



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:23 PM UTC

PDB ID : 3J6E / pdb_00003j6e
EMDB ID : EMD-5895
Title : Energy minimized average structure of Microtubules stabilized by GmpCp
Authors : Alushin, G.M.; Lander, G.C.; Kellogg, E.H.; Zhang, R.; Baker, D.; Nogales, E.
Deposited on : 2014-02-18
Resolution : 4.70 Å(reported)
Based on initial model : 1JFF

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

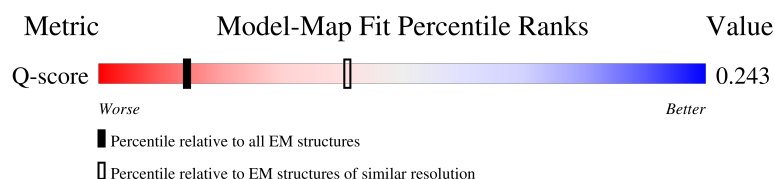
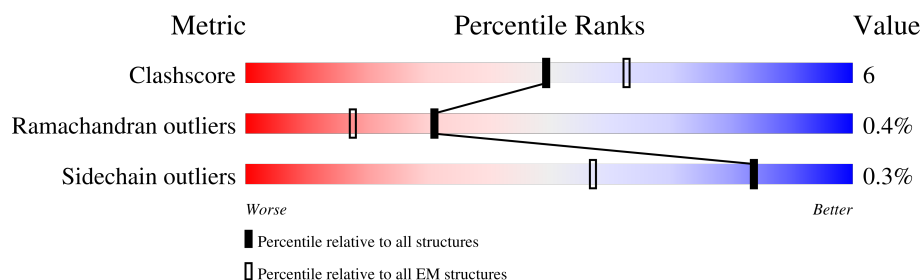
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

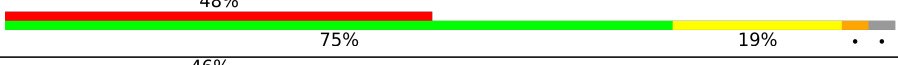
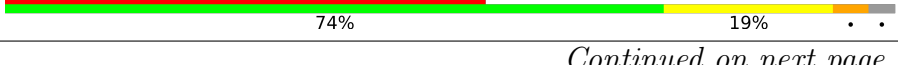
The reported resolution of this entry is 4.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1989 (4.20 - 5.20)

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

Mol	Chain	Length	Quality of chain
1	A	439	
1	C	439	
1	E	439	
1	G	439	

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Mol	Chain	Length	Quality of chain
1	I	439	48% 74%19% . .
1	K	439	55% 74%19% . .
1	M	439	68% 74%20% . .
1	O	439	57% 75%18% . .
1	Q	439	70% 74%20% . .
2	B	427	37% 78%19% .
2	D	427	49% 77%19% .
2	F	427	49% 77%19% .
2	H	427	67% 78%19% .
2	J	427	59% 78%19% .
2	L	427	69% 77%20% .
2	N	427	55% 77%19% .
2	P	427	46% 77%19% .
2	R	427	59% 77%19% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 60984 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 alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	C	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	E	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	G	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	I	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	K	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	M	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	O	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		
1	Q	428	Total	C	N	O	S	0	0
			3350	2121	570	638	21		

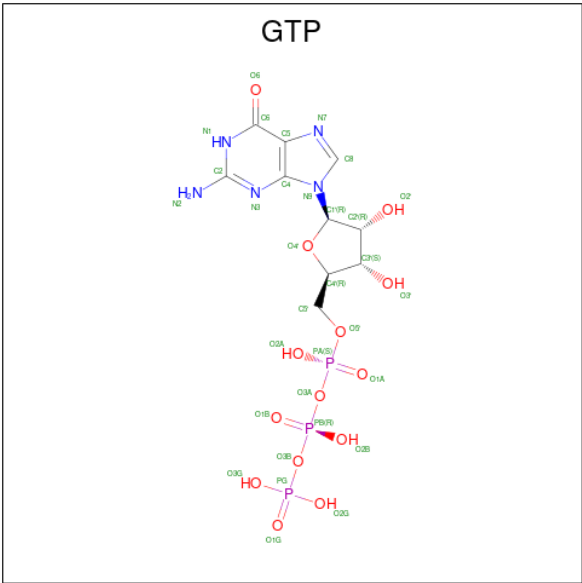
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	conflict	UNP P02550
C	265	GLY	ALA	conflict	UNP P02550
E	265	GLY	ALA	conflict	UNP P02550
G	265	GLY	ALA	conflict	UNP P02550
I	265	GLY	ALA	conflict	UNP P02550
K	265	GLY	ALA	conflict	UNP P02550
M	265	GLY	ALA	conflict	UNP P02550
O	265	GLY	ALA	conflict	UNP P02550
Q	265	GLY	ALA	conflict	UNP P02550

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	D	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	F	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	H	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	J	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	L	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	N	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	P	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		
2	R	426	Total	C	N	O	S	0	0
			3352	2105	575	647	25		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	I	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	M	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	O	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	Q	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

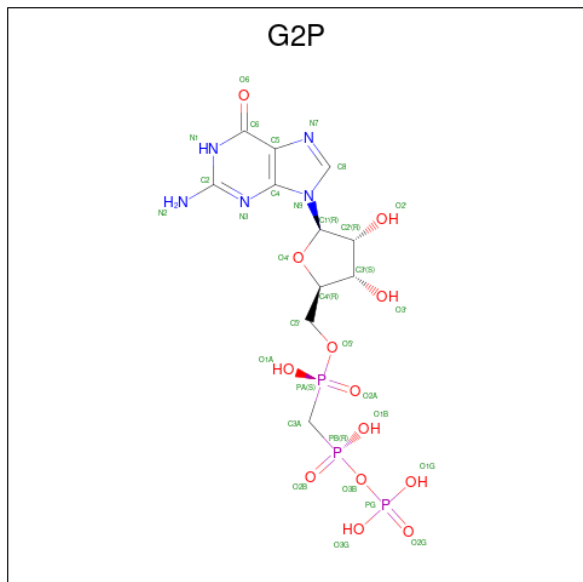
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	F	1	Total	Mg	0
			1	1	
4	G	1	Total	Mg	0
			1	1	
4	H	1	Total	Mg	0
			1	1	
4	I	1	Total	Mg	0
			1	1	
4	J	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	L	1	Total	Mg	0
			1	1	
4	M	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	N	1	Total	Mg	0
			1	1	
4	O	1	Total	Mg	0
			1	1	
4	P	1	Total	Mg	0
			1	1	
4	Q	1	Total	Mg	0
			1	1	
4	R	1	Total	Mg	0
			1	1	

- Molecule 5 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



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Mol	Chain	Residues	Atoms					AltConf
5	N	1	Total	C	N	O	P	0
			32	11	5	13	3	
5	P	1	Total	C	N	O	P	0
			32	11	5	13	3	
5	R	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	4	Total	O	0
			4	4	
6	B	4	Total	O	0
			4	4	
6	C	4	Total	O	0
			4	4	
6	D	4	Total	O	0
			4	4	
6	E	4	Total	O	0
			4	4	
6	F	4	Total	O	0
			4	4	
6	G	4	Total	O	0
			4	4	
6	H	4	Total	O	0
			4	4	
6	I	4	Total	O	0
			4	4	
6	J	4	Total	O	0
			4	4	
6	K	4	Total	O	0
			4	4	
6	L	4	Total	O	0
			4	4	
6	M	4	Total	O	0
			4	4	
6	N	4	Total	O	0
			4	4	
6	O	4	Total	O	0
			4	4	
6	P	4	Total	O	0
			4	4	

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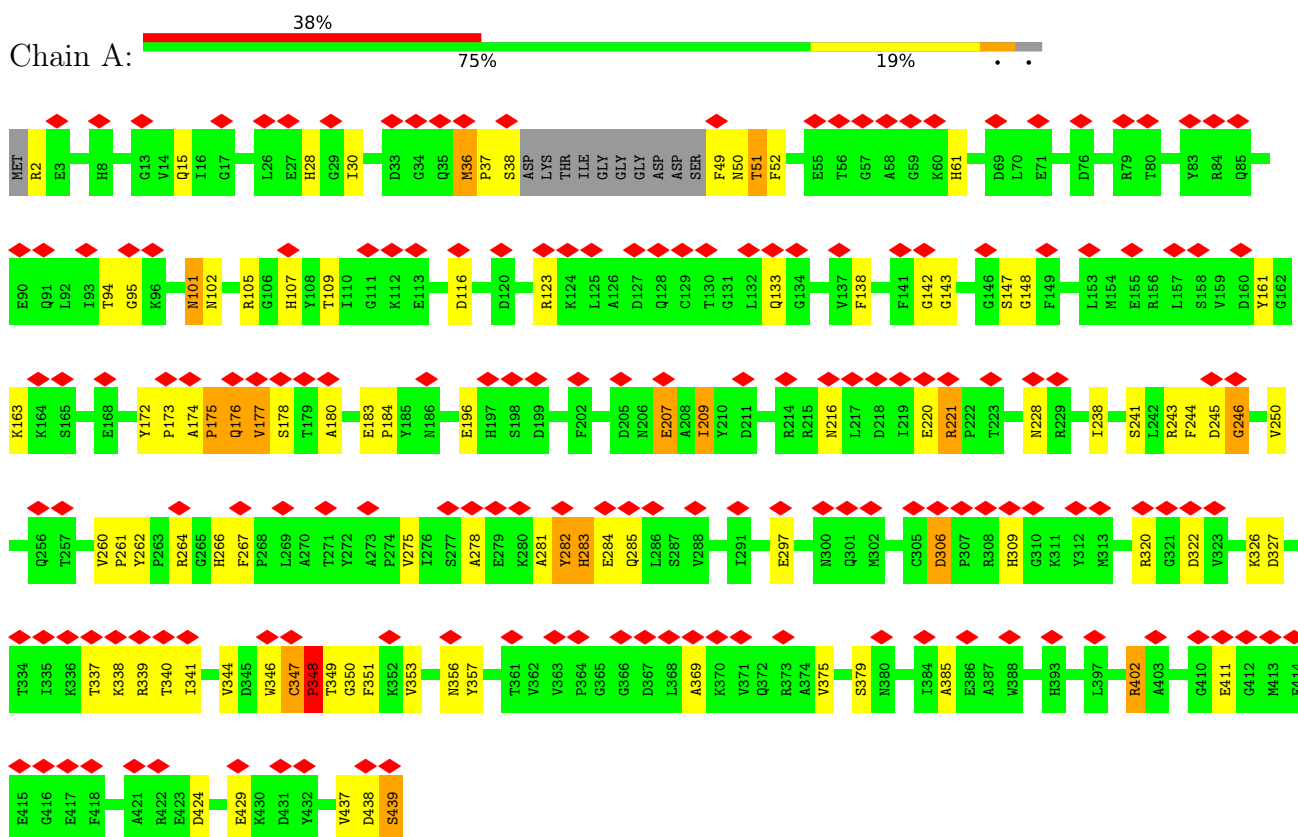
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Mol	Chain	Residues	Atoms		AltConf
6	Q	4	Total	O	0
			4	4	
6	R	4	Total	O	0
			4	4	

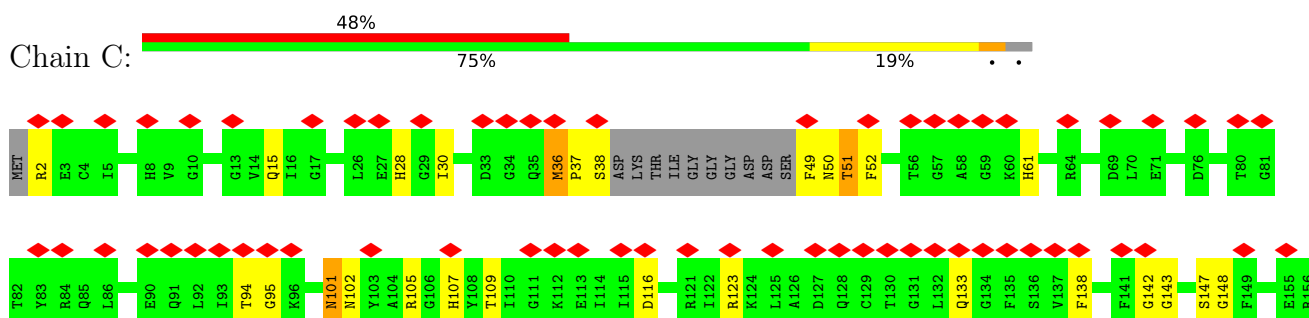
3 Residue-property plots

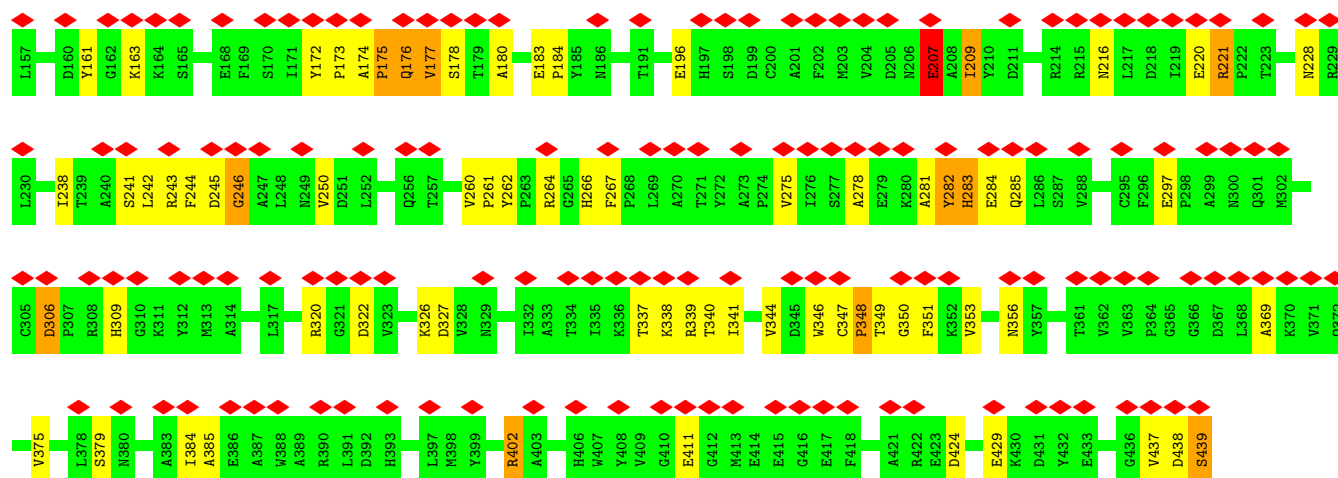
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 alpha-1A chain

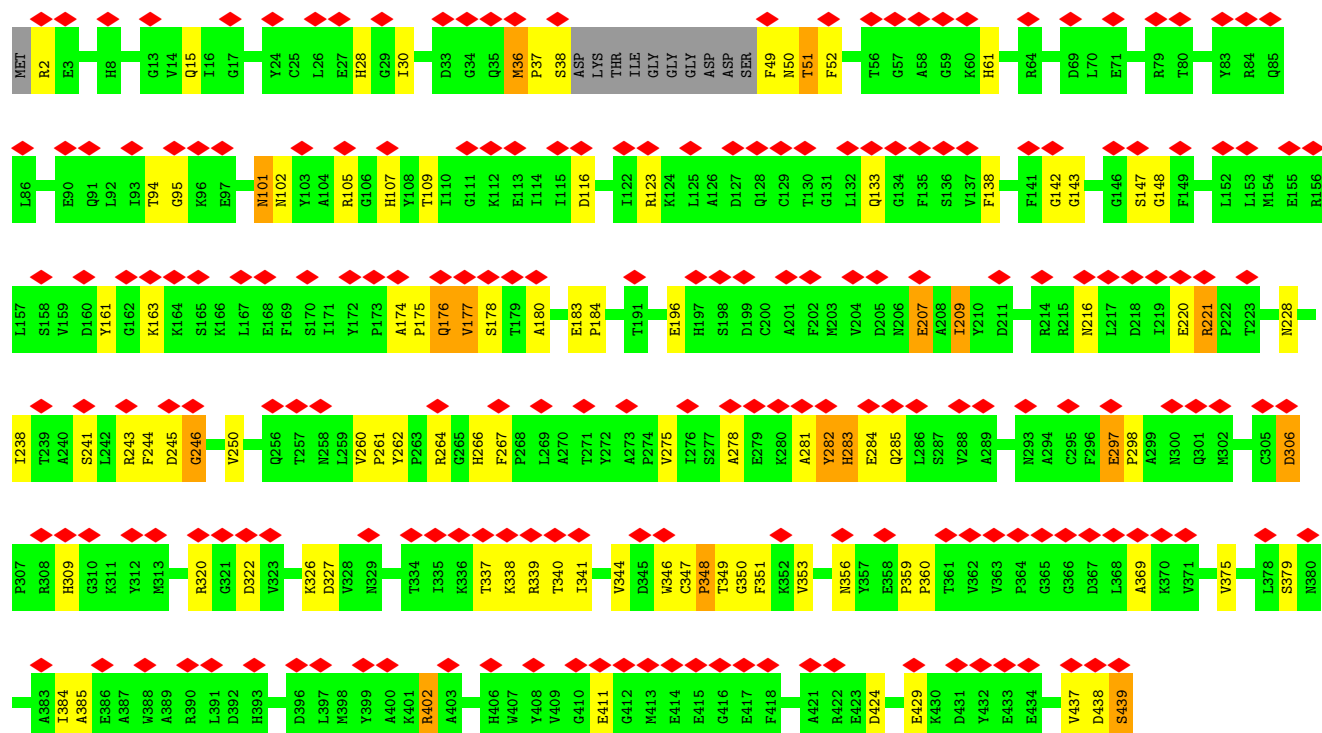
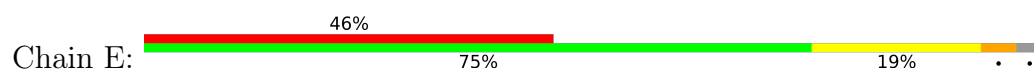


- Molecule 1: Tubulin alpha-1A chain

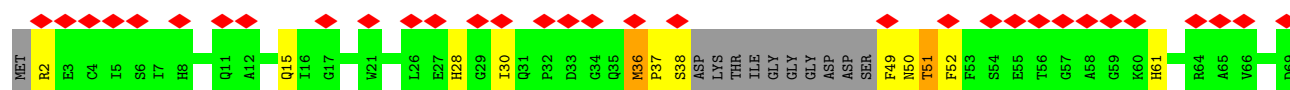
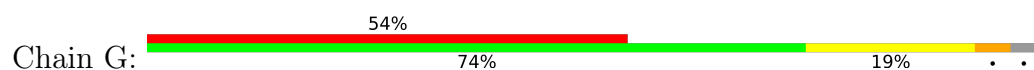


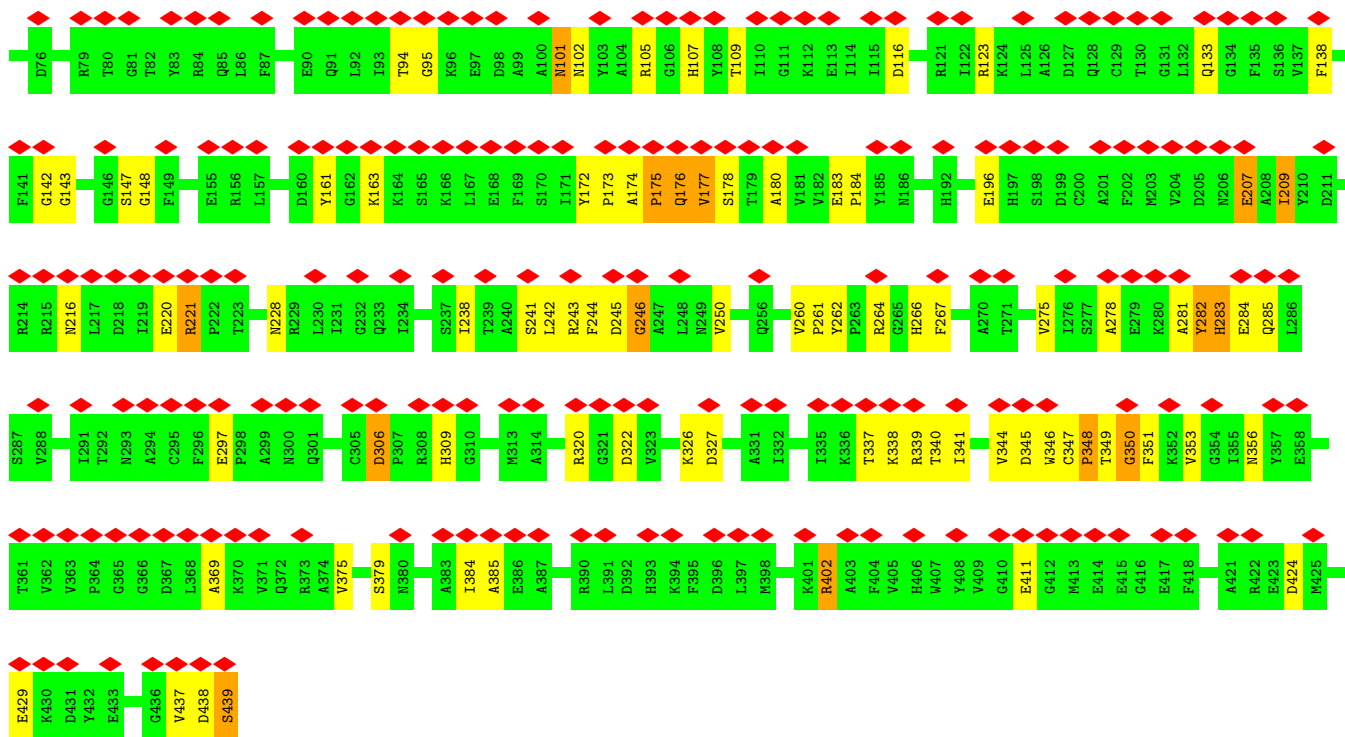


• Molecule 1: Tubulin alpha-1A chain

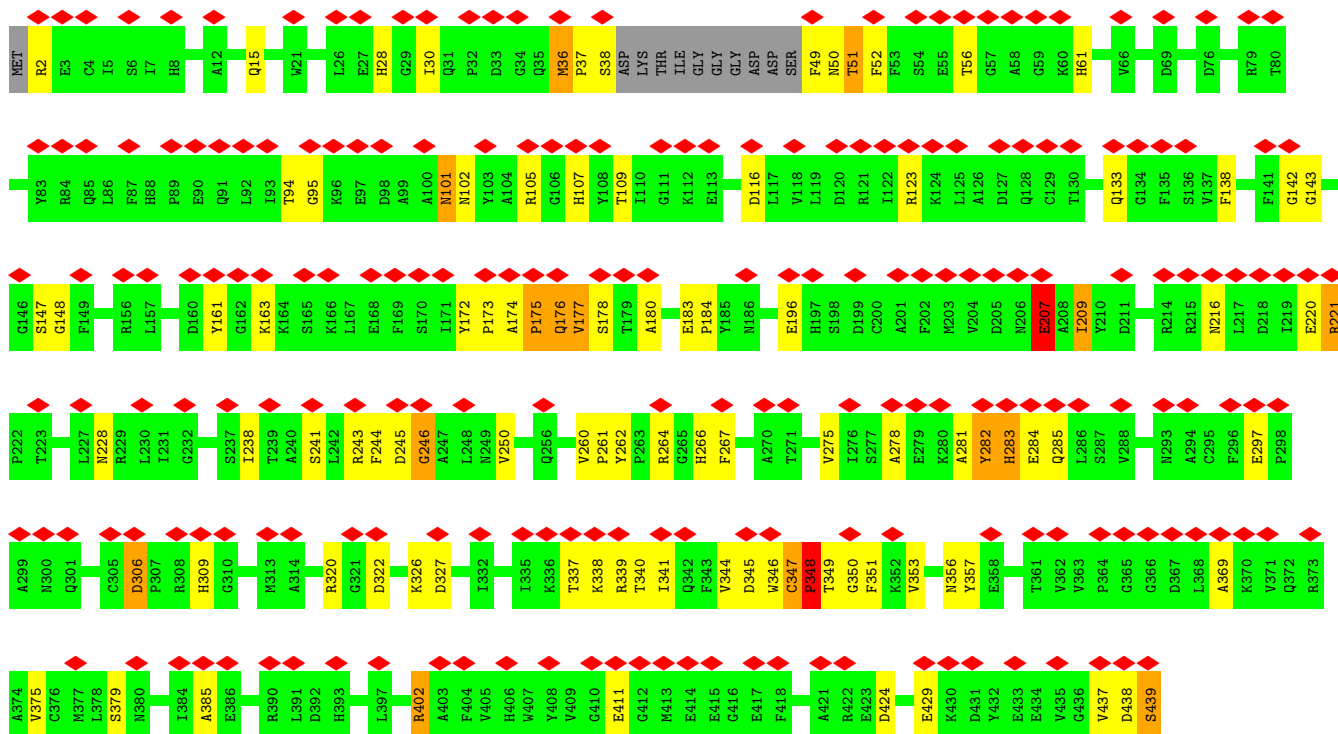
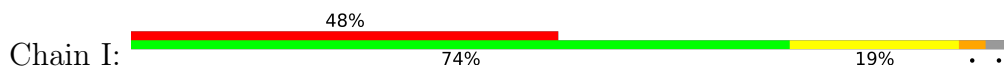


• Molecule 1: Tubulin alpha-1A chain

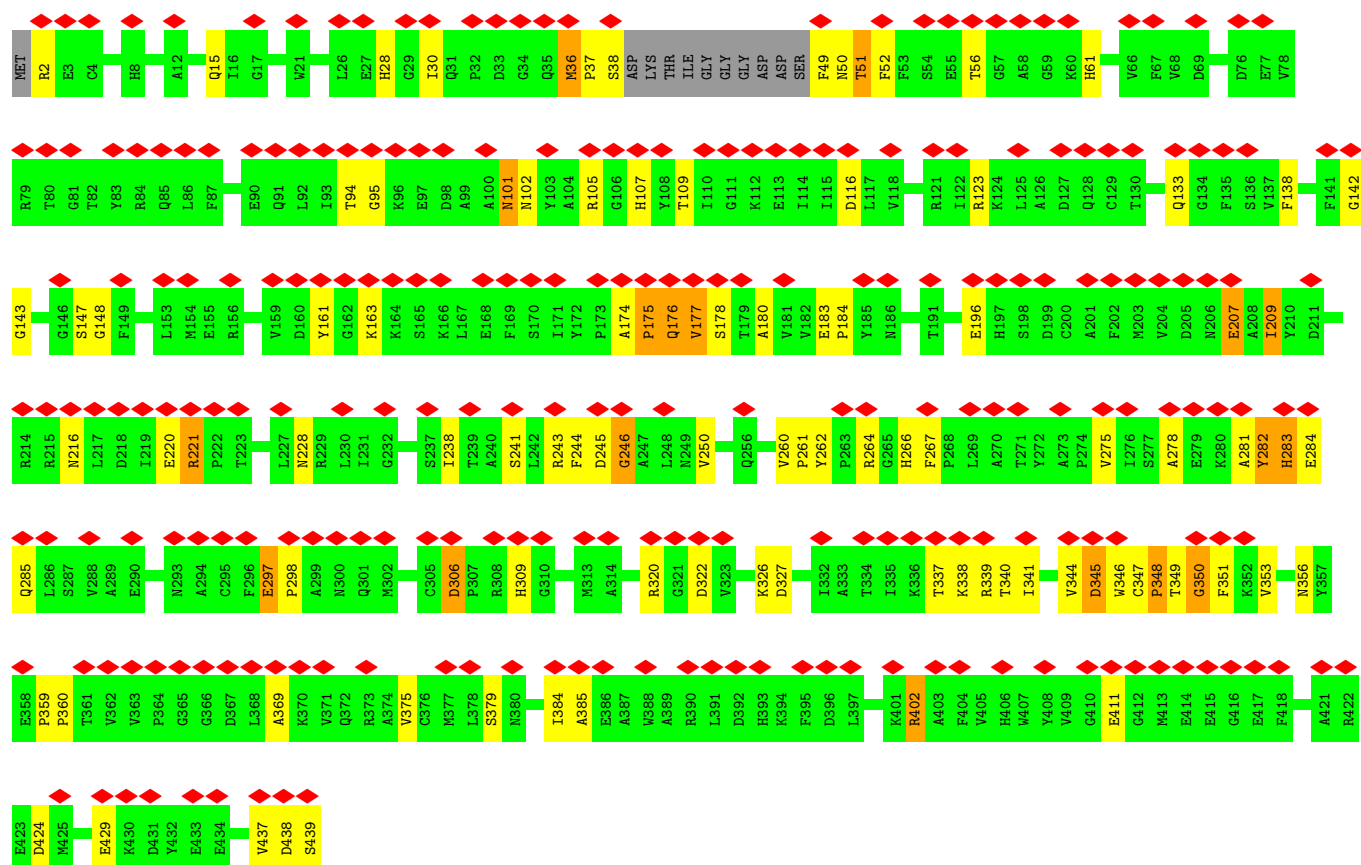
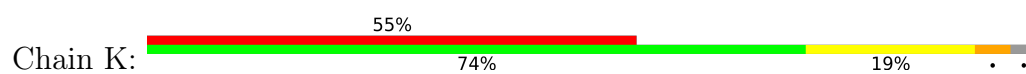




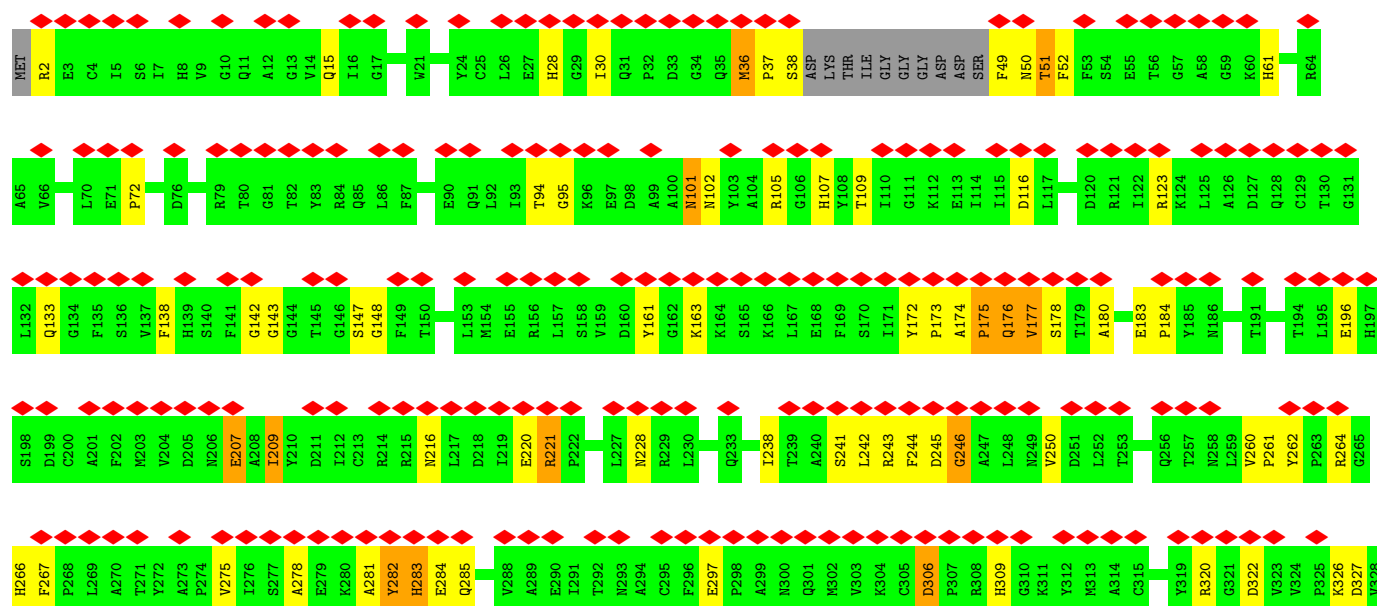
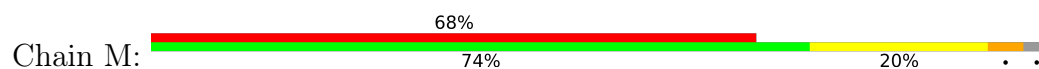
• Molecule 1: Tubulin alpha-1A chain

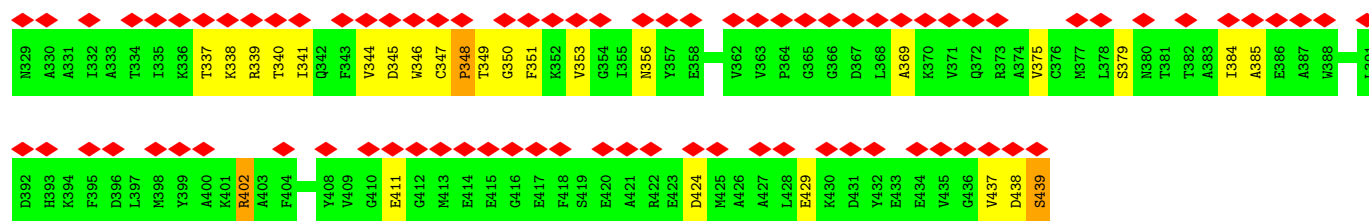


• Molecule 1: Tubulin alpha-1A chain

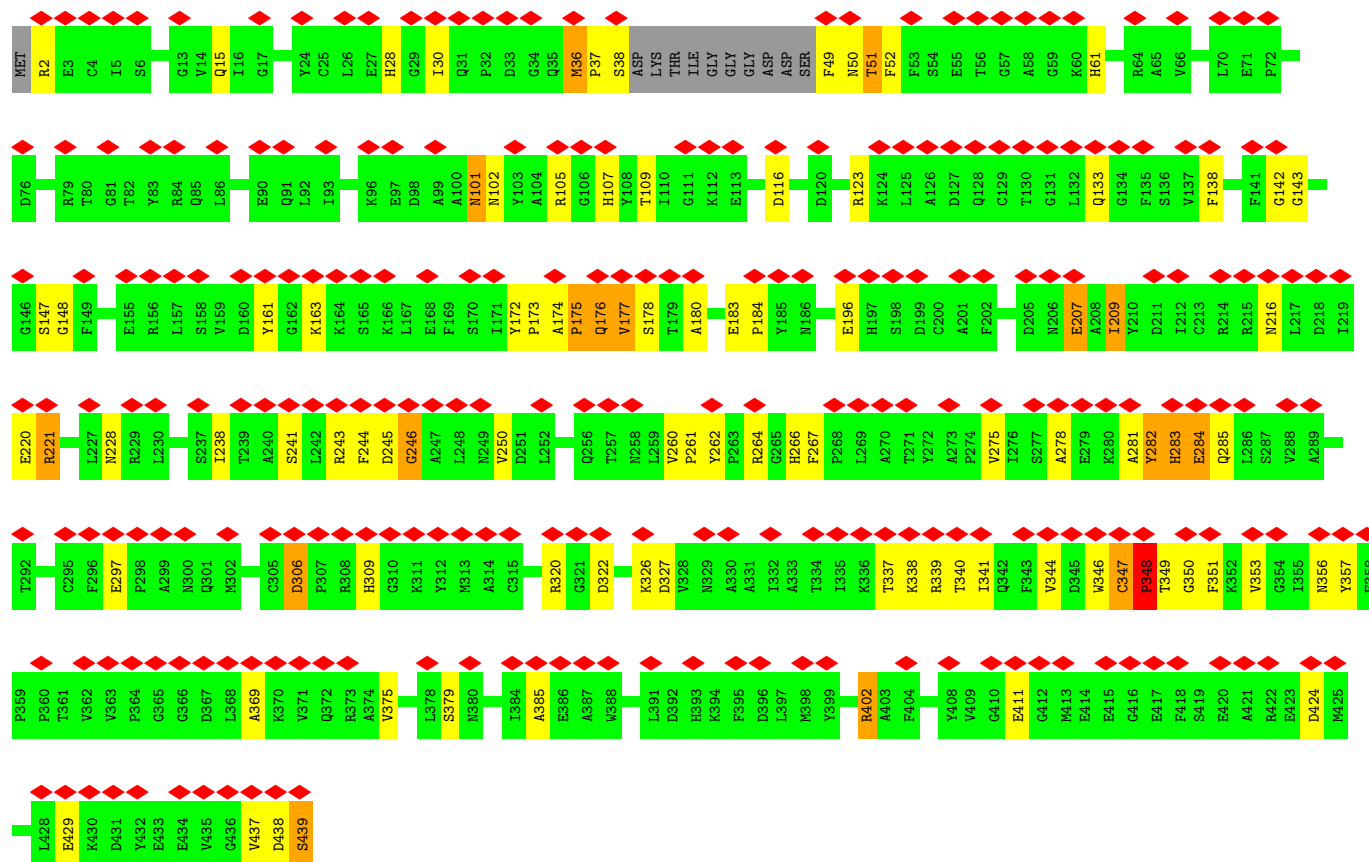
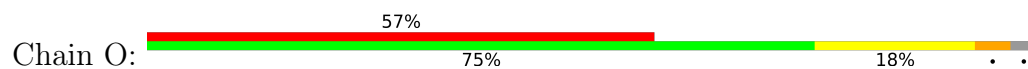


• Molecule 1: Tubulin alpha-1A chain

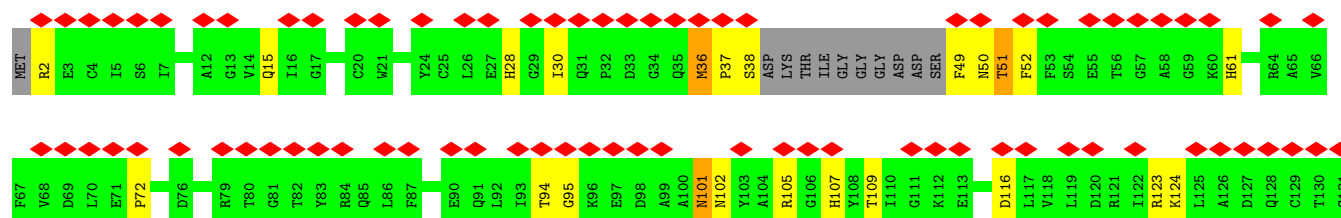
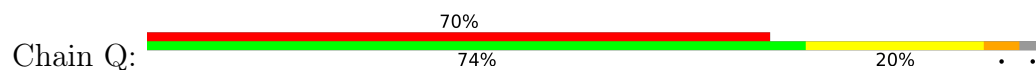


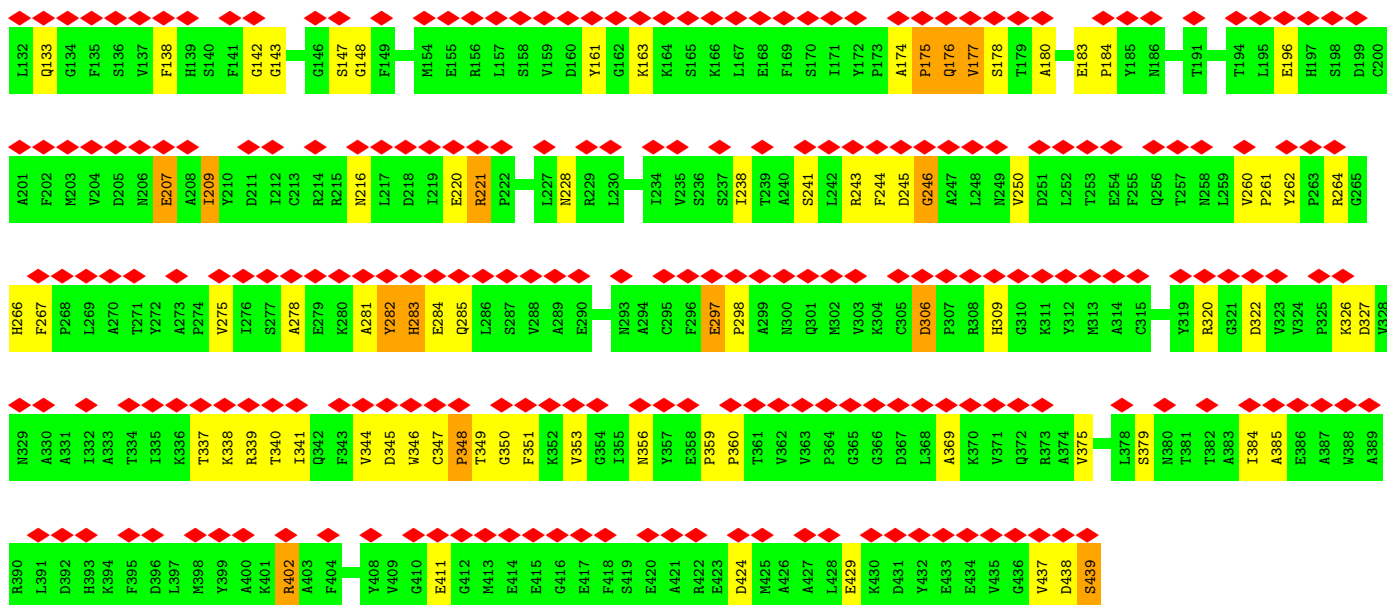


• Molecule 1: Tubulin alpha-1A chain

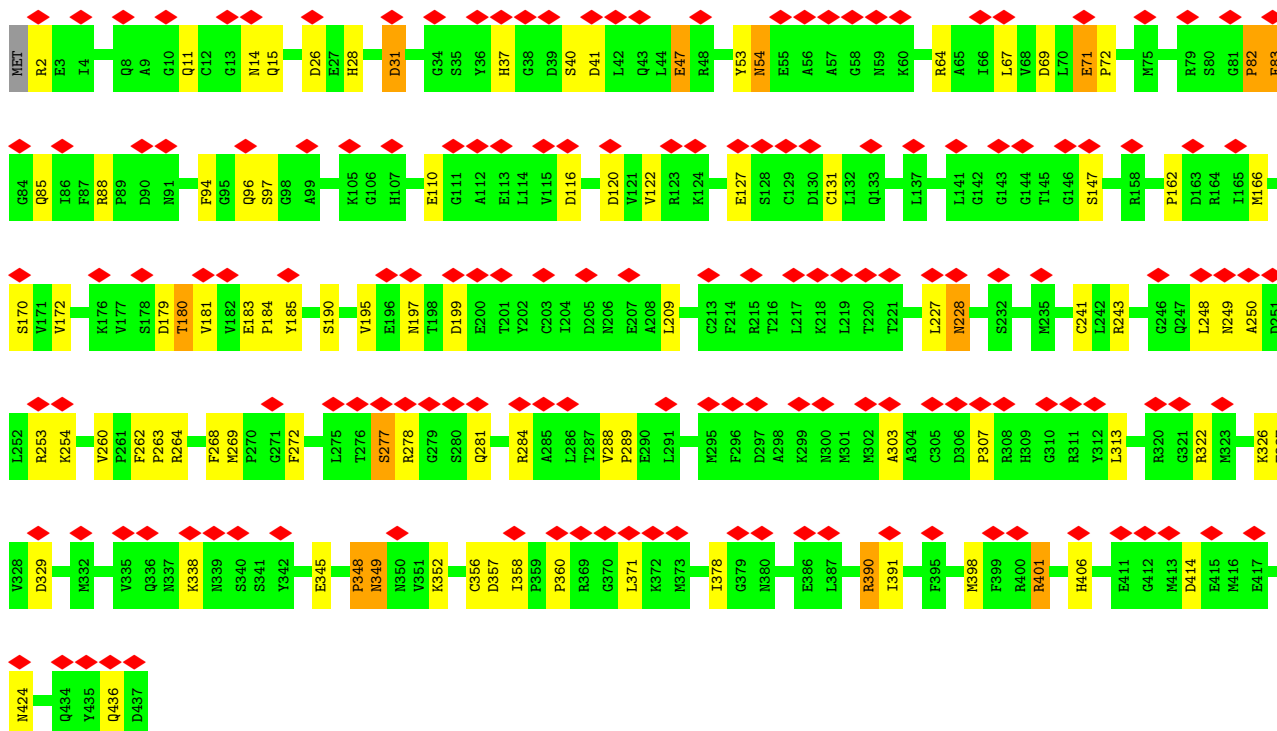
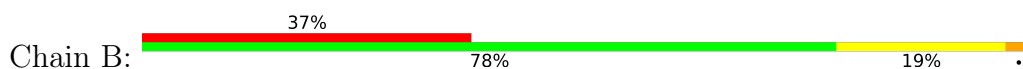


• Molecule 1: Tubulin alpha-1A chain

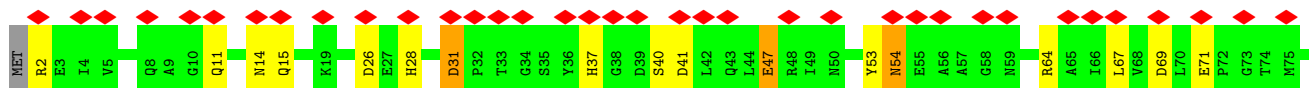
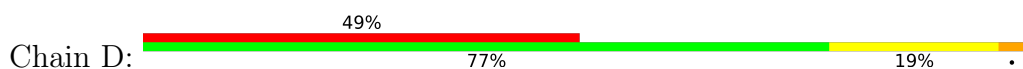


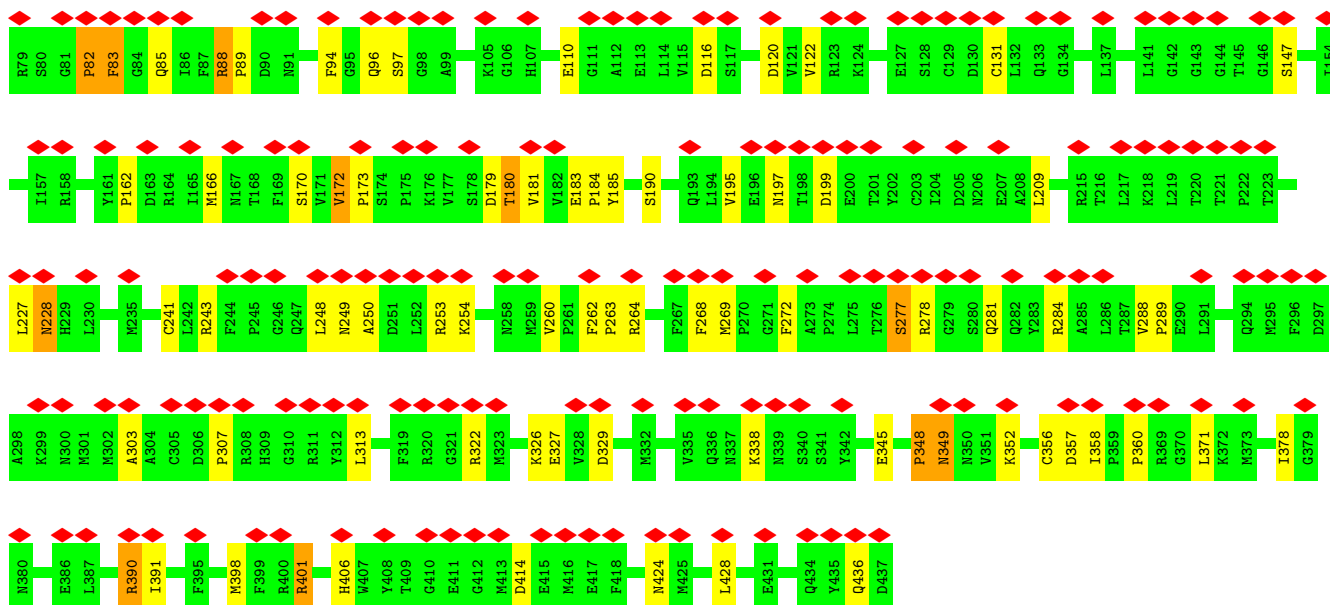


• Molecule 2: Tubulin beta chain

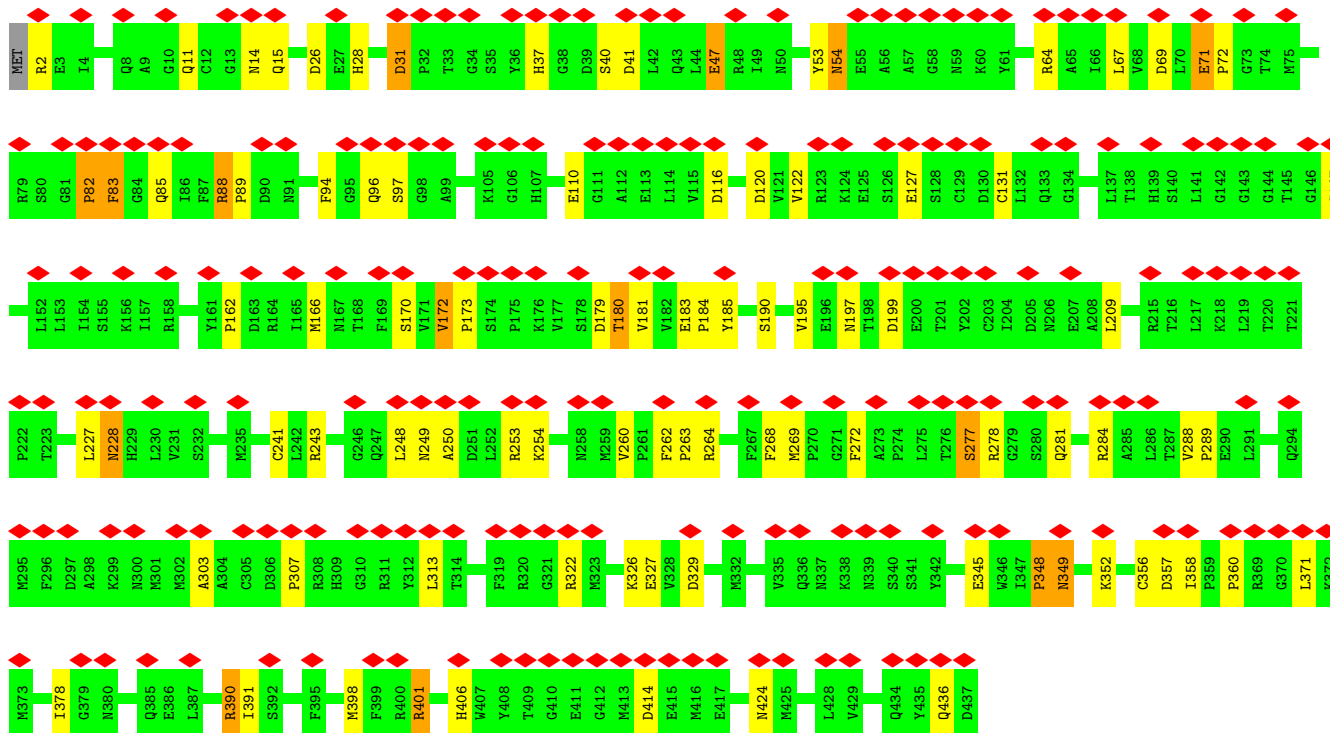
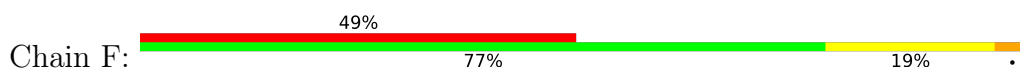


• Molecule 2: Tubulin beta chain

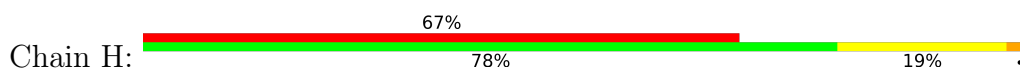


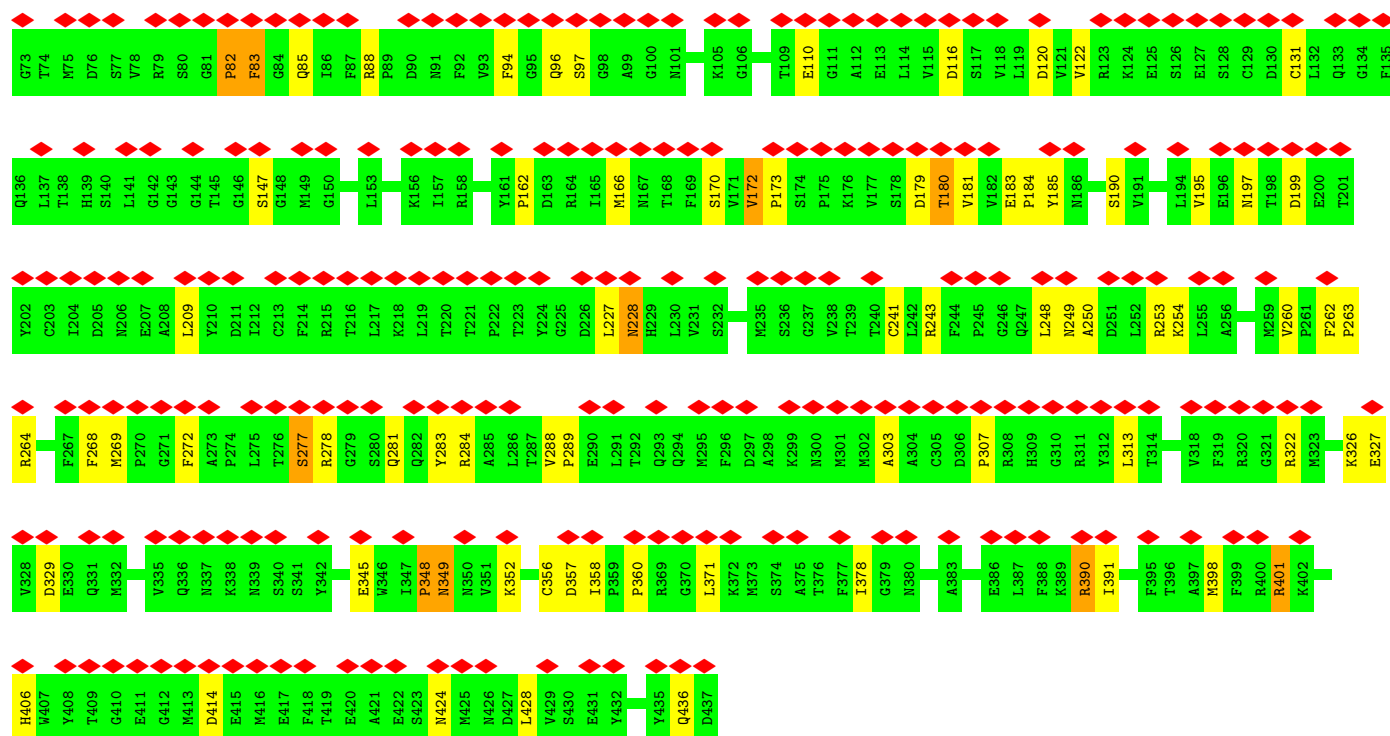


• Molecule 2: Tubulin beta chain

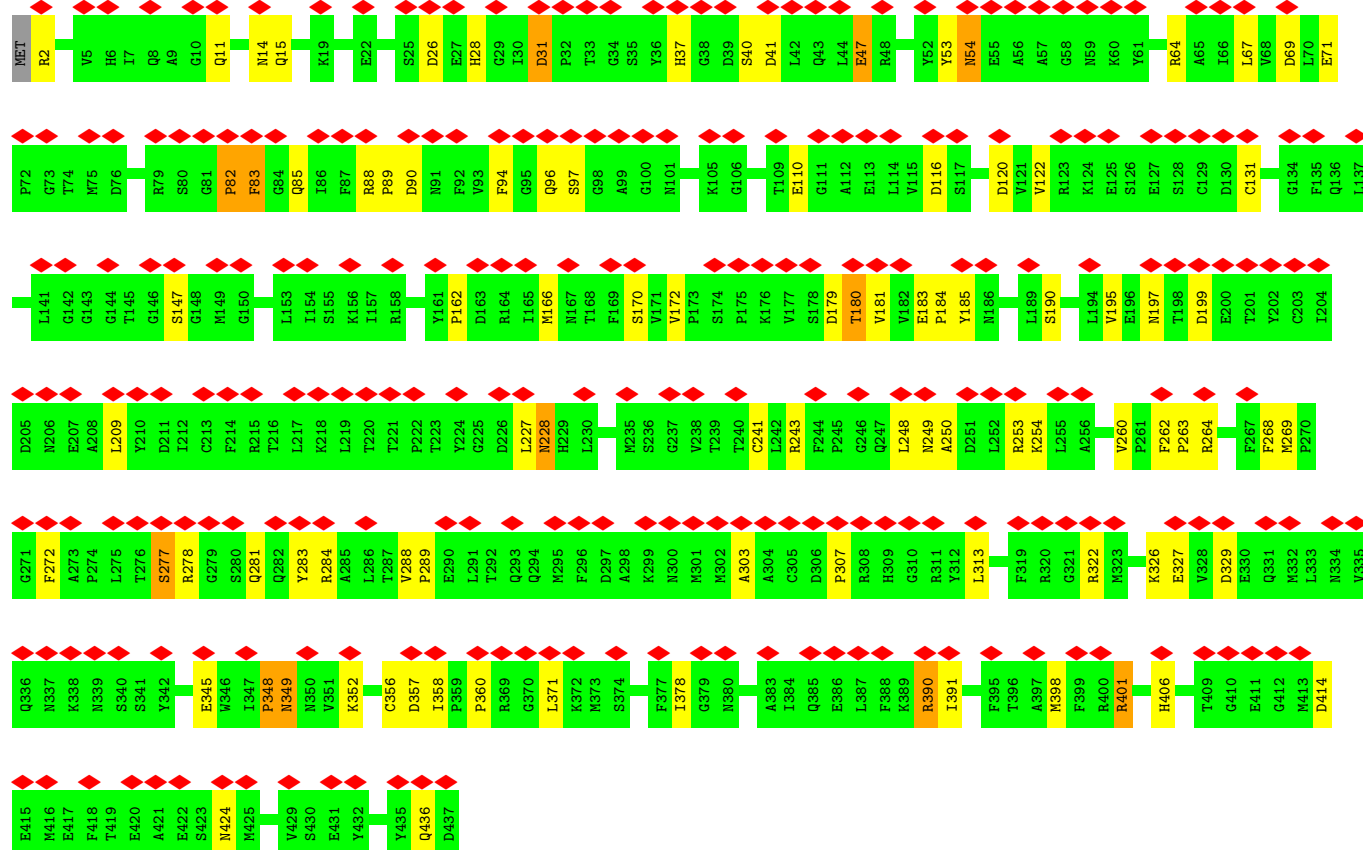
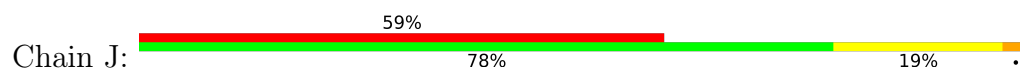


• Molecule 2: Tubulin beta chain

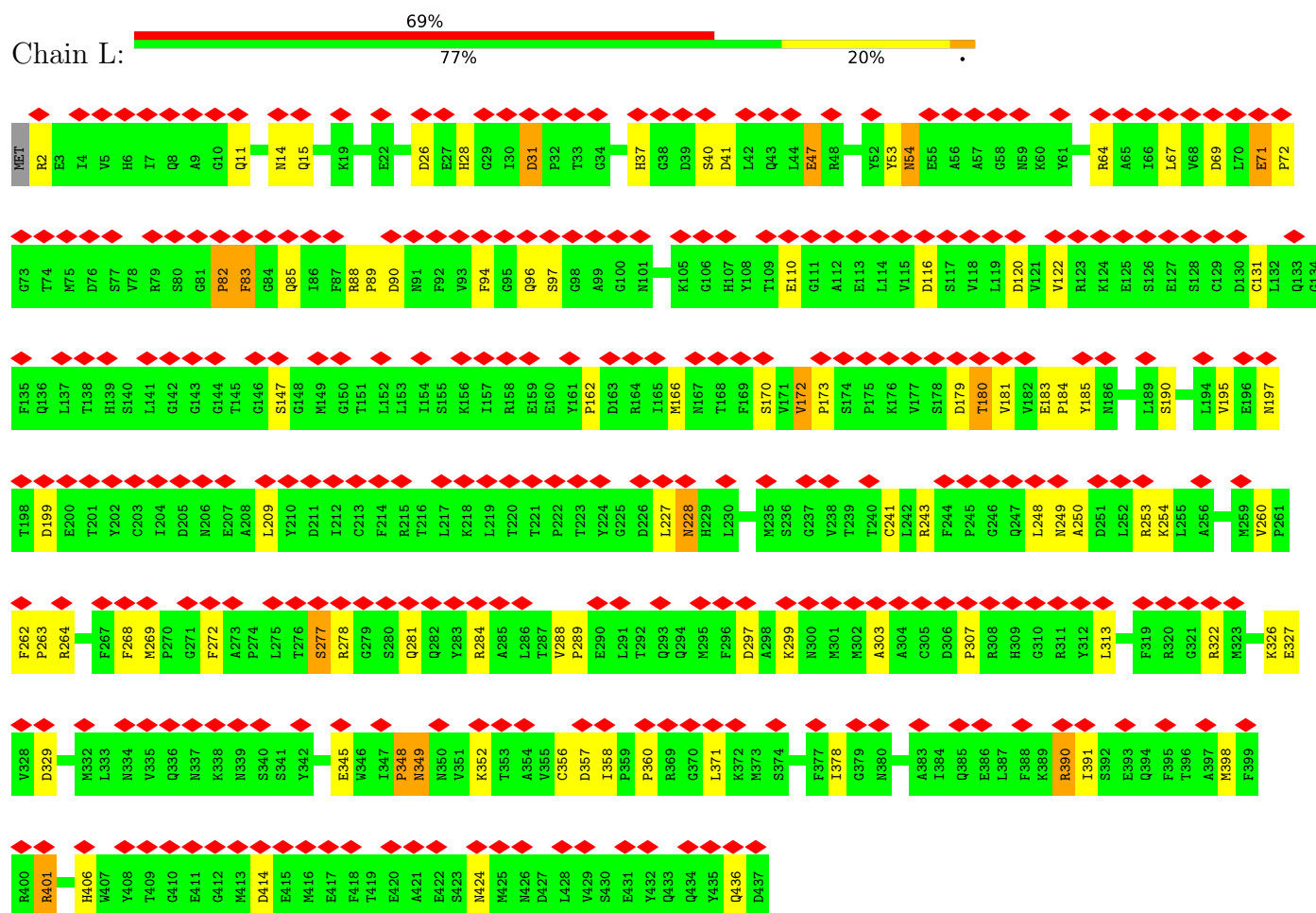




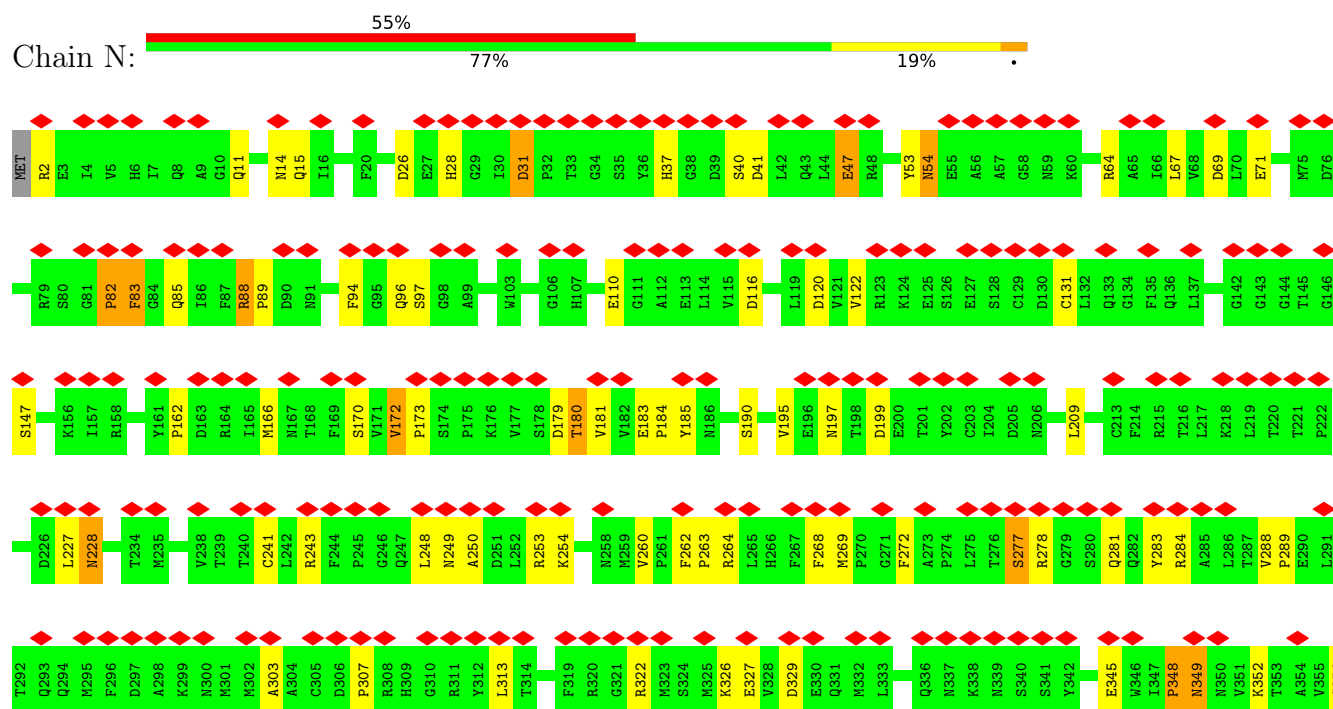
• Molecule 2: Tubulin beta chain

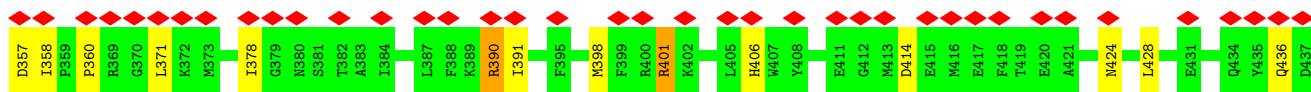


- Molecule 2: Tubulin beta chain

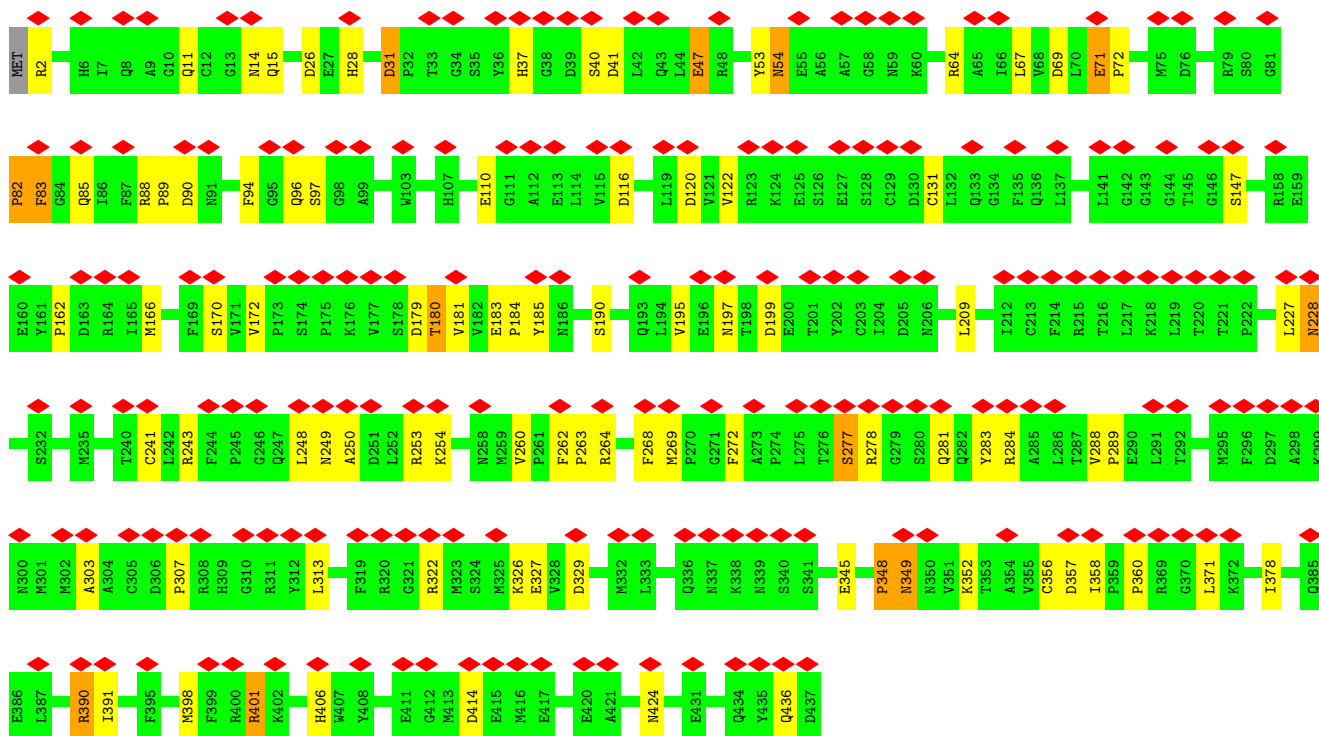
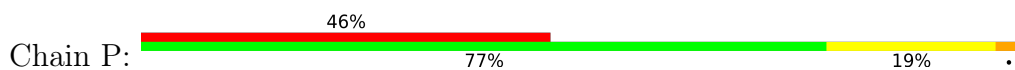


- Molecule 2: Tubulin beta chain

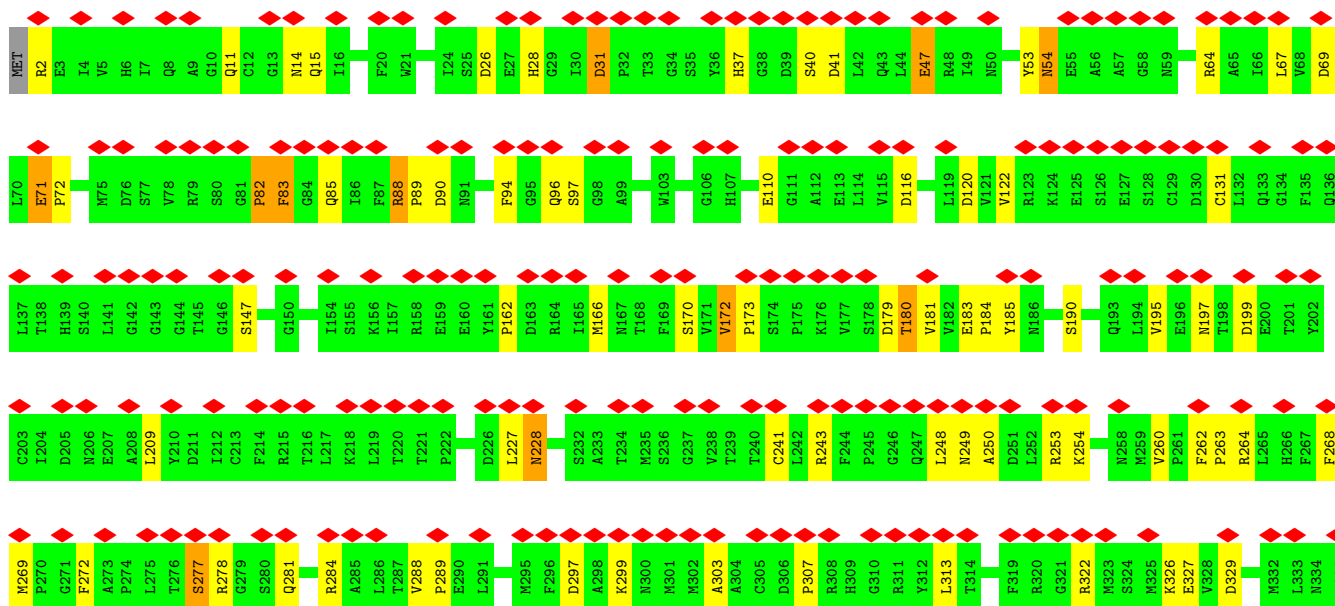
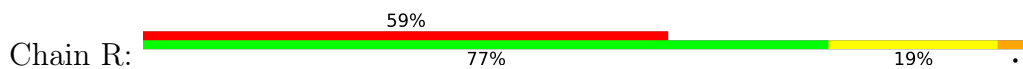


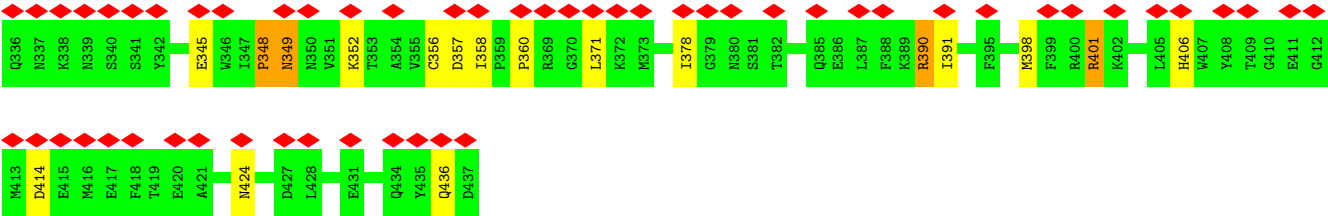


• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of particles used	57451	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	ctftilt	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25.0	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	72000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	12.334	Depositor
Minimum map value	-5.288	Depositor
Average map value	0.468	Depositor
Map value standard deviation	1.871	Depositor
Recommended contour level	4	Depositor
Map size (Å)	191.4, 114.840004, 281.88	wwPDB
Map dimensions	110, 66, 162	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7399999, 1.74, 1.74	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, GTP, G2P

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	1.52	49/3427 (1.4%)	1.79	90/4651 (1.9%)
1	C	1.52	50/3427 (1.5%)	1.79	91/4651 (2.0%)
1	E	1.52	49/3427 (1.4%)	1.79	90/4651 (1.9%)
1	G	1.52	49/3427 (1.4%)	1.78	90/4651 (1.9%)
1	I	1.52	49/3427 (1.4%)	1.79	91/4651 (2.0%)
1	K	1.52	48/3427 (1.4%)	1.79	91/4651 (2.0%)
1	M	1.52	50/3427 (1.5%)	1.79	92/4651 (2.0%)
1	O	1.52	49/3427 (1.4%)	1.78	90/4651 (1.9%)
1	Q	1.52	49/3427 (1.4%)	1.79	92/4651 (2.0%)
2	B	1.15	9/3427 (0.3%)	1.72	76/4642 (1.6%)
2	D	1.15	9/3427 (0.3%)	1.72	76/4642 (1.6%)
2	F	1.15	9/3427 (0.3%)	1.72	76/4642 (1.6%)
2	H	1.15	9/3427 (0.3%)	1.72	76/4642 (1.6%)
2	J	1.15	9/3427 (0.3%)	1.72	76/4642 (1.6%)
2	L	1.15	9/3427 (0.3%)	1.72	76/4642 (1.6%)
2	N	1.15	9/3427 (0.3%)	1.72	77/4642 (1.7%)
2	P	1.15	9/3427 (0.3%)	1.72	76/4642 (1.6%)
2	R	1.15	9/3427 (0.3%)	1.72	76/4642 (1.6%)
All	All	1.35	523/61686 (0.8%)	1.75	1502/83637 (1.8%)

All (523) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	349	THR	CA-C	-17.60	1.32	1.52
1	C	349	THR	CA-C	-17.60	1.32	1.52
1	E	349	THR	CA-C	-17.57	1.32	1.52
1	I	349	THR	CA-C	-17.57	1.32	1.52
1	O	349	THR	CA-C	-17.55	1.32	1.52
1	Q	349	THR	CA-C	-17.54	1.32	1.52
1	G	349	THR	CA-C	-17.54	1.32	1.52
1	A	349	THR	CA-C	-17.54	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	349	THR	CA-C	-17.51	1.32	1.52
1	K	50	ASN	N-CA	-14.48	1.25	1.46
1	I	50	ASN	N-CA	-14.47	1.25	1.46
1	Q	50	ASN	N-CA	-14.46	1.25	1.46
1	A	50	ASN	N-CA	-14.45	1.25	1.46
1	E	50	ASN	N-CA	-14.45	1.25	1.46
1	G	50	ASN	N-CA	-14.45	1.25	1.46
1	C	50	ASN	N-CA	-14.45	1.25	1.46
1	M	50	ASN	N-CA	-14.43	1.25	1.46
1	O	50	ASN	N-CA	-14.43	1.25	1.46
1	I	339	ARG	CA-C	-12.76	1.35	1.53
1	G	339	ARG	CA-C	-12.74	1.35	1.53
1	K	339	ARG	CA-C	-12.72	1.35	1.53
1	A	339	ARG	CA-C	-12.71	1.35	1.53
1	Q	339	ARG	CA-C	-12.71	1.35	1.53
1	M	339	ARG	CA-C	-12.70	1.35	1.53
1	E	339	ARG	CA-C	-12.67	1.35	1.53
1	O	339	ARG	CA-C	-12.67	1.35	1.53
1	C	339	ARG	CA-C	-12.67	1.35	1.53
1	C	340	THR	N-CA	-12.23	1.30	1.46
1	Q	340	THR	N-CA	-12.18	1.30	1.46
1	K	340	THR	N-CA	-12.15	1.30	1.46
1	A	340	THR	N-CA	-12.15	1.30	1.46
1	O	340	THR	N-CA	-12.14	1.30	1.46
1	E	340	THR	N-CA	-12.14	1.30	1.46
1	M	340	THR	N-CA	-12.13	1.30	1.46
1	I	340	THR	N-CA	-12.13	1.30	1.46
1	G	340	THR	N-CA	-12.12	1.30	1.46
1	G	283	HIS	CA-C	-11.76	1.36	1.53
1	M	283	HIS	CA-C	-11.73	1.36	1.53
1	K	283	HIS	CA-C	-11.73	1.36	1.53
1	E	283	HIS	CA-C	-11.72	1.36	1.53
1	A	283	HIS	CA-C	-11.71	1.36	1.53
1	I	283	HIS	CA-C	-11.71	1.36	1.53
1	Q	283	HIS	CA-C	-11.71	1.36	1.53
1	C	283	HIS	CA-C	-11.70	1.36	1.53
1	O	283	HIS	CA-C	-11.69	1.36	1.53
1	I	177	VAL	CA-C	-10.65	1.41	1.53
1	O	177	VAL	CA-C	-10.61	1.41	1.53
1	M	282	TYR	CA-C	-10.60	1.39	1.52
1	O	282	TYR	CA-C	-10.59	1.39	1.52
1	Q	177	VAL	CA-C	-10.59	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	TYR	CA-C	-10.58	1.39	1.52
1	A	177	VAL	CA-C	-10.58	1.41	1.53
1	Q	282	TYR	CA-C	-10.58	1.39	1.52
1	C	282	TYR	CA-C	-10.57	1.39	1.52
1	I	282	TYR	CA-C	-10.57	1.39	1.52
1	K	177	VAL	CA-C	-10.56	1.41	1.53
1	G	177	VAL	CA-C	-10.55	1.41	1.53
1	M	177	VAL	CA-C	-10.54	1.41	1.53
1	E	177	VAL	CA-C	-10.54	1.41	1.53
1	G	282	TYR	CA-C	-10.53	1.39	1.52
1	E	282	TYR	CA-C	-10.53	1.39	1.52
1	K	282	TYR	CA-C	-10.52	1.39	1.52
1	C	177	VAL	CA-C	-10.51	1.41	1.53
1	C	338	LYS	CA-C	-10.32	1.38	1.52
1	M	338	LYS	CA-C	-10.32	1.38	1.52
1	Q	338	LYS	CA-C	-10.31	1.38	1.52
1	A	338	LYS	CA-C	-10.31	1.38	1.52
2	J	249	ASN	CA-C	-10.30	1.42	1.53
1	I	338	LYS	CA-C	-10.29	1.38	1.52
1	O	338	LYS	CA-C	-10.29	1.38	1.52
1	K	338	LYS	CA-C	-10.29	1.38	1.52
1	E	338	LYS	CA-C	-10.28	1.38	1.52
2	R	249	ASN	CA-C	-10.27	1.42	1.53
2	B	249	ASN	CA-C	-10.26	1.42	1.53
2	L	249	ASN	CA-C	-10.26	1.42	1.53
2	N	249	ASN	CA-C	-10.26	1.42	1.53
2	P	249	ASN	CA-C	-10.25	1.42	1.53
1	G	338	LYS	CA-C	-10.24	1.38	1.52
2	H	249	ASN	CA-C	-10.24	1.42	1.53
2	D	249	ASN	CA-C	-10.24	1.42	1.53
2	F	249	ASN	CA-C	-10.24	1.42	1.53
1	E	339	ARG	N-CA	-10.04	1.34	1.45
1	C	339	ARG	N-CA	-10.02	1.34	1.45
1	A	339	ARG	N-CA	-9.98	1.34	1.45
1	M	339	ARG	N-CA	-9.98	1.34	1.45
1	K	339	ARG	N-CA	-9.98	1.34	1.45
1	O	339	ARG	N-CA	-9.98	1.34	1.45
1	Q	339	ARG	N-CA	-9.98	1.34	1.45
1	G	339	ARG	N-CA	-9.95	1.34	1.45
1	I	339	ARG	N-CA	-9.95	1.34	1.45
1	G	36	MET	CA-C	-9.94	1.40	1.52
1	Q	36	MET	CA-C	-9.89	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	MET	CA-C	-9.89	1.40	1.52
1	E	36	MET	CA-C	-9.88	1.40	1.52
1	I	36	MET	CA-C	-9.87	1.40	1.52
1	C	36	MET	CA-C	-9.87	1.40	1.52
1	O	36	MET	CA-C	-9.87	1.40	1.52
1	K	36	MET	CA-C	-9.87	1.40	1.52
1	M	36	MET	CA-C	-9.85	1.40	1.52
1	C	284	GLU	N-CA	-9.71	1.34	1.46
1	I	284	GLU	N-CA	-9.71	1.34	1.46
1	K	284	GLU	N-CA	-9.70	1.34	1.46
1	A	284	GLU	N-CA	-9.68	1.34	1.46
1	E	284	GLU	N-CA	-9.68	1.34	1.46
1	M	284	GLU	N-CA	-9.68	1.34	1.46
1	G	284	GLU	N-CA	-9.67	1.34	1.46
1	Q	284	GLU	N-CA	-9.64	1.34	1.46
1	O	284	GLU	N-CA	-9.64	1.34	1.46
1	E	37	PRO	CA-C	-9.13	1.44	1.52
1	I	37	PRO	CA-C	-9.08	1.44	1.52
1	K	37	PRO	CA-C	-9.08	1.44	1.52
1	Q	37	PRO	CA-C	-9.07	1.44	1.52
1	M	37	PRO	CA-C	-9.06	1.44	1.52
1	A	37	PRO	CA-C	-9.03	1.44	1.52
1	C	37	PRO	CA-C	-9.03	1.44	1.52
1	O	37	PRO	CA-C	-9.03	1.44	1.52
1	G	37	PRO	CA-C	-9.00	1.44	1.52
2	D	436	GLN	CA-C	-8.58	1.41	1.52
1	I	284	GLU	CA-C	-8.57	1.42	1.52
2	J	436	GLN	CA-C	-8.55	1.41	1.52
1	Q	284	GLU	CA-C	-8.55	1.42	1.52
1	O	284	GLU	CA-C	-8.54	1.42	1.52
1	G	284	GLU	CA-C	-8.53	1.42	1.52
1	Q	51	THR	N-CA	-8.53	1.34	1.46
2	H	436	GLN	CA-C	-8.53	1.41	1.52
1	K	284	GLU	CA-C	-8.53	1.42	1.52
2	N	436	GLN	CA-C	-8.53	1.41	1.52
1	K	51	THR	N-CA	-8.52	1.34	1.46
1	A	284	GLU	CA-C	-8.52	1.42	1.52
1	M	174	ALA	CA-C	-8.51	1.42	1.53
2	B	436	GLN	CA-C	-8.51	1.41	1.52
1	E	284	GLU	CA-C	-8.51	1.42	1.52
1	C	284	GLU	CA-C	-8.51	1.42	1.52
1	M	284	GLU	CA-C	-8.50	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	51	THR	N-CA	-8.50	1.34	1.46
2	F	436	GLN	CA-C	-8.49	1.41	1.52
2	R	436	GLN	CA-C	-8.49	1.41	1.52
1	A	51	THR	N-CA	-8.49	1.34	1.46
1	C	51	THR	N-CA	-8.49	1.34	1.46
1	I	174	ALA	CA-C	-8.49	1.42	1.53
1	M	51	THR	N-CA	-8.49	1.34	1.46
1	E	51	THR	N-CA	-8.49	1.34	1.46
1	I	51	THR	N-CA	-8.49	1.34	1.46
1	G	51	THR	N-CA	-8.48	1.34	1.46
1	G	174	ALA	CA-C	-8.48	1.42	1.53
1	K	174	ALA	CA-C	-8.48	1.42	1.53
1	C	174	ALA	CA-C	-8.47	1.42	1.53
2	P	436	GLN	CA-C	-8.47	1.41	1.52
1	Q	174	ALA	CA-C	-8.46	1.42	1.53
1	A	174	ALA	CA-C	-8.46	1.42	1.53
1	O	174	ALA	CA-C	-8.45	1.42	1.53
2	L	436	GLN	CA-C	-8.44	1.41	1.52
1	E	174	ALA	CA-C	-8.41	1.42	1.53
1	G	37	PRO	N-CA	-8.35	1.35	1.48
1	A	37	PRO	N-CA	-8.31	1.35	1.48
1	Q	37	PRO	N-CA	-8.31	1.35	1.48
2	H	82	PRO	CA-C	-8.30	1.42	1.52
1	M	37	PRO	N-CA	-8.30	1.35	1.48
1	E	37	PRO	N-CA	-8.30	1.35	1.48
1	O	37	PRO	N-CA	-8.30	1.35	1.48
1	I	37	PRO	N-CA	-8.29	1.35	1.48
1	K	37	PRO	N-CA	-8.29	1.35	1.48
1	C	37	PRO	N-CA	-8.28	1.35	1.48
2	P	82	PRO	CA-C	-8.28	1.42	1.52
2	L	82	PRO	CA-C	-8.27	1.42	1.52
2	D	82	PRO	CA-C	-8.26	1.42	1.52
2	B	82	PRO	CA-C	-8.26	1.42	1.52
2	J	82	PRO	CA-C	-8.25	1.42	1.52
2	R	82	PRO	CA-C	-8.23	1.42	1.52
2	N	82	PRO	CA-C	-8.21	1.42	1.52
2	F	82	PRO	CA-C	-8.20	1.42	1.52
1	Q	178	SER	CA-C	-8.12	1.43	1.52
1	E	178	SER	CA-C	-8.11	1.43	1.52
1	M	178	SER	CA-C	-8.11	1.43	1.52
1	O	178	SER	CA-C	-8.09	1.43	1.52
1	A	178	SER	CA-C	-8.08	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	SER	CA-C	-8.07	1.43	1.52
1	K	178	SER	CA-C	-8.06	1.43	1.52
1	G	178	SER	CA-C	-8.05	1.43	1.52
1	I	178	SER	CA-C	-8.04	1.43	1.52
1	O	438	ASP	CA-C	-8.03	1.42	1.52
1	G	438	ASP	CA-C	-8.00	1.42	1.52
1	Q	438	ASP	CA-C	-7.99	1.42	1.52
1	C	438	ASP	CA-C	-7.99	1.42	1.52
1	E	438	ASP	CA-C	-7.98	1.42	1.52
1	K	438	ASP	CA-C	-7.98	1.42	1.52
1	A	438	ASP	CA-C	-7.97	1.42	1.52
1	M	438	ASP	CA-C	-7.96	1.42	1.52
1	I	438	ASP	CA-C	-7.95	1.42	1.52
1	E	283	HIS	N-CA	-7.65	1.35	1.46
1	C	283	HIS	N-CA	-7.63	1.35	1.46
1	A	283	HIS	N-CA	-7.62	1.35	1.46
1	I	283	HIS	N-CA	-7.62	1.35	1.46
1	Q	283	HIS	N-CA	-7.61	1.35	1.46
2	J	96	GLN	CA-C	-7.60	1.44	1.53
1	G	283	HIS	N-CA	-7.60	1.35	1.46
2	F	96	GLN	CA-C	-7.60	1.44	1.53
1	O	283	HIS	N-CA	-7.59	1.35	1.46
2	D	96	GLN	CA-C	-7.58	1.44	1.53
2	N	96	GLN	CA-C	-7.58	1.44	1.53
1	K	283	HIS	N-CA	-7.58	1.35	1.46
2	R	96	GLN	CA-C	-7.58	1.44	1.53
1	M	283	HIS	N-CA	-7.57	1.35	1.46
2	B	96	GLN	CA-C	-7.57	1.44	1.53
2	H	96	GLN	CA-C	-7.55	1.44	1.53
2	P	96	GLN	CA-C	-7.54	1.44	1.53
1	O	349	THR	N-CA	-7.53	1.37	1.46
2	L	96	GLN	CA-C	-7.52	1.44	1.53
1	I	349	THR	N-CA	-7.50	1.37	1.46
1	K	349	THR	N-CA	-7.48	1.37	1.46
1	E	349	THR	N-CA	-7.46	1.37	1.46
1	A	349	THR	N-CA	-7.46	1.37	1.46
1	Q	349	THR	N-CA	-7.44	1.37	1.46
1	G	349	THR	N-CA	-7.43	1.37	1.46
1	C	349	THR	N-CA	-7.42	1.37	1.46
1	M	349	THR	N-CA	-7.42	1.37	1.46
1	M	437	VAL	CA-C	-7.40	1.44	1.52
1	O	437	VAL	CA-C	-7.35	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	51	THR	CA-C	-7.34	1.42	1.52
1	I	437	VAL	CA-C	-7.34	1.44	1.52
1	A	437	VAL	CA-C	-7.34	1.44	1.52
1	E	437	VAL	CA-C	-7.34	1.44	1.52
1	Q	437	VAL	CA-C	-7.33	1.44	1.52
1	G	51	THR	CA-C	-7.33	1.42	1.52
1	M	51	THR	CA-C	-7.33	1.42	1.52
1	A	51	THR	CA-C	-7.32	1.42	1.52
1	C	437	VAL	CA-C	-7.32	1.44	1.52
1	I	51	THR	CA-C	-7.32	1.42	1.52
1	Q	51	THR	CA-C	-7.32	1.42	1.52
1	O	51	THR	CA-C	-7.31	1.42	1.52
1	K	437	VAL	CA-C	-7.31	1.44	1.52
1	C	51	THR	CA-C	-7.30	1.42	1.52
1	G	348	PRO	CA-C	-7.30	1.42	1.52
1	G	437	VAL	CA-C	-7.30	1.44	1.52
1	E	51	THR	CA-C	-7.30	1.42	1.52
1	E	348	PRO	CA-C	-7.29	1.42	1.52
1	A	348	PRO	CA-C	-7.29	1.42	1.52
1	K	348	PRO	CA-C	-7.28	1.42	1.52
1	M	348	PRO	CA-C	-7.28	1.42	1.52
1	I	348	PRO	CA-C	-7.28	1.42	1.52
1	O	348	PRO	CA-C	-7.28	1.42	1.52
1	C	348	PRO	CA-C	-7.27	1.42	1.52
1	Q	348	PRO	CA-C	-7.26	1.42	1.52
1	K	281	ALA	CA-C	-7.24	1.42	1.52
1	M	281	ALA	CA-C	-7.23	1.42	1.52
1	E	281	ALA	CA-C	-7.22	1.42	1.52
1	O	281	ALA	CA-C	-7.20	1.42	1.52
1	C	281	ALA	CA-C	-7.19	1.42	1.52
1	A	281	ALA	CA-C	-7.19	1.42	1.52
1	Q	281	ALA	CA-C	-7.18	1.42	1.52
1	G	281	ALA	CA-C	-7.17	1.42	1.52
1	I	281	ALA	CA-C	-7.16	1.42	1.52
1	G	285	GLN	N-CA	-7.11	1.37	1.46
1	K	285	GLN	N-CA	-7.11	1.37	1.46
1	M	285	GLN	N-CA	-7.11	1.37	1.46
1	A	285	GLN	N-CA	-7.08	1.37	1.46
1	E	285	GLN	N-CA	-7.08	1.37	1.46
1	O	285	GLN	N-CA	-7.08	1.37	1.46
1	C	285	GLN	N-CA	-7.07	1.37	1.46
1	I	285	GLN	N-CA	-7.07	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	285	GLN	N-CA	-7.02	1.37	1.46
1	E	282	TYR	N-CA	-7.00	1.37	1.46
1	M	282	TYR	N-CA	-6.98	1.37	1.46
1	Q	351	PHE	N-CA	-6.96	1.37	1.46
1	Q	282	TYR	N-CA	-6.96	1.37	1.46
1	A	282	TYR	N-CA	-6.95	1.37	1.46
1	O	282	TYR	N-CA	-6.95	1.37	1.46
1	M	175	PRO	N-CA	-6.94	1.38	1.47
1	I	38	SER	CA-C	-6.94	1.38	1.52
1	O	38	SER	CA-C	-6.94	1.38	1.52
1	Q	38	SER	CA-C	-6.94	1.38	1.52
1	I	282	TYR	N-CA	-6.94	1.37	1.46
1	E	38	SER	CA-C	-6.93	1.38	1.52
1	I	175	PRO	N-CA	-6.93	1.38	1.47
1	A	38	SER	CA-C	-6.93	1.38	1.52
1	G	38	SER	CA-C	-6.93	1.38	1.52
1	K	175	PRO	N-CA	-6.93	1.38	1.47
1	K	282	TYR	N-CA	-6.93	1.37	1.46
1	C	175	PRO	N-CA	-6.92	1.38	1.47
1	M	38	SER	CA-C	-6.92	1.38	1.52
1	I	351	PHE	N-CA	-6.92	1.37	1.46
1	A	175	PRO	N-CA	-6.92	1.38	1.47
1	C	38	SER	CA-C	-6.91	1.38	1.52
1	O	175	PRO	N-CA	-6.91	1.38	1.47
1	Q	175	PRO	N-CA	-6.91	1.38	1.47
1	G	351	PHE	N-CA	-6.90	1.37	1.46
1	G	175	PRO	N-CA	-6.90	1.38	1.47
1	C	351	PHE	N-CA	-6.90	1.37	1.46
1	K	38	SER	CA-C	-6.90	1.38	1.52
1	A	351	PHE	N-CA	-6.89	1.37	1.46
1	G	178	SER	N-CA	-6.89	1.38	1.46
1	C	282	TYR	N-CA	-6.88	1.37	1.46
1	E	175	PRO	N-CA	-6.88	1.38	1.47
1	O	178	SER	N-CA	-6.88	1.38	1.46
1	G	282	TYR	N-CA	-6.88	1.37	1.46
1	M	351	PHE	N-CA	-6.88	1.37	1.46
1	A	178	SER	N-CA	-6.86	1.38	1.46
1	C	178	SER	N-CA	-6.86	1.38	1.46
1	K	246	GLY	N-CA	-6.86	1.39	1.45
1	K	351	PHE	N-CA	-6.86	1.37	1.46
1	C	246	GLY	N-CA	-6.85	1.39	1.45
1	O	243	ARG	CA-C	-6.85	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	178	SER	N-CA	-6.85	1.38	1.46
1	O	351	PHE	N-CA	-6.85	1.37	1.46
1	K	178	SER	N-CA	-6.83	1.38	1.46
1	M	178	SER	N-CA	-6.83	1.38	1.46
1	E	178	SER	N-CA	-6.83	1.38	1.46
1	E	351	PHE	N-CA	-6.83	1.37	1.46
1	G	243	ARG	CA-C	-6.83	1.43	1.52
1	I	243	ARG	CA-C	-6.82	1.43	1.52
1	I	246	GLY	N-CA	-6.82	1.39	1.45
1	Q	246	GLY	N-CA	-6.82	1.39	1.45
1	Q	243	ARG	CA-C	-6.82	1.43	1.52
1	A	243	ARG	CA-C	-6.82	1.43	1.52
1	E	243	ARG	CA-C	-6.81	1.43	1.52
1	Q	178	SER	N-CA	-6.81	1.38	1.46
1	K	243	ARG	CA-C	-6.80	1.43	1.52
1	A	246	GLY	N-CA	-6.79	1.39	1.45
1	G	246	GLY	N-CA	-6.78	1.39	1.45
1	C	243	ARG	CA-C	-6.77	1.43	1.52
1	M	243	ARG	CA-C	-6.77	1.43	1.52
1	O	246	GLY	N-CA	-6.76	1.39	1.45
1	I	176	GLN	N-CA	-6.73	1.38	1.46
1	G	347	CYS	CA-C	-6.72	1.44	1.52
1	E	246	GLY	N-CA	-6.72	1.39	1.45
1	Q	347	CYS	CA-C	-6.71	1.44	1.52
1	C	176	GLN	N-CA	-6.71	1.38	1.46
1	M	176	GLN	N-CA	-6.71	1.38	1.46
1	M	347	CYS	CA-C	-6.70	1.44	1.52
1	M	246	GLY	N-CA	-6.70	1.39	1.45
1	O	347	CYS	CA-C	-6.70	1.44	1.52
1	K	347	CYS	CA-C	-6.69	1.44	1.52
1	E	347	CYS	CA-C	-6.68	1.44	1.52
1	A	176	GLN	N-CA	-6.68	1.38	1.46
1	E	176	GLN	N-CA	-6.68	1.38	1.46
1	K	176	GLN	N-CA	-6.67	1.38	1.46
1	A	347	CYS	CA-C	-6.67	1.44	1.52
1	I	347	CYS	CA-C	-6.65	1.44	1.52
1	Q	176	GLN	N-CA	-6.65	1.38	1.46
1	O	176	GLN	N-CA	-6.64	1.38	1.46
1	G	176	GLN	N-CA	-6.64	1.38	1.46
1	C	347	CYS	CA-C	-6.63	1.44	1.52
1	C	50	ASN	CA-C	-6.58	1.41	1.52
1	O	50	ASN	CA-C	-6.56	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	50	ASN	CA-C	-6.55	1.41	1.52
1	A	50	ASN	CA-C	-6.55	1.41	1.52
1	G	50	ASN	CA-C	-6.54	1.41	1.52
1	I	244	PHE	CA-C	-6.54	1.44	1.52
1	Q	50	ASN	CA-C	-6.54	1.41	1.52
1	E	50	ASN	CA-C	-6.54	1.41	1.52
1	E	244	PHE	CA-C	-6.54	1.44	1.52
1	M	244	PHE	CA-C	-6.54	1.44	1.52
1	A	244	PHE	CA-C	-6.53	1.44	1.52
1	O	244	PHE	CA-C	-6.53	1.44	1.52
1	C	244	PHE	CA-C	-6.52	1.44	1.52
1	Q	244	PHE	CA-C	-6.52	1.44	1.52
1	K	50	ASN	CA-C	-6.51	1.41	1.52
1	I	50	ASN	CA-C	-6.50	1.41	1.52
1	G	244	PHE	CA-C	-6.50	1.44	1.52
1	K	244	PHE	CA-C	-6.49	1.44	1.52
1	G	348	PRO	N-CA	-6.48	1.39	1.47
1	I	348	PRO	N-CA	-6.46	1.39	1.47
1	E	348	PRO	N-CA	-6.45	1.39	1.47
1	K	348	PRO	N-CA	-6.44	1.39	1.47
1	A	348	PRO	N-CA	-6.43	1.39	1.47
1	M	348	PRO	N-CA	-6.43	1.39	1.47
1	C	348	PRO	N-CA	-6.43	1.39	1.47
1	O	348	PRO	N-CA	-6.42	1.39	1.47
1	G	282	TYR	C-N	-6.40	1.25	1.33
1	K	282	TYR	C-N	-6.39	1.25	1.33
1	M	282	TYR	C-N	-6.39	1.25	1.33
1	Q	282	TYR	C-N	-6.38	1.25	1.33
1	E	282	TYR	C-N	-6.37	1.25	1.33
1	A	282	TYR	C-N	-6.37	1.25	1.33
1	Q	348	PRO	N-CA	-6.36	1.39	1.47
1	I	282	TYR	C-N	-6.35	1.25	1.33
1	O	282	TYR	C-N	-6.33	1.25	1.33
1	C	282	TYR	C-N	-6.32	1.25	1.33
2	R	180	THR	CA-C	-6.05	1.45	1.52
2	N	180	THR	CA-C	-6.02	1.45	1.52
2	J	250	ALA	N-CA	-6.01	1.38	1.46
2	N	250	ALA	N-CA	-6.00	1.38	1.46
2	P	250	ALA	N-CA	-6.00	1.38	1.46
2	J	180	THR	CA-C	-6.00	1.45	1.52
2	B	180	THR	CA-C	-5.99	1.45	1.52
2	P	180	THR	CA-C	-5.99	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	180	THR	CA-C	-5.99	1.45	1.52
2	F	180	THR	CA-C	-5.99	1.45	1.52
2	B	250	ALA	N-CA	-5.98	1.38	1.46
2	D	250	ALA	N-CA	-5.98	1.38	1.46
2	H	250	ALA	N-CA	-5.98	1.38	1.46
2	L	250	ALA	N-CA	-5.97	1.38	1.46
2	F	250	ALA	N-CA	-5.97	1.38	1.46
2	R	250	ALA	N-CA	-5.96	1.38	1.46
2	D	180	THR	CA-C	-5.95	1.45	1.52
2	L	180	THR	CA-C	-5.91	1.45	1.52
1	C	52	PHE	N-CA	-5.91	1.37	1.45
1	M	52	PHE	N-CA	-5.91	1.37	1.45
1	Q	52	PHE	N-CA	-5.91	1.37	1.45
1	A	52	PHE	N-CA	-5.90	1.37	1.45
1	O	52	PHE	N-CA	-5.90	1.37	1.45
1	E	52	PHE	N-CA	-5.89	1.37	1.45
1	G	52	PHE	N-CA	-5.88	1.37	1.45
1	K	52	PHE	N-CA	-5.88	1.37	1.45
1	I	52	PHE	N-CA	-5.86	1.37	1.45
1	K	245	ASP	CA-C	-5.67	1.45	1.52
1	E	245	ASP	CA-C	-5.67	1.45	1.52
1	Q	245	ASP	CA-C	-5.65	1.45	1.52
1	A	245	ASP	CA-C	-5.64	1.45	1.52
1	G	245	ASP	CA-C	-5.63	1.45	1.52
1	I	245	ASP	CA-C	-5.63	1.45	1.52
1	M	245	ASP	CA-C	-5.62	1.45	1.52
1	O	245	ASP	CA-C	-5.61	1.45	1.52
1	C	245	ASP	CA-C	-5.58	1.45	1.52
1	G	337	THR	CA-C	-5.47	1.45	1.52
1	O	266	HIS	N-CA	-5.47	1.40	1.46
1	O	337	THR	CA-C	-5.47	1.45	1.52
1	K	337	THR	CA-C	-5.46	1.45	1.52
1	M	266	HIS	N-CA	-5.45	1.40	1.46
1	Q	266	HIS	N-CA	-5.45	1.40	1.46
1	M	337	THR	CA-C	-5.43	1.45	1.52
1	A	337	THR	CA-C	-5.42	1.45	1.52
1	K	266	HIS	N-CA	-5.42	1.40	1.46
1	E	337	THR	CA-C	-5.42	1.45	1.52
1	C	337	THR	CA-C	-5.41	1.45	1.52
1	E	266	HIS	N-CA	-5.41	1.40	1.46
1	G	266	HIS	N-CA	-5.41	1.40	1.46
1	I	266	HIS	N-CA	-5.41	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	HIS	N-CA	-5.41	1.40	1.46
1	Q	337	THR	CA-C	-5.41	1.45	1.52
1	I	337	THR	CA-C	-5.41	1.45	1.52
1	C	266	HIS	N-CA	-5.38	1.40	1.46
2	L	401	ARG	CD-NE	-5.35	1.38	1.46
2	J	401	ARG	CD-NE	-5.35	1.38	1.46
2	P	401	ARG	CD-NE	-5.35	1.38	1.46
1	G	177	VAL	N-CA	-5.34	1.40	1.46
1	I	285	GLN	CA-C	-5.32	1.46	1.52
2	H	401	ARG	CD-NE	-5.32	1.38	1.46
1	E	244	PHE	N-CA	-5.32	1.39	1.46
1	G	244	PHE	N-CA	-5.31	1.39	1.46
2	B	401	ARG	CD-NE	-5.31	1.38	1.46
1	C	177	VAL	N-CA	-5.31	1.40	1.46
1	K	339	ARG	C-N	-5.31	1.27	1.33
1	G	339	ARG	C-N	-5.30	1.27	1.33
1	M	339	ARG	C-N	-5.30	1.27	1.33
1	G	285	GLN	CA-C	-5.30	1.46	1.52
2	H	326	LYS	CA-C	-5.30	1.46	1.52
1	K	177	VAL	N-CA	-5.30	1.40	1.46
1	Q	339	ARG	C-N	-5.30	1.27	1.33
2	N	401	ARG	CD-NE	-5.30	1.38	1.46
2	R	401	ARG	CD-NE	-5.30	1.38	1.46
1	C	285	GLN	CA-C	-5.30	1.46	1.52
2	F	401	ARG	CD-NE	-5.30	1.38	1.46
1	Q	244	PHE	N-CA	-5.30	1.39	1.46
1	A	339	ARG	C-N	-5.29	1.27	1.33
1	E	339	ARG	C-N	-5.29	1.27	1.33
1	K	244	PHE	N-CA	-5.29	1.39	1.46
1	O	339	ARG	C-N	-5.29	1.27	1.33
1	I	339	ARG	C-N	-5.29	1.27	1.33
1	A	177	VAL	N-CA	-5.29	1.40	1.46
1	A	244	PHE	N-CA	-5.29	1.39	1.46
1	G	262	TYR	CA-C	-5.29	1.47	1.52
1	C	244	PHE	N-CA	-5.29	1.39	1.46
1	O	177	VAL	N-CA	-5.29	1.40	1.46
1	Q	285	GLN	CA-C	-5.28	1.46	1.52
2	D	326	LYS	CA-C	-5.28	1.46	1.52
1	A	285	GLN	CA-C	-5.27	1.46	1.52
1	I	244	PHE	N-CA	-5.27	1.39	1.46
1	K	344	VAL	CA-C	-5.27	1.47	1.52
2	B	326	LYS	CA-C	-5.26	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	344	VAL	CA-C	-5.26	1.47	1.52
1	I	177	VAL	N-CA	-5.26	1.40	1.46
2	N	326	LYS	CA-C	-5.26	1.46	1.52
2	J	326	LYS	CA-C	-5.25	1.46	1.52
2	D	401	ARG	CD-NE	-5.25	1.38	1.46
1	E	177	VAL	N-CA	-5.25	1.40	1.46
2	L	326	LYS	CA-C	-5.25	1.46	1.52
2	R	326	LYS	CA-C	-5.25	1.46	1.52
1	C	262	TYR	CA-C	-5.25	1.47	1.52
1	Q	177	VAL	N-CA	-5.25	1.40	1.46
1	O	244	PHE	N-CA	-5.25	1.39	1.46
1	M	244	PHE	N-CA	-5.24	1.39	1.46
2	P	326	LYS	CA-C	-5.24	1.46	1.52
1	K	285	GLN	CA-C	-5.23	1.46	1.52
1	O	285	GLN	CA-C	-5.23	1.46	1.52
1	O	344	VAL	CA-C	-5.23	1.47	1.52
1	Q	262	TYR	CA-C	-5.23	1.47	1.52
1	M	344	VAL	CA-C	-5.23	1.47	1.52
1	E	262	TYR	CA-C	-5.22	1.47	1.52
1	M	285	GLN	CA-C	-5.22	1.46	1.52
1	C	339	ARG	C-N	-5.22	1.27	1.33
1	I	262	TYR	CA-C	-5.22	1.47	1.52
1	M	177	VAL	N-CA	-5.22	1.40	1.46
2	F	326	LYS	CA-C	-5.21	1.46	1.52
1	E	344	VAL	CA-C	-5.21	1.47	1.52
1	A	262	TYR	CA-C	-5.21	1.47	1.52
1	E	285	GLN	CA-C	-5.20	1.46	1.52
1	O	262	TYR	CA-C	-5.20	1.47	1.52
1	A	344	VAL	CA-C	-5.20	1.47	1.52
1	I	344	VAL	CA-C	-5.19	1.47	1.52
1	G	344	VAL	CA-C	-5.19	1.47	1.52
1	K	262	TYR	CA-C	-5.19	1.47	1.52
1	M	262	TYR	CA-C	-5.19	1.47	1.52
1	C	344	VAL	CA-C	-5.15	1.47	1.52
2	H	349	ASN	CA-C	-5.11	1.47	1.53
2	F	349	ASN	CA-C	-5.10	1.47	1.53
2	B	349	ASN	CA-C	-5.09	1.47	1.53
2	L	349	ASN	CA-C	-5.09	1.47	1.53
1	O	283	HIS	C-N	-5.09	1.26	1.33
2	D	349	ASN	CA-C	-5.08	1.47	1.53
2	P	349	ASN	CA-C	-5.08	1.47	1.53
2	J	349	ASN	CA-C	-5.07	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	349	ASN	CA-C	-5.07	1.47	1.53
1	C	283	HIS	C-N	-5.06	1.27	1.33
1	Q	283	HIS	C-N	-5.06	1.27	1.33
2	N	349	ASN	CA-C	-5.06	1.47	1.53
1	M	283	HIS	C-N	-5.04	1.27	1.33
1	A	283	HIS	C-N	-5.03	1.27	1.33
1	G	283	HIS	C-N	-5.03	1.27	1.33
1	C	348	PRO	C-N	-5.02	1.27	1.33
1	M	348	PRO	C-N	-5.02	1.27	1.33
1	I	283	HIS	C-N	-5.01	1.27	1.33
1	E	283	HIS	C-N	-5.01	1.27	1.33

All (1502) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	228	ASN	CA-CB-CG	-11.60	101.00	112.60
2	P	228	ASN	CA-CB-CG	-11.60	101.00	112.60
2	F	228	ASN	CA-CB-CG	-11.60	101.00	112.60
2	N	228	ASN	CA-CB-CG	-11.60	101.00	112.60
2	J	228	ASN	CA-CB-CG	-11.59	101.01	112.60
2	B	228	ASN	CA-CB-CG	-11.59	101.01	112.60
2	R	228	ASN	CA-CB-CG	-11.57	101.03	112.60
2	H	228	ASN	CA-CB-CG	-11.56	101.04	112.60
2	L	228	ASN	CA-CB-CG	-11.55	101.05	112.60
1	K	338	LYS	CA-C-N	-10.85	103.91	122.67
1	K	338	LYS	C-N-CA	-10.85	103.91	122.67
1	Q	338	LYS	CA-C-N	-10.85	103.91	122.67
1	Q	338	LYS	C-N-CA	-10.85	103.91	122.67
1	C	338	LYS	CA-C-N	-10.84	103.92	122.67
1	C	338	LYS	C-N-CA	-10.84	103.92	122.67
1	O	338	LYS	CA-C-N	-10.84	103.91	122.67
1	O	338	LYS	C-N-CA	-10.84	103.91	122.67
1	G	338	LYS	CA-C-N	-10.83	103.93	122.67
1	G	338	LYS	C-N-CA	-10.83	103.93	122.67
1	A	338	LYS	CA-C-N	-10.82	103.94	122.67
1	A	338	LYS	C-N-CA	-10.82	103.94	122.67
1	E	338	LYS	CA-C-N	-10.82	103.95	122.67
1	E	338	LYS	C-N-CA	-10.82	103.95	122.67
1	I	338	LYS	CA-C-N	-10.81	103.97	122.67
1	I	338	LYS	C-N-CA	-10.81	103.97	122.67
1	M	338	LYS	CA-C-N	-10.81	103.97	122.67
1	M	338	LYS	C-N-CA	-10.81	103.97	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	283	HIS	CA-C-N	-10.65	103.37	121.89
1	E	283	HIS	C-N-CA	-10.65	103.37	121.89
1	I	283	HIS	CA-C-N	-10.65	103.37	121.89
1	I	283	HIS	C-N-CA	-10.65	103.37	121.89
1	O	283	HIS	CA-C-N	-10.63	103.39	121.89
1	O	283	HIS	C-N-CA	-10.63	103.39	121.89
1	A	283	HIS	CA-C-N	-10.63	103.39	121.89
1	A	283	HIS	C-N-CA	-10.63	103.39	121.89
1	Q	283	HIS	CA-C-N	-10.63	103.39	121.89
1	Q	283	HIS	C-N-CA	-10.63	103.39	121.89
1	K	283	HIS	CA-C-N	-10.62	103.41	121.89
1	K	283	HIS	C-N-CA	-10.62	103.41	121.89
1	M	283	HIS	CA-C-N	-10.62	103.41	121.89
1	M	283	HIS	C-N-CA	-10.62	103.41	121.89
1	C	283	HIS	CA-C-N	-10.62	103.41	121.89
1	C	283	HIS	C-N-CA	-10.62	103.41	121.89
1	G	283	HIS	CA-C-N	-10.62	103.42	121.89
1	G	283	HIS	C-N-CA	-10.62	103.42	121.89
1	E	228	ASN	CA-CB-CG	-10.00	102.60	112.60
1	I	228	ASN	CA-CB-CG	-10.00	102.60	112.60
1	O	228	ASN	CA-CB-CG	-9.97	102.63	112.60
1	C	228	ASN	CA-CB-CG	-9.97	102.63	112.60
1	A	228	ASN	CA-CB-CG	-9.96	102.64	112.60
1	G	228	ASN	CA-CB-CG	-9.95	102.65	112.60
1	M	228	ASN	CA-CB-CG	-9.95	102.65	112.60
1	Q	228	ASN	CA-CB-CG	-9.95	102.65	112.60
1	K	228	ASN	CA-CB-CG	-9.94	102.66	112.60
1	Q	339	ARG	N-CA-C	9.79	124.95	110.46
1	G	177	VAL	CB-CA-C	-9.77	100.68	111.23
1	E	177	VAL	CB-CA-C	-9.77	100.68	111.23
1	Q	177	VAL	CB-CA-C	-9.77	100.68	111.23
1	M	339	ARG	N-CA-C	9.76	124.91	110.46
1	M	177	VAL	CB-CA-C	-9.76	100.69	111.23
1	A	177	VAL	CB-CA-C	-9.75	100.70	111.23
1	K	339	ARG	N-CA-C	9.75	124.89	110.46
1	A	339	ARG	N-CA-C	9.74	124.88	110.46
1	E	339	ARG	N-CA-C	9.74	124.87	110.46
1	I	339	ARG	N-CA-C	9.73	124.87	110.46
1	O	177	VAL	CB-CA-C	-9.73	100.72	111.23
1	I	177	VAL	CB-CA-C	-9.73	100.72	111.23
1	C	177	VAL	CB-CA-C	-9.73	100.72	111.23
1	G	339	ARG	N-CA-C	9.73	124.86	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	177	VAL	CB-CA-C	-9.73	100.72	111.23
1	C	339	ARG	N-CA-C	9.72	124.84	110.46
1	O	339	ARG	N-CA-C	9.72	124.84	110.46
1	C	350	GLY	CA-C-N	-9.50	109.75	123.05
1	C	350	GLY	C-N-CA	-9.50	109.75	123.05
1	I	350	GLY	CA-C-N	-9.49	109.76	123.05
1	I	350	GLY	C-N-CA	-9.49	109.76	123.05
1	G	350	GLY	CA-C-N	-9.49	109.76	123.05
1	G	350	GLY	C-N-CA	-9.49	109.76	123.05
1	M	350	GLY	CA-C-N	-9.49	109.76	123.05
1	M	350	GLY	C-N-CA	-9.49	109.76	123.05
1	E	350	GLY	CA-C-N	-9.48	109.78	123.05
1	E	350	GLY	C-N-CA	-9.48	109.78	123.05
1	A	350	GLY	CA-C-N	-9.48	109.78	123.05
1	A	350	GLY	C-N-CA	-9.48	109.78	123.05
1	K	350	GLY	CA-C-N	-9.48	109.78	123.05
1	K	350	GLY	C-N-CA	-9.48	109.78	123.05
1	O	350	GLY	CA-C-N	-9.47	109.79	123.05
1	O	350	GLY	C-N-CA	-9.47	109.79	123.05
1	Q	350	GLY	CA-C-N	-9.45	109.82	123.05
1	Q	350	GLY	C-N-CA	-9.45	109.82	123.05
1	M	339	ARG	O-C-N	9.27	133.60	122.84
1	Q	339	ARG	O-C-N	9.27	133.60	122.84
1	O	339	ARG	O-C-N	9.27	133.59	122.84
1	E	339	ARG	O-C-N	9.26	133.59	122.84
1	A	339	ARG	O-C-N	9.25	133.57	122.84
1	G	339	ARG	O-C-N	9.25	133.57	122.84
1	C	339	ARG	O-C-N	9.23	133.55	122.84
1	K	339	ARG	O-C-N	9.22	133.53	122.84
1	I	339	ARG	O-C-N	9.22	133.53	122.84
2	J	26	ASP	CA-CB-CG	-9.04	103.56	112.60
2	D	26	ASP	CA-CB-CG	-9.02	103.58	112.60
2	L	26	ASP	CA-CB-CG	-9.02	103.58	112.60
2	R	26	ASP	CA-CB-CG	-9.02	103.58	112.60
2	F	26	ASP	CA-CB-CG	-9.02	103.58	112.60
2	P	26	ASP	CA-CB-CG	-9.02	103.58	112.60
2	B	26	ASP	CA-CB-CG	-9.01	103.59	112.60
2	H	26	ASP	CA-CB-CG	-9.01	103.59	112.60
2	N	26	ASP	CA-CB-CG	-9.00	103.60	112.60
2	H	37	HIS	CA-C-N	-8.98	114.44	122.43
2	H	37	HIS	C-N-CA	-8.98	114.44	122.43
2	F	37	HIS	CA-C-N	-8.97	114.45	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	37	HIS	C-N-CA	-8.97	114.45	122.43
2	N	37	HIS	CA-C-N	-8.96	114.46	122.43
2	N	37	HIS	C-N-CA	-8.96	114.46	122.43
2	J	37	HIS	CA-C-N	-8.95	114.46	122.43
2	J	37	HIS	C-N-CA	-8.95	114.46	122.43
2	L	37	HIS	CA-C-N	-8.95	114.46	122.43
2	L	37	HIS	C-N-CA	-8.95	114.46	122.43
2	B	37	HIS	CA-C-N	-8.95	114.47	122.43
2	B	37	HIS	C-N-CA	-8.95	114.47	122.43
2	R	37	HIS	CA-C-N	-8.94	114.47	122.43
2	R	37	HIS	C-N-CA	-8.94	114.47	122.43
2	P	37	HIS	CA-C-N	-8.93	114.48	122.43
2	P	37	HIS	C-N-CA	-8.93	114.48	122.43
2	D	37	HIS	CA-C-N	-8.91	114.50	122.43
2	D	37	HIS	C-N-CA	-8.91	114.50	122.43
2	R	249	ASN	CA-CB-CG	8.80	121.40	112.60
2	J	249	ASN	CA-CB-CG	8.77	121.37	112.60
1	G	281	ALA	CA-C-N	-8.76	108.44	120.87
1	G	281	ALA	C-N-CA	-8.76	108.44	120.87
2	N	249	ASN	CA-CB-CG	8.75	121.35	112.60
2	F	249	ASN	CA-CB-CG	8.75	121.35	112.60
2	D	249	ASN	CA-CB-CG	8.74	121.34	112.60
1	C	281	ALA	CA-C-N	-8.73	108.47	120.87
1	C	281	ALA	C-N-CA	-8.73	108.47	120.87
2	L	249	ASN	CA-CB-CG	8.73	121.33	112.60
2	B	249	ASN	CA-CB-CG	8.73	121.33	112.60
1	K	281	ALA	CA-C-N	-8.73	108.48	120.87
1	K	281	ALA	C-N-CA	-8.73	108.48	120.87
1	A	281	ALA	CA-C-N	-8.71	108.50	120.87
1	A	281	ALA	C-N-CA	-8.71	108.50	120.87
2	H	249	ASN	CA-CB-CG	8.71	121.31	112.60
1	I	281	ALA	CA-C-N	-8.71	108.51	120.87
1	I	281	ALA	C-N-CA	-8.71	108.51	120.87
2	P	249	ASN	CA-CB-CG	8.71	121.31	112.60
1	M	281	ALA	CA-C-N	-8.70	108.51	120.87
1	M	281	ALA	C-N-CA	-8.70	108.51	120.87
1	Q	281	ALA	CA-C-N	-8.69	108.53	120.87
1	Q	281	ALA	C-N-CA	-8.69	108.53	120.87
1	E	281	ALA	CA-C-N	-8.69	108.54	120.87
1	E	281	ALA	C-N-CA	-8.69	108.54	120.87
1	O	281	ALA	CA-C-N	-8.68	108.55	120.87
1	O	281	ALA	C-N-CA	-8.68	108.55	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	339	ARG	CA-C-O	8.38	132.54	121.89
1	C	339	ARG	CA-C-O	8.36	132.50	121.89
1	G	339	ARG	CA-C-O	8.35	132.49	121.89
1	A	339	ARG	CA-C-O	8.34	132.48	121.89
1	O	339	ARG	CA-C-O	8.34	132.48	121.89
2	P	436	GLN	CA-C-N	-8.34	106.69	121.70
2	P	436	GLN	C-N-CA	-8.34	106.69	121.70
1	M	339	ARG	CA-C-O	8.33	132.47	121.89
2	D	436	GLN	CA-C-N	-8.33	106.71	121.70
2	D	436	GLN	C-N-CA	-8.33	106.71	121.70
1	E	339	ARG	CA-C-O	8.33	132.47	121.89
2	F	436	GLN	CA-C-N	-8.33	106.71	121.70
2	F	436	GLN	C-N-CA	-8.33	106.71	121.70
2	J	436	GLN	CA-C-N	-8.33	106.71	121.70
2	J	436	GLN	C-N-CA	-8.33	106.71	121.70
1	K	339	ARG	CA-C-O	8.33	132.46	121.89
2	L	436	GLN	CA-C-N	-8.33	106.71	121.70
2	L	436	GLN	C-N-CA	-8.33	106.71	121.70
2	B	436	GLN	CA-C-N	-8.32	106.72	121.70
2	B	436	GLN	C-N-CA	-8.32	106.72	121.70
2	H	436	GLN	CA-C-N	-8.32	106.72	121.70
2	H	436	GLN	C-N-CA	-8.32	106.72	121.70
2	N	436	GLN	CA-C-N	-8.32	106.73	121.70
2	N	436	GLN	C-N-CA	-8.32	106.73	121.70
2	J	116	ASP	CA-CB-CG	-8.31	104.29	112.60
2	F	116	ASP	CA-CB-CG	-8.30	104.30	112.60
2	R	436	GLN	CA-C-N	-8.30	106.76	121.70
2	R	436	GLN	C-N-CA	-8.30	106.76	121.70
2	P	116	ASP	CA-CB-CG	-8.30	104.30	112.60
1	Q	339	ARG	CA-C-O	8.30	132.43	121.89
2	H	116	ASP	CA-CB-CG	-8.29	104.31	112.60
2	B	116	ASP	CA-CB-CG	-8.28	104.32	112.60
2	R	116	ASP	CA-CB-CG	-8.28	104.32	112.60
2	N	116	ASP	CA-CB-CG	-8.28	104.33	112.60
2	D	116	ASP	CA-CB-CG	-8.26	104.34	112.60
2	L	116	ASP	CA-CB-CG	-8.25	104.35	112.60
2	J	88	ARG	NE-CZ-NH1	8.18	129.68	121.50
2	F	88	ARG	NE-CZ-NH1	8.17	129.67	121.50
2	D	88	ARG	NE-CZ-NH1	8.16	129.66	121.50
2	B	88	ARG	NE-CZ-NH1	8.14	129.64	121.50
2	R	88	ARG	NE-CZ-NH1	8.13	129.63	121.50
2	H	88	ARG	NE-CZ-NH1	8.13	129.63	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	88	ARG	NE-CZ-NH1	8.12	129.62	121.50
2	N	88	ARG	NE-CZ-NH1	8.10	129.60	121.50
2	J	197	ASN	N-CA-C	8.10	122.88	112.92
2	L	88	ARG	NE-CZ-NH1	8.09	129.59	121.50
2	N	197	ASN	N-CA-C	8.09	122.87	112.92
2	R	197	ASN	N-CA-C	8.09	122.86	112.92
2	B	197	ASN	N-CA-C	8.08	122.86	112.92
2	H	197	ASN	N-CA-C	8.08	122.86	112.92
2	D	197	ASN	N-CA-C	8.07	122.85	112.92
2	P	197	ASN	N-CA-C	8.07	122.84	112.92
2	F	197	ASN	N-CA-C	8.06	122.84	112.92
2	L	197	ASN	N-CA-C	8.06	122.83	112.92
2	J	249	ASN	N-CA-C	7.99	121.00	111.02
2	N	249	ASN	N-CA-C	7.97	120.98	111.02
2	R	249	ASN	N-CA-C	7.97	120.98	111.02
2	L	249	ASN	N-CA-C	7.96	120.98	111.02
2	B	249	ASN	N-CA-C	7.95	120.96	111.02
2	F	249	ASN	N-CA-C	7.95	120.96	111.02
2	H	249	ASN	N-CA-C	7.94	120.95	111.02
2	D	249	ASN	N-CA-C	7.94	120.94	111.02
2	P	249	ASN	N-CA-C	7.93	120.93	111.02
1	K	264	ARG	N-CA-C	7.83	122.83	113.28
1	E	264	ARG	N-CA-C	7.82	122.82	113.28
1	C	264	ARG	N-CA-C	7.81	122.81	113.28
1	O	264	ARG	N-CA-C	7.80	122.80	113.28
1	A	264	ARG	N-CA-C	7.80	122.80	113.28
1	I	264	ARG	N-CA-C	7.79	122.79	113.28
1	G	264	ARG	N-CA-C	7.79	122.78	113.28
1	Q	264	ARG	N-CA-C	7.78	122.77	113.28
1	M	264	ARG	N-CA-C	7.78	122.77	113.28
1	M	28	HIS	CA-CB-CG	-7.73	106.07	113.80
1	O	28	HIS	CA-CB-CG	-7.70	106.10	113.80
1	K	28	HIS	CA-CB-CG	-7.69	106.11	113.80
1	I	28	HIS	CA-CB-CG	-7.68	106.12	113.80
1	A	28	HIS	CA-CB-CG	-7.68	106.12	113.80
1	C	28	HIS	CA-CB-CG	-7.68	106.12	113.80
1	G	28	HIS	CA-CB-CG	-7.67	106.13	113.80
1	Q	28	HIS	CA-CB-CG	-7.65	106.15	113.80
1	E	28	HIS	CA-CB-CG	-7.65	106.15	113.80
1	E	177	VAL	CA-C-N	-7.64	111.08	122.39
1	E	177	VAL	C-N-CA	-7.64	111.08	122.39
1	M	177	VAL	CA-C-N	-7.64	111.08	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	177	VAL	C-N-CA	-7.64	111.08	122.39
1	I	177	VAL	CA-C-N	-7.63	111.09	122.39
1	I	177	VAL	C-N-CA	-7.63	111.09	122.39
1	O	177	VAL	CA-C-N	-7.63	111.10	122.39
1	O	177	VAL	C-N-CA	-7.63	111.10	122.39
1	K	177	VAL	CA-C-N	-7.61	111.12	122.39
1	K	177	VAL	C-N-CA	-7.61	111.12	122.39
1	A	177	VAL	CA-C-N	-7.60	111.14	122.39
1	A	177	VAL	C-N-CA	-7.60	111.14	122.39
1	G	177	VAL	CA-C-N	-7.60	111.14	122.39
1	G	177	VAL	C-N-CA	-7.60	111.14	122.39
1	C	177	VAL	CA-C-N	-7.60	111.15	122.39
1	C	177	VAL	C-N-CA	-7.60	111.15	122.39
1	Q	177	VAL	CA-C-N	-7.58	111.17	122.39
1	Q	177	VAL	C-N-CA	-7.58	111.17	122.39
2	H	172	VAL	N-CA-C	7.47	115.30	107.76
2	H	69	ASP	CA-CB-CG	7.45	120.05	112.60
2	F	172	VAL	N-CA-C	7.44	115.28	107.76
2	J	172	VAL	N-CA-C	7.44	115.28	107.76
2	L	172	VAL	N-CA-C	7.44	115.28	107.76
2	N	172	VAL	N-CA-C	7.43	115.27	107.76
2	P	172	VAL	N-CA-C	7.42	115.26	107.76
2	B	172	VAL	N-CA-C	7.42	115.25	107.76
2	D	172	VAL	N-CA-C	7.42	115.25	107.76
2	H	424	ASN	CA-CB-CG	-7.42	105.18	112.60
1	K	402	ARG	NE-CZ-NH2	7.42	125.88	119.20
2	L	424	ASN	CA-CB-CG	-7.41	105.19	112.60
2	R	172	VAL	N-CA-C	7.41	115.25	107.76
2	F	69	ASP	CA-CB-CG	7.41	120.01	112.60
2	N	69	ASP	CA-CB-CG	7.40	120.00	112.60
2	D	424	ASN	CA-CB-CG	-7.40	105.20	112.60
2	F	424	ASN	CA-CB-CG	-7.40	105.20	112.60
1	I	402	ARG	NE-CZ-NH2	7.40	125.86	119.20
2	N	424	ASN	CA-CB-CG	-7.40	105.20	112.60
2	B	424	ASN	CA-CB-CG	-7.39	105.21	112.60
2	J	424	ASN	CA-CB-CG	-7.39	105.21	112.60
1	M	402	ARG	NE-CZ-NH2	7.39	125.85	119.20
2	P	69	ASP	CA-CB-CG	7.38	119.98	112.60
2	R	424	ASN	CA-CB-CG	-7.38	105.22	112.60
1	Q	402	ARG	NE-CZ-NH2	7.38	125.84	119.20
1	O	402	ARG	NE-CZ-NH2	7.38	125.84	119.20
1	E	402	ARG	NE-CZ-NH2	7.38	125.84	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	69	ASP	CA-CB-CG	7.37	119.97	112.60
1	A	402	ARG	NE-CZ-NH2	7.37	125.83	119.20
1	G	402	ARG	NE-CZ-NH2	7.37	125.83	119.20
2	R	69	ASP	CA-CB-CG	7.37	119.97	112.60
2	P	424	ASN	CA-CB-CG	-7.36	105.24	112.60
2	L	69	ASP	CA-CB-CG	7.36	119.96	112.60
2	D	69	ASP	CA-CB-CG	7.35	119.95	112.60
1	C	402	ARG	NE-CZ-NH2	7.34	125.80	119.20
2	J	69	ASP	CA-CB-CG	7.33	119.93	112.60
2	P	348	PRO	N-CA-C	-7.25	99.80	111.19
2	R	348	PRO	N-CA-C	-7.25	99.81	111.19
2	B	348	PRO	N-CA-C	-7.24	99.82	111.19
2	J	348	PRO	N-CA-C	-7.24	99.82	111.19
2	L	348	PRO	N-CA-C	-7.24	99.82	111.19
2	N	348	PRO	N-CA-C	-7.24	99.82	111.19
2	H	348	PRO	N-CA-C	-7.23	99.83	111.19
2	D	348	PRO	N-CA-C	-7.23	99.83	111.19
2	F	348	PRO	N-CA-C	-7.22	99.85	111.19
1	O	282	TYR	N-CA-C	-7.21	99.60	110.28
1	I	282	TYR	N-CA-C	-7.21	99.61	110.28
1	Q	348	PRO	CA-C-N	-7.21	111.73	122.39
1	Q	348	PRO	C-N-CA	-7.21	111.73	122.39
2	R	401	ARG	NE-CZ-NH1	7.20	128.70	121.50
1	G	348	PRO	CA-C-N	-7.20	111.74	122.39
1	G	348	PRO	C-N-CA	-7.20	111.74	122.39
1	C	282	TYR	N-CA-C	-7.20	99.63	110.28
1	I	348	PRO	CA-C-N	-7.20	111.74	122.39
1	I	348	PRO	C-N-CA	-7.20	111.74	122.39
1	M	348	PRO	CA-C-N	-7.19	111.75	122.39
1	M	348	PRO	C-N-CA	-7.19	111.75	122.39
1	G	282	TYR	N-CA-C	-7.19	99.64	110.28
1	A	348	PRO	CA-C-N	-7.19	111.75	122.39
1	A	348	PRO	C-N-CA	-7.19	111.75	122.39
2	D	401	ARG	NE-CZ-NH1	7.19	128.69	121.50
1	O	348	PRO	CA-C-N	-7.19	111.75	122.39
1	O	348	PRO	C-N-CA	-7.19	111.75	122.39
2	H	401	ARG	NE-CZ-NH1	7.19	128.69	121.50
1	K	282	TYR	N-CA-C	-7.18	99.65	110.28
1	M	282	TYR	N-CA-C	-7.18	99.65	110.28
1	A	282	TYR	N-CA-C	-7.18	99.65	110.28
1	K	348	PRO	CA-C-N	-7.18	111.77	122.39
1	K	348	PRO	C-N-CA	-7.18	111.77	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	401	ARG	NE-CZ-NH1	7.17	128.68	121.50
1	C	348	PRO	CA-C-N	-7.17	111.78	122.39
1	C	348	PRO	C-N-CA	-7.17	111.78	122.39
1	E	282	TYR	N-CA-C	-7.17	99.67	110.28
1	E	348	PRO	CA-C-N	-7.17	111.78	122.39
1	E	348	PRO	C-N-CA	-7.17	111.78	122.39
2	N	401	ARG	NE-CZ-NH1	7.16	128.66	121.50
1	Q	282	TYR	N-CA-C	-7.16	99.69	110.28
2	B	401	ARG	NE-CZ-NH1	7.15	128.65	121.50
2	L	401	ARG	NE-CZ-NH1	7.13	128.63	121.50
2	J	401	ARG	NE-CZ-NH1	7.11	128.61	121.50
2	F	401	ARG	NE-CZ-NH1	7.11	128.61	121.50
1	O	105	ARG	NE-CZ-NH2	-7.11	112.81	119.20
1	C	105	ARG	NE-CZ-NH2	-7.09	112.81	119.20
1	G	105	ARG	NE-CZ-NH2	-7.07	112.83	119.20
1	A	105	ARG	NE-CZ-NH2	-7.06	112.84	119.20
1	K	105	ARG	NE-CZ-NH2	-7.06	112.84	119.20
1	E	105	ARG	NE-CZ-NH2	-7.05	112.85	119.20
1	Q	105	ARG	NE-CZ-NH2	-7.05	112.85	119.20
1	I	105	ARG	NE-CZ-NH2	-7.04	112.87	119.20
1	M	105	ARG	NE-CZ-NH2	-7.03	112.88	119.20
2	N	120	ASP	CA-CB-CG	-7.01	105.58	112.60
2	R	120	ASP	CA-CB-CG	-7.01	105.59	112.60
2	J	120	ASP	CA-CB-CG	-7.01	105.59	112.60
2	D	120	ASP	CA-CB-CG	-7.00	105.60	112.60
2	H	120	ASP	CA-CB-CG	-7.00	105.60	112.60
1	E	61	HIS	CA-CB-CG	-6.99	106.81	113.80
2	P	120	ASP	CA-CB-CG	-6.99	105.61	112.60
2	B	120	ASP	CA-CB-CG	-6.99	105.61	112.60
2	F	120	ASP	CA-CB-CG	-6.98	105.62	112.60
2	L	120	ASP	CA-CB-CG	-6.98	105.62	112.60
2	R	358	ILE	N-CA-C	6.97	115.67	107.73
1	Q	61	HIS	CA-CB-CG	-6.97	106.83	113.80
1	G	61	HIS	CA-CB-CG	-6.97	106.83	113.80
2	J	358	ILE	N-CA-C	6.97	115.67	107.73
2	P	358	ILE	N-CA-C	6.96	115.67	107.73
2	F	358	ILE	N-CA-C	6.95	115.66	107.73
2	L	358	ILE	N-CA-C	6.95	115.65	107.73
1	A	61	HIS	CA-CB-CG	-6.94	106.86	113.80
1	I	61	HIS	CA-CB-CG	-6.94	106.86	113.80
2	B	358	ILE	N-CA-C	6.94	115.64	107.73
2	N	358	ILE	N-CA-C	6.93	115.63	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	358	ILE	N-CA-C	6.93	115.63	107.73
1	M	37	PRO	CA-C-N	-6.92	109.23	121.70
1	M	37	PRO	C-N-CA	-6.92	109.23	121.70
1	M	61	HIS	CA-CB-CG	-6.92	106.88	113.80
2	H	358	ILE	N-CA-C	6.92	115.61	107.73
1	C	37	PRO	CA-C-N	-6.91	109.25	121.70
1	C	37	PRO	C-N-CA	-6.91	109.25	121.70
1	C	61	HIS	CA-CB-CG	-6.91	106.89	113.80
1	E	37	PRO	CA-C-N	-6.91	109.26	121.70
1	E	37	PRO	C-N-CA	-6.91	109.26	121.70
1	K	61	HIS	CA-CB-CG	-6.91	106.89	113.80
1	Q	37	PRO	CA-C-N	-6.91	109.27	121.70
1	Q	37	PRO	C-N-CA	-6.91	109.27	121.70
1	A	37	PRO	CA-C-N	-6.90	109.27	121.70
1	A	37	PRO	C-N-CA	-6.90	109.27	121.70
1	G	37	PRO	CA-C-N	-6.90	109.28	121.70
1	G	37	PRO	C-N-CA	-6.90	109.28	121.70
1	K	37	PRO	CA-C-N	-6.89	109.29	121.70
1	K	37	PRO	C-N-CA	-6.89	109.29	121.70
1	O	61	HIS	CA-CB-CG	-6.89	106.91	113.80
1	I	37	PRO	CA-C-N	-6.89	109.30	121.70
1	I	37	PRO	C-N-CA	-6.89	109.30	121.70
1	O	37	PRO	CA-C-N	-6.87	109.33	121.70
1	O	37	PRO	C-N-CA	-6.87	109.33	121.70
1	K	284	GLU	CA-C-N	-6.84	113.35	123.00
1	K	284	GLU	C-N-CA	-6.84	113.35	123.00
1	M	284	GLU	CA-C-N	-6.84	113.35	123.00
1	M	284	GLU	C-N-CA	-6.84	113.35	123.00
1	Q	284	GLU	CA-C-N	-6.84	113.36	123.00
1	Q	284	GLU	C-N-CA	-6.84	113.36	123.00
1	G	284	GLU	CA-C-N	-6.83	113.38	123.00
1	G	284	GLU	C-N-CA	-6.83	113.38	123.00
1	I	284	GLU	CA-C-N	-6.82	113.39	123.00
1	I	284	GLU	C-N-CA	-6.82	113.39	123.00
1	O	177	VAL	N-CA-C	6.82	118.28	107.98
1	E	284	GLU	CA-C-N	-6.81	113.39	123.00
1	E	284	GLU	C-N-CA	-6.81	113.39	123.00
1	A	284	GLU	CA-C-N	-6.81	113.40	123.00
1	A	284	GLU	C-N-CA	-6.81	113.40	123.00
1	I	177	VAL	N-CA-C	6.81	118.26	107.98
1	A	177	VAL	N-CA-C	6.80	118.25	107.98
1	C	284	GLU	CA-C-N	-6.80	113.41	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	284	GLU	C-N-CA	-6.80	113.41	123.00
1	K	177	VAL	N-CA-C	6.80	118.25	107.98
1	E	177	VAL	N-CA-C	6.80	118.25	107.98
1	G	177	VAL	N-CA-C	6.80	118.24	107.98
1	O	284	GLU	CA-C-N	-6.79	113.43	123.00
1	O	284	GLU	C-N-CA	-6.79	113.43	123.00
1	M	177	VAL	N-CA-C	6.78	118.22	107.98
1	C	177	VAL	N-CA-C	6.78	118.22	107.98
1	Q	177	VAL	N-CA-C	6.78	118.22	107.98
2	N	401	ARG	NE-CZ-NH2	-6.71	113.16	119.20
2	R	249	ASN	CB-CG-ND2	6.70	126.44	116.40
2	D	401	ARG	NE-CZ-NH2	-6.68	113.19	119.20
2	H	249	ASN	CB-CG-ND2	6.68	126.42	116.40
2	J	249	ASN	CB-CG-ND2	6.68	126.42	116.40
2	B	249	ASN	CB-CG-ND2	6.67	126.41	116.40
2	F	249	ASN	CB-CG-ND2	6.67	126.41	116.40
2	L	249	ASN	CB-CG-ND2	6.67	126.41	116.40
2	N	249	ASN	CB-CG-ND2	6.67	126.40	116.40
2	D	249	ASN	CB-CG-ND2	6.67	126.40	116.40
2	P	249	ASN	CB-CG-ND2	6.67	126.40	116.40
2	H	401	ARG	NE-CZ-NH2	-6.66	113.20	119.20
2	J	401	ARG	NE-CZ-NH2	-6.66	113.21	119.20
2	R	401	ARG	NE-CZ-NH2	-6.65	113.21	119.20
2	B	401	ARG	NE-CZ-NH2	-6.64	113.22	119.20
1	G	50	ASN	CA-C-N	-6.63	109.99	121.66
1	G	50	ASN	C-N-CA	-6.63	109.99	121.66
1	M	50	ASN	CA-C-N	-6.62	110.01	121.66
1	M	50	ASN	C-N-CA	-6.62	110.01	121.66
1	E	50	ASN	CA-C-N	-6.61	110.02	121.66
1	E	50	ASN	C-N-CA	-6.61	110.02	121.66
1	K	50	ASN	CA-C-N	-6.61	110.02	121.66
1	K	50	ASN	C-N-CA	-6.61	110.02	121.66
2	F	401	ARG	NE-CZ-NH2	-6.61	113.25	119.20
1	A	50	ASN	CA-C-N	-6.61	110.03	121.66
1	A	50	ASN	C-N-CA	-6.61	110.03	121.66
1	I	50	ASN	CA-C-N	-6.61	110.03	121.66
1	I	50	ASN	C-N-CA	-6.61	110.03	121.66
1	Q	50	ASN	CA-C-N	-6.60	110.04	121.66
1	Q	50	ASN	C-N-CA	-6.60	110.04	121.66
2	L	401	ARG	NE-CZ-NH2	-6.60	113.26	119.20
2	P	401	ARG	NE-CZ-NH2	-6.59	113.27	119.20
1	C	50	ASN	CA-C-N	-6.58	110.07	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	50	ASN	C-N-CA	-6.58	110.07	121.66
1	O	50	ASN	CA-C-N	-6.57	110.09	121.66
1	O	50	ASN	C-N-CA	-6.57	110.09	121.66
1	Q	244	PHE	CA-C-N	-6.56	112.88	122.65
1	Q	244	PHE	C-N-CA	-6.56	112.88	122.65
1	I	244	PHE	CA-C-N	-6.55	112.89	122.65
1	I	244	PHE	C-N-CA	-6.55	112.89	122.65
1	E	244	PHE	CA-C-N	-6.54	112.91	122.65
1	E	244	PHE	C-N-CA	-6.54	112.91	122.65
1	C	244	PHE	CA-C-N	-6.53	112.92	122.65
1	C	244	PHE	C-N-CA	-6.53	112.92	122.65
1	O	244	PHE	CA-C-N	-6.53	112.93	122.65
1	O	244	PHE	C-N-CA	-6.53	112.93	122.65
1	A	244	PHE	CA-C-N	-6.52	112.93	122.65
1	A	244	PHE	C-N-CA	-6.52	112.93	122.65
1	G	244	PHE	CA-C-N	-6.52	112.94	122.65
1	G	244	PHE	C-N-CA	-6.52	112.94	122.65
1	M	244	PHE	CA-C-N	-6.52	112.94	122.65
1	M	244	PHE	C-N-CA	-6.52	112.94	122.65
2	F	322	ARG	N-CA-C	6.51	120.21	108.17
1	K	244	PHE	CA-C-N	-6.50	112.96	122.65
1	K	244	PHE	C-N-CA	-6.50	112.96	122.65
2	D	322	ARG	N-CA-C	6.49	120.18	108.17
2	P	322	ARG	N-CA-C	6.49	120.17	108.17
2	B	322	ARG	N-CA-C	6.48	120.17	108.17
2	N	322	ARG	N-CA-C	6.47	120.14	108.17
2	H	322	ARG	N-CA-C	6.47	120.14	108.17
2	J	322	ARG	N-CA-C	6.46	120.13	108.17
2	R	322	ARG	N-CA-C	6.46	120.13	108.17
2	L	322	ARG	N-CA-C	6.46	120.11	108.17
2	H	14	ASN	CA-CB-CG	-6.42	106.18	112.60
2	F	14	ASN	CA-CB-CG	-6.42	106.19	112.60
2	F	96	GLN	N-CA-C	6.41	121.35	109.56
2	J	14	ASN	CA-CB-CG	-6.41	106.19	112.60
2	N	96	GLN	N-CA-C	6.40	121.34	109.56
2	J	96	GLN	N-CA-C	6.40	121.33	109.56
2	N	249	ASN	CA-C-N	-6.40	109.64	120.58
2	N	249	ASN	C-N-CA	-6.40	109.64	120.58
2	R	96	GLN	N-CA-C	6.40	121.33	109.56
2	L	14	ASN	CA-CB-CG	-6.39	106.21	112.60
2	L	249	ASN	CA-C-N	-6.39	109.65	120.58
2	L	249	ASN	C-N-CA	-6.39	109.65	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	GLN	N-CA-C	6.39	121.32	109.56
2	L	96	GLN	N-CA-C	6.39	121.31	109.56
2	F	249	ASN	CA-C-N	-6.38	109.67	120.58
2	F	249	ASN	C-N-CA	-6.38	109.67	120.58
2	B	14	ASN	CA-CB-CG	-6.38	106.22	112.60
1	G	283	HIS	N-CA-C	6.38	120.37	112.58
2	P	96	GLN	N-CA-C	6.38	121.30	109.56
2	D	249	ASN	CA-C-N	-6.38	109.67	120.58
2	D	249	ASN	C-N-CA	-6.38	109.67	120.58
2	H	96	GLN	N-CA-C	6.38	121.30	109.56
2	R	249	ASN	CA-C-N	-6.38	109.67	120.58
2	R	249	ASN	C-N-CA	-6.38	109.67	120.58
2	H	249	ASN	CA-C-N	-6.38	109.68	120.58
2	H	249	ASN	C-N-CA	-6.38	109.68	120.58
2	D	96	GLN	N-CA-C	6.38	121.29	109.56
2	B	249	ASN	CA-C-N	-6.37	109.69	120.58
2	B	249	ASN	C-N-CA	-6.37	109.69	120.58
2	P	249	ASN	CA-C-N	-6.37	109.69	120.58
2	P	249	ASN	C-N-CA	-6.37	109.69	120.58
2	P	14	ASN	CA-CB-CG	-6.37	106.23	112.60
2	R	14	ASN	CA-CB-CG	-6.36	106.24	112.60
2	J	249	ASN	CA-C-N	-6.36	109.71	120.58
2	J	249	ASN	C-N-CA	-6.36	109.71	120.58
1	K	283	HIS	N-CA-C	6.36	120.34	112.58
2	N	14	ASN	CA-CB-CG	-6.36	106.24	112.60
2	D	14	ASN	CA-CB-CG	-6.36	106.24	112.60
1	E	283	HIS	N-CA-C	6.36	120.33	112.58
1	A	283	HIS	N-CA-C	6.34	120.32	112.58
1	Q	283	HIS	N-CA-C	6.34	120.32	112.58
1	K	109	THR	N-CA-C	6.34	119.00	111.33
1	M	109	THR	N-CA-C	6.33	119.00	111.33
1	I	109	THR	N-CA-C	6.33	118.98	111.33
1	I	283	HIS	N-CA-C	6.33	120.30	112.58
1	C	283	HIS	N-CA-C	6.32	120.29	112.58
1	O	283	HIS	N-CA-C	6.32	120.29	112.58
1	M	283	HIS	N-CA-C	6.31	120.28	112.58
1	C	109	THR	N-CA-C	6.31	118.97	111.33
1	A	109	THR	N-CA-C	6.31	118.97	111.33
1	Q	109	THR	N-CA-C	6.30	118.96	111.33
1	O	109	THR	N-CA-C	6.30	118.95	111.33
2	N	166	MET	CA-C-N	-6.30	112.70	122.59
2	N	166	MET	C-N-CA	-6.30	112.70	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	109	THR	N-CA-C	6.29	118.95	111.33
2	J	166	MET	CA-C-N	-6.29	112.71	122.59
2	J	166	MET	C-N-CA	-6.29	112.71	122.59
2	R	166	MET	CA-C-N	-6.29	112.72	122.59
2	R	166	MET	C-N-CA	-6.29	112.72	122.59
1	E	283	HIS	CB-CA-C	-6.28	101.66	111.39
1	E	109	THR	N-CA-C	6.28	118.93	111.33
1	M	375	VAL	N-CA-C	6.28	117.16	108.12
1	C	50	ASN	N-CA-C	6.27	120.61	113.15
1	E	176	GLN	CA-C-N	-6.26	113.11	122.01
1	E	176	GLN	C-N-CA	-6.26	113.11	122.01
1	C	283	HIS	CB-CA-C	-6.26	101.68	111.39
1	M	50	ASN	N-CA-C	6.26	120.60	113.15
1	A	283	HIS	CB-CA-C	-6.26	101.69	111.39
1	K	50	ASN	N-CA-C	6.26	120.60	113.15
1	O	50	ASN	N-CA-C	6.26	120.60	113.15
1	A	50	ASN	N-CA-C	6.26	120.60	113.15
2	B	166	MET	CA-C-N	-6.26	112.77	122.59
2	B	166	MET	C-N-CA	-6.26	112.77	122.59
1	C	375	VAL	N-CA-C	6.26	117.13	108.12
1	G	375	VAL	N-CA-C	6.26	117.13	108.12
1	M	283	HIS	CB-CA-C	-6.26	101.69	111.39
1	G	50	ASN	N-CA-C	6.25	120.59	113.15
1	K	283	HIS	CB-CA-C	-6.25	101.70	111.39
2	P	166	MET	CA-C-N	-6.25	112.77	122.59
2	P	166	MET	C-N-CA	-6.25	112.77	122.59
2	L	166	MET	CA-C-N	-6.25	112.78	122.59
2	L	166	MET	C-N-CA	-6.25	112.78	122.59
1	M	176	GLN	CA-C-N	-6.25	113.13	122.01
1	M	176	GLN	C-N-CA	-6.25	113.13	122.01
1	Q	50	ASN	N-CA-C	6.25	120.59	113.15
1	E	50	ASN	N-CA-C	6.25	120.59	113.15
1	Q	176	GLN	CA-C-N	-6.25	113.14	122.01
1	Q	176	GLN	C-N-CA	-6.25	113.14	122.01
1	G	283	HIS	CB-CA-C	-6.25	101.71	111.39
1	O	375	VAL	N-CA-C	6.25	117.11	108.12
2	F	166	MET	CA-C-N	-6.25	112.79	122.59
2	F	166	MET	C-N-CA	-6.25	112.79	122.59
1	A	375	VAL	N-CA-C	6.24	117.11	108.12
1	I	375	VAL	N-CA-C	6.24	117.11	108.12
1	O	283	HIS	CB-CA-C	-6.24	101.71	111.39
1	I	50	ASN	N-CA-C	6.24	120.58	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	166	MET	CA-C-N	-6.24	112.79	122.59
2	D	166	MET	C-N-CA	-6.24	112.79	122.59
2	P	53	TYR	N-CA-C	6.24	119.36	109.50
1	Q	283	HIS	CB-CA-C	-6.24	101.72	111.39
1	Q	375	VAL	N-CA-C	6.24	117.11	108.12
2	R	53	TYR	N-CA-C	6.24	119.36	109.50
1	G	176	GLN	CA-C-N	-6.24	113.15	122.01
1	G	176	GLN	C-N-CA	-6.24	113.15	122.01
2	L	53	TYR	N-CA-C	6.24	119.36	109.50
2	F	53	TYR	N-CA-C	6.23	119.35	109.50
1	A	176	GLN	CA-C-N	-6.23	113.16	122.01
1	A	176	GLN	C-N-CA	-6.23	113.16	122.01
1	K	176	GLN	CA-C-N	-6.23	113.16	122.01
1	K	176	GLN	C-N-CA	-6.23	113.16	122.01
1	K	375	VAL	N-CA-C	6.23	117.10	108.12
1	O	176	GLN	CA-C-N	-6.23	113.16	122.01
1	O	176	GLN	C-N-CA	-6.23	113.16	122.01
2	D	53	TYR	N-CA-C	6.23	119.34	109.50
2	B	53	TYR	N-CA-C	6.23	119.34	109.50
2	H	166	MET	CA-C-N	-6.23	112.81	122.59
2	H	166	MET	C-N-CA	-6.23	112.81	122.59
2	N	53	TYR	N-CA-C	6.22	119.34	109.50
1	C	176	GLN	CA-C-N	-6.22	113.17	122.01
1	C	176	GLN	C-N-CA	-6.22	113.17	122.01
1	I	283	HIS	CB-CA-C	-6.22	101.75	111.39
1	I	176	GLN	CA-C-N	-6.22	113.18	122.01
1	I	176	GLN	C-N-CA	-6.22	113.18	122.01
2	J	53	TYR	N-CA-C	6.22	119.32	109.50
1	E	375	VAL	N-CA-C	6.21	117.06	108.12
2	H	53	TYR	N-CA-C	6.20	119.30	109.50
1	C	228	ASN	OD1-CG-ND2	6.17	128.77	122.60
1	I	337	THR	N-CA-C	6.17	120.98	112.90
1	M	37	PRO	CA-N-CD	6.16	120.62	112.00
1	K	337	THR	N-CA-C	6.15	120.96	112.90
2	D	83	PHE	CB-CA-C	6.15	119.33	110.04
2	R	83	PHE	CB-CA-C	6.15	119.33	110.04
1	O	337	THR	N-CA-C	6.14	120.94	112.90
1	E	337	THR	N-CA-C	6.13	120.94	112.90
1	Q	337	THR	N-CA-C	6.13	120.93	112.90
2	J	83	PHE	CB-CA-C	6.13	119.30	110.04
2	N	83	PHE	CB-CA-C	6.13	119.30	110.04
1	A	337	THR	N-CA-C	6.13	120.92	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	337	THR	N-CA-C	6.13	120.93	112.90
1	Q	228	ASN	OD1-CG-ND2	6.12	128.72	122.60
2	B	83	PHE	CB-CA-C	6.12	119.28	110.04
1	E	228	ASN	OD1-CG-ND2	6.12	128.72	122.60
1	O	228	ASN	OD1-CG-ND2	6.12	128.72	122.60
1	A	37	PRO	CA-N-CD	6.12	120.57	112.00
1	E	37	PRO	CA-N-CD	6.12	120.57	112.00
2	F	83	PHE	CB-CA-C	6.12	119.28	110.04
1	Q	37	PRO	CA-N-CD	6.12	120.57	112.00
1	A	228	ASN	OD1-CG-ND2	6.11	128.71	122.60
1	M	337	THR	N-CA-C	6.11	120.91	112.90
1	G	37	PRO	CA-N-CD	6.11	120.55	112.00
1	K	37	PRO	CA-N-CD	6.11	120.55	112.00
2	P	83	PHE	CB-CA-C	6.11	119.26	110.04
1	C	37	PRO	CA-N-CD	6.10	120.54	112.00
1	I	37	PRO	CA-N-CD	6.10	120.54	112.00
1	O	37	PRO	CA-N-CD	6.10	120.54	112.00
1	I	228	ASN	OD1-CG-ND2	6.10	128.70	122.60
2	L	83	PHE	CB-CA-C	6.10	119.25	110.04
2	H	83	PHE	CB-CA-C	6.10	119.25	110.04
1	C	337	THR	N-CA-C	6.09	120.88	112.90
1	K	379	SER	N-CA-C	6.08	119.15	108.75
1	C	379	SER	N-CA-C	6.08	119.14	108.75
1	K	228	ASN	OD1-CG-ND2	6.08	128.68	122.60
1	G	282	TYR	O-C-N	6.07	130.30	122.89
1	G	379	SER	N-CA-C	6.07	119.13	108.75
1	K	282	TYR	O-C-N	6.07	130.30	122.89
1	E	379	SER	N-CA-C	6.07	119.13	108.75
1	M	228	ASN	OD1-CG-ND2	6.07	128.67	122.60
1	G	228	ASN	OD1-CG-ND2	6.07	128.67	122.60
2	H	28	HIS	CA-CB-CG	-6.07	107.73	113.80
1	I	379	SER	N-CA-C	6.07	119.12	108.75
1	M	379	SER	N-CA-C	6.07	119.13	108.75
1	O	379	SER	N-CA-C	6.07	119.12	108.75
1	Q	379	SER	N-CA-C	6.07	119.13	108.75
1	A	379	SER	N-CA-C	6.07	119.12	108.75
2	F	28	HIS	CA-CB-CG	-6.07	107.73	113.80
1	E	282	TYR	O-C-N	6.06	130.29	122.89
1	G	37	PRO	N-CA-C	6.06	123.66	112.33
2	P	28	HIS	CA-CB-CG	-6.06	107.74	113.80
1	O	142	GLY	CA-C-N	-6.06	113.60	121.96
1	O	142	GLY	C-N-CA	-6.06	113.60	121.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	142	GLY	CA-C-N	-6.05	113.61	121.96
1	K	142	GLY	C-N-CA	-6.05	113.61	121.96
2	R	28	HIS	CA-CB-CG	-6.05	107.75	113.80
1	K	37	PRO	N-CA-C	6.05	123.65	112.33
2	N	28	HIS	CA-CB-CG	-6.05	107.75	113.80
1	M	142	GLY	CA-C-N	-6.05	113.61	121.96
1	M	142	GLY	C-N-CA	-6.05	113.61	121.96
1	Q	282	TYR	O-C-N	6.05	130.27	122.89
1	M	37	PRO	N-CA-C	6.05	123.64	112.33
1	E	37	PRO	N-CA-C	6.04	123.63	112.33
1	G	142	GLY	CA-C-N	-6.04	113.62	121.96
1	G	142	GLY	C-N-CA	-6.04	113.62	121.96
1	Q	37	PRO	N-CA-C	6.04	123.63	112.33
2	B	28	HIS	CA-CB-CG	-6.04	107.76	113.80
1	A	37	PRO	N-CA-C	6.04	123.62	112.33
1	C	142	GLY	CA-C-N	-6.04	113.63	121.96
1	C	142	GLY	C-N-CA	-6.04	113.63	121.96
1	I	37	PRO	N-CA-C	6.04	123.62	112.33
1	A	142	GLY	CA-C-N	-6.03	113.64	121.96
1	A	142	GLY	C-N-CA	-6.03	113.64	121.96
2	D	28	HIS	CA-CB-CG	-6.03	107.77	113.80
1	Q	161	TYR	CA-CB-CG	-6.03	103.04	113.90
1	C	37	PRO	N-CA-C	6.03	123.61	112.33
1	C	161	TYR	CA-CB-CG	-6.03	103.05	113.90
1	C	282	TYR	O-C-N	6.03	130.25	122.89
1	O	37	PRO	N-CA-C	6.03	123.61	112.33
1	Q	142	GLY	CA-C-N	-6.03	113.64	121.96
1	Q	142	GLY	C-N-CA	-6.03	113.64	121.96
1	M	282	TYR	O-C-N	6.03	130.25	122.89
1	G	161	TYR	CA-CB-CG	-6.03	103.05	113.90
1	I	161	TYR	CA-CB-CG	-6.03	103.05	113.90
1	M	161	TYR	CA-CB-CG	-6.03	103.06	113.90
1	A	282	TYR	O-C-N	6.02	130.24	122.89
1	E	161	TYR	CA-CB-CG	-6.02	103.06	113.90
1	A	161	TYR	CA-CB-CG	-6.02	103.06	113.90
1	E	142	GLY	CA-C-N	-6.02	113.66	121.96
1	E	142	GLY	C-N-CA	-6.02	113.66	121.96
1	I	282	TYR	O-C-N	6.02	130.23	122.89
1	O	161	TYR	CA-CB-CG	-6.02	103.07	113.90
1	I	142	GLY	CA-C-N	-6.02	113.66	121.96
1	I	142	GLY	C-N-CA	-6.02	113.66	121.96
2	L	28	HIS	CA-CB-CG	-6.01	107.79	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	28	HIS	CA-CB-CG	-6.00	107.80	113.80
1	O	282	TYR	O-C-N	6.00	130.21	122.89
1	K	161	TYR	CA-CB-CG	-6.00	103.11	113.90
1	I	327	ASP	CA-CB-CG	-5.98	106.62	112.60
2	F	71	GLU	CA-C-N	5.97	126.13	119.32
2	F	71	GLU	C-N-CA	5.97	126.13	119.32
1	C	61	HIS	CA-C-N	-5.96	118.14	123.33
1	C	61	HIS	C-N-CA	-5.96	118.14	123.33
1	M	61	HIS	CA-C-N	-5.96	118.14	123.33
1	M	61	HIS	C-N-CA	-5.96	118.14	123.33
1	M	327	ASP	CA-CB-CG	-5.96	106.64	112.60
1	C	327	ASP	CA-CB-CG	-5.96	106.64	112.60
1	K	327	ASP	CA-CB-CG	-5.96	106.64	112.60
1	O	327	ASP	CA-CB-CG	-5.96	106.64	112.60
2	D	401	ARG	CD-NE-CZ	-5.95	116.06	124.40
1	G	61	HIS	CA-C-N	-5.95	118.15	123.33
1	G	61	HIS	C-N-CA	-5.95	118.15	123.33
2	N	401	ARG	CD-NE-CZ	-5.95	116.07	124.40
1	A	327	ASP	CA-CB-CG	-5.95	106.65	112.60
2	J	401	ARG	CD-NE-CZ	-5.95	116.07	124.40
2	H	401	ARG	CD-NE-CZ	-5.95	116.08	124.40
2	B	401	ARG	CD-NE-CZ	-5.94	116.08	124.40
1	G	250	VAL	N-CA-C	5.94	117.22	107.24
2	J	71	GLU	CA-C-N	5.94	126.09	119.32
2	J	71	GLU	C-N-CA	5.94	126.09	119.32
2	R	401	ARG	CD-NE-CZ	-5.94	116.08	124.40
1	E	327	ASP	CA-CB-CG	-5.94	106.66	112.60
2	P	401	ARG	CD-NE-CZ	-5.94	116.09	124.40
2	F	401	ARG	CD-NE-CZ	-5.94	116.09	124.40
2	L	401	ARG	CD-NE-CZ	-5.93	116.10	124.40
1	G	327	ASP	CA-CB-CG	-5.93	106.67	112.60
1	O	61	HIS	CA-C-N	-5.93	118.17	123.33
1	O	61	HIS	C-N-CA	-5.93	118.17	123.33
1	M	250	VAL	N-CA-C	5.92	117.19	107.24
1	K	61	HIS	CA-C-N	-5.92	118.18	123.33
1	K	61	HIS	C-N-CA	-5.92	118.18	123.33
2	L	71	GLU	CA-C-N	5.92	126.07	119.32
2	L	71	GLU	C-N-CA	5.92	126.07	119.32
1	O	250	VAL	N-CA-C	5.92	117.19	107.24
1	Q	250	VAL	N-CA-C	5.92	117.19	107.24
2	P	378	ILE	CA-C-N	-5.92	116.86	122.66
2	P	378	ILE	C-N-CA	-5.92	116.86	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	71	GLU	CA-C-N	5.92	126.06	119.32
2	N	71	GLU	C-N-CA	5.92	126.06	119.32
2	P	71	GLU	CA-C-N	5.91	126.06	119.32
2	P	71	GLU	C-N-CA	5.91	126.06	119.32
1	A	61	HIS	CA-C-N	-5.91	118.19	123.33
1	A	61	HIS	C-N-CA	-5.91	118.19	123.33
1	K	250	VAL	N-CA-C	5.91	117.17	107.24
2	N	378	ILE	CA-C-N	-5.91	116.87	122.66
2	N	378	ILE	C-N-CA	-5.91	116.87	122.66
1	A	250	VAL	N-CA-C	5.91	117.16	107.24
2	B	71	GLU	CA-C-N	5.91	126.05	119.32
2	B	71	GLU	C-N-CA	5.91	126.05	119.32
1	C	250	VAL	N-CA-C	5.91	117.16	107.24
2	J	277	SER	CA-C-N	5.90	129.00	120.38
2	J	277	SER	C-N-CA	5.90	129.00	120.38
2	R	378	ILE	CA-C-N	-5.90	116.88	122.66
2	R	378	ILE	C-N-CA	-5.90	116.88	122.66
2	H	71	GLU	CA-C-N	5.90	126.04	119.32
2	H	71	GLU	C-N-CA	5.90	126.04	119.32
1	Q	327	ASP	CA-CB-CG	-5.90	106.70	112.60
1	E	250	VAL	N-CA-C	5.90	117.14	107.24
2	R	71	GLU	CA-C-N	5.90	126.04	119.32
2	R	71	GLU	C-N-CA	5.90	126.04	119.32
2	B	378	ILE	CA-C-N	-5.89	116.88	122.66
2	B	378	ILE	C-N-CA	-5.89	116.88	122.66
2	D	71	GLU	CA-C-N	5.89	126.04	119.32
2	D	71	GLU	C-N-CA	5.89	126.04	119.32
2	F	378	ILE	CA-C-N	-5.89	116.89	122.66
2	F	378	ILE	C-N-CA	-5.89	116.89	122.66
2	L	277	SER	CA-C-N	5.88	128.97	120.38
2	L	277	SER	C-N-CA	5.88	128.97	120.38
2	L	378	ILE	CA-C-N	-5.88	116.89	122.66
2	L	378	ILE	C-N-CA	-5.88	116.89	122.66
1	Q	61	HIS	CA-C-N	-5.88	118.21	123.33
1	Q	61	HIS	C-N-CA	-5.88	118.21	123.33
1	E	61	HIS	CA-C-N	-5.88	118.21	123.33
1	E	61	HIS	C-N-CA	-5.88	118.21	123.33
1	I	250	VAL	N-CA-C	5.88	117.12	107.24
2	B	277	SER	CA-C-N	5.88	128.96	120.38
2	B	277	SER	C-N-CA	5.88	128.96	120.38
2	D	277	SER	CA-C-N	5.87	128.96	120.38
2	D	277	SER	C-N-CA	5.87	128.96	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	277	SER	CA-C-N	5.87	128.96	120.38
2	H	277	SER	C-N-CA	5.87	128.96	120.38
2	F	277	SER	CA-C-N	5.87	128.95	120.38
2	F	277	SER	C-N-CA	5.87	128.95	120.38
2	R	277	SER	CA-C-N	5.87	128.95	120.38
2	R	277	SER	C-N-CA	5.87	128.95	120.38
2	D	378	ILE	CA-C-N	-5.87	116.91	122.66
2	D	378	ILE	C-N-CA	-5.87	116.91	122.66
2	P	277	SER	CA-C-N	5.87	128.94	120.38
2	P	277	SER	C-N-CA	5.87	128.94	120.38
2	R	253	ARG	NE-CZ-NH1	5.87	127.37	121.50
1	I	61	HIS	CA-C-N	-5.86	118.23	123.33
1	I	61	HIS	C-N-CA	-5.86	118.23	123.33
2	H	378	ILE	CA-C-N	-5.85	116.93	122.66
2	H	378	ILE	C-N-CA	-5.85	116.93	122.66
2	N	277	SER	CA-C-N	5.85	128.92	120.38
2	N	277	SER	C-N-CA	5.85	128.92	120.38
2	H	253	ARG	NE-CZ-NH1	5.84	127.34	121.50
2	J	378	ILE	CA-C-N	-5.84	116.94	122.66
2	J	378	ILE	C-N-CA	-5.84	116.94	122.66
2	L	253	ARG	NE-CZ-NH1	5.83	127.33	121.50
2	D	253	ARG	NE-CZ-NH1	5.82	127.32	121.50
1	C	285	GLN	CA-C-N	-5.82	114.97	123.00
1	C	285	GLN	C-N-CA	-5.82	114.97	123.00
1	M	285	GLN	CA-C-N	-5.82	114.97	123.00
1	M	285	GLN	C-N-CA	-5.82	114.97	123.00
1	O	285	GLN	CA-C-N	-5.82	114.97	123.00
1	O	285	GLN	C-N-CA	-5.82	114.97	123.00
2	B	253	ARG	NE-CZ-NH1	5.81	127.31	121.50
1	Q	285	GLN	CA-C-N	-5.81	114.98	123.00
1	Q	285	GLN	C-N-CA	-5.81	114.98	123.00
2	N	253	ARG	NE-CZ-NH1	5.80	127.31	121.50
2	J	253	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	E	285	GLN	CA-C-N	-5.80	115.00	123.00
1	E	285	GLN	C-N-CA	-5.80	115.00	123.00
1	M	37	PRO	N-CA-CB	-5.80	98.23	102.35
2	P	253	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	Q	37	PRO	N-CA-CB	-5.79	98.24	102.35
1	A	285	GLN	CA-C-N	-5.79	115.00	123.00
1	A	285	GLN	C-N-CA	-5.79	115.00	123.00
1	G	285	GLN	CA-C-N	-5.79	115.01	123.00
1	G	285	GLN	C-N-CA	-5.79	115.01	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	253	ARG	NE-CZ-NH1	5.79	127.29	121.50
1	K	37	PRO	N-CA-CB	-5.79	98.24	102.35
1	A	37	PRO	N-CA-CB	-5.78	98.24	102.35
1	E	37	PRO	N-CA-CB	-5.78	98.25	102.35
1	K	285	GLN	CA-C-N	-5.78	115.03	123.00
1	K	285	GLN	C-N-CA	-5.78	115.03	123.00
1	M	243	ARG	CA-C-N	-5.78	113.16	121.42
1	M	243	ARG	C-N-CA	-5.78	113.16	121.42
1	I	285	GLN	CA-C-N	-5.77	115.04	123.00
1	I	285	GLN	C-N-CA	-5.77	115.04	123.00
1	I	37	PRO	N-CA-CB	-5.76	98.26	102.35
1	K	243	ARG	CA-C-N	-5.76	113.18	121.42
1	K	243	ARG	C-N-CA	-5.76	113.18	121.42
1	M	250	VAL	CB-CA-C	-5.76	103.87	110.73
1	A	243	ARG	CA-C-N	-5.76	113.19	121.42
1	A	243	ARG	C-N-CA	-5.76	113.19	121.42
1	C	243	ARG	CA-C-N	-5.76	113.19	121.42
1	C	243	ARG	C-N-CA	-5.76	113.19	121.42
1	C	37	PRO	N-CA-CB	-5.75	98.27	102.35
1	G	250	VAL	CB-CA-C	-5.75	103.89	110.73
1	O	243	ARG	CA-C-N	-5.75	113.20	121.42
1	O	243	ARG	C-N-CA	-5.75	113.20	121.42
1	Q	243	ARG	CA-C-N	-5.75	113.20	121.42
1	Q	243	ARG	C-N-CA	-5.75	113.20	121.42
1	G	243	ARG	CA-C-N	-5.75	113.20	121.42
1	G	243	ARG	C-N-CA	-5.75	113.20	121.42
1	O	37	PRO	N-CA-CB	-5.75	98.27	102.35
1	E	243	ARG	CA-C-N	-5.74	113.21	121.42
1	E	243	ARG	C-N-CA	-5.74	113.21	121.42
1	E	250	VAL	CB-CA-C	-5.74	103.90	110.73
1	G	37	PRO	N-CA-CB	-5.74	98.27	102.35
1	O	250	VAL	CB-CA-C	-5.74	103.90	110.73
1	I	322	ASP	N-CA-C	5.74	118.50	108.52
1	A	250	VAL	CB-CA-C	-5.74	103.90	110.73
1	I	243	ARG	CA-C-N	-5.73	113.22	121.42
1	I	243	ARG	C-N-CA	-5.73	113.22	121.42
1	K	250	VAL	CB-CA-C	-5.73	103.91	110.73
1	E	322	ASP	N-CA-C	5.73	118.48	108.52
1	Q	250	VAL	CB-CA-C	-5.72	103.92	110.73
1	Q	322	ASP	N-CA-C	5.72	118.47	108.52
1	A	322	ASP	N-CA-C	5.72	118.47	108.52
1	I	123	ARG	NE-CZ-NH2	-5.72	114.06	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	322	ASP	N-CA-C	5.72	118.47	108.52
1	I	250	VAL	CB-CA-C	-5.71	103.93	110.73
1	O	322	ASP	N-CA-C	5.71	118.46	108.52
1	C	322	ASP	N-CA-C	5.71	118.45	108.52
1	C	250	VAL	CB-CA-C	-5.71	103.94	110.73
1	G	322	ASP	N-CA-C	5.70	118.44	108.52
1	K	322	ASP	N-CA-C	5.70	118.44	108.52
2	P	243	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	G	123	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	M	123	ARG	NE-CZ-NH2	-5.69	114.08	119.20
2	P	272	PHE	N-CA-C	5.69	118.48	108.75
2	N	272	PHE	N-CA-C	5.69	118.47	108.75
2	J	272	PHE	N-CA-C	5.69	118.47	108.75
2	D	272	PHE	N-CA-C	5.68	118.47	108.75
2	F	272	PHE	N-CA-C	5.68	118.47	108.75
2	P	88	ARG	CA-C-N	5.68	126.06	119.47
2	P	88	ARG	C-N-CA	5.68	126.06	119.47
2	J	88	ARG	CA-C-N	5.68	126.06	119.47
2	J	88	ARG	C-N-CA	5.68	126.06	119.47
2	B	272	PHE	N-CA-C	5.68	118.46	108.75
2	L	272	PHE	N-CA-C	5.68	118.46	108.75
2	F	88	ARG	CA-C-N	5.67	126.05	119.47
2	F	88	ARG	C-N-CA	5.67	126.05	119.47
1	A	123	ARG	NE-CZ-NH2	-5.67	114.09	119.20
2	R	272	PHE	N-CA-C	5.67	118.45	108.75
2	D	88	ARG	CA-C-N	5.67	126.05	119.47
2	D	88	ARG	C-N-CA	5.67	126.05	119.47
1	O	101	ASN	CB-CA-C	-5.67	103.84	111.89
1	Q	123	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	E	101	ASN	CB-CA-C	-5.67	103.85	111.89
2	F	243	ARG	NE-CZ-NH2	5.66	124.30	119.20
2	L	243	ARG	NE-CZ-NH2	5.66	124.30	119.20
2	H	272	PHE	N-CA-C	5.66	118.43	108.75
2	B	88	ARG	CA-C-N	5.66	126.03	119.47
2	B	88	ARG	C-N-CA	5.66	126.03	119.47
1	E	123	ARG	NE-CZ-NH2	-5.66	114.11	119.20
2	R	88	ARG	CA-C-N	5.66	126.03	119.47
2	R	88	ARG	C-N-CA	5.66	126.03	119.47
1	K	101	ASN	CB-CA-C	-5.65	103.86	111.89
1	M	101	ASN	CB-CA-C	-5.65	103.87	111.89
1	A	101	ASN	CB-CA-C	-5.65	103.87	111.89
1	G	101	ASN	CB-CA-C	-5.65	103.87	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	243	ARG	NE-CZ-NH2	5.65	124.28	119.20
1	Q	101	ASN	CB-CA-C	-5.64	103.88	111.89
2	H	243	ARG	NE-CZ-NH2	5.64	124.28	119.20
2	B	243	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	O	123	ARG	NE-CZ-NH2	-5.64	114.12	119.20
2	F	54	ASN	CA-C-N	-5.63	114.70	122.30
2	F	54	ASN	C-N-CA	-5.63	114.70	122.30
1	C	101	ASN	CB-CA-C	-5.63	103.89	111.89
1	C	123	ARG	NE-CZ-NH2	-5.63	114.13	119.20
2	L	88	ARG	CA-C-N	5.63	126.00	119.47
2	L	88	ARG	C-N-CA	5.63	126.00	119.47
2	J	243	ARG	NE-CZ-NH2	5.63	124.27	119.20
2	N	88	ARG	CA-C-N	5.62	126.00	119.47
2	N	88	ARG	C-N-CA	5.62	126.00	119.47
2	J	54	ASN	CA-C-N	-5.62	114.71	122.30
2	J	54	ASN	C-N-CA	-5.62	114.71	122.30
1	K	123	ARG	NE-CZ-NH2	-5.62	114.14	119.20
2	L	243	ARG	NH1-CZ-NH2	-5.62	111.99	119.30
2	H	199	ASP	CA-CB-CG	-5.62	106.98	112.60
2	N	243	ARG	NH1-CZ-NH2	-5.62	112.00	119.30
2	F	329	ASP	CA-CB-CG	-5.62	106.98	112.60
2	F	243	ARG	NH1-CZ-NH2	-5.61	112.00	119.30
1	I	101	ASN	CB-CA-C	-5.61	103.92	111.89
2	N	54	ASN	CA-C-N	-5.61	114.73	122.30
2	N	54	ASN	C-N-CA	-5.61	114.73	122.30
2	P	243	ARG	NH1-CZ-NH2	-5.61	112.01	119.30
2	R	199	ASP	CA-CB-CG	-5.61	106.99	112.60
2	H	88	ARG	CA-C-N	5.60	125.97	119.47
2	H	88	ARG	C-N-CA	5.60	125.97	119.47
2	B	54	ASN	CA-C-N	-5.60	114.74	122.30
2	B	54	ASN	C-N-CA	-5.60	114.74	122.30
2	D	243	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	I	306	ASP	CA-C-N	5.60	125.27	119.56
1	I	306	ASP	C-N-CA	5.60	125.27	119.56
2	P	54	ASN	CA-C-N	-5.60	114.74	122.30
2	P	54	ASN	C-N-CA	-5.60	114.74	122.30
2	R	243	ARG	NE-CZ-NH2	5.60	124.24	119.20
2	B	243	ARG	NH1-CZ-NH2	-5.60	112.02	119.30
2	H	54	ASN	CA-C-N	-5.60	114.74	122.30
2	H	54	ASN	C-N-CA	-5.60	114.74	122.30
2	D	54	ASN	CA-C-N	-5.59	114.75	122.30
2	D	54	ASN	C-N-CA	-5.59	114.75	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	199	ASP	CA-CB-CG	-5.59	107.01	112.60
2	H	243	ARG	NH1-CZ-NH2	-5.59	112.03	119.30
1	M	320	ARG	NH1-CZ-NH2	-5.59	112.03	119.30
2	D	329	ASP	CA-CB-CG	-5.59	107.01	112.60
2	N	199	ASP	CA-CB-CG	-5.59	107.01	112.60
2	P	199	ASP	CA-CB-CG	-5.59	107.01	112.60
2	H	329	ASP	CA-CB-CG	-5.58	107.02	112.60
2	R	54	ASN	CA-C-N	-5.58	114.76	122.30
2	R	54	ASN	C-N-CA	-5.58	114.76	122.30
2	B	329	ASP	CA-CB-CG	-5.58	107.02	112.60
1	C	306	ASP	CA-C-N	5.58	125.25	119.56
1	C	306	ASP	C-N-CA	5.58	125.25	119.56
2	L	329	ASP	CA-CB-CG	-5.58	107.02	112.60
1	M	306	ASP	CA-C-N	5.58	125.25	119.56
1	M	306	ASP	C-N-CA	5.58	125.25	119.56
1	I	320	ARG	NH1-CZ-NH2	-5.58	112.05	119.30
2	L	54	ASN	CA-C-N	-5.58	114.77	122.30
2	L	54	ASN	C-N-CA	-5.58	114.77	122.30
2	B	199	ASP	CA-CB-CG	-5.58	107.02	112.60
2	J	329	ASP	CA-CB-CG	-5.58	107.02	112.60
2	J	243	ARG	NH1-CZ-NH2	-5.58	112.05	119.30
1	Q	306	ASP	CA-C-N	5.58	125.25	119.56
1	Q	306	ASP	C-N-CA	5.58	125.25	119.56
1	E	320	ARG	NH1-CZ-NH2	-5.57	112.06	119.30
1	E	306	ASP	CA-C-N	5.57	125.24	119.56
1	E	306	ASP	C-N-CA	5.57	125.24	119.56
2	J	199	ASP	CA-CB-CG	-5.57	107.03	112.60
2	L	199	ASP	CA-CB-CG	-5.57	107.03	112.60
2	N	329	ASP	CA-CB-CG	-5.56	107.04	112.60
2	D	243	ARG	NH1-CZ-NH2	-5.56	112.07	119.30
2	R	243	ARG	NH1-CZ-NH2	-5.56	112.07	119.30
1	A	306	ASP	CA-C-N	5.55	125.22	119.56
1	A	306	ASP	C-N-CA	5.55	125.22	119.56
1	A	320	ARG	NH1-CZ-NH2	-5.55	112.08	119.30
1	C	320	ARG	NH1-CZ-NH2	-5.55	112.09	119.30
2	P	329	ASP	CA-CB-CG	-5.55	107.05	112.60
1	K	320	ARG	NH1-CZ-NH2	-5.55	112.09	119.30
2	F	199	ASP	CA-CB-CG	-5.54	107.06	112.60
1	Q	320	ARG	NH1-CZ-NH2	-5.54	112.09	119.30
2	R	329	ASP	CA-CB-CG	-5.54	107.06	112.60
1	K	306	ASP	CA-C-N	5.54	125.21	119.56
1	K	306	ASP	C-N-CA	5.54	125.21	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	320	ARG	NH1-CZ-NH2	-5.54	112.10	119.30
1	G	320	ARG	NH1-CZ-NH2	-5.53	112.11	119.30
1	O	306	ASP	CA-C-N	5.53	125.20	119.56
1	O	306	ASP	C-N-CA	5.53	125.20	119.56
1	C	267	PHE	N-CA-C	5.52	118.63	109.79
1	Q	28	HIS	N-CA-C	5.52	120.72	112.94
1	G	306	ASP	CA-C-N	5.52	125.19	119.56
1	G	306	ASP	C-N-CA	5.52	125.19	119.56
1	M	102	ASN	CA-CB-CG	5.51	118.11	112.60
1	M	267	PHE	N-CA-C	5.51	118.61	109.79
1	E	267	PHE	N-CA-C	5.51	118.61	109.79
1	K	353	VAL	N-CA-C	5.51	115.79	107.75
1	E	353	VAL	N-CA-C	5.50	115.78	107.75
1	O	353	VAL	N-CA-C	5.50	115.78	107.75
1	A	267	PHE	N-CA-C	5.49	118.58	109.79
1	K	28	HIS	N-CA-C	5.49	120.68	112.94
1	Q	353	VAL	N-CA-C	5.49	115.77	107.75
1	E	28	HIS	N-CA-C	5.49	120.67	112.94
1	G	28	HIS	N-CA-C	5.49	120.67	112.94
1	I	102	ASN	CA-CB-CG	5.49	118.09	112.60
1	I	267	PHE	N-CA-C	5.49	118.57	109.79
1	O	267	PHE	N-CA-C	5.49	118.57	109.79
1	Q	267	PHE	N-CA-C	5.49	118.57	109.79
1	A	102	ASN	CA-CB-CG	5.48	118.08	112.60
1	A	353	VAL	N-CA-C	5.48	115.75	107.75
1	G	267	PHE	N-CA-C	5.48	118.56	109.79
1	G	102	ASN	CA-CB-CG	5.48	118.08	112.60
1	M	353	VAL	N-CA-C	5.48	115.75	107.75
1	C	353	VAL	N-CA-C	5.48	115.75	107.75
1	E	102	ASN	CA-CB-CG	5.48	118.08	112.60
1	A	28	HIS	N-CA-C	5.47	120.66	112.94
1	G	353	VAL	N-CA-C	5.47	115.73	107.75
1	I	28	HIS	N-CA-C	5.46	120.64	112.94
1	M	28	HIS	N-CA-C	5.46	120.64	112.94
1	O	28	HIS	N-CA-C	5.46	120.64	112.94
1	K	267	PHE	N-CA-C	5.46	118.53	109.79
1	I	353	VAL	N-CA-C	5.46	115.72	107.75
1	Q	102	ASN	CA-CB-CG	5.45	118.05	112.60
1	C	102	ASN	CA-CB-CG	5.45	118.05	112.60
1	C	28	HIS	N-CA-C	5.44	120.62	112.94
1	M	175	PRO	CA-C-N	-5.44	112.06	120.88
1	M	175	PRO	C-N-CA	-5.44	112.06	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	102	ASN	CA-CB-CG	5.43	118.03	112.60
1	K	102	ASN	CA-CB-CG	5.43	118.03	112.60
1	Q	175	PRO	CA-C-N	-5.42	112.09	120.88
1	Q	175	PRO	C-N-CA	-5.42	112.09	120.88
1	K	175	PRO	CA-C-N	-5.42	112.11	120.88
1	K	175	PRO	C-N-CA	-5.42	112.11	120.88
1	G	209	ILE	CB-CA-C	-5.42	104.83	112.14
1	C	175	PRO	CA-C-N	-5.41	112.11	120.88
1	C	175	PRO	C-N-CA	-5.41	112.11	120.88
2	L	88	ARG	CD-NE-CZ	5.41	131.97	124.40
1	E	175	PRO	CA-C-N	-5.41	112.12	120.88
1	E	175	PRO	C-N-CA	-5.41	112.12	120.88
1	G	175	PRO	CA-C-N	-5.41	112.12	120.88
1	G	175	PRO	C-N-CA	-5.41	112.12	120.88
2	P	88	ARG	CD-NE-CZ	5.41	131.97	124.40
1	A	175	PRO	CA-C-N	-5.41	112.12	120.88
1	A	175	PRO	C-N-CA	-5.41	112.12	120.88
2	J	88	ARG	CD-NE-CZ	5.41	131.97	124.40
2	N	88	ARG	CD-NE-CZ	5.40	131.96	124.40
1	I	175	PRO	CA-C-N	-5.40	112.13	120.88
1	I	175	PRO	C-N-CA	-5.40	112.13	120.88
1	O	175	PRO	CA-C-N	-5.40	112.13	120.88
1	O	175	PRO	C-N-CA	-5.40	112.13	120.88
1	E	209	ILE	CB-CA-C	-5.40	104.85	112.14
2	B	88	ARG	CD-NE-CZ	5.40	131.96	124.40
1	I	209	ILE	CB-CA-C	-5.39	104.86	112.14
1	O	209	ILE	CB-CA-C	-5.39	104.86	112.14
2	D	88	ARG	CD-NE-CZ	5.39	131.95	124.40
1	A	209	ILE	CB-CA-C	-5.39	104.86	112.14
1	M	209	ILE	CB-CA-C	-5.39	104.87	112.14
2	H	88	ARG	CD-NE-CZ	5.39	131.94	124.40
2	R	88	ARG	CD-NE-CZ	5.39	131.94	124.40
2	F	88	ARG	CD-NE-CZ	5.38	131.93	124.40
1	K	138	PHE	CA-CB-CG	-5.38	108.42	113.80
1	C	209	ILE	CB-CA-C	-5.38	104.88	112.14
1	K	320	ARG	NE-CZ-NH2	5.37	124.04	119.20
1	M	138	PHE	CA-CB-CG	-5.37	108.43	113.80
1	Q	209	ILE	CB-CA-C	-5.37	104.89	112.14
1	M	320	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	I	138	PHE	CA-CB-CG	-5.36	108.44	113.80
1	K	209	ILE	CB-CA-C	-5.36	104.90	112.14
1	O	138	PHE	CA-CB-CG	-5.36	108.44	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	138	PHE	CA-CB-CG	-5.35	108.45	113.80
1	A	138	PHE	CA-CB-CG	-5.35	108.45	113.80
1	G	424	ASP	CA-CB-CG	5.35	117.95	112.60
2	J	345	GLU	N-CA-C	5.35	119.29	112.87
1	Q	320	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	C	138	PHE	CA-CB-CG	-5.34	108.45	113.80
1	C	424	ASP	CA-CB-CG	5.34	117.94	112.60
2	D	345	GLU	N-CA-C	5.34	119.28	112.87
2	B	345	GLU	N-CA-C	5.33	119.27	112.87
1	O	320	ARG	NE-CZ-NH2	5.33	124.00	119.20
2	F	345	GLU	N-CA-C	5.33	119.27	112.87
2	D	357	ASP	N-CA-C	5.33	119.77	113.16
1	G	138	PHE	CA-CB-CG	-5.33	108.47	113.80
2	R	345	GLU	N-CA-C	5.33	119.27	112.87
2	N	345	GLU	N-CA-C	5.33	119.26	112.87
2	P	357	ASP	N-CA-C	5.32	119.76	113.16
2	H	345	GLU	N-CA-C	5.32	119.26	112.87
1	A	320	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	Q	424	ASP	CA-CB-CG	5.32	117.92	112.60
1	I	320	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	M	163	LYS	N-CA-C	5.31	119.39	113.01
1	K	163	LYS	N-CA-C	5.31	119.38	113.01
2	P	345	GLU	N-CA-C	5.31	119.24	112.87
1	A	424	ASP	CA-CB-CG	5.31	117.91	112.60
2	F	357	ASP	N-CA-C	5.31	119.74	113.16
1	M	424	ASP	CA-CB-CG	5.31	117.91	112.60
2	N	110	GLU	N-CA-C	5.31	116.75	111.07
2	L	357	ASP	N-CA-C	5.30	119.74	113.16
1	Q	138	PHE	CA-CB-CG	-5.30	108.50	113.80
2	R	357	ASP	N-CA-C	5.30	119.74	113.16
1	A	163	LYS	N-CA-C	5.30	119.37	113.01
2	B	357	ASP	N-CA-C	5.30	119.73	113.16
2	J	357	ASP	N-CA-C	5.30	119.73	113.16
2	F	110	GLU	N-CA-C	5.30	116.74	111.07
2	L	345	GLU	N-CA-C	5.30	119.23	112.87
2	N	357	ASP	N-CA-C	5.30	119.73	113.16
1	O	424	ASP	CA-CB-CG	5.30	117.90	112.60
1	E	320	ARG	NE-CZ-NH2	5.29	123.97	119.20
1	G	320	ARG	NE-CZ-NH2	5.29	123.97	119.20
2	D	110	GLU	N-CA-C	5.29	116.73	111.07
1	Q	163	LYS	N-CA-C	5.29	119.36	113.01
1	E	424	ASP	CA-CB-CG	5.29	117.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	163	LYS	N-CA-C	5.29	119.36	113.01
1	G	163	LYS	N-CA-C	5.29	119.36	113.01
2	J	110	GLU	N-CA-C	5.29	116.73	111.07
2	P	436	GLN	O-C-N	5.29	127.59	122.09
2	H	357	ASP	N-CA-C	5.28	119.71	113.16
2	R	110	GLU	N-CA-C	5.28	116.72	111.07
2	P	110	GLU	N-CA-C	5.28	116.72	111.07
1	I	424	ASP	CA-CB-CG	5.28	117.88	112.60
1	O	163	LYS	N-CA-C	5.28	119.34	113.01
2	B	110	GLU	N-CA-C	5.28	116.72	111.07
2	H	110	GLU	N-CA-C	5.28	116.71	111.07
1	C	163	LYS	N-CA-C	5.27	119.34	113.01
2	N	436	GLN	O-C-N	5.27	127.57	122.09
2	L	110	GLU	N-CA-C	5.26	116.70	111.07
1	E	163	LYS	N-CA-C	5.26	119.33	113.01
1	C	320	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	K	424	ASP	CA-CB-CG	5.25	117.86	112.60
2	L	436	GLN	O-C-N	5.25	127.55	122.09
2	H	436	GLN	O-C-N	5.25	127.55	122.09
1	O	221	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	E	221	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	E	439	SER	N-CA-C	5.23	125.65	111.00
2	L	391	ILE	N-CA-C	5.23	115.45	110.53
2	J	436	GLN	O-C-N	5.23	127.53	122.09
2	R	391	ILE	N-CA-C	5.23	115.44	110.53
1	A	221	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	C	439	SER	N-CA-C	5.22	125.62	111.00
1	I	411	GLU	CA-CB-CG	5.22	124.54	114.10
1	A	439	SER	N-CA-C	5.22	125.62	111.00
2	B	436	GLN	O-C-N	5.22	127.52	122.09
1	Q	221	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	C	221	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	O	439	SER	N-CA-C	5.22	125.61	111.00
1	G	439	SER	N-CA-C	5.22	125.61	111.00
1	I	439	SER	N-CA-C	5.22	125.60	111.00
1	K	439	SER	N-CA-C	5.22	125.61	111.00
2	P	391	ILE	N-CA-C	5.22	115.43	110.53
2	J	391	ILE	N-CA-C	5.21	115.43	110.53
1	K	221	ARG	N-CA-C	5.21	119.34	108.39
1	Q	439	SER	N-CA-C	5.21	125.60	111.00
2	F	436	GLN	O-C-N	5.21	127.51	122.09
1	A	411	GLU	CA-CB-CG	5.21	124.52	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	221	ARG	NE-CZ-NH1	-5.21	116.29	121.50
2	H	391	ILE	N-CA-C	5.21	115.43	110.53
1	M	439	SER	N-CA-C	5.21	125.59	111.00
1	Q	411	GLU	CA-CB-CG	5.21	124.52	114.10
1	I	221	ARG	N-CA-C	5.21	119.33	108.39
1	E	221	ARG	N-CA-C	5.21	119.32	108.39
1	E	411	GLU	CA-CB-CG	5.21	124.51	114.10
1	G	221	ARG	N-CA-C	5.21	119.32	108.39
1	G	411	GLU	CA-CB-CG	5.21	124.51	114.10
1	O	411	GLU	CA-CB-CG	5.21	124.51	114.10
2	D	436	GLN	O-C-N	5.20	127.50	122.09
2	N	391	ILE	N-CA-C	5.20	115.42	110.53
1	O	221	ARG	N-CA-C	5.20	119.32	108.39
1	A	221	ARG	N-CA-C	5.20	119.31	108.39
1	M	411	GLU	CA-CB-CG	5.20	124.50	114.10
1	C	221	ARG	N-CA-C	5.20	119.31	108.39
1	C	411	GLU	CA-CB-CG	5.20	124.50	114.10
1	K	411	GLU	CA-CB-CG	5.20	124.49	114.10
1	M	221	ARG	N-CA-C	5.20	119.30	108.39
1	I	221	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	Q	221	ARG	N-CA-C	5.19	119.30	108.39
1	E	51	THR	CA-C-N	-5.19	114.00	122.26
1	E	51	THR	C-N-CA	-5.19	114.00	122.26
1	M	51	THR	CA-C-N	-5.19	114.00	122.26
1	M	51	THR	C-N-CA	-5.19	114.00	122.26
1	C	51	THR	CA-C-N	-5.19	114.01	122.26
1	C	51	THR	C-N-CA	-5.19	114.01	122.26
1	M	221	ARG	NE-CZ-NH1	-5.19	116.31	121.50
2	F	94	PHE	N-CA-C	5.19	116.72	108.79
2	B	391	ILE	N-CA-C	5.18	115.40	110.53
2	D	47	GLU	N-CA-C	5.18	121.84	110.80
2	D	248	LEU	N-CA-C	5.18	117.90	109.24
2	D	391	ILE	N-CA-C	5.18	115.40	110.53
2	J	248	LEU	N-CA-C	5.18	117.89	109.24
2	J	264	ARG	CA-C-N	-5.18	115.09	123.23
2	J	264	ARG	C-N-CA	-5.18	115.09	123.23
2	R	436	GLN	O-C-N	5.18	127.48	122.09
1	Q	51	THR	CA-C-N	-5.18	114.03	122.26
1	Q	51	THR	C-N-CA	-5.18	114.03	122.26
1	I	51	THR	CA-C-N	-5.18	114.03	122.26
1	I	51	THR	C-N-CA	-5.18	114.03	122.26
1	A	51	THR	CA-C-N	-5.17	114.03	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	THR	C-N-CA	-5.17	114.03	122.26
2	P	248	LEU	N-CA-C	5.17	117.88	109.24
2	F	264	ARG	CA-C-N	-5.17	115.11	123.23
2	F	264	ARG	C-N-CA	-5.17	115.11	123.23
2	B	248	LEU	N-CA-C	5.17	117.88	109.24
2	H	47	GLU	N-CA-C	5.17	121.81	110.80
1	K	51	THR	CA-C-N	-5.17	114.04	122.26
1	K	51	THR	C-N-CA	-5.17	114.04	122.26
1	E	116	ASP	CA-CB-CG	-5.17	107.43	112.60
1	I	116	ASP	CA-CB-CG	-5.17	107.43	112.60
2	P	264	ARG	CA-C-N	-5.17	115.12	123.23
2	P	264	ARG	C-N-CA	-5.17	115.12	123.23
1	G	51	THR	CA-C-N	-5.17	114.05	122.26
1	G	51	THR	C-N-CA	-5.17	114.05	122.26
1	K	221	ARG	NE-CZ-NH1	-5.17	116.33	121.50
2	L	94	PHE	N-CA-C	5.17	116.69	108.79
2	R	248	LEU	N-CA-C	5.17	117.87	109.24
2	B	47	GLU	N-CA-C	5.16	121.80	110.80
2	B	94	PHE	N-CA-C	5.16	116.69	108.79
2	F	47	GLU	N-CA-C	5.16	121.80	110.80
2	J	47	GLU	N-CA-C	5.16	121.80	110.80
1	M	116	ASP	CA-CB-CG	-5.16	107.44	112.60
2	N	248	LEU	N-CA-C	5.16	117.86	109.24
2	H	248	LEU	N-CA-C	5.16	117.86	109.24
2	F	248	LEU	N-CA-C	5.16	117.85	109.24
2	N	47	GLU	N-CA-C	5.16	121.79	110.80
2	P	260	VAL	CA-C-N	5.16	124.85	119.64
2	P	260	VAL	C-N-CA	5.16	124.85	119.64
2	R	264	ARG	CA-C-N	-5.16	115.13	123.23
2	R	264	ARG	C-N-CA	-5.16	115.13	123.23
1	A	116	ASP	CA-CB-CG	-5.16	107.44	112.60
2	B	264	ARG	CA-C-N	-5.16	115.13	123.23
2	B	264	ARG	C-N-CA	-5.16	115.13	123.23
2	N	94	PHE	N-CA-C	5.16	116.68	108.79
2	P	47	GLU	N-CA-C	5.16	121.78	110.80
2	J	390	ARG	NE-CZ-NH2	5.16	123.84	119.20
2	R	47	GLU	N-CA-C	5.16	121.78	110.80
2	H	94	PHE	N-CA-C	5.15	116.68	108.79
2	J	94	PHE	N-CA-C	5.15	116.67	108.79
1	E	209	ILE	CA-CB-CG2	-5.15	101.74	110.50
2	L	248	LEU	N-CA-C	5.15	117.84	109.24
2	L	264	ARG	CA-C-N	-5.15	115.14	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	264	ARG	C-N-CA	-5.15	115.14	123.23
2	N	264	ARG	CA-C-N	-5.15	115.14	123.23
2	N	264	ARG	C-N-CA	-5.15	115.14	123.23
1	O	51	THR	CA-C-N	-5.15	114.07	122.26
1	O	51	THR	C-N-CA	-5.15	114.07	122.26
1	Q	116	ASP	CA-CB-CG	-5.15	107.45	112.60
2	F	391	ILE	N-CA-C	5.15	115.37	110.53
2	L	47	GLU	N-CA-C	5.15	121.77	110.80
1	C	209	ILE	CA-CB-CG2	-5.15	101.75	110.50
2	F	185	TYR	CA-CB-CG	5.15	123.17	113.90
1	K	116	ASP	CA-CB-CG	-5.15	107.45	112.60
2	D	94	PHE	N-CA-C	5.15	116.66	108.79
2	H	264	ARG	CA-C-N	-5.15	115.15	123.23
2	H	264	ARG	C-N-CA	-5.15	115.15	123.23
2	R	94	PHE	N-CA-C	5.15	116.66	108.79
2	D	264	ARG	CA-C-N	-5.14	115.15	123.23
2	D	264	ARG	C-N-CA	-5.14	115.15	123.23
2	J	260	VAL	CA-C-N	5.14	124.83	119.64
2	J	260	VAL	C-N-CA	5.14	124.83	119.64
2	D	162	PRO	CA-C-N	-5.14	114.42	122.65
2	D	162	PRO	C-N-CA	-5.14	114.42	122.65
2	L	185	TYR	CA-CB-CG	5.14	123.16	113.90
2	N	185	TYR	CA-CB-CG	5.14	123.16	113.90
2	P	94	PHE	N-CA-C	5.14	116.66	108.79
1	A	209	ILE	CA-CB-CG2	-5.14	101.76	110.50
1	K	209	ILE	CA-CB-CG2	-5.14	101.76	110.50
1	O	116	ASP	CA-CB-CG	-5.14	107.46	112.60
1	K	297	GLU	CA-C-N	5.14	125.43	119.47
1	K	297	GLU	C-N-CA	5.14	125.43	119.47
2	N	162	PRO	CA-C-N	-5.14	114.43	122.65
2	N	162	PRO	C-N-CA	-5.14	114.43	122.65
2	P	185	TYR	CA-CB-CG	5.14	123.14	113.90
2	B	162	PRO	CA-C-N	-5.13	114.44	122.65
2	B	162	PRO	C-N-CA	-5.13	114.44	122.65
1	G	209	ILE	CA-CB-CG2	-5.13	101.77	110.50
1	O	297	GLU	CA-C-N	5.13	125.43	119.47
1	O	297	GLU	C-N-CA	5.13	125.43	119.47
2	B	185	TYR	CA-CB-CG	5.13	123.14	113.90
1	C	116	ASP	CA-CB-CG	-5.13	107.47	112.60
2	F	162	PRO	CA-C-N	-5.13	114.44	122.65
2	F	162	PRO	C-N-CA	-5.13	114.44	122.65
2	J	185	TYR	CA-CB-CG	5.13	123.13	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	209	ILE	CA-CB-CG2	-5.13	101.78	110.50
1	O	209	ILE	CA-CB-CG2	-5.13	101.78	110.50
1	I	196	GLU	N-CA-C	5.13	116.95	111.36
1	I	209	ILE	CA-CB-CG2	-5.13	101.78	110.50
2	H	162	PRO	CA-C-N	-5.12	114.45	122.65
2	H	162	PRO	C-N-CA	-5.12	114.45	122.65
2	N	390	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	Q	209	ILE	CA-CB-CG2	-5.12	101.79	110.50
2	R	185	TYR	CA-CB-CG	5.12	123.12	113.90
2	R	268	PHE	N-CA-C	5.12	117.92	109.72
1	C	196	GLU	N-CA-C	5.12	116.94	111.36
1	G	116	ASP	CA-CB-CG	-5.12	107.48	112.60
2	H	260	VAL	CA-C-N	5.12	124.81	119.64
2	H	260	VAL	C-N-CA	5.12	124.81	119.64
2	J	268	PHE	N-CA-C	5.12	117.92	109.72
1	K	196	GLU	N-CA-C	5.12	116.94	111.36
2	P	162	PRO	CA-C-N	-5.12	114.45	122.65
2	P	162	PRO	C-N-CA	-5.12	114.45	122.65
2	R	162	PRO	CA-C-N	-5.12	114.46	122.65
2	R	162	PRO	C-N-CA	-5.12	114.46	122.65
1	G	196	GLU	N-CA-C	5.12	116.94	111.36
2	H	406	HIS	CA-CB-CG	5.12	118.92	113.80
2	D	390	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	F	268	PHE	N-CA-C	5.12	117.91	109.72
2	L	162	PRO	CA-C-N	-5.12	114.46	122.65
2	L	162	PRO	C-N-CA	-5.12	114.46	122.65
2	R	390	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	B	260	VAL	CA-C-N	5.12	124.81	119.64
2	B	260	VAL	C-N-CA	5.12	124.81	119.64
1	C	107	HIS	CA-C-N	-5.12	111.77	121.54
1	C	107	HIS	C-N-CA	-5.12	111.77	121.54
2	H	185	TYR	CA-CB-CG	5.12	123.11	113.90
2	J	162	PRO	CA-C-N	-5.12	114.47	122.65
2	J	162	PRO	C-N-CA	-5.12	114.47	122.65
1	A	297	GLU	CA-C-N	5.11	125.40	119.47
1	A	297	GLU	C-N-CA	5.11	125.40	119.47
1	C	351	PHE	CB-CA-C	-5.11	101.81	110.19
2	L	260	VAL	CA-C-N	5.11	124.80	119.64
2	L	260	VAL	C-N-CA	5.11	124.80	119.64
2	P	122	VAL	CB-CA-C	-5.11	105.33	111.88
1	Q	107	HIS	CA-C-N	-5.11	111.78	121.54
1	Q	107	HIS	C-N-CA	-5.11	111.78	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	390	ARG	NE-CZ-NH2	5.11	123.80	119.20
2	D	185	TYR	CA-CB-CG	5.11	123.10	113.90
2	F	260	VAL	CA-C-N	5.11	124.80	119.64
2	F	260	VAL	C-N-CA	5.11	124.80	119.64
1	K	107	HIS	CA-C-N	-5.11	111.78	121.54
1	K	107	HIS	C-N-CA	-5.11	111.78	121.54
1	M	297	GLU	CA-C-N	5.11	125.40	119.47
1	M	297	GLU	C-N-CA	5.11	125.40	119.47
1	Q	196	GLU	N-CA-C	5.11	116.93	111.36
1	G	107	HIS	CA-C-N	-5.11	111.78	121.54
1	G	107	HIS	C-N-CA	-5.11	111.78	121.54
1	I	351	PHE	CB-CA-C	-5.11	101.81	110.19
2	L	406	HIS	CA-CB-CG	5.11	118.91	113.80
1	G	351	PHE	CB-CA-C	-5.11	101.82	110.19
2	F	401	ARG	CB-CG-CD	-5.10	99.56	111.30
1	O	107	HIS	CA-C-N	-5.10	111.79	121.54
1	O	107	HIS	C-N-CA	-5.10	111.79	121.54
1	A	196	GLU	N-CA-C	5.10	116.92	111.36
2	B	268	PHE	N-CA-C	5.10	117.88	109.72
1	I	297	GLU	CA-C-N	5.10	125.39	119.47
1	I	297	GLU	C-N-CA	5.10	125.39	119.47
1	O	196	GLU	N-CA-C	5.10	116.92	111.36
1	C	297	GLU	CA-C-N	5.10	125.39	119.47
1	C	297	GLU	C-N-CA	5.10	125.39	119.47
1	I	107	HIS	CA-C-N	-5.10	111.80	121.54
1	I	107	HIS	C-N-CA	-5.10	111.80	121.54
2	J	406	HIS	CA-CB-CG	5.10	118.90	113.80
1	A	107	HIS	CA-C-N	-5.09	111.81	121.54
1	A	107	HIS	C-N-CA	-5.09	111.81	121.54
2	D	401	ARG	CB-CG-CD	-5.09	99.58	111.30
1	Q	297	GLU	CA-C-N	5.09	125.38	119.47
1	Q	297	GLU	C-N-CA	5.09	125.38	119.47
2	R	406	HIS	CA-CB-CG	5.09	118.89	113.80
2	N	401	ARG	CB-CG-CD	-5.09	99.59	111.30
2	B	401	ARG	CB-CG-CD	-5.09	99.59	111.30
2	F	390	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	H	122	VAL	CB-CA-C	-5.09	105.36	111.88
2	H	401	ARG	CB-CG-CD	-5.09	99.59	111.30
2	R	401	ARG	CB-CG-CD	-5.09	99.59	111.30
1	A	351	PHE	CB-CA-C	-5.09	101.84	110.19
2	D	260	VAL	CA-C-N	5.09	124.78	119.64
2	D	260	VAL	C-N-CA	5.09	124.78	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	406	HIS	CA-CB-CG	5.09	118.89	113.80
2	H	390	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	M	107	HIS	CA-C-N	-5.09	111.82	121.54
1	M	107	HIS	C-N-CA	-5.09	111.82	121.54
1	M	351	PHE	CB-CA-C	-5.09	101.84	110.19
2	N	268	PHE	N-CA-C	5.09	117.86	109.72
1	O	351	PHE	CB-CA-C	-5.09	101.84	110.19
1	Q	351	PHE	CB-CA-C	-5.09	101.84	110.19
1	E	351	PHE	CB-CA-C	-5.09	101.85	110.19
2	F	122	VAL	CB-CA-C	-5.09	105.37	111.88
2	J	88	ARG	NE-CZ-NH2	-5.09	114.62	119.20
2	R	260	VAL	CA-C-N	5.09	124.78	119.64
2	R	260	VAL	C-N-CA	5.09	124.78	119.64
2	P	401	ARG	CB-CG-CD	-5.08	99.60	111.30
2	F	406	HIS	CA-CB-CG	5.08	118.88	113.80
2	N	88	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	O	309	HIS	CA-CB-CG	-5.08	108.72	113.80
2	B	122	VAL	CB-CA-C	-5.08	105.38	111.88
2	B	406	HIS	CA-CB-CG	5.08	118.88	113.80
1	E	107	HIS	CA-C-N	-5.08	111.83	121.54
1	E	107	HIS	C-N-CA	-5.08	111.83	121.54
1	K	351	PHE	CB-CA-C	-5.08	101.86	110.19
2	P	268	PHE	N-CA-C	5.08	117.85	109.72
2	D	268	PHE	N-CA-C	5.08	117.85	109.72
1	E	297	GLU	CA-C-N	5.08	125.36	119.47
1	E	297	GLU	C-N-CA	5.08	125.36	119.47
2	L	401	ARG	CB-CG-CD	-5.08	99.62	111.30
2	P	414	ASP	CA-CB-CG	5.08	117.68	112.60
1	G	297	GLU	CA-C-N	5.08	125.36	119.47
1	G	297	GLU	C-N-CA	5.08	125.36	119.47
2	P	31	ASP	CA-C-N	5.08	124.80	119.82
2	P	31	ASP	C-N-CA	5.08	124.80	119.82
2	H	268	PHE	N-CA-C	5.08	117.84	109.72
2	N	260	VAL	CA-C-N	5.08	124.77	119.64
2	N	260	VAL	C-N-CA	5.08	124.77	119.64
1	E	196	GLU	N-CA-C	5.07	116.89	111.36
2	R	122	VAL	CB-CA-C	-5.07	105.39	111.88
2	L	390	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	M	309	HIS	CA-CB-CG	-5.07	108.73	113.80
1	I	309	HIS	CA-CB-CG	-5.07	108.73	113.80
2	J	401	ARG	CB-CG-CD	-5.07	99.64	111.30
2	F	88	ARG	NE-CZ-NH2	-5.07	114.64	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	179	ASP	CA-C-N	-5.07	114.71	122.87
2	F	179	ASP	C-N-CA	-5.07	114.71	122.87
2	N	31	ASP	CA-C-N	5.06	124.78	119.82
2	N	31	ASP	C-N-CA	5.06	124.78	119.82
2	D	122	VAL	CB-CA-C	-5.06	105.40	111.88
2	D	179	ASP	CA-C-N	-5.06	114.72	122.87
2	D	179	ASP	C-N-CA	-5.06	114.72	122.87
2	F	31	ASP	CA-C-N	5.06	124.78	119.82
2	F	31	ASP	C-N-CA	5.06	124.78	119.82
2	J	122	VAL	CB-CA-C	-5.06	105.40	111.88
2	L	268	PHE	N-CA-C	5.06	117.82	109.72
1	M	196	GLU	N-CA-C	5.06	116.88	111.36
2	P	313	LEU	N-CA-C	-5.06	105.95	112.68
2	P	88	ARG	NE-CZ-NH2	-5.06	114.65	119.20
1	Q	309	HIS	CA-CB-CG	-5.06	108.74	113.80
2	J	31	ASP	CA-C-N	5.06	124.78	119.82
2	J	31	ASP	C-N-CA	5.06	124.78	119.82
1	K	309	HIS	CA-CB-CG	-5.06	108.74	113.80
1	A	309	HIS	CA-CB-CG	-5.05	108.75	113.80
2	N	122	VAL	CB-CA-C	-5.05	105.41	111.88
2	P	390	ARG	NE-CZ-NH2	5.05	123.75	119.20
2	B	313	LEU	N-CA-C	-5.05	105.96	112.68
2	H	179	ASP	CA-C-N	-5.05	114.73	122.87
2	H	179	ASP	C-N-CA	-5.05	114.73	122.87
2	N	406	HIS	CA-CB-CG	5.05	118.85	113.80
2	J	179	ASP	CA-C-N	-5.05	114.74	122.87
2	J	179	ASP	C-N-CA	-5.05	114.74	122.87
2	R	313	LEU	N-CA-C	-5.05	105.96	112.68
2	L	122	VAL	CB-CA-C	-5.05	105.42	111.88
2	R	31	ASP	CA-C-N	5.05	124.77	119.82
2	R	31	ASP	C-N-CA	5.05	124.77	119.82
2	D	313	LEU	N-CA-C	-5.05	105.97	112.68
2	N	313	LEU	N-CA-C	-5.05	105.97	112.68
2	D	88	ARG	NE-CZ-NH2	-5.05	114.66	119.20
1	E	309	HIS	CA-CB-CG	-5.05	108.75	113.80
2	J	170	SER	N-CA-C	5.05	116.91	108.99
2	L	179	ASP	CA-C-N	-5.05	114.75	122.87
2	L	179	ASP	C-N-CA	-5.05	114.75	122.87
2	H	313	LEU	N-CA-C	-5.04	105.97	112.68
2	B	31	ASP	CA-C-N	5.04	124.76	119.82
2	B	31	ASP	C-N-CA	5.04	124.76	119.82
2	B	88	ARG	NE-CZ-NH2	-5.04	114.66	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	414	ASP	CA-CB-CG	5.04	117.64	112.60
2	H	88	ARG	NE-CZ-NH2	-5.04	114.66	119.20
2	J	313	LEU	N-CA-C	-5.04	105.97	112.68
2	R	88	ARG	NE-CZ-NH2	-5.04	114.66	119.20
2	B	414	ASP	CA-CB-CG	5.04	117.64	112.60
2	D	31	ASP	CA-C-N	5.04	124.76	119.82
2	D	31	ASP	C-N-CA	5.04	124.76	119.82
2	F	313	LEU	N-CA-C	-5.04	105.97	112.68
2	H	31	ASP	CA-C-N	5.04	124.76	119.82
2	H	31	ASP	C-N-CA	5.04	124.76	119.82
2	L	31	ASP	CA-C-N	5.04	124.76	119.82
2	L	31	ASP	C-N-CA	5.04	124.76	119.82
2	P	406	HIS	CA-CB-CG	5.04	118.84	113.80
2	L	414	ASP	CA-CB-CG	5.04	117.64	112.60
2	H	414	ASP	CA-CB-CG	5.04	117.64	112.60
2	N	179	ASP	CA-C-N	-5.04	114.76	122.87
2	N	179	ASP	C-N-CA	-5.04	114.76	122.87
1	C	309	HIS	CA-CB-CG	-5.03	108.77	113.80
1	G	309	HIS	CA-CB-CG	-5.03	108.77	113.80
2	L	313	LEU	N-CA-C	-5.03	105.98	112.68
2	P	179	ASP	CA-C-N	-5.03	114.77	122.87
2	P	179	ASP	C-N-CA	-5.03	114.77	122.87
2	B	179	ASP	CA-C-N	-5.03	114.77	122.87
2	B	179	ASP	C-N-CA	-5.03	114.77	122.87
2	F	414	ASP	CA-CB-CG	5.03	117.63	112.60
1	Q	72	PRO	N-CA-C	5.03	121.24	113.75
2	N	170	SER	N-CA-C	5.03	116.88	108.99
2	P	170	SER	N-CA-C	5.03	116.88	108.99
2	F	170	SER	N-CA-C	5.02	116.88	108.99
2	B	170	SER	N-CA-C	5.02	116.88	108.99
2	L	170	SER	N-CA-C	5.02	116.87	108.99
2	R	170	SER	N-CA-C	5.02	116.88	108.99
2	J	414	ASP	CA-CB-CG	5.02	117.62	112.60
1	Q	345	ASP	N-CA-C	5.01	118.17	111.75
1	M	72	PRO	N-CA-C	5.01	121.22	113.75
2	R	179	ASP	CA-C-N	-5.01	114.80	122.87
2	R	179	ASP	C-N-CA	-5.01	114.80	122.87
2	N	414	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	207	GLU	CA-CB-CG	-5.01	104.08	114.10
2	R	414	ASP	CA-CB-CG	5.01	117.61	112.60
1	I	207	GLU	CA-CB-CG	-5.01	104.09	114.10
2	N	268	PHE	CA-CB-CG	-5.00	108.80	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	170	SER	N-CA-C	5.00	116.84	108.99
2	H	170	SER	N-CA-C	5.00	116.84	108.99
1	K	345	ASP	N-CA-C	5.00	118.15	111.75
2	L	88	ARG	NE-CZ-NH2	-5.00	114.70	119.20
1	M	345	ASP	N-CA-C	5.00	118.15	111.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3350	0	3254	38	0
1	C	3350	0	3254	38	0
1	E	3350	0	3254	37	0
1	G	3350	0	3254	42	0
1	I	3350	0	3254	41	0
1	K	3350	0	3254	42	0
1	M	3350	0	3254	38	0
1	O	3350	0	3254	37	0
1	Q	3350	0	3254	39	0
2	B	3352	0	3229	40	0
2	D	3352	0	3229	43	0
2	F	3352	0	3229	42	0
2	H	3352	0	3229	40	0
2	J	3352	0	3229	40	0
2	L	3352	0	3229	41	0
2	N	3352	0	3229	41	0
2	P	3352	0	3229	41	0
2	R	3352	0	3229	42	0
3	A	32	0	12	0	0
3	C	32	0	12	0	0
3	E	32	0	12	0	0
3	G	32	0	12	0	0
3	I	32	0	12	0	0
3	K	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	32	0	12	0	0
3	O	32	0	12	0	0
3	Q	32	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
5	B	32	0	13	4	0
5	D	32	0	13	4	0
5	F	32	0	13	4	0
5	H	32	0	13	4	0
5	J	32	0	13	4	0
5	L	32	0	13	4	0
5	N	32	0	13	4	0
5	P	32	0	13	4	0
5	R	32	0	13	4	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
6	E	4	0	0	0	0
6	F	4	0	0	0	0
6	G	4	0	0	0	0
6	H	4	0	0	0	0
6	I	4	0	0	0	0
6	J	4	0	0	0	0
6	K	4	0	0	0	0
6	L	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	4	0	0	0	0
6	N	4	0	0	0	0
6	O	4	0	0	0	0
6	P	4	0	0	0	0
6	Q	4	0	0	0	0
6	R	4	0	0	0	0
All	All	60984	0	58572	685	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 6.

All (685) 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)
2:D:228:ASN:HD21	5:D:501:G2P:H1	1.13	0.95
2:N:228:ASN:HD21	5:N:501:G2P:H1	1.13	0.95
2:H:228:ASN:HD21	5:H:501:G2P:H1	1.13	0.95
2:L:228:ASN:HD21	5:L:501:G2P:H1	1.13	0.93
1:K:341:ILE:HG13	1:K:341:ILE:O	1.67	0.93
1:E:341:ILE:O	1:E:341:ILE:HG13	1.67	0.93
1:I:341:ILE:HG13	1:I:341:ILE:O	1.67	0.93
1:Q:341:ILE:HG13	1:Q:341:ILE:O	1.67	0.93
1:A:341:ILE:HG13	1:A:341:ILE:O	1.67	0.93
1:O:341:ILE:O	1:O:341:ILE:HG13	1.67	0.93
2:R:228:ASN:HD21	5:R:501:G2P:H1	1.13	0.93
2:F:228:ASN:HD21	5:F:501:G2P:H1	1.13	0.92
1:G:341:ILE:O	1:G:341:ILE:HG13	1.67	0.92
1:M:341:ILE:HG13	1:M:341:ILE:O	1.67	0.92
1:C:341:ILE:HG13	1:C:341:ILE:O	1.67	0.92
2:B:228:ASN:HD21	5:B:501:G2P:H1	1.13	0.91
2:P:228:ASN:HD21	5:P:501:G2P:H1	1.13	0.91
2:J:228:ASN:HD21	5:J:501:G2P:H1	1.13	0.90
1:M:439:SER:O	1:M:439:SER:OG	2.05	0.71
2:J:401:ARG:HD3	2:J:401:ARG:N	2.07	0.70
2:B:401:ARG:N	2:B:401:ARG:HD3	2.07	0.70
1:O:439:SER:O	1:O:439:SER:OG	2.05	0.70
2:P:401:ARG:HD3	2:P:401:ARG:N	2.07	0.70
2:F:401:ARG:HD3	2:F:401:ARG:N	2.07	0.69
2:R:401:ARG:HD3	2:R:401:ARG:N	2.07	0.69
2:L:401:ARG:HD3	2:L:401:ARG:N	2.07	0.69
1:Q:439:SER:O	1:Q:439:SER:OG	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:SER:OG	1:I:148:GLY:N	2.26	0.68
2:D:401:ARG:HD3	2:D:401:ARG:N	2.07	0.68
1:E:147:SER:OG	1:E:148:GLY:N	2.26	0.68
1:K:147:SER:OG	1:K:148:GLY:N	2.26	0.68
2:N:401:ARG:HD3	2:N:401:ARG:N	2.07	0.68
1:Q:147:SER:OG	1:Q:148:GLY:N	2.26	0.68
1:O:147:SER:OG	1:O:148:GLY:N	2.26	0.68
1:A:147:SER:OG	1:A:148:GLY:N	2.26	0.67
2:H:401:ARG:HD3	2:H:401:ARG:N	2.07	0.67
1:G:177:VAL:HG23	1:G:207:GLU:OE1	1.95	0.67
1:C:177:VAL:HG23	1:C:207:GLU:OE1	1.95	0.67
1:M:177:VAL:HG23	1:M:207:GLU:OE1	1.95	0.67
1:A:177:VAL:HG23	1:A:207:GLU:OE1	1.95	0.67
1:O:177:VAL:HG23	1:O:207:GLU:OE1	1.95	0.67
1:I:177:VAL:HG23	1:I:207:GLU:OE1	1.95	0.66
2:B:85:GLN:CD	2:B:85:GLN:H	2.04	0.66
2:P:85:GLN:CD	2:P:85:GLN:H	2.04	0.66
2:J:85:GLN:H	2:J:85:GLN:CD	2.04	0.66
2:R:85:GLN:H	2:R:85:GLN:CD	2.04	0.66
1:E:177:VAL:HG23	1:E:207:GLU:OE1	1.95	0.66
2:F:85:GLN:CD	2:F:85:GLN:H	2.04	0.66
1:Q:177:VAL:HG23	1:Q:207:GLU:OE1	1.95	0.66
2:L:85:GLN:CD	2:L:85:GLN:H	2.04	0.66
1:A:439:SER:O	1:A:439:SER:OG	2.05	0.66
1:G:147:SER:OG	1:G:148:GLY:N	2.26	0.66
1:K:177:VAL:HG23	1:K:207:GLU:OE1	1.95	0.66
1:C:147:SER:OG	1:C:148:GLY:N	2.26	0.66
2:H:85:GLN:H	2:H:85:GLN:CD	2.04	0.66
1:M:147:SER:OG	1:M:148:GLY:N	2.26	0.66
2:N:85:GLN:CD	2:N:85:GLN:H	2.03	0.66
2:D:85:GLN:CD	2:D:85:GLN:H	2.04	0.65
2:L:401:ARG:N	2:L:401:ARG:CD	2.56	0.65
2:F:401:ARG:N	2:F:401:ARG:CD	2.56	0.65
2:R:401:ARG:N	2:R:401:ARG:CD	2.56	0.65
2:B:401:ARG:N	2:B:401:ARG:CD	2.56	0.64
2:P:401:ARG:N	2:P:401:ARG:CD	2.56	0.64
2:J:401:ARG:N	2:J:401:ARG:CD	2.56	0.64
1:E:439:SER:O	1:E:439:SER:OG	2.05	0.64
2:H:401:ARG:N	2:H:401:ARG:CD	2.56	0.63
2:D:401:ARG:N	2:D:401:ARG:CD	2.56	0.63
2:N:401:ARG:N	2:N:401:ARG:CD	2.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ILE:HG12	1:A:36:MET:SD	2.41	0.61
1:O:30:ILE:HG12	1:O:36:MET:SD	2.41	0.61
1:I:30:ILE:HG12	1:I:36:MET:SD	2.41	0.61
1:Q:30:ILE:HG12	1:Q:36:MET:SD	2.41	0.61
1:E:30:ILE:HG12	1:E:36:MET:SD	2.41	0.61
1:K:30:ILE:HG12	1:K:36:MET:SD	2.41	0.61
1:C:30:ILE:HG12	1:C:36:MET:SD	2.41	0.60
1:M:30:ILE:HG12	1:M:36:MET:SD	2.41	0.60
1:G:30:ILE:HG12	1:G:36:MET:SD	2.41	0.60
2:D:228:ASN:ND2	5:D:501:G2P:H1	1.93	0.60
2:N:228:ASN:ND2	5:N:501:G2P:H1	1.93	0.60
1:M:207:GLU:N	1:M:207:GLU:OE2	2.35	0.60
1:C:207:GLU:N	1:C:207:GLU:OE2	2.35	0.60
1:G:207:GLU:OE2	1:G:207:GLU:N	2.35	0.60
1:K:2:ARG:HA	1:K:133:GLN:HG3	1.84	0.60
1:Q:2:ARG:HA	1:Q:133:GLN:HG3	1.84	0.60
1:A:207:GLU:N	1:A:207:GLU:OE2	2.35	0.59
1:E:2:ARG:HA	1:E:133:GLN:HG3	1.84	0.59
1:I:207:GLU:OE2	1:I:207:GLU:N	2.35	0.59
2:L:228:ASN:ND2	5:L:501:G2P:H1	1.93	0.59
1:O:207:GLU:N	1:O:207:GLU:OE2	2.35	0.59
1:C:2:ARG:HA	1:C:133:GLN:HG3	1.84	0.59
1:M:2:ARG:HA	1:M:133:GLN:HG3	1.84	0.59
1:A:2:ARG:HA	1:A:133:GLN:HG3	1.84	0.59
1:E:207:GLU:OE2	1:E:207:GLU:N	2.35	0.59
1:G:2:ARG:HA	1:G:133:GLN:HG3	1.84	0.59
1:I:2:ARG:HA	1:I:133:GLN:HG3	1.83	0.59
1:O:2:ARG:HA	1:O:133:GLN:HG3	1.84	0.59
1:K:207:GLU:N	1:K:207:GLU:OE2	2.35	0.59
1:Q:207:GLU:OE2	1:Q:207:GLU:N	2.35	0.59
2:R:228:ASN:ND2	5:R:501:G2P:H1	1.93	0.59
2:F:228:ASN:ND2	5:F:501:G2P:H1	1.93	0.59
2:F:390:ARG:HA	2:F:390:ARG:NE	2.18	0.58
2:L:390:ARG:NE	2:L:390:ARG:HA	2.18	0.58
2:R:390:ARG:HA	2:R:390:ARG:NE	2.18	0.58
2:H:390:ARG:HA	2:H:390:ARG:NE	2.18	0.58
2:D:390:ARG:HA	2:D:390:ARG:NE	2.18	0.57
2:N:390:ARG:HA	2:N:390:ARG:NE	2.18	0.57
2:J:390:ARG:HA	2:J:390:ARG:NE	2.18	0.57
2:P:390:ARG:HA	2:P:390:ARG:NE	2.18	0.57
2:B:390:ARG:HA	2:B:390:ARG:NE	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ILE:O	1:A:341:ILE:CG1	2.43	0.57
1:O:341:ILE:O	1:O:341:ILE:CG1	2.43	0.56
1:I:341:ILE:O	1:I:341:ILE:CG1	2.43	0.56
2:N:85:GLN:CD	2:N:85:GLN:N	2.64	0.56
2:D:85:GLN:CD	2:D:85:GLN:N	2.64	0.56
2:H:85:GLN:CD	2:H:85:GLN:N	2.64	0.56
2:H:228:ASN:ND2	5:H:501:G2P:H1	1.93	0.55
1:C:246:GLY:HA3	1:C:356:ASN:HA	1.89	0.55
1:G:246:GLY:HA3	1:G:356:ASN:HA	1.89	0.55
2:J:228:ASN:ND2	5:J:501:G2P:H1	1.93	0.55
1:M:246:GLY:HA3	1:M:356:ASN:HA	1.89	0.55
2:P:228:ASN:ND2	5:P:501:G2P:H1	1.93	0.55
2:B:228:ASN:ND2	5:B:501:G2P:H1	1.93	0.55
2:B:85:GLN:CD	2:B:85:GLN:N	2.64	0.55
1:K:246:GLY:HA3	1:K:356:ASN:HA	1.89	0.54
2:B:269:MET:SD	2:B:307:PRO:HG3	2.48	0.54
1:E:246:GLY:HA3	1:E:356:ASN:HA	1.89	0.54
2:P:269:MET:SD	2:P:307:PRO:HG3	2.48	0.54
1:Q:246:GLY:HA3	1:Q:356:ASN:HA	1.89	0.54
1:A:246:GLY:HA3	1:A:356:ASN:HA	1.89	0.54
2:F:269:MET:SD	2:F:307:PRO:HG3	2.48	0.54
2:J:269:MET:SD	2:J:307:PRO:HG3	2.48	0.54
1:O:246:GLY:HA3	1:O:356:ASN:HA	1.89	0.54
2:R:269:MET:SD	2:R:307:PRO:HG3	2.48	0.54
2:H:269:MET:SD	2:H:307:PRO:HG3	2.48	0.54
1:I:246:GLY:HA3	1:I:356:ASN:HA	1.89	0.54
2:L:269:MET:SD	2:L:307:PRO:HG3	2.48	0.54
2:D:269:MET:SD	2:D:307:PRO:HG3	2.48	0.54
2:N:269:MET:SD	2:N:307:PRO:HG3	2.48	0.54
2:H:277:SER:OG	2:H:278:ARG:N	2.41	0.54
2:N:277:SER:OG	2:N:278:ARG:N	2.41	0.54
2:D:277:SER:OG	2:D:278:ARG:N	2.41	0.54
1:C:341:ILE:O	1:C:341:ILE:CG1	2.43	0.53
1:M:341:ILE:O	1:M:341:ILE:CG1	2.43	0.53
2:P:85:GLN:CD	2:P:85:GLN:N	2.64	0.53
2:J:85:GLN:CD	2:J:85:GLN:N	2.64	0.53
2:F:85:GLN:CD	2:F:85:GLN:N	2.64	0.53
2:P:283:TYR:CE1	2:R:89:PRO:HD3	2.44	0.53
2:R:85:GLN:CD	2:R:85:GLN:N	2.64	0.53
2:L:85:GLN:CD	2:L:85:GLN:N	2.64	0.53
2:F:277:SER:OG	2:F:278:ARG:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:277:SER:OG	2:L:278:ARG:N	2.41	0.53
2:R:277:SER:OG	2:R:278:ARG:N	2.41	0.53
1:E:346:TRP:H	1:E:346:TRP:CD1	2.27	0.53
1:G:341:ILE:O	1:G:341:ILE:CG1	2.43	0.53
1:Q:346:TRP:H	1:Q:346:TRP:CD1	2.27	0.52
1:K:346:TRP:H	1:K:346:TRP:CD1	2.27	0.52
1:I:346:TRP:H	1:I:346:TRP:CD1	2.28	0.52
1:O:346:TRP:H	1:O:346:TRP:CD1	2.27	0.52
1:A:346:TRP:H	1:A:346:TRP:CD1	2.27	0.52
2:D:288:VAL:HB	2:D:327:GLU:HG2	1.91	0.52
1:G:346:TRP:CD1	1:G:346:TRP:H	2.27	0.52
2:H:288:VAL:HB	2:H:327:GLU:HG2	1.91	0.52
2:L:2:ARG:N	2:L:131:CYS:O	2.43	0.52
2:J:288:VAL:HB	2:J:327:GLU:HG2	1.91	0.52
2:N:288:VAL:HB	2:N:327:GLU:HG2	1.91	0.52
2:R:2:ARG:N	2:R:131:CYS:O	2.43	0.52
2:B:288:VAL:HB	2:B:327:GLU:HG2	1.91	0.51
2:F:2:ARG:N	2:F:131:CYS:O	2.43	0.51
2:P:288:VAL:HB	2:P:327:GLU:HG2	1.91	0.51
2:H:283:TYR:CE1	2:J:89:PRO:HD3	2.46	0.51
1:M:346:TRP:H	1:M:346:TRP:CD1	2.28	0.51
1:K:143:GLY:O	1:K:147:SER:OG	2.28	0.51
1:Q:143:GLY:O	1:Q:147:SER:OG	2.28	0.51
2:B:277:SER:OG	2:B:278:ARG:N	2.41	0.51
1:I:346:TRP:CD1	1:I:346:TRP:N	2.78	0.51
2:L:288:VAL:HB	2:L:327:GLU:HG2	1.91	0.51
2:N:2:ARG:N	2:N:131:CYS:O	2.43	0.51
2:P:277:SER:OG	2:P:278:ARG:N	2.41	0.51
2:R:288:VAL:HB	2:R:327:GLU:HG2	1.91	0.51
1:A:346:TRP:CD1	1:A:346:TRP:N	2.78	0.51
1:C:346:TRP:N	1:C:346:TRP:CD1	2.78	0.51
2:D:2:ARG:N	2:D:131:CYS:O	2.43	0.51
2:F:288:VAL:HB	2:F:327:GLU:HG2	1.91	0.51
2:H:2:ARG:N	2:H:131:CYS:O	2.43	0.51
2:H:284:ARG:NH1	2:J:90:ASP:OD2	2.43	0.51
2:J:2:ARG:N	2:J:131:CYS:O	2.43	0.51
2:J:277:SER:OG	2:J:278:ARG:N	2.41	0.51
1:M:346:TRP:CD1	1:M:346:TRP:N	2.78	0.51
1:O:346:TRP:CD1	1:O:346:TRP:N	2.78	0.51
1:C:346:TRP:CD1	1:C:346:TRP:H	2.27	0.51
2:F:401:ARG:NH2	1:K:345:ASP:OD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:N	2:B:131:CYS:O	2.43	0.51
1:K:346:TRP:CD1	1:K:346:TRP:N	2.78	0.51
2:P:2:ARG:N	2:P:131:CYS:O	2.43	0.51
1:C:282:TYR:O	1:C:283:HIS:HB2	2.11	0.51
1:M:282:TYR:O	1:M:283:HIS:HB2	2.11	0.51
1:E:346:TRP:CD1	1:E:346:TRP:N	2.78	0.50
2:D:401:ARG:NH2	1:G:345:ASP:OD2	2.43	0.50
2:J:283:TYR:CE1	2:L:89:PRO:HD3	2.46	0.50
1:Q:346:TRP:CD1	1:Q:346:TRP:N	2.78	0.50
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.94	0.50
1:G:282:TYR:O	1:G:283:HIS:HB2	2.11	0.50
1:G:346:TRP:CD1	1:G:346:TRP:N	2.78	0.50
1:M:180:ALA:HB3	1:M:183:GLU:HG3	1.94	0.50
1:A:143:GLY:O	1:A:147:SER:OG	2.28	0.50
1:G:180:ALA:HB3	1:G:183:GLU:HG3	1.94	0.50
1:O:143:GLY:O	1:O:147:SER:OG	2.28	0.50
2:D:360:PRO:HG2	2:D:371:LEU:HB2	1.93	0.50
2:N:360:PRO:HG2	2:N:371:LEU:HB2	1.93	0.50
1:E:180:ALA:HB3	1:E:183:GLU:HG3	1.94	0.50
1:E:326:LYS:HD2	1:E:326:LYS:C	2.37	0.50
1:I:326:LYS:C	1:I:326:LYS:HD2	2.37	0.50
1:K:180:ALA:HB3	1:K:183:GLU:HG3	1.94	0.50
2:N:283:TYR:CE1	2:P:89:PRO:HD3	2.47	0.50
1:Q:180:ALA:HB3	1:Q:183:GLU:HG3	1.94	0.50
1:Q:326:LYS:HD2	1:Q:326:LYS:C	2.37	0.50
1:I:143:GLY:O	1:I:147:SER:OG	2.28	0.50
1:K:326:LYS:C	1:K:326:LYS:HD2	2.37	0.50
1:O:326:LYS:HD2	1:O:326:LYS:C	2.37	0.50
1:A:282:TYR:O	1:A:283:HIS:HB2	2.11	0.50
1:A:326:LYS:C	1:A:326:LYS:HD2	2.37	0.50
2:H:360:PRO:HG2	2:H:371:LEU:HB2	1.93	0.50
1:I:282:TYR:O	1:I:283:HIS:HB2	2.11	0.50
2:L:195:VAL:O	2:L:195:VAL:HG22	2.12	0.50
1:O:282:TYR:O	1:O:283:HIS:HB2	2.11	0.50
2:B:195:VAL:O	2:B:195:VAL:HG22	2.12	0.49
2:P:195:VAL:HG22	2:P:195:VAL:O	2.12	0.49
2:B:360:PRO:HG2	2:B:371:LEU:HB2	1.93	0.49
2:F:195:VAL:HG22	2:F:195:VAL:O	2.12	0.49
2:J:195:VAL:HG22	2:J:195:VAL:O	2.12	0.49
2:R:195:VAL:HG22	2:R:195:VAL:O	2.12	0.49
2:J:360:PRO:HG2	2:J:371:LEU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:282:TYR:O	1:K:283:HIS:HB2	2.11	0.49
2:P:360:PRO:HG2	2:P:371:LEU:HB2	1.93	0.49
1:Q:282:TYR:O	1:Q:283:HIS:HB2	2.11	0.49
2:D:181:VAL:O	2:D:398:MET:SD	2.71	0.49
1:E:282:TYR:O	1:E:283:HIS:HB2	2.12	0.49
2:H:181:VAL:O	2:H:398:MET:SD	2.71	0.49
2:N:181:VAL:O	2:N:398:MET:SD	2.71	0.49
1:C:326:LYS:HD2	1:C:326:LYS:C	2.37	0.49
1:G:326:LYS:HD2	1:G:326:LYS:C	2.37	0.49
2:J:181:VAL:O	2:J:398:MET:SD	2.71	0.49
1:M:326:LYS:C	1:M:326:LYS:HD2	2.37	0.49
1:E:306:ASP:C	1:E:306:ASP:OD1	2.56	0.49
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.94	0.49
2:F:360:PRO:HG2	2:F:371:LEU:HB2	1.93	0.49
1:Q:306:ASP:OD1	1:Q:306:ASP:C	2.56	0.49
2:R:360:PRO:HG2	2:R:371:LEU:HB2	1.93	0.49
2:B:181:VAL:O	2:B:398:MET:SD	2.71	0.48
2:B:401:ARG:NH2	1:I:345:ASP:OD2	2.45	0.48
1:G:15:GLN:OE1	1:G:15:GLN:HA	2.14	0.48
1:I:180:ALA:HB3	1:I:183:GLU:HG3	1.94	0.48
1:K:306:ASP:OD1	1:K:306:ASP:C	2.56	0.48
2:L:360:PRO:HG2	2:L:371:LEU:HB2	1.93	0.48
1:M:15:GLN:HA	1:M:15:GLN:OE1	2.13	0.48
2:P:181:VAL:O	2:P:398:MET:SD	2.71	0.48
1:C:15:GLN:OE1	1:C:15:GLN:HA	2.14	0.48
1:O:180:ALA:HB3	1:O:183:GLU:HG3	1.94	0.48
2:L:181:VAL:O	2:L:398:MET:SD	2.71	0.48
2:D:195:VAL:O	2:D:195:VAL:HG22	2.12	0.48
1:E:143:GLY:O	1:E:147:SER:OG	2.28	0.48
2:N:195:VAL:O	2:N:195:VAL:HG22	2.12	0.48
2:H:348:PRO:O	2:H:349:ASN:HB2	2.14	0.48
2:N:348:PRO:O	2:N:349:ASN:HB2	2.14	0.48
2:D:348:PRO:O	2:D:349:ASN:HB2	2.14	0.48
2:F:181:VAL:O	2:F:398:MET:SD	2.71	0.48
2:H:195:VAL:HG22	2:H:195:VAL:O	2.12	0.48
1:O:15:GLN:OE1	1:O:15:GLN:HA	2.13	0.48
1:A:15:GLN:HA	1:A:15:GLN:OE1	2.13	0.48
2:F:348:PRO:O	2:F:349:ASN:HB2	2.14	0.48
2:H:40:SER:OG	2:H:41:ASP:N	2.46	0.48
2:R:181:VAL:O	2:R:398:MET:SD	2.71	0.48
2:B:401:ARG:HA	2:B:401:ARG:HD2	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:40:SER:OG	2:F:41:ASP:N	2.46	0.47
1:I:15:GLN:HA	1:I:15:GLN:OE1	2.13	0.47
2:R:348:PRO:O	2:R:349:ASN:HB2	2.14	0.47
2:N:40:SER:OG	2:N:41:ASP:N	2.46	0.47
2:N:284:ARG:NH1	2:P:90:ASP:OD2	2.47	0.47
2:R:40:SER:OG	2:R:41:ASP:N	2.46	0.47
2:D:31:ASP:C	2:D:31:ASP:OD1	2.57	0.47
2:D:40:SER:OG	2:D:41:ASP:N	2.46	0.47
2:L:40:SER:OG	2:L:41:ASP:N	2.46	0.47
2:L:348:PRO:O	2:L:349:ASN:HB2	2.14	0.47
1:Q:15:GLN:OE1	1:Q:15:GLN:HA	2.13	0.47
2:H:31:ASP:OD1	2:H:31:ASP:C	2.58	0.47
1:K:15:GLN:HA	1:K:15:GLN:OE1	2.13	0.47
2:N:31:ASP:OD1	2:N:31:ASP:C	2.58	0.47
1:E:15:GLN:OE1	1:E:15:GLN:HA	2.14	0.47
1:G:439:SER:O	1:G:439:SER:OG	2.05	0.47
1:A:306:ASP:OD1	1:A:306:ASP:C	2.56	0.47
2:D:401:ARG:HA	2:D:401:ARG:HD2	1.61	0.47
2:J:348:PRO:O	2:J:349:ASN:HB2	2.14	0.47
2:N:401:ARG:HA	2:N:401:ARG:HD2	1.61	0.47
2:P:348:PRO:O	2:P:349:ASN:HB2	2.14	0.47
1:C:439:SER:O	1:C:439:SER:OG	2.05	0.47
2:J:31:ASP:OD1	2:J:31:ASP:C	2.58	0.47
1:O:306:ASP:C	1:O:306:ASP:OD1	2.56	0.47
2:B:348:PRO:O	2:B:349:ASN:HB2	2.14	0.47
1:I:101:ASN:OD1	2:J:254:LYS:NZ	2.48	0.47
1:A:101:ASN:OD1	2:B:254:LYS:NZ	2.48	0.46
2:B:31:ASP:OD1	2:B:31:ASP:C	2.58	0.46
2:B:338:LYS:NZ	2:F:127:GLU:OE2	2.44	0.46
2:J:40:SER:OG	2:J:41:ASP:N	2.46	0.46
1:O:101:ASN:OD1	2:P:254:LYS:NZ	2.48	0.46
2:P:31:ASP:C	2:P:31:ASP:OD1	2.58	0.46
2:B:40:SER:OG	2:B:41:ASP:N	2.46	0.46
2:P:40:SER:OG	2:P:41:ASP:N	2.46	0.46
1:I:306:ASP:OD1	1:I:306:ASP:C	2.56	0.46
2:F:31:ASP:C	2:F:31:ASP:OD1	2.58	0.46
1:I:220:GLU:OE2	1:I:221:ARG:NH1	2.49	0.46
1:K:220:GLU:OE2	1:K:221:ARG:NH1	2.49	0.46
2:R:31:ASP:C	2:R:31:ASP:OD1	2.58	0.46
1:C:306:ASP:C	1:C:306:ASP:OD1	2.56	0.46
1:E:238:ILE:O	1:E:238:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:238:ILE:O	1:K:238:ILE:HG22	2.16	0.46
2:L:31:ASP:OD1	2:L:31:ASP:C	2.57	0.46
2:P:71:GLU:HA	2:P:72:PRO:HD3	1.75	0.46
1:Q:220:GLU:OE2	1:Q:221:ARG:NH1	2.49	0.46
1:Q:238:ILE:O	1:Q:238:ILE:HG22	2.16	0.46
1:E:220:GLU:OE2	1:E:221:ARG:NH1	2.49	0.46
1:M:306:ASP:C	1:M:306:ASP:OD1	2.56	0.46
1:O:220:GLU:OE2	1:O:221:ARG:NH1	2.49	0.46
1:A:220:GLU:OE2	1:A:221:ARG:NH1	2.49	0.46
2:B:180:THR:HG23	2:B:183:GLU:HB2	1.98	0.46
2:D:180:THR:HG23	2:D:183:GLU:HB2	1.98	0.46
1:E:101:ASN:OD1	2:F:254:LYS:NZ	2.48	0.46
1:G:306:ASP:OD1	1:G:306:ASP:C	2.56	0.46
2:H:180:THR:HG23	2:H:183:GLU:HB2	1.98	0.46
2:N:180:THR:HG23	2:N:183:GLU:HB2	1.98	0.46
2:P:180:THR:HG23	2:P:183:GLU:HB2	1.98	0.46
1:Q:101:ASN:OD1	2:R:254:LYS:NZ	2.48	0.46
1:E:49:PHE:C	1:E:51:THR:H	2.24	0.46
1:G:220:GLU:OE2	1:G:221:ARG:NH1	2.49	0.46
2:B:71:GLU:HA	2:B:72:PRO:HD3	1.75	0.46
1:E:278:ALA:HA	1:E:369:ALA:HB2	1.98	0.46
1:I:241:SER:O	1:I:356:ASN:ND2	2.48	0.46
2:J:180:THR:HG23	2:J:183:GLU:HB2	1.98	0.46
1:K:241:SER:O	1:K:356:ASN:ND2	2.48	0.46
2:L:180:THR:HG23	2:L:183:GLU:HB2	1.98	0.46
1:Q:49:PHE:C	1:Q:51:THR:H	2.24	0.46
2:F:390:ARG:HA	2:F:390:ARG:HE	1.80	0.46
1:I:238:ILE:O	1:I:238:ILE:HG22	2.16	0.46
1:K:101:ASN:OD1	2:L:254:LYS:NZ	2.48	0.46
1:M:220:GLU:OE2	1:M:221:ARG:NH1	2.49	0.46
2:P:67:LEU:N	2:P:67:LEU:HD12	2.31	0.46
1:Q:278:ALA:HA	1:Q:369:ALA:HB2	1.98	0.46
2:B:67:LEU:N	2:B:67:LEU:HD12	2.31	0.45
1:C:220:GLU:OE2	1:C:221:ARG:NH1	2.49	0.45
1:E:341:ILE:O	1:E:341:ILE:CG1	2.43	0.45
1:I:278:ALA:HA	1:I:369:ALA:HB2	1.98	0.45
1:K:278:ALA:HA	1:K:369:ALA:HB2	1.98	0.45
1:O:238:ILE:O	1:O:238:ILE:HG22	2.16	0.45
1:A:238:ILE:O	1:A:238:ILE:HG22	2.16	0.45
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.98	0.45
2:B:390:ARG:HA	2:B:390:ARG:HE	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:180:THR:HG23	2:F:183:GLU:HB2	1.98	0.45
1:G:278:ALA:HA	1:G:369:ALA:HB2	1.98	0.45
1:O:278:ALA:HA	1:O:369:ALA:HB2	1.98	0.45
2:R:390:ARG:HA	2:R:390:ARG:HE	1.80	0.45
1:G:385:ALA:HB1	1:G:429:GLU:HG3	1.98	0.45
1:I:49:PHE:C	1:I:51:THR:H	2.24	0.45
2:J:67:LEU:N	2:J:67:LEU:HD12	2.31	0.45
1:K:49:PHE:C	1:K:51:THR:H	2.24	0.45
2:P:390:ARG:HA	2:P:390:ARG:HE	1.80	0.45
2:R:180:THR:HG23	2:R:183:GLU:HB2	1.98	0.45
1:C:385:ALA:HB1	1:C:429:GLU:HG3	1.98	0.45
2:D:390:ARG:HA	2:D:390:ARG:HE	1.80	0.45
2:H:390:ARG:HA	2:H:390:ARG:HE	1.80	0.45
1:M:385:ALA:HB1	1:M:429:GLU:HG3	1.98	0.45
2:N:390:ARG:HA	2:N:390:ARG:HE	1.80	0.45
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.98	0.45
2:J:390:ARG:HA	2:J:390:ARG:HE	1.80	0.45
1:K:216:ASN:HB3	1:K:275:VAL:O	2.16	0.45
2:L:67:LEU:N	2:L:67:LEU:HD12	2.31	0.45
2:L:390:ARG:HA	2:L:390:ARG:HE	1.80	0.45
1:M:238:ILE:O	1:M:238:ILE:HG22	2.16	0.45
1:M:278:ALA:HA	1:M:369:ALA:HB2	1.98	0.45
1:O:49:PHE:C	1:O:51:THR:H	2.24	0.45
1:Q:341:ILE:O	1:Q:341:ILE:CG1	2.43	0.45
1:A:49:PHE:C	1:A:51:THR:H	2.24	0.45
1:C:238:ILE:O	1:C:238:ILE:HG22	2.16	0.45
1:G:238:ILE:O	1:G:238:ILE:HG22	2.16	0.45
1:M:216:ASN:HB3	1:M:275:VAL:O	2.16	0.45
1:C:216:ASN:HB3	1:C:275:VAL:O	2.16	0.45
2:H:67:LEU:HD12	2:H:67:LEU:N	2.31	0.45
1:I:385:ALA:HB1	1:I:429:GLU:HG3	1.98	0.45
1:O:385:ALA:HB1	1:O:429:GLU:HG3	1.98	0.45
1:Q:216:ASN:HB3	1:Q:275:VAL:O	2.16	0.45
1:A:385:ALA:HB1	1:A:429:GLU:HG3	1.98	0.45
1:E:216:ASN:HB3	1:E:275:VAL:O	2.16	0.45
1:G:49:PHE:C	1:G:51:THR:H	2.24	0.45
1:I:216:ASN:HB3	1:I:275:VAL:O	2.16	0.45
2:P:54:ASN:OD1	2:P:64:ARG:NH1	2.50	0.45
2:R:67:LEU:HD12	2:R:67:LEU:N	2.32	0.45
1:A:216:ASN:HB3	1:A:275:VAL:O	2.16	0.45
2:B:54:ASN:OD1	2:B:64:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:GLU:N	2:B:184:PRO:CD	2.80	0.45
1:C:143:GLY:O	1:C:147:SER:OG	2.28	0.45
2:F:67:LEU:HD12	2:F:67:LEU:N	2.32	0.45
2:L:172:VAL:HA	2:L:173:PRO:HD3	1.82	0.45
2:L:183:GLU:N	2:L:184:PRO:CD	2.80	0.45
1:M:143:GLY:O	1:M:147:SER:OG	2.28	0.45
1:O:216:ASN:HB3	1:O:275:VAL:O	2.16	0.45
2:P:183:GLU:N	2:P:184:PRO:CD	2.80	0.45
2:R:172:VAL:HA	2:R:173:PRO:HD3	1.82	0.45
1:C:49:PHE:C	1:C:51:THR:H	2.24	0.45
2:F:172:VAL:HA	2:F:173:PRO:HD3	1.82	0.45
1:G:216:ASN:HB3	1:G:275:VAL:O	2.16	0.45
2:H:54:ASN:OD1	2:H:64:ARG:NH1	2.50	0.45
2:J:54:ASN:OD1	2:J:64:ARG:NH1	2.50	0.45
1:K:385:ALA:HB1	1:K:429:GLU:HG3	1.98	0.45
2:N:67:LEU:N	2:N:67:LEU:HD12	2.31	0.45
2:R:183:GLU:N	2:R:184:PRO:CD	2.80	0.45
1:C:241:SER:O	1:C:356:ASN:ND2	2.48	0.44
2:D:67:LEU:N	2:D:67:LEU:HD12	2.31	0.44
2:F:183:GLU:N	2:F:184:PRO:CD	2.80	0.44
2:J:183:GLU:N	2:J:184:PRO:CD	2.80	0.44
1:M:49:PHE:C	1:M:51:THR:H	2.24	0.44
1:M:241:SER:O	1:M:356:ASN:ND2	2.48	0.44
1:Q:385:ALA:HB1	1:Q:429:GLU:HG3	1.98	0.44
2:D:172:VAL:HA	2:D:173:PRO:HD3	1.82	0.44
1:E:241:SER:O	1:E:356:ASN:ND2	2.48	0.44
1:E:385:ALA:HB1	1:E:429:GLU:HG3	1.98	0.44
1:K:341:ILE:O	1:K:341:ILE:CG1	2.43	0.44
2:L:54:ASN:OD1	2:L:64:ARG:NH1	2.50	0.44
2:L:71:GLU:HA	2:L:72:PRO:HD3	1.75	0.44
2:N:172:VAL:HA	2:N:173:PRO:HD3	1.82	0.44
1:A:241:SER:O	1:A:356:ASN:ND2	2.48	0.44
1:C:49:PHE:C	1:C:51:THR:N	2.73	0.44
2:H:172:VAL:HA	2:H:173:PRO:HD3	1.82	0.44
1:I:209:ILE:O	1:I:209:ILE:HG22	2.16	0.44
2:N:54:ASN:OD1	2:N:64:ARG:NH1	2.50	0.44
2:R:54:ASN:OD1	2:R:64:ARG:NH1	2.50	0.44
1:A:209:ILE:O	1:A:209:ILE:HG22	2.16	0.44
2:D:54:ASN:OD1	2:D:64:ARG:NH1	2.50	0.44
2:D:269:MET:O	2:D:269:MET:HG2	2.18	0.44
2:F:54:ASN:OD1	2:F:64:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:GLY:O	1:G:147:SER:OG	2.28	0.44
2:H:269:MET:O	2:H:269:MET:HG2	2.18	0.44
2:J:269:MET:O	2:J:269:MET:HG2	2.18	0.44
1:M:49:PHE:C	1:M:51:THR:N	2.73	0.44
2:N:269:MET:O	2:N:269:MET:HG2	2.18	0.44
1:O:241:SER:O	1:O:356:ASN:ND2	2.48	0.44
2:B:269:MET:O	2:B:269:MET:HG2	2.18	0.44
1:G:241:SER:O	1:G:356:ASN:ND2	2.48	0.44
2:H:183:GLU:N	2:H:184:PRO:CD	2.80	0.44
1:O:209:ILE:O	1:O:209:ILE:HG22	2.16	0.44
2:P:269:MET:O	2:P:269:MET:HG2	2.18	0.44
1:Q:241:SER:O	1:Q:356:ASN:ND2	2.48	0.44
2:F:269:MET:O	2:F:269:MET:HG2	2.18	0.44
1:G:101:ASN:OD1	2:H:254:LYS:NZ	2.48	0.44
2:H:209:LEU:HB3	2:H:227:LEU:HD22	2.00	0.44
2:J:209:LEU:HB3	2:J:227:LEU:HD22	2.00	0.44
2:D:209:LEU:HB3	2:D:227:LEU:HD22	2.00	0.44
2:J:284:ARG:NH1	2:L:90:ASP:OD2	2.50	0.44
2:L:269:MET:O	2:L:269:MET:HG2	2.18	0.44
2:R:269:MET:O	2:R:269:MET:HG2	2.18	0.44
2:B:209:LEU:HB3	2:B:227:LEU:HD22	2.00	0.44
2:D:183:GLU:N	2:D:184:PRO:CD	2.80	0.44
1:G:49:PHE:C	1:G:51:THR:N	2.73	0.44
1:I:175:PRO:O	2:J:349:ASN:ND2	2.51	0.44
2:N:183:GLU:N	2:N:184:PRO:CD	2.80	0.44
2:F:209:LEU:HB3	2:F:227:LEU:HD22	2.00	0.44
2:N:209:LEU:HB3	2:N:227:LEU:HD22	2.00	0.44
2:P:209:LEU:HB3	2:P:227:LEU:HD22	2.00	0.44
2:R:209:LEU:HB3	2:R:227:LEU:HD22	2.00	0.44
1:A:175:PRO:O	2:B:349:ASN:ND2	2.51	0.43
1:E:209:ILE:O	1:E:209:ILE:HG22	2.16	0.43
2:L:209:LEU:HB3	2:L:227:LEU:HD22	2.00	0.43
1:M:101:ASN:OD1	2:N:254:LYS:NZ	2.48	0.43
1:O:175:PRO:O	2:P:349:ASN:ND2	2.51	0.43
2:R:71:GLU:HA	2:R:72:PRO:HD3	1.75	0.43
1:C:101:ASN:OD1	2:D:254:LYS:NZ	2.48	0.43
2:D:181:VAL:HG12	1:G:350:GLY:HA2	2.00	0.43
2:B:269:MET:HG3	2:B:303:ALA:HB3	2.01	0.43
2:F:71:GLU:HA	2:F:72:PRO:HD3	1.75	0.43
2:H:269:MET:HG3	2:H:303:ALA:HB3	2.01	0.43
2:J:269:MET:HG3	2:J:303:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:269:MET:HG3	2:P:303:ALA:HB3	2.01	0.43
2:R:269:MET:HG3	2:R:303:ALA:HB3	2.01	0.43
1:A:49:PHE:C	1:A:51:THR:N	2.73	0.43
2:D:269:MET:HG3	2:D:303:ALA:HB3	2.01	0.43
2:F:269:MET:HG3	2:F:303:ALA:HB3	2.01	0.43
2:L:269:MET:HG3	2:L:303:ALA:HB3	2.01	0.43
2:N:269:MET:HG3	2:N:303:ALA:HB3	2.01	0.43
2:N:281:GLN:HA	2:N:284:ARG:HG2	2.01	0.43
2:D:281:GLN:HA	2:D:284:ARG:HG2	2.01	0.43
2:H:281:GLN:HA	2:H:284:ARG:HG2	2.01	0.43
2:R:281:GLN:HA	2:R:284:ARG:HG2	2.01	0.43
2:F:281:GLN:HA	2:F:284:ARG:HG2	2.01	0.43
2:L:281:GLN:HA	2:L:284:ARG:HG2	2.01	0.43
1:O:49:PHE:C	1:O:51:THR:N	2.73	0.43
2:P:281:GLN:HA	2:P:284:ARG:HG2	2.01	0.43
2:B:281:GLN:HA	2:B:284:ARG:HG2	2.01	0.43
2:P:284:ARG:NH1	2:R:90:ASP:OD2	2.51	0.43
2:B:241:CYS:SG	2:B:356:CYS:HB3	2.59	0.43
2:H:241:CYS:SG	2:H:356:CYS:HB3	2.59	0.43
2:J:241:CYS:SG	2:J:356:CYS:HB3	2.59	0.43
2:J:281:GLN:HA	2:J:284:ARG:HG2	2.01	0.43
2:N:241:CYS:SG	2:N:356:CYS:HB3	2.59	0.43
2:D:241:CYS:SG	2:D:356:CYS:HB3	2.59	0.42
2:F:241:CYS:SG	2:F:356:CYS:HB3	2.59	0.42
1:G:209:ILE:O	1:G:209:ILE:HG22	2.16	0.42
2:P:241:CYS:SG	2:P:356:CYS:HB3	2.59	0.42
2:R:241:CYS:SG	2:R:356:CYS:HB3	2.59	0.42
1:C:402:ARG:HA	1:C:402:ARG:HD3	1.87	0.42
1:I:49:PHE:C	1:I:51:THR:N	2.73	0.42
2:L:15:GLN:NE2	5:L:501:G2P:O6	2.53	0.42
1:M:402:ARG:HA	1:M:402:ARG:HD3	1.87	0.42
2:R:15:GLN:NE2	5:R:501:G2P:O6	2.53	0.42
2:B:15:GLN:NE2	5:B:501:G2P:O6	2.53	0.42
2:F:15:GLN:NE2	5:F:501:G2P:O6	2.53	0.42
2:L:241:CYS:SG	2:L:356:CYS:HB3	2.59	0.42
2:P:15:GLN:NE2	5:P:501:G2P:O6	2.53	0.42
1:A:402:ARG:HA	1:A:402:ARG:HD3	1.87	0.42
1:G:175:PRO:O	2:H:349:ASN:ND2	2.51	0.42
1:K:176:GLN:HE21	1:K:176:GLN:HB2	1.67	0.42
1:O:284:GLU:OE2	1:Q:124:LYS:NZ	2.37	0.42
1:O:402:ARG:HA	1:O:402:ARG:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.42
1:E:49:PHE:C	1:E:51:THR:N	2.73	0.42
1:I:183:GLU:N	1:I:184:PRO:CD	2.83	0.42
2:J:15:GLN:NE2	5:J:501:G2P:O6	2.53	0.42
1:O:183:GLU:N	1:O:184:PRO:CD	2.83	0.42
1:Q:402:ARG:HA	1:Q:402:ARG:HD3	1.87	0.42
1:C:175:PRO:O	2:D:349:ASN:ND2	2.51	0.42
1:C:209:ILE:O	1:C:209:ILE:HG22	2.16	0.42
1:E:402:ARG:HA	1:E:402:ARG:HD3	1.87	0.42
1:K:209:ILE:O	1:K:209:ILE:HG22	2.16	0.42
1:M:209:ILE:O	1:M:209:ILE:HG22	2.16	0.42
2:D:15:GLN:NE2	5:D:501:G2P:O6	2.53	0.42
2:F:401:ARG:NH1	1:K:345:ASP:OD2	2.53	0.42
1:I:402:ARG:HA	1:I:402:ARG:HD3	1.87	0.42
1:M:175:PRO:O	2:N:349:ASN:ND2	2.51	0.42
2:N:15:GLN:NE2	5:N:501:G2P:O6	2.53	0.42
1:C:183:GLU:N	1:C:184:PRO:CD	2.83	0.42
1:E:346:TRP:H	1:E:346:TRP:HD1	1.68	0.42
1:G:260:VAL:HA	1:G:261:PRO:HD2	1.87	0.42
1:M:183:GLU:N	1:M:184:PRO:CD	2.83	0.42
1:Q:49:PHE:C	1:Q:51:THR:N	2.73	0.42
1:Q:209:ILE:O	1:Q:209:ILE:HG22	2.16	0.42
1:G:402:ARG:HA	1:G:402:ARG:HD3	1.87	0.42
1:K:346:TRP:H	1:K:346:TRP:HD1	1.68	0.42
1:K:402:ARG:HA	1:K:402:ARG:HD3	1.87	0.42
2:L:82:PRO:O	2:L:83:PHE:HB2	2.20	0.42
2:L:262:PHE:HA	2:L:263:PRO:HD3	1.93	0.42
1:Q:346:TRP:H	1:Q:346:TRP:HD1	1.68	0.42
2:R:82:PRO:O	2:R:83:PHE:HB2	2.20	0.42
2:D:82:PRO:O	2:D:83:PHE:HB2	2.20	0.42
2:D:401:ARG:NH1	1:G:345:ASP:OD2	2.53	0.42
1:G:183:GLU:N	1:G:184:PRO:CD	2.83	0.42
1:G:283:HIS:HA	1:I:56:THR:HG21	2.01	0.42
2:H:15:GLN:NE2	5:H:501:G2P:O6	2.53	0.42
1:I:346:TRP:H	1:I:346:TRP:HD1	1.68	0.42
1:K:260:VAL:HA	1:K:261:PRO:HD2	1.87	0.42
2:B:147:SER:HB2	2:B:190:SER:HB3	2.02	0.41
1:G:172:TYR:HA	1:G:173:PRO:HD3	1.87	0.41
2:H:82:PRO:O	2:H:83:PHE:HB2	2.20	0.41
2:H:147:SER:HB2	2:H:190:SER:HB3	2.02	0.41
1:I:260:VAL:HA	1:I:261:PRO:HD2	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:147:SER:HB2	2:J:190:SER:HB3	2.02	0.41
2:J:262:PHE:HA	2:J:263:PRO:HD3	1.93	0.41
2:J:288:VAL:N	2:J:289:PRO:CD	2.83	0.41
2:L:147:SER:HB2	2:L:190:SER:HB3	2.02	0.41
2:N:82:PRO:O	2:N:83:PHE:HB2	2.20	0.41
1:Q:359:PRO:HA	1:Q:360:PRO:HD3	1.76	0.41
2:B:288:VAL:N	2:B:289:PRO:CD	2.83	0.41
1:C:94:THR:OG1	1:C:95:GLY:N	2.53	0.41
1:E:183:GLU:N	1:E:184:PRO:CD	2.83	0.41
1:E:359:PRO:HA	1:E:360:PRO:HD3	1.76	0.41
2:F:82:PRO:O	2:F:83:PHE:HB2	2.20	0.41
1:G:49:PHE:HD1	1:G:49:PHE:HA	1.72	0.41
2:J:82:PRO:O	2:J:83:PHE:HB2	2.20	0.41
1:M:94:THR:OG1	1:M:95:GLY:N	2.53	0.41
1:M:260:VAL:HA	1:M:261:PRO:HD2	1.87	0.41
2:N:147:SER:HB2	2:N:190:SER:HB3	2.02	0.41
2:P:147:SER:HB2	2:P:190:SER:HB3	2.02	0.41
2:P:288:VAL:N	2:P:289:PRO:CD	2.83	0.41
2:R:147:SER:HB2	2:R:190:SER:HB3	2.02	0.41
2:B:82:PRO:O	2:B:83:PHE:HB2	2.20	0.41
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.87	0.41
1:C:260:VAL:HA	1:C:261:PRO:HD2	1.87	0.41
2:D:147:SER:HB2	2:D:190:SER:HB3	2.02	0.41
2:D:428:LEU:HA	2:D:428:LEU:HD23	1.86	0.41
2:F:147:SER:HB2	2:F:190:SER:HB3	2.02	0.41
1:G:94:THR:OG1	1:G:95:GLY:N	2.53	0.41
1:K:297:GLU:HA	1:K:298:PRO:HD3	1.92	0.41
2:L:398:MET:HE2	2:L:398:MET:HB3	1.91	0.41
1:M:49:PHE:HD1	1:M:49:PHE:HA	1.72	0.41
2:N:428:LEU:HA	2:N:428:LEU:HD23	1.86	0.41
1:Q:183:GLU:N	1:Q:184:PRO:CD	2.83	0.41
1:C:49:PHE:HD1	1:C:49:PHE:HA	1.72	0.41
2:H:262:PHE:HA	2:H:263:PRO:HD3	1.93	0.41
1:K:49:PHE:C	1:K:51:THR:N	2.73	0.41
1:M:172:TYR:HA	1:M:173:PRO:HD3	1.88	0.41
1:O:260:VAL:HA	1:O:261:PRO:HD2	1.87	0.41
2:P:82:PRO:O	2:P:83:PHE:HB2	2.20	0.41
2:R:262:PHE:HA	2:R:263:PRO:HD3	1.93	0.41
1:A:347:CYS:HA	1:A:348:PRO:HD3	1.87	0.41
1:K:183:GLU:N	1:K:184:PRO:CD	2.83	0.41
1:O:347:CYS:HA	1:O:348:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:260:VAL:HA	1:Q:261:PRO:HD2	1.87	0.41
2:F:262:PHE:HA	2:F:263:PRO:HD3	1.93	0.41
1:K:238:ILE:O	1:K:238:ILE:CG2	2.67	0.41
1:K:359:PRO:HA	1:K:360:PRO:HD3	1.76	0.41
2:P:262:PHE:HA	2:P:263:PRO:HD3	1.93	0.41
1:Q:94:THR:OG1	1:Q:95:GLY:N	2.53	0.41
1:Q:238:ILE:O	1:Q:238:ILE:CG2	2.67	0.41
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.87	0.41
1:E:94:THR:OG1	1:E:95:GLY:N	2.53	0.41
1:E:238:ILE:O	1:E:238:ILE:CG2	2.67	0.41
1:E:260:VAL:HA	1:E:261:PRO:HD2	1.87	0.41
2:F:11:GLN:HB3	5:F:501:G2P:O2A	2.21	0.41
2:F:288:VAL:N	2:F:289:PRO:CD	2.83	0.41
1:I:283:HIS:HA	1:K:56:THR:HG21	2.03	0.41
2:J:398:MET:HE2	2:J:398:MET:HB3	1.91	0.41
1:K:94:THR:OG1	1:K:95:GLY:N	2.53	0.41
1:A:260:VAL:HA	1:A:261:PRO:HD2	1.87	0.41
2:B:262:PHE:HA	2:B:263:PRO:HD3	1.93	0.41
2:F:88:ARG:HA	2:F:89:PRO:HD3	1.83	0.41
2:H:428:LEU:HA	2:H:428:LEU:HD23	1.86	0.41
1:I:172:TYR:HA	1:I:173:PRO:HD3	1.87	0.41
1:I:439:SER:O	1:I:439:SER:OG	2.05	0.41
1:O:172:TYR:HA	1:O:173:PRO:HD3	1.87	0.41
2:R:288:VAL:N	2:R:289:PRO:CD	2.83	0.41
1:A:176:GLN:HB3	1:A:207:GLU:HG2	2.03	0.41
2:B:11:GLN:HB3	5:B:501:G2P:O2A	2.21	0.41
1:C:176:GLN:HB3	1:C:207:GLU:HG2	2.03	0.41
2:D:262:PHE:HA	2:D:263:PRO:HD3	1.93	0.41
2:D:288:VAL:N	2:D:289:PRO:CD	2.83	0.41
1:E:176:GLN:HB3	1:E:207:GLU:HG2	2.03	0.41
1:I:176:GLN:HB3	1:I:207:GLU:HG2	2.03	0.41
1:I:238:ILE:O	1:I:238:ILE:CG2	2.67	0.41
1:I:347:CYS:HA	1:I:348:PRO:HD3	1.87	0.41
2:L:11:GLN:HB3	5:L:501:G2P:O2A	2.21	0.41
1:M:176:GLN:HB3	1:M:207:GLU:HG2	2.03	0.41
2:N:262:PHE:HA	2:N:263:PRO:HD3	1.93	0.41
2:N:288:VAL:N	2:N:289:PRO:CD	2.83	0.41
1:O:176:GLN:HB3	1:O:207:GLU:HG2	2.03	0.41
1:O:238:ILE:O	1:O:238:ILE:CG2	2.67	0.41
1:Q:175:PRO:O	2:R:349:ASN:ND2	2.51	0.41
1:Q:297:GLU:HA	1:Q:298:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:11:GLN:HB3	5:R:501:G2P:O2A	2.21	0.41
2:R:398:MET:HE2	2:R:398:MET:HB3	1.91	0.41
1:A:238:ILE:O	1:A:238:ILE:CG2	2.67	0.41
2:B:127:GLU:OE2	2:D:338:LYS:NZ	2.50	0.41
2:D:88:ARG:HA	2:D:89:PRO:HD3	1.83	0.41
1:G:176:GLN:HB3	1:G:207:GLU:HG2	2.03	0.41
1:G:238:ILE:O	1:G:238:ILE:CG2	2.67	0.41
1:G:242:LEU:HD23	1:G:242:LEU:HA	1.81	0.41
2:L:288:VAL:N	2:L:289:PRO:CD	2.84	0.41
2:P:11:GLN:HB3	5:P:501:G2P:O2A	2.21	0.41
1:Q:176:GLN:HB3	1:Q:207:GLU:HG2	2.03	0.41
1:C:242:LEU:HD23	1:C:242:LEU:HA	1.81	0.40
2:D:11:GLN:HB3	5:D:501:G2P:O2A	2.21	0.40
2:H:398:MET:HE2	2:H:398:MET:HB3	1.91	0.40
1:K:176:GLN:HB3	1:K:207:GLU:HG2	2.03	0.40
1:M:238:ILE:O	1:M:238:ILE:CG2	2.67	0.40
2:N:11:GLN:HB3	5:N:501:G2P:O2A	2.21	0.40
2:N:88:ARG:HA	2:N:89:PRO:HD3	1.83	0.40
2:R:88:ARG:HA	2:R:89:PRO:HD3	1.83	0.40
1:C:238:ILE:O	1:C:238:ILE:CG2	2.67	0.40
1:E:297:GLU:HA	1:E:298:PRO:HD3	1.92	0.40
2:F:181:VAL:HG12	1:K:350:GLY:HA2	2.04	0.40
2:F:398:MET:HE2	2:F:398:MET:HB3	1.91	0.40
2:H:288:VAL:N	2:H:289:PRO:CD	2.83	0.40
2:J:11:GLN:HB3	5:J:501:G2P:O2A	2.21	0.40
1:K:175:PRO:O	2:L:349:ASN:ND2	2.51	0.40
1:M:242:LEU:HD23	1:M:242:LEU:HA	1.82	0.40
2:P:398:MET:HE2	2:P:398:MET:HB3	1.91	0.40
1:A:176:GLN:HE21	1:A:176:GLN:HB2	1.67	0.40
1:G:384:ILE:O	1:G:384:ILE:HG12	2.21	0.40
1:I:94:THR:OG1	1:I:95:GLY:N	2.53	0.40
1:O:356:ASN:OD1	1:O:357:TYR:N	2.54	0.40
1:A:356:ASN:OD1	1:A:357:TYR:N	2.54	0.40
2:H:11:GLN:HB3	5:H:501:G2P:O2A	2.21	0.40
1:I:356:ASN:OD1	1:I:357:TYR:N	2.54	0.40
1:M:384:ILE:O	1:M:384:ILE:HG12	2.21	0.40
1:Q:384:ILE:O	1:Q:384:ILE:HG12	2.21	0.40
1:A:94:THR:OG1	1:A:95:GLY:N	2.53	0.40
1:C:384:ILE:O	1:C:384:ILE:HG12	2.21	0.40
1:E:384:ILE:O	1:E:384:ILE:HG12	2.21	0.40
1:K:384:ILE:O	1:K:384:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:297:ASP:OD2	2:L:299:LYS:NZ	2.55	0.40
2:R:297:ASP:OD2	2:R:299:LYS:NZ	2.55	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	424/439 (97%)	405 (96%)	18 (4%)	1 (0%)	43	78
1	C	424/439 (97%)	405 (96%)	18 (4%)	1 (0%)	43	78
1	E	424/439 (97%)	405 (96%)	18 (4%)	1 (0%)	43	78
1	G	424/439 (97%)	405 (96%)	18 (4%)	1 (0%)	43	78
1	I	424/439 (97%)	405 (96%)	18 (4%)	1 (0%)	43	78
1	K	424/439 (97%)	405 (96%)	18 (4%)	1 (0%)	43	78
1	M	424/439 (97%)	405 (96%)	18 (4%)	1 (0%)	43	78
1	O	424/439 (97%)	405 (96%)	18 (4%)	1 (0%)	43	78
1	Q	424/439 (97%)	405 (96%)	18 (4%)	1 (0%)	43	78
2	B	424/427 (99%)	411 (97%)	11 (3%)	2 (0%)	24	63
2	D	424/427 (99%)	411 (97%)	11 (3%)	2 (0%)	24	63
2	F	424/427 (99%)	411 (97%)	11 (3%)	2 (0%)	24	63
2	H	424/427 (99%)	411 (97%)	11 (3%)	2 (0%)	24	63
2	J	424/427 (99%)	411 (97%)	11 (3%)	2 (0%)	24	63
2	L	424/427 (99%)	411 (97%)	11 (3%)	2 (0%)	24	63
2	N	424/427 (99%)	411 (97%)	11 (3%)	2 (0%)	24	63
2	P	424/427 (99%)	411 (97%)	11 (3%)	2 (0%)	24	63
2	R	424/427 (99%)	411 (97%)	11 (3%)	2 (0%)	24	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	7632/7794 (98%)	7344 (96%)	261 (3%)	27 (0%)	31 67

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	PRO
2	B	97	SER
1	C	348	PRO
2	D	97	SER
1	E	348	PRO
2	F	97	SER
1	G	348	PRO
2	H	97	SER
1	I	348	PRO
2	J	97	SER
1	K	348	PRO
2	L	97	SER
1	M	348	PRO
2	N	97	SER
1	O	348	PRO
2	P	97	SER
1	Q	348	PRO
2	R	97	SER
2	B	47	GLU
2	D	47	GLU
2	F	47	GLU
2	H	47	GLU
2	J	47	GLU
2	L	47	GLU
2	N	47	GLU
2	P	47	GLU
2	R	47	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	C	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	E	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	G	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	I	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	K	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	M	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	O	360/368 (98%)	359 (100%)	1 (0%)	86	84
1	Q	360/368 (98%)	359 (100%)	1 (0%)	86	84
2	B	367/368 (100%)	366 (100%)	1 (0%)	86	84
2	D	367/368 (100%)	366 (100%)	1 (0%)	86	84
2	F	367/368 (100%)	366 (100%)	1 (0%)	86	84
2	H	367/368 (100%)	366 (100%)	1 (0%)	86	84
2	J	367/368 (100%)	366 (100%)	1 (0%)	86	84
2	L	367/368 (100%)	366 (100%)	1 (0%)	86	84
2	N	367/368 (100%)	366 (100%)	1 (0%)	86	84
2	P	367/368 (100%)	366 (100%)	1 (0%)	86	84
2	R	367/368 (100%)	366 (100%)	1 (0%)	86	84
All	All	6543/6624 (99%)	6525 (100%)	18 (0%)	84	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
2	B	352	LYS
1	C	207	GLU
2	D	352	LYS
1	E	207	GLU
2	F	352	LYS
1	G	207	GLU
2	H	352	LYS
1	I	207	GLU
2	J	352	LYS
1	K	207	GLU
2	L	352	LYS
1	M	207	GLU
2	N	352	LYS

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Mol	Chain	Res	Type
1	O	207	GLU
2	P	352	LYS
1	Q	207	GLU
2	R	352	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	216	ASN
2	B	11	GLN
2	B	15	GLN
2	B	102	ASN
2	B	192	HIS
2	B	247	GLN
2	B	309	HIS
2	B	339	ASN
2	B	385	GLN
2	B	433	GLN
1	C	31	GLN
1	C	216	ASN
2	D	11	GLN
2	D	15	GLN
2	D	102	ASN
2	D	192	HIS
2	D	309	HIS
2	D	339	ASN
2	D	385	GLN
2	D	433	GLN
1	E	31	GLN
1	E	216	ASN
2	F	11	GLN
2	F	15	GLN
2	F	102	ASN
2	F	192	HIS
2	F	247	GLN
2	F	309	HIS
2	F	339	ASN
2	F	385	GLN
2	F	433	GLN
1	G	31	GLN
1	G	216	ASN

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Mol	Chain	Res	Type
1	G	285	GLN
1	G	393	HIS
2	H	11	GLN
2	H	15	GLN
2	H	192	HIS
2	H	247	GLN
2	H	309	HIS
2	H	339	ASN
2	H	385	GLN
2	H	433	GLN
1	I	31	GLN
1	I	107	HIS
1	I	216	ASN
1	I	285	GLN
2	J	11	GLN
2	J	15	GLN
2	J	192	HIS
2	J	247	GLN
2	J	309	HIS
2	J	339	ASN
2	J	385	GLN
2	J	433	GLN
1	K	31	GLN
1	K	216	ASN
2	L	11	GLN
2	L	15	GLN
2	L	192	HIS
2	L	247	GLN
2	L	309	HIS
2	L	339	ASN
2	L	385	GLN
2	L	433	GLN
1	M	31	GLN
1	M	216	ASN
1	M	285	GLN
2	N	11	GLN
2	N	15	GLN
2	N	102	ASN
2	N	192	HIS
2	N	309	HIS
2	N	339	ASN
2	N	385	GLN

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Mol	Chain	Res	Type
2	N	433	GLN
1	O	31	GLN
1	O	216	ASN
1	O	285	GLN
2	P	11	GLN
2	P	15	GLN
2	P	102	ASN
2	P	192	HIS
2	P	247	GLN
2	P	309	HIS
2	P	339	ASN
2	P	385	GLN
2	P	433	GLN
1	Q	31	GLN
1	Q	216	ASN
2	R	11	GLN
2	R	15	GLN
2	R	102	ASN
2	R	192	HIS
2	R	247	GLN
2	R	309	HIS
2	R	339	ASN
2	R	385	GLN
2	R	433	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 18 are monoatomic - leaving 18 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
3	GTP	G	501	4	33,34,34	1.88	3 (9%)	50,54,54	0.91	3 (6%)
5	G2P	R	501	4	30,34,34	3.74	24 (80%)	46,54,54	3.12	22 (47%)
3	GTP	O	501	4	33,34,34	1.88	3 (9%)	50,54,54	0.91	3 (6%)
5	G2P	J	501	4	30,34,34	3.75	24 (80%)	46,54,54	3.12	22 (47%)
5	G2P	N	501	4	30,34,34	3.74	24 (80%)	46,54,54	3.12	22 (47%)
5	G2P	P	501	4	30,34,34	3.75	24 (80%)	46,54,54	3.12	22 (47%)
5	G2P	L	501	4	30,34,34	3.74	24 (80%)	46,54,54	3.13	22 (47%)
3	GTP	A	501	4	33,34,34	1.87	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	C	501	4	33,34,34	1.88	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	M	501	4	33,34,34	1.88	3 (9%)	50,54,54	0.91	3 (6%)
5	G2P	F	501	4	30,34,34	3.75	24 (80%)	46,54,54	3.12	22 (47%)
3	GTP	K	501	4	33,34,34	1.88	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	Q	501	4	33,34,34	1.88	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	I	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
5	G2P	H	501	4	30,34,34	3.74	24 (80%)	46,54,54	3.12	22 (47%)
3	GTP	E	501	4	33,34,34	1.88	3 (9%)	50,54,54	0.91	3 (6%)
5	G2P	D	501	4	30,34,34	3.75	24 (80%)	46,54,54	3.12	22 (47%)
5	G2P	B	501	4	30,34,34	3.74	24 (80%)	46,54,54	3.12	22 (47%)

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
3	GTP	G	501	4	-	4/22/38/38	0/3/3/3
5	G2P	R	501	4	-	5/19/38/38	0/3/3/3
3	GTP	O	501	4	-	4/22/38/38	0/3/3/3
5	G2P	J	501	4	-	5/19/38/38	0/3/3/3
5	G2P	N	501	4	-	5/19/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	G2P	P	501	4	-	5/19/38/38	0/3/3/3
5	G2P	L	501	4	-	5/19/38/38	0/3/3/3
3	GTP	A	501	4	-	4/22/38/38	0/3/3/3
3	GTP	C	501	4	-	4/22/38/38	0/3/3/3
3	GTP	M	501	4	-	4/22/38/38	0/3/3/3
5	G2P	F	501	4	-	5/19/38/38	0/3/3/3
3	GTP	K	501	4	-	4/22/38/38	0/3/3/3
3	GTP	Q	501	4	-	4/22/38/38	0/3/3/3
3	GTP	I	501	4	-	4/22/38/38	0/3/3/3
5	G2P	H	501	4	-	5/19/38/38	0/3/3/3
3	GTP	E	501	4	-	4/22/38/38	0/3/3/3
5	G2P	D	501	4	-	5/19/38/38	0/3/3/3
5	G2P	B	501	4	-	5/19/38/38	0/3/3/3

All (243) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	501	G2P	O3'-C3'	7.68	1.62	1.43
5	B	501	G2P	O3'-C3'	7.67	1.61	1.43
5	F	501	G2P	O3'-C3'	7.66	1.61	1.43
5	D	501	G2P	O3'-C3'	7.66	1.61	1.43
5	N	501	G2P	O3'-C3'	7.64	1.61	1.43
5	J	501	G2P	O3'-C3'	7.64	1.61	1.43
5	R	501	G2P	O3'-C3'	7.64	1.61	1.43
5	L	501	G2P	O3'-C3'	7.63	1.61	1.43
5	H	501	G2P	O3'-C3'	7.63	1.61	1.43
5	R	501	G2P	C2-N2	7.17	1.51	1.34
5	N	501	G2P	C2-N2	7.14	1.50	1.34
5	P	501	G2P	C2-N2	7.14	1.50	1.34
5	D	501	G2P	C2-N2	7.14	1.50	1.34
5	H	501	G2P	C2-N2	7.13	1.50	1.34
5	F	501	G2P	C2-N2	7.13	1.50	1.34
5	L	501	G2P	C2-N2	7.13	1.50	1.34
5	B	501	G2P	C2-N2	7.13	1.50	1.34
5	J	501	G2P	C2-N2	7.11	1.50	1.34
3	K	501	GTP	PA-O3A	-6.06	1.53	1.59
3	G	501	GTP	PA-O3A	-6.02	1.53	1.59
3	A	501	GTP	PA-O3A	-6.00	1.53	1.59
3	C	501	GTP	PA-O3A	-5.97	1.53	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	501	GTP	PA-O3A	-5.96	1.53	1.59
3	O	501	GTP	PA-O3A	-5.96	1.53	1.59
3	E	501	GTP	PA-O3A	-5.94	1.53	1.59
5	J	501	G2P	C2-N3	5.94	1.47	1.33
3	Q	501	GTP	PA-O3A	-5.92	1.53	1.59
5	F	501	G2P	C2-N3	5.91	1.47	1.33
3	I	501	GTP	PA-O3A	-5.90	1.53	1.59
5	L	501	G2P	C2-N3	5.90	1.47	1.33
5	P	501	G2P	C2-N3	5.90	1.47	1.33
5	D	501	G2P	C2-N3	5.90	1.47	1.33
5	N	501	G2P	C2-N3	5.89	1.47	1.33
5	R	501	G2P	C2-N3	5.88	1.47	1.33
5	H	501	G2P	C2-N3	5.88	1.47	1.33
5	B	501	G2P	C2-N3	5.88	1.47	1.33
3	I	501	GTP	PB-O3A	-5.84	1.53	1.59
5	F	501	G2P	O2'-C2'	-5.82	1.28	1.43
5	R	501	G2P	O2'-C2'	-5.82	1.28	1.43
5	L	501	G2P	O2'-C2'	-5.82	1.28	1.43
5	P	501	G2P	O2'-C2'	-5.81	1.28	1.43
5	J	501	G2P	O2'-C2'	-5.81	1.28	1.43
5	D	501	G2P	O2'-C2'	-5.81	1.28	1.43
5	B	501	G2P	O2'-C2'	-5.80	1.28	1.43
5	N	501	G2P	O2'-C2'	-5.79	1.28	1.43
5	H	501	G2P	O2'-C2'	-5.78	1.28	1.43
3	M	501	GTP	PB-O3A	-5.76	1.53	1.59
3	E	501	GTP	PB-O3A	-5.76	1.53	1.59
3	Q	501	GTP	PB-O3A	-5.74	1.53	1.59
3	C	501	GTP	PB-O3A	-5.74	1.53	1.59
3	O	501	GTP	PB-O3A	-5.73	1.53	1.59
3	G	501	GTP	PB-O3A	-5.69	1.53	1.59
3	K	501	GTP	PB-O3A	-5.67	1.53	1.59
3	A	501	GTP	PB-O3A	-5.65	1.53	1.59
3	I	501	GTP	PB-O3B	5.41	1.65	1.59
3	E	501	GTP	PB-O3B	5.39	1.65	1.59
3	Q	501	GTP	PB-O3B	5.35	1.65	1.59
3	C	501	GTP	PB-O3B	5.35	1.65	1.59
3	M	501	GTP	PB-O3B	5.34	1.65	1.59
3	G	501	GTP	PB-O3B	5.34	1.65	1.59
3	O	501	GTP	PB-O3B	5.34	1.65	1.59
3	K	501	GTP	PB-O3B	5.33	1.65	1.59
3	A	501	GTP	PB-O3B	5.28	1.65	1.59
5	F	501	G2P	C4-N9	-4.98	1.25	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	501	G2P	PB-O2B	4.98	1.63	1.51
5	R	501	G2P	C4-N9	-4.97	1.25	1.38
5	N	501	G2P	PB-O2B	4.96	1.63	1.51
5	J	501	G2P	PB-O2B	4.96	1.63	1.51
5	P	501	G2P	PB-O2B	4.96	1.63	1.51
5	D	501	G2P	C4-N9	-4.96	1.25	1.38
5	D	501	G2P	PB-O2B	4.95	1.63	1.51
5	L	501	G2P	C4-N9	-4.95	1.25	1.38
5	R	501	G2P	PB-O2B	4.95	1.63	1.51
5	B	501	G2P	C4-N9	-4.95	1.25	1.38
5	J	501	G2P	C4-N9	-4.94	1.25	1.38
5	N	501	G2P	C4-N9	-4.94	1.25	1.38
5	B	501	G2P	PB-O2B	4.94	1.63	1.51
5	H	501	G2P	C4-N9	-4.94	1.25	1.38
5	H	501	G2P	PB-O2B	4.94	1.63	1.51
5	F	501	G2P	PB-O2B	4.92	1.63	1.51
5	P	501	G2P	C4-N9	-4.92	1.25	1.38
5	H	501	G2P	C4-N3	4.56	1.44	1.34
5	F	501	G2P	C4-N3	4.56	1.44	1.34
5	B	501	G2P	C4-N3	4.54	1.44	1.34
5	D	501	G2P	C4-N3	4.54	1.44	1.34
5	J	501	G2P	C4-N3	4.54	1.44	1.34
5	N	501	G2P	C4-N3	4.53	1.44	1.34
5	R	501	G2P	C4-N3	4.52	1.44	1.34
5	P	501	G2P	C4-N3	4.52	1.44	1.34
5	L	501	G2P	C4-N3	4.51	1.44	1.34
5	J	501	G2P	O5'-C5'	-4.47	1.27	1.44
5	R	501	G2P	O5'-C5'	-4.46	1.27	1.44
5	P	501	G2P	O5'-C5'	-4.46	1.27	1.44
5	H	501	G2P	O5'-C5'	-4.46	1.27	1.44
5	F	501	G2P	O5'-C5'	-4.46	1.27	1.44
5	D	501	G2P	O5'-C5'	-4.46	1.27	1.44
5	L	501	G2P	O5'-C5'	-4.45	1.27	1.44
5	N	501	G2P	O5'-C5'	-4.45	1.27	1.44
5	B	501	G2P	O5'-C5'	-4.44	1.27	1.44
5	J	501	G2P	PA-O2A	-4.33	1.41	1.51
5	P	501	G2P	PA-O2A	-4.33	1.41	1.51
5	H	501	G2P	PA-O2A	-4.31	1.41	1.51
5	F	501	G2P	PA-O2A	-4.31	1.41	1.51
5	N	501	G2P	C2-N1	4.30	1.48	1.37
5	H	501	G2P	C2-N1	4.30	1.48	1.37
5	D	501	G2P	PA-O2A	-4.30	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	501	G2P	PA-O2A	-4.29	1.41	1.51
5	L	501	G2P	PA-O2A	-4.29	1.41	1.51
5	P	501	G2P	C2-N1	4.28	1.48	1.37
5	D	501	G2P	C2-N1	4.28	1.48	1.37
5	B	501	G2P	C2-N1	4.28	1.48	1.37
5	R	501	G2P	PA-O2A	-4.28	1.41	1.51
5	F	501	G2P	C2-N1	4.27	1.48	1.37
5	J	501	G2P	C2-N1	4.27	1.48	1.37
5	L	501	G2P	C2-N1	4.27	1.48	1.37
5	B	501	G2P	PA-O2A	-4.27	1.41	1.51
5	R	501	G2P	C2-N1	4.24	1.47	1.37
5	L	501	G2P	C8-N9	-4.04	1.28	1.37
5	P	501	G2P	C8-N9	-4.04	1.28	1.37
5	R	501	G2P	C8-N9	-4.03	1.28	1.37
5	N	501	G2P	C8-N9	-4.03	1.28	1.37
5	B	501	G2P	C8-N9	-4.02	1.28	1.37
5	H	501	G2P	C8-N9	-4.01	1.28	1.37
5	D	501	G2P	C8-N9	-4.01	1.28	1.37
5	J	501	G2P	C8-N9	-4.00	1.28	1.37
5	F	501	G2P	C8-N9	-4.00	1.28	1.37
5	L	501	G2P	C2'-C1'	3.49	1.64	1.53
5	R	501	G2P	C2'-C1'	3.48	1.64	1.53
5	B	501	G2P	C2'-C1'	3.47	1.64	1.53
5	F	501	G2P	C2'-C1'	3.47	1.64	1.53
5	D	501	G2P	C2'-C1'	3.47	1.64	1.53
5	N	501	G2P	C2'-C1'	3.47	1.64	1.53
5	J	501	G2P	C2'-C1'	3.46	1.64	1.53
5	H	501	G2P	C2'-C1'	3.45	1.64	1.53
5	P	501	G2P	C2'-C1'	3.45	1.64	1.53
5	H	501	G2P	C3'-C4'	3.26	1.61	1.53
5	L	501	G2P	C3'-C4'	3.25	1.61	1.53
5	J	501	G2P	C3'-C4'	3.24	1.61	1.53
5	D	501	G2P	C3'-C4'	3.24	1.61	1.53
5	B	501	G2P	C3'-C4'	3.23	1.61	1.53
5	P	501	G2P	C3'-C4'	3.23	1.61	1.53
5	R	501	G2P	C3'-C4'	3.23	1.61	1.53
5	N	501	G2P	C3'-C4'	3.22	1.61	1.53
5	F	501	G2P	C3'-C4'	3.21	1.61	1.53
5	J	501	G2P	O6-C6	-2.83	1.18	1.23
5	L	501	G2P	O6-C6	-2.82	1.18	1.23
5	B	501	G2P	PG-O2G	-2.82	1.41	1.50
5	N	501	G2P	PG-O2G	-2.81	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	501	G2P	PG-O2G	-2.81	1.41	1.50
5	H	501	G2P	PG-O2G	-2.81	1.41	1.50
5	D	501	G2P	PG-O2G	-2.80	1.41	1.50
5	F	501	G2P	PG-O2G	-2.80	1.41	1.50
5	P	501	G2P	O6-C6	-2.80	1.18	1.23
5	H	501	G2P	C1'-N9	-2.80	1.39	1.47
5	P	501	G2P	C1'-N9	-2.80	1.39	1.47
5	J	501	G2P	PG-O2G	-2.79	1.41	1.50
5	N	501	G2P	O6-C6	-2.79	1.18	1.23
5	L	501	G2P	PG-O2G	-2.79	1.41	1.50
5	D	501	G2P	O6-C6	-2.79	1.18	1.23
5	J	501	G2P	C1'-N9	-2.79	1.39	1.47
5	D	501	G2P	C1'-N9	-2.79	1.39	1.47
5	F	501	G2P	C1'-N9	-2.78	1.39	1.47
5	R	501	G2P	PG-O2G	-2.78	1.41	1.50
5	F	501	G2P	O6-C6	-2.78	1.18	1.23
5	N	501	G2P	C1'-N9	-2.78	1.39	1.47
5	H	501	G2P	O6-C6	-2.78	1.18	1.23
5	R	501	G2P	O6-C6	-2.78	1.18	1.23
5	B	501	G2P	O6-C6	-2.78	1.18	1.23
5	R	501	G2P	C1'-N9	-2.77	1.39	1.47
5	B	501	G2P	C1'-N9	-2.77	1.39	1.47
5	L	501	G2P	C1'-N9	-2.77	1.39	1.47
5	H	501	G2P	O4'-C4'	2.76	1.51	1.45
5	B	501	G2P	O4'-C4'	2.76	1.51	1.45
5	F	501	G2P	O4'-C4'	2.75	1.51	1.45
5	P	501	G2P	O4'-C4'	2.75	1.51	1.45
5	L	501	G2P	O4'-C4'	2.74	1.51	1.45
5	D	501	G2P	O4'-C4'	2.74	1.51	1.45
5	N	501	G2P	O4'-C4'	2.74	1.51	1.45
5	J	501	G2P	O4'-C4'	2.74	1.51	1.45
5	R	501	G2P	O4'-C4'	2.74	1.51	1.45
5	F	501	G2P	C8-N7	-2.69	1.25	1.32
5	H	501	G2P	C8-N7	-2.69	1.25	1.32
5	P	501	G2P	C8-N7	-2.68	1.25	1.32
5	D	501	G2P	C8-N7	-2.67	1.25	1.32
5	J	501	G2P	C8-N7	-2.67	1.25	1.32
5	R	501	G2P	C8-N7	-2.67	1.25	1.32
5	N	501	G2P	C8-N7	-2.66	1.25	1.32
5	B	501	G2P	C8-N7	-2.66	1.25	1.32
5	L	501	G2P	C8-N7	-2.66	1.25	1.32
5	F	501	G2P	PA-O1A	2.53	1.62	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	501	G2P	PA-O1A	2.53	1.62	1.56
5	R	501	G2P	PA-O1A	2.52	1.62	1.56
5	J	501	G2P	PA-O1A	2.50	1.62	1.56
5	N	501	G2P	PA-O1A	2.50	1.62	1.56
5	P	501	G2P	PA-O1A	2.50	1.62	1.56
5	D	501	G2P	PA-O1A	2.49	1.62	1.56
5	L	501	G2P	PA-O1A	2.49	1.62	1.56
5	B	501	G2P	PA-O1A	2.47	1.62	1.56
5	N	501	G2P	PG-O1G	2.43	1.63	1.54
5	H	501	G2P	PG-O1G	2.42	1.63	1.54
5	R	501	G2P	PG-O1G	2.42	1.63	1.54
5	B	501	G2P	PG-O1G	2.42	1.63	1.54
5	D	501	G2P	PG-O1G	2.42	1.63	1.54
5	F	501	G2P	PG-O1G	2.41	1.63	1.54
5	P	501	G2P	PG-O1G	2.41	1.63	1.54
5	L	501	G2P	PG-O1G	2.41	1.63	1.54
5	J	501	G2P	PG-O1G	2.41	1.63	1.54
5	P	501	G2P	C2'-C3'	-2.33	1.47	1.53
5	H	501	G2P	C5-C6	2.33	1.53	1.44
5	F	501	G2P	C5-C6	2.31	1.53	1.44
5	F	501	G2P	C2'-C3'	-2.31	1.47	1.53
5	J	501	G2P	C2'-C3'	-2.30	1.47	1.53
5	D	501	G2P	C5-C6	2.30	1.53	1.44
5	J	501	G2P	C5-C6	2.30	1.53	1.44
5	D	501	G2P	C2'-C3'	-2.30	1.47	1.53
5	L	501	G2P	C5-C6	2.30	1.53	1.44
5	B	501	G2P	C2'-C3'	-2.29	1.47	1.53
5	P	501	G2P	C5-C6	2.29	1.53	1.44
5	R	501	G2P	C2'-C3'	-2.29	1.47	1.53
5	H	501	G2P	C2'-C3'	-2.29	1.47	1.53
5	L	501	G2P	C2'-C3'	-2.29	1.47	1.53
5	N	501	G2P	C2'-C3'	-2.29	1.47	1.53
5	R	501	G2P	C5-C6	2.28	1.52	1.44
5	B	501	G2P	C5-C6	2.28	1.52	1.44
5	N	501	G2P	C5-C6	2.28	1.52	1.44
5	R	501	G2P	C5-C4	2.18	1.44	1.38
5	L	501	G2P	C5-C4	2.17	1.44	1.38
5	B	501	G2P	C5-C4	2.17	1.44	1.38
5	P	501	G2P	C5-C4	2.16	1.44	1.38
5	D	501	G2P	C5-C4	2.15	1.44	1.38
5	N	501	G2P	C5-C4	2.15	1.44	1.38
5	J	501	G2P	C5-C4	2.14	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	501	G2P	C5-C4	2.14	1.44	1.38
5	F	501	G2P	C5-C4	2.14	1.44	1.38
5	R	501	G2P	PB-O3B	2.10	1.60	1.58
5	L	501	G2P	PB-O3B	2.08	1.60	1.58
5	N	501	G2P	PB-O3B	2.07	1.60	1.58
5	F	501	G2P	PB-O3B	2.06	1.60	1.58
5	H	501	G2P	PB-O3B	2.06	1.60	1.58
5	D	501	G2P	PB-O3B	2.05	1.60	1.58
5	J	501	G2P	PB-O3B	2.05	1.60	1.58
5	P	501	G2P	PB-O3B	2.02	1.60	1.58
5	B	501	G2P	PB-O3B	2.00	1.60	1.58

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	501	G2P	O4'-C4'-C3'	-7.82	89.64	105.15
5	J	501	G2P	O4'-C4'-C3'	-7.81	89.64	105.15
5	L	501	G2P	O4'-C4'-C3'	-7.81	89.65	105.15
5	B	501	G2P	O4'-C4'-C3'	-7.81	89.65	105.15
5	D	501	G2P	O4'-C4'-C3'	-7.81	89.65	105.15
5	H	501	G2P	O4'-C4'-C3'	-7.81	89.66	105.15
5	F	501	G2P	O4'-C4'-C3'	-7.80	89.68	105.15
5	N	501	G2P	O4'-C4'-C3'	-7.79	89.69	105.15
5	R	501	G2P	O4'-C4'-C3'	-7.79	89.70	105.15
5	P	501	G2P	O2A-PA-C3A	6.35	125.77	109.05
5	R	501	G2P	O2A-PA-C3A	6.34	125.76	109.05
5	B	501	G2P	O2A-PA-C3A	6.34	125.76	109.05
5	H	501	G2P	O2A-PA-C3A	6.34	125.75	109.05
5	L	501	G2P	O2A-PA-C3A	6.34	125.74	109.05
5	N	501	G2P	O2A-PA-C3A	6.34	125.74	109.05
5	J	501	G2P	O2A-PA-C3A	6.34	125.74	109.05
5	D	501	G2P	O2A-PA-C3A	6.33	125.73	109.05
5	F	501	G2P	O2A-PA-C3A	6.33	125.72	109.05
5	R	501	G2P	C2-N3-C4	6.21	122.99	112.30
5	B	501	G2P	C2-N3-C4	6.21	122.99	112.30
5	L	501	G2P	C2-N3-C4	6.21	122.99	112.30
5	F	501	G2P	C2-N3-C4	6.20	122.97	112.30
5	J	501	G2P	C2-N3-C4	6.19	122.97	112.30
5	D	501	G2P	C2-N3-C4	6.19	122.96	112.30
5	H	501	G2P	C2-N3-C4	6.19	122.96	112.30
5	N	501	G2P	C2-N3-C4	6.19	122.95	112.30
5	P	501	G2P	C2-N3-C4	6.17	122.92	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	501	G2P	N1-C2-N3	-5.95	112.43	123.32
5	L	501	G2P	N1-C2-N3	-5.94	112.46	123.32
5	B	501	G2P	N1-C2-N3	-5.93	112.47	123.32
5	D	501	G2P	N1-C2-N3	-5.92	112.48	123.32
5	F	501	G2P	N1-C2-N3	-5.92	112.48	123.32
5	H	501	G2P	N1-C2-N3	-5.92	112.50	123.32
5	N	501	G2P	N1-C2-N3	-5.91	112.50	123.32
5	R	501	G2P	N1-C2-N3	-5.91	112.50	123.32
5	P	501	G2P	N1-C2-N3	-5.90	112.52	123.32
5	N	501	G2P	N2-C2-N3	5.67	130.74	119.67
5	L	501	G2P	N2-C2-N3	5.66	130.73	119.67
5	B	501	G2P	N2-C2-N3	5.66	130.71	119.67
5	H	501	G2P	N2-C2-N3	5.66	130.71	119.67
5	J	501	G2P	N2-C2-N3	5.65	130.71	119.67
5	D	501	G2P	N2-C2-N3	5.65	130.70	119.67
5	F	501	G2P	N2-C2-N3	5.65	130.69	119.67
5	P	501	G2P	N2-C2-N3	5.65	130.69	119.67
5	R	501	G2P	N2-C2-N3	5.63	130.66	119.67
5	R	501	G2P	N9-C4-N3	5.45	136.86	125.95
5	L	501	G2P	N9-C4-N3	5.44	136.84	125.95
5	N	501	G2P	N9-C4-N3	5.43	136.80	125.95
5	B	501	G2P	N9-C4-N3	5.43	136.80	125.95
5	F	501	G2P	N9-C4-N3	5.42	136.80	125.95
5	D	501	G2P	N9-C4-N3	5.42	136.79	125.95
5	P	501	G2P	N9-C4-N3	5.41	136.77	125.95
5	H	501	G2P	N9-C4-N3	5.41	136.76	125.95
5	J	501	G2P	N9-C4-N3	5.40	136.75	125.95
5	R	501	G2P	O1B-PB-O2B	5.03	126.34	109.95
5	B	501	G2P	O1B-PB-O2B	5.03	126.33	109.95
5	D	501	G2P	O1B-PB-O2B	5.03	126.31	109.95
5	P	501	G2P	O1B-PB-O2B	5.02	126.30	109.95
5	H	501	G2P	O1B-PB-O2B	5.02	126.30	109.95
5	N	501	G2P	O1B-PB-O2B	5.02	126.30	109.95
5	F	501	G2P	O1B-PB-O2B	5.02	126.29	109.95
5	J	501	G2P	O1B-PB-O2B	5.02	126.29	109.95
5	L	501	G2P	O1B-PB-O2B	5.02	126.27	109.95
5	H	501	G2P	O2'-C2'-C3'	-4.54	97.25	111.82
5	J	501	G2P	O2'-C2'-C3'	-4.54	97.28	111.82
5	N	501	G2P	O2'-C2'-C3'	-4.54	97.28	111.82
5	L	501	G2P	O2'-C2'-C3'	-4.53	97.29	111.82
5	R	501	G2P	O2'-C2'-C3'	-4.53	97.29	111.82
5	D	501	G2P	O2'-C2'-C3'	-4.53	97.29	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	G2P	O2'-C2'-C3'	-4.53	97.30	111.82
5	P	501	G2P	O2'-C2'-C3'	-4.52	97.33	111.82
5	F	501	G2P	O2'-C2'-C3'	-4.51	97.37	111.82
5	L	501	G2P	C3'-C2'-C1'	-4.25	93.42	101.46
5	J	501	G2P	C3'-C2'-C1'	-4.24	93.44	101.46
5	B	501	G2P	C3'-C2'-C1'	-4.23	93.46	101.46
5	D	501	G2P	C3'-C2'-C1'	-4.22	93.47	101.46
5	R	501	G2P	C3'-C2'-C1'	-4.22	93.48	101.46
5	F	501	G2P	C3'-C2'-C1'	-4.22	93.49	101.46
5	H	501	G2P	C3'-C2'-C1'	-4.21	93.49	101.46
5	N	501	G2P	C3'-C2'-C1'	-4.21	93.50	101.46
5	P	501	G2P	C3'-C2'-C1'	-4.20	93.52	101.46
5	R	501	G2P	C5-C4-N3	-4.12	121.84	128.39
5	L	501	G2P	C5-C4-N3	-4.10	121.87	128.39
5	B	501	G2P	C5-C4-N3	-4.10	121.87	128.39
5	F	501	G2P	C5-C4-N3	-4.09	121.88	128.39
5	J	501	G2P	C5-C4-N3	-4.09	121.88	128.39
5	D	501	G2P	C5-C4-N3	-4.09	121.88	128.39
5	N	501	G2P	C5-C4-N3	-4.09	121.88	128.39
5	H	501	G2P	C5-C4-N3	-4.08	121.90	128.39
5	P	501	G2P	C5-C4-N3	-4.06	121.93	128.39
5	P	501	G2P	O2B-PB-C3A	-4.02	98.47	109.05
5	H	501	G2P	O2B-PB-C3A	-4.01	98.48	109.05
5	B	501	G2P	O2B-PB-C3A	-4.01	98.50	109.05
5	D	501	G2P	O2B-PB-C3A	-4.00	98.50	109.05
5	J	501	G2P	O2B-PB-C3A	-4.00	98.51	109.05
5	N	501	G2P	O2B-PB-C3A	-4.00	98.52	109.05
5	F	501	G2P	O2B-PB-C3A	-4.00	98.52	109.05
5	L	501	G2P	O2B-PB-C3A	-4.00	98.53	109.05
5	R	501	G2P	O2B-PB-C3A	-3.99	98.53	109.05
5	P	501	G2P	C4'-O4'-C1'	3.81	117.87	109.47
5	L	501	G2P	C4'-O4'-C1'	3.80	117.86	109.47
5	N	501	G2P	C4'-O4'-C1'	3.80	117.86	109.47
5	R	501	G2P	C4'-O4'-C1'	3.80	117.86	109.47
5	B	501	G2P	C4'-O4'-C1'	3.80	117.85	109.47
5	D	501	G2P	C4'-O4'-C1'	3.80	117.85	109.47
5	J	501	G2P	C4'-O4'-C1'	3.79	117.84	109.47
5	H	501	G2P	C4'-O4'-C1'	3.79	117.83	109.47
5	F	501	G2P	C4'-O4'-C1'	3.78	117.80	109.47
5	L	501	G2P	C8-N9-C4	3.69	112.95	106.03
5	R	501	G2P	C8-N9-C4	3.69	112.94	106.03
5	N	501	G2P	C8-N9-C4	3.68	112.93	106.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	501	G2P	C8-N9-C4	3.68	112.92	106.03
5	P	501	G2P	C8-N9-C4	3.67	112.90	106.03
5	D	501	G2P	C8-N9-C4	3.66	112.89	106.03
5	B	501	G2P	C8-N9-C4	3.65	112.88	106.03
5	J	501	G2P	C8-N9-C4	3.64	112.84	106.03
5	H	501	G2P	C8-N9-C4	3.63	112.83	106.03
5	P	501	G2P	O4'-C1'-C2'	-3.59	98.93	106.62
5	N	501	G2P	O4'-C1'-C2'	-3.59	98.93	106.62
5	H	501	G2P	O4'-C1'-C2'	-3.59	98.94	106.62
5	F	501	G2P	O4'-C1'-C2'	-3.58	98.95	106.62
5	D	501	G2P	O4'-C1'-C2'	-3.58	98.95	106.62
5	B	501	G2P	O4'-C1'-C2'	-3.58	98.96	106.62
5	L	501	G2P	O4'-C1'-C2'	-3.58	98.96	106.62
5	R	501	G2P	O4'-C1'-C2'	-3.58	98.96	106.62
5	J	501	G2P	O4'-C1'-C2'	-3.57	98.97	106.62
5	J	501	G2P	O2'-C2'-C1'	3.05	120.61	110.10
5	R	501	G2P	O2'-C2'-C1'	3.05	120.59	110.10
5	L	501	G2P	O2'-C2'-C1'	3.04	120.58	110.10
5	N	501	G2P	O2'-C2'-C1'	3.04	120.58	110.10
5	D	501	G2P	O2'-C2'-C1'	3.04	120.57	110.10
5	P	501	G2P	O2'-C2'-C1'	3.04	120.56	110.10
5	F	501	G2P	O2'-C2'-C1'	3.04	120.56	110.10
5	B	501	G2P	O2'-C2'-C1'	3.03	120.54	110.10
5	H	501	G2P	O2'-C2'-C1'	3.03	120.53	110.10
5	H	501	G2P	O6-C6-C5	-2.67	119.49	126.53
5	B	501	G2P	O6-C6-C5	-2.66	119.50	126.53
3	G	501	GTP	O2G-PG-O3B	2.66	113.55	104.64
3	A	501	GTP	O2G-PG-O3B	2.66	113.55	104.64
3	E	501	GTP	O2G-PG-O3B	2.66	113.54	104.64
5	D	501	G2P	O6-C6-C5	-2.65	119.53	126.53
5	N	501	G2P	O6-C6-C5	-2.65	119.53	126.53
3	I	501	GTP	O2G-PG-O3B	2.65	113.51	104.64
3	Q	501	GTP	O2G-PG-O3B	2.65	113.51	104.64
3	C	501	GTP	O2G-PG-O3B	2.64	113.50	104.64
3	K	501	GTP	O2G-PG-O3B	2.64	113.50	104.64
5	L	501	G2P	O6-C6-C5	-2.64	119.56	126.53
3	O	501	GTP	O2G-PG-O3B	2.64	113.49	104.64
5	R	501	G2P	O6-C6-C5	-2.64	119.56	126.53
5	F	501	G2P	O6-C6-C5	-2.64	119.56	126.53
5	P	501	G2P	O6-C6-C5	-2.64	119.56	126.53
5	J	501	G2P	O6-C6-C5	-2.64	119.57	126.53
3	M	501	GTP	O2G-PG-O3B	2.63	113.46	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	501	G2P	C5-C4-N9	-2.44	101.29	105.66
5	L	501	G2P	C5-C4-N9	-2.44	101.29	105.66
5	R	501	G2P	C5-C4-N9	-2.43	101.30	105.66
5	N	501	G2P	C5-C4-N9	-2.43	101.31	105.66
5	F	501	G2P	C5-C4-N9	-2.42	101.32	105.66
5	D	501	G2P	C5-C4-N9	-2.42	101.32	105.66
5	B	501	G2P	C5-C4-N9	-2.42	101.32	105.66
5	H	501	G2P	C5-C4-N9	-2.41	101.33	105.66
5	J	501	G2P	C5-C4-N9	-2.40	101.36	105.66
5	H	501	G2P	O3'-C3'-C2'	2.33	119.28	111.82
5	J	501	G2P	O3'-C3'-C2'	2.32	119.25	111.82
5	D	501	G2P	O3'-C3'-C2'	2.31	119.22	111.82
5	L	501	G2P	O3'-C3'-C2'	2.31	119.22	111.82
5	N	501	G2P	O3'-C3'-C2'	2.30	119.20	111.82
5	B	501	G2P	O3'-C3'-C2'	2.30	119.18	111.82
5	F	501	G2P	O3'-C3'-C2'	2.30	119.18	111.82
5	R	501	G2P	O3'-C3'-C2'	2.30	119.18	111.82
5	P	501	G2P	O3'-C3'-C2'	2.29	119.17	111.82
5	L	501	G2P	C1'-N9-C4	-2.23	119.89	126.49
5	N	501	G2P	C1'-N9-C4	-2.23	119.90	126.49
5	P	501	G2P	C1'-N9-C4	-2.23	119.91	126.49
5	R	501	G2P	C1'-N9-C4	-2.22	119.91	126.49
5	B	501	G2P	C1'-N9-C4	-2.22	119.92	126.49
5	F	501	G2P	C1'-N9-C4	-2.22	119.93	126.49
5	D	501	G2P	C1'-N9-C4	-2.22	119.94	126.49
5	H	501	G2P	C1'-N9-C4	-2.22	119.94	126.49
5	J	501	G2P	C1'-N9-C4	-2.21	119.95	126.49
5	H	501	G2P	O6-C6-N1	2.16	124.17	120.11
5	J	501	G2P	O6-C6-N1	2.15	124.16	120.11
5	B	501	G2P	O6-C6-N1	2.15	124.15	120.11
5	D	501	G2P	O6-C6-N1	2.15	124.15	120.11
5	L	501	G2P	O6-C6-N1	2.15	124.15	120.11
5	R	501	G2P	O6-C6-N1	2.14	124.13	120.11
5	N	501	G2P	O6-C6-N1	2.13	124.12	120.11
5	F	501	G2P	O6-C6-N1	2.12	124.11	120.11
5	P	501	G2P	O6-C6-N1	2.12	124.11	120.11
3	Q	501	GTP	O5'-C5'-C4'	2.11	116.18	108.99
3	G	501	GTP	O5'-C5'-C4'	2.11	116.17	108.99
3	A	501	GTP	O5'-C5'-C4'	2.11	116.17	108.99
5	F	501	G2P	O4'-C4'-C5'	2.11	116.08	109.33
5	B	501	G2P	O4'-C4'-C5'	2.10	116.08	109.33
3	O	501	GTP	O5'-C5'-C4'	2.10	116.15	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	GTP	O5'-C5'-C4'	2.10	116.15	108.99
3	I	501	GTP	O5'-C5'-C4'	2.10	116.15	108.99
5	D	501	G2P	O4'-C4'-C5'	2.10	116.06	109.33
3	K	501	GTP	O5'-C5'-C4'	2.10	116.14	108.99
3	M	501	GTP	O5'-C5'-C4'	2.10	116.14	108.99
5	R	501	G2P	O4'-C4'-C5'	2.10	116.05	109.33
5	F	501	G2P	O3'-C3'-C4'	2.10	117.10	111.08
3	E	501	GTP	O5'-C5'-C4'	2.09	116.12	108.99
5	L	501	G2P	O4'-C4'-C5'	2.09	116.03	109.33
5	P	501	G2P	O4'-C4'-C5'	2.09	116.03	109.33
5	H	501	G2P	O4'-C4'-C5'	2.09	116.03	109.33
5	L	501	G2P	O3'-C3'-C4'	2.09	117.08	111.08
5	N	501	G2P	O4'-C4'-C5'	2.09	116.01	109.33
5	J	501	G2P	O4'-C4'-C5'	2.08	116.01	109.33
5	B	501	G2P	O3'-C3'-C4'	2.08	117.06	111.08
5	D	501	G2P	O3'-C3'-C4'	2.08	117.04	111.08
5	R	501	G2P	O3'-C3'-C4'	2.07	117.04	111.08
5	J	501	G2P	O3'-C3'-C4'	2.07	117.04	111.08
5	N	501	G2P	O3'-C3'-C4'	2.07	117.04	111.08
5	H	501	G2P	O3'-C3'-C4'	2.07	117.03	111.08
5	P	501	G2P	O3'-C3'-C4'	2.07	117.03	111.08
3	M	501	GTP	O3G-PG-O3B	2.03	111.45	104.64
3	K	501	GTP	O3G-PG-O3B	2.03	111.44	104.64
3	E	501	GTP	O3G-PG-O3B	2.03	111.44	104.64
3	G	501	GTP	O3G-PG-O3B	2.03	111.43	104.64
3	C	501	GTP	O3G-PG-O3B	2.02	111.43	104.64
3	I	501	GTP	O3G-PG-O3B	2.02	111.42	104.64
3	Q	501	GTP	O3G-PG-O3B	2.02	111.42	104.64
3	A	501	GTP	O3G-PG-O3B	2.02	111.41	104.64
3	O	501	GTP	O3G-PG-O3B	2.01	111.39	104.64

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GTP	C3'-C4'-C5'-O5'
3	C	501	GTP	C3'-C4'-C5'-O5'
3	E	501	GTP	C3'-C4'-C5'-O5'
3	G	501	GTP	C3'-C4'-C5'-O5'
3	I	501	GTP	C3'-C4'-C5'-O5'
3	K	501	GTP	C3'-C4'-C5'-O5'
3	M	501	GTP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	O	501	GTP	C3'-C4'-C5'-O5'
3	Q	501	GTP	C3'-C4'-C5'-O5'
3	K	501	GTP	O4'-C4'-C5'-O5'
3	A	501	GTP	C5'-O5'-PA-O1A
3	C	501	GTP	C5'-O5'-PA-O1A
3	E	501	GTP	C5'-O5'-PA-O1A
3	G	501	GTP	C5'-O5'-PA-O1A
3	I	501	GTP	C5'-O5'-PA-O1A
3	K	501	GTP	C5'-O5'-PA-O1A
3	M	501	GTP	C5'-O5'-PA-O1A
3	O	501	GTP	C5'-O5'-PA-O1A
3	Q	501	GTP	C5'-O5'-PA-O1A
3	A	501	GTP	O4'-C4'-C5'-O5'
3	C	501	GTP	O4'-C4'-C5'-O5'
3	E	501	GTP	O4'-C4'-C5'-O5'
3	G	501	GTP	O4'-C4'-C5'-O5'
3	I	501	GTP	O4'-C4'-C5'-O5'
3	M	501	GTP	O4'-C4'-C5'-O5'
3	O	501	GTP	O4'-C4'-C5'-O5'
3	Q	501	GTP	O4'-C4'-C5'-O5'
5	B	501	G2P	C3'-C4'-C5'-O5'
5	D	501	G2P	C3'-C4'-C5'-O5'
5	F	501	G2P	C3'-C4'-C5'-O5'
5	H	501	G2P	C3'-C4'-C5'-O5'
5	J	501	G2P	C3'-C4'-C5'-O5'
5	L	501	G2P	C3'-C4'-C5'-O5'
5	N	501	G2P	C3'-C4'-C5'-O5'
5	P	501	G2P	C3'-C4'-C5'-O5'
5	R	501	G2P	C3'-C4'-C5'-O5'
5	B	501	G2P	C5'-O5'-PA-O1A
5	D	501	G2P	C5'-O5'-PA-O1A
5	F	501	G2P	C5'-O5'-PA-O1A
5	H	501	G2P	C5'-O5'-PA-O1A
5	J	501	G2P	C5'-O5'-PA-O1A
5	L	501	G2P	C5'-O5'-PA-O1A
5	N	501	G2P	C5'-O5'-PA-O1A
5	P	501	G2P	C5'-O5'-PA-O1A
5	R	501	G2P	C5'-O5'-PA-O1A
5	B	501	G2P	PB-O3B-PG-O1G
5	B	501	G2P	PB-O3B-PG-O3G
5	D	501	G2P	PB-O3B-PG-O1G
5	D	501	G2P	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
5	F	501	G2P	PB-O3B-PG-O1G
5	F	501	G2P	PB-O3B-PG-O3G
5	H	501	G2P	PB-O3B-PG-O1G
5	H	501	G2P	PB-O3B-PG-O3G
5	J	501	G2P	PB-O3B-PG-O1G
5	J	501	G2P	PB-O3B-PG-O3G
5	L	501	G2P	PB-O3B-PG-O1G
5	L	501	G2P	PB-O3B-PG-O3G
5	N	501	G2P	PB-O3B-PG-O1G
5	N	501	G2P	PB-O3B-PG-O3G
5	P	501	G2P	PB-O3B-PG-O1G
5	P	501	G2P	PB-O3B-PG-O3G
5	R	501	G2P	PB-O3B-PG-O1G
5	R	501	G2P	PB-O3B-PG-O3G
5	B	501	G2P	C5'-O5'-PA-C3A
5	D	501	G2P	C5'-O5'-PA-C3A
5	F	501	G2P	C5'-O5'-PA-C3A
5	H	501	G2P	C5'-O5'-PA-C3A
5	J	501	G2P	C5'-O5'-PA-C3A
5	L	501	G2P	C5'-O5'-PA-C3A
5	N	501	G2P	C5'-O5'-PA-C3A
5	P	501	G2P	C5'-O5'-PA-C3A
5	R	501	G2P	C5'-O5'-PA-C3A
3	A	501	GTP	PG-O3B-PB-O2B
3	C	501	GTP	PG-O3B-PB-O2B
3	E	501	GTP	PG-O3B-PB-O2B
3	G	501	GTP	PG-O3B-PB-O2B
3	I	501	GTP	PG-O3B-PB-O2B
3	K	501	GTP	PG-O3B-PB-O2B
3	M	501	GTP	PG-O3B-PB-O2B
3	O	501	GTP	PG-O3B-PB-O2B
3	Q	501	GTP	PG-O3B-PB-O2B

There are no ring outliers.

9 monomers are involved in 36 short contacts:

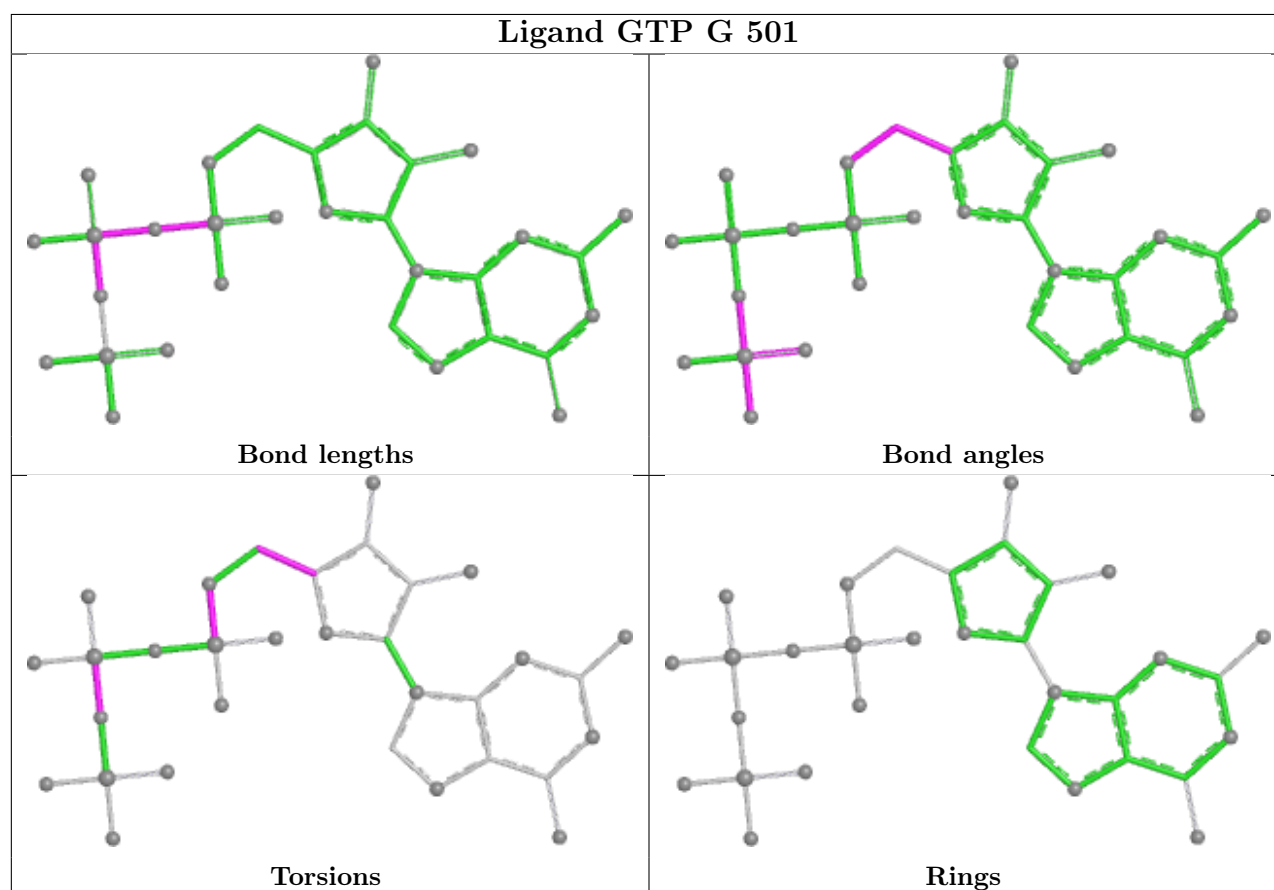
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	501	G2P	4	0
5	J	501	G2P	4	0
5	N	501	G2P	4	0
5	P	501	G2P	4	0
5	L	501	G2P	4	0

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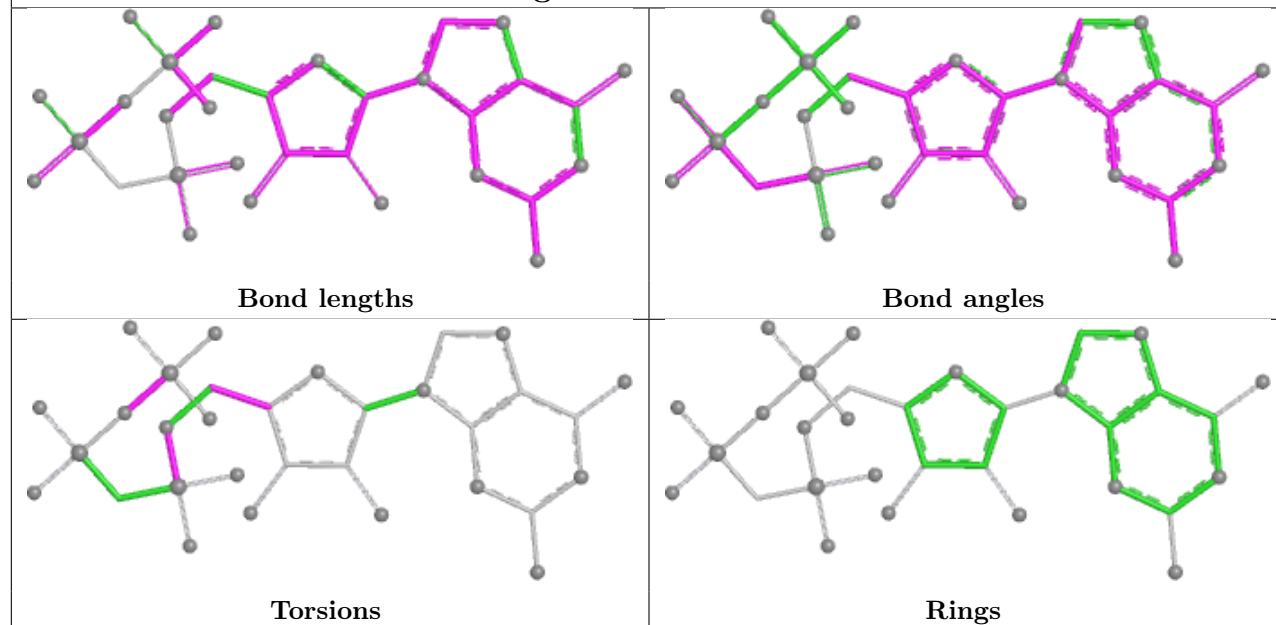
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	501	G2P	4	0
5	H	501	G2P	4	0
5	D	501	G2P	4	0
5	B	501	G2P	4	0

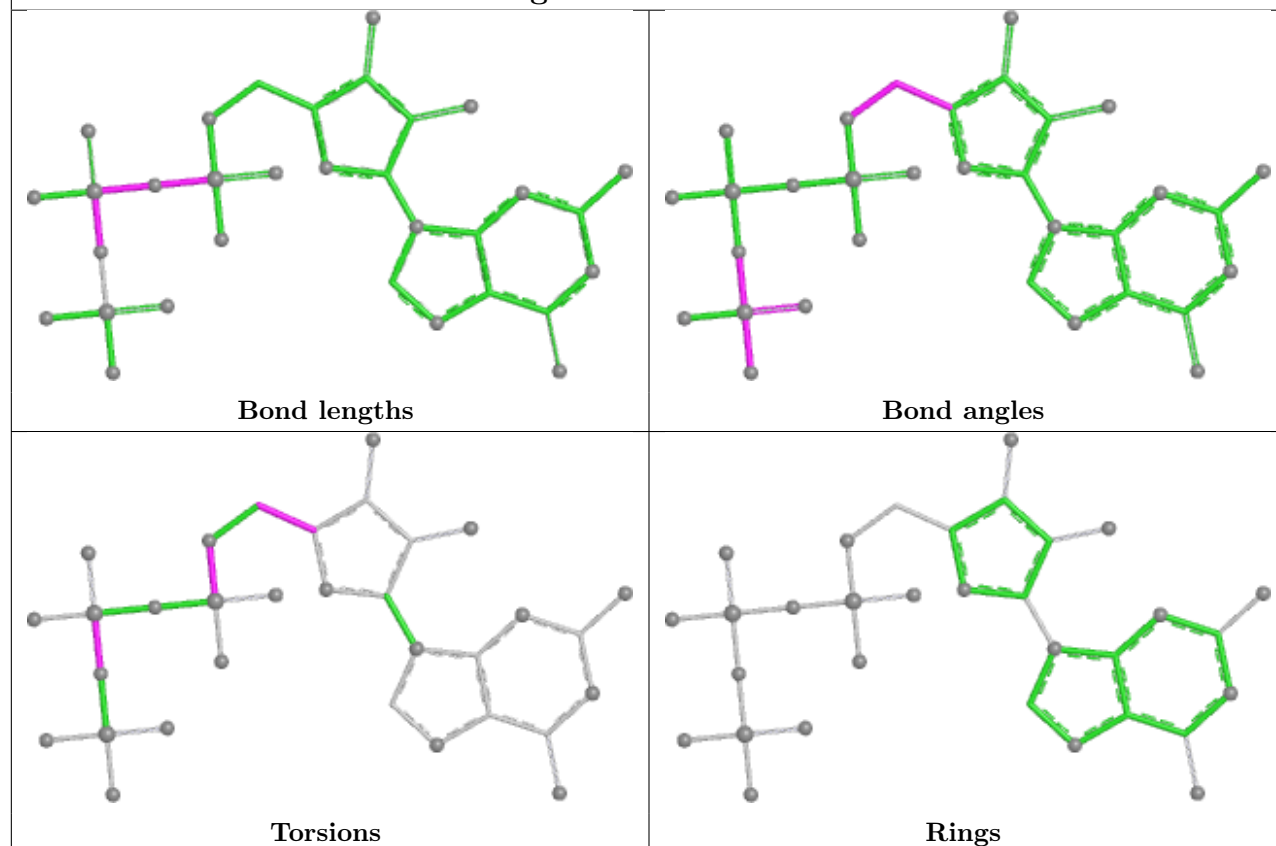
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

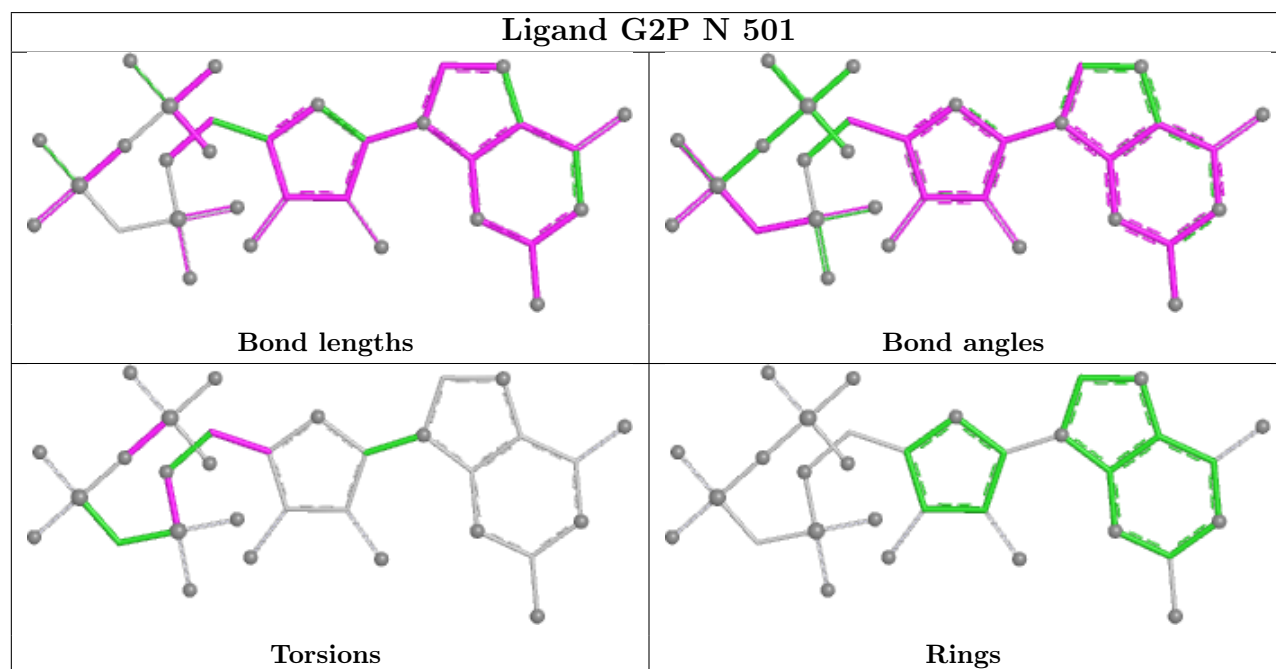
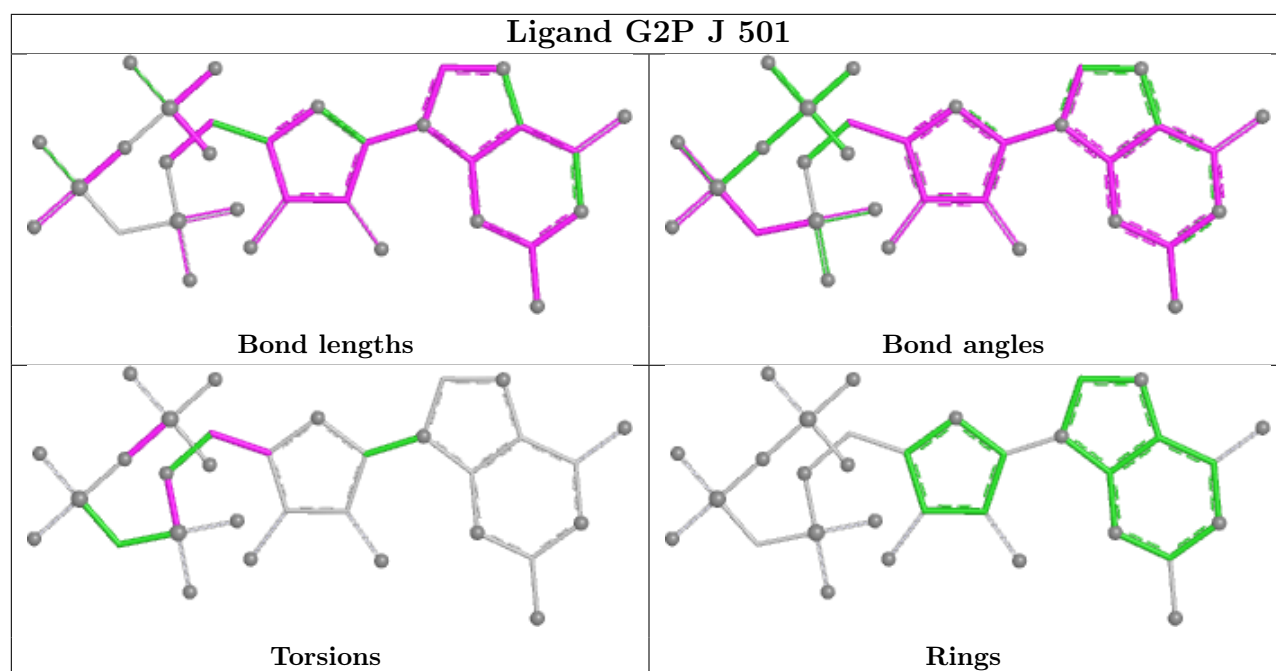


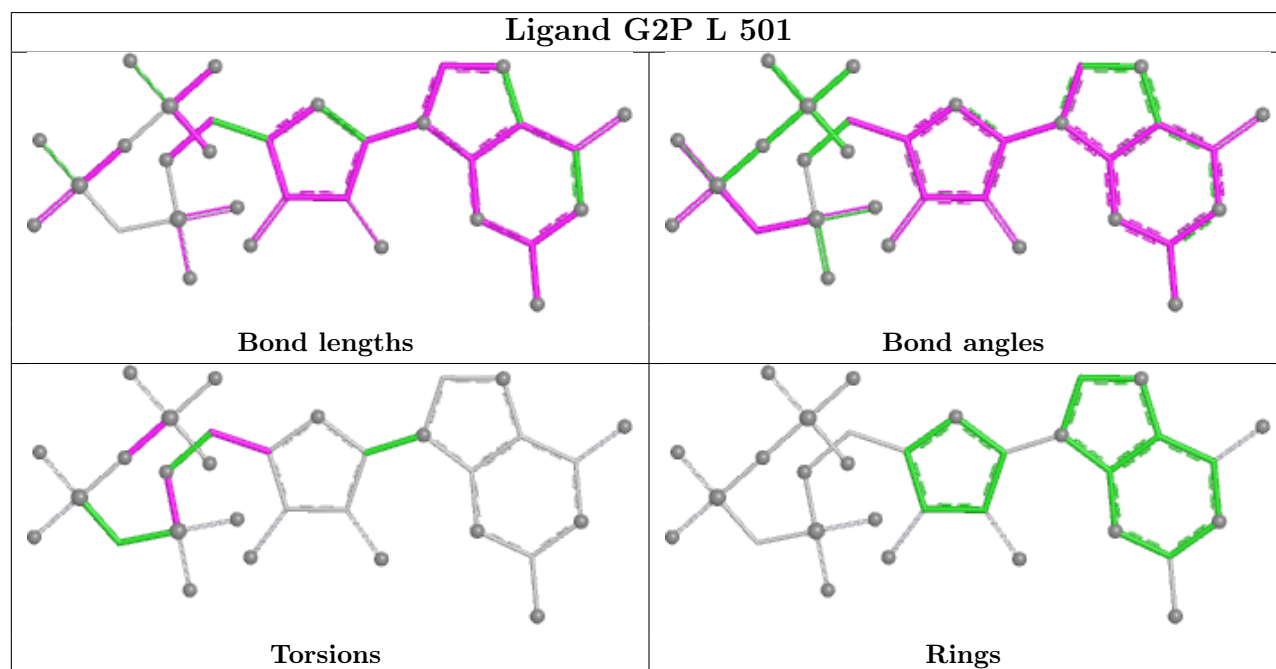
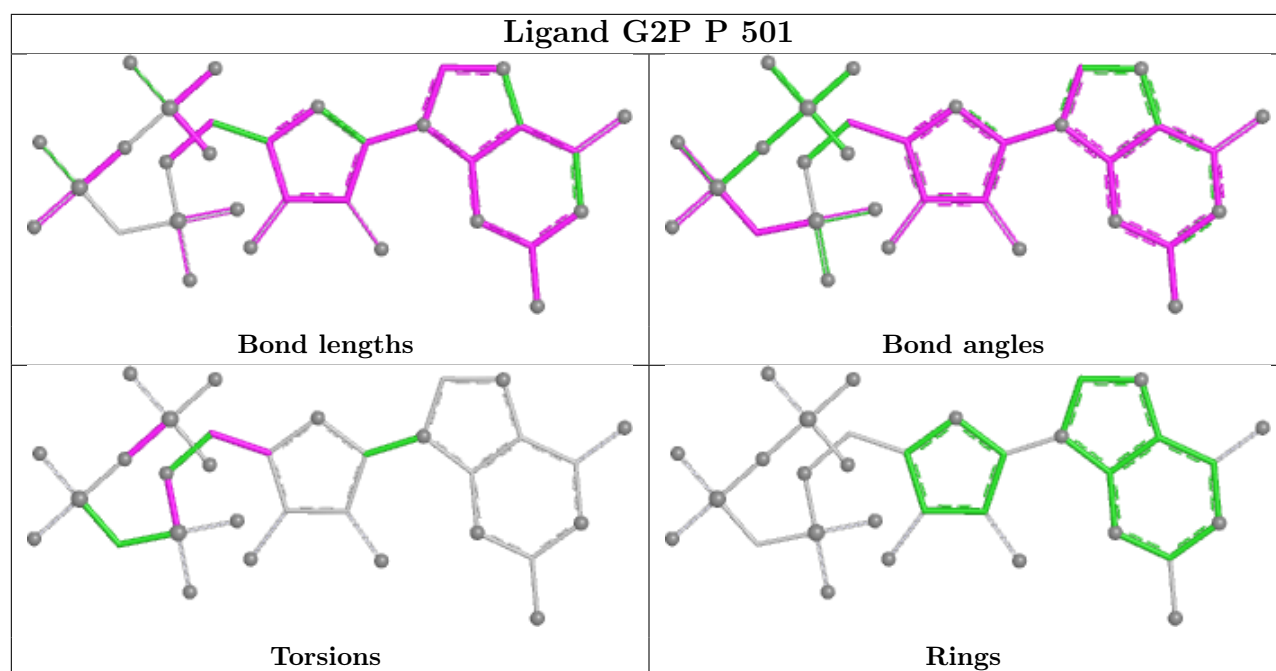
Ligand G2P R 501



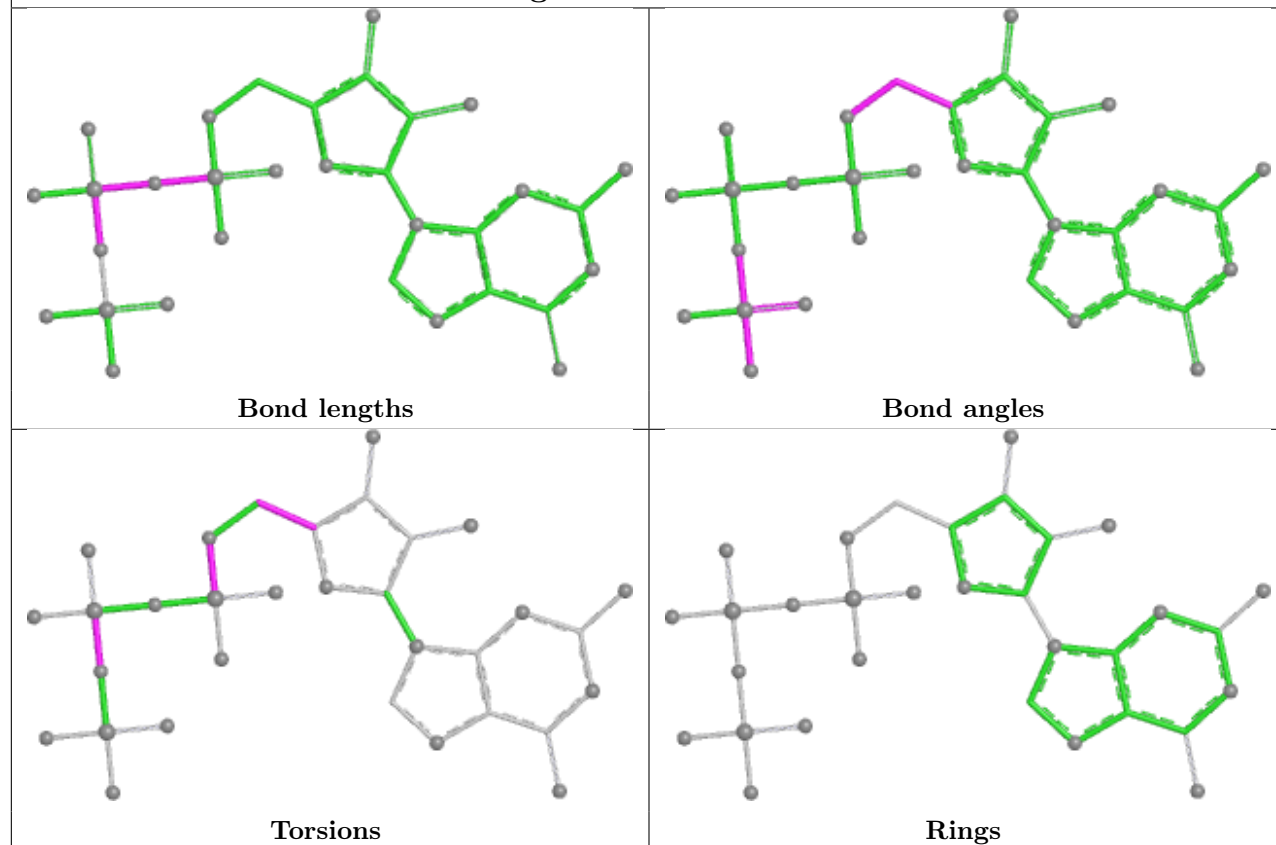
Ligand GTP O 501



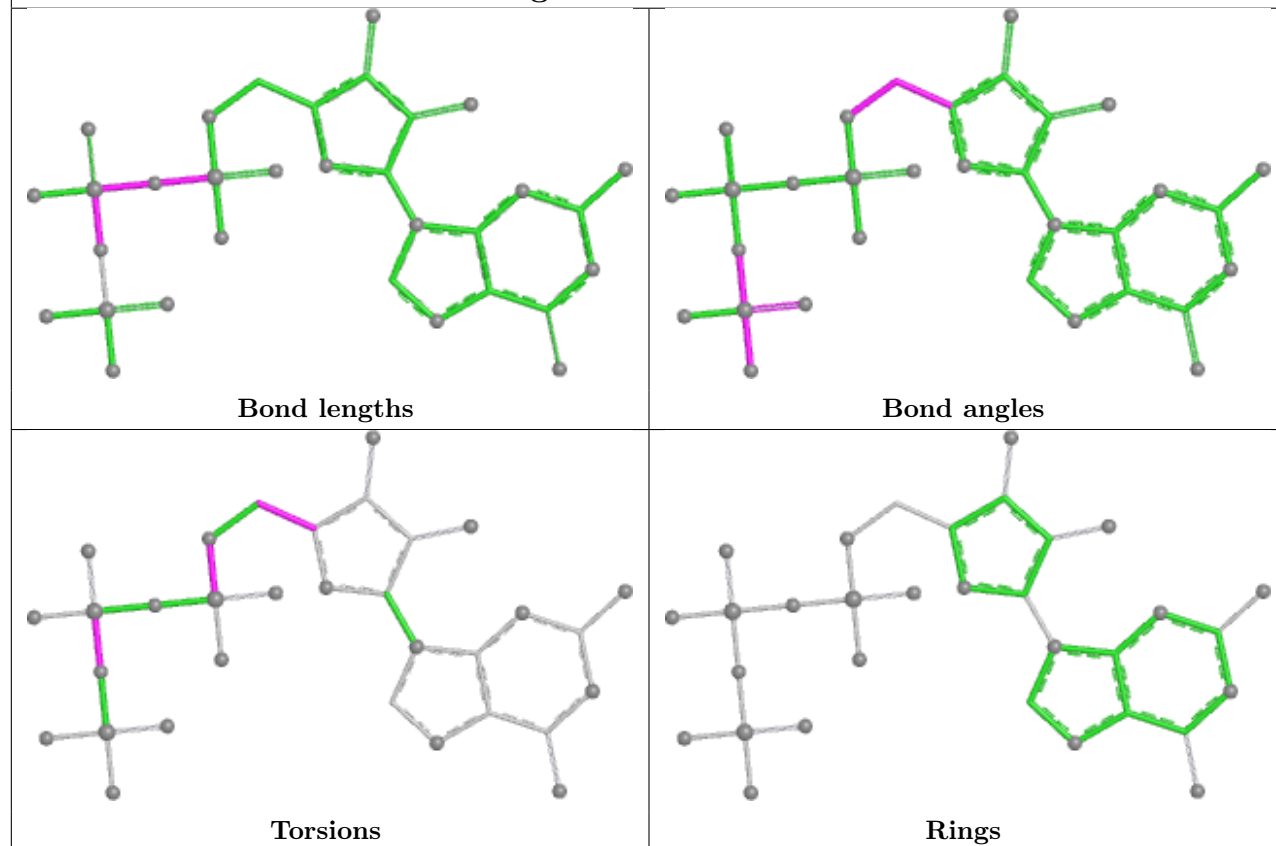


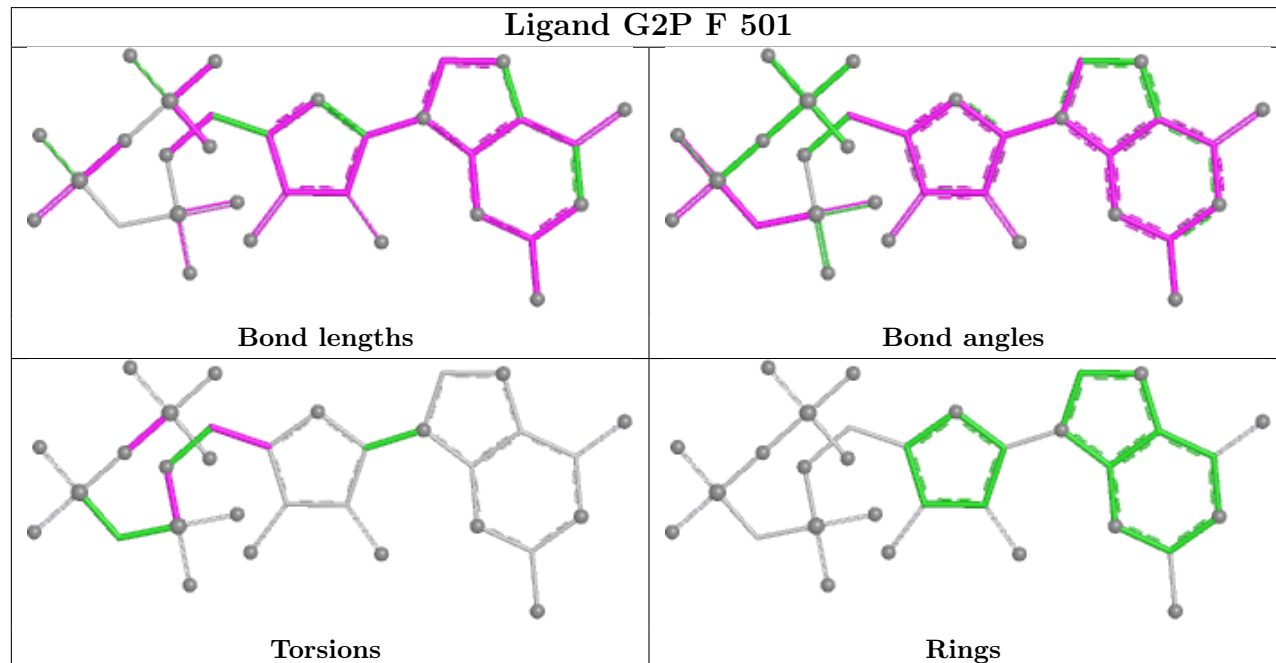
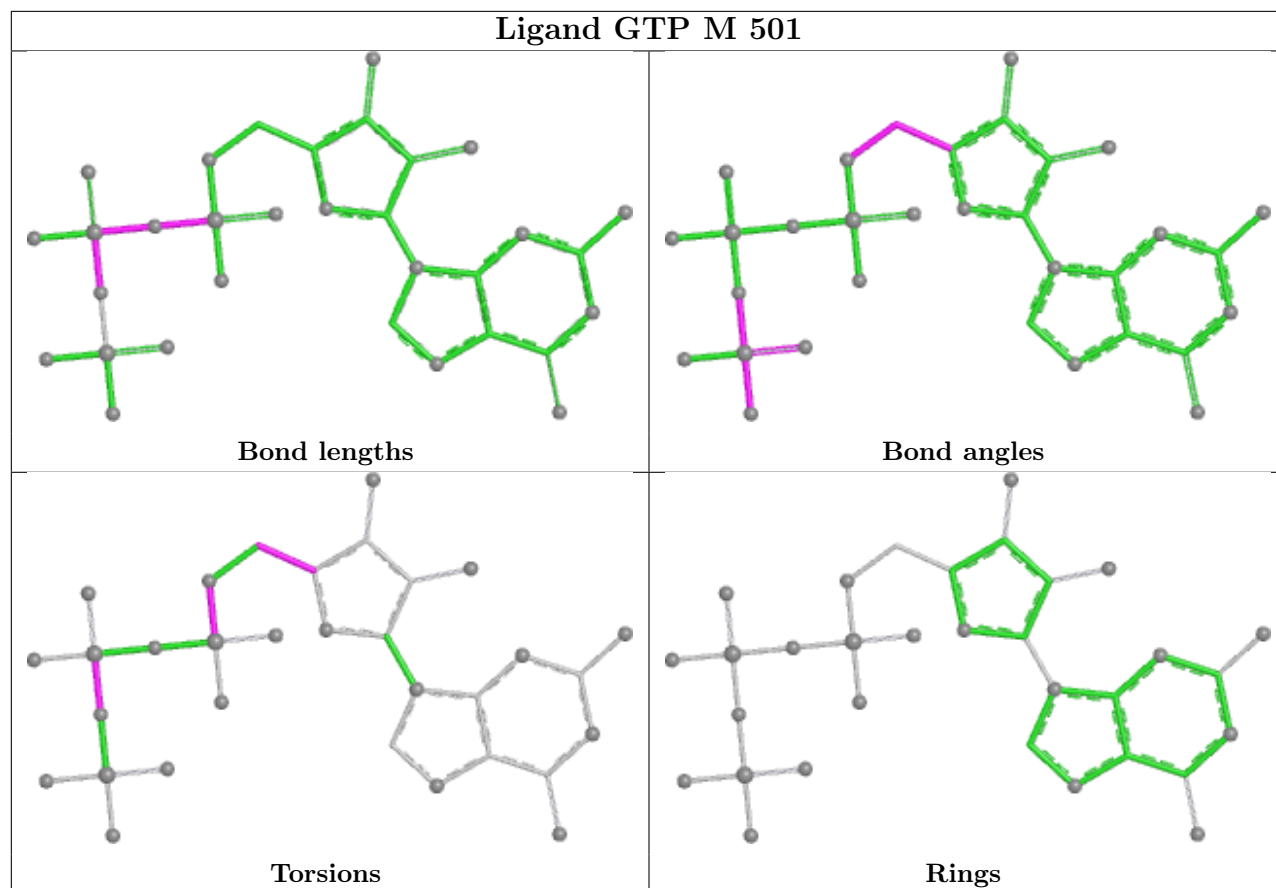


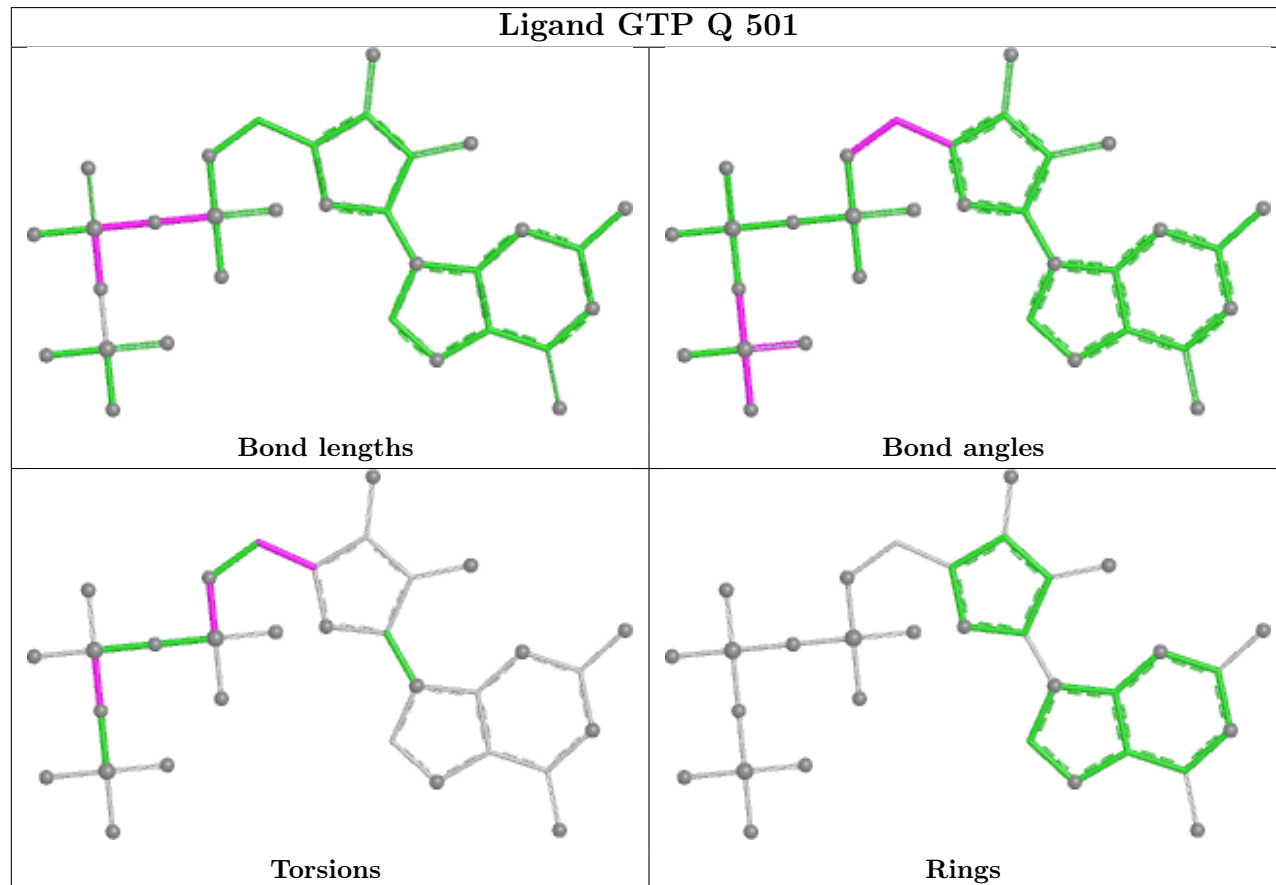
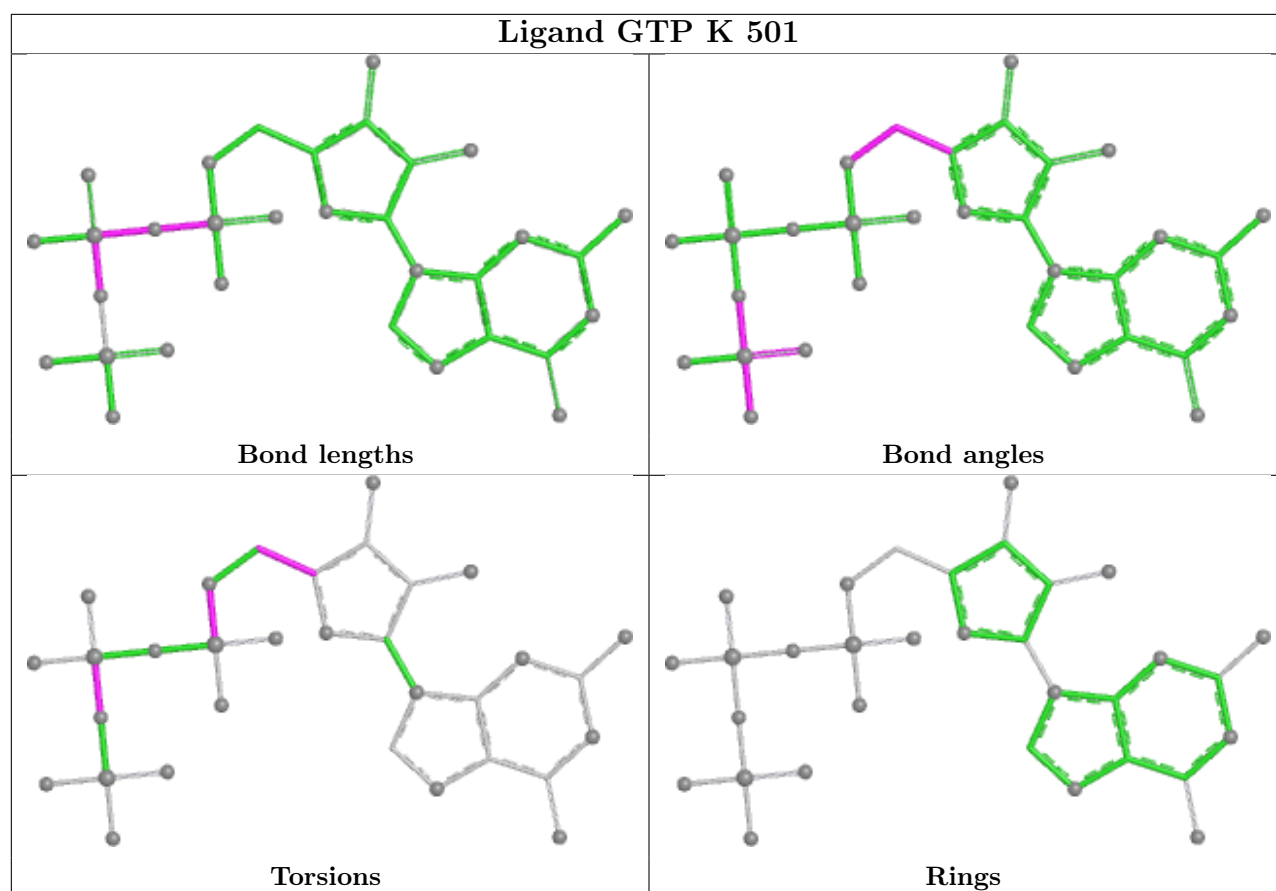
Ligand GTP A 501



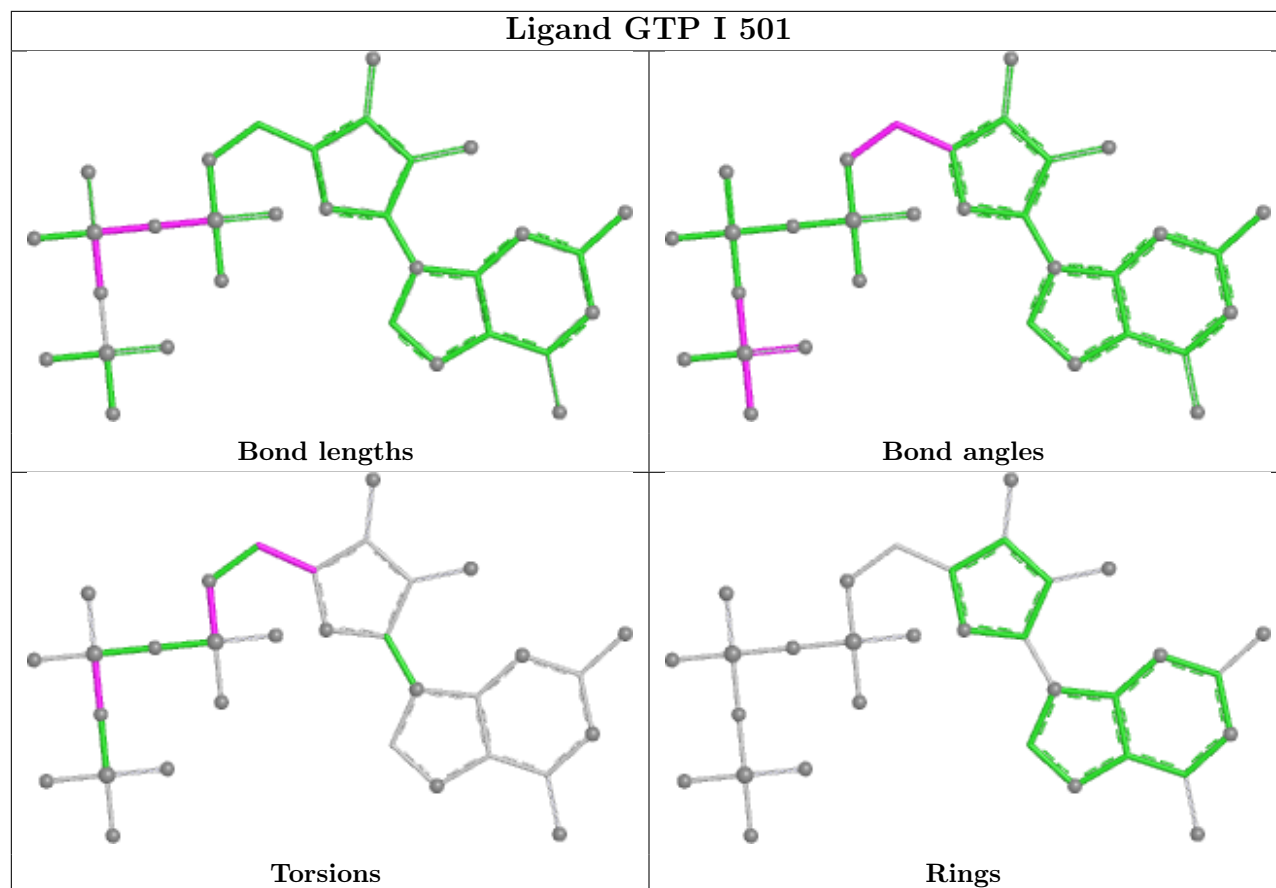
Ligand GTP C 501



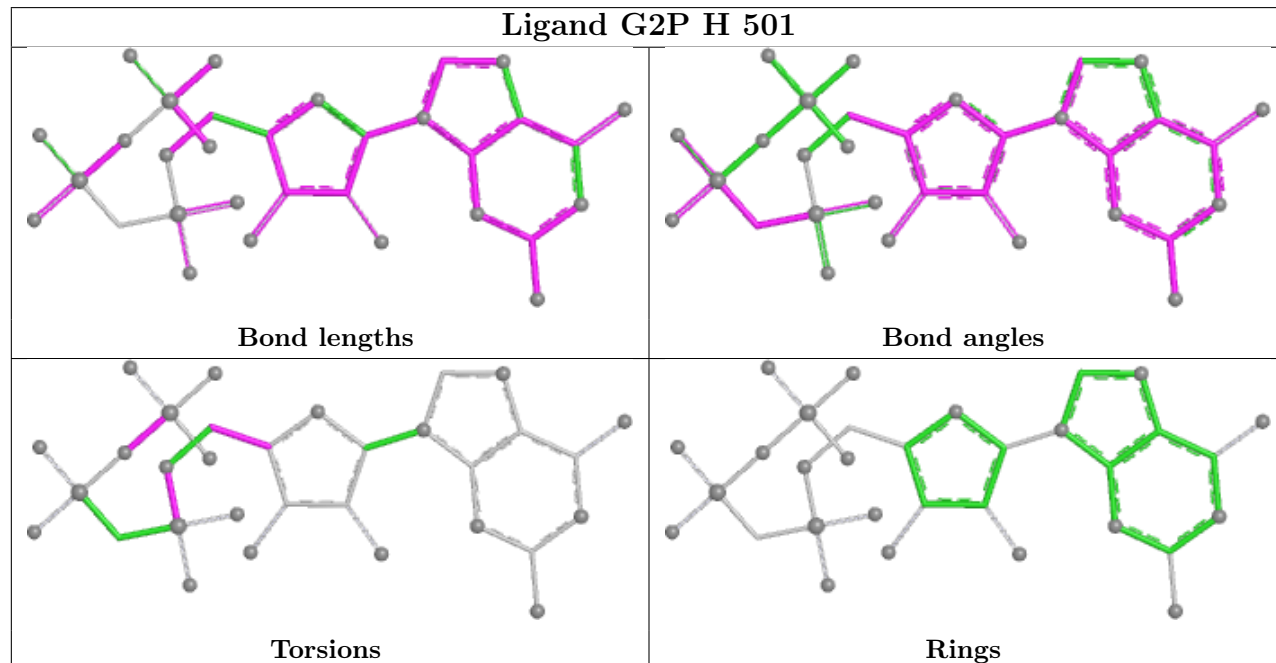




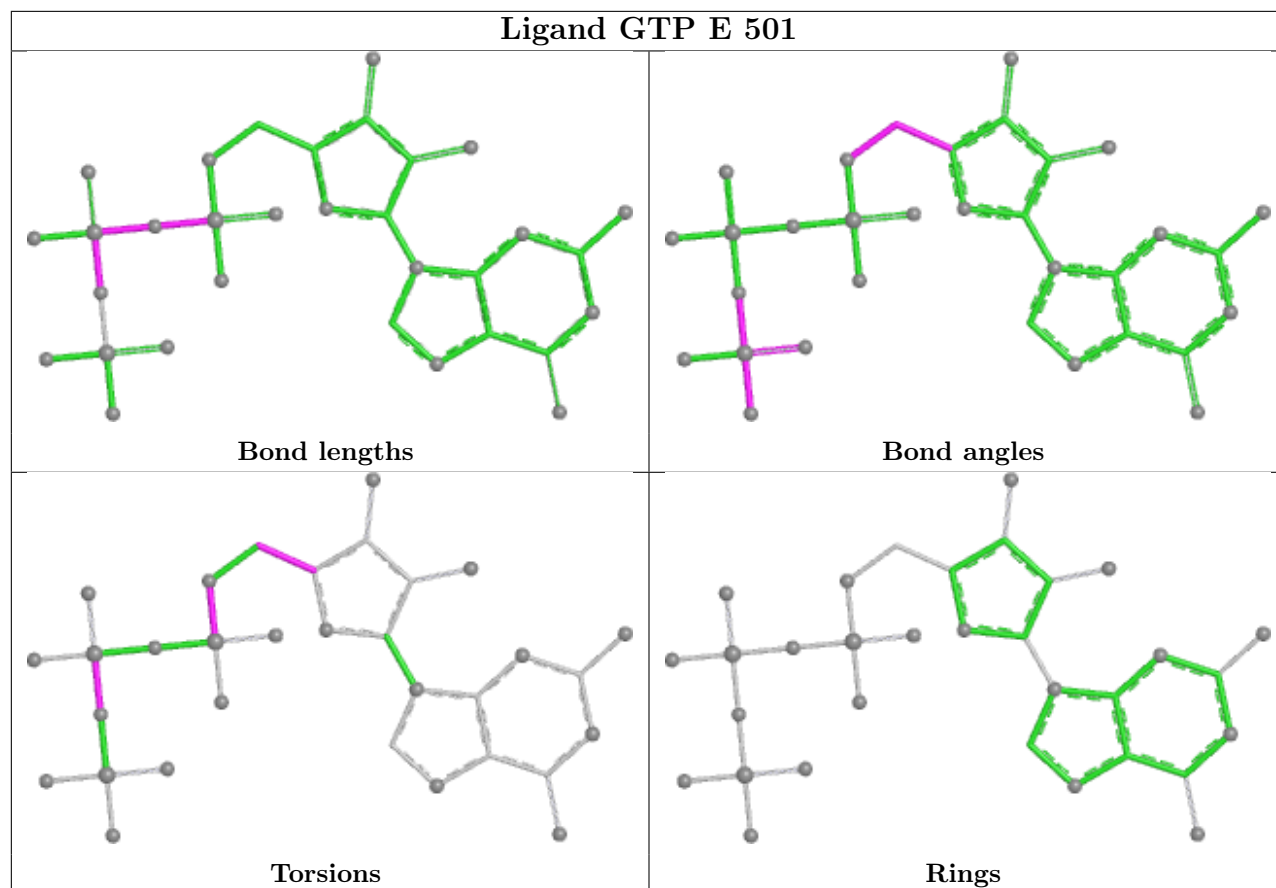
Ligand GTP I 501



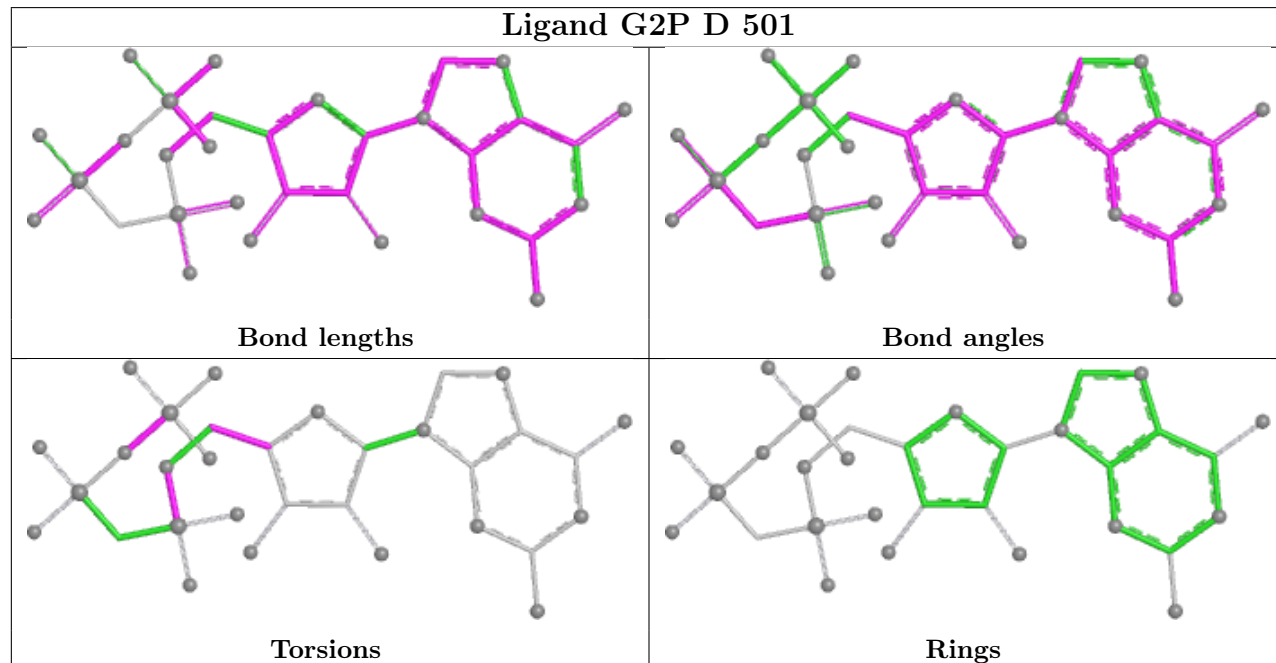
Ligand G2P H 501

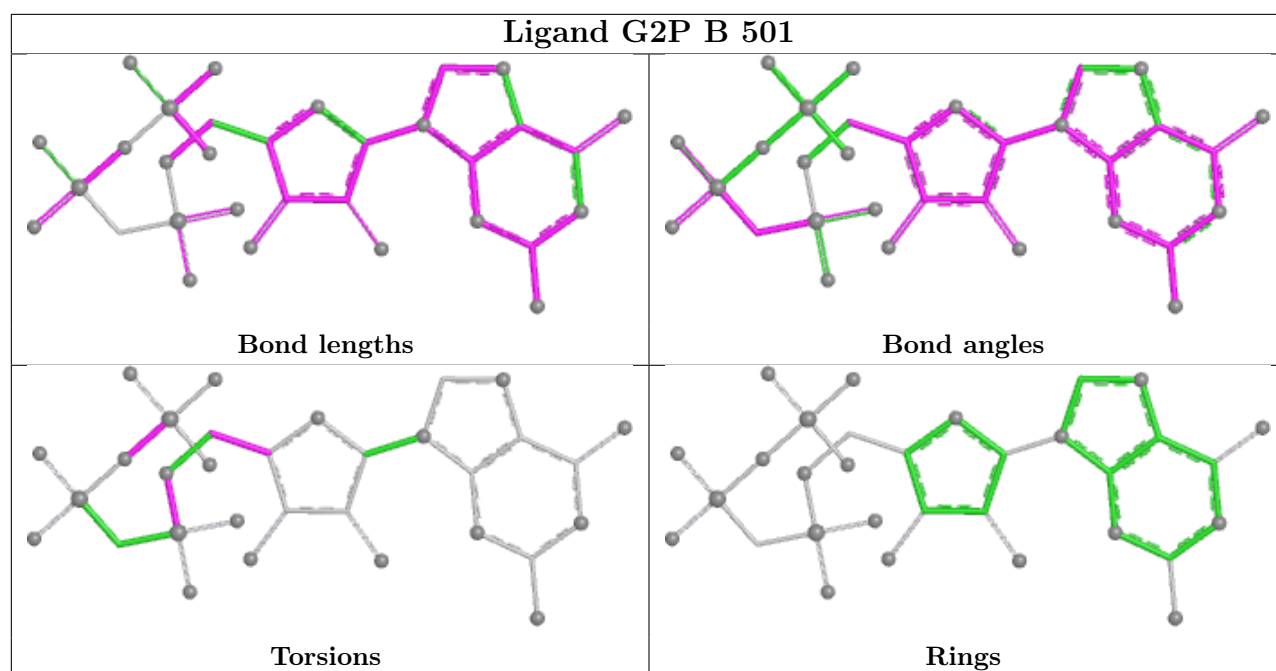


Ligand GTP E 501



Ligand G2P D 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

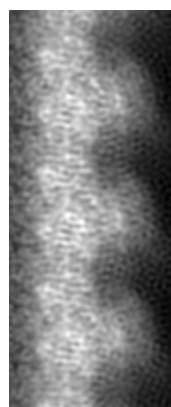
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5895. These allow visual inspection of the internal detail of the map and identification of artifacts.

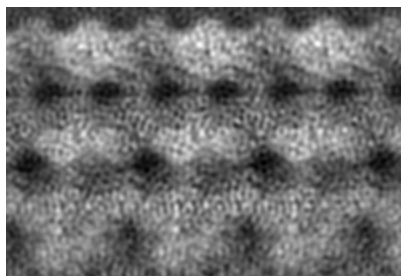
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

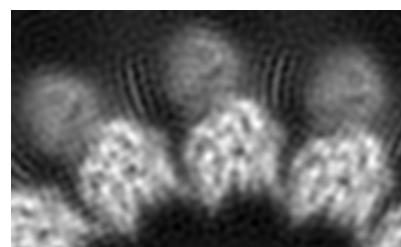
6.1.1 Primary map



X



Y

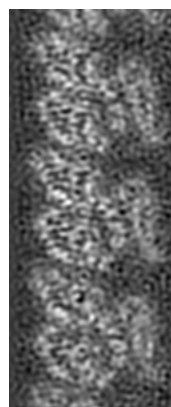


Z

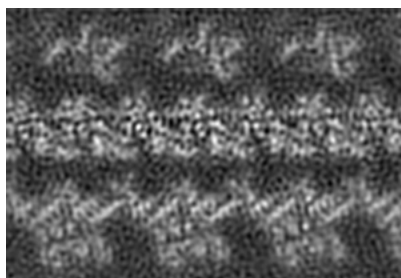
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

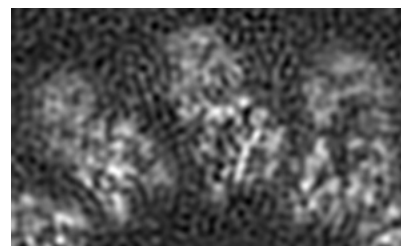
6.2.1 Primary map



X Index: 55



Y Index: 33

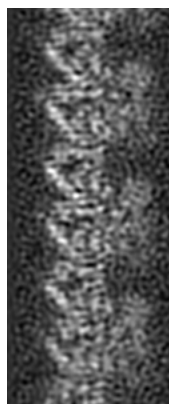


Z Index: 81

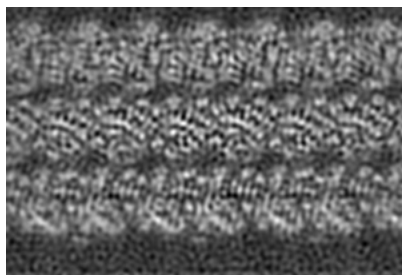
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

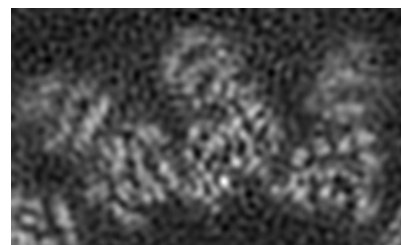
6.3.1 Primary map



X Index: 59



Y Index: 22

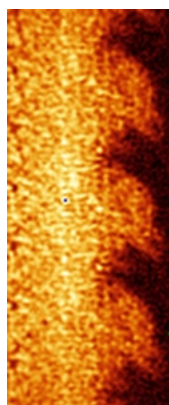


Z Index: 73

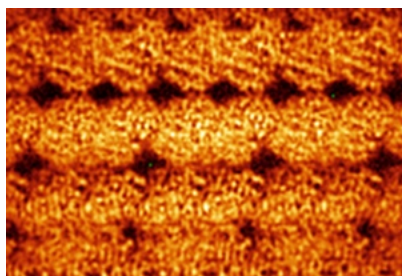
The images above show the largest variance slices of the map in three orthogonal directions.

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

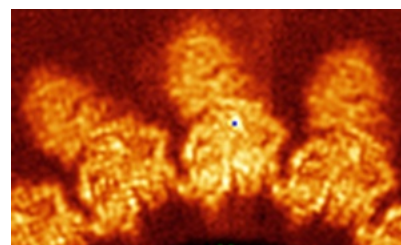
6.4.1 Primary map



X



Y

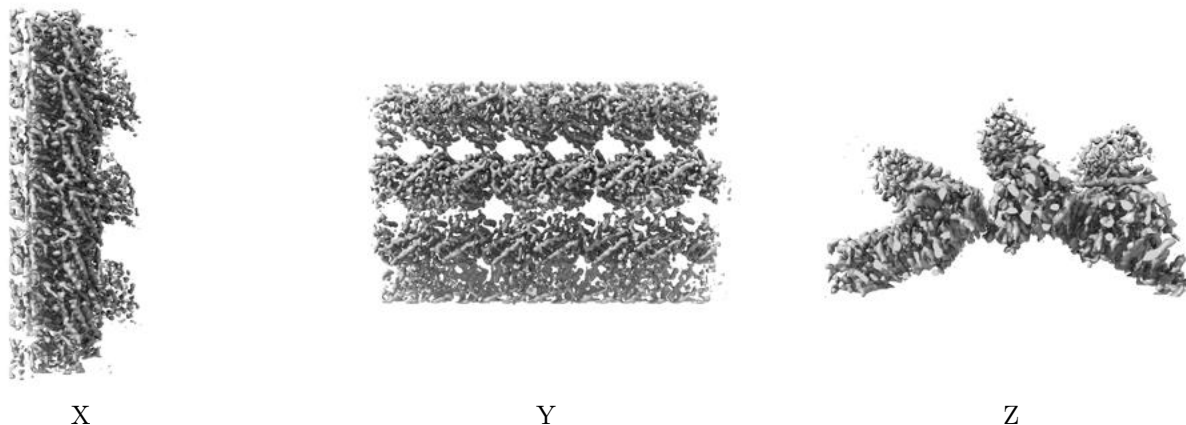


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

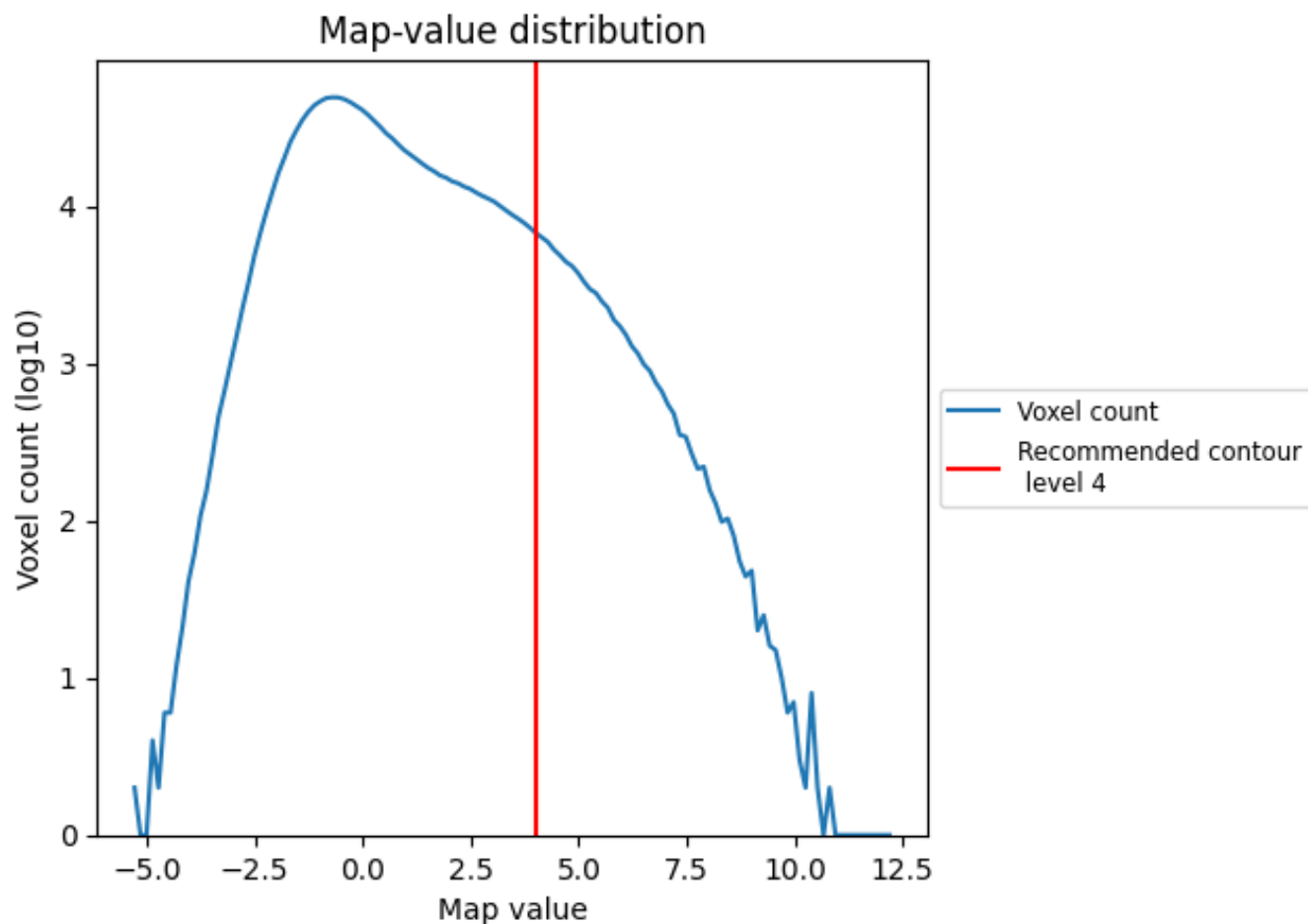
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

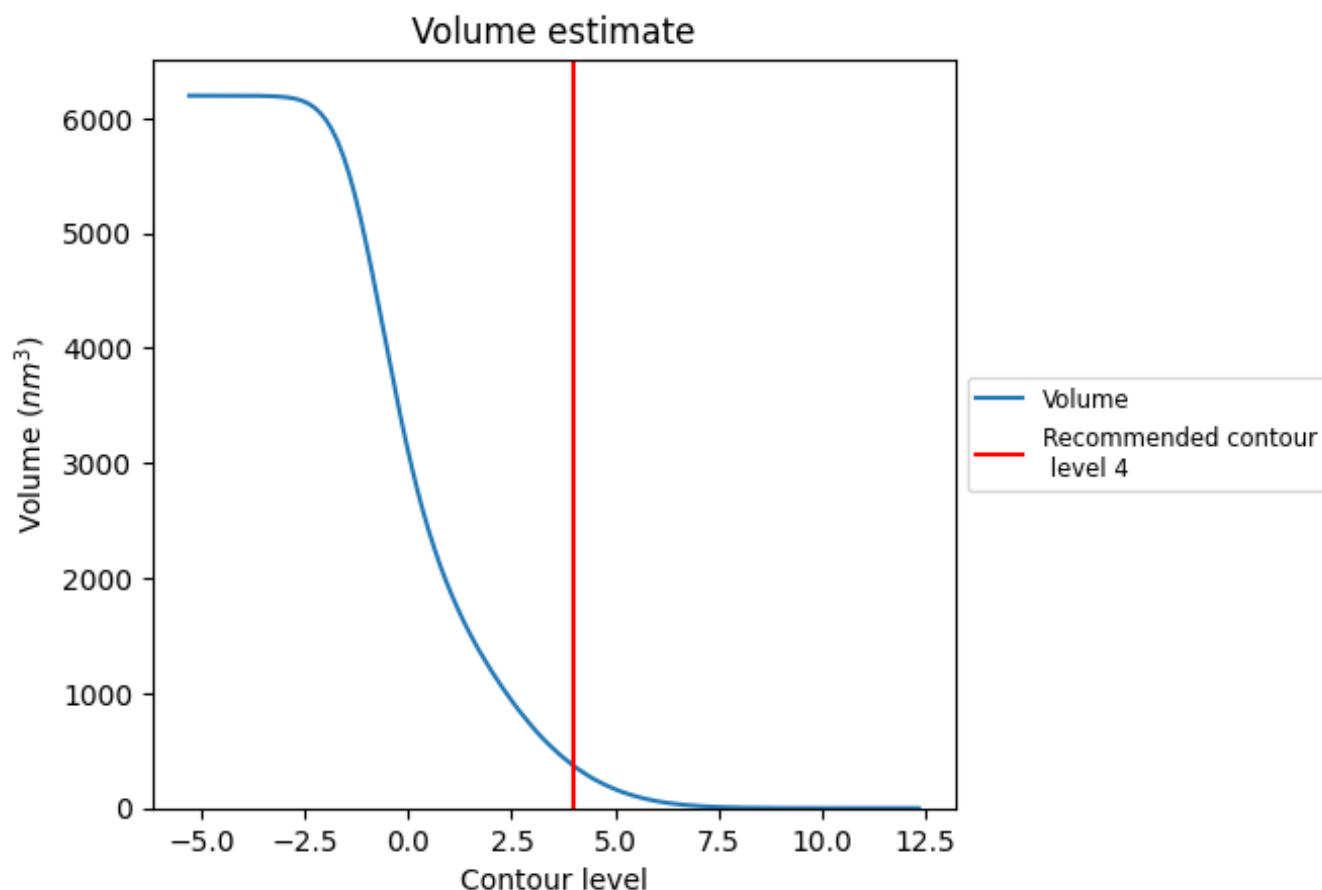
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 367 nm³; this corresponds to an approximate mass of 332 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation

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

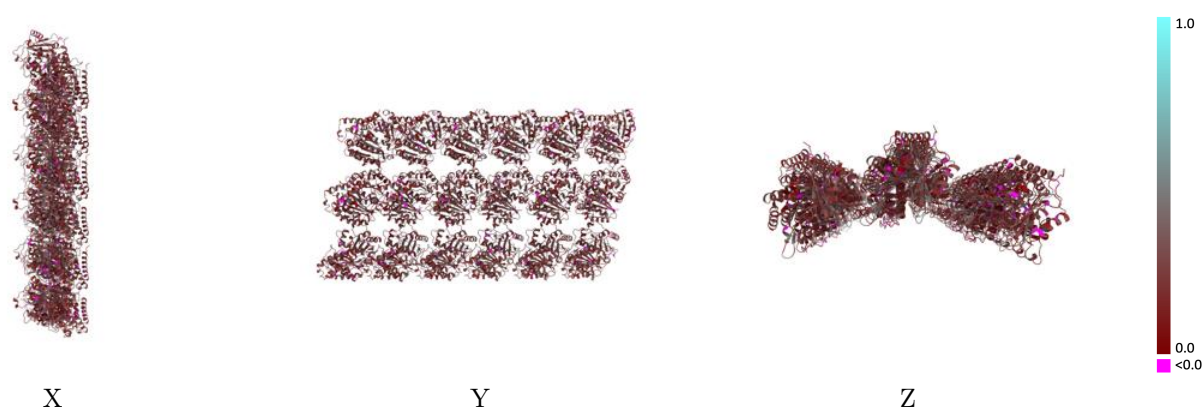
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5895 and PDB model 3J6E. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)

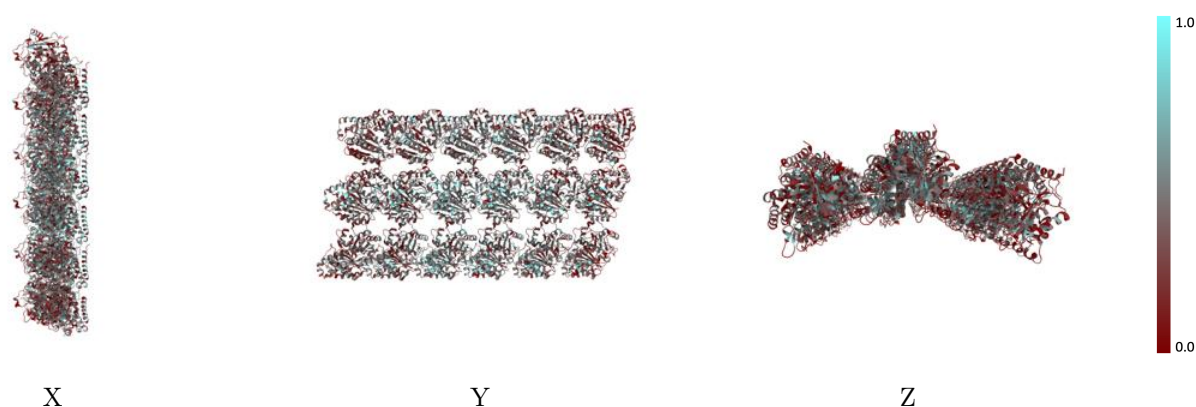
This section was not generated.

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



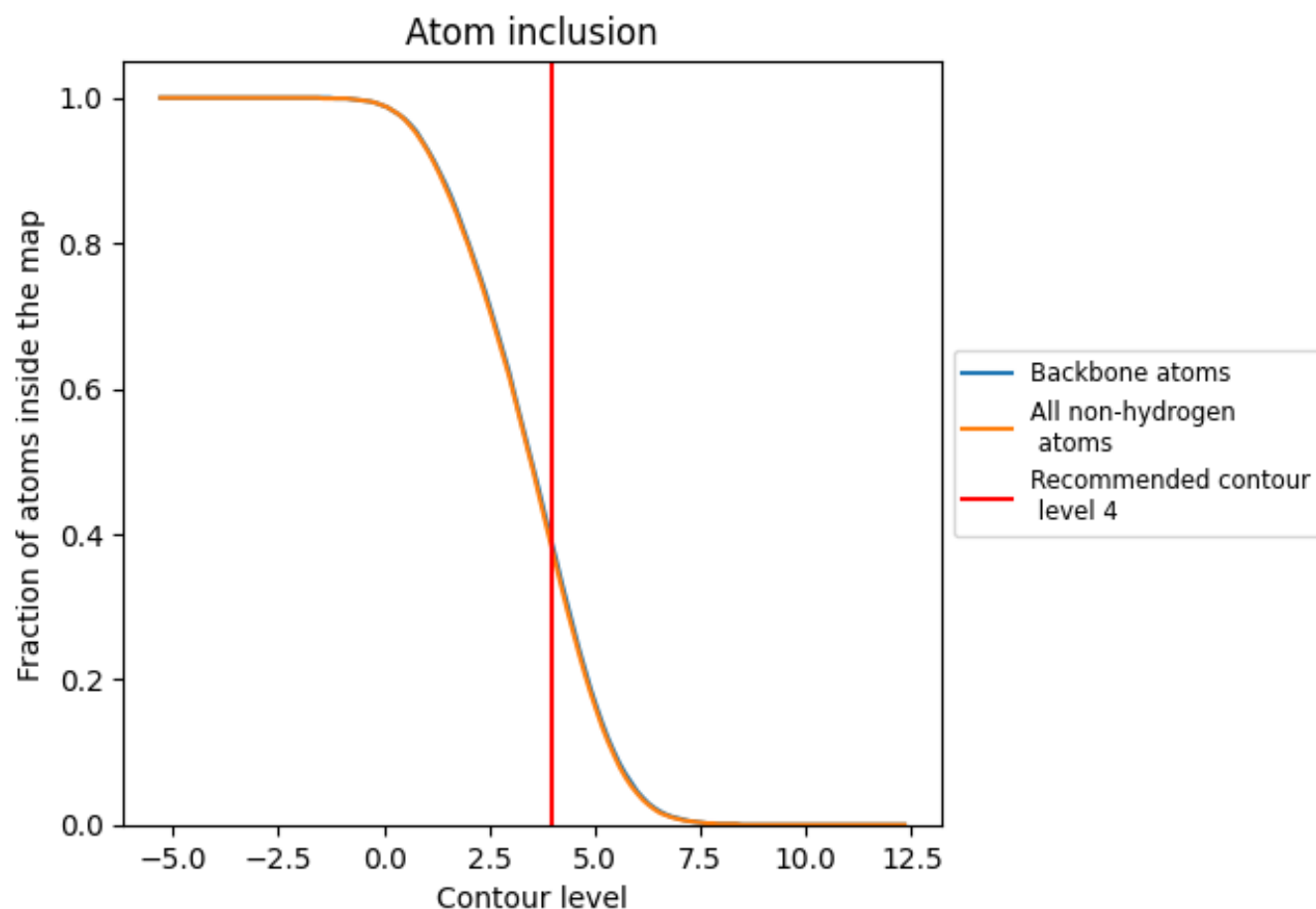
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3750	0.2430
A	0.4570	0.2580
B	0.4690	0.2630
C	0.4100	0.2520
D	0.4260	0.2570
E	0.4150	0.2490
F	0.4200	0.2570
G	0.3690	0.2340
H	0.3150	0.2310
I	0.4090	0.2400
J	0.3620	0.2370
K	0.3680	0.2380
L	0.3150	0.2370
M	0.3100	0.2360
N	0.3740	0.2400
O	0.3640	0.2420
P	0.4150	0.2420
Q	0.3040	0.2310
R	0.3660	0.2340

1.0

0.0

<0.0