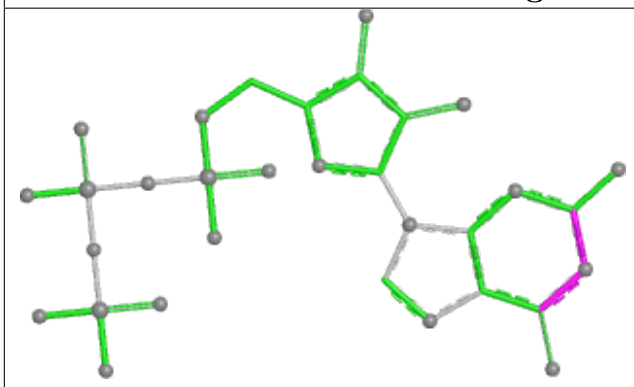
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	501	GTP	1	0

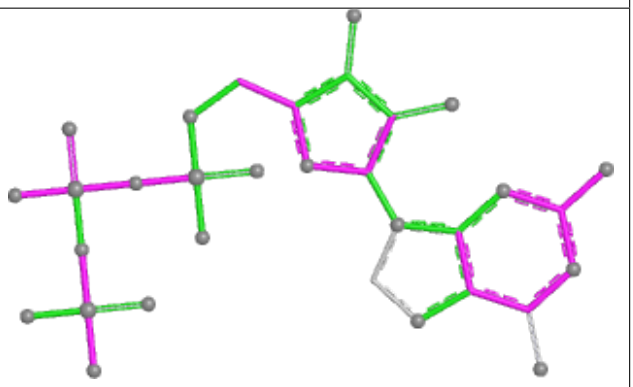
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

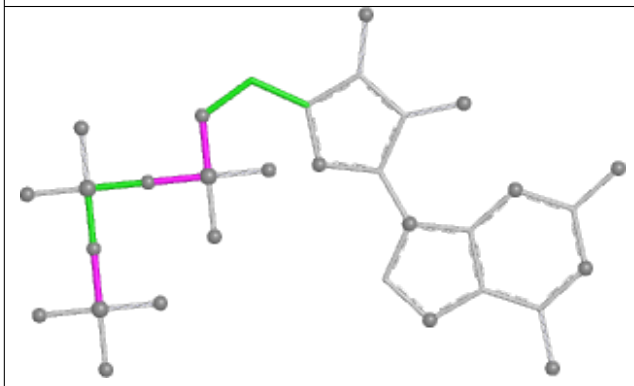
Ligand GTP L 501



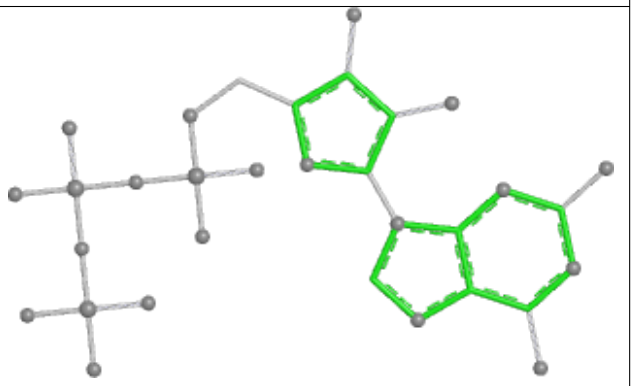
Bond lengths



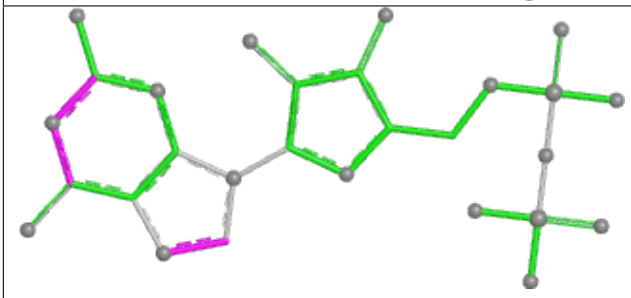
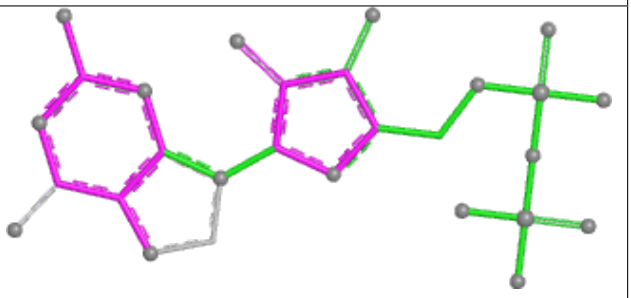
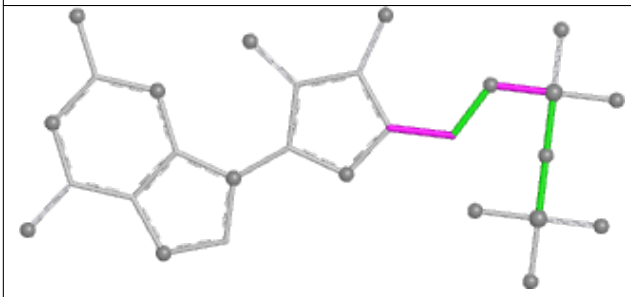
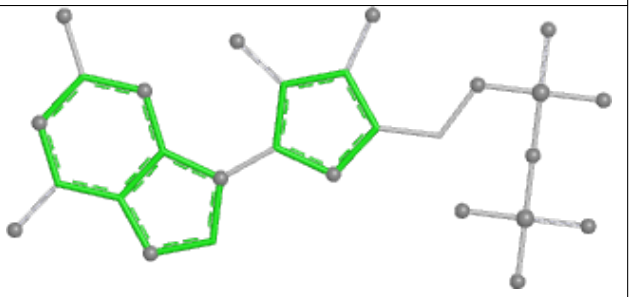
Bond angles

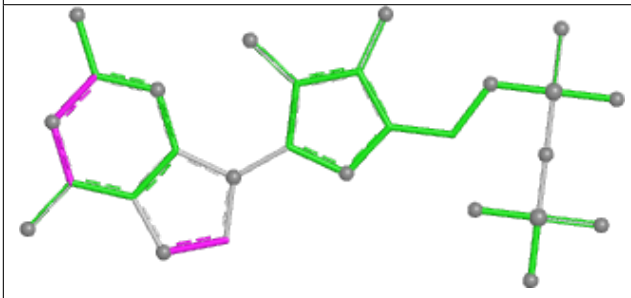
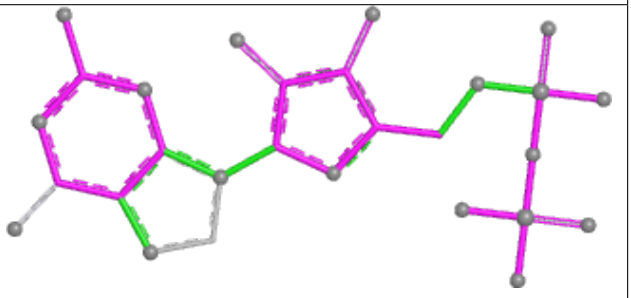
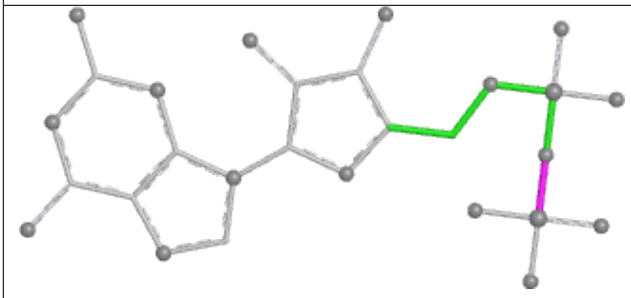
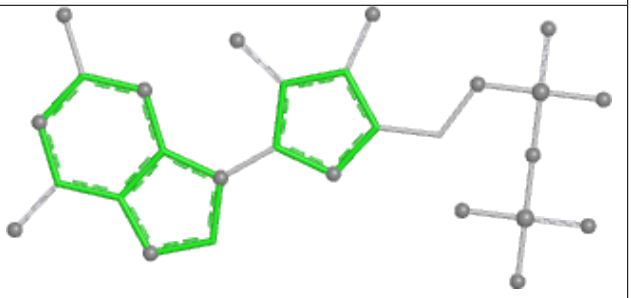


Torsions



Rings

Ligand GDP G 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand GDP C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

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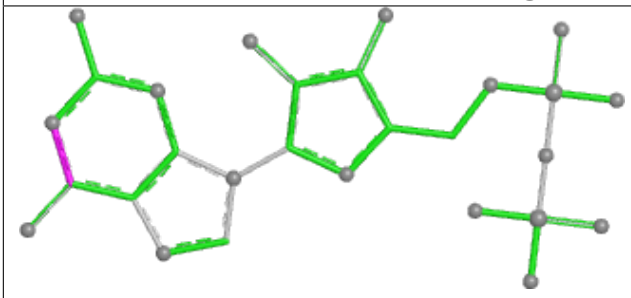
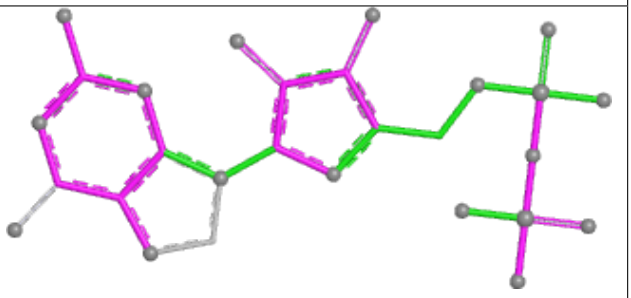
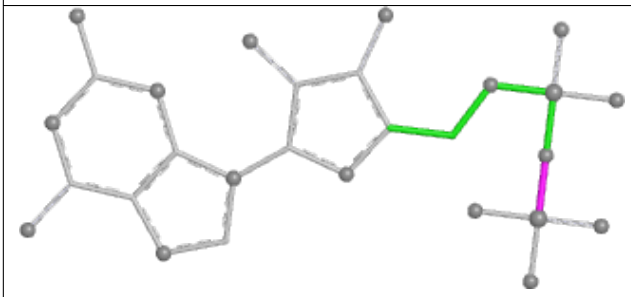
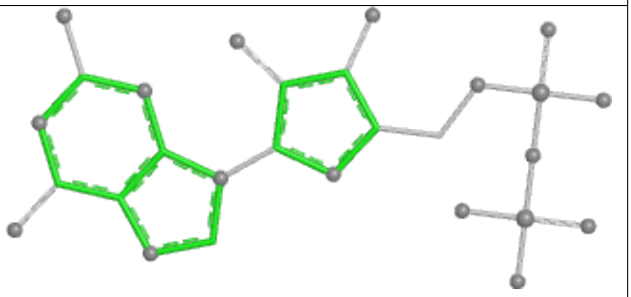
 Bond lengths	 Bond angles
 Torsions	 Rings

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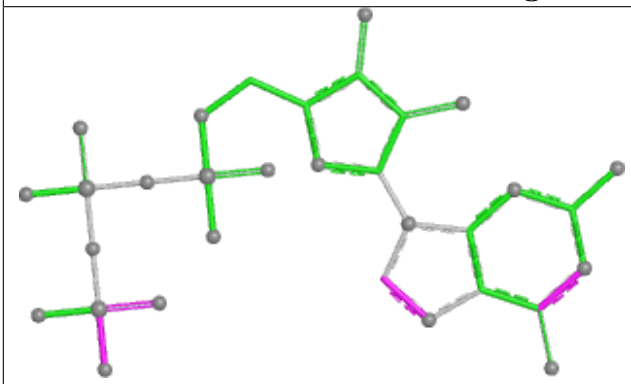
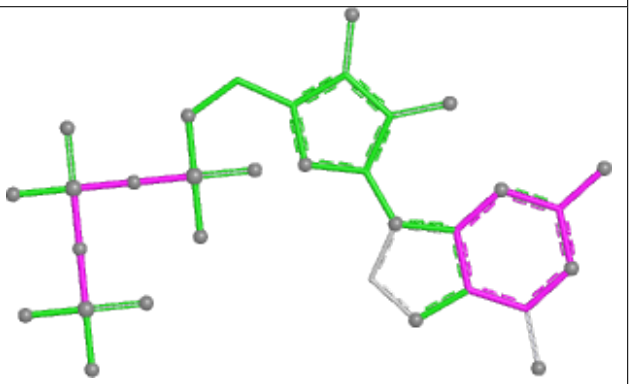
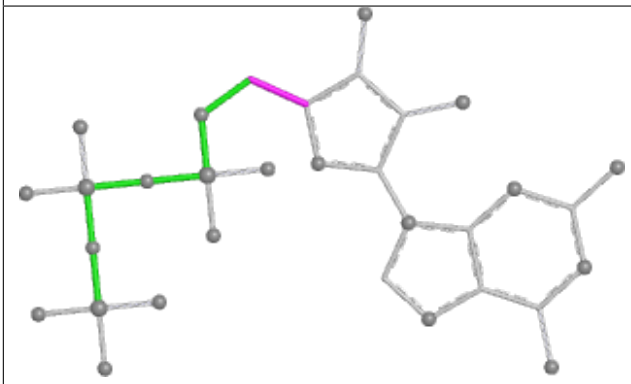
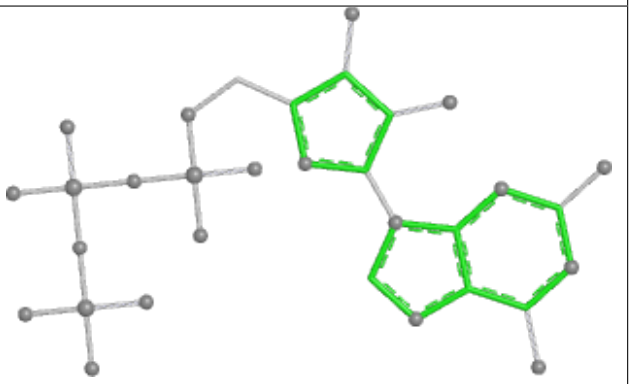
 Bond lengths	 Bond angles
 Torsions	 Rings

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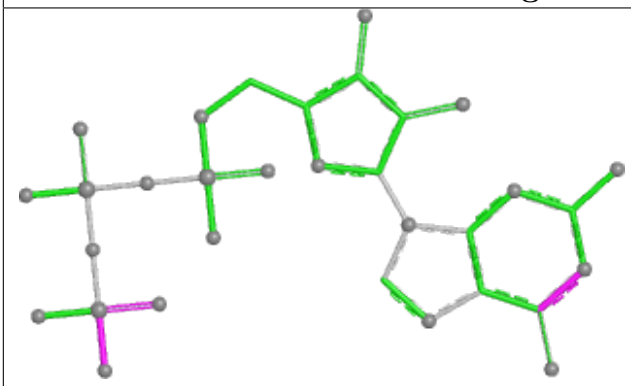
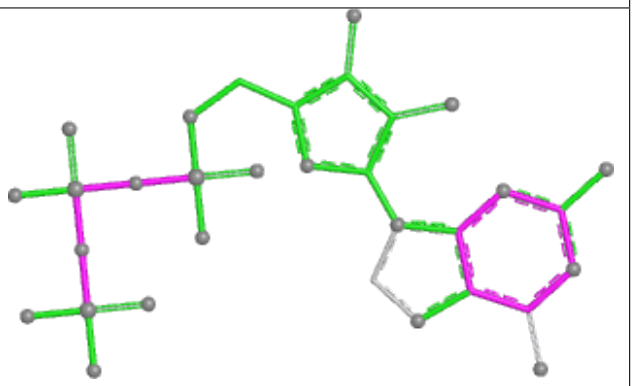
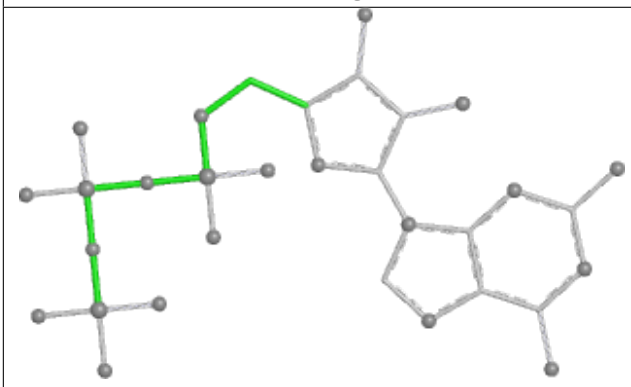
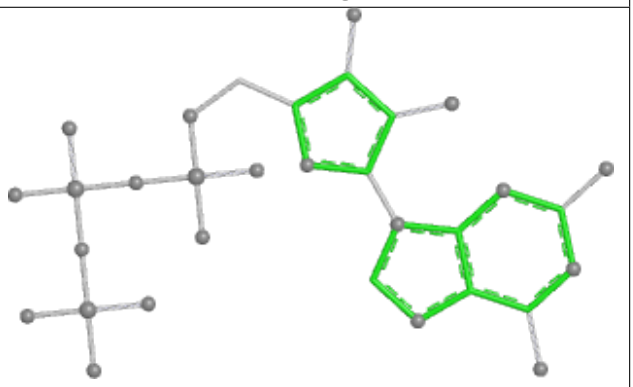
 Bond lengths	 Bond angles
 Torsions	 Rings

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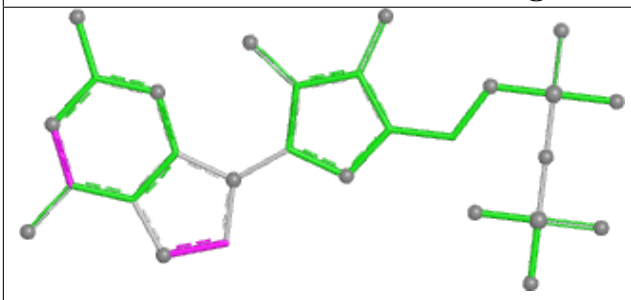
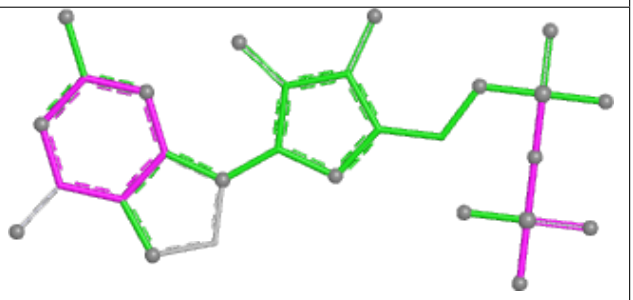
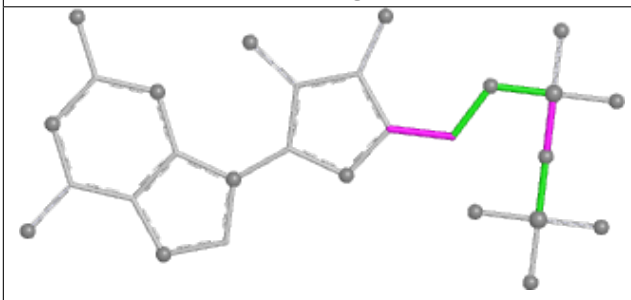
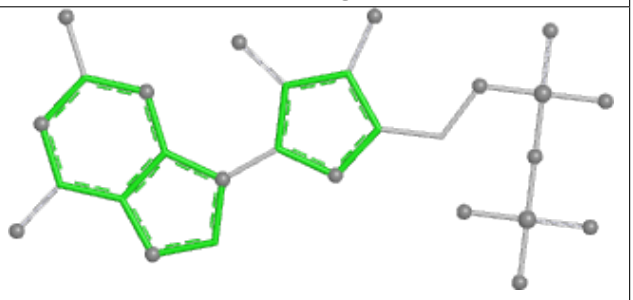
 Bond lengths	 Bond angles
 Torsions	 Rings

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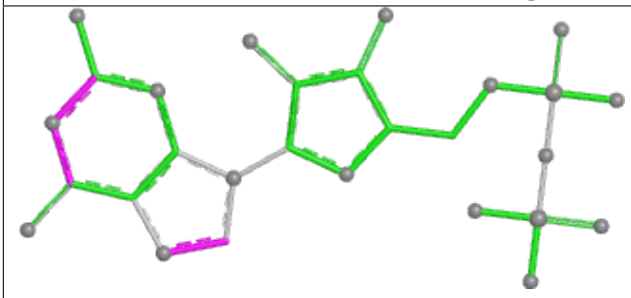
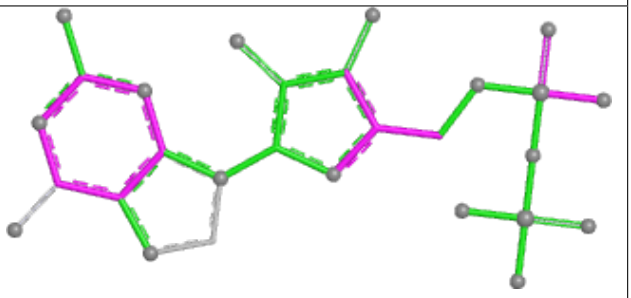
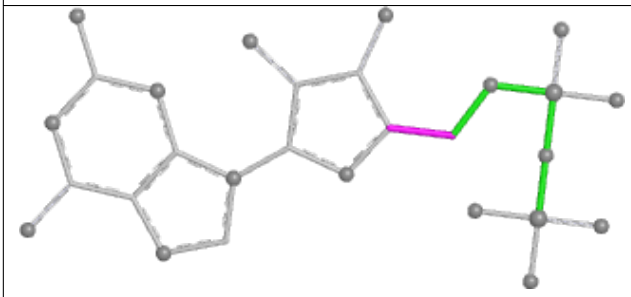
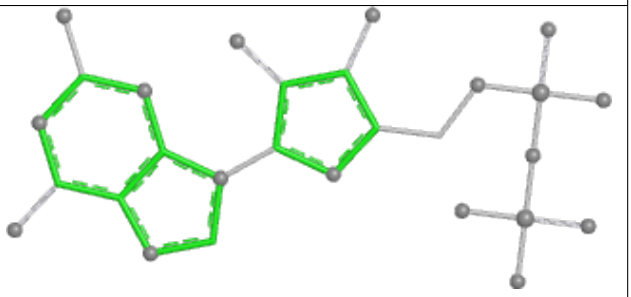
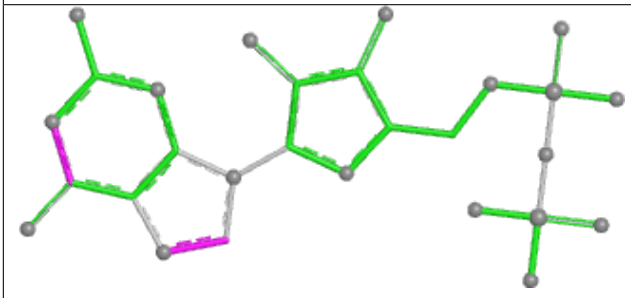
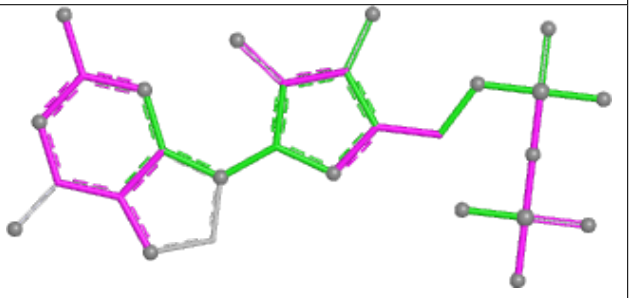
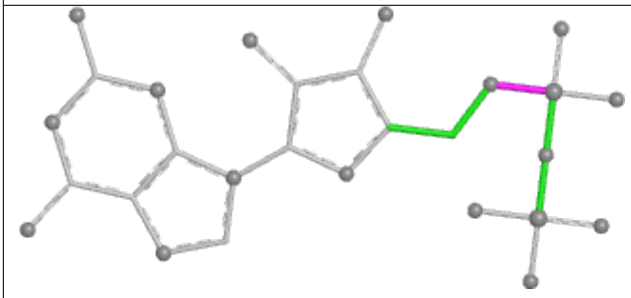
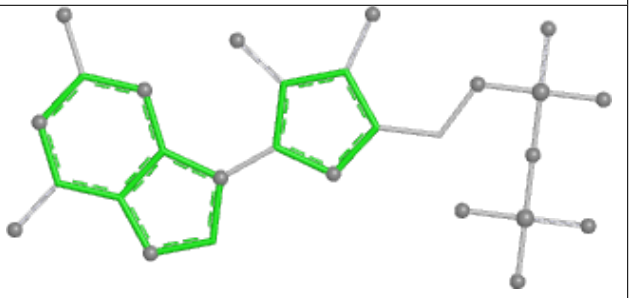
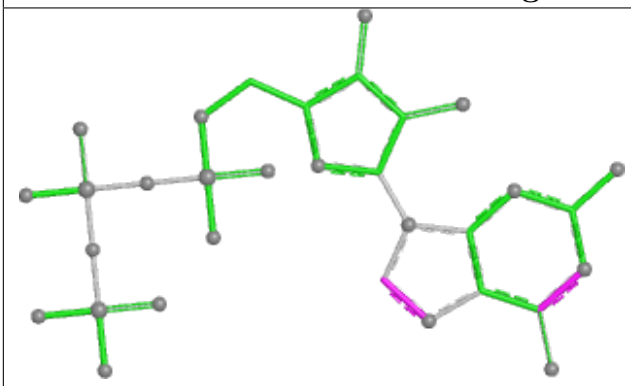
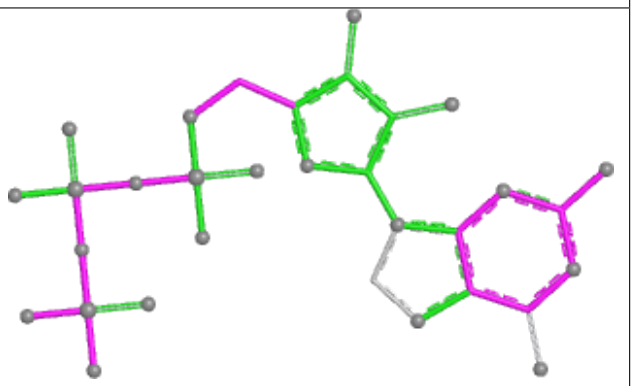
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP D 501



Bond lengths



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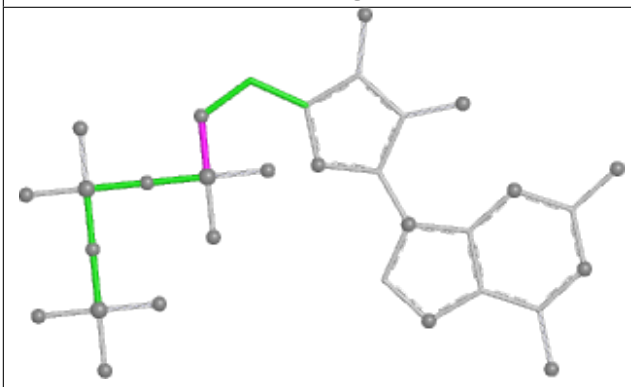

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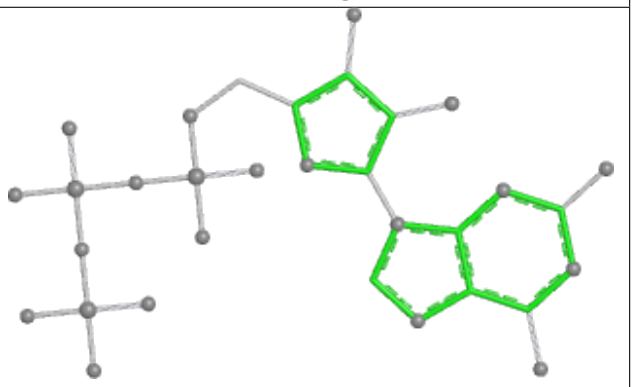
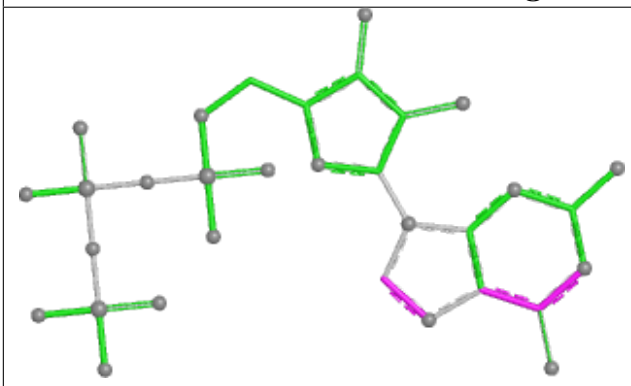


Rings

Ligand GTP F 501



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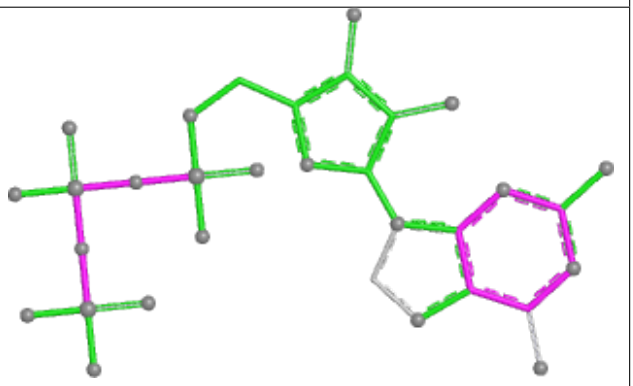

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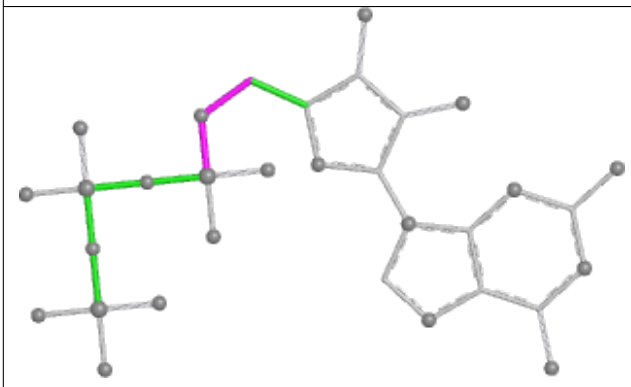
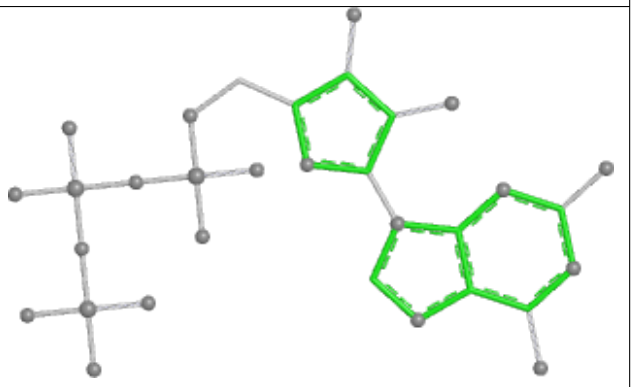
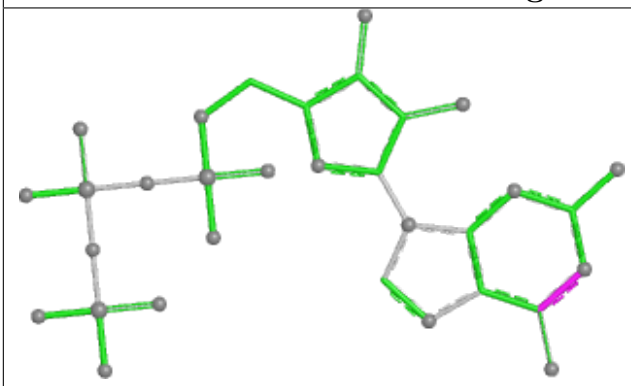
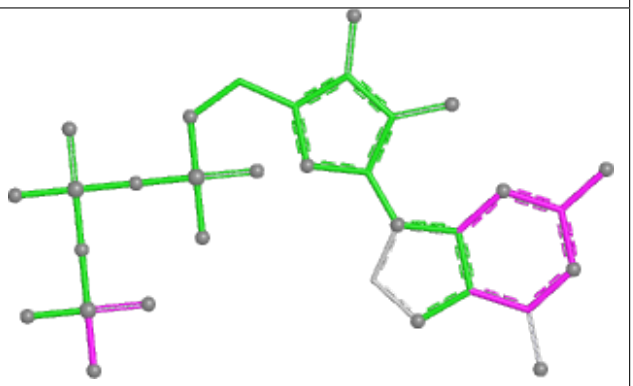
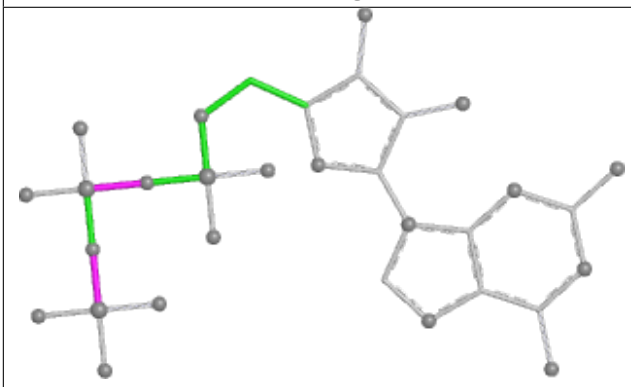
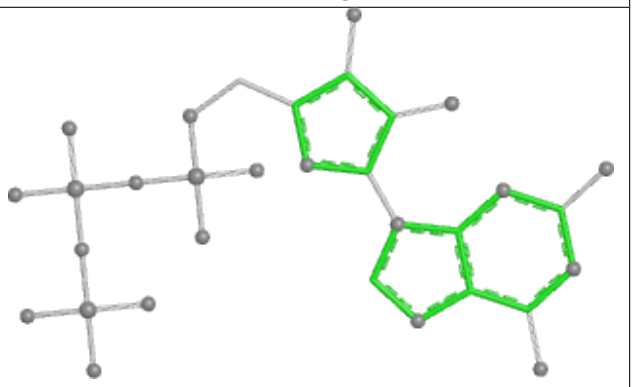
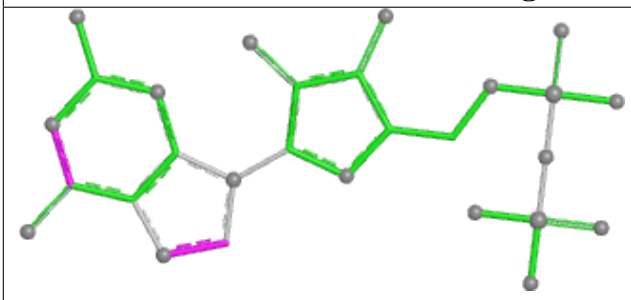
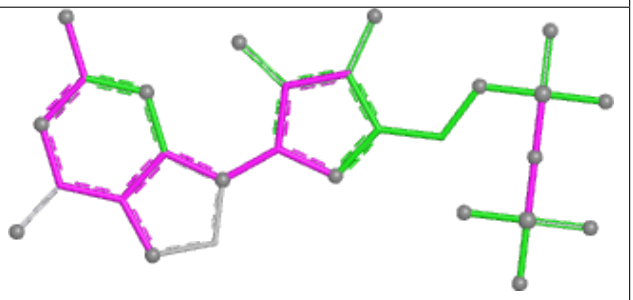
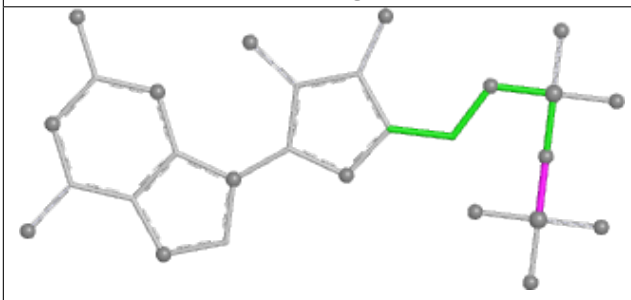
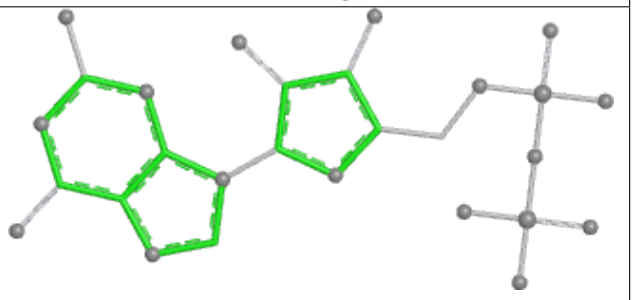


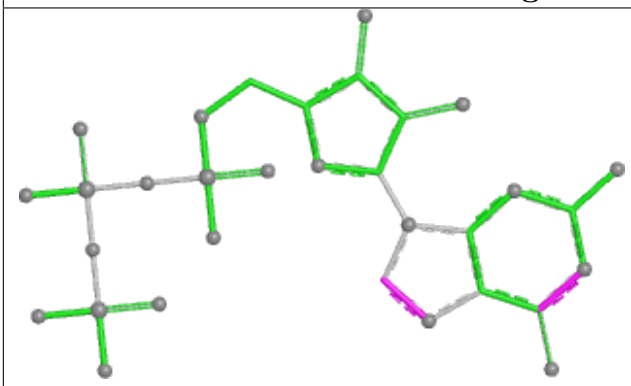
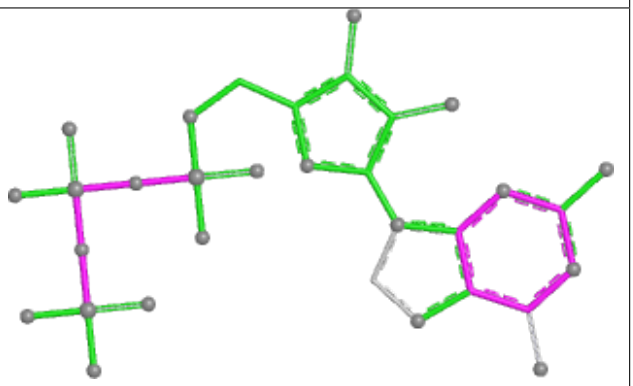
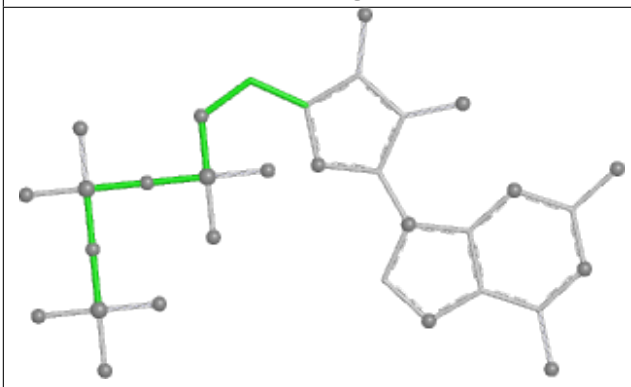
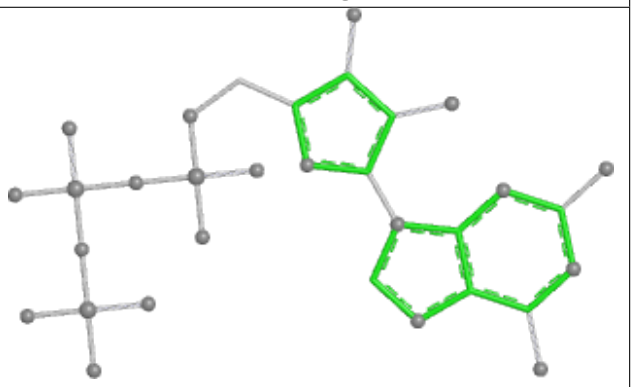
Torsions



Rings

Ligand GTP J 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP K 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP H 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

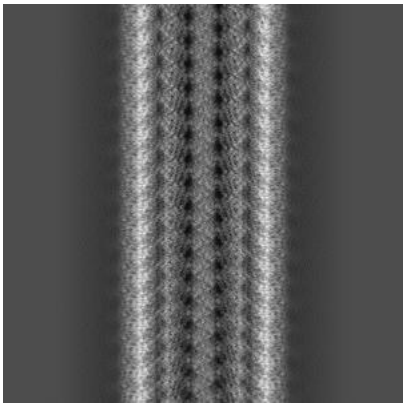
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7522. These allow visual inspection of the internal detail of the map and identification of artifacts.

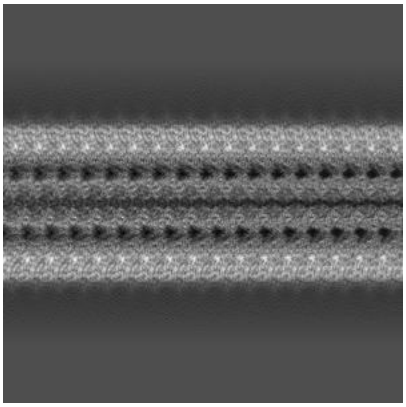
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

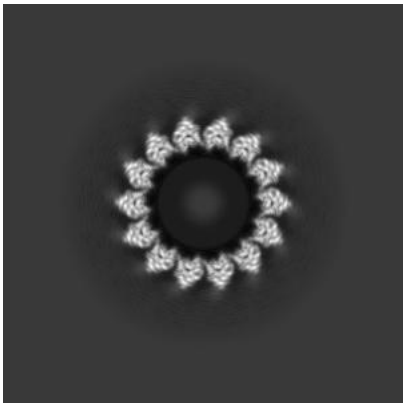
6.1.1 Primary map



X



Y

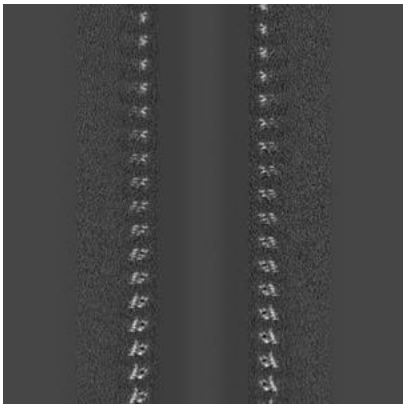


Z

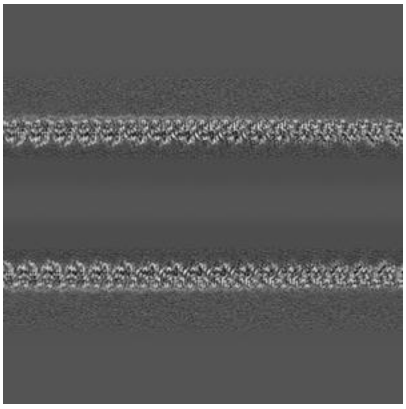
The images above show the map projected in three orthogonal directions.

6.2 Central slices

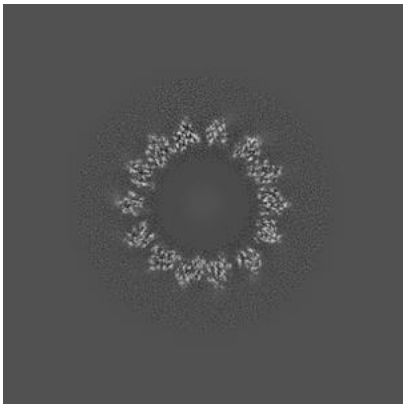
6.2.1 Primary map



X Index: 256



Y Index: 256

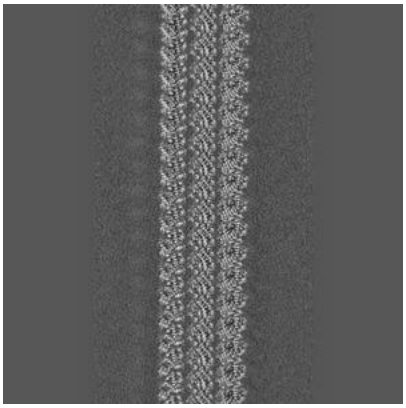


Z Index: 256

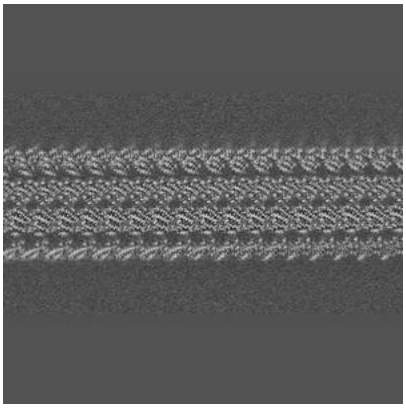
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

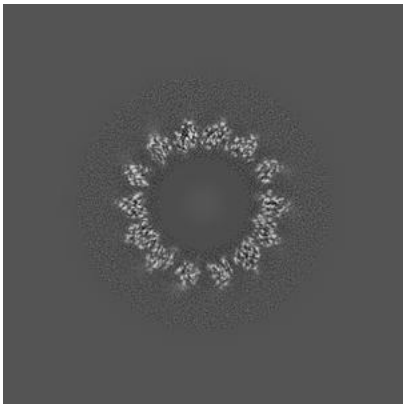
6.3.1 Primary map



X Index: 174



Y Index: 337

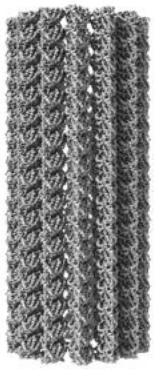


Z Index: 237

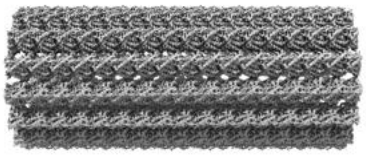
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

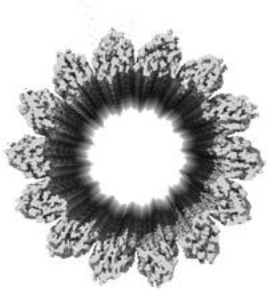
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

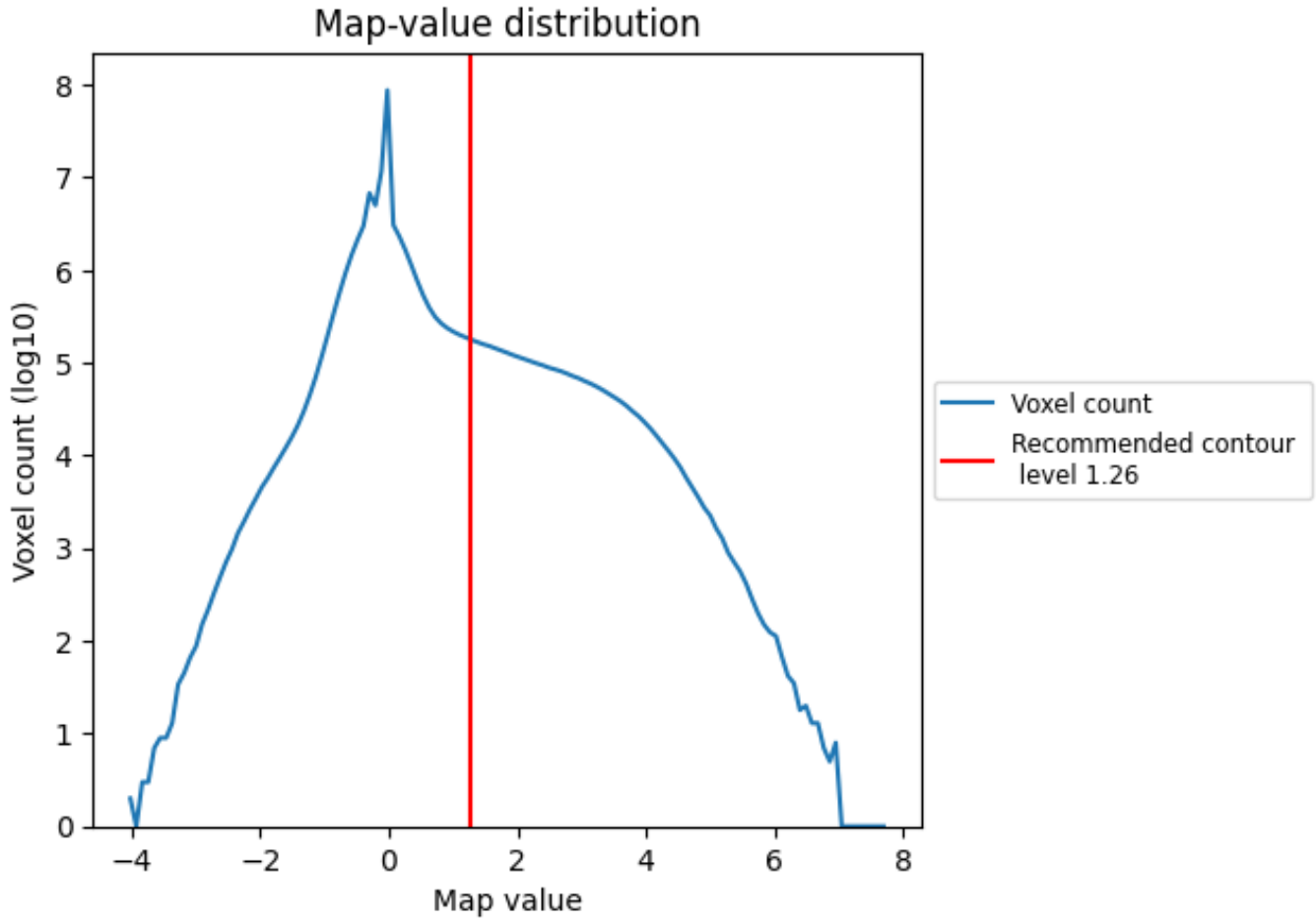
6.5 Mask visualisation (i)

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

7 Map analysis

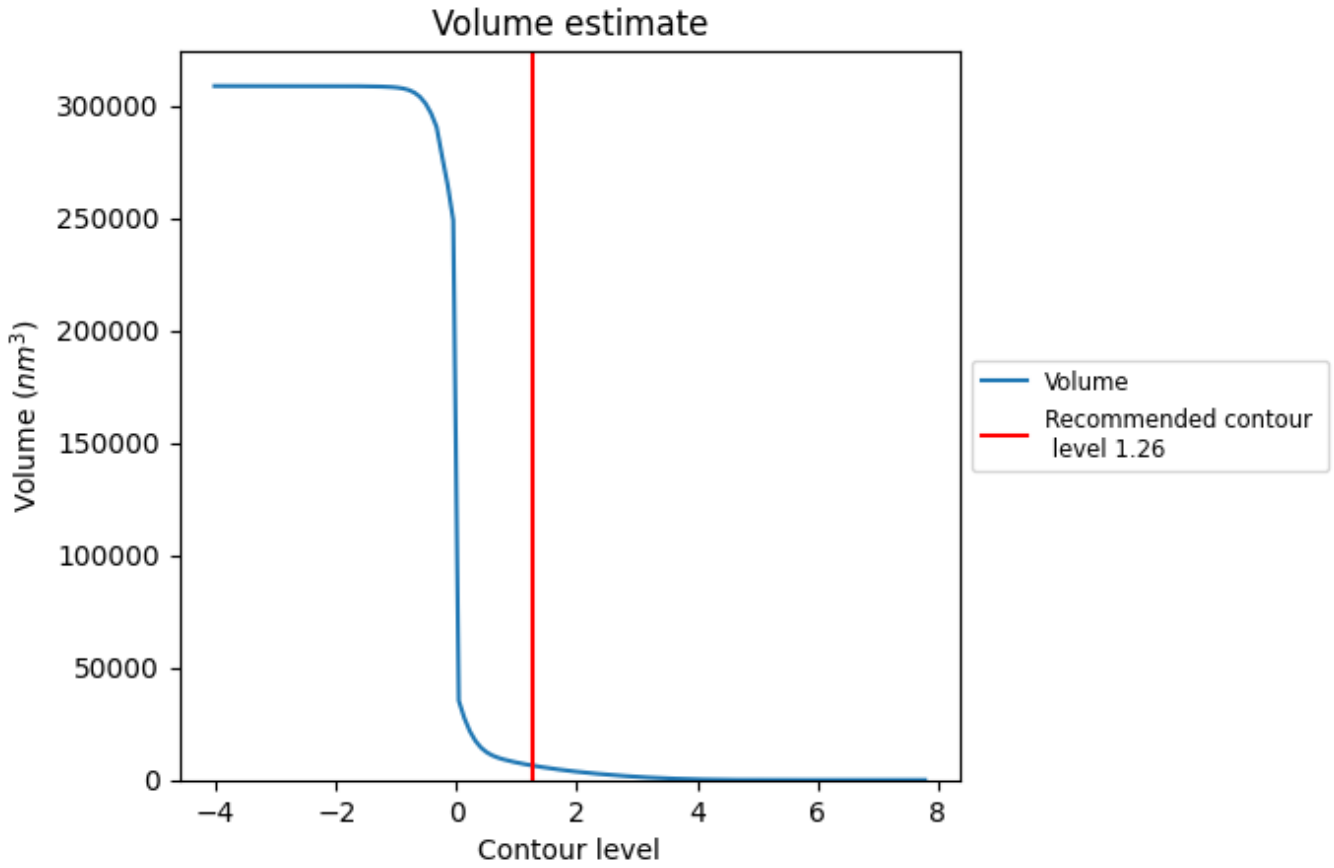
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

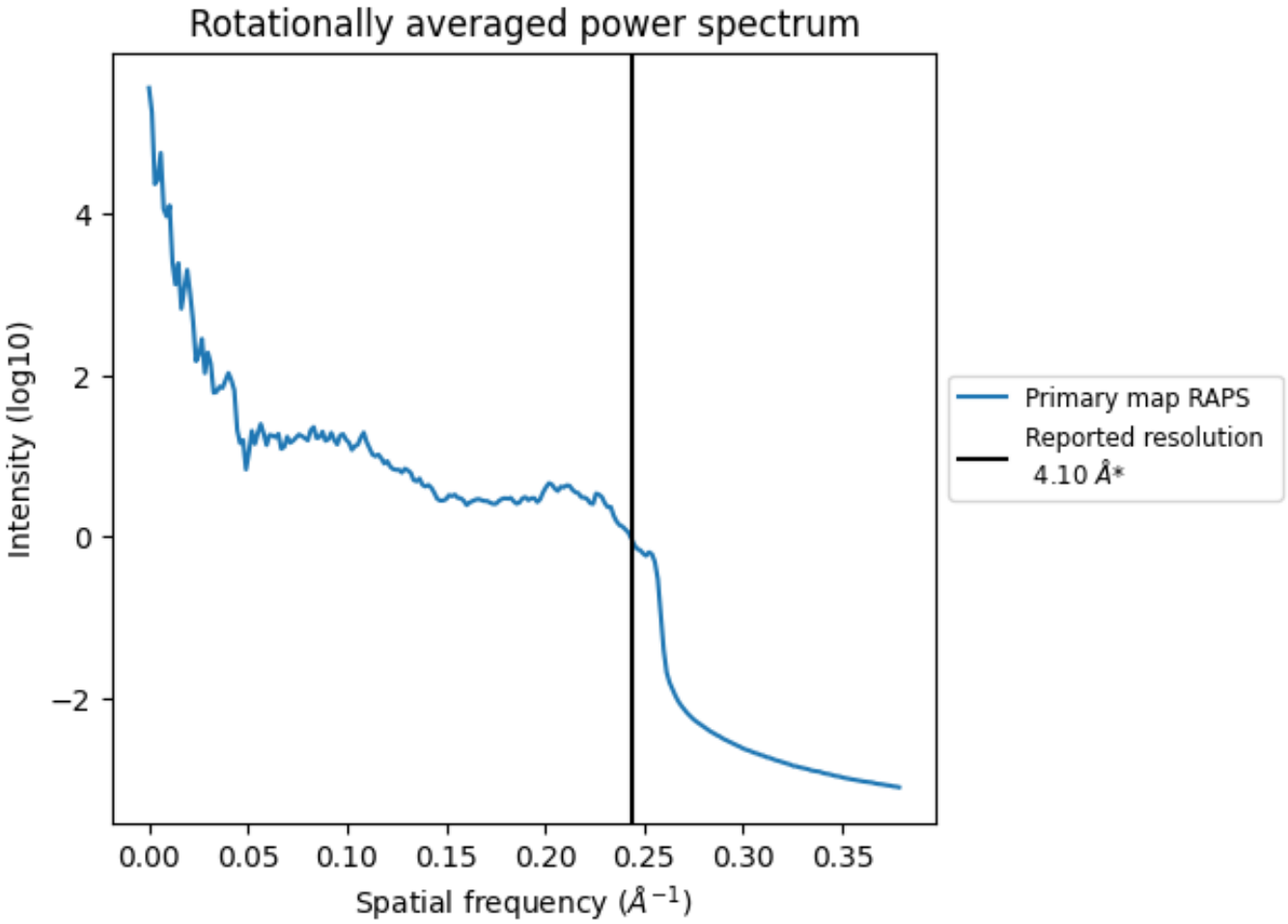
7.2 Volume estimate



The volume at the recommended contour level is 6436 nm^3; this corresponds to an approximate mass of 5814 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 (i)



*Reported resolution corresponds to spatial frequency of 0.244 Å^{-1}

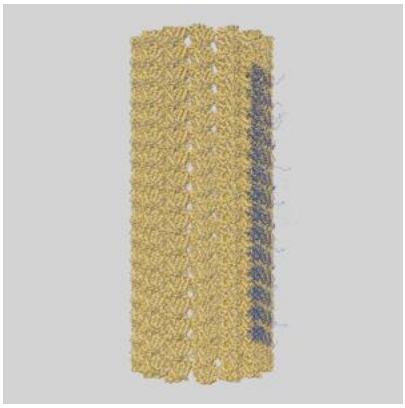
8 Fourier-Shell correlation (i)

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

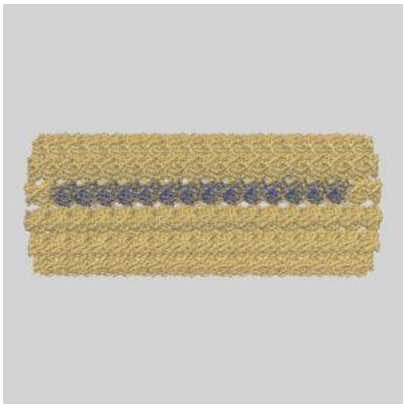
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7522 and PDB model 7PQP. Per-residue inclusion information can be found in section 3 on page 8.

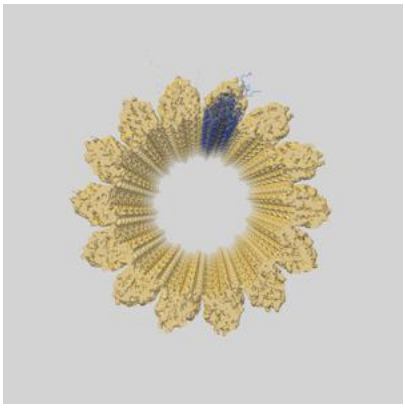
9.1 Map-model overlay



X



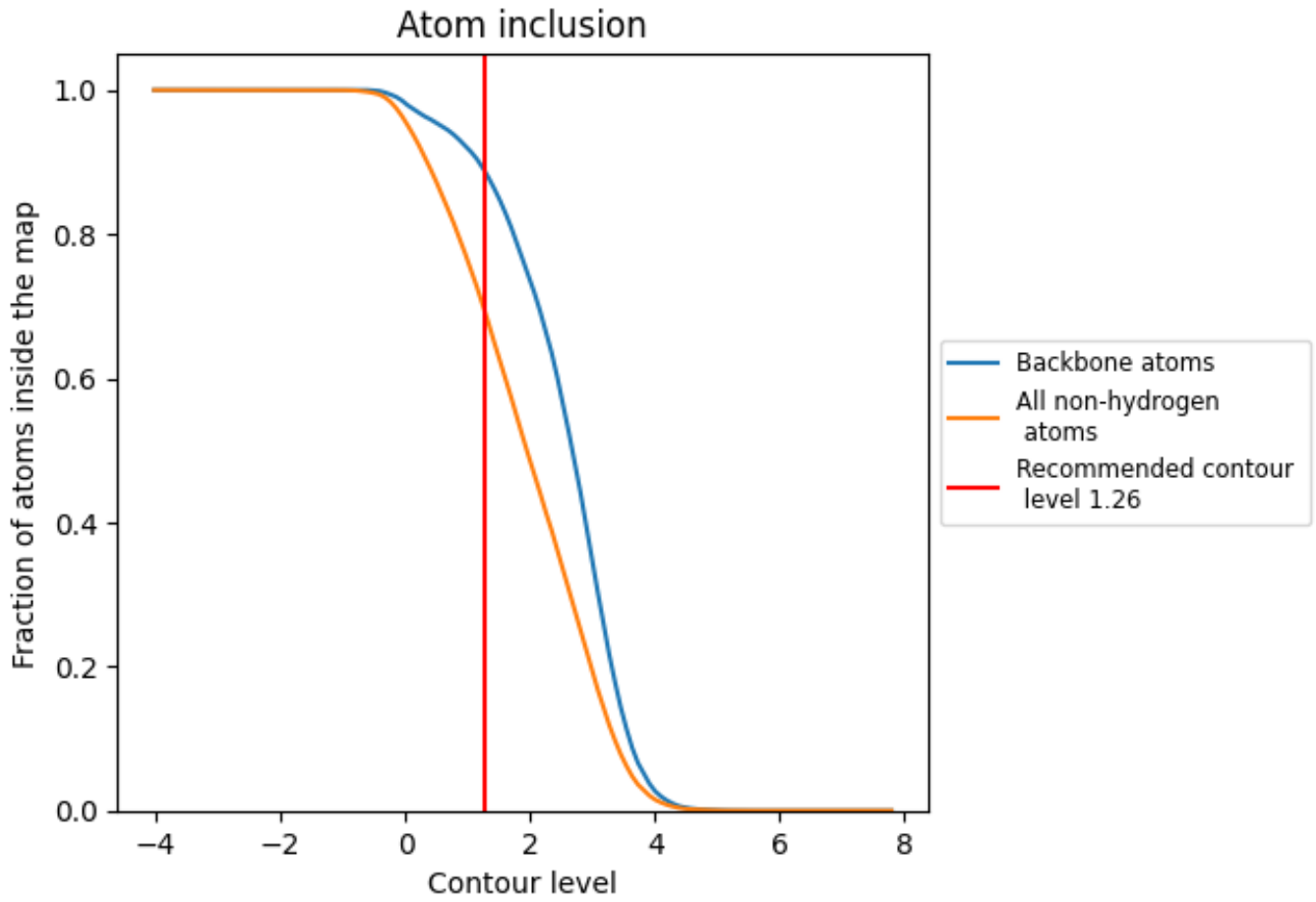
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.26 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 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.