



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 01:54 PM UTC

PDB ID : 3J6G / pdb_00003j6g
EMDB ID : EMD-5897
Title : Minimized average structure of microtubules stabilized by taxol
Authors : Alushin, G.M.; Lander, G.C.; Kellogg, E.H.; Zhang, R.; Baker, D.; Nogales, E.
Deposited on : 2014-02-19
Resolution : 5.50 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:

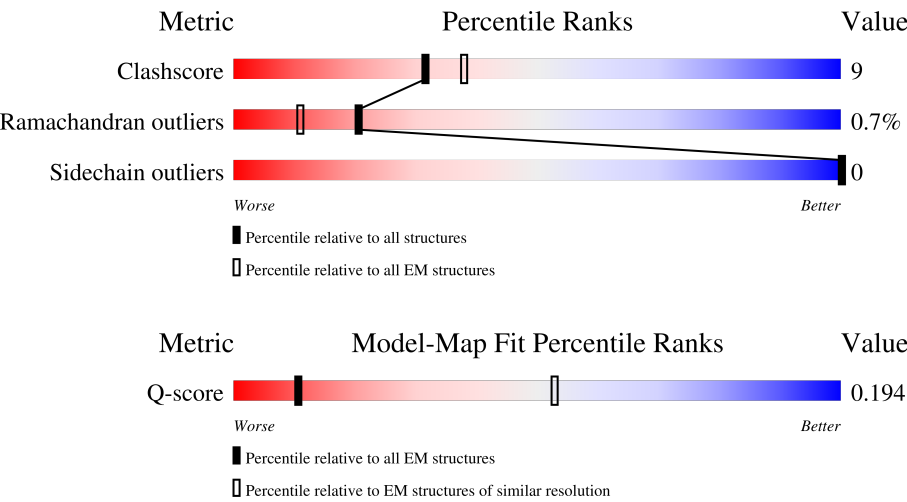
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 5.50 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	520 (5.00 - 6.00)

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	48% 63% 26% 8% ..
1	C	439	54% 62% 27% 8% ..
1	E	439	54% 63% 26% 8% ..
1	G	439	63% 63% 26% 8% ..

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Mol	Chain	Length	Quality of chain
1	I	439	54% 63% 26% 7% . .
1	K	439	61% 63% 26% 7% . .
1	M	439	73% 63% 26% 8% . .
1	O	439	66% 63% 27% 7% . .
1	Q	439	72% 63% 26% 8% . .
2	B	427	50% 65% 30% .
2	D	427	55% 67% 29% .
2	F	427	54% 67% 28% .
2	H	427	71% 66% 29% .
2	J	427	63% 65% 30% 5%
2	L	427	72% 67% 29% .
2	N	427	62% 66% 30% .
2	P	427	56% 65% 30% 5%
2	R	427	63% 66% 29% 5%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 61461 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		

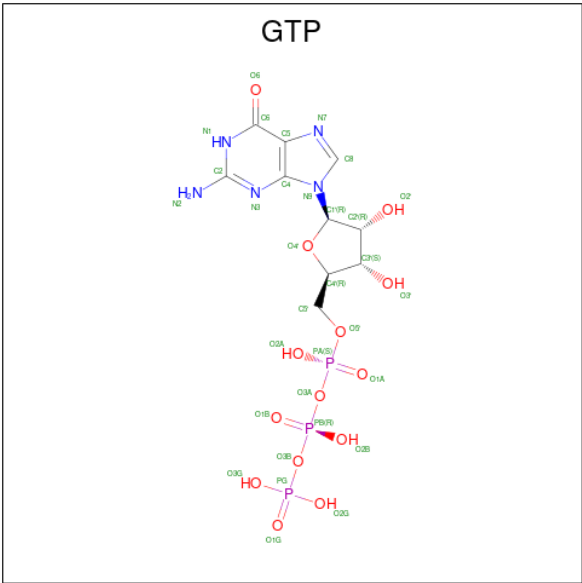
There are 9 discrepancies between the modelled and reference sequences:

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).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	E	1	Total	C	N	O	P	0
			32	10	5	14	3	

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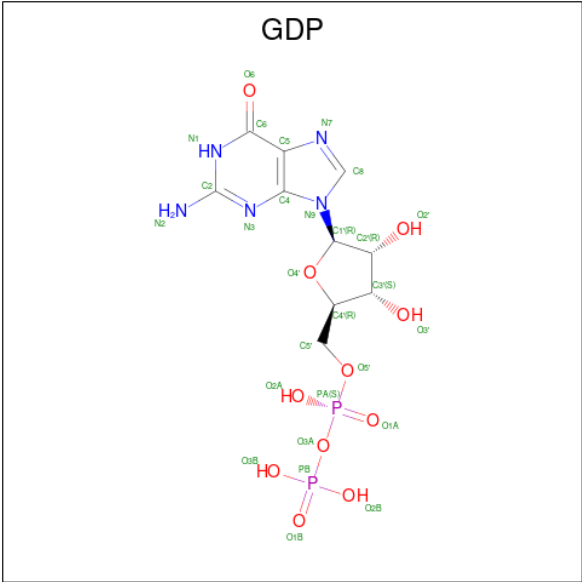
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Mol	Chain	Residues	Atoms					AltConf
3	G	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	I	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	K	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	M	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	O	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	Q	1	Total	C	N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

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

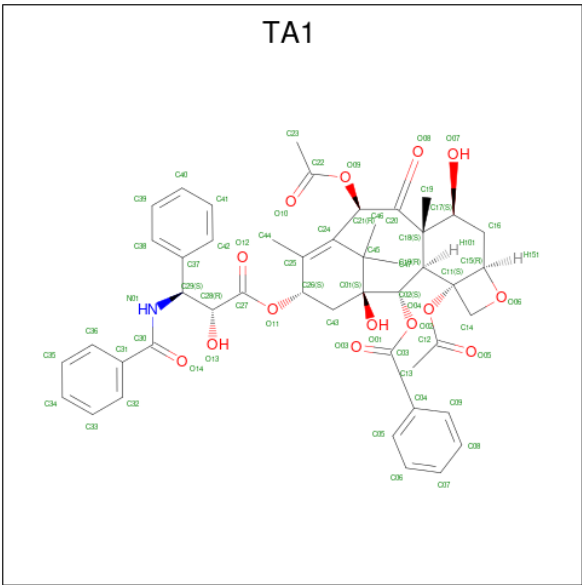
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	G	1	Total	Mg	0
			1	1	
4	I	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	M	1	Total	Mg	0
			1	1	
4	O	1	Total	Mg	0
			1	1	
4	Q	1	Total	Mg	0
			1	1	

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



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	D	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	F	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	H	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	J	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	L	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	N	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	P	1	Total	C	N	O	P	0
			28	10	5	11	2	
5	R	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 6 is TAXOL (CCD ID: TA1) (formula: C₄₇H₅₁NO₁₄).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			62	47	1	14	
6	D	1	Total	C	N	O	0
			62	47	1	14	
6	F	1	Total	C	N	O	0
			62	47	1	14	
6	H	1	Total	C	N	O	0
			62	47	1	14	
6	J	1	Total	C	N	O	0
			62	47	1	14	
6	L	1	Total	C	N	O	0
			62	47	1	14	
6	N	1	Total	C	N	O	0
			62	47	1	14	
6	P	1	Total	C	N	O	0
			62	47	1	14	
6	R	1	Total	C	N	O	0
			62	47	1	14	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	4	Total	O	0
			4	4	
7	C	4	Total	O	0
			4	4	
7	E	4	Total	O	0
			4	4	

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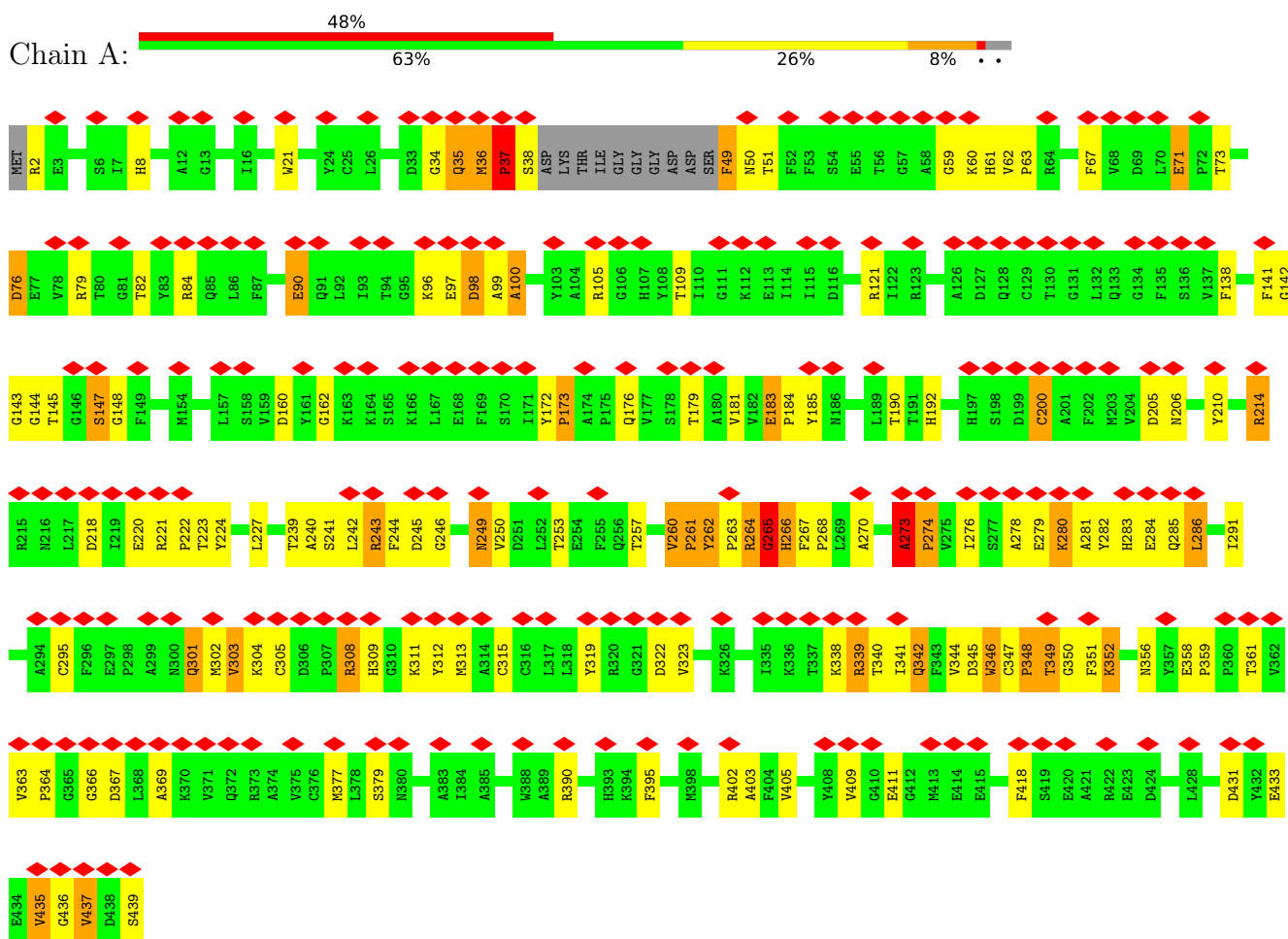
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Mol	Chain	Residues	Atoms		AltConf
7	G	4	Total 4	O 4	0
7	I	4	Total 4	O 4	0
7	K	4	Total 4	O 4	0
7	M	4	Total 4	O 4	0
7	O	4	Total 4	O 4	0
7	Q	4	Total 4	O 4	0

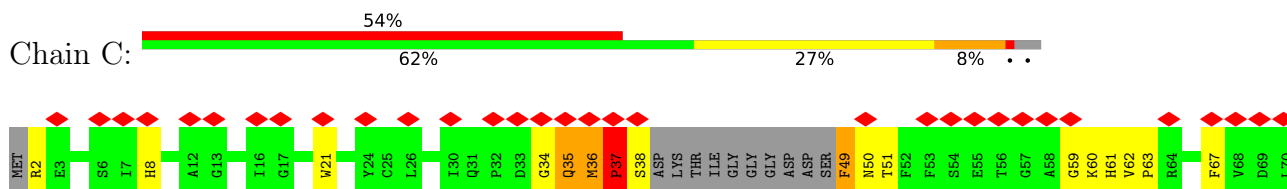
3 Residue-property plots

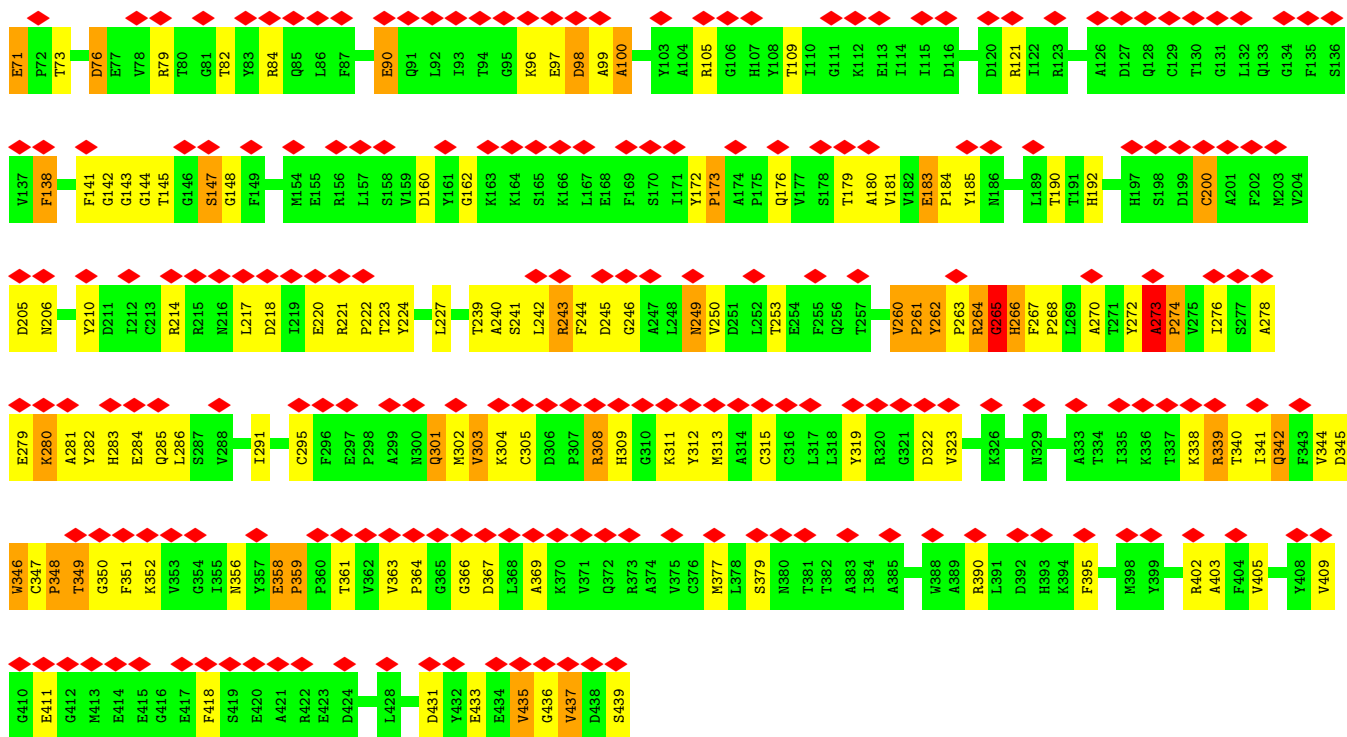
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

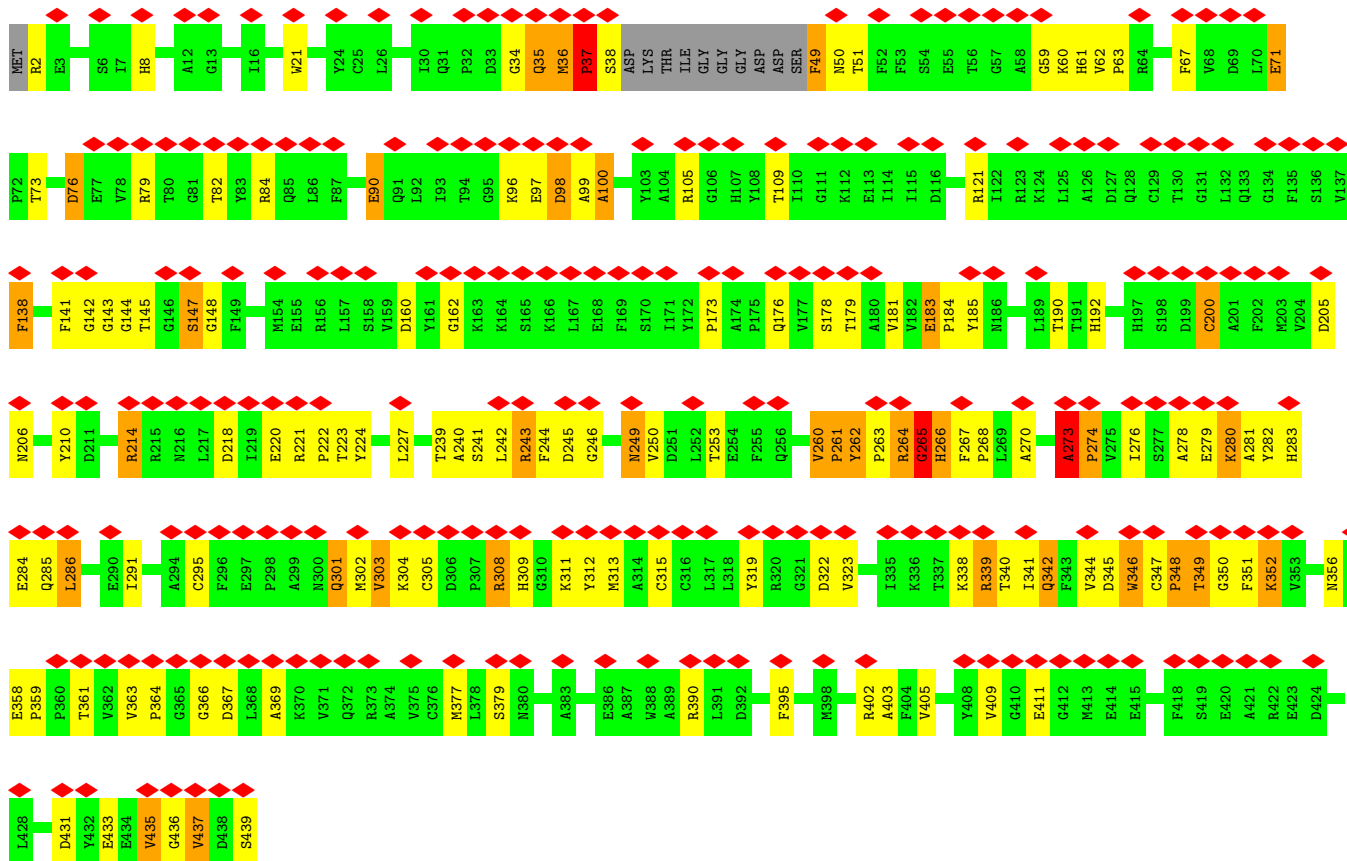


- Molecule 1: Tubulin alpha-1A chain

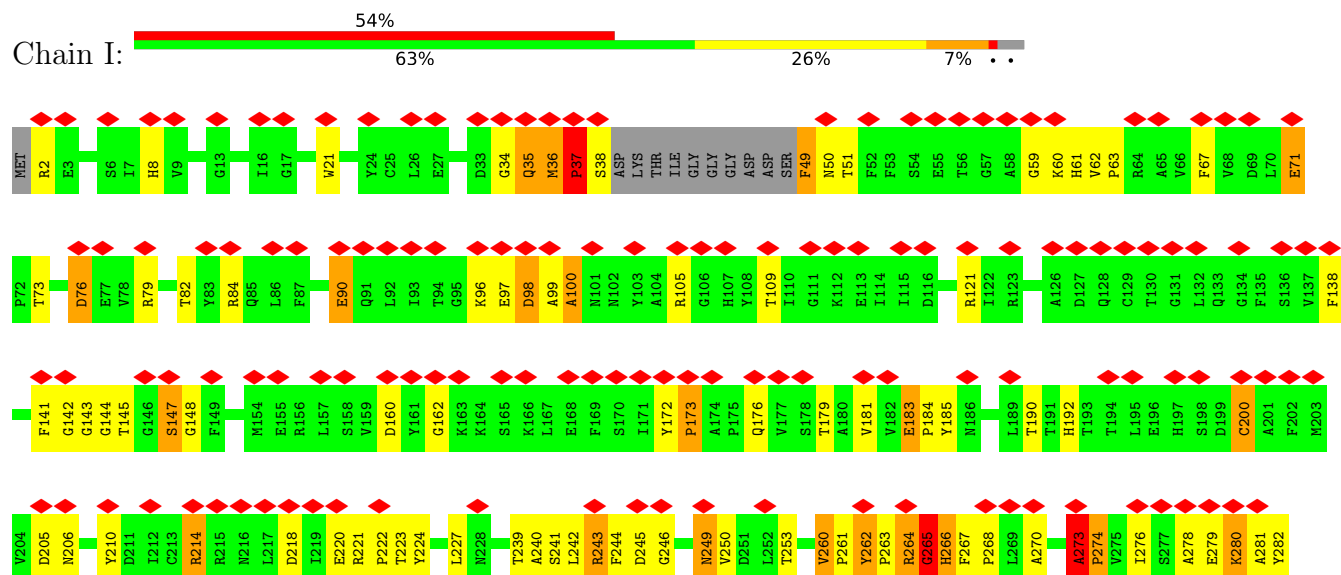


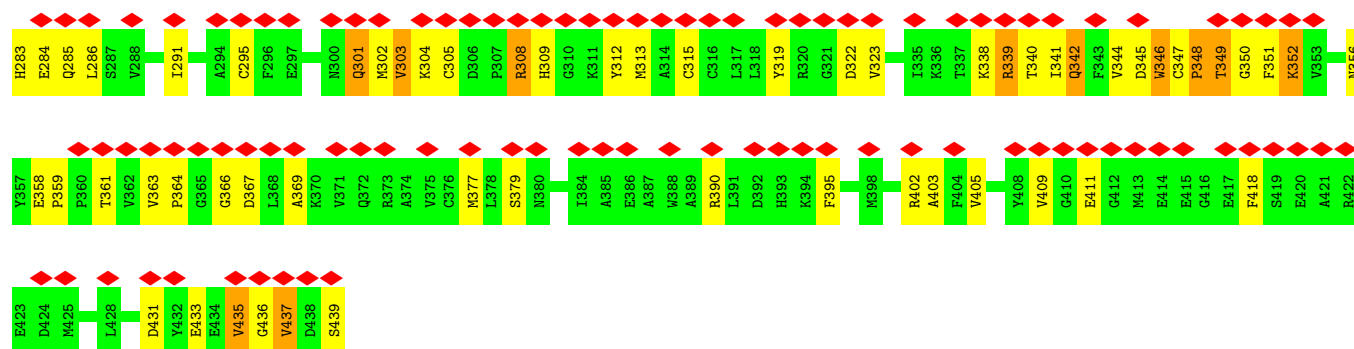


• Molecule 1: Tubulin alpha-1A chain

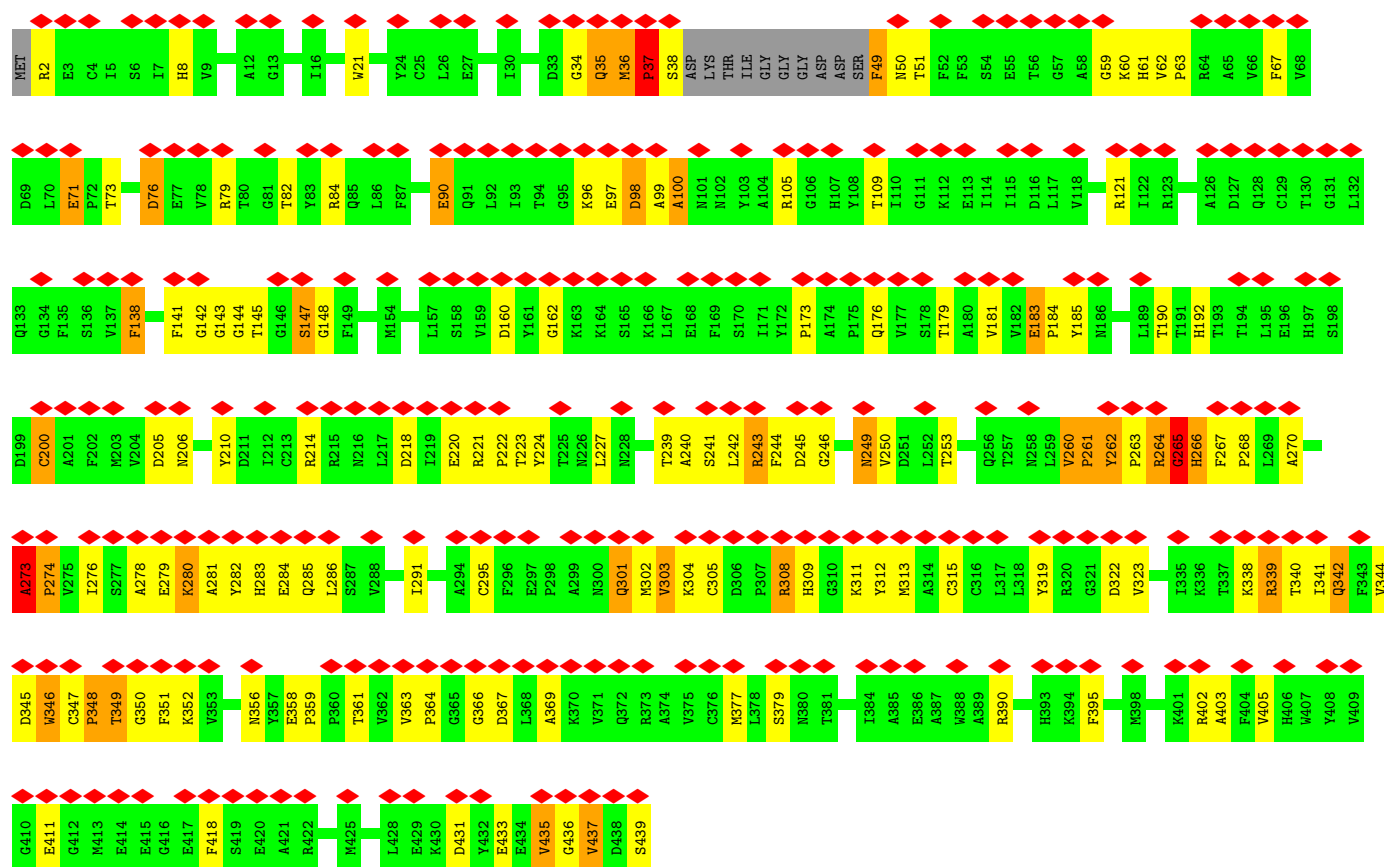


Chain G:

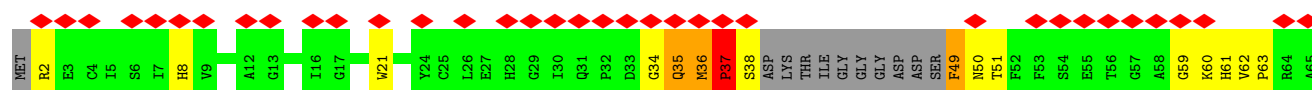
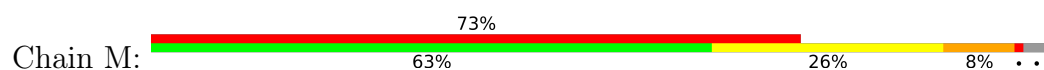


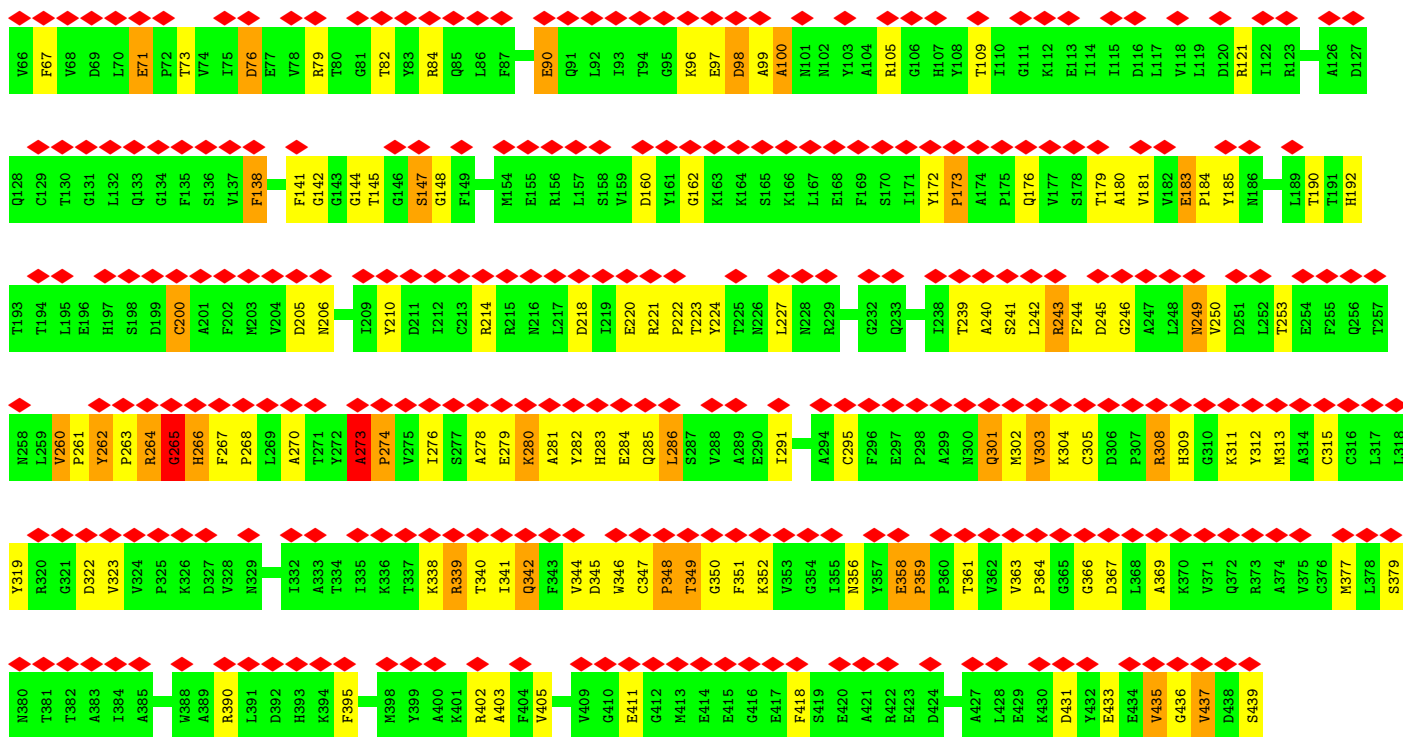


• Molecule 1: Tubulin alpha-1A chain

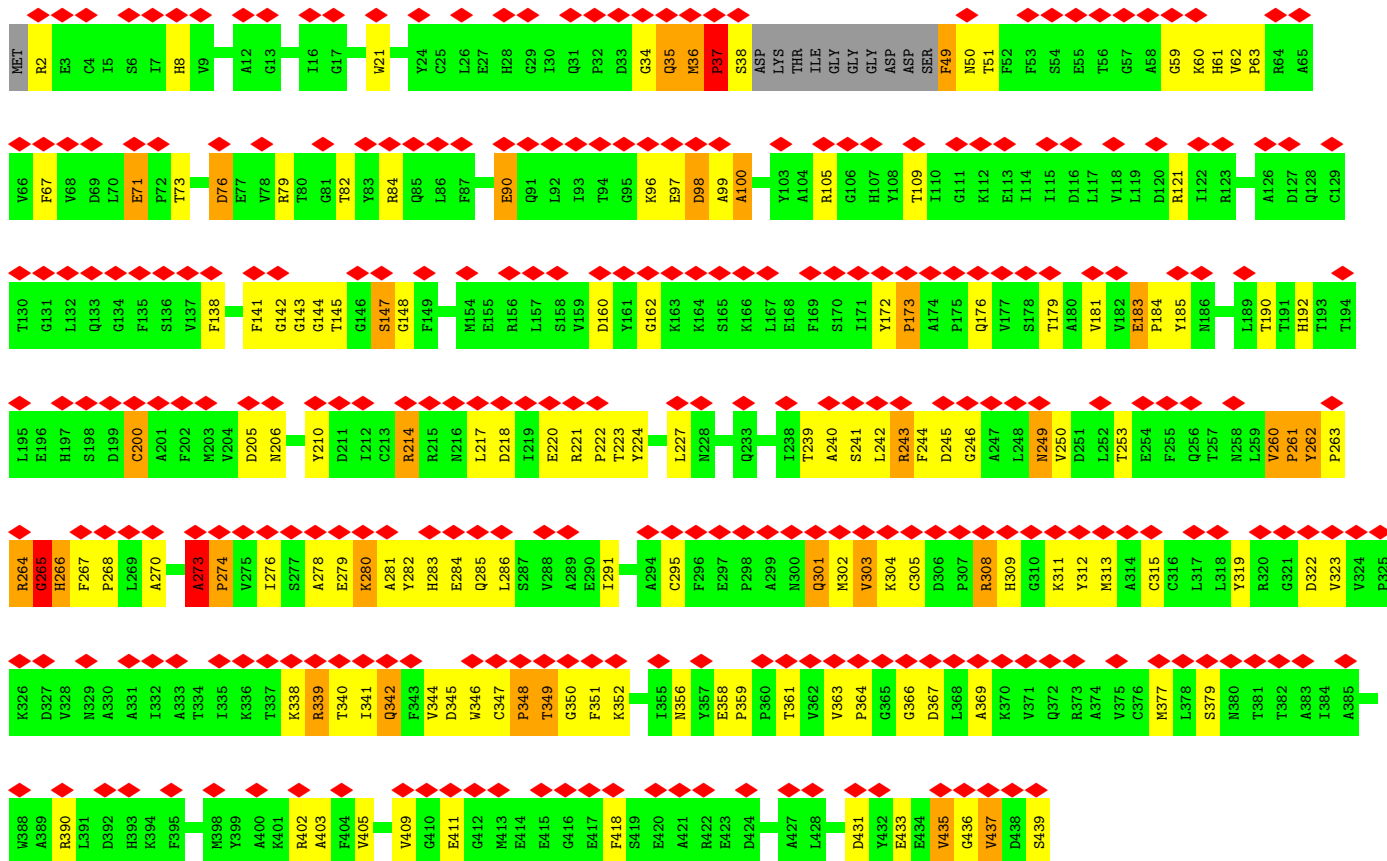


• Molecule 1: Tubulin alpha-1A chain

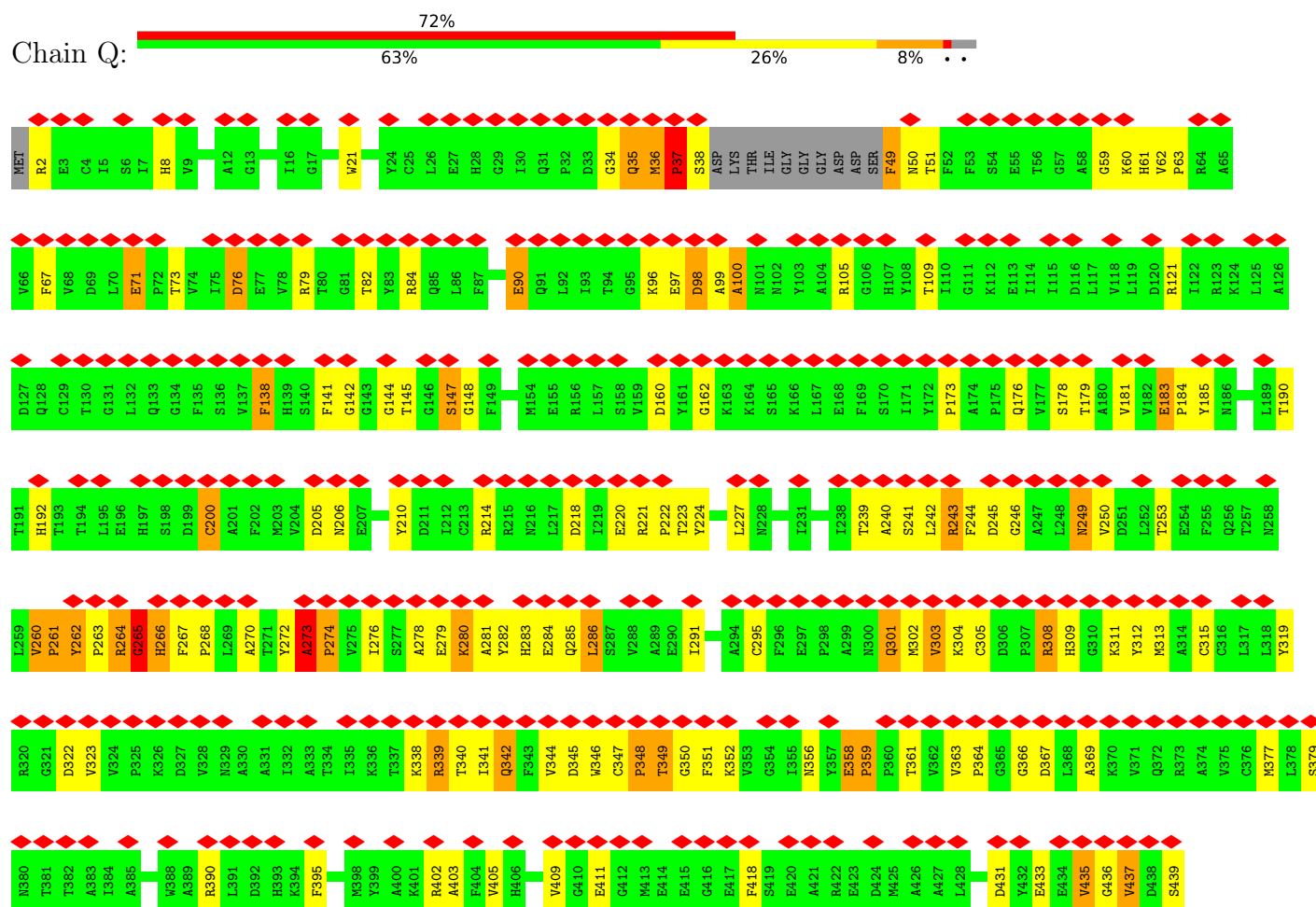




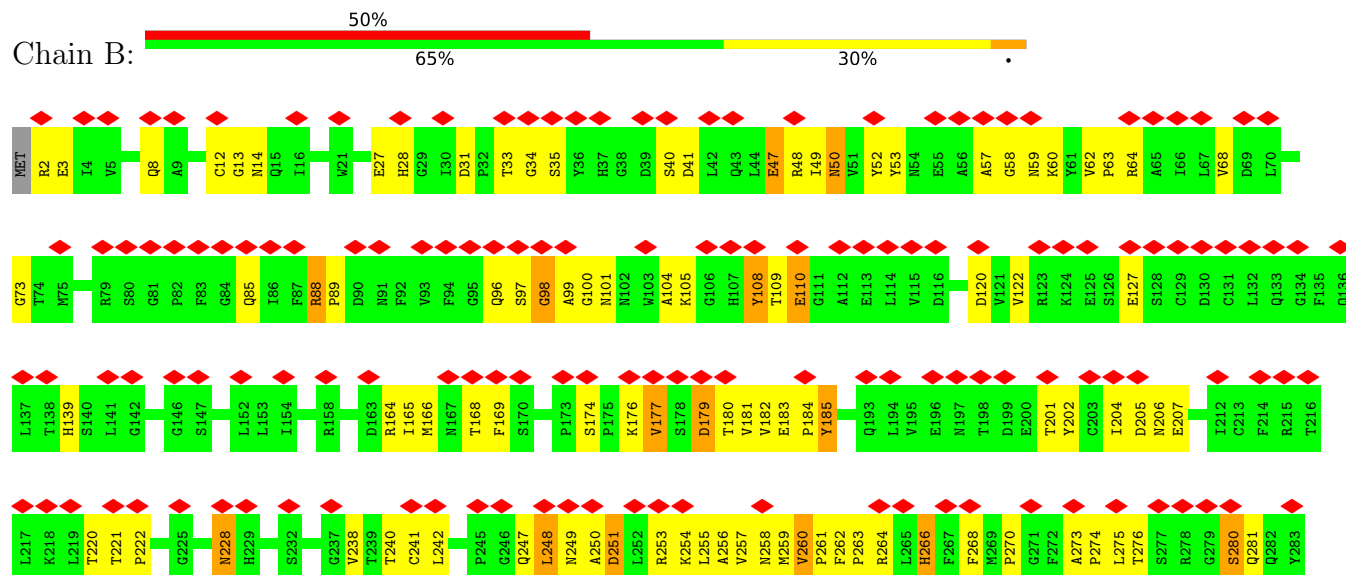
• Molecule 1: Tubulin alpha-1A chain

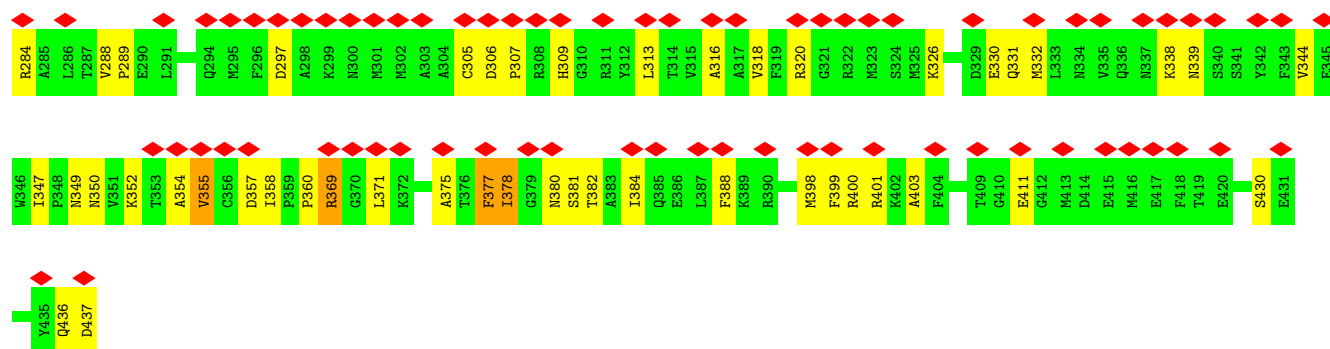


- Molecule 1: Tubulin alpha-1A chain

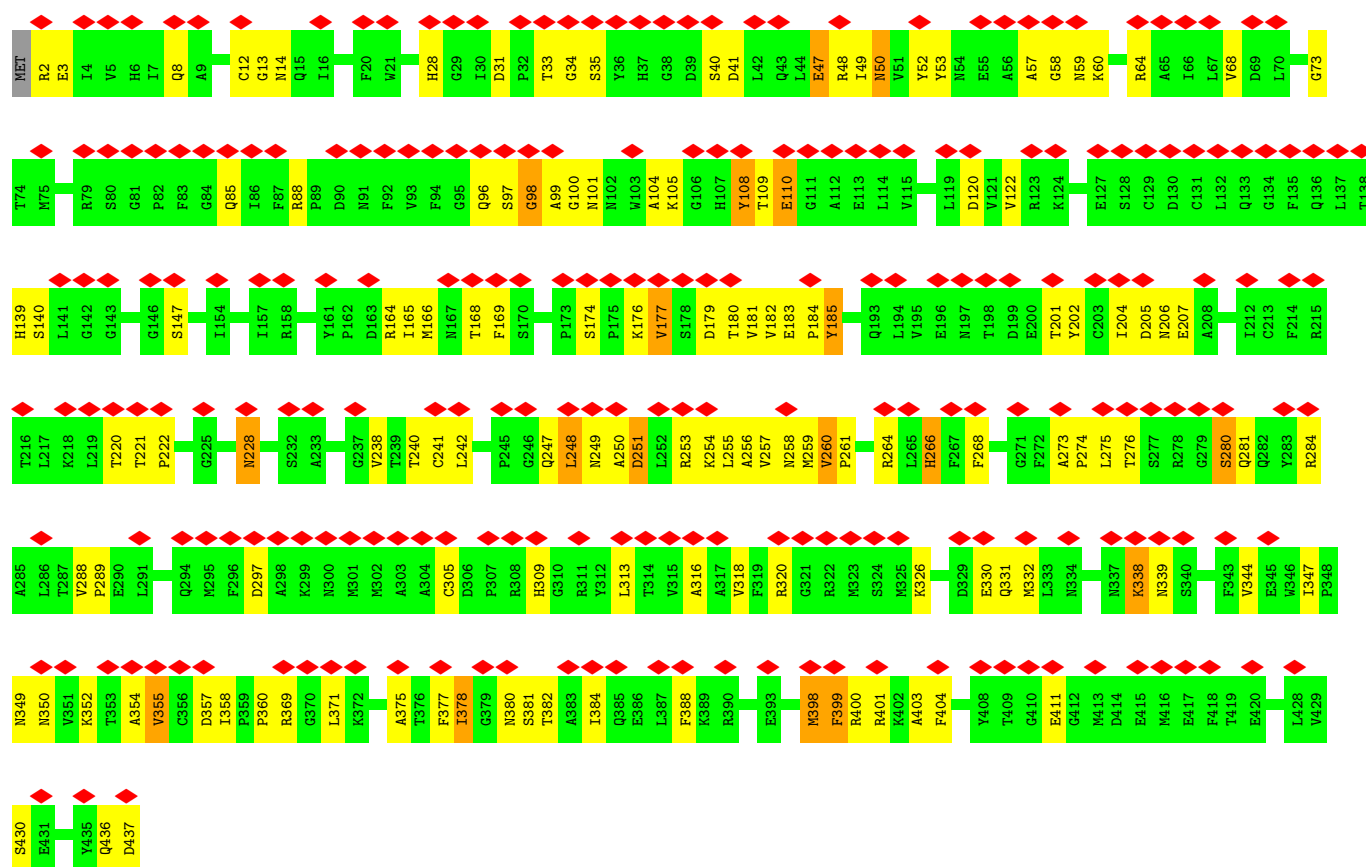


- Molecule 2: Tubulin beta chain

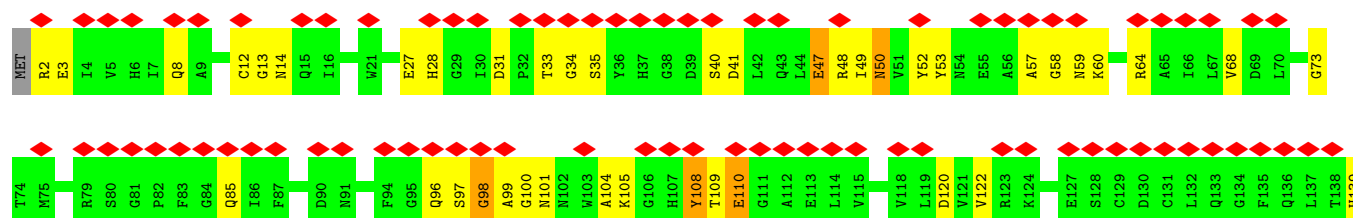


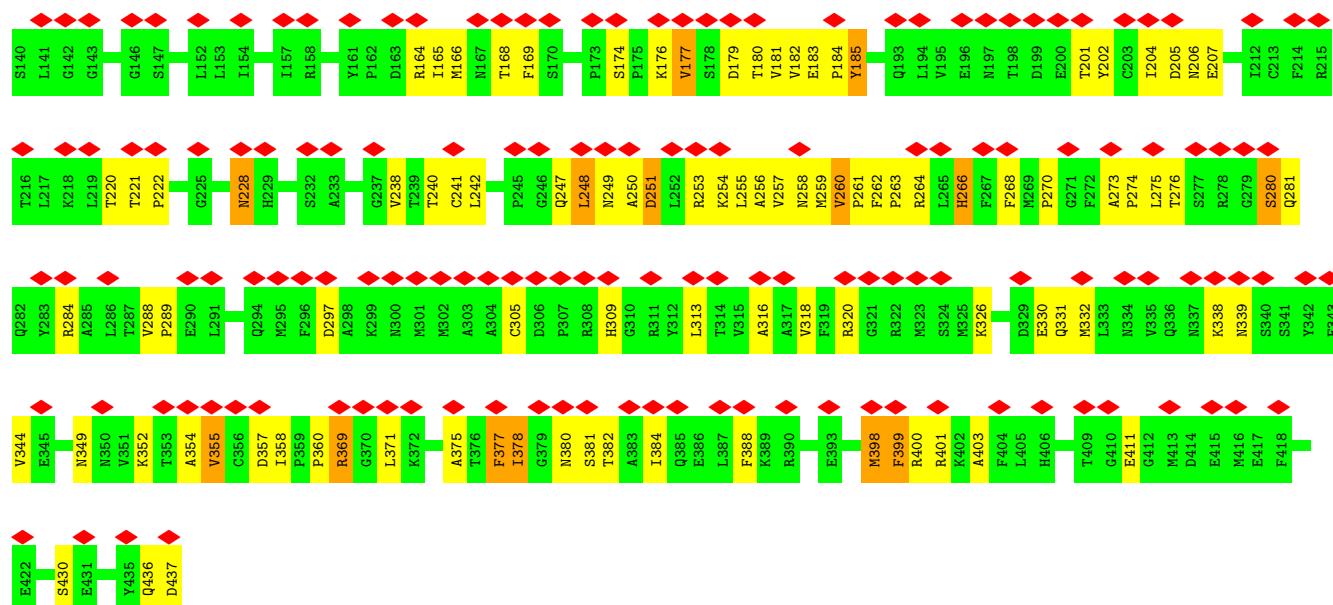


• Molecule 2: Tubulin beta chain

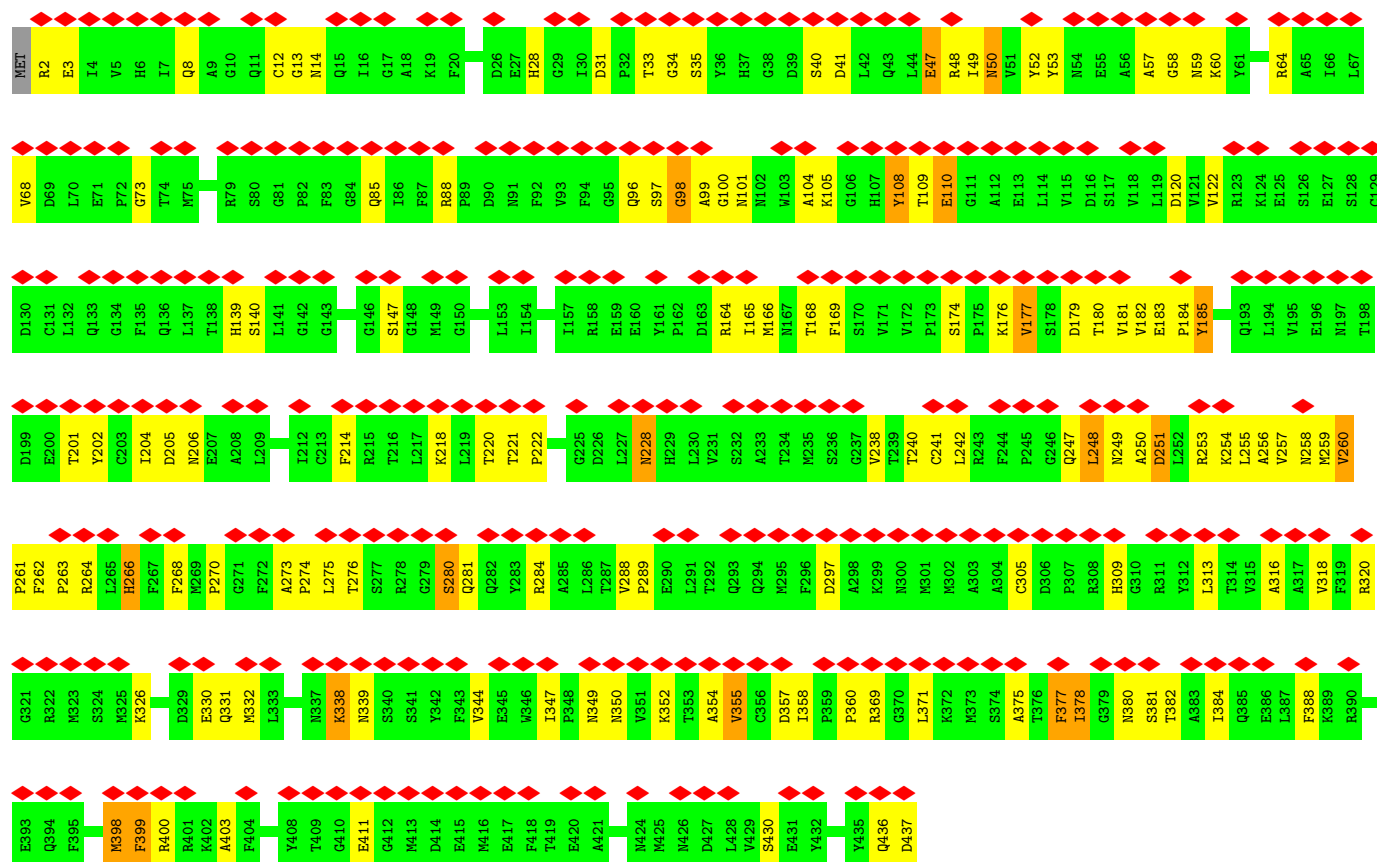


• Molecule 2: Tubulin beta chain





• Molecule 2: Tubulin beta chain



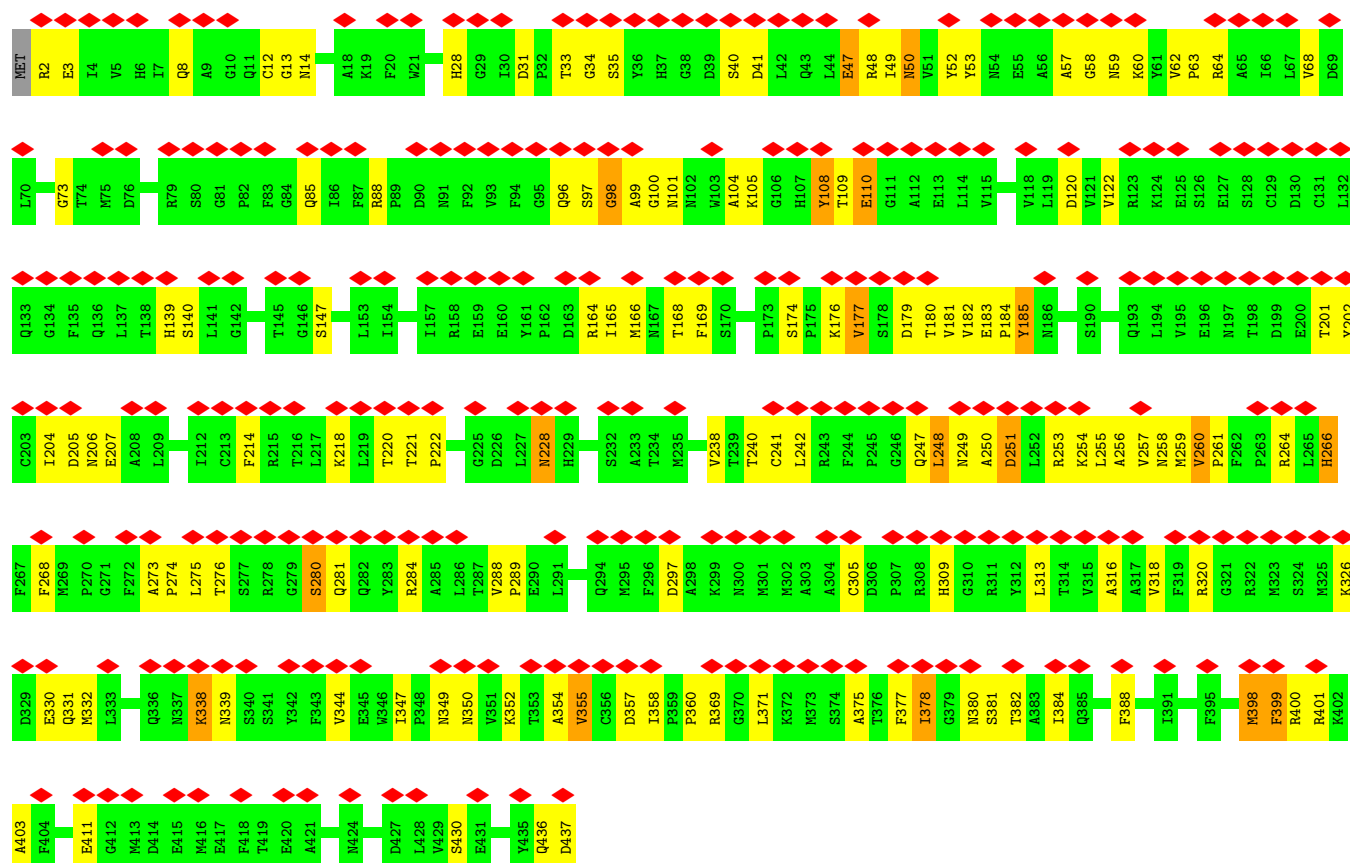
• Molecule 2: Tubulin beta chain



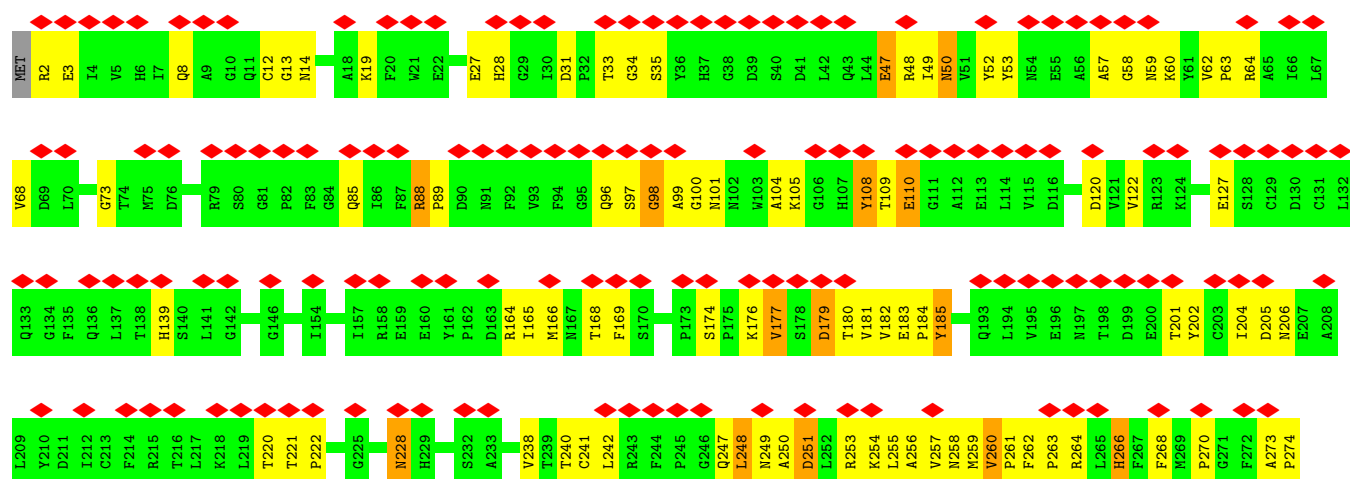


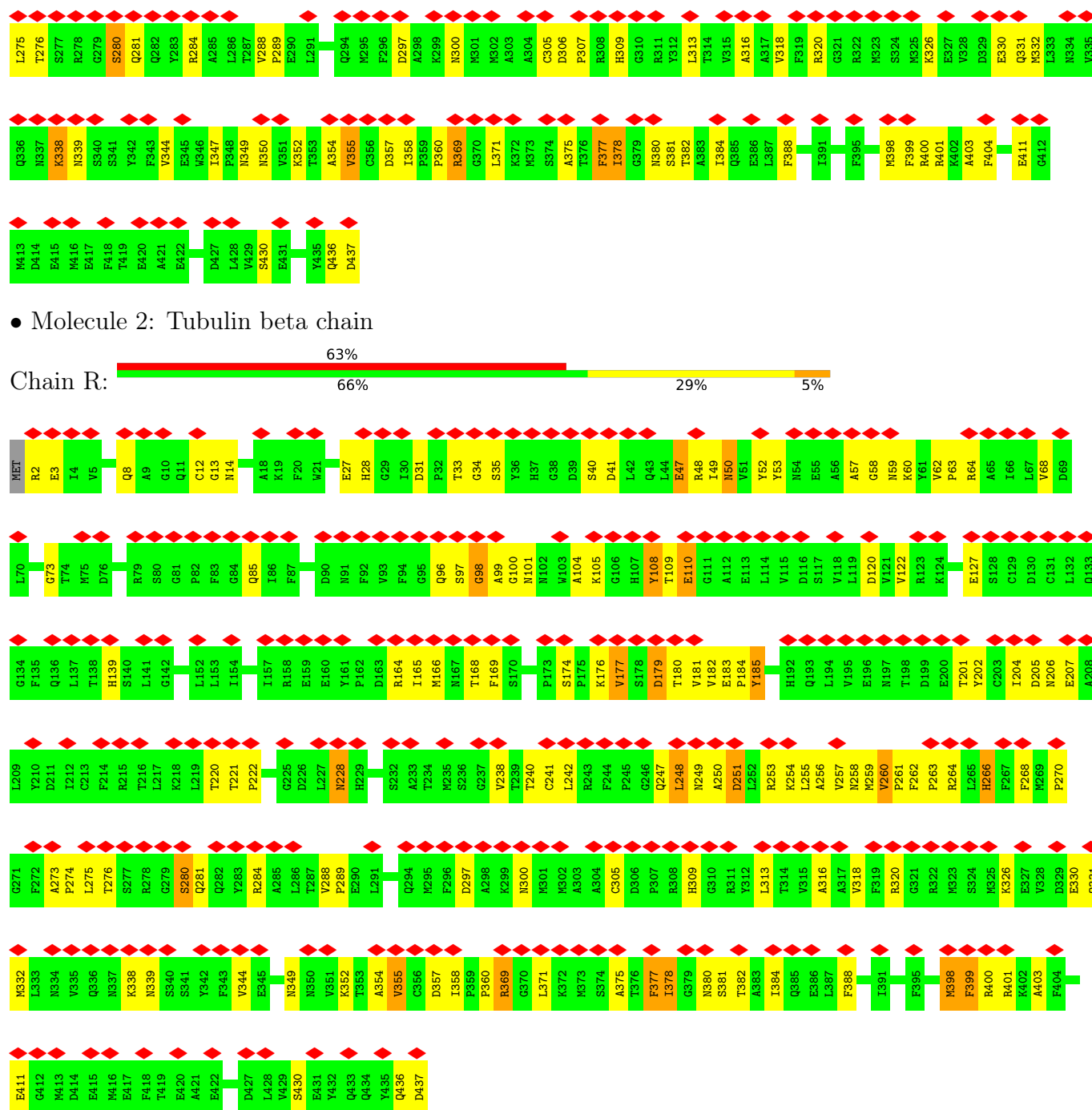


• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain





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	24357	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	10.347	Depositor
Minimum map value	-4.274	Depositor
Average map value	0.500	Depositor
Map value standard deviation	1.793	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: TA1, GDP, GTP, MG

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	1.88	77/3427 (2.2%)	2.14	150/4651 (3.2%)
1	C	1.88	76/3427 (2.2%)	2.14	150/4651 (3.2%)
1	E	1.88	78/3427 (2.3%)	2.14	149/4651 (3.2%)
1	G	1.88	76/3427 (2.2%)	2.14	150/4651 (3.2%)
1	I	1.88	75/3427 (2.2%)	2.14	148/4651 (3.2%)
1	K	1.88	74/3427 (2.2%)	2.14	149/4651 (3.2%)
1	M	1.88	75/3427 (2.2%)	2.14	150/4651 (3.2%)
1	O	1.88	75/3427 (2.2%)	2.14	150/4651 (3.2%)
1	Q	1.88	78/3427 (2.3%)	2.14	151/4651 (3.2%)
2	B	1.67	58/3427 (1.7%)	1.94	125/4642 (2.7%)
2	D	1.67	58/3427 (1.7%)	1.94	125/4642 (2.7%)
2	F	1.67	59/3427 (1.7%)	1.95	123/4642 (2.6%)
2	H	1.67	58/3427 (1.7%)	1.94	122/4642 (2.6%)
2	J	1.67	58/3427 (1.7%)	1.95	126/4642 (2.7%)
2	L	1.67	59/3427 (1.7%)	1.94	127/4642 (2.7%)
2	N	1.67	58/3427 (1.7%)	1.94	125/4642 (2.7%)
2	P	1.67	57/3427 (1.7%)	1.94	125/4642 (2.7%)
2	R	1.67	58/3427 (1.7%)	1.95	125/4642 (2.7%)
All	All	1.78	1207/61686 (2.0%)	2.05	2470/83637 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	C	0	6
1	E	0	6
1	G	0	6
1	I	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	6
1	M	0	6
1	O	0	6
1	Q	0	6
All	All	0	54

All (1207) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	249	ASN	CA-C	-24.64	1.21	1.52
2	F	249	ASN	CA-C	-24.61	1.21	1.52
2	R	249	ASN	CA-C	-24.60	1.21	1.52
2	H	249	ASN	CA-C	-24.59	1.21	1.52
2	B	249	ASN	CA-C	-24.59	1.21	1.52
2	P	249	ASN	CA-C	-24.59	1.21	1.52
2	N	249	ASN	CA-C	-24.59	1.21	1.52
2	L	249	ASN	CA-C	-24.58	1.21	1.52
2	J	249	ASN	CA-C	-24.56	1.21	1.52
1	K	266	HIS	N-CA	-20.58	1.22	1.46
1	E	266	HIS	N-CA	-20.55	1.22	1.46
1	G	266	HIS	N-CA	-20.55	1.22	1.46
1	C	266	HIS	N-CA	-20.54	1.22	1.46
1	A	266	HIS	N-CA	-20.53	1.22	1.46
1	I	266	HIS	N-CA	-20.53	1.22	1.46
1	O	266	HIS	N-CA	-20.53	1.22	1.46
1	M	266	HIS	N-CA	-20.51	1.22	1.46
1	Q	266	HIS	N-CA	-20.47	1.22	1.46
2	D	3	GLU	N-CA	-19.42	1.21	1.45
2	N	3	GLU	N-CA	-19.41	1.21	1.45
2	R	3	GLU	N-CA	-19.41	1.21	1.45
2	H	3	GLU	N-CA	-19.39	1.21	1.45
2	B	3	GLU	N-CA	-19.38	1.21	1.45
2	P	3	GLU	N-CA	-19.38	1.21	1.45
2	F	3	GLU	N-CA	-19.37	1.21	1.45
2	J	3	GLU	N-CA	-19.37	1.21	1.45
2	L	3	GLU	N-CA	-19.35	1.21	1.45
1	K	36	MET	CA-C	-19.00	1.28	1.52
1	E	36	MET	CA-C	-18.94	1.28	1.52
1	I	36	MET	CA-C	-18.92	1.28	1.52
1	A	36	MET	CA-C	-18.92	1.28	1.52
1	M	36	MET	CA-C	-18.92	1.28	1.52
1	O	36	MET	CA-C	-18.92	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	36	MET	CA-C	-18.92	1.28	1.52
1	G	36	MET	CA-C	-18.88	1.29	1.52
1	Q	36	MET	CA-C	-18.86	1.29	1.52
1	Q	264	ARG	CA-C	-17.26	1.35	1.53
1	K	264	ARG	CA-C	-17.25	1.35	1.53
1	C	264	ARG	CA-C	-17.25	1.35	1.53
1	A	264	ARG	CA-C	-17.23	1.35	1.53
1	I	264	ARG	CA-C	-17.22	1.35	1.53
1	M	264	ARG	CA-C	-17.21	1.35	1.53
1	O	264	ARG	CA-C	-17.20	1.35	1.53
1	E	264	ARG	CA-C	-17.19	1.35	1.53
1	G	264	ARG	CA-C	-17.16	1.35	1.53
1	G	283	HIS	CA-C	-16.62	1.31	1.53
1	I	283	HIS	CA-C	-16.60	1.31	1.53
1	E	283	HIS	CA-C	-16.59	1.31	1.53
1	C	283	HIS	CA-C	-16.59	1.31	1.53
1	A	283	HIS	CA-C	-16.59	1.31	1.53
1	Q	283	HIS	CA-C	-16.58	1.31	1.53
1	M	283	HIS	CA-C	-16.57	1.31	1.53
1	K	283	HIS	CA-C	-16.57	1.31	1.53
1	O	283	HIS	CA-C	-16.51	1.31	1.53
1	O	349	THR	CA-C	-15.86	1.36	1.53
1	K	349	THR	CA-C	-15.85	1.36	1.53
1	G	349	THR	CA-C	-15.82	1.36	1.53
1	M	349	THR	CA-C	-15.80	1.36	1.53
1	A	349	THR	CA-C	-15.79	1.36	1.53
1	Q	349	THR	CA-C	-15.78	1.36	1.53
1	C	349	THR	CA-C	-15.78	1.36	1.53
1	I	349	THR	CA-C	-15.77	1.36	1.53
1	E	349	THR	CA-C	-15.77	1.36	1.53
1	G	284	GLU	CA-C	-13.62	1.36	1.52
1	M	284	GLU	CA-C	-13.60	1.36	1.52
1	K	284	GLU	CA-C	-13.60	1.36	1.52
1	Q	284	GLU	N-CA	-13.57	1.29	1.46
1	O	284	GLU	CA-C	-13.57	1.36	1.52
2	N	436	GLN	CA-C	-13.56	1.35	1.52
1	A	284	GLU	CA-C	-13.56	1.36	1.52
1	C	284	GLU	CA-C	-13.55	1.36	1.52
1	E	284	GLU	N-CA	-13.55	1.29	1.46
1	G	284	GLU	N-CA	-13.55	1.29	1.46
2	B	436	GLN	CA-C	-13.55	1.35	1.52
2	H	436	GLN	CA-C	-13.54	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	436	GLN	CA-C	-13.54	1.35	1.52
1	K	284	GLU	N-CA	-13.53	1.29	1.46
1	C	284	GLU	N-CA	-13.53	1.29	1.46
1	I	284	GLU	N-CA	-13.53	1.29	1.46
2	P	436	GLN	CA-C	-13.52	1.35	1.52
2	F	436	GLN	CA-C	-13.52	1.35	1.52
1	A	284	GLU	N-CA	-13.51	1.29	1.46
2	D	436	GLN	CA-C	-13.51	1.35	1.52
1	E	284	GLU	CA-C	-13.51	1.36	1.52
1	I	284	GLU	CA-C	-13.50	1.36	1.52
1	Q	284	GLU	CA-C	-13.50	1.36	1.52
2	J	436	GLN	CA-C	-13.50	1.35	1.52
2	L	436	GLN	CA-C	-13.50	1.35	1.52
2	J	99	ALA	CA-C	-13.49	1.35	1.52
2	L	99	ALA	CA-C	-13.49	1.35	1.52
2	D	99	ALA	CA-C	-13.49	1.35	1.52
1	M	284	GLU	N-CA	-13.49	1.29	1.46
1	O	284	GLU	N-CA	-13.49	1.29	1.46
2	B	99	ALA	CA-C	-13.48	1.35	1.52
2	H	99	ALA	CA-C	-13.47	1.35	1.52
2	P	99	ALA	CA-C	-13.47	1.35	1.52
2	N	99	ALA	CA-C	-13.46	1.35	1.52
2	R	99	ALA	CA-C	-13.44	1.35	1.52
2	F	99	ALA	CA-C	-13.44	1.35	1.52
1	G	347	CYS	CA-C	-12.76	1.42	1.52
1	O	347	CYS	CA-C	-12.75	1.42	1.52
1	E	282	TYR	CA-C	-12.74	1.35	1.52
1	I	282	TYR	CA-C	-12.73	1.35	1.52
1	O	282	TYR	CA-C	-12.73	1.35	1.52
1	C	282	TYR	CA-C	-12.73	1.35	1.52
1	A	282	TYR	CA-C	-12.72	1.35	1.52
1	G	282	TYR	CA-C	-12.72	1.35	1.52
1	K	282	TYR	CA-C	-12.72	1.35	1.52
1	M	282	TYR	CA-C	-12.72	1.35	1.52
1	Q	347	CYS	CA-C	-12.71	1.42	1.52
1	C	347	CYS	CA-C	-12.70	1.42	1.52
1	M	347	CYS	CA-C	-12.68	1.42	1.52
1	Q	282	TYR	CA-C	-12.67	1.35	1.52
1	A	347	CYS	CA-C	-12.67	1.42	1.52
1	K	347	CYS	CA-C	-12.67	1.42	1.52
1	E	347	CYS	CA-C	-12.66	1.42	1.52
1	I	347	CYS	CA-C	-12.65	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	282	TYR	N-CA	-12.12	1.30	1.46
1	G	282	TYR	N-CA	-12.11	1.30	1.46
1	O	282	TYR	N-CA	-12.10	1.30	1.46
1	Q	282	TYR	N-CA	-12.10	1.30	1.46
1	K	282	TYR	N-CA	-12.10	1.30	1.46
1	A	282	TYR	N-CA	-12.08	1.30	1.46
1	M	282	TYR	N-CA	-12.08	1.30	1.46
1	I	282	TYR	N-CA	-12.06	1.30	1.46
1	E	285	GLN	N-CA	-12.04	1.32	1.46
1	M	285	GLN	N-CA	-12.03	1.32	1.46
1	C	282	TYR	N-CA	-12.02	1.30	1.46
1	I	285	GLN	N-CA	-12.00	1.32	1.46
1	G	285	GLN	N-CA	-12.00	1.32	1.46
1	O	285	GLN	N-CA	-11.99	1.32	1.46
1	A	285	GLN	N-CA	-11.98	1.32	1.46
1	Q	285	GLN	N-CA	-11.98	1.32	1.46
1	C	285	GLN	N-CA	-11.97	1.32	1.46
1	K	285	GLN	N-CA	-11.94	1.32	1.46
1	E	348	PRO	CA-C	-11.80	1.35	1.52
1	M	348	PRO	CA-C	-11.79	1.35	1.52
1	Q	348	PRO	CA-C	-11.77	1.35	1.52
1	A	348	PRO	CA-C	-11.77	1.35	1.52
1	I	348	PRO	CA-C	-11.76	1.35	1.52
1	G	348	PRO	CA-C	-11.75	1.35	1.52
1	O	348	PRO	CA-C	-11.75	1.35	1.52
1	C	348	PRO	CA-C	-11.74	1.35	1.52
1	K	348	PRO	CA-C	-11.72	1.35	1.52
1	Q	280	LYS	CA-C	-11.28	1.37	1.52
1	E	280	LYS	CA-C	-11.27	1.37	1.52
1	A	280	LYS	CA-C	-11.27	1.37	1.52
1	K	280	LYS	CA-C	-11.27	1.37	1.52
1	M	280	LYS	CA-C	-11.27	1.37	1.52
1	G	280	LYS	CA-C	-11.26	1.37	1.52
1	O	280	LYS	CA-C	-11.26	1.37	1.52
1	C	280	LYS	CA-C	-11.25	1.37	1.52
1	I	280	LYS	CA-C	-11.20	1.37	1.52
1	Q	437	VAL	CA-C	-11.12	1.39	1.52
1	I	437	VAL	CA-C	-11.11	1.39	1.52
1	M	437	VAL	CA-C	-11.09	1.39	1.52
1	A	437	VAL	CA-C	-11.09	1.39	1.52
1	C	437	VAL	CA-C	-11.09	1.39	1.52
1	K	437	VAL	CA-C	-11.07	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	437	VAL	CA-C	-11.06	1.39	1.52
1	G	437	VAL	CA-C	-11.05	1.39	1.52
1	E	437	VAL	CA-C	-11.05	1.39	1.52
1	G	339	ARG	CA-C	-10.96	1.37	1.52
1	K	339	ARG	CA-C	-10.94	1.37	1.52
1	E	339	ARG	CA-C	-10.94	1.37	1.52
1	O	339	ARG	CA-C	-10.92	1.37	1.52
1	A	339	ARG	CA-C	-10.92	1.37	1.52
1	I	339	ARG	CA-C	-10.91	1.37	1.52
1	C	339	ARG	CA-C	-10.91	1.37	1.52
2	F	179	ASP	CA-C	-10.88	1.43	1.52
1	M	339	ARG	CA-C	-10.88	1.37	1.52
2	L	179	ASP	CA-C	-10.87	1.43	1.52
2	P	179	ASP	CA-C	-10.86	1.43	1.52
1	Q	339	ARG	CA-C	-10.85	1.37	1.52
1	O	98	ASP	CA-C	-10.85	1.38	1.52
1	K	98	ASP	CA-C	-10.83	1.38	1.52
2	D	179	ASP	CA-C	-10.83	1.43	1.52
1	C	98	ASP	CA-C	-10.82	1.38	1.52
2	H	179	ASP	CA-C	-10.82	1.43	1.52
2	R	179	ASP	CA-C	-10.82	1.43	1.52
2	B	179	ASP	CA-C	-10.82	1.43	1.52
1	M	98	ASP	CA-C	-10.82	1.38	1.52
1	G	98	ASP	CA-C	-10.81	1.38	1.52
1	E	98	ASP	CA-C	-10.81	1.38	1.52
2	J	179	ASP	CA-C	-10.81	1.43	1.52
1	A	98	ASP	CA-C	-10.81	1.38	1.52
1	O	283	HIS	N-CA	-10.80	1.31	1.46
1	Q	98	ASP	CA-C	-10.80	1.38	1.52
1	I	98	ASP	CA-C	-10.80	1.38	1.52
1	M	283	HIS	N-CA	-10.79	1.31	1.46
1	C	283	HIS	N-CA	-10.75	1.31	1.46
1	A	283	HIS	N-CA	-10.75	1.31	1.46
1	E	283	HIS	N-CA	-10.74	1.31	1.46
2	N	179	ASP	CA-C	-10.74	1.43	1.52
1	I	283	HIS	N-CA	-10.74	1.31	1.46
1	K	283	HIS	N-CA	-10.74	1.31	1.46
1	Q	283	HIS	N-CA	-10.73	1.31	1.46
1	G	283	HIS	N-CA	-10.71	1.31	1.46
1	Q	436	GLY	CA-C	-10.66	1.36	1.51
1	I	436	GLY	CA-C	-10.65	1.36	1.51
1	M	436	GLY	CA-C	-10.65	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	436	GLY	CA-C	-10.64	1.36	1.51
1	O	436	GLY	CA-C	-10.63	1.36	1.51
1	K	436	GLY	CA-C	-10.63	1.36	1.51
1	E	436	GLY	CA-C	-10.62	1.36	1.51
1	G	436	GLY	CA-C	-10.62	1.36	1.51
1	C	436	GLY	CA-C	-10.58	1.36	1.51
1	C	437	VAL	N-CA	-10.35	1.34	1.46
1	G	437	VAL	N-CA	-10.35	1.34	1.46
1	E	437	VAL	N-CA	-10.34	1.34	1.46
1	A	437	VAL	N-CA	-10.31	1.34	1.46
1	Q	437	VAL	N-CA	-10.31	1.34	1.46
1	I	437	VAL	N-CA	-10.29	1.34	1.46
1	K	437	VAL	N-CA	-10.28	1.34	1.46
1	O	437	VAL	N-CA	-10.26	1.34	1.46
1	M	437	VAL	N-CA	-10.26	1.34	1.46
1	O	340	THR	N-CA	-9.89	1.31	1.46
1	C	340	THR	N-CA	-9.87	1.31	1.46
1	Q	340	THR	N-CA	-9.86	1.31	1.46
1	G	340	THR	N-CA	-9.85	1.31	1.46
1	M	340	THR	N-CA	-9.85	1.31	1.46
1	I	340	THR	N-CA	-9.85	1.31	1.46
1	E	340	THR	N-CA	-9.84	1.31	1.46
1	A	340	THR	N-CA	-9.84	1.31	1.46
1	K	340	THR	N-CA	-9.83	1.31	1.46
1	Q	279	GLU	CA-C	-9.20	1.40	1.52
1	M	279	GLU	CA-C	-9.18	1.40	1.52
1	A	279	GLU	CA-C	-9.16	1.40	1.52
1	I	279	GLU	CA-C	-9.16	1.40	1.52
1	C	279	GLU	CA-C	-9.14	1.40	1.52
1	E	279	GLU	CA-C	-9.14	1.40	1.52
1	G	279	GLU	CA-C	-9.14	1.40	1.52
1	K	279	GLU	CA-C	-9.14	1.40	1.52
1	O	279	GLU	CA-C	-9.14	1.40	1.52
2	P	220	THR	CA-C	-8.99	1.40	1.52
2	N	220	THR	CA-C	-8.98	1.40	1.52
2	D	220	THR	CA-C	-8.98	1.40	1.52
2	B	220	THR	CA-C	-8.95	1.40	1.52
2	H	220	THR	CA-C	-8.94	1.40	1.52
2	R	220	THR	CA-C	-8.94	1.40	1.52
2	J	220	THR	CA-C	-8.92	1.40	1.52
2	L	220	THR	CA-C	-8.91	1.40	1.52
2	F	220	THR	CA-C	-8.85	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	180	THR	CA-C	-8.79	1.42	1.52
2	F	180	THR	CA-C	-8.78	1.42	1.52
1	C	38	SER	N-CA	-8.75	1.29	1.46
1	G	38	SER	N-CA	-8.75	1.29	1.46
1	A	38	SER	N-CA	-8.75	1.29	1.46
1	I	38	SER	N-CA	-8.75	1.29	1.46
1	K	38	SER	N-CA	-8.75	1.29	1.46
1	M	38	SER	N-CA	-8.75	1.29	1.46
2	B	180	THR	CA-C	-8.74	1.42	1.52
1	E	38	SER	N-CA	-8.74	1.29	1.46
2	D	180	THR	CA-C	-8.74	1.42	1.52
1	O	38	SER	N-CA	-8.74	1.29	1.46
2	N	180	THR	CA-C	-8.74	1.42	1.52
1	Q	38	SER	N-CA	-8.74	1.29	1.46
2	P	180	THR	CA-C	-8.73	1.42	1.52
2	L	180	THR	CA-C	-8.71	1.42	1.52
2	H	180	THR	CA-C	-8.71	1.42	1.52
2	J	180	THR	CA-C	-8.71	1.42	1.52
1	C	350	GLY	N-CA	-8.69	1.32	1.45
2	J	354	ALA	CA-C	-8.68	1.44	1.53
1	Q	350	GLY	N-CA	-8.68	1.32	1.45
1	I	350	GLY	N-CA	-8.68	1.32	1.45
1	E	350	GLY	N-CA	-8.68	1.32	1.45
1	A	350	GLY	N-CA	-8.66	1.32	1.45
1	O	350	GLY	N-CA	-8.65	1.32	1.45
2	D	354	ALA	CA-C	-8.64	1.44	1.53
1	M	350	GLY	N-CA	-8.64	1.32	1.45
1	K	350	GLY	N-CA	-8.64	1.32	1.45
2	N	354	ALA	CA-C	-8.63	1.44	1.53
1	G	308	ARG	CA-C	-8.62	1.41	1.52
1	G	350	GLY	N-CA	-8.61	1.32	1.45
2	B	354	ALA	CA-C	-8.60	1.44	1.53
1	Q	308	ARG	CA-C	-8.60	1.41	1.52
2	H	354	ALA	CA-C	-8.60	1.44	1.53
2	L	354	ALA	CA-C	-8.60	1.44	1.53
1	M	308	ARG	CA-C	-8.60	1.41	1.52
2	P	354	ALA	CA-C	-8.59	1.44	1.53
1	A	308	ARG	CA-C	-8.59	1.41	1.52
2	F	354	ALA	CA-C	-8.58	1.44	1.53
1	C	281	ALA	N-CA	-8.58	1.33	1.46
1	I	308	ARG	CA-C	-8.58	1.41	1.52
1	K	308	ARG	CA-C	-8.58	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	354	ALA	CA-C	-8.57	1.44	1.53
1	E	308	ARG	CA-C	-8.57	1.41	1.52
1	Q	281	ALA	N-CA	-8.57	1.33	1.46
1	A	281	ALA	N-CA	-8.56	1.33	1.46
1	E	281	ALA	N-CA	-8.55	1.33	1.46
1	O	281	ALA	N-CA	-8.55	1.33	1.46
1	M	281	ALA	N-CA	-8.55	1.33	1.46
1	O	308	ARG	CA-C	-8.55	1.41	1.52
1	C	308	ARG	CA-C	-8.54	1.41	1.52
1	Q	339	ARG	N-CA	-8.54	1.35	1.46
1	I	339	ARG	N-CA	-8.52	1.35	1.46
1	G	339	ARG	N-CA	-8.52	1.35	1.46
1	K	281	ALA	N-CA	-8.52	1.33	1.46
1	G	281	ALA	N-CA	-8.52	1.33	1.46
1	I	281	ALA	N-CA	-8.51	1.33	1.46
1	K	339	ARG	N-CA	-8.50	1.35	1.46
1	M	339	ARG	N-CA	-8.50	1.35	1.46
1	I	281	ALA	CA-C	-8.50	1.33	1.52
1	C	339	ARG	N-CA	-8.50	1.35	1.46
1	E	281	ALA	CA-C	-8.49	1.33	1.52
1	G	281	ALA	CA-C	-8.49	1.33	1.52
1	A	339	ARG	N-CA	-8.49	1.35	1.46
1	O	339	ARG	N-CA	-8.49	1.35	1.46
1	K	281	ALA	CA-C	-8.49	1.33	1.52
1	E	339	ARG	N-CA	-8.48	1.35	1.46
1	M	281	ALA	CA-C	-8.47	1.33	1.52
1	A	281	ALA	CA-C	-8.46	1.33	1.52
1	C	281	ALA	CA-C	-8.45	1.33	1.52
1	O	281	ALA	CA-C	-8.45	1.33	1.52
1	Q	281	ALA	CA-C	-8.45	1.33	1.52
2	F	100	GLY	N-CA	-8.44	1.33	1.45
2	L	100	GLY	N-CA	-8.43	1.33	1.45
2	J	100	GLY	N-CA	-8.42	1.33	1.45
2	R	100	GLY	N-CA	-8.38	1.33	1.45
2	R	221	THR	N-CA	-8.24	1.37	1.46
2	H	221	THR	N-CA	-8.21	1.38	1.46
2	P	221	THR	N-CA	-8.20	1.38	1.46
2	N	221	THR	N-CA	-8.20	1.38	1.46
2	B	221	THR	N-CA	-8.19	1.38	1.46
2	D	221	THR	N-CA	-8.18	1.38	1.46
2	F	221	THR	N-CA	-8.15	1.38	1.46
1	O	99	ALA	N-CA	-8.15	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	99	ALA	N-CA	-8.14	1.35	1.46
2	N	100	GLY	N-CA	-8.14	1.33	1.45
2	J	221	THR	N-CA	-8.14	1.38	1.46
2	B	100	GLY	N-CA	-8.14	1.33	1.45
1	K	97	GLU	N-CA	-8.13	1.36	1.46
1	E	99	ALA	N-CA	-8.12	1.35	1.46
2	L	221	THR	N-CA	-8.12	1.38	1.46
2	H	100	GLY	N-CA	-8.12	1.33	1.45
1	A	99	ALA	N-CA	-8.12	1.35	1.46
1	K	99	ALA	N-CA	-8.11	1.35	1.46
1	M	348	PRO	N-CA	-8.11	1.36	1.47
2	D	100	GLY	N-CA	-8.10	1.33	1.45
1	C	99	ALA	N-CA	-8.09	1.35	1.46
1	I	99	ALA	N-CA	-8.09	1.35	1.46
1	Q	99	ALA	N-CA	-8.09	1.35	1.46
1	Q	348	PRO	N-CA	-8.09	1.36	1.47
1	C	97	GLU	N-CA	-8.09	1.36	1.46
2	P	100	GLY	N-CA	-8.09	1.33	1.45
1	O	97	GLU	N-CA	-8.08	1.36	1.46
1	G	99	ALA	N-CA	-8.08	1.35	1.46
2	R	59	ASN	CA-C	-8.08	1.43	1.53
1	A	97	GLU	N-CA	-8.07	1.36	1.46
1	C	348	PRO	N-CA	-8.07	1.36	1.47
1	A	348	PRO	N-CA	-8.07	1.36	1.47
1	E	348	PRO	N-CA	-8.07	1.36	1.47
1	M	97	GLU	N-CA	-8.06	1.36	1.46
2	L	273	ALA	CA-C	-8.06	1.42	1.52
1	I	97	GLU	N-CA	-8.06	1.36	1.46
2	P	59	ASN	CA-C	-8.05	1.43	1.53
1	E	97	GLU	N-CA	-8.05	1.36	1.46
2	H	273	ALA	CA-C	-8.05	1.42	1.52
2	J	59	ASN	CA-C	-8.05	1.43	1.53
1	K	348	PRO	N-CA	-8.05	1.37	1.47
2	B	59	ASN	CA-C	-8.04	1.43	1.53
1	G	348	PRO	N-CA	-8.04	1.37	1.47
1	O	348	PRO	N-CA	-8.04	1.37	1.47
2	F	59	ASN	CA-C	-8.04	1.43	1.53
2	D	59	ASN	CA-C	-8.04	1.43	1.53
1	Q	97	GLU	N-CA	-8.04	1.36	1.46
2	H	59	ASN	CA-C	-8.04	1.43	1.53
2	L	59	ASN	CA-C	-8.03	1.43	1.53
2	P	273	ALA	CA-C	-8.03	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	348	PRO	N-CA	-8.03	1.37	1.47
2	J	57	ALA	CA-C	-8.03	1.42	1.52
2	B	273	ALA	CA-C	-8.02	1.42	1.52
2	F	57	ALA	CA-C	-8.02	1.42	1.52
2	R	273	ALA	CA-C	-8.02	1.42	1.52
1	G	97	GLU	N-CA	-8.01	1.36	1.46
2	J	273	ALA	CA-C	-8.01	1.42	1.52
2	N	273	ALA	CA-C	-8.00	1.42	1.52
2	H	57	ALA	CA-C	-8.00	1.42	1.52
2	B	57	ALA	CA-C	-8.00	1.42	1.52
2	R	57	ALA	CA-C	-7.99	1.42	1.52
2	N	59	ASN	CA-C	-7.99	1.43	1.53
2	F	273	ALA	CA-C	-7.98	1.42	1.52
2	D	273	ALA	CA-C	-7.98	1.42	1.52
2	D	57	ALA	CA-C	-7.97	1.42	1.52
2	P	57	ALA	CA-C	-7.97	1.42	1.52
2	N	222	PRO	N-CA	-7.97	1.37	1.47
2	N	57	ALA	CA-C	-7.96	1.42	1.52
2	L	222	PRO	N-CA	-7.95	1.37	1.47
2	L	57	ALA	CA-C	-7.94	1.42	1.52
2	P	222	PRO	N-CA	-7.93	1.37	1.47
2	B	222	PRO	N-CA	-7.92	1.37	1.47
2	F	222	PRO	N-CA	-7.92	1.37	1.47
2	D	222	PRO	N-CA	-7.92	1.37	1.47
2	J	222	PRO	N-CA	-7.91	1.37	1.47
2	H	222	PRO	N-CA	-7.91	1.37	1.47
2	R	222	PRO	N-CA	-7.90	1.37	1.47
1	K	35	GLN	CA-C	-7.80	1.42	1.52
1	Q	35	GLN	CA-C	-7.79	1.42	1.52
1	A	35	GLN	CA-C	-7.78	1.42	1.52
1	C	35	GLN	CA-C	-7.78	1.42	1.52
1	E	35	GLN	CA-C	-7.78	1.42	1.52
1	M	35	GLN	CA-C	-7.77	1.42	1.52
1	O	35	GLN	CA-C	-7.77	1.42	1.52
1	I	35	GLN	CA-C	-7.76	1.42	1.52
2	F	257	VAL	CA-C	-7.74	1.43	1.52
1	G	35	GLN	CA-C	-7.74	1.42	1.52
2	J	257	VAL	CA-C	-7.72	1.43	1.52
2	R	257	VAL	CA-C	-7.71	1.43	1.52
2	D	257	VAL	CA-C	-7.70	1.43	1.52
2	B	257	VAL	CA-C	-7.69	1.43	1.52
2	P	257	VAL	CA-C	-7.69	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	257	VAL	CA-C	-7.67	1.43	1.52
2	L	257	VAL	CA-C	-7.65	1.43	1.52
2	N	257	VAL	CA-C	-7.65	1.43	1.52
2	F	437	ASP	N-CA	-7.64	1.31	1.46
2	F	58	GLY	CA-C	-7.64	1.41	1.51
2	H	437	ASP	N-CA	-7.63	1.31	1.46
2	H	58	GLY	CA-C	-7.63	1.41	1.51
2	N	437	ASP	N-CA	-7.62	1.31	1.46
2	P	58	GLY	CA-C	-7.62	1.41	1.51
2	N	58	GLY	CA-C	-7.62	1.41	1.51
2	B	58	GLY	CA-C	-7.61	1.41	1.51
2	D	58	GLY	CA-C	-7.60	1.41	1.51
2	R	58	GLY	CA-C	-7.59	1.41	1.51
2	J	58	GLY	CA-C	-7.59	1.41	1.51
2	P	437	ASP	N-CA	-7.58	1.31	1.46
2	R	437	ASP	N-CA	-7.58	1.31	1.46
2	B	437	ASP	N-CA	-7.58	1.31	1.46
2	D	437	ASP	N-CA	-7.56	1.31	1.46
2	L	437	ASP	N-CA	-7.55	1.31	1.46
2	J	437	ASP	N-CA	-7.54	1.31	1.46
2	L	58	GLY	CA-C	-7.54	1.41	1.51
2	L	355	VAL	N-CA	-7.48	1.37	1.46
2	D	355	VAL	N-CA	-7.46	1.37	1.46
2	J	274	PRO	N-CA	-7.46	1.38	1.47
2	D	274	PRO	N-CA	-7.46	1.38	1.47
2	L	274	PRO	N-CA	-7.45	1.38	1.47
2	B	274	PRO	N-CA	-7.45	1.38	1.47
1	O	96	LYS	CA-C	-7.45	1.43	1.52
2	R	355	VAL	N-CA	-7.44	1.37	1.46
2	F	274	PRO	N-CA	-7.44	1.38	1.47
1	E	96	LYS	CA-C	-7.44	1.43	1.52
2	H	274	PRO	N-CA	-7.44	1.38	1.47
2	F	355	VAL	N-CA	-7.43	1.37	1.46
2	H	355	VAL	N-CA	-7.42	1.37	1.46
2	P	355	VAL	N-CA	-7.42	1.37	1.46
2	B	355	VAL	N-CA	-7.42	1.37	1.46
2	R	274	PRO	N-CA	-7.41	1.38	1.47
1	A	96	LYS	CA-C	-7.41	1.43	1.52
2	J	355	VAL	N-CA	-7.41	1.37	1.46
2	N	274	PRO	N-CA	-7.41	1.38	1.47
1	G	96	LYS	CA-C	-7.40	1.43	1.52
2	N	355	VAL	N-CA	-7.40	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	98	ASP	N-CA	-7.40	1.36	1.46
1	Q	96	LYS	CA-C	-7.39	1.43	1.52
1	Q	98	ASP	N-CA	-7.39	1.36	1.46
1	K	98	ASP	N-CA	-7.39	1.36	1.46
2	P	274	PRO	N-CA	-7.39	1.38	1.47
1	I	98	ASP	N-CA	-7.39	1.36	1.46
1	C	96	LYS	CA-C	-7.38	1.43	1.52
1	K	96	LYS	CA-C	-7.38	1.43	1.52
1	I	96	LYS	CA-C	-7.38	1.43	1.52
1	G	98	ASP	N-CA	-7.37	1.36	1.46
1	K	338	LYS	CA-C	-7.37	1.42	1.52
1	A	98	ASP	N-CA	-7.36	1.36	1.46
1	M	96	LYS	CA-C	-7.35	1.43	1.52
1	M	338	LYS	CA-C	-7.35	1.42	1.52
1	M	98	ASP	N-CA	-7.34	1.36	1.46
1	G	338	LYS	CA-C	-7.33	1.42	1.52
1	C	338	LYS	CA-C	-7.33	1.42	1.52
1	I	338	LYS	CA-C	-7.32	1.42	1.52
1	O	98	ASP	N-CA	-7.32	1.36	1.46
1	A	338	LYS	CA-C	-7.32	1.42	1.52
1	Q	338	LYS	CA-C	-7.32	1.42	1.52
1	E	338	LYS	CA-C	-7.32	1.42	1.52
1	C	98	ASP	N-CA	-7.31	1.36	1.46
1	O	338	LYS	CA-C	-7.30	1.42	1.52
1	O	435	VAL	CA-C	-7.26	1.42	1.52
1	I	435	VAL	CA-C	-7.24	1.42	1.52
1	E	435	VAL	CA-C	-7.24	1.42	1.52
1	Q	435	VAL	CA-C	-7.23	1.42	1.52
1	G	435	VAL	CA-C	-7.23	1.42	1.52
1	A	435	VAL	CA-C	-7.23	1.42	1.52
1	K	435	VAL	CA-C	-7.21	1.42	1.52
1	C	435	VAL	CA-C	-7.20	1.42	1.52
1	M	435	VAL	CA-C	-7.19	1.42	1.52
1	C	280	LYS	N-CA	-7.05	1.37	1.46
2	R	100	GLY	CA-C	-7.05	1.42	1.51
1	G	280	LYS	N-CA	-7.04	1.37	1.46
1	M	349	THR	N-CA	-7.04	1.34	1.46
1	A	349	THR	N-CA	-7.04	1.34	1.46
1	E	349	THR	N-CA	-7.04	1.34	1.46
1	K	280	LYS	N-CA	-7.03	1.37	1.46
1	C	349	THR	N-CA	-7.03	1.34	1.46
1	G	349	THR	N-CA	-7.02	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	349	THR	N-CA	-7.02	1.34	1.46
1	I	349	THR	N-CA	-7.02	1.34	1.46
1	A	280	LYS	N-CA	-7.01	1.37	1.46
1	Q	349	THR	N-CA	-7.01	1.34	1.46
1	I	280	LYS	N-CA	-7.00	1.37	1.46
2	L	100	GLY	CA-C	-7.00	1.42	1.51
1	M	280	LYS	N-CA	-7.00	1.37	1.46
1	K	349	THR	N-CA	-7.00	1.34	1.46
1	E	280	LYS	N-CA	-7.00	1.37	1.46
1	Q	280	LYS	N-CA	-7.00	1.37	1.46
1	O	280	LYS	N-CA	-6.99	1.37	1.46
2	F	100	GLY	CA-C	-6.98	1.42	1.51
2	J	100	GLY	CA-C	-6.97	1.42	1.51
1	I	285	GLN	CA-C	-6.96	1.45	1.52
1	K	285	GLN	CA-C	-6.96	1.45	1.52
2	R	280	SER	CA-C	-6.95	1.43	1.52
1	Q	285	GLN	CA-C	-6.94	1.45	1.52
2	H	280	SER	CA-C	-6.92	1.43	1.52
1	G	285	GLN	CA-C	-6.92	1.45	1.52
1	E	285	GLN	CA-C	-6.91	1.45	1.52
1	M	285	GLN	CA-C	-6.91	1.45	1.52
1	A	285	GLN	CA-C	-6.91	1.45	1.52
1	C	285	GLN	CA-C	-6.90	1.45	1.52
2	N	256	ALA	CA-C	-6.89	1.43	1.52
2	D	256	ALA	CA-C	-6.89	1.43	1.52
2	J	280	SER	CA-C	-6.89	1.43	1.52
1	O	285	GLN	CA-C	-6.88	1.45	1.52
2	B	280	SER	CA-C	-6.88	1.43	1.52
2	N	280	SER	CA-C	-6.88	1.43	1.52
2	P	251	ASP	N-CA	-6.88	1.37	1.46
2	R	251	ASP	N-CA	-6.87	1.37	1.46
2	F	280	SER	CA-C	-6.87	1.43	1.52
2	P	280	SER	CA-C	-6.86	1.43	1.52
2	B	256	ALA	CA-C	-6.86	1.43	1.52
2	J	256	ALA	CA-C	-6.85	1.43	1.52
2	N	34	GLY	CA-C	-6.84	1.42	1.51
2	D	251	ASP	N-CA	-6.84	1.37	1.46
2	R	256	ALA	CA-C	-6.84	1.43	1.52
2	D	280	SER	CA-C	-6.84	1.43	1.52
2	L	280	SER	CA-C	-6.84	1.43	1.52
2	F	251	ASP	N-CA	-6.83	1.37	1.46
2	H	256	ALA	CA-C	-6.83	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	256	ALA	CA-C	-6.83	1.43	1.52
2	H	34	GLY	CA-C	-6.83	1.42	1.51
2	L	34	GLY	CA-C	-6.83	1.42	1.51
2	L	256	ALA	CA-C	-6.82	1.43	1.52
2	L	251	ASP	N-CA	-6.82	1.37	1.46
2	P	256	ALA	CA-C	-6.82	1.43	1.52
2	B	251	ASP	N-CA	-6.82	1.37	1.46
2	J	34	GLY	CA-C	-6.82	1.42	1.51
2	B	34	GLY	CA-C	-6.81	1.42	1.51
1	C	49	PHE	CA-C	-6.81	1.38	1.52
2	J	251	ASP	N-CA	-6.81	1.37	1.46
1	I	49	PHE	CA-C	-6.80	1.38	1.52
2	R	34	GLY	CA-C	-6.80	1.42	1.51
2	P	34	GLY	CA-C	-6.80	1.42	1.51
2	D	221	THR	CA-C	-6.79	1.44	1.52
2	D	34	GLY	CA-C	-6.79	1.42	1.51
1	O	49	PHE	CA-C	-6.79	1.38	1.52
2	L	221	THR	CA-C	-6.79	1.44	1.52
2	N	251	ASP	N-CA	-6.79	1.37	1.46
1	G	49	PHE	CA-C	-6.79	1.38	1.52
2	F	34	GLY	CA-C	-6.79	1.42	1.51
1	E	49	PHE	CA-C	-6.78	1.38	1.52
1	A	49	PHE	CA-C	-6.78	1.38	1.52
2	H	251	ASP	N-CA	-6.77	1.37	1.46
1	K	49	PHE	CA-C	-6.77	1.38	1.52
1	Q	49	PHE	CA-C	-6.77	1.38	1.52
1	M	49	PHE	CA-C	-6.77	1.38	1.52
2	F	221	THR	CA-C	-6.76	1.44	1.52
2	N	221	THR	CA-C	-6.76	1.44	1.52
2	P	221	THR	CA-C	-6.75	1.44	1.52
2	H	221	THR	CA-C	-6.75	1.44	1.52
2	B	221	THR	CA-C	-6.74	1.44	1.52
2	P	100	GLY	CA-C	-6.73	1.42	1.51
2	R	221	THR	CA-C	-6.73	1.44	1.52
2	J	221	THR	CA-C	-6.72	1.44	1.52
2	H	100	GLY	CA-C	-6.71	1.42	1.51
2	B	100	GLY	CA-C	-6.67	1.42	1.51
2	N	100	GLY	CA-C	-6.67	1.42	1.51
1	O	348	PRO	C-N	-6.67	1.25	1.33
2	D	100	GLY	CA-C	-6.65	1.42	1.51
1	G	348	PRO	C-N	-6.65	1.25	1.33
1	C	348	PRO	C-N	-6.65	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	348	PRO	C-N	-6.64	1.25	1.33
2	P	349	ASN	CA-C	-6.63	1.45	1.53
1	M	348	PRO	C-N	-6.62	1.25	1.33
2	N	349	ASN	CA-C	-6.62	1.45	1.53
2	R	349	ASN	CA-C	-6.62	1.45	1.53
1	A	348	PRO	C-N	-6.61	1.25	1.33
1	E	348	PRO	C-N	-6.61	1.25	1.33
1	I	348	PRO	C-N	-6.61	1.25	1.33
2	H	349	ASN	CA-C	-6.60	1.45	1.53
2	B	349	ASN	CA-C	-6.60	1.45	1.53
2	L	349	ASN	CA-C	-6.59	1.45	1.53
2	D	349	ASN	CA-C	-6.58	1.46	1.53
2	F	349	ASN	CA-C	-6.56	1.46	1.53
1	Q	348	PRO	C-N	-6.56	1.25	1.33
2	J	349	ASN	CA-C	-6.53	1.46	1.53
1	C	241	SER	N-CA	-6.50	1.38	1.46
1	M	241	SER	N-CA	-6.50	1.38	1.46
1	G	241	SER	N-CA	-6.48	1.38	1.46
1	A	241	SER	N-CA	-6.47	1.38	1.46
1	O	241	SER	N-CA	-6.47	1.38	1.46
1	K	241	SER	N-CA	-6.47	1.38	1.46
1	E	241	SER	N-CA	-6.46	1.38	1.46
2	J	101	ASN	N-CA	-6.43	1.37	1.46
1	Q	241	SER	N-CA	-6.43	1.38	1.46
2	N	101	ASN	N-CA	-6.42	1.37	1.46
2	L	101	ASN	N-CA	-6.42	1.37	1.46
2	H	101	ASN	N-CA	-6.41	1.37	1.46
2	P	101	ASN	N-CA	-6.41	1.37	1.46
2	B	101	ASN	N-CA	-6.40	1.37	1.46
2	R	101	ASN	N-CA	-6.39	1.37	1.46
1	I	241	SER	N-CA	-6.39	1.38	1.46
2	D	101	ASN	N-CA	-6.38	1.37	1.46
1	Q	50	ASN	N-CA	-6.37	1.36	1.46
1	K	50	ASN	N-CA	-6.36	1.36	1.46
1	E	50	ASN	N-CA	-6.36	1.36	1.46
1	G	50	ASN	N-CA	-6.35	1.36	1.46
1	I	50	ASN	N-CA	-6.35	1.36	1.46
2	F	101	ASN	N-CA	-6.35	1.37	1.46
1	A	50	ASN	N-CA	-6.34	1.36	1.46
1	M	50	ASN	N-CA	-6.34	1.36	1.46
1	C	50	ASN	N-CA	-6.34	1.36	1.46
1	O	50	ASN	N-CA	-6.34	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	371	LEU	CA-C	-6.34	1.44	1.52
2	N	59	ASN	N-CA	-6.33	1.37	1.46
1	C	309	HIS	N-CA	-6.32	1.38	1.46
2	F	371	LEU	CA-C	-6.32	1.44	1.52
2	L	371	LEU	CA-C	-6.32	1.44	1.52
2	D	371	LEU	CA-C	-6.31	1.44	1.52
2	H	59	ASN	N-CA	-6.31	1.37	1.46
2	N	371	LEU	CA-C	-6.31	1.44	1.52
2	R	371	LEU	CA-C	-6.31	1.44	1.52
2	P	59	ASN	N-CA	-6.31	1.37	1.46
2	L	59	ASN	N-CA	-6.30	1.37	1.46
2	B	371	LEU	CA-C	-6.30	1.44	1.52
2	J	59	ASN	N-CA	-6.29	1.37	1.46
1	A	309	HIS	N-CA	-6.28	1.38	1.46
2	B	59	ASN	N-CA	-6.28	1.37	1.46
2	D	59	ASN	N-CA	-6.28	1.37	1.46
1	M	309	HIS	N-CA	-6.28	1.38	1.46
2	J	371	LEU	CA-C	-6.27	1.44	1.52
2	F	59	ASN	N-CA	-6.27	1.37	1.46
1	K	309	HIS	N-CA	-6.27	1.38	1.46
1	O	309	HIS	N-CA	-6.27	1.38	1.46
1	I	309	HIS	N-CA	-6.25	1.38	1.46
2	H	255	LEU	CA-C	-6.25	1.44	1.52
2	N	110	GLU	CA-C	-6.25	1.44	1.52
1	Q	309	HIS	N-CA	-6.25	1.38	1.46
1	E	309	HIS	N-CA	-6.25	1.38	1.46
1	Q	36	MET	N-CA	-6.24	1.37	1.46
1	G	309	HIS	N-CA	-6.24	1.38	1.46
1	I	364	PRO	CA-C	-6.23	1.45	1.52
2	L	110	GLU	CA-C	-6.23	1.44	1.52
1	E	36	MET	N-CA	-6.22	1.37	1.46
2	H	371	LEU	CA-C	-6.22	1.44	1.52
1	O	364	PRO	CA-C	-6.22	1.45	1.52
1	Q	364	PRO	CA-C	-6.22	1.45	1.52
1	M	36	MET	N-CA	-6.21	1.37	1.46
2	R	110	GLU	CA-C	-6.21	1.44	1.52
2	R	59	ASN	N-CA	-6.21	1.37	1.46
1	C	36	MET	N-CA	-6.21	1.37	1.46
1	A	36	MET	N-CA	-6.20	1.37	1.46
2	B	110	GLU	CA-C	-6.20	1.44	1.52
1	E	364	PRO	CA-C	-6.20	1.45	1.52
1	C	364	PRO	CA-C	-6.20	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	255	LEU	CA-C	-6.20	1.45	1.52
1	K	36	MET	N-CA	-6.20	1.37	1.46
1	K	82	THR	CA-C	-6.20	1.44	1.53
2	J	110	GLU	CA-C	-6.20	1.44	1.52
1	O	82	THR	CA-C	-6.20	1.44	1.53
1	I	36	MET	N-CA	-6.19	1.37	1.46
1	O	36	MET	N-CA	-6.19	1.37	1.46
2	L	60	LYS	N-CA	-6.19	1.38	1.46
1	A	364	PRO	CA-C	-6.19	1.45	1.52
2	R	60	LYS	N-CA	-6.19	1.38	1.46
2	N	60	LYS	N-CA	-6.18	1.38	1.46
2	F	110	GLU	CA-C	-6.18	1.44	1.52
2	F	258	ASN	N-CA	-6.18	1.38	1.46
1	G	36	MET	N-CA	-6.18	1.37	1.46
1	M	364	PRO	CA-C	-6.18	1.45	1.52
2	J	255	LEU	CA-C	-6.18	1.45	1.52
2	P	110	GLU	CA-C	-6.17	1.44	1.52
2	B	255	LEU	CA-C	-6.17	1.45	1.52
1	K	364	PRO	CA-C	-6.17	1.45	1.52
2	L	255	LEU	CA-C	-6.17	1.45	1.52
2	D	110	GLU	CA-C	-6.17	1.44	1.52
2	F	60	LYS	N-CA	-6.16	1.38	1.46
1	G	82	THR	CA-C	-6.16	1.44	1.53
1	G	364	PRO	CA-C	-6.16	1.45	1.52
2	L	257	VAL	N-CA	-6.16	1.39	1.46
2	R	257	VAL	N-CA	-6.16	1.39	1.46
2	P	257	VAL	N-CA	-6.16	1.39	1.46
2	D	255	LEU	CA-C	-6.16	1.45	1.52
2	P	60	LYS	N-CA	-6.16	1.38	1.46
1	A	82	THR	CA-C	-6.16	1.44	1.53
1	I	82	THR	CA-C	-6.16	1.44	1.53
2	L	258	ASN	N-CA	-6.16	1.38	1.46
2	B	60	LYS	N-CA	-6.15	1.38	1.46
2	D	258	ASN	N-CA	-6.15	1.38	1.46
2	R	255	LEU	CA-C	-6.15	1.45	1.52
1	Q	97	GLU	CA-C	-6.15	1.45	1.52
2	D	257	VAL	N-CA	-6.15	1.39	1.46
2	N	257	VAL	N-CA	-6.15	1.39	1.46
1	Q	82	THR	CA-C	-6.15	1.44	1.53
2	B	258	ASN	N-CA	-6.15	1.38	1.46
2	H	110	GLU	CA-C	-6.15	1.44	1.52
1	C	82	THR	CA-C	-6.14	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	257	VAL	N-CA	-6.14	1.39	1.46
1	I	349	THR	C-N	-6.13	1.24	1.33
2	J	257	VAL	N-CA	-6.13	1.39	1.46
2	J	258	ASN	N-CA	-6.13	1.38	1.46
2	F	255	LEU	CA-C	-6.13	1.45	1.52
2	B	257	VAL	N-CA	-6.13	1.39	1.46
1	E	82	THR	CA-C	-6.13	1.44	1.53
1	E	97	GLU	CA-C	-6.12	1.45	1.52
1	G	97	GLU	CA-C	-6.12	1.45	1.52
2	H	60	LYS	N-CA	-6.12	1.38	1.46
2	R	258	ASN	N-CA	-6.12	1.38	1.46
1	C	349	THR	C-N	-6.12	1.24	1.33
2	P	255	LEU	CA-C	-6.12	1.45	1.52
2	H	257	VAL	N-CA	-6.12	1.39	1.46
2	H	258	ASN	N-CA	-6.12	1.38	1.46
1	Q	349	THR	C-N	-6.12	1.24	1.33
1	G	349	THR	C-N	-6.11	1.24	1.33
1	O	97	GLU	CA-C	-6.11	1.45	1.52
1	M	349	THR	C-N	-6.11	1.24	1.33
1	E	349	THR	C-N	-6.11	1.24	1.33
2	N	258	ASN	N-CA	-6.11	1.38	1.46
2	D	60	LYS	N-CA	-6.10	1.38	1.46
2	J	60	LYS	N-CA	-6.10	1.38	1.46
1	K	301	GLN	CA-C	-6.10	1.44	1.52
1	O	349	THR	C-N	-6.10	1.24	1.33
2	P	258	ASN	N-CA	-6.10	1.38	1.46
1	M	82	THR	CA-C	-6.09	1.44	1.53
1	K	349	THR	C-N	-6.09	1.24	1.33
1	I	97	GLU	CA-C	-6.09	1.45	1.52
1	A	97	GLU	CA-C	-6.09	1.45	1.52
1	A	349	THR	C-N	-6.09	1.24	1.33
1	I	301	GLN	CA-C	-6.08	1.44	1.52
1	C	97	GLU	CA-C	-6.08	1.45	1.52
1	K	97	GLU	CA-C	-6.06	1.45	1.52
1	M	97	GLU	CA-C	-6.06	1.45	1.52
1	E	301	GLN	CA-C	-6.05	1.44	1.52
1	I	283	HIS	C-N	-6.04	1.25	1.33
1	A	301	GLN	CA-C	-6.04	1.44	1.52
1	G	301	GLN	CA-C	-6.03	1.44	1.52
1	Q	301	GLN	CA-C	-6.01	1.44	1.52
1	C	301	GLN	CA-C	-6.01	1.44	1.52
1	E	283	HIS	C-N	-6.00	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	301	GLN	CA-C	-5.99	1.44	1.52
1	K	240	ALA	CA-C	-5.99	1.45	1.52
1	Q	283	HIS	C-N	-5.99	1.25	1.33
1	C	283	HIS	C-N	-5.98	1.25	1.33
1	O	145	THR	CA-C	-5.98	1.45	1.52
1	O	301	GLN	CA-C	-5.98	1.44	1.52
1	O	283	HIS	C-N	-5.97	1.25	1.33
1	Q	145	THR	CA-C	-5.97	1.45	1.52
1	M	145	THR	CA-C	-5.97	1.45	1.52
1	K	145	THR	CA-C	-5.96	1.45	1.52
1	I	145	THR	CA-C	-5.96	1.45	1.52
1	A	283	HIS	C-N	-5.96	1.25	1.33
1	G	283	HIS	C-N	-5.95	1.25	1.33
1	K	283	HIS	C-N	-5.95	1.25	1.33
1	G	145	THR	CA-C	-5.95	1.45	1.52
1	A	145	THR	CA-C	-5.95	1.45	1.52
1	E	145	THR	CA-C	-5.93	1.45	1.52
1	M	240	ALA	CA-C	-5.92	1.45	1.52
1	A	240	ALA	CA-C	-5.92	1.45	1.52
1	C	308	ARG	N-CA	-5.91	1.39	1.46
1	G	240	ALA	CA-C	-5.91	1.45	1.52
1	O	240	ALA	CA-C	-5.91	1.45	1.52
1	Q	240	ALA	CA-C	-5.91	1.45	1.52
1	C	145	THR	CA-C	-5.90	1.45	1.52
1	E	240	ALA	CA-C	-5.90	1.45	1.52
1	M	283	HIS	C-N	-5.88	1.25	1.33
1	K	308	ARG	N-CA	-5.88	1.39	1.46
1	I	240	ALA	CA-C	-5.87	1.45	1.52
1	M	308	ARG	N-CA	-5.87	1.39	1.46
1	G	262	TYR	CA-C	-5.87	1.46	1.52
2	B	240	THR	CA-C	-5.87	1.44	1.52
2	P	240	THR	CA-C	-5.86	1.44	1.52
2	H	240	THR	CA-C	-5.86	1.44	1.52
1	C	240	ALA	CA-C	-5.86	1.45	1.52
1	I	308	ARG	N-CA	-5.86	1.39	1.46
2	D	240	THR	CA-C	-5.85	1.44	1.52
1	E	308	ARG	N-CA	-5.85	1.39	1.46
1	O	308	ARG	N-CA	-5.85	1.39	1.46
1	Q	308	ARG	N-CA	-5.85	1.39	1.46
1	K	262	TYR	CA-C	-5.85	1.46	1.52
1	A	308	ARG	N-CA	-5.84	1.39	1.46
2	D	181	VAL	N-CA	-5.84	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	262	TYR	CA-C	-5.83	1.46	1.52
1	M	262	TYR	CA-C	-5.83	1.46	1.52
2	N	240	THR	CA-C	-5.83	1.44	1.52
2	F	240	THR	CA-C	-5.83	1.44	1.52
2	L	240	THR	CA-C	-5.83	1.44	1.52
1	C	262	TYR	CA-C	-5.82	1.46	1.52
2	B	181	VAL	N-CA	-5.82	1.39	1.46
2	L	181	VAL	N-CA	-5.82	1.39	1.46
2	F	181	VAL	N-CA	-5.81	1.39	1.46
2	H	181	VAL	N-CA	-5.81	1.39	1.46
2	J	240	THR	CA-C	-5.81	1.44	1.52
2	P	181	VAL	N-CA	-5.81	1.39	1.46
1	Q	262	TYR	CA-C	-5.81	1.46	1.52
2	R	240	THR	CA-C	-5.81	1.44	1.52
2	R	358	ILE	N-CA	-5.81	1.41	1.46
1	A	262	TYR	CA-C	-5.80	1.46	1.52
2	R	181	VAL	N-CA	-5.80	1.39	1.46
1	G	308	ARG	N-CA	-5.80	1.39	1.46
2	N	358	ILE	N-CA	-5.80	1.41	1.46
2	J	260	VAL	N-CA	-5.79	1.41	1.46
2	N	181	VAL	N-CA	-5.79	1.39	1.46
2	F	358	ILE	N-CA	-5.78	1.41	1.46
2	J	181	VAL	N-CA	-5.78	1.39	1.46
2	H	358	ILE	N-CA	-5.77	1.41	1.46
1	E	262	TYR	CA-C	-5.77	1.46	1.52
2	N	260	VAL	N-CA	-5.77	1.41	1.46
2	B	358	ILE	N-CA	-5.76	1.41	1.46
2	D	358	ILE	N-CA	-5.76	1.41	1.46
2	F	260	VAL	N-CA	-5.76	1.41	1.46
2	H	260	VAL	N-CA	-5.76	1.41	1.46
2	J	358	ILE	N-CA	-5.76	1.41	1.46
2	P	260	VAL	N-CA	-5.75	1.41	1.46
2	P	358	ILE	N-CA	-5.75	1.41	1.46
1	O	262	TYR	CA-C	-5.75	1.46	1.52
2	L	358	ILE	N-CA	-5.75	1.41	1.46
2	B	260	VAL	N-CA	-5.73	1.41	1.46
2	P	177	VAL	CA-C	-5.72	1.45	1.52
1	G	147	SER	N-CA	-5.72	1.39	1.46
2	D	177	VAL	CA-C	-5.72	1.45	1.52
1	I	147	SER	N-CA	-5.71	1.39	1.46
2	R	260	VAL	N-CA	-5.71	1.41	1.46
1	Q	147	SER	N-CA	-5.70	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	60	LYS	CA-C	-5.70	1.45	1.52
1	O	147	SER	N-CA	-5.70	1.39	1.46
1	M	60	LYS	CA-C	-5.70	1.45	1.52
2	J	242	LEU	N-CA	-5.69	1.39	1.46
2	F	177	VAL	CA-C	-5.69	1.45	1.52
1	K	147	SER	N-CA	-5.69	1.39	1.46
2	L	260	VAL	N-CA	-5.69	1.41	1.46
2	B	177	VAL	CA-C	-5.69	1.45	1.52
1	A	147	SER	N-CA	-5.68	1.39	1.46
2	D	260	VAL	N-CA	-5.68	1.41	1.46
1	M	147	SER	N-CA	-5.68	1.39	1.46
1	E	147	SER	N-CA	-5.68	1.39	1.46
2	H	242	LEU	N-CA	-5.68	1.39	1.46
2	P	248	LEU	CA-C	-5.67	1.45	1.53
2	R	177	VAL	CA-C	-5.67	1.45	1.52
2	B	242	LEU	N-CA	-5.66	1.39	1.46
2	R	242	LEU	N-CA	-5.66	1.39	1.46
2	N	248	LEU	CA-C	-5.66	1.45	1.53
2	J	177	VAL	CA-C	-5.66	1.45	1.52
2	P	242	LEU	N-CA	-5.66	1.39	1.46
2	N	177	VAL	CA-C	-5.66	1.45	1.52
2	N	242	LEU	N-CA	-5.65	1.39	1.46
1	C	147	SER	N-CA	-5.65	1.39	1.46
2	L	248	LEU	CA-C	-5.65	1.45	1.53
1	G	367	ASP	N-CA	-5.65	1.39	1.46
2	R	248	LEU	CA-C	-5.65	1.45	1.53
2	L	242	LEU	N-CA	-5.65	1.39	1.46
1	C	60	LYS	CA-C	-5.64	1.45	1.52
2	D	242	LEU	N-CA	-5.64	1.39	1.46
1	I	60	LYS	CA-C	-5.64	1.45	1.52
1	I	367	ASP	N-CA	-5.64	1.39	1.46
1	A	60	LYS	CA-C	-5.64	1.45	1.52
1	E	60	LYS	CA-C	-5.64	1.45	1.52
1	Q	60	LYS	CA-C	-5.64	1.45	1.52
2	F	242	LEU	N-CA	-5.64	1.39	1.46
2	H	177	VAL	CA-C	-5.64	1.45	1.52
2	L	177	VAL	CA-C	-5.64	1.45	1.52
1	O	60	LYS	CA-C	-5.63	1.45	1.52
1	G	60	LYS	CA-C	-5.63	1.45	1.52
1	O	367	ASP	N-CA	-5.63	1.39	1.46
2	B	248	LEU	CA-C	-5.62	1.45	1.53
1	C	367	ASP	N-CA	-5.61	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	248	LEU	CA-C	-5.61	1.45	1.53
2	H	248	LEU	CA-C	-5.61	1.45	1.53
1	A	367	ASP	N-CA	-5.61	1.39	1.46
2	D	248	LEU	CA-C	-5.61	1.45	1.53
2	P	259	MET	N-CA	-5.59	1.38	1.46
1	E	50	ASN	CA-C	-5.59	1.45	1.53
1	G	50	ASN	CA-C	-5.59	1.45	1.53
1	Q	50	ASN	CA-C	-5.59	1.45	1.53
2	J	248	LEU	CA-C	-5.58	1.45	1.53
1	K	50	ASN	CA-C	-5.58	1.45	1.53
1	Q	37	PRO	N-CA	-5.58	1.40	1.47
1	M	367	ASP	N-CA	-5.58	1.40	1.46
1	O	50	ASN	CA-C	-5.58	1.45	1.53
1	A	50	ASN	CA-C	-5.58	1.45	1.53
1	I	50	ASN	CA-C	-5.58	1.45	1.53
1	C	50	ASN	CA-C	-5.57	1.45	1.53
1	E	37	PRO	N-CA	-5.57	1.40	1.47
1	E	367	ASP	N-CA	-5.57	1.40	1.46
1	K	367	ASP	N-CA	-5.57	1.40	1.46
1	Q	367	ASP	N-CA	-5.56	1.40	1.46
1	M	37	PRO	N-CA	-5.56	1.40	1.47
1	M	361	THR	CA-C	-5.56	1.45	1.52
2	N	259	MET	N-CA	-5.56	1.38	1.46
2	B	259	MET	N-CA	-5.55	1.38	1.46
2	R	259	MET	N-CA	-5.55	1.38	1.46
2	F	259	MET	N-CA	-5.54	1.38	1.46
1	C	37	PRO	N-CA	-5.54	1.40	1.47
1	G	37	PRO	N-CA	-5.54	1.40	1.47
2	H	259	MET	N-CA	-5.54	1.38	1.46
1	M	50	ASN	CA-C	-5.54	1.45	1.53
1	G	361	THR	CA-C	-5.53	1.45	1.52
1	A	361	THR	CA-C	-5.53	1.45	1.52
1	A	37	PRO	N-CA	-5.53	1.40	1.47
2	L	259	MET	N-CA	-5.52	1.38	1.46
1	O	37	PRO	N-CA	-5.52	1.40	1.47
1	O	361	THR	CA-C	-5.52	1.45	1.52
2	D	259	MET	N-CA	-5.51	1.38	1.46
1	I	37	PRO	N-CA	-5.51	1.40	1.47
1	I	361	THR	CA-C	-5.51	1.45	1.52
1	E	361	THR	CA-C	-5.50	1.45	1.52
1	C	361	THR	CA-C	-5.50	1.45	1.52
2	R	99	ALA	C-N	-5.50	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	259	MET	N-CA	-5.50	1.38	1.46
1	K	361	THR	CA-C	-5.50	1.45	1.52
1	K	37	PRO	N-CA	-5.49	1.40	1.47
2	J	99	ALA	C-N	-5.48	1.26	1.33
1	Q	361	THR	CA-C	-5.47	1.45	1.52
2	F	99	ALA	C-N	-5.45	1.26	1.33
2	N	180	THR	N-CA	-5.42	1.39	1.45
1	M	403	ALA	CA-C	-5.41	1.45	1.52
1	M	49	PHE	N-CA	-5.41	1.35	1.46
1	O	49	PHE	N-CA	-5.41	1.35	1.46
2	L	99	ALA	C-N	-5.40	1.27	1.33
1	E	403	ALA	CA-C	-5.40	1.45	1.52
2	F	174	SER	CA-C	-5.39	1.46	1.53
1	K	49	PHE	N-CA	-5.39	1.36	1.46
2	L	436	GLN	C-N	-5.38	1.25	1.33
2	R	259	MET	CA-C	-5.37	1.45	1.52
2	D	436	GLN	C-N	-5.37	1.25	1.33
2	N	174	SER	CA-C	-5.37	1.46	1.53
2	J	174	SER	CA-C	-5.37	1.46	1.53
2	R	403	ALA	CA-C	-5.37	1.45	1.52
1	A	403	ALA	CA-C	-5.37	1.45	1.52
2	H	180	THR	N-CA	-5.37	1.39	1.45
2	J	259	MET	CA-C	-5.37	1.45	1.52
1	C	49	PHE	N-CA	-5.36	1.36	1.46
1	G	49	PHE	N-CA	-5.36	1.36	1.46
1	O	403	ALA	CA-C	-5.36	1.45	1.52
1	A	49	PHE	N-CA	-5.36	1.36	1.46
1	C	403	ALA	CA-C	-5.36	1.45	1.52
1	Q	403	ALA	CA-C	-5.36	1.45	1.52
1	Q	49	PHE	N-CA	-5.36	1.36	1.46
2	R	174	SER	CA-C	-5.36	1.46	1.53
1	I	403	ALA	CA-C	-5.36	1.45	1.52
2	R	436	GLN	C-N	-5.36	1.25	1.33
2	N	436	GLN	C-N	-5.35	1.25	1.33
1	G	403	ALA	CA-C	-5.35	1.45	1.52
2	R	180	THR	N-CA	-5.35	1.39	1.45
1	E	49	PHE	N-CA	-5.34	1.36	1.46
2	B	180	THR	N-CA	-5.34	1.39	1.45
2	H	174	SER	CA-C	-5.34	1.46	1.53
2	P	180	THR	N-CA	-5.34	1.39	1.45
2	D	180	THR	N-CA	-5.34	1.39	1.45
2	F	180	THR	N-CA	-5.33	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	403	ALA	CA-C	-5.33	1.45	1.52
2	N	258	ASN	CA-C	-5.33	1.45	1.52
1	I	49	PHE	N-CA	-5.33	1.36	1.46
2	L	174	SER	CA-C	-5.33	1.46	1.53
2	L	180	THR	N-CA	-5.33	1.39	1.45
2	P	174	SER	CA-C	-5.33	1.46	1.53
1	Q	363	VAL	CA-C	-5.33	1.48	1.53
2	D	174	SER	CA-C	-5.33	1.46	1.53
2	L	259	MET	CA-C	-5.33	1.45	1.52
2	B	259	MET	CA-C	-5.33	1.45	1.52
2	D	403	ALA	CA-C	-5.33	1.45	1.52
2	P	436	GLN	C-N	-5.33	1.25	1.33
2	F	259	MET	CA-C	-5.32	1.45	1.52
2	L	403	ALA	CA-C	-5.32	1.45	1.52
2	P	259	MET	CA-C	-5.32	1.45	1.52
1	C	363	VAL	CA-C	-5.32	1.48	1.53
2	F	436	GLN	C-N	-5.32	1.25	1.33
2	N	403	ALA	CA-C	-5.32	1.45	1.52
2	B	174	SER	CA-C	-5.32	1.46	1.53
2	B	403	ALA	CA-C	-5.32	1.45	1.52
2	H	403	ALA	CA-C	-5.32	1.45	1.52
2	B	436	GLN	C-N	-5.32	1.25	1.33
2	J	436	GLN	C-N	-5.31	1.25	1.33
2	N	259	MET	CA-C	-5.31	1.45	1.52
2	D	259	MET	CA-C	-5.31	1.45	1.52
2	P	403	ALA	CA-C	-5.31	1.45	1.52
2	D	258	ASN	CA-C	-5.31	1.45	1.52
1	E	411	GLU	N-CA	-5.30	1.39	1.46
2	H	258	ASN	CA-C	-5.30	1.45	1.52
2	J	258	ASN	CA-C	-5.30	1.45	1.52
2	L	258	ASN	CA-C	-5.30	1.45	1.52
2	H	259	MET	CA-C	-5.30	1.45	1.52
2	J	180	THR	N-CA	-5.30	1.39	1.45
1	M	363	VAL	CA-C	-5.30	1.49	1.53
1	A	363	VAL	CA-C	-5.30	1.49	1.53
2	F	258	ASN	CA-C	-5.30	1.45	1.52
2	P	258	ASN	CA-C	-5.29	1.45	1.52
1	E	363	VAL	CA-C	-5.29	1.49	1.53
1	K	411	GLU	N-CA	-5.29	1.39	1.46
1	G	363	VAL	CA-C	-5.29	1.49	1.53
2	F	403	ALA	CA-C	-5.28	1.45	1.52
2	B	258	ASN	CA-C	-5.28	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	411	GLU	N-CA	-5.28	1.39	1.46
1	K	363	VAL	N-CA	-5.28	1.42	1.46
2	J	403	ALA	CA-C	-5.27	1.45	1.52
1	O	411	GLU	N-CA	-5.27	1.39	1.46
2	R	258	ASN	CA-C	-5.27	1.45	1.52
1	G	350	GLY	CA-C	-5.27	1.44	1.51
1	C	411	GLU	N-CA	-5.26	1.39	1.46
1	Q	411	GLU	N-CA	-5.26	1.39	1.46
2	H	436	GLN	C-N	-5.26	1.25	1.33
1	M	411	GLU	N-CA	-5.26	1.39	1.46
1	I	363	VAL	CA-C	-5.26	1.49	1.53
1	I	411	GLU	N-CA	-5.25	1.39	1.46
2	H	360	PRO	N-CA	-5.25	1.41	1.46
2	N	360	PRO	N-CA	-5.25	1.41	1.46
1	O	363	VAL	CA-C	-5.25	1.49	1.53
1	I	241	SER	CA-C	-5.24	1.46	1.52
1	A	411	GLU	N-CA	-5.24	1.39	1.46
2	F	360	PRO	N-CA	-5.23	1.41	1.46
2	L	360	PRO	N-CA	-5.23	1.41	1.46
1	M	241	SER	CA-C	-5.23	1.46	1.52
2	D	360	PRO	N-CA	-5.23	1.41	1.46
2	F	275	LEU	N-CA	-5.22	1.39	1.46
1	K	363	VAL	CA-C	-5.22	1.49	1.53
1	M	363	VAL	N-CA	-5.22	1.42	1.46
2	R	241	CYS	CA-C	-5.22	1.45	1.52
1	O	241	SER	CA-C	-5.21	1.46	1.52
2	D	241	CYS	CA-C	-5.21	1.45	1.52
2	P	360	PRO	N-CA	-5.21	1.41	1.46
1	C	34	GLY	CA-C	-5.20	1.44	1.51
2	N	275	LEU	N-CA	-5.20	1.39	1.46
2	B	360	PRO	N-CA	-5.20	1.41	1.46
1	C	162	GLY	CA-C	-5.20	1.45	1.52
2	F	400	ARG	CA-C	-5.20	1.46	1.52
2	J	241	CYS	CA-C	-5.20	1.45	1.52
1	C	241	SER	CA-C	-5.19	1.46	1.52
2	L	241	CYS	CA-C	-5.19	1.45	1.52
1	O	350	GLY	CA-C	-5.19	1.44	1.51
2	P	241	CYS	CA-C	-5.19	1.45	1.52
1	A	241	SER	CA-C	-5.19	1.46	1.52
2	H	275	LEU	N-CA	-5.19	1.39	1.46
2	R	275	LEU	N-CA	-5.18	1.39	1.46
1	A	350	GLY	CA-C	-5.18	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	350	GLY	CA-C	-5.18	1.44	1.51
2	R	360	PRO	N-CA	-5.18	1.41	1.46
2	B	241	CYS	CA-C	-5.18	1.45	1.52
1	E	366	GLY	N-CA	-5.18	1.39	1.45
1	Q	241	SER	CA-C	-5.18	1.46	1.52
1	Q	363	VAL	N-CA	-5.18	1.42	1.46
2	J	360	PRO	N-CA	-5.18	1.41	1.46
1	K	241	SER	CA-C	-5.17	1.46	1.52
1	Q	162	GLY	CA-C	-5.17	1.45	1.52
2	H	399	PHE	CA-C	-5.17	1.46	1.52
2	R	399	PHE	CA-C	-5.17	1.46	1.52
1	K	350	GLY	CA-C	-5.17	1.44	1.51
1	C	284	GLU	C-N	-5.17	1.26	1.33
2	D	399	PHE	CA-C	-5.17	1.46	1.52
2	B	275	LEU	N-CA	-5.17	1.39	1.46
1	M	350	GLY	CA-C	-5.16	1.44	1.51
2	N	241	CYS	CA-C	-5.16	1.45	1.52
1	A	363	VAL	N-CA	-5.16	1.42	1.46
1	A	34	GLY	CA-C	-5.16	1.44	1.51
1	E	241	SER	CA-C	-5.16	1.46	1.52
2	P	399	PHE	CA-C	-5.16	1.46	1.52
1	C	363	VAL	N-CA	-5.16	1.42	1.46
1	G	241	SER	CA-C	-5.16	1.46	1.52
2	H	241	CYS	CA-C	-5.16	1.45	1.52
2	J	220	THR	C-N	-5.16	1.27	1.33
2	D	400	ARG	CA-C	-5.15	1.46	1.52
1	I	350	GLY	CA-C	-5.15	1.44	1.51
2	P	275	LEU	N-CA	-5.15	1.39	1.46
2	F	241	CYS	CA-C	-5.15	1.45	1.52
2	N	399	PHE	CA-C	-5.15	1.46	1.52
2	N	400	ARG	CA-C	-5.15	1.46	1.52
1	Q	366	GLY	N-CA	-5.15	1.39	1.45
1	A	366	GLY	N-CA	-5.15	1.39	1.45
2	B	399	PHE	CA-C	-5.15	1.46	1.52
1	Q	350	GLY	CA-C	-5.15	1.44	1.51
1	A	162	GLY	CA-C	-5.14	1.45	1.52
2	B	400	ARG	CA-C	-5.14	1.46	1.52
2	R	400	ARG	CA-C	-5.14	1.46	1.52
2	P	400	ARG	CA-C	-5.14	1.46	1.52
2	D	275	LEU	N-CA	-5.14	1.39	1.46
1	O	162	GLY	CA-C	-5.14	1.46	1.52
1	E	284	GLU	C-N	-5.14	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	34	GLY	CA-C	-5.14	1.44	1.51
2	F	399	PHE	CA-C	-5.14	1.46	1.52
1	G	162	GLY	CA-C	-5.14	1.46	1.52
1	G	366	GLY	N-CA	-5.14	1.39	1.45
1	E	363	VAL	N-CA	-5.13	1.42	1.46
1	G	34	GLY	CA-C	-5.13	1.44	1.51
1	Q	34	GLY	CA-C	-5.13	1.44	1.51
1	M	366	GLY	N-CA	-5.13	1.39	1.45
2	D	220	THR	C-N	-5.13	1.27	1.33
1	O	34	GLY	CA-C	-5.13	1.44	1.51
1	C	366	GLY	N-CA	-5.13	1.39	1.45
1	E	34	GLY	CA-C	-5.13	1.44	1.51
2	J	400	ARG	CA-C	-5.13	1.46	1.52
2	L	399	PHE	CA-C	-5.13	1.46	1.52
1	O	363	VAL	N-CA	-5.13	1.42	1.46
1	C	350	GLY	CA-C	-5.13	1.44	1.51
1	I	162	GLY	CA-C	-5.13	1.46	1.52
1	I	173	PRO	N-CA	-5.13	1.41	1.47
1	I	34	GLY	CA-C	-5.12	1.44	1.51
1	G	363	VAL	N-CA	-5.12	1.42	1.46
2	L	400	ARG	CA-C	-5.12	1.46	1.52
1	O	366	GLY	N-CA	-5.12	1.39	1.45
1	E	162	GLY	CA-C	-5.12	1.46	1.52
1	I	363	VAL	N-CA	-5.12	1.42	1.46
2	J	275	LEU	N-CA	-5.12	1.39	1.46
1	M	284	GLU	C-N	-5.12	1.26	1.33
2	L	275	LEU	N-CA	-5.12	1.39	1.46
1	K	34	GLY	CA-C	-5.12	1.44	1.51
1	K	162	GLY	CA-C	-5.12	1.46	1.52
2	J	399	PHE	CA-C	-5.12	1.46	1.52
1	A	284	GLU	C-N	-5.11	1.26	1.33
2	J	241	CYS	N-CA	-5.11	1.39	1.46
1	K	366	GLY	N-CA	-5.11	1.39	1.45
1	M	162	GLY	CA-C	-5.11	1.46	1.52
1	I	284	GLU	C-N	-5.11	1.26	1.33
1	I	366	GLY	N-CA	-5.11	1.39	1.45
2	N	35	SER	N-CA	-5.11	1.40	1.45
2	N	241	CYS	N-CA	-5.11	1.39	1.46
1	Q	284	GLU	C-N	-5.11	1.26	1.33
2	H	35	SER	N-CA	-5.11	1.40	1.45
1	G	173	PRO	N-CA	-5.10	1.41	1.47
1	G	284	GLU	C-N	-5.10	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	181	VAL	CA-C	-5.10	1.46	1.52
1	O	284	GLU	C-N	-5.10	1.26	1.33
2	B	220	THR	C-N	-5.10	1.27	1.33
2	D	241	CYS	N-CA	-5.10	1.39	1.46
2	H	220	THR	C-N	-5.10	1.27	1.33
2	L	220	THR	C-N	-5.10	1.27	1.33
2	F	241	CYS	N-CA	-5.09	1.39	1.46
2	H	181	VAL	CA-C	-5.09	1.46	1.52
2	N	220	THR	C-N	-5.09	1.27	1.33
2	P	241	CYS	N-CA	-5.09	1.39	1.46
1	E	261	PRO	N-CA	-5.09	1.40	1.47
1	Q	261	PRO	N-CA	-5.09	1.40	1.47
2	B	241	CYS	N-CA	-5.08	1.39	1.46
2	H	241	CYS	N-CA	-5.08	1.39	1.46
1	I	409	VAL	CA-C	-5.08	1.46	1.52
2	D	35	SER	N-CA	-5.08	1.40	1.45
2	F	220	THR	C-N	-5.08	1.27	1.33
2	R	35	SER	N-CA	-5.08	1.40	1.45
1	K	284	GLU	C-N	-5.08	1.26	1.33
2	R	220	THR	C-N	-5.08	1.27	1.33
1	A	173	PRO	N-CA	-5.07	1.41	1.47
2	D	181	VAL	CA-C	-5.07	1.46	1.52
1	M	173	PRO	N-CA	-5.07	1.41	1.47
1	C	173	PRO	N-CA	-5.07	1.41	1.47
1	E	286	LEU	N-CA	-5.06	1.40	1.46
1	Q	409	VAL	CA-C	-5.06	1.46	1.52
1	O	261	PRO	N-CA	-5.06	1.40	1.47
1	K	173	PRO	N-CA	-5.06	1.41	1.47
2	B	35	SER	N-CA	-5.06	1.40	1.45
2	L	181	VAL	CA-C	-5.06	1.46	1.52
2	P	35	SER	N-CA	-5.06	1.40	1.45
1	Q	173	PRO	N-CA	-5.06	1.41	1.47
1	G	436	GLY	N-CA	-5.05	1.38	1.45
1	M	436	GLY	N-CA	-5.05	1.38	1.45
1	C	339	ARG	C-N	-5.05	1.26	1.33
1	G	339	ARG	C-N	-5.05	1.26	1.33
1	Q	436	GLY	N-CA	-5.05	1.38	1.45
2	B	181	VAL	CA-C	-5.05	1.46	1.52
1	K	436	GLY	N-CA	-5.05	1.38	1.45
2	P	220	THR	C-N	-5.05	1.27	1.33
2	L	241	CYS	N-CA	-5.05	1.39	1.46
2	R	181	VAL	CA-C	-5.05	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	35	SER	N-CA	-5.04	1.40	1.45
1	C	261	PRO	N-CA	-5.04	1.40	1.47
1	C	436	GLY	N-CA	-5.04	1.38	1.45
1	O	200	CYS	CA-C	-5.03	1.46	1.52
2	R	241	CYS	N-CA	-5.03	1.39	1.46
1	E	173	PRO	N-CA	-5.03	1.41	1.47
1	I	339	ARG	C-N	-5.03	1.26	1.33
2	N	281	GLN	N-CA	-5.03	1.40	1.46
2	L	35	SER	N-CA	-5.03	1.40	1.45
1	E	178	SER	CA-C	-5.02	1.46	1.52
2	H	281	GLN	N-CA	-5.02	1.40	1.46
1	I	436	GLY	N-CA	-5.02	1.38	1.45
1	Q	339	ARG	C-N	-5.02	1.26	1.33
1	E	409	VAL	CA-C	-5.02	1.46	1.52
2	F	181	VAL	CA-C	-5.02	1.46	1.52
2	L	281	GLN	N-CA	-5.02	1.40	1.46
1	M	339	ARG	C-N	-5.02	1.26	1.33
1	K	261	PRO	N-CA	-5.02	1.40	1.47
1	A	261	PRO	N-CA	-5.01	1.41	1.47
1	A	286	LEU	N-CA	-5.01	1.40	1.46
2	F	281	GLN	N-CA	-5.01	1.40	1.46
1	Q	178	SER	CA-C	-5.01	1.46	1.52
1	Q	286	LEU	N-CA	-5.01	1.40	1.46
2	D	281	GLN	N-CA	-5.01	1.40	1.46
1	G	409	VAL	CA-C	-5.01	1.46	1.52
1	E	436	GLY	N-CA	-5.01	1.38	1.45
1	A	339	ARG	C-N	-5.01	1.26	1.33
2	B	281	GLN	N-CA	-5.01	1.40	1.46
2	J	35	SER	N-CA	-5.01	1.40	1.45
1	A	436	GLY	N-CA	-5.01	1.38	1.45
1	E	339	ARG	C-N	-5.01	1.26	1.33
1	A	409	VAL	CA-C	-5.01	1.46	1.52
2	H	400	ARG	CA-C	-5.01	1.46	1.52
2	P	181	VAL	CA-C	-5.01	1.46	1.52
1	C	409	VAL	CA-C	-5.00	1.46	1.52
1	O	173	PRO	N-CA	-5.00	1.41	1.47
1	O	409	VAL	CA-C	-5.00	1.46	1.52
1	G	261	PRO	N-CA	-5.00	1.41	1.47
1	M	286	LEU	N-CA	-5.00	1.40	1.46
2	N	181	VAL	CA-C	-5.00	1.46	1.52

All (2470) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	273	ALA	CA-C-N	-18.29	96.98	119.84
1	I	273	ALA	C-N-CA	-18.29	96.98	119.84
1	G	273	ALA	CA-C-N	-18.27	97.00	119.84
1	G	273	ALA	C-N-CA	-18.27	97.00	119.84
1	C	273	ALA	CA-C-N	-18.26	97.01	119.84
1	C	273	ALA	C-N-CA	-18.26	97.01	119.84
1	O	273	ALA	CA-C-N	-18.26	97.01	119.84
1	O	273	ALA	C-N-CA	-18.26	97.01	119.84
1	A	273	ALA	CA-C-N	-18.26	97.02	119.84
1	A	273	ALA	C-N-CA	-18.26	97.02	119.84
1	E	273	ALA	CA-C-N	-18.25	97.02	119.84
1	E	273	ALA	C-N-CA	-18.25	97.02	119.84
1	Q	273	ALA	CA-C-N	-18.25	97.03	119.84
1	Q	273	ALA	C-N-CA	-18.25	97.03	119.84
1	K	273	ALA	CA-C-N	-18.24	97.04	119.84
1	K	273	ALA	C-N-CA	-18.24	97.04	119.84
1	M	273	ALA	CA-C-N	-18.23	97.05	119.84
1	M	273	ALA	C-N-CA	-18.23	97.05	119.84
1	O	98	ASP	CA-CB-CG	15.31	127.91	112.60
1	I	98	ASP	CA-CB-CG	15.31	127.91	112.60
1	E	98	ASP	CA-CB-CG	15.30	127.90	112.60
1	A	98	ASP	CA-CB-CG	15.28	127.88	112.60
1	Q	98	ASP	CA-CB-CG	15.27	127.87	112.60
1	K	98	ASP	CA-CB-CG	15.27	127.87	112.60
1	M	98	ASP	CA-CB-CG	15.26	127.86	112.60
1	G	98	ASP	CA-CB-CG	15.24	127.84	112.60
1	C	98	ASP	CA-CB-CG	15.22	127.82	112.60
2	N	378	ILE	CA-C-N	-14.19	109.90	121.82
2	N	378	ILE	C-N-CA	-14.19	109.90	121.82
2	D	378	ILE	CA-C-N	-14.18	109.91	121.82
2	D	378	ILE	C-N-CA	-14.18	109.91	121.82
2	B	378	ILE	CA-C-N	-14.17	109.92	121.82
2	B	378	ILE	C-N-CA	-14.17	109.92	121.82
2	R	378	ILE	CA-C-N	-14.16	109.92	121.82
2	R	378	ILE	C-N-CA	-14.16	109.92	121.82
2	P	378	ILE	CA-C-N	-14.16	109.93	121.82
2	P	378	ILE	C-N-CA	-14.16	109.93	121.82
2	J	378	ILE	CA-C-N	-14.14	109.94	121.82
2	J	378	ILE	C-N-CA	-14.14	109.94	121.82
2	L	378	ILE	CA-C-N	-14.14	109.94	121.82
2	L	378	ILE	C-N-CA	-14.14	109.94	121.82
2	H	378	ILE	CA-C-N	-14.13	109.95	121.82
2	H	378	ILE	C-N-CA	-14.13	109.95	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	378	ILE	CA-C-N	-14.12	109.96	121.82
2	F	378	ILE	C-N-CA	-14.12	109.96	121.82
1	K	301	GLN	N-CA-C	12.68	128.20	112.23
1	O	301	GLN	N-CA-C	12.67	128.19	112.23
1	I	301	GLN	N-CA-C	12.65	128.18	112.23
2	J	436	GLN	O-C-N	12.65	135.53	122.12
1	A	301	GLN	N-CA-C	12.65	128.17	112.23
1	G	301	GLN	N-CA-C	12.64	128.16	112.23
2	N	436	GLN	O-C-N	12.64	135.52	122.12
1	C	301	GLN	N-CA-C	12.63	128.15	112.23
2	L	436	GLN	O-C-N	12.63	135.51	122.12
2	R	436	GLN	O-C-N	12.63	135.50	122.12
2	D	436	GLN	O-C-N	12.62	135.50	122.12
1	Q	301	GLN	N-CA-C	12.62	128.14	112.23
2	B	436	GLN	O-C-N	12.62	135.50	122.12
1	M	301	GLN	N-CA-C	12.62	128.13	112.23
2	F	436	GLN	O-C-N	12.62	135.50	122.12
2	P	436	GLN	O-C-N	12.62	135.50	122.12
1	E	301	GLN	N-CA-C	12.61	128.12	112.23
2	H	436	GLN	O-C-N	12.60	135.47	122.12
1	K	436	GLY	CA-C-N	-12.27	104.85	120.56
1	K	436	GLY	C-N-CA	-12.27	104.85	120.56
1	C	436	GLY	CA-C-N	-12.26	104.86	120.56
1	C	436	GLY	C-N-CA	-12.26	104.86	120.56
1	I	436	GLY	CA-C-N	-12.25	104.88	120.56
1	I	436	GLY	C-N-CA	-12.25	104.88	120.56
1	M	436	GLY	CA-C-N	-12.25	104.88	120.56
1	M	436	GLY	C-N-CA	-12.25	104.88	120.56
1	A	436	GLY	CA-C-N	-12.25	104.88	120.56
1	A	436	GLY	C-N-CA	-12.25	104.88	120.56
1	O	436	GLY	CA-C-N	-12.24	104.90	120.56
1	O	436	GLY	C-N-CA	-12.24	104.90	120.56
1	Q	436	GLY	CA-C-N	-12.24	104.90	120.56
1	Q	436	GLY	C-N-CA	-12.24	104.90	120.56
1	E	436	GLY	CA-C-N	-12.23	104.90	120.56
1	E	436	GLY	C-N-CA	-12.23	104.90	120.56
1	G	436	GLY	CA-C-N	-12.21	104.94	120.56
1	G	436	GLY	C-N-CA	-12.21	104.94	120.56
2	H	110	GLU	N-CA-C	11.84	124.27	111.36
2	J	110	GLU	N-CA-C	11.84	124.27	111.36
2	F	110	GLU	N-CA-C	11.84	124.27	111.36
2	N	110	GLU	N-CA-C	11.84	124.27	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	110	GLU	N-CA-C	11.83	124.26	111.36
2	D	110	GLU	N-CA-C	11.83	124.25	111.36
2	P	110	GLU	N-CA-C	11.82	124.24	111.36
2	L	110	GLU	N-CA-C	11.81	124.24	111.36
2	R	110	GLU	N-CA-C	11.81	124.23	111.36
1	K	437	VAL	N-CA-C	11.68	121.50	110.53
1	I	437	VAL	N-CA-C	11.65	121.48	110.53
1	C	437	VAL	N-CA-C	11.65	121.48	110.53
1	I	282	TYR	CA-C-N	-11.64	105.91	123.14
1	I	282	TYR	C-N-CA	-11.64	105.91	123.14
1	G	437	VAL	N-CA-C	11.64	121.47	110.53
1	Q	282	TYR	CA-C-N	-11.64	105.92	123.14
1	Q	282	TYR	C-N-CA	-11.64	105.92	123.14
1	K	282	TYR	CA-C-N	-11.64	105.92	123.14
1	K	282	TYR	C-N-CA	-11.64	105.92	123.14
1	A	437	VAL	N-CA-C	11.63	121.46	110.53
1	E	437	VAL	N-CA-C	11.63	121.46	110.53
1	C	282	TYR	CA-C-N	-11.63	105.93	123.14
1	C	282	TYR	C-N-CA	-11.63	105.93	123.14
1	A	282	TYR	CA-C-N	-11.62	105.94	123.14
1	A	282	TYR	C-N-CA	-11.62	105.94	123.14
1	M	49	PHE	CA-C-N	-11.62	107.46	123.03
1	M	49	PHE	C-N-CA	-11.62	107.46	123.03
1	O	282	TYR	CA-C-N	-11.62	105.95	123.14
1	O	282	TYR	C-N-CA	-11.62	105.95	123.14
1	Q	437	VAL	N-CA-C	11.61	121.44	110.53
1	G	282	TYR	CA-C-N	-11.61	105.96	123.14
1	G	282	TYR	C-N-CA	-11.61	105.96	123.14
1	M	282	TYR	CA-C-N	-11.61	105.96	123.14
1	M	282	TYR	C-N-CA	-11.61	105.96	123.14
1	O	437	VAL	N-CA-C	11.61	121.44	110.53
1	E	282	TYR	CA-C-N	-11.60	105.97	123.14
1	E	282	TYR	C-N-CA	-11.60	105.97	123.14
1	O	49	PHE	CA-C-N	-11.60	107.48	123.03
1	O	49	PHE	C-N-CA	-11.60	107.48	123.03
1	M	437	VAL	N-CA-C	11.59	121.43	110.53
1	A	49	PHE	CA-C-N	-11.58	107.51	123.03
1	A	49	PHE	C-N-CA	-11.58	107.51	123.03
1	I	49	PHE	CA-C-N	-11.58	107.51	123.03
1	I	49	PHE	C-N-CA	-11.58	107.51	123.03
1	C	49	PHE	CA-C-N	-11.57	107.53	123.03
1	C	49	PHE	C-N-CA	-11.57	107.53	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	49	PHE	CA-C-N	-11.57	107.53	123.03
1	E	49	PHE	C-N-CA	-11.57	107.53	123.03
1	G	49	PHE	CA-C-N	-11.56	107.53	123.03
1	G	49	PHE	C-N-CA	-11.56	107.53	123.03
1	K	49	PHE	CA-C-N	-11.56	107.54	123.03
1	K	49	PHE	C-N-CA	-11.56	107.54	123.03
1	Q	49	PHE	CA-C-N	-11.55	107.55	123.03
1	Q	49	PHE	C-N-CA	-11.55	107.55	123.03
1	I	274	PRO	CA-N-CD	-11.13	96.42	112.00
1	G	274	PRO	CA-N-CD	-11.12	96.43	112.00
1	E	274	PRO	CA-N-CD	-11.12	96.44	112.00
1	A	274	PRO	CA-N-CD	-11.11	96.44	112.00
1	O	274	PRO	CA-N-CD	-11.12	96.44	112.00
1	K	274	PRO	CA-N-CD	-11.11	96.44	112.00
1	Q	274	PRO	CA-N-CD	-11.11	96.44	112.00
1	M	274	PRO	CA-N-CD	-11.11	96.45	112.00
1	C	274	PRO	CA-N-CD	-11.10	96.46	112.00
1	C	142	GLY	CA-C-N	-10.97	109.56	122.83
1	C	142	GLY	C-N-CA	-10.97	109.56	122.83
2	L	34	GLY	N-CA-C	10.96	128.19	114.37
1	I	142	GLY	CA-C-N	-10.96	109.57	122.83
1	I	142	GLY	C-N-CA	-10.96	109.57	122.83
1	M	142	GLY	CA-C-N	-10.96	109.57	122.83
1	M	142	GLY	C-N-CA	-10.96	109.57	122.83
1	G	142	GLY	CA-C-N	-10.95	109.58	122.83
1	G	142	GLY	C-N-CA	-10.95	109.58	122.83
1	K	142	GLY	CA-C-N	-10.95	109.58	122.83
1	K	142	GLY	C-N-CA	-10.95	109.58	122.83
2	J	34	GLY	N-CA-C	10.95	128.16	114.37
1	A	142	GLY	CA-C-N	-10.94	109.59	122.83
1	A	142	GLY	C-N-CA	-10.94	109.59	122.83
1	C	281	ALA	CA-C-N	-10.94	102.08	120.68
1	C	281	ALA	C-N-CA	-10.94	102.08	120.68
2	F	34	GLY	N-CA-C	10.94	128.15	114.37
1	O	142	GLY	CA-C-N	-10.93	109.60	122.83
1	O	142	GLY	C-N-CA	-10.93	109.60	122.83
1	E	142	GLY	CA-C-N	-10.93	109.60	122.83
1	E	142	GLY	C-N-CA	-10.93	109.60	122.83
2	H	34	GLY	N-CA-C	10.93	128.14	114.37
2	P	34	GLY	N-CA-C	10.93	128.14	114.37
2	B	34	GLY	N-CA-C	10.92	128.13	114.37
1	A	281	ALA	CA-C-N	-10.92	102.11	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ALA	C-N-CA	-10.92	102.11	120.68
2	D	34	GLY	N-CA-C	10.92	128.13	114.37
1	G	281	ALA	CA-C-N	-10.92	102.11	120.68
1	G	281	ALA	C-N-CA	-10.92	102.11	120.68
1	I	281	ALA	CA-C-N	-10.92	102.12	120.68
1	I	281	ALA	C-N-CA	-10.92	102.12	120.68
1	M	281	ALA	CA-C-N	-10.92	102.12	120.68
1	M	281	ALA	C-N-CA	-10.92	102.12	120.68
1	O	281	ALA	CA-C-N	-10.91	102.13	120.68
1	O	281	ALA	C-N-CA	-10.91	102.13	120.68
1	Q	281	ALA	CA-C-N	-10.91	102.13	120.68
1	Q	281	ALA	C-N-CA	-10.91	102.13	120.68
1	Q	142	GLY	CA-C-N	-10.91	109.63	122.83
1	Q	142	GLY	C-N-CA	-10.91	109.63	122.83
1	K	281	ALA	CA-C-N	-10.90	102.14	120.68
1	K	281	ALA	C-N-CA	-10.90	102.14	120.68
2	N	34	GLY	N-CA-C	10.90	128.11	114.37
1	E	281	ALA	CA-C-N	-10.89	102.17	120.68
1	E	281	ALA	C-N-CA	-10.89	102.17	120.68
2	R	34	GLY	N-CA-C	10.88	128.08	114.37
2	L	266	HIS	CA-CB-CG	-10.71	103.09	113.80
2	N	266	HIS	CA-CB-CG	-10.71	103.09	113.80
2	H	266	HIS	CA-CB-CG	-10.69	103.11	113.80
2	B	266	HIS	CA-CB-CG	-10.69	103.11	113.80
2	R	266	HIS	CA-CB-CG	-10.69	103.11	113.80
2	D	266	HIS	CA-CB-CG	-10.68	103.12	113.80
2	P	266	HIS	CA-CB-CG	-10.68	103.12	113.80
2	J	266	HIS	CA-CB-CG	-10.67	103.13	113.80
2	F	266	HIS	CA-CB-CG	-10.67	103.13	113.80
1	O	283	HIS	CA-C-N	-10.56	103.52	121.89
1	O	283	HIS	C-N-CA	-10.56	103.52	121.89
1	C	283	HIS	CA-C-N	-10.55	103.53	121.89
1	C	283	HIS	C-N-CA	-10.55	103.53	121.89
1	M	283	HIS	CA-C-N	-10.55	103.53	121.89
1	M	283	HIS	C-N-CA	-10.55	103.53	121.89
1	Q	283	HIS	CA-C-N	-10.54	103.54	121.89
1	Q	283	HIS	C-N-CA	-10.54	103.54	121.89
1	A	283	HIS	CA-C-N	-10.53	103.56	121.89
1	A	283	HIS	C-N-CA	-10.53	103.56	121.89
1	E	283	HIS	CA-C-N	-10.53	103.56	121.89
1	E	283	HIS	C-N-CA	-10.53	103.56	121.89
1	K	283	HIS	CA-C-N	-10.53	103.57	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	283	HIS	C-N-CA	-10.53	103.57	121.89
1	I	283	HIS	CA-C-N	-10.51	103.60	121.89
1	I	283	HIS	C-N-CA	-10.51	103.60	121.89
1	G	283	HIS	CA-C-N	-10.49	103.64	121.89
1	G	283	HIS	C-N-CA	-10.49	103.64	121.89
1	Q	308	ARG	N-CA-C	10.42	123.69	111.71
1	M	308	ARG	N-CA-C	10.41	123.68	111.71
1	E	308	ARG	N-CA-C	10.41	123.68	111.71
1	C	308	ARG	N-CA-C	10.40	123.67	111.71
1	A	308	ARG	N-CA-C	10.39	123.66	111.71
1	G	308	ARG	N-CA-C	10.39	123.66	111.71
1	I	308	ARG	N-CA-C	10.38	123.65	111.71
1	K	308	ARG	N-CA-C	10.37	123.63	111.71
1	O	308	ARG	N-CA-C	10.37	123.63	111.71
1	I	97	GLU	CA-C-N	10.26	141.13	121.54
1	I	97	GLU	C-N-CA	10.26	141.13	121.54
1	C	97	GLU	CA-C-N	10.24	141.11	121.54
1	C	97	GLU	C-N-CA	10.24	141.11	121.54
1	E	97	GLU	CA-C-N	10.24	141.11	121.54
1	E	97	GLU	C-N-CA	10.24	141.11	121.54
1	M	97	GLU	CA-C-N	10.24	141.11	121.54
1	M	97	GLU	C-N-CA	10.24	141.11	121.54
1	G	97	GLU	CA-C-N	10.23	141.08	121.54
1	G	97	GLU	C-N-CA	10.23	141.08	121.54
1	Q	97	GLU	CA-C-N	10.23	141.09	121.54
1	Q	97	GLU	C-N-CA	10.23	141.09	121.54
1	A	97	GLU	CA-C-N	10.23	141.08	121.54
1	A	97	GLU	C-N-CA	10.23	141.08	121.54
1	O	97	GLU	CA-C-N	10.22	141.06	121.54
1	O	97	GLU	C-N-CA	10.22	141.06	121.54
1	K	97	GLU	CA-C-N	10.21	141.05	121.54
1	K	97	GLU	C-N-CA	10.21	141.05	121.54
1	Q	67	PHE	CE1-CZ-CE2	10.18	138.33	120.00
1	A	67	PHE	CE1-CZ-CE2	10.17	138.31	120.00
1	C	67	PHE	CE1-CZ-CE2	10.17	138.31	120.00
1	M	67	PHE	CE1-CZ-CE2	10.17	138.30	120.00
1	E	67	PHE	CE1-CZ-CE2	10.16	138.29	120.00
1	G	67	PHE	CE1-CZ-CE2	10.16	138.29	120.00
1	O	67	PHE	CE1-CZ-CE2	10.14	138.26	120.00
1	I	265	GLY	CA-C-N	-10.14	107.74	122.44
1	I	265	GLY	C-N-CA	-10.14	107.74	122.44
1	K	67	PHE	CE1-CZ-CE2	10.13	138.24	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	67	PHE	CE1-CZ-CE2	10.12	138.23	120.00
1	A	265	GLY	CA-C-N	-10.12	107.77	122.44
1	A	265	GLY	C-N-CA	-10.12	107.77	122.44
1	C	265	GLY	CA-C-N	-10.12	107.77	122.44
1	C	265	GLY	C-N-CA	-10.12	107.77	122.44
1	G	265	GLY	CA-C-N	-10.12	107.77	122.44
1	G	265	GLY	C-N-CA	-10.12	107.77	122.44
1	K	265	GLY	CA-C-N	-10.12	107.77	122.44
1	K	265	GLY	C-N-CA	-10.12	107.77	122.44
1	Q	265	GLY	CA-C-N	-10.12	107.77	122.44
1	Q	265	GLY	C-N-CA	-10.12	107.77	122.44
1	M	265	GLY	CA-C-N	-10.11	107.77	122.44
1	M	265	GLY	C-N-CA	-10.11	107.77	122.44
1	E	265	GLY	CA-C-N	-10.11	107.78	122.44
1	E	265	GLY	C-N-CA	-10.11	107.78	122.44
1	O	265	GLY	CA-C-N	-10.10	107.79	122.44
1	O	265	GLY	C-N-CA	-10.10	107.79	122.44
2	N	28	HIS	CA-CB-CG	-10.10	103.70	113.80
2	D	28	HIS	CA-CB-CG	-10.09	103.71	113.80
2	F	28	HIS	CA-CB-CG	-10.09	103.71	113.80
2	J	28	HIS	CA-CB-CG	-10.09	103.71	113.80
2	B	28	HIS	CA-CB-CG	-10.07	103.73	113.80
2	P	28	HIS	CA-CB-CG	-10.06	103.74	113.80
2	R	28	HIS	CA-CB-CG	-10.06	103.74	113.80
1	O	339	ARG	N-CA-C	10.06	125.38	110.30
1	M	339	ARG	N-CA-C	10.05	125.38	110.30
1	E	339	ARG	N-CA-C	10.04	125.37	110.30
1	Q	339	ARG	N-CA-C	10.04	125.37	110.30
1	K	339	ARG	N-CA-C	10.04	125.36	110.30
1	G	339	ARG	N-CA-C	10.04	125.36	110.30
2	H	28	HIS	CA-CB-CG	-10.04	103.76	113.80
2	L	28	HIS	CA-CB-CG	-10.04	103.76	113.80
1	A	339	ARG	N-CA-C	10.03	125.34	110.30
1	I	339	ARG	N-CA-C	10.03	125.34	110.30
1	C	339	ARG	N-CA-C	10.02	125.33	110.30
1	K	346	TRP	CD2-CE3-CZ3	-9.73	105.96	118.60
1	M	346	TRP	CD2-CE3-CZ3	-9.72	105.96	118.60
1	C	346	TRP	CD2-CE3-CZ3	-9.71	105.98	118.60
1	I	346	TRP	CD2-CE3-CZ3	-9.71	105.98	118.60
1	E	346	TRP	CD2-CE3-CZ3	-9.70	105.99	118.60
1	A	346	TRP	CD2-CE3-CZ3	-9.69	106.01	118.60
1	Q	346	TRP	CD2-CE3-CZ3	-9.68	106.01	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	346	TRP	CD2-CE3-CZ3	-9.67	106.03	118.60
1	O	346	TRP	CD2-CE3-CZ3	-9.67	106.03	118.60
1	G	281	ALA	N-CA-C	9.53	124.17	113.21
1	I	281	ALA	N-CA-C	9.53	124.17	113.21
1	Q	281	ALA	N-CA-C	9.53	124.17	113.21
1	C	281	ALA	N-CA-C	9.52	124.16	113.21
1	A	281	ALA	N-CA-C	9.52	124.15	113.21
1	E	281	ALA	N-CA-C	9.51	124.14	113.21
1	K	281	ALA	N-CA-C	9.50	124.14	113.21
2	F	260	VAL	N-CA-C	9.50	117.76	107.60
2	H	260	VAL	N-CA-C	9.46	117.72	107.60
1	O	281	ALA	N-CA-C	9.46	124.09	113.21
2	N	260	VAL	N-CA-C	9.46	117.72	107.60
1	M	281	ALA	N-CA-C	9.46	124.08	113.21
2	P	260	VAL	N-CA-C	9.45	117.72	107.60
2	J	260	VAL	N-CA-C	9.45	117.71	107.60
2	B	260	VAL	N-CA-C	9.45	117.71	107.60
2	L	260	VAL	N-CA-C	9.42	117.68	107.60
2	R	260	VAL	N-CA-C	9.42	117.68	107.60
1	G	98	ASP	N-CA-CB	-9.41	94.58	110.49
1	Q	98	ASP	N-CA-CB	-9.41	94.59	110.49
1	C	98	ASP	N-CA-CB	-9.41	94.59	110.49
2	D	260	VAL	N-CA-C	9.41	117.66	107.60
1	M	98	ASP	N-CA-CB	-9.41	94.59	110.49
1	K	98	ASP	N-CA-CB	-9.40	94.60	110.49
1	A	98	ASP	N-CA-CB	-9.40	94.61	110.49
1	O	98	ASP	N-CA-CB	-9.39	94.62	110.49
1	E	98	ASP	N-CA-CB	-9.39	94.63	110.49
1	I	98	ASP	N-CA-CB	-9.38	94.63	110.49
2	N	437	ASP	CA-CB-CG	9.38	121.97	112.60
2	R	437	ASP	CA-CB-CG	9.37	121.97	112.60
2	L	437	ASP	CA-CB-CG	9.36	121.96	112.60
2	D	437	ASP	CA-CB-CG	9.35	121.95	112.60
2	J	437	ASP	CA-CB-CG	9.35	121.94	112.60
2	B	437	ASP	CA-CB-CG	9.34	121.94	112.60
2	P	437	ASP	CA-CB-CG	9.33	121.93	112.60
2	F	437	ASP	CA-CB-CG	9.32	121.92	112.60
2	H	437	ASP	CA-CB-CG	9.31	121.92	112.60
2	P	220	THR	N-CA-C	9.16	124.90	112.90
2	L	220	THR	N-CA-C	9.15	124.89	112.90
2	H	220	THR	N-CA-C	9.15	124.89	112.90
2	B	220	THR	N-CA-C	9.15	124.88	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	220	THR	N-CA-C	9.15	124.88	112.90
2	J	220	THR	N-CA-C	9.14	124.88	112.90
2	D	220	THR	N-CA-C	9.13	124.86	112.90
2	F	220	THR	N-CA-C	9.13	124.86	112.90
2	R	220	THR	N-CA-C	9.10	124.82	112.90
1	K	339	ARG	CA-C-O	9.06	130.59	120.80
1	C	309	HIS	CA-C-N	-9.03	113.00	122.30
1	C	309	HIS	C-N-CA	-9.03	113.00	122.30
1	G	339	ARG	CA-C-O	9.02	130.55	120.80
1	E	339	ARG	CA-C-O	9.02	130.54	120.80
1	K	100	ALA	N-CA-C	9.02	123.81	111.54
1	A	339	ARG	CA-C-O	9.02	130.54	120.80
1	E	100	ALA	N-CA-C	9.01	123.80	111.54
1	Q	309	HIS	CA-C-N	-9.01	113.02	122.30
1	Q	309	HIS	C-N-CA	-9.01	113.02	122.30
1	A	100	ALA	N-CA-C	9.01	123.79	111.54
1	C	100	ALA	N-CA-C	9.01	123.79	111.54
1	I	100	ALA	N-CA-C	9.01	123.79	111.54
1	I	309	HIS	CA-C-N	-9.01	113.03	122.30
1	I	309	HIS	C-N-CA	-9.01	113.03	122.30
1	K	309	HIS	CA-C-N	-9.01	113.03	122.30
1	K	309	HIS	C-N-CA	-9.01	113.03	122.30
1	O	339	ARG	CA-C-O	9.01	130.53	120.80
1	M	100	ALA	N-CA-C	9.00	123.78	111.54
1	Q	100	ALA	N-CA-C	9.00	123.78	111.54
1	O	100	ALA	N-CA-C	9.00	123.78	111.54
1	C	339	ARG	CA-C-O	9.00	130.52	120.80
1	M	309	HIS	CA-C-N	-9.00	113.03	122.30
1	M	309	HIS	C-N-CA	-9.00	113.03	122.30
1	I	339	ARG	CA-C-O	8.99	130.51	120.80
1	M	339	ARG	CA-C-O	8.99	130.51	120.80
1	A	309	HIS	CA-C-N	-8.99	113.04	122.30
1	A	309	HIS	C-N-CA	-8.99	113.04	122.30
1	G	309	HIS	CA-C-N	-8.99	113.04	122.30
1	G	309	HIS	C-N-CA	-8.99	113.04	122.30
1	G	100	ALA	N-CA-C	8.98	123.75	111.54
1	O	308	ARG	CA-C-N	-8.98	108.59	122.60
1	O	308	ARG	C-N-CA	-8.98	108.59	122.60
1	K	308	ARG	CA-C-N	-8.98	108.59	122.60
1	K	308	ARG	C-N-CA	-8.98	108.59	122.60
1	E	309	HIS	CA-C-N	-8.97	113.06	122.30
1	E	309	HIS	C-N-CA	-8.97	113.06	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	308	ARG	CA-C-N	-8.97	108.61	122.60
1	E	308	ARG	C-N-CA	-8.97	108.61	122.60
1	Q	339	ARG	CA-C-O	8.97	130.49	120.80
1	O	309	HIS	CA-C-N	-8.96	113.07	122.30
1	O	309	HIS	C-N-CA	-8.96	113.07	122.30
2	F	220	THR	CA-C-N	-8.96	111.40	122.42
2	F	220	THR	C-N-CA	-8.96	111.40	122.42
1	C	308	ARG	CA-C-N	-8.96	108.63	122.60
1	C	308	ARG	C-N-CA	-8.96	108.63	122.60
1	Q	308	ARG	CA-C-N	-8.96	108.63	122.60
1	Q	308	ARG	C-N-CA	-8.96	108.63	122.60
1	A	308	ARG	CA-C-N	-8.95	108.64	122.60
1	A	308	ARG	C-N-CA	-8.95	108.64	122.60
1	K	347	CYS	CA-C-N	-8.95	108.66	119.84
1	K	347	CYS	C-N-CA	-8.95	108.66	119.84
1	G	308	ARG	CA-C-N	-8.94	108.65	122.60
1	G	308	ARG	C-N-CA	-8.94	108.65	122.60
1	I	347	CYS	CA-C-N	-8.94	108.66	119.84
1	I	347	CYS	C-N-CA	-8.94	108.66	119.84
1	C	141	PHE	CA-CB-CG	8.94	122.74	113.80
2	L	220	THR	CA-C-N	-8.93	111.43	122.42
2	L	220	THR	C-N-CA	-8.93	111.43	122.42
1	M	308	ARG	CA-C-N	-8.93	108.67	122.60
1	M	308	ARG	C-N-CA	-8.93	108.67	122.60
1	Q	347	CYS	CA-C-N	-8.93	108.67	119.84
1	Q	347	CYS	C-N-CA	-8.93	108.67	119.84
1	C	347	CYS	CA-C-N	-8.93	108.68	119.84
1	C	347	CYS	C-N-CA	-8.93	108.68	119.84
1	I	308	ARG	CA-C-N	-8.93	108.67	122.60
1	I	308	ARG	C-N-CA	-8.93	108.67	122.60
1	G	347	CYS	CA-C-N	-8.93	108.68	119.84
1	G	347	CYS	C-N-CA	-8.93	108.68	119.84
1	G	141	PHE	CA-CB-CG	8.93	122.73	113.80
2	H	220	THR	CA-C-N	-8.92	111.45	122.42
2	H	220	THR	C-N-CA	-8.92	111.45	122.42
1	A	347	CYS	CA-C-N	-8.92	108.69	119.84
1	A	347	CYS	C-N-CA	-8.92	108.69	119.84
1	O	347	CYS	CA-C-N	-8.91	108.70	119.84
1	O	347	CYS	C-N-CA	-8.91	108.70	119.84
2	J	220	THR	CA-C-N	-8.91	111.46	122.42
2	J	220	THR	C-N-CA	-8.91	111.46	122.42
2	B	220	THR	CA-C-N	-8.90	111.47	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	220	THR	C-N-CA	-8.90	111.47	122.42
1	M	347	CYS	CA-C-N	-8.90	108.71	119.84
1	M	347	CYS	C-N-CA	-8.90	108.71	119.84
2	R	220	THR	CA-C-N	-8.90	111.47	122.42
2	R	220	THR	C-N-CA	-8.90	111.47	122.42
1	M	141	PHE	CA-CB-CG	8.90	122.70	113.80
1	A	141	PHE	CA-CB-CG	8.89	122.69	113.80
1	E	141	PHE	CA-CB-CG	8.89	122.69	113.80
1	Q	141	PHE	CA-CB-CG	8.89	122.69	113.80
2	D	220	THR	CA-C-N	-8.88	111.49	122.42
2	D	220	THR	C-N-CA	-8.88	111.49	122.42
2	D	320	ARG	NH1-CZ-NH2	-8.88	107.75	119.30
2	N	220	THR	CA-C-N	-8.88	111.50	122.42
2	N	220	THR	C-N-CA	-8.88	111.50	122.42
1	E	347	CYS	CA-C-N	-8.88	108.75	119.84
1	E	347	CYS	C-N-CA	-8.88	108.75	119.84
2	P	220	THR	CA-C-N	-8.88	111.50	122.42
2	P	220	THR	C-N-CA	-8.88	111.50	122.42
1	K	141	PHE	CA-CB-CG	8.87	122.67	113.80
1	O	141	PHE	CA-CB-CG	8.86	122.66	113.80
2	B	320	ARG	NH1-CZ-NH2	-8.85	107.80	119.30
1	I	141	PHE	CA-CB-CG	8.85	122.65	113.80
2	N	320	ARG	NH1-CZ-NH2	-8.85	107.80	119.30
2	H	320	ARG	NH1-CZ-NH2	-8.85	107.80	119.30
2	J	320	ARG	NH1-CZ-NH2	-8.85	107.80	119.30
2	R	320	ARG	NH1-CZ-NH2	-8.85	107.80	119.30
2	P	320	ARG	NH1-CZ-NH2	-8.84	107.81	119.30
2	F	320	ARG	NH1-CZ-NH2	-8.83	107.82	119.30
2	L	320	ARG	NH1-CZ-NH2	-8.82	107.83	119.30
1	O	273	ALA	CA-C-O	-8.78	108.13	120.16
1	I	273	ALA	CA-C-O	-8.76	108.16	120.16
1	A	273	ALA	CA-C-O	-8.75	108.17	120.16
1	E	273	ALA	CA-C-O	-8.75	108.17	120.16
1	M	273	ALA	CA-C-O	-8.75	108.18	120.16
1	K	273	ALA	CA-C-O	-8.74	108.18	120.16
1	C	273	ALA	CA-C-O	-8.74	108.19	120.16
1	G	273	ALA	CA-C-O	-8.74	108.19	120.16
1	Q	273	ALA	CA-C-O	-8.73	108.20	120.16
2	P	436	GLN	N-CA-C	8.61	120.67	111.28
2	L	436	GLN	N-CA-C	8.58	120.63	111.28
2	B	436	GLN	N-CA-C	8.57	120.62	111.28
2	H	436	GLN	N-CA-C	8.57	120.62	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	436	GLN	N-CA-C	8.56	120.61	111.28
2	N	436	GLN	N-CA-C	8.55	120.60	111.28
2	F	436	GLN	N-CA-C	8.54	120.59	111.28
2	R	436	GLN	N-CA-C	8.54	120.59	111.28
2	D	436	GLN	N-CA-C	8.53	120.57	111.28
1	Q	276	ILE	N-CA-C	8.47	120.03	108.17
1	E	276	ILE	N-CA-C	8.45	120.05	107.80
1	C	276	ILE	N-CA-C	8.44	120.04	107.80
1	O	276	ILE	N-CA-C	8.44	120.03	107.80
1	K	276	ILE	N-CA-C	8.44	120.03	107.80
1	G	276	ILE	N-CA-C	8.43	120.02	107.80
1	M	276	ILE	N-CA-C	8.43	120.02	107.80
1	A	276	ILE	N-CA-C	8.43	120.02	107.80
2	D	355	VAL	N-CA-C	8.41	120.27	107.99
1	I	276	ILE	N-CA-C	8.41	119.99	107.80
2	H	355	VAL	N-CA-C	8.41	120.26	107.99
2	L	355	VAL	N-CA-C	8.40	120.25	107.99
2	R	355	VAL	N-CA-C	8.40	120.25	107.99
2	N	355	VAL	N-CA-C	8.39	120.24	107.99
2	J	355	VAL	N-CA-C	8.39	120.24	107.99
2	F	99	ALA	CA-C-N	-8.38	106.75	121.00
2	F	99	ALA	C-N-CA	-8.38	106.75	121.00
2	B	355	VAL	N-CA-C	8.38	120.22	107.99
2	J	99	ALA	CA-C-N	-8.37	106.77	121.00
2	J	99	ALA	C-N-CA	-8.37	106.77	121.00
2	P	355	VAL	N-CA-C	8.37	120.21	107.99
2	F	355	VAL	N-CA-C	8.36	120.20	107.99
2	L	99	ALA	CA-C-N	-8.36	106.78	121.00
2	L	99	ALA	C-N-CA	-8.36	106.78	121.00
2	R	99	ALA	CA-C-N	-8.36	106.79	121.00
2	R	99	ALA	C-N-CA	-8.36	106.79	121.00
2	J	228	ASN	CA-CB-CG	-8.28	104.32	112.60
2	D	228	ASN	CA-CB-CG	-8.28	104.32	112.60
2	P	228	ASN	CA-CB-CG	-8.27	104.33	112.60
2	R	228	ASN	CA-CB-CG	-8.27	104.33	112.60
2	B	228	ASN	CA-CB-CG	-8.26	104.34	112.60
2	H	228	ASN	CA-CB-CG	-8.26	104.34	112.60
1	E	49	PHE	CA-CB-CG	-8.26	105.54	113.80
2	L	228	ASN	CA-CB-CG	-8.25	104.35	112.60
2	F	228	ASN	CA-CB-CG	-8.24	104.36	112.60
1	G	49	PHE	CA-CB-CG	-8.24	105.56	113.80
1	C	49	PHE	CA-CB-CG	-8.24	105.56	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	228	ASN	CA-CB-CG	-8.24	104.36	112.60
1	I	49	PHE	CA-CB-CG	-8.24	105.56	113.80
1	A	49	PHE	CA-CB-CG	-8.23	105.57	113.80
1	M	49	PHE	CA-CB-CG	-8.23	105.57	113.80
1	Q	284	GLU	CA-C-N	-8.23	109.33	121.76
1	Q	284	GLU	C-N-CA	-8.23	109.33	121.76
1	O	49	PHE	CA-CB-CG	-8.22	105.58	113.80
1	Q	49	PHE	CA-CB-CG	-8.22	105.58	113.80
1	I	284	GLU	CA-C-N	-8.21	109.37	121.76
1	I	284	GLU	C-N-CA	-8.21	109.37	121.76
1	A	284	GLU	CA-C-N	-8.20	109.38	121.76
1	A	284	GLU	C-N-CA	-8.20	109.38	121.76
1	K	284	GLU	CA-C-N	-8.20	109.38	121.76
1	K	284	GLU	C-N-CA	-8.20	109.38	121.76
1	O	284	GLU	CA-C-N	-8.20	109.38	121.76
1	O	284	GLU	C-N-CA	-8.20	109.38	121.76
1	K	49	PHE	CA-CB-CG	-8.20	105.60	113.80
1	G	284	GLU	CA-C-N	-8.20	109.38	121.76
1	G	284	GLU	C-N-CA	-8.20	109.38	121.76
1	E	284	GLU	CA-C-N	-8.19	109.39	121.76
1	E	284	GLU	C-N-CA	-8.19	109.39	121.76
1	C	284	GLU	CA-C-N	-8.18	109.40	121.76
1	C	284	GLU	C-N-CA	-8.18	109.40	121.76
1	M	284	GLU	CA-C-N	-8.18	109.40	121.76
1	M	284	GLU	C-N-CA	-8.18	109.40	121.76
1	I	109	THR	N-CA-C	8.16	121.21	111.33
1	E	109	THR	N-CA-C	8.16	121.20	111.33
1	A	109	THR	N-CA-C	8.15	121.20	111.33
1	O	109	THR	N-CA-C	8.15	121.19	111.33
1	C	109	THR	N-CA-C	8.14	121.18	111.33
1	M	109	THR	N-CA-C	8.14	121.17	111.33
1	Q	109	THR	N-CA-C	8.13	121.17	111.33
1	K	109	THR	N-CA-C	8.13	121.17	111.33
1	G	109	THR	N-CA-C	8.10	121.12	111.33
1	K	348	PRO	CA-C-N	-8.08	106.70	122.62
1	K	348	PRO	C-N-CA	-8.08	106.70	122.62
1	G	348	PRO	CA-C-N	-8.08	106.71	122.62
1	G	348	PRO	C-N-CA	-8.08	106.71	122.62
1	I	348	PRO	CA-N-CD	8.07	123.30	112.00
1	Q	348	PRO	CA-C-N	-8.07	106.72	122.62
1	Q	348	PRO	C-N-CA	-8.07	106.72	122.62
1	A	348	PRO	CA-C-N	-8.07	106.73	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	PRO	C-N-CA	-8.07	106.73	122.62
1	E	348	PRO	CA-C-N	-8.07	106.72	122.62
1	E	348	PRO	C-N-CA	-8.07	106.72	122.62
1	Q	348	PRO	CA-N-CD	8.07	123.29	112.00
1	M	348	PRO	CA-C-N	-8.06	106.73	122.62
1	M	348	PRO	C-N-CA	-8.06	106.73	122.62
1	A	348	PRO	CA-N-CD	8.06	123.28	112.00
1	M	348	PRO	CA-N-CD	8.06	123.29	112.00
1	C	348	PRO	CA-C-N	-8.06	106.75	122.62
1	C	348	PRO	C-N-CA	-8.06	106.75	122.62
1	G	348	PRO	CA-N-CD	8.06	123.28	112.00
1	O	348	PRO	CA-C-N	-8.06	106.75	122.62
1	C	348	PRO	CA-N-CD	8.05	123.28	112.00
1	K	348	PRO	CA-N-CD	8.05	123.28	112.00
1	O	348	PRO	C-N-CA	-8.06	106.75	122.62
1	I	348	PRO	CA-C-N	-8.05	106.76	122.62
1	I	348	PRO	C-N-CA	-8.05	106.76	122.62
1	O	348	PRO	CA-N-CD	8.05	123.27	112.00
1	E	348	PRO	CA-N-CD	8.03	123.25	112.00
2	N	164	ARG	NE-CZ-NH2	8.01	126.41	119.20
1	K	192	HIS	CA-CB-CG	-8.01	105.79	113.80
1	Q	192	HIS	CA-CB-CG	-8.01	105.79	113.80
1	A	192	HIS	CA-CB-CG	-8.00	105.80	113.80
1	O	192	HIS	CA-CB-CG	-8.00	105.80	113.80
2	P	164	ARG	NE-CZ-NH2	7.99	126.39	119.20
1	E	192	HIS	CA-CB-CG	-7.98	105.82	113.80
2	F	164	ARG	NE-CZ-NH2	7.98	126.38	119.20
1	I	192	HIS	CA-CB-CG	-7.98	105.82	113.80
1	G	192	HIS	CA-CB-CG	-7.97	105.83	113.80
1	M	192	HIS	CA-CB-CG	-7.97	105.83	113.80
2	B	164	ARG	NE-CZ-NH2	7.96	126.37	119.20
2	J	164	ARG	NE-CZ-NH2	7.96	126.37	119.20
2	L	164	ARG	NE-CZ-NH2	7.95	126.36	119.20
1	C	192	HIS	CA-CB-CG	-7.95	105.85	113.80
2	D	164	ARG	NE-CZ-NH2	7.95	126.35	119.20
2	R	164	ARG	NE-CZ-NH2	7.95	126.35	119.20
1	K	98	ASP	N-CA-C	7.94	127.71	110.80
1	Q	98	ASP	N-CA-C	7.94	127.71	110.80
1	O	98	ASP	N-CA-C	7.93	127.70	110.80
2	H	164	ARG	NE-CZ-NH2	7.92	126.33	119.20
1	A	98	ASP	N-CA-C	7.92	127.67	110.80
1	E	98	ASP	N-CA-C	7.92	127.66	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	98	ASP	N-CA-C	7.91	127.66	110.80
1	G	98	ASP	N-CA-C	7.91	127.65	110.80
1	M	98	ASP	N-CA-C	7.91	127.64	110.80
1	I	98	ASP	N-CA-C	7.90	127.62	110.80
1	I	346	TRP	CE3-CZ3-CH2	7.89	131.36	121.10
1	C	346	TRP	CE3-CZ3-CH2	7.87	131.33	121.10
1	K	346	TRP	CE3-CZ3-CH2	7.86	131.32	121.10
1	M	346	TRP	CE3-CZ3-CH2	7.86	131.32	121.10
1	E	346	TRP	CE3-CZ3-CH2	7.85	131.30	121.10
2	F	47	GLU	N-CA-C	7.84	120.73	111.71
2	P	259	MET	N-CA-C	7.84	122.61	112.89
1	A	346	TRP	CE3-CZ3-CH2	7.84	131.29	121.10
2	N	47	GLU	N-CA-C	7.83	120.72	111.71
1	Q	346	TRP	CE3-CZ3-CH2	7.83	131.28	121.10
1	O	346	TRP	CE3-CZ3-CH2	7.82	131.27	121.10
2	R	259	MET	N-CA-C	7.82	122.59	112.89
1	G	346	TRP	CE3-CZ3-CH2	7.81	131.25	121.10
2	P	47	GLU	N-CA-C	7.81	120.69	111.71
2	H	47	GLU	N-CA-C	7.80	120.68	111.71
2	B	47	GLU	N-CA-C	7.80	120.68	111.71
2	B	259	MET	N-CA-C	7.80	122.56	112.89
1	I	274	PRO	N-CD-CG	7.80	114.90	103.20
2	F	259	MET	N-CA-C	7.80	122.56	112.89
2	R	47	GLU	N-CA-C	7.80	120.68	111.71
2	D	47	GLU	N-CA-C	7.79	120.67	111.71
1	E	274	PRO	N-CD-CG	7.79	114.89	103.20
1	K	274	PRO	N-CD-CG	7.79	114.88	103.20
2	L	47	GLU	N-CA-C	7.79	120.66	111.71
2	L	259	MET	N-CA-C	7.79	122.54	112.89
2	D	259	MET	N-CA-C	7.78	122.54	112.89
1	G	274	PRO	N-CD-CG	7.78	114.88	103.20
2	J	47	GLU	N-CA-C	7.77	120.65	111.71
2	J	259	MET	N-CA-C	7.77	122.53	112.89
1	A	274	PRO	N-CD-CG	7.77	114.86	103.20
2	N	259	MET	N-CA-C	7.77	122.52	112.89
1	C	274	PRO	N-CD-CG	7.77	114.85	103.20
1	O	274	PRO	N-CD-CG	7.77	114.85	103.20
1	M	274	PRO	N-CD-CG	7.77	114.85	103.20
1	Q	274	PRO	N-CD-CG	7.76	114.84	103.20
2	H	259	MET	N-CA-C	7.75	122.50	112.89
1	E	363	VAL	N-CA-C	7.48	115.31	107.76
2	N	99	ALA	CA-C-N	-7.47	106.76	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	99	ALA	C-N-CA	-7.47	106.76	121.41
2	P	99	ALA	CA-C-N	-7.47	106.76	121.41
2	P	99	ALA	C-N-CA	-7.47	106.76	121.41
1	O	363	VAL	N-CA-C	7.46	115.30	107.76
2	D	99	ALA	CA-C-N	-7.46	106.79	121.41
2	D	99	ALA	C-N-CA	-7.46	106.79	121.41
2	B	99	ALA	CA-C-N	-7.46	106.79	121.41
2	B	99	ALA	C-N-CA	-7.46	106.79	121.41
1	K	363	VAL	N-CA-C	7.46	115.29	107.76
2	H	99	ALA	CA-C-N	-7.46	106.80	121.41
2	H	99	ALA	C-N-CA	-7.46	106.80	121.41
1	C	358	GLU	CA-C-N	7.45	125.10	119.66
1	C	358	GLU	C-N-CA	7.45	125.10	119.66
1	O	283	HIS	O-C-N	7.45	132.70	123.01
1	Q	363	VAL	N-CA-C	7.45	115.29	107.76
1	M	358	GLU	CA-C-N	7.45	125.10	119.66
1	M	358	GLU	C-N-CA	7.45	125.10	119.66
1	A	363	VAL	N-CA-C	7.44	115.27	107.76
1	C	363	VAL	N-CA-C	7.43	115.27	107.76
1	I	363	VAL	N-CA-C	7.42	115.26	107.76
1	Q	283	HIS	O-C-N	7.42	132.66	123.01
1	C	283	HIS	O-C-N	7.42	132.65	123.01
1	E	358	GLU	CA-C-N	7.41	125.07	119.66
1	E	358	GLU	C-N-CA	7.41	125.07	119.66
1	K	349	THR	CA-C-N	-7.40	106.90	121.41
1	K	349	THR	C-N-CA	-7.40	106.90	121.41
1	Q	349	THR	CA-C-N	-7.40	106.90	121.41
1	Q	349	THR	C-N-CA	-7.40	106.90	121.41
1	A	358	GLU	CA-C-N	7.40	125.06	119.66
1	A	358	GLU	C-N-CA	7.40	125.06	119.66
1	M	283	HIS	O-C-N	7.40	132.63	123.01
1	M	363	VAL	N-CA-C	7.40	115.23	107.76
1	G	363	VAL	N-CA-C	7.40	115.23	107.76
1	A	283	HIS	O-C-N	7.39	132.62	123.01
1	A	349	THR	CA-C-N	-7.39	106.93	121.41
1	A	349	THR	C-N-CA	-7.39	106.93	121.41
1	I	358	GLU	CA-C-N	7.39	125.05	119.66
1	I	358	GLU	C-N-CA	7.39	125.05	119.66
1	K	283	HIS	O-C-N	7.39	132.62	123.01
1	G	349	THR	CA-C-N	-7.39	106.93	121.41
1	G	349	THR	C-N-CA	-7.39	106.93	121.41
1	O	358	GLU	CA-C-N	7.39	125.05	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	358	GLU	C-N-CA	7.39	125.05	119.66
1	Q	358	GLU	CA-C-N	7.39	125.05	119.66
1	Q	358	GLU	C-N-CA	7.39	125.05	119.66
1	M	349	THR	CA-C-N	-7.38	106.94	121.41
1	M	349	THR	C-N-CA	-7.38	106.94	121.41
1	C	349	THR	CA-C-N	-7.38	106.94	121.41
1	C	349	THR	C-N-CA	-7.38	106.94	121.41
1	E	283	HIS	O-C-N	7.38	132.60	123.01
1	I	349	THR	CA-C-N	-7.38	106.94	121.41
1	I	349	THR	C-N-CA	-7.38	106.94	121.41
1	O	349	THR	CA-C-N	-7.38	106.94	121.41
1	O	349	THR	C-N-CA	-7.38	106.94	121.41
1	E	349	THR	CA-C-N	-7.36	106.98	121.41
1	E	349	THR	C-N-CA	-7.36	106.98	121.41
1	I	283	HIS	O-C-N	7.36	132.57	123.01
1	G	358	GLU	CA-C-N	7.35	125.02	119.66
1	G	358	GLU	C-N-CA	7.35	125.02	119.66
1	K	358	GLU	CA-C-N	7.34	125.02	119.66
1	K	358	GLU	C-N-CA	7.34	125.02	119.66
1	G	283	HIS	O-C-N	7.34	132.55	123.01
1	K	266	HIS	CB-CA-C	-7.29	99.98	110.62
1	M	266	HIS	CB-CA-C	-7.27	100.00	110.62
2	H	273	ALA	N-CA-C	7.27	125.88	109.81
1	I	82	THR	N-CA-C	-7.27	100.74	110.55
2	J	273	ALA	N-CA-C	7.27	125.88	109.81
2	F	273	ALA	N-CA-C	7.27	125.87	109.81
2	L	273	ALA	N-CA-C	7.27	125.87	109.81
1	M	82	THR	N-CA-C	-7.27	100.74	110.55
1	C	266	HIS	CB-CA-C	-7.27	100.01	110.62
2	B	273	ALA	N-CA-C	7.26	125.85	109.81
1	A	266	HIS	CB-CA-C	-7.26	100.03	110.62
1	E	82	THR	N-CA-C	-7.26	100.75	110.55
1	I	266	HIS	CB-CA-C	-7.26	100.03	110.62
2	P	273	ALA	N-CA-C	7.25	125.84	109.81
2	R	273	ALA	N-CA-C	7.25	125.84	109.81
1	G	266	HIS	CB-CA-C	-7.25	100.04	110.62
2	N	273	ALA	N-CA-C	7.25	125.82	109.81
1	A	82	THR	N-CA-C	-7.25	100.77	110.55
1	E	266	HIS	CB-CA-C	-7.24	100.05	110.62
1	G	82	THR	N-CA-C	-7.24	100.77	110.55
2	D	273	ALA	N-CA-C	7.24	125.81	109.81
1	O	82	THR	N-CA-C	-7.24	100.77	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	THR	N-CA-C	-7.24	100.78	110.55
1	Q	266	HIS	CB-CA-C	-7.23	100.06	110.62
1	Q	82	THR	N-CA-C	-7.23	100.78	110.55
1	K	82	THR	N-CA-C	-7.23	100.80	110.55
1	O	266	HIS	CB-CA-C	-7.22	100.08	110.62
2	D	339	ASN	N-CA-C	7.12	119.30	109.54
2	F	339	ASN	N-CA-C	7.11	119.28	109.54
2	L	339	ASN	N-CA-C	7.10	119.27	109.54
1	M	274	PRO	N-CA-CB	7.10	110.71	103.25
1	C	274	PRO	N-CA-CB	7.09	110.70	103.25
2	J	339	ASN	N-CA-C	7.09	119.25	109.54
1	K	36	MET	CA-C-O	7.09	129.88	120.16
2	B	339	ASN	N-CA-C	7.09	119.25	109.54
1	O	36	MET	CA-C-O	7.09	129.87	120.16
2	R	339	ASN	N-CA-C	7.09	119.25	109.54
1	C	36	MET	CA-C-O	7.08	129.86	120.16
1	O	274	PRO	N-CA-CB	7.08	110.69	103.25
2	P	339	ASN	N-CA-C	7.08	119.24	109.54
2	N	339	ASN	N-CA-C	7.08	119.24	109.54
1	E	274	PRO	N-CA-CB	7.08	110.68	103.25
1	A	274	PRO	N-CA-CB	7.08	110.68	103.25
1	G	274	PRO	N-CA-CB	7.08	110.68	103.25
1	Q	274	PRO	N-CA-CB	7.08	110.68	103.25
2	H	339	ASN	N-CA-C	7.07	119.23	109.54
1	A	36	MET	CA-C-O	7.07	129.84	120.16
1	K	274	PRO	N-CA-CB	7.07	110.67	103.25
1	Q	36	MET	CA-C-O	7.07	129.84	120.16
1	M	36	MET	CA-C-O	7.06	129.84	120.16
2	D	64	ARG	NE-CZ-NH2	7.06	125.56	119.20
2	J	64	ARG	NE-CZ-NH2	7.06	125.55	119.20
1	I	36	MET	CA-C-O	7.05	129.82	120.16
2	P	64	ARG	NE-CZ-NH2	7.05	125.54	119.20
1	E	36	MET	CA-C-O	7.04	129.81	120.16
1	I	274	PRO	N-CA-CB	7.04	110.65	103.25
1	G	36	MET	CA-C-O	7.04	129.80	120.16
2	B	64	ARG	NE-CZ-NH2	7.04	125.53	119.20
2	F	64	ARG	NE-CZ-NH2	7.02	125.52	119.20
2	H	64	ARG	NE-CZ-NH2	7.02	125.52	119.20
2	N	64	ARG	NE-CZ-NH2	7.01	125.51	119.20
2	R	64	ARG	NE-CZ-NH2	7.01	125.51	119.20
2	L	64	ARG	NE-CZ-NH2	6.99	125.50	119.20
2	D	320	ARG	NE-CZ-NH1	6.98	128.48	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	59	ASN	CA-C-N	-6.97	112.49	122.94
2	D	59	ASN	C-N-CA	-6.97	112.49	122.94
2	N	320	ARG	NE-CZ-NH1	6.96	128.46	121.50
1	Q	221	ARG	NE-CZ-NH2	-6.95	112.94	119.20
1	E	221	ARG	NE-CZ-NH2	-6.95	112.95	119.20
1	G	221	ARG	NE-CZ-NH2	-6.95	112.95	119.20
1	I	221	ARG	NE-CZ-NH2	-6.95	112.95	119.20
2	J	320	ARG	NE-CZ-NH1	6.95	128.45	121.50
2	N	59	ASN	CA-C-N	-6.95	112.52	122.94
2	N	59	ASN	C-N-CA	-6.95	112.52	122.94
2	R	68	VAL	N-CA-C	6.95	117.87	107.80
1	K	221	ARG	NE-CZ-NH2	-6.94	112.95	119.20
2	P	68	VAL	N-CA-C	6.94	117.87	107.80
2	R	59	ASN	CA-C-N	-6.94	112.53	122.94
2	R	59	ASN	C-N-CA	-6.94	112.53	122.94
2	B	59	ASN	CA-C-N	-6.94	112.53	122.94
2	B	59	ASN	C-N-CA	-6.94	112.53	122.94
2	H	59	ASN	CA-C-N	-6.94	112.53	122.94
2	H	59	ASN	C-N-CA	-6.94	112.53	122.94
2	B	320	ARG	NE-CZ-NH1	6.94	128.44	121.50
2	L	68	VAL	N-CA-C	6.94	117.86	107.80
2	N	68	VAL	N-CA-C	6.94	117.86	107.80
2	F	68	VAL	N-CA-C	6.94	117.86	107.80
2	H	320	ARG	NE-CZ-NH1	6.94	128.44	121.50
2	L	59	ASN	CA-C-N	-6.94	112.53	122.94
2	L	59	ASN	C-N-CA	-6.94	112.53	122.94
2	P	320	ARG	NE-CZ-NH1	6.94	128.44	121.50
1	C	206	ASN	CA-CB-CG	-6.93	105.67	112.60
2	L	320	ARG	NE-CZ-NH1	6.93	128.43	121.50
2	D	68	VAL	N-CA-C	6.93	117.84	107.80
1	I	206	ASN	CA-CB-CG	-6.93	105.67	112.60
1	A	221	ARG	NE-CZ-NH2	-6.92	112.97	119.20
2	B	68	VAL	N-CA-C	6.92	117.84	107.80
2	F	48	ARG	NE-CZ-NH2	6.92	125.43	119.20
2	J	59	ASN	CA-C-N	-6.92	112.56	122.94
2	J	59	ASN	C-N-CA	-6.92	112.56	122.94
2	H	68	VAL	N-CA-C	6.92	117.83	107.80
2	J	68	VAL	N-CA-C	6.92	117.83	107.80
2	L	34	GLY	CA-C-N	-6.92	110.15	122.74
2	L	34	GLY	C-N-CA	-6.92	110.15	122.74
1	M	221	ARG	NE-CZ-NH2	-6.92	112.97	119.20
2	F	34	GLY	CA-C-N	-6.92	110.16	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	34	GLY	C-N-CA	-6.92	110.16	122.74
2	F	59	ASN	CA-C-N	-6.91	112.57	122.94
2	F	59	ASN	C-N-CA	-6.91	112.57	122.94
2	P	59	ASN	CA-C-N	-6.91	112.57	122.94
2	P	59	ASN	C-N-CA	-6.91	112.57	122.94
2	R	320	ARG	NE-CZ-NH1	6.91	128.41	121.50
1	O	221	ARG	NE-CZ-NH2	-6.90	112.99	119.20
2	B	34	GLY	CA-C-N	-6.90	110.18	122.74
2	B	34	GLY	C-N-CA	-6.90	110.18	122.74
2	J	34	GLY	CA-C-N	-6.90	110.18	122.74
2	J	34	GLY	C-N-CA	-6.90	110.18	122.74
2	D	34	GLY	CA-C-N	-6.90	110.19	122.74
2	D	34	GLY	C-N-CA	-6.90	110.19	122.74
2	F	320	ARG	NE-CZ-NH1	6.90	128.40	121.50
2	H	34	GLY	CA-C-N	-6.90	110.19	122.74
2	H	34	GLY	C-N-CA	-6.90	110.19	122.74
2	N	48	ARG	NE-CZ-NH2	6.90	125.41	119.20
2	B	48	ARG	NE-CZ-NH2	6.89	125.40	119.20
1	O	206	ASN	CA-CB-CG	-6.89	105.71	112.60
2	R	34	GLY	CA-C-N	-6.89	110.19	122.74
2	R	34	GLY	C-N-CA	-6.89	110.19	122.74
1	M	206	ASN	CA-CB-CG	-6.89	105.71	112.60
1	A	206	ASN	CA-CB-CG	-6.89	105.71	112.60
1	E	206	ASN	CA-CB-CG	-6.89	105.71	112.60
2	P	48	ARG	NE-CZ-NH2	6.89	125.40	119.20
1	G	206	ASN	CA-CB-CG	-6.89	105.71	112.60
1	Q	206	ASN	CA-CB-CG	-6.89	105.71	112.60
2	D	48	ARG	NE-CZ-NH2	6.88	125.40	119.20
1	K	206	ASN	CA-CB-CG	-6.88	105.72	112.60
2	N	34	GLY	CA-C-N	-6.88	110.21	122.74
2	N	34	GLY	C-N-CA	-6.88	110.21	122.74
1	C	221	ARG	NE-CZ-NH2	-6.88	113.00	119.20
2	J	48	ARG	NE-CZ-NH2	6.88	125.39	119.20
2	P	34	GLY	CA-C-N	-6.88	110.22	122.74
2	P	34	GLY	C-N-CA	-6.88	110.22	122.74
2	R	48	ARG	NE-CZ-NH2	6.87	125.39	119.20
2	L	48	ARG	NE-CZ-NH2	6.87	125.38	119.20
2	H	48	ARG	NE-CZ-NH2	6.86	125.38	119.20
2	N	50	ASN	CA-C-N	6.86	130.16	120.42
2	N	50	ASN	C-N-CA	6.86	130.16	120.42
1	E	21	TRP	CA-CB-CG	-6.85	100.58	113.60
2	D	50	ASN	CA-C-N	6.85	130.15	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	50	ASN	C-N-CA	6.85	130.15	120.42
1	K	262	TYR	CB-CG-CD1	-6.85	110.53	120.80
1	Q	21	TRP	CA-CB-CG	-6.85	100.59	113.60
1	I	21	TRP	CA-CB-CG	-6.85	100.59	113.60
1	G	262	TYR	CB-CG-CD1	-6.84	110.53	120.80
2	N	99	ALA	O-C-N	6.84	129.95	122.15
1	A	21	TRP	CA-CB-CG	-6.84	100.60	113.60
1	K	21	TRP	CA-CB-CG	-6.84	100.60	113.60
1	O	21	TRP	CA-CB-CG	-6.84	100.60	113.60
1	A	262	TYR	CB-CG-CD1	-6.84	110.54	120.80
1	G	76	ASP	CA-CB-CG	6.84	119.44	112.60
1	C	21	TRP	CA-CB-CG	-6.84	100.61	113.60
1	E	262	TYR	CB-CG-CD1	-6.84	110.55	120.80
1	M	21	TRP	CA-CB-CG	-6.83	100.62	113.60
1	I	262	TYR	CB-CG-CD1	-6.83	110.55	120.80
1	O	262	TYR	CB-CG-CD1	-6.83	110.55	120.80
2	R	50	ASN	CA-C-N	6.83	130.12	120.42
2	R	50	ASN	C-N-CA	6.83	130.12	120.42
1	C	262	TYR	CB-CG-CD1	-6.83	110.56	120.80
1	E	160	ASP	N-CA-C	6.83	120.09	111.69
1	O	76	ASP	CA-CB-CG	6.83	119.43	112.60
2	F	99	ALA	O-C-N	6.83	129.93	122.15
1	G	21	TRP	CA-CB-CG	-6.83	100.63	113.60
1	Q	73	THR	N-CA-C	6.83	119.30	111.11
1	E	73	THR	N-CA-C	6.82	119.30	111.11
1	G	73	THR	N-CA-C	6.82	119.30	111.11
2	J	50	ASN	CA-C-N	6.82	130.11	120.42
2	J	50	ASN	C-N-CA	6.82	130.11	120.42
1	E	76	ASP	CA-CB-CG	6.82	119.42	112.60
2	J	99	ALA	O-C-N	6.82	129.93	122.15
1	Q	262	TYR	CB-CG-CD1	-6.82	110.57	120.80
2	B	50	ASN	CA-C-N	6.82	130.10	120.42
2	B	50	ASN	C-N-CA	6.82	130.10	120.42
1	M	262	TYR	CB-CG-CD1	-6.82	110.57	120.80
2	R	99	ALA	O-C-N	6.82	129.92	122.15
1	A	73	THR	N-CA-C	6.82	119.29	111.11
1	K	73	THR	N-CA-C	6.82	119.29	111.11
1	K	241	SER	CA-C-N	-6.81	110.47	120.28
1	K	241	SER	C-N-CA	-6.81	110.47	120.28
1	C	73	THR	N-CA-C	6.81	119.28	111.11
1	C	76	ASP	CA-CB-CG	6.81	119.41	112.60
1	I	160	ASP	N-CA-C	6.81	120.07	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	99	ALA	O-C-N	6.81	129.91	122.15
2	H	50	ASN	CA-C-N	6.81	130.09	120.42
2	H	50	ASN	C-N-CA	6.81	130.09	120.42
2	P	50	ASN	CA-C-N	6.81	130.09	120.42
2	P	50	ASN	C-N-CA	6.81	130.09	120.42
1	A	76	ASP	CA-CB-CG	6.81	119.41	112.60
2	B	99	ALA	O-C-N	6.81	129.91	122.15
1	I	59	GLY	CA-C-N	-6.81	113.39	122.99
1	I	59	GLY	C-N-CA	-6.81	113.39	122.99
1	M	241	SER	CA-C-N	-6.81	110.48	120.28
1	M	241	SER	C-N-CA	-6.81	110.48	120.28
1	I	73	THR	N-CA-C	6.80	119.28	111.11
1	K	160	ASP	N-CA-C	6.80	120.06	111.69
1	O	241	SER	CA-C-N	-6.80	110.48	120.28
1	O	241	SER	C-N-CA	-6.80	110.48	120.28
2	L	50	ASN	CA-C-N	6.80	130.08	120.42
2	L	50	ASN	C-N-CA	6.80	130.08	120.42
1	Q	241	SER	CA-C-N	-6.80	110.48	120.28
1	Q	241	SER	C-N-CA	-6.80	110.48	120.28
1	M	73	THR	N-CA-C	6.80	119.27	111.11
1	E	241	SER	CA-C-N	-6.80	110.49	120.28
1	E	241	SER	C-N-CA	-6.80	110.49	120.28
1	K	76	ASP	CA-CB-CG	6.80	119.40	112.60
2	L	377	PHE	CA-C-N	-6.80	114.06	123.10
2	L	377	PHE	C-N-CA	-6.80	114.06	123.10
1	G	241	SER	CA-C-N	-6.79	110.50	120.28
1	G	241	SER	C-N-CA	-6.79	110.50	120.28
2	L	99	ALA	O-C-N	6.79	129.90	122.15
1	C	59	GLY	CA-C-N	-6.79	113.41	122.99
1	C	59	GLY	C-N-CA	-6.79	113.41	122.99
1	O	160	ASP	N-CA-C	6.79	120.05	111.69
1	A	241	SER	CA-C-N	-6.79	110.50	120.28
1	A	241	SER	C-N-CA	-6.79	110.50	120.28
1	C	241	SER	CA-C-N	-6.79	110.50	120.28
1	C	241	SER	C-N-CA	-6.79	110.50	120.28
1	E	59	GLY	CA-C-N	-6.79	113.42	122.99
1	E	59	GLY	C-N-CA	-6.79	113.42	122.99
1	I	76	ASP	CA-CB-CG	6.79	119.39	112.60
1	A	160	ASP	N-CA-C	6.79	120.04	111.69
1	C	160	ASP	N-CA-C	6.78	120.03	111.69
1	A	59	GLY	CA-C-N	-6.78	113.43	122.99
1	A	59	GLY	C-N-CA	-6.78	113.43	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	377	PHE	CA-C-N	-6.78	114.08	123.10
2	N	377	PHE	C-N-CA	-6.78	114.08	123.10
2	H	99	ALA	O-C-N	6.78	129.88	122.15
1	I	241	SER	CA-C-N	-6.78	110.52	120.28
1	I	241	SER	C-N-CA	-6.78	110.52	120.28
1	Q	76	ASP	CA-CB-CG	6.78	119.38	112.60
2	D	99	ALA	O-C-N	6.78	129.87	122.15
2	F	50	ASN	CA-C-N	6.78	130.04	120.42
2	F	50	ASN	C-N-CA	6.78	130.04	120.42
1	G	160	ASP	N-CA-C	6.78	120.02	111.69
1	M	160	ASP	N-CA-C	6.78	120.02	111.69
2	J	377	PHE	CA-C-N	-6.77	114.09	123.10
2	J	377	PHE	C-N-CA	-6.77	114.09	123.10
1	O	59	GLY	CA-C-N	-6.77	113.44	122.99
1	O	59	GLY	C-N-CA	-6.77	113.44	122.99
1	Q	160	ASP	N-CA-C	6.77	120.02	111.69
1	Q	59	GLY	CA-C-N	-6.77	113.44	122.99
1	Q	59	GLY	C-N-CA	-6.77	113.44	122.99
1	M	76	ASP	CA-CB-CG	6.77	119.37	112.60
1	C	200	CYS	CA-C-N	-6.77	113.45	122.99
1	C	200	CYS	C-N-CA	-6.77	113.45	122.99
2	B	377	PHE	CA-C-N	-6.76	114.10	123.10
2	B	377	PHE	C-N-CA	-6.76	114.10	123.10
1	O	73	THR	N-CA-C	6.76	119.23	111.11
1	O	200	CYS	CA-C-N	-6.76	113.45	122.99
1	O	200	CYS	C-N-CA	-6.76	113.45	122.99
1	M	59	GLY	CA-C-N	-6.76	113.46	122.99
1	M	59	GLY	C-N-CA	-6.76	113.46	122.99
1	E	200	CYS	CA-C-N	-6.76	113.46	122.99
1	E	200	CYS	C-N-CA	-6.76	113.46	122.99
1	A	200	CYS	CA-C-N	-6.75	113.47	122.99
1	A	200	CYS	C-N-CA	-6.75	113.47	122.99
1	K	59	GLY	CA-C-N	-6.75	113.47	122.99
1	K	59	GLY	C-N-CA	-6.75	113.47	122.99
1	K	200	CYS	CA-C-N	-6.75	113.47	122.99
1	K	200	CYS	C-N-CA	-6.75	113.47	122.99
1	M	200	CYS	CA-C-N	-6.75	113.47	122.99
1	M	200	CYS	C-N-CA	-6.75	113.47	122.99
1	G	59	GLY	CA-C-N	-6.75	113.47	122.99
1	G	59	GLY	C-N-CA	-6.75	113.47	122.99
2	H	377	PHE	CA-C-N	-6.75	114.13	123.10
2	H	377	PHE	C-N-CA	-6.75	114.13	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	377	PHE	CA-C-N	-6.75	114.13	123.10
2	P	377	PHE	C-N-CA	-6.75	114.13	123.10
1	Q	200	CYS	CA-C-N	-6.75	113.48	122.99
1	Q	200	CYS	C-N-CA	-6.75	113.48	122.99
2	R	377	PHE	CA-C-N	-6.74	114.14	123.10
2	R	377	PHE	C-N-CA	-6.74	114.14	123.10
2	D	377	PHE	CA-C-N	-6.73	114.14	123.10
2	D	377	PHE	C-N-CA	-6.73	114.14	123.10
2	F	377	PHE	CA-C-N	-6.73	114.15	123.10
2	F	377	PHE	C-N-CA	-6.73	114.15	123.10
2	L	206	ASN	CA-CB-CG	-6.73	105.87	112.60
1	G	200	CYS	CA-C-N	-6.73	113.50	122.99
1	G	200	CYS	C-N-CA	-6.73	113.50	122.99
1	I	200	CYS	CA-C-N	-6.73	113.50	122.99
1	I	200	CYS	C-N-CA	-6.73	113.50	122.99
2	P	206	ASN	CA-CB-CG	-6.73	105.87	112.60
2	B	206	ASN	CA-CB-CG	-6.72	105.88	112.60
2	D	206	ASN	CA-CB-CG	-6.72	105.88	112.60
2	J	206	ASN	CA-CB-CG	-6.71	105.89	112.60
2	N	206	ASN	CA-CB-CG	-6.71	105.89	112.60
2	F	206	ASN	CA-CB-CG	-6.71	105.89	112.60
2	F	52	TYR	CA-C-N	-6.70	112.18	122.62
2	F	52	TYR	C-N-CA	-6.70	112.18	122.62
1	M	340	THR	N-CA-C	-6.69	102.25	110.61
1	O	340	THR	N-CA-C	-6.69	102.24	110.61
1	A	340	THR	N-CA-C	-6.69	102.25	110.61
2	R	52	TYR	CA-C-N	-6.69	112.18	122.62
2	R	52	TYR	C-N-CA	-6.69	112.18	122.62
2	H	206	ASN	CA-CB-CG	-6.69	105.91	112.60
1	E	340	THR	N-CA-C	-6.68	102.25	110.61
2	N	52	TYR	CA-C-N	-6.68	112.19	122.62
2	N	52	TYR	C-N-CA	-6.68	112.19	122.62
2	R	206	ASN	CA-CB-CG	-6.68	105.92	112.60
2	J	52	TYR	CA-C-N	-6.68	112.20	122.62
2	J	52	TYR	C-N-CA	-6.68	112.20	122.62
2	D	52	TYR	CA-C-N	-6.67	112.21	122.62
2	D	52	TYR	C-N-CA	-6.67	112.21	122.62
2	B	52	TYR	CA-C-N	-6.67	112.21	122.62
2	B	52	TYR	C-N-CA	-6.67	112.21	122.62
1	G	340	THR	N-CA-C	-6.67	102.27	110.61
2	P	52	TYR	CA-C-N	-6.67	112.22	122.62
2	P	52	TYR	C-N-CA	-6.67	112.22	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	340	THR	N-CA-C	-6.67	102.28	110.61
2	H	52	TYR	CA-C-N	-6.66	112.22	122.62
2	H	52	TYR	C-N-CA	-6.66	112.22	122.62
1	M	96	LYS	CA-C-N	-6.66	112.53	122.39
1	M	96	LYS	C-N-CA	-6.66	112.53	122.39
1	C	96	LYS	CA-C-N	-6.66	112.53	122.39
1	C	96	LYS	C-N-CA	-6.66	112.53	122.39
1	C	340	THR	N-CA-C	-6.66	102.28	110.61
1	I	340	THR	N-CA-C	-6.66	102.29	110.61
1	K	340	THR	N-CA-C	-6.65	102.29	110.61
2	L	52	TYR	CA-C-N	-6.65	112.25	122.62
2	L	52	TYR	C-N-CA	-6.65	112.25	122.62
1	A	96	LYS	CA-C-N	-6.64	112.56	122.39
1	A	96	LYS	C-N-CA	-6.64	112.56	122.39
1	O	96	LYS	CA-C-N	-6.64	112.56	122.39
1	O	96	LYS	C-N-CA	-6.64	112.56	122.39
1	G	96	LYS	CA-C-N	-6.64	112.57	122.39
1	G	96	LYS	C-N-CA	-6.64	112.57	122.39
1	E	96	LYS	CA-C-N	-6.63	112.57	122.39
1	E	96	LYS	C-N-CA	-6.63	112.57	122.39
1	Q	96	LYS	CA-C-N	-6.63	112.57	122.39
1	Q	96	LYS	C-N-CA	-6.63	112.57	122.39
1	I	96	LYS	CA-C-N	-6.63	112.58	122.39
1	I	96	LYS	C-N-CA	-6.63	112.58	122.39
1	K	96	LYS	CA-C-N	-6.63	112.58	122.39
1	K	96	LYS	C-N-CA	-6.63	112.58	122.39
1	K	338	LYS	N-CA-C	6.59	121.17	113.20
1	C	338	LYS	N-CA-C	6.58	121.17	113.20
1	G	348	PRO	N-CA-C	6.58	126.02	112.47
2	R	358	ILE	N-CA-C	6.58	114.28	108.63
1	O	245	ASP	N-CA-C	6.57	120.58	110.20
1	C	348	PRO	N-CA-C	6.57	126.00	112.47
2	J	249	ASN	CA-CB-CG	-6.57	106.03	112.60
2	D	249	ASN	CA-CB-CG	-6.56	106.04	112.60
1	M	348	PRO	N-CA-C	6.56	125.99	112.47
1	Q	338	LYS	N-CA-C	6.56	121.14	113.20
1	A	348	PRO	N-CA-C	6.56	125.98	112.47
1	G	338	LYS	N-CA-C	6.56	121.14	113.20
1	O	338	LYS	N-CA-C	6.56	121.14	113.20
2	D	358	ILE	N-CA-C	6.55	114.27	108.63
1	E	348	PRO	N-CA-C	6.55	125.97	112.47
1	Q	348	PRO	N-CA-C	6.55	125.97	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	LYS	N-CA-C	6.55	121.13	113.20
1	O	348	PRO	N-CA-C	6.55	125.96	112.47
2	J	358	ILE	N-CA-C	6.55	114.26	108.63
1	I	348	PRO	N-CA-C	6.55	125.95	112.47
1	K	348	PRO	N-CA-C	6.55	125.96	112.47
2	L	249	ASN	CA-CB-CG	-6.54	106.06	112.60
2	R	249	ASN	CA-CB-CG	-6.54	106.06	112.60
2	B	358	ILE	N-CA-C	6.54	114.25	108.63
1	G	431	ASP	CA-CB-CG	-6.54	106.06	112.60
1	M	245	ASP	N-CA-C	6.54	120.53	110.20
1	M	338	LYS	N-CA-C	6.54	121.11	113.20
2	B	249	ASN	CA-CB-CG	-6.54	106.06	112.60
2	L	108	TYR	CA-C-N	-6.54	113.79	121.64
2	L	108	TYR	C-N-CA	-6.54	113.79	121.64
1	Q	305	CYS	N-CA-C	-6.54	99.72	108.74
1	Q	262	TYR	CB-CA-C	-6.54	98.74	108.87
1	O	262	TYR	CB-CA-C	-6.53	98.74	108.87
2	P	249	ASN	CA-CB-CG	-6.53	106.07	112.60
1	E	245	ASP	N-CA-C	6.53	120.52	110.20
1	A	245	ASP	N-CA-C	6.53	120.52	110.20
1	C	431	ASP	CA-CB-CG	-6.53	106.07	112.60
1	E	338	LYS	N-CA-C	6.53	121.10	113.20
2	F	358	ILE	N-CA-C	6.53	114.25	108.63
2	H	358	ILE	N-CA-C	6.53	114.25	108.63
1	K	262	TYR	CB-CA-C	-6.53	98.75	108.87
1	K	305	CYS	N-CA-C	-6.53	99.73	108.74
1	K	245	ASP	N-CA-C	6.53	120.52	110.20
1	I	245	ASP	N-CA-C	6.52	120.51	110.20
1	G	245	ASP	N-CA-C	6.52	120.51	110.20
1	A	262	TYR	CB-CA-C	-6.52	98.77	108.87
1	G	262	TYR	CB-CA-C	-6.52	98.77	108.87
1	I	338	LYS	N-CA-C	6.52	121.09	113.20
2	D	108	TYR	CA-C-N	-6.51	113.82	121.64
2	D	108	TYR	C-N-CA	-6.51	113.82	121.64
1	M	262	TYR	CB-CA-C	-6.51	98.77	108.87
1	C	245	ASP	N-CA-C	6.51	120.49	110.20
2	F	249	ASN	CA-CB-CG	-6.51	106.09	112.60
1	G	305	CYS	N-CA-C	-6.51	99.75	108.74
1	I	262	TYR	CB-CA-C	-6.51	98.78	108.87
2	F	108	TYR	CA-C-N	-6.51	113.83	121.64
2	F	108	TYR	C-N-CA	-6.51	113.83	121.64
2	N	249	ASN	CA-CB-CG	-6.51	106.09	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	431	ASP	CA-CB-CG	-6.51	106.09	112.60
1	C	262	TYR	CB-CA-C	-6.51	98.78	108.87
2	J	108	TYR	CA-C-N	-6.51	113.83	121.64
2	J	108	TYR	C-N-CA	-6.51	113.83	121.64
1	M	305	CYS	N-CA-C	-6.51	99.76	108.74
1	Q	431	ASP	CA-CB-CG	-6.50	106.09	112.60
2	L	358	ILE	N-CA-C	6.50	114.22	108.63
1	O	431	ASP	CA-CB-CG	-6.50	106.10	112.60
1	Q	245	ASP	N-CA-C	6.50	120.47	110.20
1	A	305	CYS	N-CA-C	-6.50	99.77	108.74
1	A	431	ASP	CA-CB-CG	-6.50	106.10	112.60
2	P	358	ILE	N-CA-C	6.50	114.22	108.63
2	R	108	TYR	CA-C-N	-6.50	113.84	121.64
2	R	108	TYR	C-N-CA	-6.50	113.84	121.64
1	M	431	ASP	CA-CB-CG	-6.50	106.11	112.60
2	H	249	ASN	CA-CB-CG	-6.49	106.11	112.60
2	B	108	TYR	CA-C-N	-6.49	113.85	121.64
2	B	108	TYR	C-N-CA	-6.49	113.85	121.64
1	C	305	CYS	N-CA-C	-6.49	99.78	108.74
1	I	305	CYS	N-CA-C	-6.49	99.78	108.74
1	E	262	TYR	CB-CA-C	-6.49	98.81	108.87
2	H	108	TYR	CA-C-N	-6.49	113.85	121.64
2	H	108	TYR	C-N-CA	-6.49	113.85	121.64
1	O	305	CYS	N-CA-C	-6.49	99.79	108.74
2	N	358	ILE	N-CA-C	6.49	114.21	108.63
2	N	108	TYR	CA-C-N	-6.49	113.86	121.64
2	N	108	TYR	C-N-CA	-6.49	113.86	121.64
2	N	258	ASN	N-CA-C	6.49	120.93	112.89
1	E	305	CYS	N-CA-C	-6.48	99.79	108.74
1	I	431	ASP	CA-CB-CG	-6.48	106.12	112.60
2	J	258	ASN	N-CA-C	6.48	120.93	112.89
2	F	258	ASN	N-CA-C	6.48	120.92	112.89
2	P	108	TYR	CA-C-N	-6.48	113.87	121.64
2	P	108	TYR	C-N-CA	-6.48	113.87	121.64
1	G	97	GLU	CA-C-O	6.47	128.10	120.20
1	Q	339	ARG	O-C-N	6.47	131.93	123.07
1	K	431	ASP	CA-CB-CG	-6.47	106.13	112.60
2	R	258	ASN	N-CA-C	6.46	120.91	112.89
2	B	258	ASN	N-CA-C	6.46	120.90	112.89
1	M	282	TYR	CA-CB-CG	-6.46	102.27	113.90
2	L	258	ASN	N-CA-C	6.46	120.90	112.89
2	L	164	ARG	NH1-CZ-NH2	-6.46	110.91	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	97	GLU	CA-C-O	6.46	128.08	120.20
2	P	258	ASN	N-CA-C	6.46	120.89	112.89
2	H	258	ASN	N-CA-C	6.45	120.89	112.89
2	N	253	ARG	NE-CZ-NH2	6.45	125.00	119.20
1	C	339	ARG	O-C-N	6.45	131.90	123.07
1	G	282	TYR	CA-CB-CG	-6.45	102.30	113.90
1	E	282	TYR	CA-CB-CG	-6.44	102.30	113.90
1	M	339	ARG	O-C-N	6.44	131.90	123.07
2	R	164	ARG	NH1-CZ-NH2	-6.44	110.93	119.30
1	E	97	GLU	CA-C-O	6.44	128.06	120.20
1	A	282	TYR	CA-CB-CG	-6.44	102.31	113.90
1	C	97	GLU	CA-C-O	6.43	128.05	120.20
1	K	282	TYR	CA-CB-CG	-6.43	102.32	113.90
1	Q	282	TYR	CA-CB-CG	-6.43	102.32	113.90
2	J	164	ARG	NH1-CZ-NH2	-6.43	110.94	119.30
1	C	282	TYR	CA-CB-CG	-6.43	102.33	113.90
1	O	282	TYR	CA-CB-CG	-6.43	102.33	113.90
2	D	258	ASN	N-CA-C	6.42	120.85	112.89
1	A	97	GLU	CA-C-O	6.42	128.03	120.20
1	A	339	ARG	O-C-N	6.42	131.87	123.07
1	I	97	GLU	CA-C-O	6.42	128.03	120.20
1	Q	97	GLU	CA-C-O	6.42	128.03	120.20
1	M	97	GLU	CA-C-O	6.42	128.03	120.20
1	I	282	TYR	CA-CB-CG	-6.41	102.36	113.90
1	I	339	ARG	O-C-N	6.41	131.86	123.07
2	B	164	ARG	NH1-CZ-NH2	-6.41	110.97	119.30
2	D	164	ARG	NH1-CZ-NH2	-6.41	110.97	119.30
1	K	339	ARG	O-C-N	6.41	131.84	123.07
1	O	339	ARG	O-C-N	6.41	131.84	123.07
1	E	339	ARG	O-C-N	6.40	131.84	123.07
2	R	253	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	E	253	THR	N-CA-C	-6.39	104.52	112.90
1	K	97	GLU	CA-C-O	6.39	128.00	120.20
2	F	164	ARG	NH1-CZ-NH2	-6.39	111.00	119.30
1	G	339	ARG	O-C-N	6.38	131.82	123.07
2	N	164	ARG	NH1-CZ-NH2	-6.38	111.00	119.30
2	F	253	ARG	NE-CZ-NH2	6.38	124.94	119.20
2	P	164	ARG	NH1-CZ-NH2	-6.38	111.01	119.30
2	P	253	ARG	NE-CZ-NH2	6.38	124.94	119.20
1	G	253	THR	N-CA-C	-6.37	104.55	112.90
2	H	253	ARG	NE-CZ-NH2	6.37	124.93	119.20
1	O	253	THR	N-CA-C	-6.37	104.56	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	164	ARG	NH1-CZ-NH2	-6.37	111.03	119.30
1	M	253	THR	N-CA-C	-6.36	104.57	112.90
1	I	253	THR	N-CA-C	-6.36	104.57	112.90
2	J	253	ARG	NE-CZ-NH2	6.36	124.92	119.20
2	B	253	ARG	NE-CZ-NH2	6.35	124.92	119.20
1	A	253	THR	N-CA-C	-6.35	104.58	112.90
1	I	435	VAL	N-CA-C	6.35	119.03	111.09
2	L	253	ARG	NE-CZ-NH2	6.35	124.92	119.20
1	M	260	VAL	N-CA-CB	-6.35	102.32	111.21
1	I	162	GLY	N-CA-C	6.35	120.58	112.83
1	M	162	GLY	N-CA-C	6.35	120.57	112.83
2	D	253	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	C	260	VAL	N-CA-CB	-6.34	102.33	111.21
1	C	162	GLY	N-CA-C	6.34	120.56	112.83
1	E	260	VAL	N-CA-CB	-6.34	102.34	111.21
1	E	105	ARG	NE-CZ-NH2	-6.33	113.50	119.20
1	M	105	ARG	NE-CZ-NH2	-6.33	113.50	119.20
1	G	162	GLY	N-CA-C	6.33	120.55	112.83
1	O	162	GLY	N-CA-C	6.33	120.55	112.83
1	G	260	VAL	N-CA-CB	-6.33	102.35	111.21
1	Q	253	THR	N-CA-C	-6.33	104.61	112.90
1	A	260	VAL	N-CA-CB	-6.33	102.36	111.21
1	Q	260	VAL	N-CA-CB	-6.33	102.35	111.21
1	O	105	ARG	NE-CZ-NH2	-6.32	113.51	119.20
1	K	346	TRP	CE2-CD2-CE3	6.32	125.12	118.80
1	A	105	ARG	NE-CZ-NH2	-6.32	113.51	119.20
1	K	253	THR	N-CA-C	-6.32	104.62	112.90
1	M	346	TRP	CE2-CD2-CE3	6.32	125.12	118.80
1	O	260	VAL	N-CA-CB	-6.32	102.36	111.21
1	A	162	GLY	N-CA-C	6.32	120.54	112.83
1	C	346	TRP	CE2-CD2-CE3	6.32	125.12	118.80
1	I	346	TRP	CE2-CD2-CE3	6.32	125.12	118.80
1	O	435	VAL	N-CA-C	6.32	118.99	111.09
1	Q	162	GLY	N-CA-C	6.32	120.54	112.83
1	C	253	THR	N-CA-C	-6.32	104.63	112.90
1	E	346	TRP	CE2-CD2-CE3	6.32	125.12	118.80
1	K	435	VAL	N-CA-C	6.32	118.98	111.09
1	Q	105	ARG	NE-CZ-NH2	-6.32	113.52	119.20
1	I	105	ARG	NE-CZ-NH2	-6.31	113.52	119.20
1	E	435	VAL	N-CA-C	6.31	118.97	111.09
1	I	260	VAL	N-CA-CB	-6.31	102.38	111.21
1	K	260	VAL	N-CA-CB	-6.31	102.38	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	346	TRP	CE2-CD2-CE3	6.31	125.11	118.80
1	G	346	TRP	CE2-CD2-CE3	6.30	125.10	118.80
1	K	105	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	A	346	TRP	CE2-CD2-CE3	6.30	125.10	118.80
1	A	435	VAL	N-CA-C	6.30	118.97	111.09
1	Q	435	VAL	N-CA-C	6.30	118.97	111.09
2	D	249	ASN	CA-C-O	6.30	128.16	120.92
1	M	435	VAL	N-CA-C	6.30	118.97	111.09
2	R	249	ASN	CA-C-O	6.30	128.16	120.92
1	K	162	GLY	N-CA-C	6.30	120.51	112.83
1	E	162	GLY	N-CA-C	6.30	120.51	112.83
2	B	249	ASN	CA-C-O	6.29	128.16	120.92
1	C	105	ARG	NE-CZ-NH2	-6.29	113.54	119.20
1	G	435	VAL	N-CA-C	6.29	118.95	111.09
1	Q	346	TRP	CE2-CD2-CE3	6.29	125.08	118.80
2	H	249	ASN	CA-C-O	6.28	128.15	120.92
2	J	249	ASN	CA-C-O	6.28	128.15	120.92
1	C	435	VAL	N-CA-C	6.28	118.94	111.09
2	L	249	ASN	CA-C-O	6.28	128.14	120.92
1	G	105	ARG	NE-CZ-NH2	-6.27	113.55	119.20
2	F	249	ASN	CA-C-O	6.26	128.12	120.92
2	P	249	ASN	CA-C-O	6.25	128.11	120.92
1	I	183	GLU	O-C-N	-6.24	114.85	120.71
1	M	183	GLU	O-C-N	-6.24	114.85	120.71
1	M	37	PRO	CA-C-N	-6.23	110.49	121.70
1	M	37	PRO	C-N-CA	-6.23	110.49	121.70
2	N	249	ASN	CA-C-O	6.23	128.08	120.92
1	Q	183	GLU	O-C-N	-6.22	114.86	120.71
1	I	37	PRO	CA-C-N	-6.22	110.51	121.70
1	I	37	PRO	C-N-CA	-6.22	110.51	121.70
1	A	183	GLU	O-C-N	-6.21	114.87	120.71
1	E	37	PRO	CA-C-N	-6.21	110.52	121.70
1	E	37	PRO	C-N-CA	-6.21	110.52	121.70
1	G	37	PRO	CA-C-N	-6.21	110.52	121.70
1	G	37	PRO	C-N-CA	-6.21	110.52	121.70
1	C	183	GLU	O-C-N	-6.21	114.87	120.71
1	A	37	PRO	CA-C-N	-6.20	110.54	121.70
1	A	37	PRO	C-N-CA	-6.20	110.54	121.70
1	C	37	PRO	CA-C-N	-6.20	110.54	121.70
1	C	37	PRO	C-N-CA	-6.20	110.54	121.70
1	K	183	GLU	O-C-N	-6.20	114.88	120.71
1	Q	37	PRO	CA-C-N	-6.20	110.54	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	37	PRO	C-N-CA	-6.20	110.54	121.70
1	O	183	GLU	O-C-N	-6.19	114.89	120.71
1	K	37	PRO	CA-C-N	-6.19	110.55	121.70
1	K	37	PRO	C-N-CA	-6.19	110.55	121.70
1	O	37	PRO	CA-C-N	-6.19	110.55	121.70
1	O	37	PRO	C-N-CA	-6.19	110.55	121.70
1	E	183	GLU	O-C-N	-6.19	114.89	120.71
1	G	183	GLU	O-C-N	-6.18	114.90	120.71
1	C	303	VAL	CA-C-N	-6.18	112.16	122.17
1	C	303	VAL	C-N-CA	-6.18	112.16	122.17
1	I	303	VAL	CA-C-N	-6.17	112.17	122.17
1	I	303	VAL	C-N-CA	-6.17	112.17	122.17
1	Q	303	VAL	CA-C-N	-6.17	112.17	122.17
1	Q	303	VAL	C-N-CA	-6.17	112.17	122.17
1	A	303	VAL	CA-C-N	-6.17	112.18	122.17
1	A	303	VAL	C-N-CA	-6.17	112.18	122.17
1	G	303	VAL	CA-C-N	-6.16	112.19	122.17
1	G	303	VAL	C-N-CA	-6.16	112.19	122.17
1	O	303	VAL	CA-C-N	-6.15	112.20	122.17
1	O	303	VAL	C-N-CA	-6.15	112.20	122.17
1	K	303	VAL	CA-C-N	-6.15	112.21	122.17
1	K	303	VAL	C-N-CA	-6.15	112.21	122.17
1	E	303	VAL	CA-C-N	-6.15	112.21	122.17
1	E	303	VAL	C-N-CA	-6.15	112.21	122.17
1	M	303	VAL	CA-C-N	-6.14	112.22	122.17
1	M	303	VAL	C-N-CA	-6.14	112.22	122.17
2	N	96	GLN	CA-C-N	6.09	132.67	121.70
2	N	96	GLN	C-N-CA	6.09	132.67	121.70
1	Q	71	GLU	N-CA-C	-6.08	101.13	110.32
2	L	96	GLN	CA-C-N	6.08	132.64	121.70
2	L	96	GLN	C-N-CA	6.08	132.64	121.70
2	D	96	GLN	CA-C-N	6.08	132.64	121.70
2	D	96	GLN	C-N-CA	6.08	132.64	121.70
2	F	96	GLN	CA-C-N	6.08	132.64	121.70
2	F	96	GLN	C-N-CA	6.08	132.64	121.70
1	C	71	GLU	N-CA-C	-6.08	101.14	110.32
1	O	71	GLU	N-CA-C	-6.07	101.15	110.32
2	H	96	GLN	CA-C-N	6.07	132.62	121.70
2	H	96	GLN	C-N-CA	6.07	132.62	121.70
1	A	71	GLU	N-CA-C	-6.07	101.16	110.32
2	P	96	GLN	CA-C-N	6.07	132.62	121.70
2	P	96	GLN	C-N-CA	6.07	132.62	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	67	PHE	CD1-CE1-CZ	-6.07	109.08	120.00
2	B	96	GLN	CA-C-N	6.06	132.62	121.70
2	B	96	GLN	C-N-CA	6.06	132.62	121.70
1	M	71	GLU	N-CA-C	-6.06	101.17	110.32
1	A	67	PHE	CD1-CE1-CZ	-6.06	109.09	120.00
1	O	67	PHE	CD1-CE1-CZ	-6.06	109.10	120.00
1	I	71	GLU	N-CA-C	-6.06	101.18	110.32
2	J	96	GLN	CA-C-N	6.05	132.60	121.70
2	J	96	GLN	C-N-CA	6.05	132.60	121.70
2	R	96	GLN	CA-C-N	6.05	132.59	121.70
2	R	96	GLN	C-N-CA	6.05	132.59	121.70
1	G	71	GLU	N-CA-C	-6.05	101.19	110.32
1	M	67	PHE	CD1-CE1-CZ	-6.05	109.11	120.00
1	K	67	PHE	CD1-CE1-CZ	-6.05	109.12	120.00
1	C	67	PHE	CD1-CE1-CZ	-6.04	109.12	120.00
1	E	71	GLU	N-CA-C	-6.04	101.20	110.32
1	K	71	GLU	N-CA-C	-6.04	101.20	110.32
1	Q	67	PHE	CD1-CE1-CZ	-6.04	109.13	120.00
1	G	67	PHE	CD1-CE1-CZ	-6.03	109.14	120.00
1	I	67	PHE	CD1-CE1-CZ	-6.03	109.14	120.00
1	C	242	LEU	CA-C-N	-6.03	111.15	120.31
1	C	242	LEU	C-N-CA	-6.03	111.15	120.31
1	E	242	LEU	CA-C-N	-6.02	111.16	120.31
1	E	242	LEU	C-N-CA	-6.02	111.16	120.31
1	G	242	LEU	CA-C-N	-6.01	111.17	120.31
1	G	242	LEU	C-N-CA	-6.01	111.17	120.31
1	K	242	LEU	CA-C-N	-6.01	111.17	120.31
1	K	242	LEU	C-N-CA	-6.01	111.17	120.31
1	K	341	ILE	N-CA-C	6.01	121.84	109.34
1	G	249	ASN	CA-C-N	6.00	130.84	123.10
1	G	249	ASN	C-N-CA	6.00	130.84	123.10
1	M	242	LEU	CA-C-N	-6.00	111.19	120.31
1	M	242	LEU	C-N-CA	-6.00	111.19	120.31
1	Q	341	ILE	N-CA-C	6.00	121.82	109.34
1	E	249	ASN	CA-C-N	6.00	130.84	123.10
1	E	249	ASN	C-N-CA	6.00	130.84	123.10
1	M	341	ILE	N-CA-C	6.00	121.82	109.34
1	A	341	ILE	N-CA-C	5.99	121.81	109.34
1	G	341	ILE	N-CA-C	5.99	121.80	109.34
1	A	242	LEU	CA-C-N	-5.99	111.20	120.31
1	A	242	LEU	C-N-CA	-5.99	111.20	120.31
1	O	341	ILE	N-CA-C	5.99	121.80	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	242	LEU	CA-C-N	-5.99	111.20	120.31
1	Q	242	LEU	C-N-CA	-5.99	111.20	120.31
1	A	249	ASN	CA-C-N	5.99	130.82	123.10
1	A	249	ASN	C-N-CA	5.99	130.82	123.10
1	I	249	ASN	CA-C-N	5.98	130.82	123.10
1	I	249	ASN	C-N-CA	5.98	130.82	123.10
1	M	249	ASN	CA-C-N	5.98	130.82	123.10
1	M	249	ASN	C-N-CA	5.98	130.82	123.10
1	Q	249	ASN	CA-C-N	5.98	130.82	123.10
1	Q	249	ASN	C-N-CA	5.98	130.82	123.10
1	O	242	LEU	CA-C-N	-5.98	111.22	120.31
1	O	242	LEU	C-N-CA	-5.98	111.22	120.31
1	I	341	ILE	N-CA-C	5.98	121.77	109.34
1	C	341	ILE	N-CA-C	5.98	121.77	109.34
1	E	341	ILE	N-CA-C	5.97	121.76	109.34
1	I	242	LEU	CA-C-N	-5.97	111.24	120.31
1	I	242	LEU	C-N-CA	-5.97	111.24	120.31
1	O	249	ASN	CA-C-N	5.97	130.80	123.10
1	O	249	ASN	C-N-CA	5.97	130.80	123.10
1	C	249	ASN	CA-C-N	5.96	130.79	123.10
1	C	249	ASN	C-N-CA	5.96	130.79	123.10
1	K	249	ASN	CA-C-N	5.96	130.79	123.10
1	K	249	ASN	C-N-CA	5.96	130.79	123.10
1	Q	348	PRO	N-CA-CB	-5.95	97.00	103.25
1	I	348	PRO	N-CA-CB	-5.95	97.00	103.25
1	A	348	PRO	N-CA-CB	-5.93	97.02	103.25
1	G	348	PRO	N-CA-CB	-5.93	97.03	103.25
2	R	309	HIS	CA-C-N	-5.93	116.40	122.27
2	R	309	HIS	C-N-CA	-5.93	116.40	122.27
2	B	309	HIS	CA-C-N	-5.92	116.40	122.27
2	B	309	HIS	C-N-CA	-5.92	116.40	122.27
1	C	260	VAL	N-CA-C	5.92	121.67	108.88
1	E	260	VAL	N-CA-C	5.92	121.67	108.88
2	N	309	HIS	CA-C-N	-5.92	116.41	122.27
2	N	309	HIS	C-N-CA	-5.92	116.41	122.27
1	O	260	VAL	N-CA-C	5.92	121.67	108.88
1	K	348	PRO	N-CA-CB	-5.92	97.04	103.25
1	O	348	PRO	N-CA-CB	-5.92	97.04	103.25
1	I	260	VAL	N-CA-C	5.92	121.66	108.88
1	M	260	VAL	N-CA-C	5.92	121.66	108.88
2	R	369	ARG	NE-CZ-NH2	-5.92	113.88	119.20
1	A	260	VAL	N-CA-C	5.91	121.65	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	348	PRO	N-CA-CB	-5.91	97.04	103.25
2	J	369	ARG	NE-CZ-NH2	-5.91	113.88	119.20
1	K	260	VAL	N-CA-C	5.91	121.65	108.88
1	C	348	PRO	N-CA-CB	-5.91	97.04	103.25
2	F	309	HIS	CA-C-N	-5.91	116.42	122.27
2	F	309	HIS	C-N-CA	-5.91	116.42	122.27
1	G	260	VAL	N-CA-C	5.91	121.65	108.88
2	J	309	HIS	CA-C-N	-5.91	116.42	122.27
2	J	309	HIS	C-N-CA	-5.91	116.42	122.27
1	M	348	PRO	N-CA-CB	-5.91	97.04	103.25
2	D	369	ARG	NE-CZ-NH2	-5.91	113.89	119.20
1	Q	260	VAL	N-CA-C	5.91	121.64	108.88
2	H	268	PHE	N-CA-C	5.90	119.34	109.95
2	P	309	HIS	CA-C-N	-5.90	116.43	122.27
2	P	309	HIS	C-N-CA	-5.90	116.43	122.27
2	J	268	PHE	N-CA-C	5.90	119.32	109.95
2	F	369	ARG	NE-CZ-NH2	-5.89	113.90	119.20
2	N	369	ARG	NE-CZ-NH2	-5.89	113.90	119.20
2	R	268	PHE	N-CA-C	5.89	119.32	109.95
2	F	268	PHE	N-CA-C	5.89	119.31	109.95
2	H	309	HIS	CA-C-N	-5.89	116.44	122.27
2	H	309	HIS	C-N-CA	-5.89	116.44	122.27
2	L	369	ARG	NE-CZ-NH2	-5.89	113.90	119.20
2	B	268	PHE	N-CA-C	5.88	119.30	109.95
2	B	369	ARG	NE-CZ-NH2	-5.88	113.91	119.20
2	H	369	ARG	NE-CZ-NH2	-5.88	113.91	119.20
2	P	268	PHE	N-CA-C	5.88	119.29	109.95
2	D	268	PHE	N-CA-C	5.87	119.29	109.95
1	O	239	THR	N-CA-C	5.87	120.95	113.55
2	L	309	HIS	CA-C-N	-5.87	116.46	122.27
2	L	309	HIS	C-N-CA	-5.87	116.46	122.27
2	P	369	ARG	NE-CZ-NH2	-5.87	113.92	119.20
2	D	309	HIS	CA-C-N	-5.87	116.46	122.27
2	D	309	HIS	C-N-CA	-5.87	116.46	122.27
2	L	238	VAL	N-CA-C	5.87	115.99	110.30
2	L	268	PHE	N-CA-C	5.86	119.27	109.95
2	N	268	PHE	N-CA-C	5.86	119.27	109.95
2	N	122	VAL	CB-CA-C	-5.86	104.47	111.97
1	C	239	THR	N-CA-C	5.86	120.93	113.55
2	H	122	VAL	CB-CA-C	-5.85	104.48	111.97
1	G	239	THR	N-CA-C	5.85	120.92	113.55
2	R	122	VAL	CB-CA-C	-5.84	104.49	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	238	VAL	N-CA-C	5.84	115.96	110.30
2	L	122	VAL	CB-CA-C	-5.84	104.50	111.97
1	Q	239	THR	N-CA-C	5.84	120.91	113.55
2	N	59	ASN	CA-CB-CG	5.84	118.44	112.60
1	G	190	THR	N-CA-C	5.83	117.31	111.07
2	B	122	VAL	CB-CA-C	-5.82	104.52	111.97
2	J	122	VAL	CB-CA-C	-5.82	104.52	111.97
2	J	238	VAL	N-CA-C	5.82	115.95	110.30
1	A	239	THR	N-CA-C	5.82	120.89	113.55
1	K	190	THR	N-CA-C	5.82	117.30	111.07
1	M	190	THR	N-CA-C	5.82	117.30	111.07
1	M	239	THR	N-CA-C	5.82	120.88	113.55
1	M	67	PHE	CZ-CE2-CD2	-5.82	109.53	120.00
1	K	239	THR	N-CA-C	5.81	120.87	113.55
1	Q	67	PHE	CZ-CE2-CD2	-5.81	109.54	120.00
1	E	190	THR	N-CA-C	5.81	117.29	111.07
1	A	190	THR	N-CA-C	5.81	117.28	111.07
2	F	122	VAL	CB-CA-C	-5.81	104.54	111.97
1	C	67	PHE	CZ-CE2-CD2	-5.80	109.55	120.00
2	F	281	GLN	N-CA-C	5.80	119.18	111.75
2	H	59	ASN	CA-CB-CG	5.80	118.40	112.60
1	I	190	THR	N-CA-C	5.80	117.28	111.07
2	L	59	ASN	CA-CB-CG	5.80	118.41	112.60
2	B	238	VAL	N-CA-C	5.80	115.93	110.30
1	G	34	GLY	CA-C-N	-5.80	112.83	120.95
1	G	34	GLY	C-N-CA	-5.80	112.83	120.95
2	J	176	LYS	N-CA-C	5.80	120.20	113.18
1	O	34	GLY	CA-C-N	-5.80	112.83	120.95
1	O	34	GLY	C-N-CA	-5.80	112.83	120.95
2	D	281	GLN	N-CA-C	5.80	119.17	111.75
2	F	59	ASN	CA-CB-CG	5.80	118.40	112.60
1	O	190	THR	N-CA-C	5.80	117.27	111.07
2	P	59	ASN	CA-CB-CG	5.80	118.40	112.60
1	A	67	PHE	CZ-CE2-CD2	-5.80	109.56	120.00
1	K	34	GLY	CA-C-N	-5.80	112.83	120.95
1	K	34	GLY	C-N-CA	-5.80	112.83	120.95
2	L	176	LYS	N-CA-C	5.80	120.20	113.18
2	D	122	VAL	CB-CA-C	-5.80	104.55	111.97
1	G	67	PHE	CZ-CE2-CD2	-5.80	109.57	120.00
1	E	239	THR	N-CA-C	5.79	120.85	113.55
2	P	122	VAL	CB-CA-C	-5.79	104.55	111.97
2	D	238	VAL	N-CA-C	5.79	115.92	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	281	GLN	N-CA-C	5.79	119.16	111.75
2	P	338	LYS	CA-C-N	-5.79	114.53	122.87
2	P	338	LYS	C-N-CA	-5.79	114.53	122.87
2	H	176	LYS	N-CA-C	5.79	120.19	113.18
1	I	34	GLY	CA-C-N	-5.79	112.84	120.95
1	I	34	GLY	C-N-CA	-5.79	112.84	120.95
1	Q	190	THR	N-CA-C	5.79	117.27	111.07
1	E	34	GLY	CA-C-N	-5.79	112.85	120.95
1	E	34	GLY	C-N-CA	-5.79	112.85	120.95
2	D	59	ASN	CA-CB-CG	5.79	118.39	112.60
2	H	257	VAL	CA-C-N	-5.79	111.02	121.14
2	H	257	VAL	C-N-CA	-5.79	111.02	121.14
2	J	59	ASN	CA-CB-CG	5.79	118.39	112.60
2	N	281	GLN	N-CA-C	5.79	119.16	111.75
2	B	281	GLN	N-CA-C	5.78	119.15	111.75
2	P	281	GLN	N-CA-C	5.78	119.15	111.75
1	C	190	THR	N-CA-C	5.78	117.26	111.07
1	M	34	GLY	CA-C-N	-5.78	112.86	120.95
1	M	34	GLY	C-N-CA	-5.78	112.86	120.95
1	I	239	THR	N-CA-C	5.78	120.83	113.55
2	N	238	VAL	N-CA-C	5.78	115.90	110.30
2	N	176	LYS	N-CA-C	5.78	120.17	113.18
2	P	176	LYS	N-CA-C	5.78	120.17	113.18
2	B	176	LYS	N-CA-C	5.77	120.17	113.18
1	K	67	PHE	CZ-CE2-CD2	-5.77	109.61	120.00
1	E	67	PHE	CZ-CE2-CD2	-5.77	109.61	120.00
2	N	257	VAL	CA-C-N	-5.77	111.04	121.14
2	N	257	VAL	C-N-CA	-5.77	111.04	121.14
2	P	238	VAL	N-CA-C	5.77	115.90	110.30
1	I	67	PHE	CZ-CE2-CD2	-5.77	109.61	120.00
2	F	176	LYS	N-CA-C	5.77	120.16	113.18
2	F	338	LYS	CA-C-N	-5.77	114.56	122.87
2	F	338	LYS	C-N-CA	-5.77	114.56	122.87
1	A	34	GLY	CA-C-N	-5.77	112.88	120.95
1	A	34	GLY	C-N-CA	-5.77	112.88	120.95
2	B	59	ASN	CA-CB-CG	5.77	118.37	112.60
1	C	34	GLY	CA-C-N	-5.77	112.87	120.95
1	C	34	GLY	C-N-CA	-5.77	112.87	120.95
1	O	67	PHE	CZ-CE2-CD2	-5.77	109.62	120.00
2	R	257	VAL	CA-C-N	-5.76	111.05	121.14
2	R	257	VAL	C-N-CA	-5.76	111.05	121.14
2	D	176	LYS	N-CA-C	5.76	120.15	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	281	GLN	N-CA-C	5.76	119.12	111.75
2	L	281	GLN	N-CA-C	5.76	119.12	111.75
1	Q	34	GLY	CA-C-N	-5.76	112.88	120.95
1	Q	34	GLY	C-N-CA	-5.76	112.88	120.95
2	R	281	GLN	N-CA-C	5.76	119.12	111.75
1	K	8	HIS	CA-CB-CG	-5.76	108.04	113.80
1	K	97	GLU	N-CA-C	5.76	117.82	108.26
1	Q	97	GLU	N-CA-C	5.76	117.82	108.26
2	B	257	VAL	CA-C-N	-5.76	111.07	121.14
2	B	257	VAL	C-N-CA	-5.76	111.07	121.14
1	E	97	GLU	N-CA-C	5.76	117.82	108.26
1	I	97	GLU	N-CA-C	5.76	117.81	108.26
2	J	257	VAL	CA-C-N	-5.76	111.06	121.14
2	J	257	VAL	C-N-CA	-5.76	111.06	121.14
2	J	338	LYS	CA-C-N	-5.75	114.58	122.87
2	J	338	LYS	C-N-CA	-5.75	114.58	122.87
1	G	8	HIS	CA-CB-CG	-5.75	108.05	113.80
2	H	338	LYS	CA-C-N	-5.75	114.59	122.87
2	H	338	LYS	C-N-CA	-5.75	114.59	122.87
2	L	338	LYS	CA-C-N	-5.75	114.58	122.87
2	L	338	LYS	C-N-CA	-5.75	114.58	122.87
2	R	176	LYS	N-CA-C	5.75	120.14	113.18
2	R	238	VAL	N-CA-C	5.75	115.88	110.30
2	N	338	LYS	CA-C-N	-5.75	114.59	122.87
2	N	338	LYS	C-N-CA	-5.75	114.59	122.87
2	P	257	VAL	CA-C-N	-5.75	111.08	121.14
2	P	257	VAL	C-N-CA	-5.75	111.08	121.14
2	L	257	VAL	CA-C-N	-5.75	111.08	121.14
2	L	257	VAL	C-N-CA	-5.75	111.08	121.14
2	R	338	LYS	CA-C-N	-5.75	114.60	122.87
2	R	338	LYS	C-N-CA	-5.75	114.60	122.87
2	B	338	LYS	CA-C-N	-5.74	114.60	122.87
2	B	338	LYS	C-N-CA	-5.74	114.60	122.87
1	C	8	HIS	CA-CB-CG	-5.74	108.06	113.80
1	C	97	GLU	N-CA-C	5.74	117.79	108.26
1	A	97	GLU	N-CA-C	5.74	117.79	108.26
2	F	257	VAL	CA-C-N	-5.74	111.10	121.14
2	F	257	VAL	C-N-CA	-5.74	111.10	121.14
2	D	257	VAL	CA-C-N	-5.74	111.10	121.14
2	D	257	VAL	C-N-CA	-5.74	111.10	121.14
1	G	97	GLU	N-CA-C	5.73	117.78	108.26
1	M	97	GLU	N-CA-C	5.73	117.78	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	97	GLU	N-CA-C	5.73	117.77	108.26
2	F	238	VAL	N-CA-C	5.73	115.86	110.30
2	R	59	ASN	CA-CB-CG	5.73	118.33	112.60
2	D	338	LYS	CA-C-N	-5.73	114.62	122.87
2	D	338	LYS	C-N-CA	-5.73	114.62	122.87
2	R	33	THR	CA-C-N	-5.72	115.35	123.08
2	R	33	THR	C-N-CA	-5.72	115.35	123.08
2	N	33	THR	CA-C-N	-5.72	115.36	123.08
2	N	33	THR	C-N-CA	-5.72	115.36	123.08
2	F	47	GLU	CA-C-N	-5.72	114.11	122.86
2	F	47	GLU	C-N-CA	-5.72	114.11	122.86
2	J	64	ARG	NH1-CZ-NH2	-5.72	111.86	119.30
2	P	64	ARG	NH1-CZ-NH2	-5.72	111.87	119.30
1	E	8	HIS	CA-CB-CG	-5.72	108.08	113.80
1	A	8	HIS	CA-CB-CG	-5.71	108.08	113.80
2	H	47	GLU	CA-C-N	-5.71	114.12	122.86
2	H	47	GLU	C-N-CA	-5.71	114.12	122.86
2	R	64	ARG	NH1-CZ-NH2	-5.71	111.88	119.30
2	D	64	ARG	NH1-CZ-NH2	-5.71	111.88	119.30
2	F	33	THR	CA-C-N	-5.71	115.38	123.08
2	F	33	THR	C-N-CA	-5.71	115.38	123.08
2	F	64	ARG	NH1-CZ-NH2	-5.71	111.88	119.30
2	J	33	THR	CA-C-N	-5.70	115.38	123.08
2	J	33	THR	C-N-CA	-5.70	115.38	123.08
1	O	8	HIS	CA-CB-CG	-5.70	108.10	113.80
2	N	47	GLU	CA-C-N	-5.70	114.14	122.86
2	N	47	GLU	C-N-CA	-5.70	114.14	122.86
2	B	47	GLU	CA-C-N	-5.70	114.14	122.86
2	B	47	GLU	C-N-CA	-5.70	114.14	122.86
2	D	47	GLU	CA-C-N	-5.70	114.14	122.86
2	D	47	GLU	C-N-CA	-5.70	114.14	122.86
2	P	47	GLU	CA-C-N	-5.70	114.14	122.86
2	P	47	GLU	C-N-CA	-5.70	114.14	122.86
1	I	8	HIS	CA-CB-CG	-5.70	108.10	113.80
2	J	47	GLU	CA-C-N	-5.69	114.15	122.86
2	J	47	GLU	C-N-CA	-5.69	114.15	122.86
2	R	47	GLU	CA-C-N	-5.69	114.15	122.86
2	R	47	GLU	C-N-CA	-5.69	114.15	122.86
2	B	64	ARG	NH1-CZ-NH2	-5.69	111.90	119.30
2	B	33	THR	CA-C-N	-5.69	115.40	123.08
2	B	33	THR	C-N-CA	-5.69	115.40	123.08
1	M	8	HIS	CA-CB-CG	-5.68	108.11	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	64	ARG	NH1-CZ-NH2	-5.68	111.91	119.30
2	D	33	THR	CA-C-N	-5.68	115.41	123.08
2	D	33	THR	C-N-CA	-5.68	115.41	123.08
2	N	222	PRO	N-CA-C	5.68	119.38	110.80
2	H	64	ARG	NH1-CZ-NH2	-5.68	111.92	119.30
2	L	33	THR	CA-C-N	-5.68	115.41	123.08
2	L	33	THR	C-N-CA	-5.68	115.41	123.08
1	M	352	LYS	N-CA-C	5.68	118.48	109.96
2	P	33	THR	CA-C-N	-5.68	115.41	123.08
2	P	33	THR	C-N-CA	-5.68	115.41	123.08
2	P	222	PRO	N-CA-C	5.68	119.37	110.80
1	Q	8	HIS	CA-CB-CG	-5.68	108.12	113.80
2	L	47	GLU	CA-C-N	-5.68	114.17	122.86
2	L	47	GLU	C-N-CA	-5.68	114.17	122.86
2	N	64	ARG	NH1-CZ-NH2	-5.68	111.92	119.30
1	G	250	VAL	CA-C-N	-5.67	112.86	122.67
1	G	250	VAL	C-N-CA	-5.67	112.86	122.67
1	K	250	VAL	CA-C-N	-5.67	112.85	122.67
1	K	250	VAL	C-N-CA	-5.67	112.85	122.67
1	O	250	VAL	CA-C-N	-5.67	112.85	122.67
1	O	250	VAL	C-N-CA	-5.67	112.85	122.67
1	C	250	VAL	CA-C-N	-5.67	112.86	122.67
1	C	250	VAL	C-N-CA	-5.67	112.86	122.67
1	I	250	VAL	CA-C-N	-5.67	112.86	122.67
1	I	250	VAL	C-N-CA	-5.67	112.86	122.67
2	F	371	LEU	CA-C-N	-5.67	111.05	120.68
2	F	371	LEU	C-N-CA	-5.67	111.05	120.68
2	J	371	LEU	CA-C-N	-5.67	111.05	120.68
2	J	371	LEU	C-N-CA	-5.67	111.05	120.68
2	B	222	PRO	N-CA-C	5.66	119.35	110.80
1	Q	352	LYS	N-CA-C	5.66	118.46	109.96
1	A	250	VAL	CA-C-N	-5.66	112.88	122.67
1	A	250	VAL	C-N-CA	-5.66	112.88	122.67
1	K	352	LYS	N-CA-C	5.66	118.45	109.96
1	K	263	PRO	CA-C-N	-5.66	114.19	122.06
1	K	263	PRO	C-N-CA	-5.66	114.19	122.06
2	H	33	THR	CA-C-N	-5.66	115.44	123.08
2	H	33	THR	C-N-CA	-5.66	115.44	123.08
1	Q	250	VAL	CA-C-N	-5.66	112.88	122.67
1	Q	250	VAL	C-N-CA	-5.66	112.88	122.67
1	A	352	LYS	N-CA-C	5.66	118.44	109.96
1	E	352	LYS	N-CA-C	5.66	118.44	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	222	PRO	N-CA-C	5.66	119.34	110.80
2	J	222	PRO	N-CA-C	5.66	119.34	110.80
2	L	371	LEU	CA-C-N	-5.66	111.06	120.68
2	L	371	LEU	C-N-CA	-5.66	111.06	120.68
1	E	250	VAL	CA-C-N	-5.65	112.89	122.67
1	E	250	VAL	C-N-CA	-5.65	112.89	122.67
2	H	371	LEU	CA-C-N	-5.65	111.07	120.68
2	H	371	LEU	C-N-CA	-5.65	111.07	120.68
1	I	352	LYS	N-CA-C	5.65	118.44	109.96
2	R	371	LEU	CA-C-N	-5.65	111.07	120.68
2	R	371	LEU	C-N-CA	-5.65	111.07	120.68
2	D	222	PRO	N-CA-C	5.65	119.33	110.80
2	N	371	LEU	CA-C-N	-5.65	111.07	120.68
2	N	371	LEU	C-N-CA	-5.65	111.07	120.68
1	C	352	LYS	N-CA-C	5.65	118.43	109.96
2	B	371	LEU	CA-C-N	-5.65	111.08	120.68
2	B	371	LEU	C-N-CA	-5.65	111.08	120.68
1	C	263	PRO	CA-C-N	-5.65	114.21	122.06
1	C	263	PRO	C-N-CA	-5.65	114.21	122.06
2	D	371	LEU	CA-C-N	-5.65	111.08	120.68
2	D	371	LEU	C-N-CA	-5.65	111.08	120.68
1	G	352	LYS	N-CA-C	5.65	118.43	109.96
1	E	390	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	M	250	VAL	CA-C-N	-5.64	112.91	122.67
1	M	250	VAL	C-N-CA	-5.64	112.91	122.67
1	K	390	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	M	390	ARG	NE-CZ-NH2	5.64	124.27	119.20
1	Q	263	PRO	CA-C-N	-5.64	114.22	122.06
1	Q	263	PRO	C-N-CA	-5.64	114.22	122.06
1	O	352	LYS	N-CA-C	5.64	118.42	109.96
1	A	263	PRO	CA-C-N	-5.63	114.23	122.06
1	A	263	PRO	C-N-CA	-5.63	114.23	122.06
2	P	371	LEU	CA-C-N	-5.63	111.11	120.68
2	P	371	LEU	C-N-CA	-5.63	111.11	120.68
2	R	222	PRO	N-CA-C	5.63	119.30	110.80
1	A	390	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	I	263	PRO	CA-C-N	-5.63	114.24	122.06
1	I	263	PRO	C-N-CA	-5.63	114.24	122.06
1	E	263	PRO	CA-C-N	-5.63	114.24	122.06
1	E	263	PRO	C-N-CA	-5.63	114.24	122.06
1	M	263	PRO	CA-C-N	-5.63	114.24	122.06
1	M	263	PRO	C-N-CA	-5.63	114.24	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	263	PRO	CA-C-N	-5.62	114.25	122.06
1	G	263	PRO	C-N-CA	-5.62	114.25	122.06
1	I	390	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	O	263	PRO	CA-C-N	-5.61	114.26	122.06
1	O	263	PRO	C-N-CA	-5.61	114.26	122.06
1	Q	390	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	C	390	ARG	NE-CZ-NH2	5.60	124.24	119.20
2	H	98	GLY	O-C-N	5.60	130.45	122.61
2	L	98	GLY	O-C-N	5.60	130.45	122.61
1	G	390	ARG	NE-CZ-NH2	5.59	124.23	119.20
2	J	352	LYS	CA-C-N	-5.59	112.50	122.07
2	J	352	LYS	C-N-CA	-5.59	112.50	122.07
2	P	98	GLY	O-C-N	5.59	130.44	122.61
2	B	98	GLY	O-C-N	5.59	130.44	122.61
2	J	98	GLY	O-C-N	5.59	130.44	122.61
2	D	98	GLY	O-C-N	5.59	130.44	122.61
1	O	390	ARG	NE-CZ-NH2	5.58	124.23	119.20
1	C	243	ARG	N-CA-C	5.58	118.30	111.82
2	D	352	LYS	CA-C-N	-5.58	112.53	122.07
2	D	352	LYS	C-N-CA	-5.58	112.53	122.07
2	F	98	GLY	O-C-N	5.58	130.42	122.61
1	G	243	ARG	N-CA-C	5.58	118.29	111.82
1	K	243	ARG	N-CA-C	5.58	118.29	111.82
2	N	98	GLY	O-C-N	5.58	130.42	122.61
2	P	352	LYS	CA-C-N	-5.58	112.53	122.07
2	P	352	LYS	C-N-CA	-5.58	112.53	122.07
1	E	243	ARG	N-CA-C	5.57	118.28	111.82
2	L	352	LYS	CA-C-N	-5.57	112.55	122.07
2	L	352	LYS	C-N-CA	-5.57	112.55	122.07
2	B	352	LYS	CA-C-N	-5.57	112.55	122.07
2	B	352	LYS	C-N-CA	-5.57	112.55	122.07
2	F	352	LYS	CA-C-N	-5.57	112.55	122.07
2	F	352	LYS	C-N-CA	-5.57	112.55	122.07
1	I	243	ARG	N-CA-C	5.57	118.28	111.82
2	R	98	GLY	O-C-N	5.56	130.40	122.61
2	H	352	LYS	CA-C-N	-5.56	112.56	122.07
2	H	352	LYS	C-N-CA	-5.56	112.56	122.07
2	N	352	LYS	CA-C-N	-5.56	112.57	122.07
2	N	352	LYS	C-N-CA	-5.56	112.57	122.07
1	A	243	ARG	N-CA-C	5.55	118.26	111.82
1	Q	243	ARG	N-CA-C	5.55	118.26	111.82
1	O	243	ARG	N-CA-C	5.55	118.26	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	352	LYS	CA-C-N	-5.54	112.59	122.07
2	R	352	LYS	C-N-CA	-5.54	112.59	122.07
2	F	139	HIS	N-CA-C	5.53	115.85	108.38
1	M	243	ARG	N-CA-C	5.53	118.23	111.82
2	L	169	PHE	CA-C-N	-5.52	114.01	122.62
2	L	169	PHE	C-N-CA	-5.52	114.01	122.62
2	B	139	HIS	N-CA-C	5.51	115.83	108.38
2	R	179	ASP	CA-CB-CG	5.51	118.11	112.60
2	D	139	HIS	N-CA-C	5.51	115.82	108.38
2	J	139	HIS	N-CA-C	5.51	115.82	108.38
2	L	179	ASP	CA-CB-CG	5.51	118.11	112.60
2	N	179	ASP	CA-CB-CG	5.51	118.11	112.60
2	D	179	ASP	CA-CB-CG	5.50	118.10	112.60
2	B	179	ASP	CA-CB-CG	5.50	118.10	112.60
2	P	179	ASP	CA-CB-CG	5.50	118.10	112.60
2	R	14	ASN	CA-CB-CG	-5.50	107.10	112.60
2	P	139	HIS	N-CA-C	5.50	115.80	108.38
1	M	359	PRO	O-C-N	5.50	123.84	121.31
2	D	169	PHE	CA-C-N	-5.49	114.05	122.62
2	D	169	PHE	C-N-CA	-5.49	114.05	122.62
2	L	14	ASN	CA-CB-CG	-5.49	107.11	112.60
2	L	139	HIS	N-CA-C	5.49	115.80	108.38
2	R	58	GLY	O-C-N	5.49	128.92	122.38
2	D	14	ASN	CA-CB-CG	-5.49	107.11	112.60
2	N	139	HIS	N-CA-C	5.49	115.79	108.38
2	H	139	HIS	N-CA-C	5.49	115.79	108.38
2	J	14	ASN	CA-CB-CG	-5.49	107.11	112.60
2	L	50	ASN	N-CA-C	5.49	122.49	110.80
2	F	179	ASP	CA-CB-CG	5.49	118.09	112.60
2	N	14	ASN	CA-CB-CG	-5.49	107.11	112.60
2	P	169	PHE	CA-C-N	-5.49	114.06	122.62
2	P	169	PHE	C-N-CA	-5.49	114.06	122.62
2	B	169	PHE	CA-C-N	-5.49	114.06	122.62
2	B	169	PHE	C-N-CA	-5.49	114.06	122.62
2	D	58	GLY	O-C-N	5.49	128.91	122.38
2	R	169	PHE	CA-C-N	-5.48	114.06	122.62
2	R	169	PHE	C-N-CA	-5.48	114.06	122.62
2	B	14	ASN	CA-CB-CG	-5.48	107.12	112.60
2	N	169	PHE	CA-C-N	-5.48	114.07	122.62
2	N	169	PHE	C-N-CA	-5.48	114.07	122.62
2	F	169	PHE	CA-C-N	-5.48	114.07	122.62
2	F	169	PHE	C-N-CA	-5.48	114.07	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	50	ASN	N-CA-C	5.48	122.47	110.80
2	J	169	PHE	CA-C-N	-5.48	114.07	122.62
2	J	169	PHE	C-N-CA	-5.48	114.07	122.62
2	F	14	ASN	CA-CB-CG	-5.48	107.12	112.60
2	H	14	ASN	CA-CB-CG	-5.48	107.12	112.60
2	L	58	GLY	O-C-N	5.48	128.90	122.38
2	R	50	ASN	N-CA-C	5.48	122.47	110.80
2	J	179	ASP	CA-CB-CG	5.48	118.08	112.60
2	P	14	ASN	CA-CB-CG	-5.48	107.12	112.60
2	R	139	HIS	N-CA-C	5.47	115.77	108.38
2	H	58	GLY	O-C-N	5.47	128.89	122.38
2	J	50	ASN	N-CA-C	5.47	122.46	110.80
2	B	58	GLY	O-C-N	5.47	128.89	122.38
2	D	352	LYS	N-CA-C	5.46	117.64	108.73
2	H	179	ASP	CA-CB-CG	5.46	118.06	112.60
2	B	50	ASN	N-CA-C	5.46	122.43	110.80
2	F	50	ASN	N-CA-C	5.46	122.43	110.80
2	F	58	GLY	O-C-N	5.46	128.88	122.38
2	F	352	LYS	N-CA-C	5.46	117.63	108.73
2	D	50	ASN	N-CA-C	5.46	122.42	110.80
2	H	169	PHE	CA-C-N	-5.46	114.11	122.62
2	H	169	PHE	C-N-CA	-5.46	114.11	122.62
2	N	50	ASN	N-CA-C	5.46	122.42	110.80
2	J	58	GLY	O-C-N	5.45	128.87	122.38
2	P	50	ASN	N-CA-C	5.45	122.41	110.80
2	H	352	LYS	N-CA-C	5.45	117.61	108.73
2	P	58	GLY	O-C-N	5.45	128.86	122.38
2	N	58	GLY	O-C-N	5.44	128.86	122.38
1	Q	284	GLU	O-C-N	5.44	130.13	123.44
2	N	352	LYS	N-CA-C	5.44	117.59	108.73
2	B	352	LYS	N-CA-C	5.43	117.59	108.73
1	C	99	ALA	N-CA-C	5.43	119.90	113.16
1	I	138	PHE	CA-CB-CG	-5.43	108.37	113.80
1	E	99	ALA	N-CA-C	5.43	119.89	113.16
2	L	352	LYS	N-CA-C	5.43	117.57	108.73
1	M	99	ALA	N-CA-C	5.43	119.89	113.16
1	O	138	PHE	CA-CB-CG	-5.43	108.37	113.80
2	J	352	LYS	N-CA-C	5.42	117.57	108.73
1	K	138	PHE	CA-CB-CG	-5.42	108.38	113.80
1	O	99	ALA	N-CA-C	5.42	119.89	113.16
1	C	319	TYR	N-CA-C	5.42	118.32	109.59
1	O	359	PRO	O-C-N	5.42	123.80	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	319	TYR	N-CA-C	5.42	118.32	109.59
1	A	138	PHE	CA-CB-CG	-5.42	108.38	113.80
1	C	359	PRO	O-C-N	5.42	123.80	121.31
1	I	284	GLU	O-C-N	5.42	130.10	123.44
1	Q	359	PRO	O-C-N	5.42	123.80	121.31
1	G	379	SER	N-CA-C	5.42	117.49	108.99
1	I	319	TYR	N-CA-C	5.41	118.31	109.59
1	O	284	GLU	CA-C-O	5.41	127.52	120.21
2	P	352	LYS	N-CA-C	5.41	117.56	108.73
1	I	176	GLN	N-CA-C	5.41	119.99	112.90
1	G	138	PHE	CA-CB-CG	-5.41	108.39	113.80
1	G	359	PRO	O-C-N	5.41	123.80	121.31
1	Q	176	GLN	N-CA-C	5.41	119.99	112.90
1	A	99	ALA	N-CA-C	5.41	119.87	113.16
1	A	284	GLU	O-C-N	5.41	130.09	123.44
1	C	284	GLU	O-C-N	5.41	130.09	123.44
1	E	284	GLU	O-C-N	5.41	130.09	123.44
1	I	359	PRO	O-C-N	5.41	123.80	121.31
1	Q	99	ALA	N-CA-C	5.41	119.86	113.16
1	K	99	ALA	N-CA-C	5.40	119.86	113.16
1	K	319	TYR	N-CA-C	5.40	118.29	109.59
1	C	176	GLN	N-CA-C	5.40	119.97	112.90
1	G	284	GLU	CA-C-O	5.40	127.50	120.21
1	K	176	GLN	N-CA-C	5.40	119.97	112.90
1	O	379	SER	N-CA-C	5.40	117.47	108.99
1	I	99	ALA	N-CA-C	5.40	119.86	113.16
1	O	319	TYR	N-CA-C	5.40	118.28	109.59
1	A	319	TYR	N-CA-C	5.40	118.28	109.59
1	M	319	TYR	N-CA-C	5.40	118.28	109.59
2	R	352	LYS	N-CA-C	5.40	117.53	108.73
1	M	138	PHE	CA-CB-CG	-5.39	108.41	113.80
2	P	297	ASP	CA-C-N	5.39	128.25	120.38
2	P	297	ASP	C-N-CA	5.39	128.25	120.38
1	Q	138	PHE	CA-CB-CG	-5.39	108.41	113.80
1	A	359	PRO	O-C-N	5.39	123.79	121.31
1	C	138	PHE	CA-CB-CG	-5.39	108.41	113.80
2	J	166	MET	CA-C-N	-5.39	114.12	122.59
2	J	166	MET	C-N-CA	-5.39	114.12	122.59
2	R	166	MET	CA-C-N	-5.39	114.13	122.59
2	R	166	MET	C-N-CA	-5.39	114.13	122.59
1	A	176	GLN	N-CA-C	5.39	119.96	112.90
1	M	284	GLU	O-C-N	5.39	130.07	123.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	138	PHE	CA-CB-CG	-5.39	108.41	113.80
1	E	176	GLN	N-CA-C	5.39	119.96	112.90
1	G	319	TYR	N-CA-C	5.39	118.26	109.59
1	K	379	SER	N-CA-C	5.39	117.45	108.99
1	M	176	GLN	N-CA-C	5.39	119.96	112.90
2	N	57	ALA	CA-C-N	-5.39	113.32	121.51
2	N	57	ALA	C-N-CA	-5.39	113.32	121.51
2	D	297	ASP	CA-C-N	5.38	128.24	120.38
2	D	297	ASP	C-N-CA	5.38	128.24	120.38
1	O	176	GLN	N-CA-C	5.38	119.95	112.90
1	A	379	SER	N-CA-C	5.38	117.44	108.99
2	H	222	PRO	N-CA-C	5.38	119.32	111.03
1	Q	379	SER	N-CA-C	5.38	117.44	108.99
1	G	435	VAL	CA-C-N	-5.38	110.86	121.41
1	G	435	VAL	C-N-CA	-5.38	110.86	121.41
1	O	284	GLU	O-C-N	5.38	130.06	123.44
1	E	359	PRO	O-C-N	5.38	123.78	121.31
1	E	379	SER	N-CA-C	5.38	117.44	108.99
1	G	176	GLN	N-CA-C	5.38	119.95	112.90
2	L	398	MET	N-CA-C	5.38	117.14	111.28
2	D	57	ALA	CA-C-N	-5.38	113.33	121.51
2	D	57	ALA	C-N-CA	-5.38	113.33	121.51
1	E	435	VAL	CA-C-N	-5.38	110.87	121.41
1	E	435	VAL	C-N-CA	-5.38	110.87	121.41
1	G	99	ALA	N-CA-C	5.38	119.83	113.16
2	L	222	PRO	N-CA-C	5.38	119.31	111.03
2	P	258	ASN	CA-CB-CG	-5.38	107.22	112.60
2	B	166	MET	CA-C-N	-5.38	114.15	122.59
2	B	166	MET	C-N-CA	-5.38	114.15	122.59
2	D	398	MET	N-CA-C	5.38	117.14	111.28
1	E	319	TYR	N-CA-C	5.38	118.25	109.59
1	G	284	GLU	O-C-N	5.38	130.05	123.44
2	L	297	ASP	CA-C-N	5.38	128.23	120.38
2	L	297	ASP	C-N-CA	5.38	128.23	120.38
1	I	435	VAL	CA-C-N	-5.38	110.88	121.41
1	I	435	VAL	C-N-CA	-5.38	110.88	121.41
1	K	284	GLU	O-C-N	5.38	130.05	123.44
1	C	379	SER	N-CA-C	5.37	117.43	108.99
1	C	435	VAL	CA-C-N	-5.37	110.88	121.41
1	C	435	VAL	C-N-CA	-5.37	110.88	121.41
2	F	166	MET	CA-C-N	-5.37	114.16	122.59
2	F	166	MET	C-N-CA	-5.37	114.16	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	297	ASP	CA-C-N	5.37	128.22	120.38
2	J	297	ASP	C-N-CA	5.37	128.22	120.38
1	K	435	VAL	CA-C-N	-5.37	110.88	121.41
1	K	435	VAL	C-N-CA	-5.37	110.88	121.41
2	H	398	MET	N-CA-C	5.37	117.13	111.28
1	A	435	VAL	CA-C-N	-5.37	110.89	121.41
1	A	435	VAL	C-N-CA	-5.37	110.89	121.41
2	D	166	MET	CA-C-N	-5.37	114.16	122.59
2	D	166	MET	C-N-CA	-5.37	114.16	122.59
2	H	166	MET	CA-C-N	-5.37	114.16	122.59
2	H	166	MET	C-N-CA	-5.37	114.16	122.59
1	I	379	SER	N-CA-C	5.37	117.42	108.99
2	N	166	MET	CA-C-N	-5.37	114.16	122.59
2	N	166	MET	C-N-CA	-5.37	114.16	122.59
2	N	297	ASP	CA-C-N	5.37	128.22	120.38
2	N	297	ASP	C-N-CA	5.37	128.22	120.38
1	A	284	GLU	CA-C-O	5.37	127.46	120.21
2	B	398	MET	N-CA-C	5.37	117.13	111.28
2	L	57	ALA	CA-C-N	-5.37	113.36	121.51
2	L	57	ALA	C-N-CA	-5.37	113.36	121.51
2	H	57	ALA	CA-C-N	-5.36	113.36	121.51
2	H	57	ALA	C-N-CA	-5.36	113.36	121.51
2	B	57	ALA	CA-C-N	-5.36	113.36	121.51
2	B	57	ALA	C-N-CA	-5.36	113.36	121.51
2	F	57	ALA	CA-C-N	-5.36	113.36	121.51
2	F	57	ALA	C-N-CA	-5.36	113.36	121.51
2	H	297	ASP	CA-C-N	5.36	128.21	120.38
2	H	297	ASP	C-N-CA	5.36	128.21	120.38
2	R	297	ASP	CA-C-N	5.36	128.21	120.38
2	R	297	ASP	C-N-CA	5.36	128.21	120.38
1	C	284	GLU	CA-C-O	5.36	127.45	120.21
1	K	284	GLU	CA-C-O	5.36	127.45	120.21
1	M	284	GLU	CA-C-O	5.36	127.45	120.21
2	P	166	MET	CA-C-N	-5.36	114.17	122.59
2	P	166	MET	C-N-CA	-5.36	114.17	122.59
2	B	297	ASP	CA-C-N	5.36	128.20	120.38
2	B	297	ASP	C-N-CA	5.36	128.20	120.38
2	F	398	MET	N-CA-C	5.36	117.12	111.28
2	J	57	ALA	CA-C-N	-5.36	113.37	121.51
2	J	57	ALA	C-N-CA	-5.36	113.37	121.51
1	O	435	VAL	CA-C-N	-5.36	110.91	121.41
1	O	435	VAL	C-N-CA	-5.36	110.91	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	398	MET	N-CA-C	5.36	117.12	111.28
1	E	284	GLU	CA-C-O	5.36	127.44	120.21
2	F	297	ASP	CA-C-N	5.36	128.20	120.38
2	F	297	ASP	C-N-CA	5.36	128.20	120.38
1	M	435	VAL	CA-C-N	-5.36	110.91	121.41
1	M	435	VAL	C-N-CA	-5.36	110.91	121.41
1	M	379	SER	N-CA-C	5.35	117.39	108.99
1	O	36	MET	CA-C-N	5.35	126.53	119.84
1	O	36	MET	C-N-CA	5.35	126.53	119.84
2	P	57	ALA	CA-C-N	-5.35	113.37	121.51
2	P	57	ALA	C-N-CA	-5.35	113.37	121.51
1	K	36	MET	CA-C-N	5.35	126.53	119.84
1	K	36	MET	C-N-CA	5.35	126.53	119.84
2	P	398	MET	N-CA-C	5.35	117.11	111.28
1	Q	284	GLU	CA-C-O	5.35	127.43	120.21
1	I	284	GLU	CA-C-O	5.35	127.43	120.21
2	J	398	MET	N-CA-C	5.35	117.11	111.28
2	L	166	MET	CA-C-N	-5.35	114.20	122.59
2	L	166	MET	C-N-CA	-5.35	114.20	122.59
1	O	179	THR	CA-C-N	-5.34	112.53	121.94
1	O	179	THR	C-N-CA	-5.34	112.53	121.94
2	P	360	PRO	CA-C-N	-5.34	113.28	120.87
2	P	360	PRO	C-N-CA	-5.34	113.28	120.87
1	I	179	THR	CA-C-N	-5.34	112.54	121.94
1	I	179	THR	C-N-CA	-5.34	112.54	121.94
2	L	380	ASN	CA-CB-CG	5.34	117.94	112.60
2	N	360	PRO	CA-C-N	-5.34	113.28	120.87
2	N	360	PRO	C-N-CA	-5.34	113.28	120.87
2	R	165	ILE	CA-C-N	-5.34	115.89	122.84
2	R	165	ILE	C-N-CA	-5.34	115.89	122.84
2	H	258	ASN	CA-CB-CG	-5.34	107.26	112.60
2	R	57	ALA	CA-C-N	-5.34	113.39	121.51
2	R	57	ALA	C-N-CA	-5.34	113.39	121.51
2	R	380	ASN	CA-CB-CG	5.34	117.94	112.60
1	Q	435	VAL	CA-C-N	-5.34	110.95	121.41
1	Q	435	VAL	C-N-CA	-5.34	110.95	121.41
2	R	430	SER	CB-CA-C	-5.34	100.75	110.63
1	C	179	THR	CA-C-N	-5.34	112.55	121.94
1	C	179	THR	C-N-CA	-5.34	112.55	121.94
1	E	36	MET	CA-C-N	5.34	126.51	119.84
1	E	36	MET	C-N-CA	5.34	126.51	119.84
1	K	339	ARG	CB-CA-C	-5.33	102.64	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	179	THR	CA-C-N	-5.33	112.55	121.94
1	E	179	THR	C-N-CA	-5.33	112.55	121.94
2	F	380	ASN	CA-CB-CG	5.33	117.93	112.60
2	R	258	ASN	CA-CB-CG	-5.33	107.27	112.60
1	G	210	TYR	CB-CA-C	-5.33	101.94	110.79
1	I	210	TYR	CB-CA-C	-5.33	101.94	110.79
2	L	400	ARG	CA-C-O	-5.33	115.19	120.90
2	N	398	MET	N-CA-C	5.33	117.09	111.28
1	A	179	THR	CA-C-N	-5.33	112.56	121.94
1	A	179	THR	C-N-CA	-5.33	112.56	121.94
2	B	258	ASN	CA-CB-CG	-5.33	107.27	112.60
1	G	36	MET	CA-C-N	5.33	126.50	119.84
1	G	36	MET	C-N-CA	5.33	126.50	119.84
2	D	8	GLN	CA-C-N	-5.33	113.21	122.37
2	D	8	GLN	C-N-CA	-5.33	113.21	122.37
1	Q	179	THR	CA-C-N	-5.33	112.57	121.94
1	Q	179	THR	C-N-CA	-5.33	112.57	121.94
1	Q	210	TYR	CB-CA-C	-5.33	101.95	110.79
1	A	36	MET	CA-C-N	5.32	126.50	119.84
1	A	36	MET	C-N-CA	5.32	126.50	119.84
2	F	258	ASN	CA-CB-CG	-5.32	107.28	112.60
1	G	179	THR	CA-C-N	-5.32	112.57	121.94
1	G	179	THR	C-N-CA	-5.32	112.57	121.94
2	L	360	PRO	CA-C-N	-5.32	113.31	120.87
2	L	360	PRO	C-N-CA	-5.32	113.31	120.87
1	Q	339	ARG	CB-CA-C	-5.32	102.66	110.06
1	I	36	MET	CA-C-N	5.32	126.49	119.84
1	I	36	MET	C-N-CA	5.32	126.49	119.84
2	J	8	GLN	CA-C-N	-5.32	113.22	122.37
2	J	8	GLN	C-N-CA	-5.32	113.22	122.37
2	J	380	ASN	CA-CB-CG	5.32	117.92	112.60
1	K	359	PRO	O-C-N	5.32	123.76	121.31
1	C	339	ARG	CB-CA-C	-5.32	102.67	110.06
2	F	430	SER	CB-CA-C	-5.32	100.79	110.63
2	B	380	ASN	CA-CB-CG	5.32	117.92	112.60
2	F	360	PRO	CA-C-N	-5.32	113.32	120.87
2	F	360	PRO	C-N-CA	-5.32	113.32	120.87
2	L	258	ASN	CA-CB-CG	-5.32	107.28	112.60
1	C	210	TYR	CB-CA-C	-5.32	101.97	110.79
2	D	380	ASN	CA-CB-CG	5.32	117.92	112.60
1	M	210	TYR	CB-CA-C	-5.32	101.97	110.79
1	Q	36	MET	CA-C-N	5.32	126.48	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	36	MET	C-N-CA	5.32	126.48	119.84
1	A	210	TYR	CB-CA-C	-5.31	101.97	110.79
2	J	430	SER	CB-CA-C	-5.31	100.80	110.63
1	M	339	ARG	CB-CA-C	-5.31	102.67	110.06
2	N	430	SER	CB-CA-C	-5.31	100.80	110.63
2	P	165	ILE	CA-C-N	-5.31	115.93	122.84
2	P	165	ILE	C-N-CA	-5.31	115.93	122.84
2	B	430	SER	CB-CA-C	-5.31	100.80	110.63
1	K	179	THR	CA-C-N	-5.31	112.59	121.94
1	K	179	THR	C-N-CA	-5.31	112.59	121.94
2	P	430	SER	CB-CA-C	-5.31	100.80	110.63
2	H	360	PRO	CA-C-N	-5.31	113.33	120.87
2	H	360	PRO	C-N-CA	-5.31	113.33	120.87
2	B	360	PRO	CA-C-N	-5.31	113.33	120.87
2	B	360	PRO	C-N-CA	-5.31	113.33	120.87
2	D	258	ASN	CA-CB-CG	-5.31	107.29	112.60
2	J	400	ARG	CA-C-O	-5.31	115.22	120.90
2	L	31	ASP	CA-CB-CG	5.31	117.91	112.60
2	B	8	GLN	CA-C-N	-5.31	113.24	122.37
2	B	8	GLN	C-N-CA	-5.31	113.24	122.37
1	G	339	ARG	CB-CA-C	-5.31	102.68	110.06
2	H	430	SER	CB-CA-C	-5.31	100.81	110.63
1	I	84	ARG	N-CA-C	5.31	119.24	112.87
1	M	36	MET	CA-C-N	5.31	126.47	119.84
1	M	36	MET	C-N-CA	5.31	126.47	119.84
1	E	210	TYR	CB-CA-C	-5.31	101.98	110.79
2	R	264	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	A	339	ARG	CB-CA-C	-5.30	102.69	110.06
2	D	430	SER	CB-CA-C	-5.30	100.82	110.63
2	P	380	ASN	CA-CB-CG	5.30	117.90	112.60
2	F	31	ASP	CA-CB-CG	5.30	117.90	112.60
2	J	258	ASN	CA-CB-CG	-5.30	107.30	112.60
1	M	179	THR	CA-C-N	-5.30	112.61	121.94
1	M	179	THR	C-N-CA	-5.30	112.61	121.94
2	N	8	GLN	CA-C-N	-5.30	113.25	122.37
2	N	8	GLN	C-N-CA	-5.30	113.25	122.37
2	P	31	ASP	CA-CB-CG	5.30	117.90	112.60
2	D	165	ILE	CA-C-N	-5.30	115.95	122.84
2	D	165	ILE	C-N-CA	-5.30	115.95	122.84
2	N	380	ASN	CA-CB-CG	5.30	117.90	112.60
2	R	240	THR	N-CA-C	5.30	119.01	112.54
2	B	165	ILE	CA-C-N	-5.30	115.95	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	165	ILE	C-N-CA	-5.30	115.95	122.84
1	E	339	ARG	CB-CA-C	-5.30	102.69	110.06
1	K	84	ARG	N-CA-C	5.30	119.23	112.87
2	F	400	ARG	CA-C-O	-5.30	115.23	120.90
2	J	240	THR	N-CA-C	5.30	119.00	112.54
2	N	31	ASP	CA-CB-CG	5.30	117.90	112.60
2	N	240	THR	N-CA-C	5.30	119.00	112.54
1	O	210	TYR	CB-CA-C	-5.30	102.00	110.79
2	F	240	THR	N-CA-C	5.29	119.00	112.54
2	D	400	ARG	CA-C-O	-5.29	115.24	120.90
2	F	8	GLN	CA-C-N	-5.29	113.27	122.37
2	F	8	GLN	C-N-CA	-5.29	113.27	122.37
2	H	8	GLN	CA-C-N	-5.29	113.27	122.37
2	H	8	GLN	C-N-CA	-5.29	113.27	122.37
1	I	339	ARG	CB-CA-C	-5.29	102.71	110.06
1	O	339	ARG	CB-CA-C	-5.29	102.70	110.06
2	B	400	ARG	CA-C-O	-5.29	115.24	120.90
1	K	210	TYR	CB-CA-C	-5.29	102.01	110.79
2	B	31	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	36	MET	CA-C-N	5.29	126.45	119.84
1	C	36	MET	C-N-CA	5.29	126.45	119.84
2	L	8	GLN	CA-C-N	-5.29	113.28	122.37
2	L	8	GLN	C-N-CA	-5.29	113.28	122.37
2	N	400	ARG	CA-C-O	-5.29	115.24	120.90
1	E	51	THR	N-CA-C	-5.29	106.77	113.43
2	F	165	ILE	CA-C-N	-5.29	115.97	122.84
2	F	165	ILE	C-N-CA	-5.29	115.97	122.84
2	P	8	GLN	CA-C-N	-5.29	113.28	122.37
2	P	8	GLN	C-N-CA	-5.29	113.28	122.37
2	P	264	ARG	NE-CZ-NH2	-5.29	114.44	119.20
2	R	8	GLN	CA-C-N	-5.29	113.28	122.37
2	R	8	GLN	C-N-CA	-5.29	113.28	122.37
2	R	31	ASP	CA-CB-CG	5.29	117.89	112.60
2	H	165	ILE	CA-C-N	-5.28	115.97	122.84
2	H	165	ILE	C-N-CA	-5.28	115.97	122.84
2	H	380	ASN	CA-CB-CG	5.28	117.88	112.60
1	Q	51	THR	N-CA-C	-5.28	106.77	113.43
2	R	360	PRO	CA-C-N	-5.28	113.37	120.87
2	R	360	PRO	C-N-CA	-5.28	113.37	120.87
2	D	240	THR	N-CA-C	5.28	118.98	112.54
2	D	360	PRO	CA-C-N	-5.28	113.37	120.87
2	D	360	PRO	C-N-CA	-5.28	113.37	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	165	ILE	CA-C-N	-5.28	115.97	122.84
2	N	165	ILE	C-N-CA	-5.28	115.97	122.84
2	P	400	ARG	CA-C-O	-5.28	115.25	120.90
2	J	360	PRO	CA-C-N	-5.28	113.38	120.87
2	J	360	PRO	C-N-CA	-5.28	113.38	120.87
2	B	240	THR	N-CA-C	5.28	118.98	112.54
1	C	84	ARG	N-CA-C	5.28	119.20	112.87
2	D	31	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	84	ARG	N-CA-C	5.27	119.19	112.87
2	N	185	TYR	CB-CA-C	-5.27	102.61	110.88
1	Q	84	ARG	N-CA-C	5.27	119.20	112.87
1	G	84	ARG	N-CA-C	5.27	119.19	112.87
2	J	165	ILE	CA-C-N	-5.27	115.99	122.84
2	J	165	ILE	C-N-CA	-5.27	115.99	122.84
2	N	258	ASN	CA-CB-CG	-5.27	107.33	112.60
1	O	322	ASP	N-CA-C	5.27	118.17	108.58
2	J	185	TYR	CB-CA-C	-5.27	102.61	110.88
2	B	185	TYR	CB-CA-C	-5.26	102.62	110.88
2	J	31	ASP	CA-CB-CG	5.26	117.86	112.60
1	Q	322	ASP	N-CA-C	5.26	118.16	108.58
2	F	280	SER	N-CA-C	5.26	117.76	111.71
2	R	185	TYR	CB-CA-C	-5.26	102.62	110.88
2	H	240	THR	N-CA-C	5.26	118.96	112.54
2	L	165	ILE	CA-C-N	-5.26	116.00	122.84
2	L	165	ILE	C-N-CA	-5.26	116.00	122.84
2	P	185	TYR	CB-CA-C	-5.26	102.62	110.88
2	F	185	TYR	CB-CA-C	-5.26	102.62	110.88
1	C	322	ASP	N-CA-C	5.26	118.15	108.58
1	G	51	THR	N-CA-C	-5.26	106.81	113.43
1	M	322	ASP	N-CA-C	5.26	118.15	108.58
1	O	51	THR	N-CA-C	-5.26	106.81	113.43
2	P	240	THR	N-CA-C	5.26	118.95	112.54
2	H	185	TYR	CB-CA-C	-5.25	102.63	110.88
1	A	51	THR	N-CA-C	-5.25	106.81	113.43
2	D	185	TYR	CB-CA-C	-5.25	102.63	110.88
2	D	280	SER	N-CA-C	5.25	117.75	111.71
1	I	322	ASP	N-CA-C	5.25	118.14	108.58
1	A	322	ASP	N-CA-C	5.25	118.14	108.58
2	B	264	ARG	NE-CZ-NH2	-5.25	114.47	119.20
1	C	51	THR	N-CA-C	-5.25	106.81	113.43
2	H	31	ASP	CA-CB-CG	5.25	117.85	112.60
1	K	322	ASP	N-CA-C	5.25	118.14	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	185	TYR	CB-CA-C	-5.25	102.64	110.88
1	M	84	ARG	N-CA-C	5.25	119.17	112.87
1	E	322	ASP	N-CA-C	5.25	118.13	108.58
2	L	264	ARG	NE-CZ-NH2	-5.25	114.48	119.20
2	N	264	ARG	NE-CZ-NH2	-5.25	114.48	119.20
2	R	400	ARG	CA-C-O	-5.25	115.29	120.90
1	E	84	ARG	N-CA-C	5.24	119.16	112.87
2	H	284	ARG	N-CA-C	5.24	117.79	109.24
2	L	240	THR	N-CA-C	5.24	118.94	112.54
2	R	280	SER	N-CA-C	5.24	117.74	111.71
1	G	322	ASP	N-CA-C	5.24	118.12	108.58
1	K	51	THR	N-CA-C	-5.24	106.83	113.43
2	P	284	ARG	N-CA-C	5.24	117.78	109.24
2	F	264	ARG	NE-CZ-NH2	-5.24	114.49	119.20
1	I	51	THR	N-CA-C	-5.23	106.84	113.43
1	O	84	ARG	N-CA-C	5.23	119.15	112.87
2	J	264	ARG	NE-CZ-NH2	-5.23	114.49	119.20
2	B	280	SER	N-CA-C	5.23	117.72	111.71
2	N	280	SER	N-CA-C	5.23	117.72	111.71
2	P	280	SER	N-CA-C	5.22	117.72	111.71
2	R	284	ARG	N-CA-C	5.22	117.75	109.24
2	B	284	ARG	N-CA-C	5.22	117.75	109.24
2	D	284	ARG	N-CA-C	5.22	117.75	109.24
2	H	264	ARG	NE-CZ-NH2	-5.22	114.50	119.20
2	J	284	ARG	N-CA-C	5.22	117.75	109.24
2	F	284	ARG	N-CA-C	5.22	117.75	109.24
2	L	284	ARG	N-CA-C	5.22	117.74	109.24
1	M	51	THR	N-CA-C	-5.22	106.86	113.43
2	D	264	ARG	NE-CZ-NH2	-5.21	114.51	119.20
2	H	280	SER	N-CA-C	5.21	117.70	111.71
2	L	280	SER	N-CA-C	5.21	117.70	111.71
2	J	280	SER	N-CA-C	5.20	117.69	111.71
2	D	110	GLU	CA-C-N	-5.20	109.28	121.34
2	D	110	GLU	C-N-CA	-5.20	109.28	121.34
2	N	284	ARG	N-CA-C	5.20	117.72	109.24
2	F	110	GLU	CA-C-N	-5.20	109.29	121.34
2	F	110	GLU	C-N-CA	-5.20	109.29	121.34
2	N	110	GLU	CA-C-N	-5.20	109.29	121.34
2	N	110	GLU	C-N-CA	-5.20	109.29	121.34
1	K	323	VAL	N-CA-C	5.19	115.59	108.12
2	P	110	GLU	CA-C-N	-5.19	109.30	121.34
2	P	110	GLU	C-N-CA	-5.19	109.30	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	110	GLU	CA-C-N	-5.18	109.31	121.34
2	H	110	GLU	C-N-CA	-5.18	109.31	121.34
2	J	110	GLU	CA-C-N	-5.18	109.32	121.34
2	J	110	GLU	C-N-CA	-5.18	109.32	121.34
2	B	110	GLU	CA-C-N	-5.18	109.32	121.34
2	B	110	GLU	C-N-CA	-5.18	109.32	121.34
1	C	323	VAL	N-CA-C	5.17	115.57	108.12
1	E	220	GLU	CB-CG-CD	-5.17	103.80	112.60
1	M	323	VAL	N-CA-C	5.17	115.57	108.12
1	G	323	VAL	N-CA-C	5.17	115.57	108.12
1	I	220	GLU	CB-CG-CD	-5.17	103.81	112.60
2	R	110	GLU	CA-C-N	-5.17	109.34	121.34
2	R	110	GLU	C-N-CA	-5.17	109.34	121.34
2	F	100	GLY	O-C-N	5.17	128.39	122.34
1	M	243	ARG	CB-CG-CD	-5.17	99.42	111.30
1	O	243	ARG	CB-CG-CD	-5.17	99.42	111.30
1	Q	220	GLU	CB-CG-CD	-5.17	103.82	112.60
2	L	120	ASP	CA-CB-CG	-5.17	107.44	112.60
1	C	243	ARG	CB-CG-CD	-5.16	99.42	111.30
1	I	90	GLU	CB-CG-CD	5.16	121.38	112.60
1	O	90	GLU	CB-CG-CD	5.16	121.38	112.60
1	O	323	VAL	N-CA-C	5.16	115.56	108.12
1	A	243	ARG	CB-CG-CD	-5.16	99.43	111.30
1	K	243	ARG	CB-CG-CD	-5.16	99.43	111.30
1	C	220	GLU	CB-CG-CD	-5.16	103.83	112.60
1	G	243	ARG	CB-CG-CD	-5.16	99.43	111.30
2	L	110	GLU	CA-C-N	-5.16	109.37	121.34
2	L	110	GLU	C-N-CA	-5.16	109.37	121.34
2	N	120	ASP	CA-CB-CG	-5.16	107.44	112.60
1	G	364	PRO	CA-C-N	-5.16	114.49	122.69
1	G	364	PRO	C-N-CA	-5.16	114.49	122.69
1	K	220	GLU	CB-CG-CD	-5.16	103.83	112.60
1	A	323	VAL	N-CA-C	5.16	115.54	108.12
1	I	243	ARG	CB-CG-CD	-5.15	99.45	111.30
1	O	220	GLU	CB-CG-CD	-5.15	103.84	112.60
2	F	120	ASP	CA-CB-CG	-5.15	107.45	112.60
2	J	120	ASP	CA-CB-CG	-5.15	107.45	112.60
1	E	243	ARG	CB-CG-CD	-5.15	99.45	111.30
1	I	323	VAL	N-CA-C	5.15	115.53	108.12
1	Q	243	ARG	CB-CG-CD	-5.15	99.46	111.30
1	A	220	GLU	CB-CG-CD	-5.15	103.85	112.60
2	B	120	ASP	CA-CB-CG	-5.15	107.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	430	SER	CB-CA-C	-5.15	100.79	110.67
1	A	90	GLU	CB-CG-CD	5.14	121.34	112.60
2	R	204	ILE	N-CA-C	5.14	115.26	107.75
1	C	90	GLU	CB-CG-CD	5.14	121.34	112.60
1	E	364	PRO	CA-C-N	-5.14	114.51	122.69
1	E	364	PRO	C-N-CA	-5.14	114.51	122.69
1	K	363	VAL	CB-CA-C	-5.14	105.21	110.71
1	Q	323	VAL	N-CA-C	5.14	115.53	108.12
2	R	120	ASP	CA-CB-CG	-5.14	107.46	112.60
1	G	90	GLU	CB-CG-CD	5.14	121.34	112.60
2	H	120	ASP	CA-CB-CG	-5.14	107.46	112.60
1	O	363	VAL	CB-CA-C	-5.14	105.21	110.71
1	E	363	VAL	CB-CA-C	-5.14	105.21	110.71
2	N	357	ASP	N-CA-C	5.14	118.33	111.75
1	Q	90	GLU	CB-CG-CD	5.14	121.33	112.60
2	H	250	ALA	CA-C-N	-5.13	113.00	120.75
2	H	250	ALA	C-N-CA	-5.13	113.00	120.75
2	J	100	GLY	O-C-N	5.13	128.35	122.34
2	J	357	ASP	N-CA-C	5.13	118.32	111.75
2	L	250	ALA	CA-C-N	-5.13	113.00	120.75
2	L	250	ALA	C-N-CA	-5.13	113.00	120.75
1	M	90	GLU	CB-CG-CD	5.13	121.33	112.60
1	Q	363	VAL	CB-CA-C	-5.13	105.22	110.71
1	A	363	VAL	CB-CA-C	-5.13	105.22	110.71
1	E	323	VAL	N-CA-C	5.13	115.51	108.12
1	K	364	PRO	CA-C-N	-5.13	114.53	122.69
1	K	364	PRO	C-N-CA	-5.13	114.53	122.69
1	M	363	VAL	CB-CA-C	-5.13	105.22	110.71
1	E	90	GLU	CB-CG-CD	5.13	121.32	112.60
1	I	363	VAL	CB-CA-C	-5.13	105.22	110.71
1	A	364	PRO	CA-C-N	-5.13	114.54	122.69
1	A	364	PRO	C-N-CA	-5.13	114.54	122.69
1	G	220	GLU	CB-CG-CD	-5.13	103.88	112.60
1	G	363	VAL	CB-CA-C	-5.13	105.22	110.71
1	I	364	PRO	CA-C-N	-5.13	114.53	122.69
1	I	364	PRO	C-N-CA	-5.13	114.53	122.69
1	M	364	PRO	CA-C-N	-5.13	114.54	122.69
1	M	364	PRO	C-N-CA	-5.13	114.54	122.69
2	R	357	ASP	N-CA-C	5.13	118.31	111.75
2	B	357	ASP	N-CA-C	5.13	118.31	111.75
2	H	58	GLY	CA-C-N	-5.13	115.21	122.34
2	H	58	GLY	C-N-CA	-5.13	115.21	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	220	GLU	CB-CG-CD	-5.13	103.88	112.60
1	K	90	GLU	CB-CG-CD	5.12	121.31	112.60
2	L	100	GLY	O-C-N	5.12	128.34	122.34
2	D	120	ASP	CA-CB-CG	-5.12	107.48	112.60
2	J	250	ALA	CA-C-N	-5.12	113.02	120.75
2	J	250	ALA	C-N-CA	-5.12	113.02	120.75
2	L	204	ILE	N-CA-C	5.12	115.23	107.75
1	O	364	PRO	CA-C-N	-5.12	114.55	122.69
1	O	364	PRO	C-N-CA	-5.12	114.55	122.69
1	Q	364	PRO	CA-C-N	-5.12	114.55	122.69
1	Q	364	PRO	C-N-CA	-5.12	114.55	122.69
2	P	120	ASP	CA-CB-CG	-5.12	107.48	112.60
2	R	58	GLY	CA-C-N	-5.12	115.22	122.34
2	R	58	GLY	C-N-CA	-5.12	115.22	122.34
1	C	363	VAL	CB-CA-C	-5.12	105.23	110.71
2	F	357	ASP	N-CA-C	5.12	118.30	111.75
2	H	204	ILE	N-CA-C	5.12	115.22	107.75
2	B	250	ALA	CA-C-N	-5.11	113.03	120.75
2	B	250	ALA	C-N-CA	-5.11	113.03	120.75
2	D	357	ASP	N-CA-C	5.11	118.30	111.75
2	F	204	ILE	N-CA-C	5.11	115.22	107.75
1	C	364	PRO	CA-C-N	-5.11	114.56	122.69
1	C	364	PRO	C-N-CA	-5.11	114.56	122.69
2	P	250	ALA	CA-C-N	-5.11	113.03	120.75
2	P	250	ALA	C-N-CA	-5.11	113.03	120.75
2	L	357	ASP	N-CA-C	5.11	118.29	111.75
2	R	250	ALA	CA-C-N	-5.11	113.04	120.75
2	R	250	ALA	C-N-CA	-5.11	113.04	120.75
2	F	250	ALA	CA-C-N	-5.11	113.04	120.75
2	F	250	ALA	C-N-CA	-5.11	113.04	120.75
2	H	357	ASP	N-CA-C	5.10	118.28	111.75
2	B	204	ILE	N-CA-C	5.10	115.19	107.75
2	P	58	GLY	CA-C-N	-5.10	115.25	122.34
2	P	58	GLY	C-N-CA	-5.10	115.25	122.34
2	P	357	ASP	N-CA-C	5.10	118.28	111.75
2	D	250	ALA	CA-C-N	-5.10	113.05	120.75
2	D	250	ALA	C-N-CA	-5.10	113.05	120.75
2	N	250	ALA	CA-C-N	-5.10	113.05	120.75
2	N	250	ALA	C-N-CA	-5.10	113.05	120.75
2	B	58	GLY	CA-C-N	-5.09	115.26	122.34
2	B	58	GLY	C-N-CA	-5.09	115.26	122.34
2	F	58	GLY	CA-C-N	-5.09	115.26	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	58	GLY	C-N-CA	-5.09	115.26	122.34
2	L	58	GLY	CA-C-N	-5.09	115.26	122.34
2	L	58	GLY	C-N-CA	-5.09	115.26	122.34
2	J	204	ILE	N-CA-C	5.09	115.18	107.75
2	R	100	GLY	O-C-N	5.09	128.29	122.34
2	H	247	GLN	CA-C-N	-5.09	114.99	123.33
2	H	247	GLN	C-N-CA	-5.09	114.99	123.33
2	R	320	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	F	247	GLN	CA-C-N	-5.09	114.99	123.33
2	F	247	GLN	C-N-CA	-5.09	114.99	123.33
1	O	390	ARG	NH1-CZ-NH2	-5.08	112.69	119.30
1	I	390	ARG	NH1-CZ-NH2	-5.08	112.69	119.30
2	N	204	ILE	N-CA-C	5.08	115.17	107.75
2	D	247	GLN	CA-C-N	-5.08	115.00	123.33
2	D	247	GLN	C-N-CA	-5.08	115.00	123.33
1	K	390	ARG	NH1-CZ-NH2	-5.08	112.70	119.30
2	J	58	GLY	CA-C-N	-5.08	115.28	122.34
2	J	58	GLY	C-N-CA	-5.08	115.28	122.34
2	F	320	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	M	418	PHE	CA-CB-CG	-5.08	108.72	113.80
2	P	204	ILE	N-CA-C	5.07	115.16	107.75
2	P	247	GLN	CA-C-N	-5.07	115.01	123.33
2	P	247	GLN	C-N-CA	-5.07	115.01	123.33
2	B	247	GLN	CA-C-N	-5.07	115.01	123.33
2	B	247	GLN	C-N-CA	-5.07	115.01	123.33
1	C	390	ARG	NH1-CZ-NH2	-5.07	112.71	119.30
2	D	58	GLY	CA-C-N	-5.07	115.29	122.34
2	D	58	GLY	C-N-CA	-5.07	115.29	122.34
1	G	35	GLN	O-C-N	5.07	129.17	122.93
2	D	204	ILE	N-CA-C	5.07	115.15	107.75
2	J	247	GLN	CA-C-N	-5.07	115.02	123.33
2	J	247	GLN	C-N-CA	-5.07	115.02	123.33
2	R	247	GLN	CA-C-N	-5.07	115.02	123.33
2	R	247	GLN	C-N-CA	-5.07	115.02	123.33
1	A	390	ARG	NH1-CZ-NH2	-5.07	112.72	119.30
2	H	177	VAL	CA-C-N	-5.07	111.89	122.07
2	H	177	VAL	C-N-CA	-5.07	111.89	122.07
1	E	390	ARG	NH1-CZ-NH2	-5.06	112.72	119.30
2	L	247	GLN	CA-C-N	-5.06	115.03	123.33
2	L	247	GLN	C-N-CA	-5.06	115.03	123.33
2	N	247	GLN	CA-C-N	-5.06	115.03	123.33
2	N	247	GLN	C-N-CA	-5.06	115.03	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	60	LYS	CA-C-N	-5.06	115.86	122.99
2	P	60	LYS	C-N-CA	-5.06	115.86	122.99
2	D	320	ARG	NE-CZ-NH2	5.06	123.75	119.20
2	B	320	ARG	NE-CZ-NH2	5.05	123.75	119.20
2	J	60	LYS	CA-C-N	-5.05	115.86	122.99
2	J	60	LYS	C-N-CA	-5.05	115.86	122.99
2	N	58	GLY	CA-C-N	-5.05	115.32	122.34
2	N	58	GLY	C-N-CA	-5.05	115.32	122.34
2	F	177	VAL	CA-C-N	-5.05	111.92	122.07
2	F	177	VAL	C-N-CA	-5.05	111.92	122.07
1	K	418	PHE	CA-CB-CG	-5.05	108.75	113.80
2	R	60	LYS	CA-C-N	-5.05	115.87	122.99
2	R	60	LYS	C-N-CA	-5.05	115.87	122.99
2	H	320	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	Q	390	ARG	NH1-CZ-NH2	-5.05	112.73	119.30
1	Q	418	PHE	CA-CB-CG	-5.05	108.75	113.80
2	D	355	VAL	CB-CA-C	-5.05	104.07	110.98
2	D	60	LYS	CA-C-N	-5.04	115.88	122.99
2	D	60	LYS	C-N-CA	-5.04	115.88	122.99
2	J	320	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	M	35	GLN	O-C-N	5.04	129.13	122.93
2	P	320	ARG	NE-CZ-NH2	5.04	123.74	119.20
2	R	177	VAL	CA-C-N	-5.04	111.93	122.07
2	R	177	VAL	C-N-CA	-5.04	111.93	122.07
2	F	320	ARG	CA-CB-CG	5.04	124.18	114.10
2	J	320	ARG	CA-CB-CG	5.04	124.18	114.10
2	B	177	VAL	CA-C-N	-5.04	111.94	122.07
2	B	177	VAL	C-N-CA	-5.04	111.94	122.07
2	H	88	ARG	CA-C-N	5.04	125.32	119.47
2	H	88	ARG	C-N-CA	5.04	125.32	119.47
1	Q	311	LYS	N-CA-C	-5.04	102.33	110.14
2	J	177	VAL	CA-C-N	-5.04	111.94	122.07
2	J	177	VAL	C-N-CA	-5.04	111.94	122.07
2	N	88	ARG	CA-C-N	5.04	125.31	119.47
2	N	88	ARG	C-N-CA	5.04	125.31	119.47
2	N	355	VAL	CB-CA-C	-5.04	104.08	110.98
1	G	311	LYS	N-CA-C	-5.04	102.33	110.14
2	L	88	ARG	CA-C-N	5.04	125.31	119.47
2	L	88	ARG	C-N-CA	5.04	125.31	119.47
2	L	177	VAL	CA-C-N	-5.04	111.95	122.07
2	L	177	VAL	C-N-CA	-5.04	111.95	122.07
2	P	320	ARG	CA-CB-CG	5.04	124.17	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	390	ARG	NH1-CZ-NH2	-5.04	112.75	119.30
1	G	214	ARG	NH1-CZ-NH2	5.03	125.84	119.30
1	G	390	ARG	NH1-CZ-NH2	-5.03	112.76	119.30
2	L	207	GLU	CB-CA-C	5.03	119.41	110.85
1	O	35	GLN	O-C-N	5.03	129.12	122.93
1	O	311	LYS	N-CA-C	-5.03	102.34	110.14
2	N	320	ARG	NE-CZ-NH2	5.03	123.73	119.20
2	H	60	LYS	CA-C-N	-5.03	115.90	122.99
2	H	60	LYS	C-N-CA	-5.03	115.90	122.99
1	I	418	PHE	CA-CB-CG	-5.03	108.77	113.80
2	L	320	ARG	CA-CB-CG	5.03	124.16	114.10
2	L	320	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	M	311	LYS	N-CA-C	-5.03	102.34	110.14
2	N	320	ARG	CA-CB-CG	5.03	124.16	114.10
2	D	88	ARG	CA-C-N	5.03	125.30	119.47
2	D	88	ARG	C-N-CA	5.03	125.30	119.47
2	N	177	VAL	CA-C-N	-5.03	111.96	122.07
2	N	177	VAL	C-N-CA	-5.03	111.96	122.07
1	O	214	ARG	NH1-CZ-NH2	5.03	125.84	119.30
2	R	355	VAL	CB-CA-C	-5.03	104.09	110.98
2	B	60	LYS	CA-C-N	-5.03	115.90	122.99
2	B	60	LYS	C-N-CA	-5.03	115.90	122.99
2	B	320	ARG	CA-CB-CG	5.03	124.16	114.10
2	D	177	VAL	CA-C-N	-5.03	111.97	122.07
2	D	177	VAL	C-N-CA	-5.03	111.97	122.07
1	I	214	ARG	NH1-CZ-NH2	5.03	125.84	119.30
2	J	300	ASN	CA-CB-CG	-5.03	107.57	112.60
2	R	320	ARG	CA-CB-CG	5.03	124.16	114.10
2	P	88	ARG	CA-C-N	5.03	125.30	119.47
2	P	88	ARG	C-N-CA	5.03	125.30	119.47
2	L	60	LYS	CA-C-N	-5.02	115.91	122.99
2	L	60	LYS	C-N-CA	-5.02	115.91	122.99
1	C	311	LYS	N-CA-C	-5.02	102.35	110.14
2	J	355	VAL	CB-CA-C	-5.02	104.10	110.98
1	K	311	LYS	N-CA-C	-5.02	102.36	110.14
2	L	355	VAL	CB-CA-C	-5.02	104.10	110.98
1	A	418	PHE	CA-CB-CG	-5.02	108.78	113.80
2	D	320	ARG	CA-CB-CG	5.02	124.14	114.10
2	H	320	ARG	CA-CB-CG	5.02	124.14	114.10
2	N	207	GLU	CB-CA-C	5.02	119.38	110.85
1	E	35	GLN	O-C-N	5.02	129.10	122.93
2	R	300	ASN	CA-CB-CG	-5.02	107.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	88	ARG	CA-C-N	5.02	125.29	119.47
2	B	88	ARG	C-N-CA	5.02	125.29	119.47
2	J	88	ARG	CA-C-N	5.02	125.29	119.47
2	J	88	ARG	C-N-CA	5.02	125.29	119.47
1	A	214	ARG	NH1-CZ-NH2	5.01	125.82	119.30
1	A	311	LYS	N-CA-C	-5.01	102.37	110.14
1	E	214	ARG	NH1-CZ-NH2	5.01	125.82	119.30
1	K	21	TRP	CZ3-CH2-CZ2	-5.01	114.98	121.50
2	B	355	VAL	CB-CA-C	-5.01	104.11	110.98
2	F	207	GLU	CB-CA-C	5.01	119.37	110.85
2	P	355	VAL	CB-CA-C	-5.01	104.11	110.98
1	C	272	TYR	CA-C-N	-5.01	109.58	121.80
1	C	272	TYR	C-N-CA	-5.01	109.58	121.80
1	O	418	PHE	CA-CB-CG	-5.01	108.79	113.80
2	P	300	ASN	CA-CB-CG	-5.01	107.59	112.60
2	R	207	GLU	CB-CA-C	5.01	119.36	110.85
2	D	207	GLU	CB-CA-C	5.01	119.36	110.85
1	A	35	GLN	O-C-N	5.00	129.09	122.93
2	P	177	VAL	CA-C-N	-5.00	112.01	122.07
2	P	177	VAL	C-N-CA	-5.00	112.01	122.07
1	Q	272	TYR	CA-C-N	-5.00	109.59	121.80
1	Q	272	TYR	C-N-CA	-5.00	109.59	121.80
2	B	207	GLU	CB-CA-C	5.00	119.36	110.85
1	E	311	LYS	N-CA-C	-5.00	102.39	110.14
2	F	60	LYS	CA-C-N	-5.00	115.94	122.99
2	F	60	LYS	C-N-CA	-5.00	115.94	122.99
1	G	21	TRP	CZ3-CH2-CZ2	-5.00	114.99	121.50
2	L	215	ARG	N-CA-C	5.00	116.73	111.28
1	C	418	PHE	CA-CB-CG	-5.00	108.80	113.80
1	M	250	VAL	N-CA-C	5.00	115.78	108.53
2	N	60	LYS	CA-C-N	-5.00	115.94	122.99
2	N	60	LYS	C-N-CA	-5.00	115.94	122.99
1	Q	35	GLN	O-C-N	5.00	129.08	122.93

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	PHE	Sidechain
1	A	264	ARG	Peptide
1	A	265	GLY	Peptide
1	A	273	ALA	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
1	A	37	PRO	Peptide
1	C	244	PHE	Sidechain
1	C	264	ARG	Peptide
1	C	265	GLY	Peptide
1	C	273	ALA	Peptide,Mainchain
1	C	37	PRO	Peptide
1	E	244	PHE	Sidechain
1	E	264	ARG	Peptide
1	E	265	GLY	Peptide
1	E	273	ALA	Peptide,Mainchain
1	E	37	PRO	Peptide
1	G	244	PHE	Sidechain
1	G	264	ARG	Peptide
1	G	265	GLY	Peptide
1	G	273	ALA	Peptide,Mainchain
1	G	37	PRO	Peptide
1	I	244	PHE	Sidechain
1	I	264	ARG	Peptide
1	I	265	GLY	Peptide
1	I	273	ALA	Peptide,Mainchain
1	I	37	PRO	Peptide
1	K	244	PHE	Sidechain
1	K	264	ARG	Peptide
1	K	265	GLY	Peptide
1	K	273	ALA	Peptide,Mainchain
1	K	37	PRO	Peptide
1	M	244	PHE	Sidechain
1	M	264	ARG	Peptide
1	M	265	GLY	Peptide
1	M	273	ALA	Peptide,Mainchain
1	M	37	PRO	Peptide
1	O	244	PHE	Sidechain
1	O	264	ARG	Peptide
1	O	265	GLY	Peptide
1	O	273	ALA	Peptide,Mainchain
1	O	37	PRO	Peptide
1	Q	244	PHE	Sidechain
1	Q	264	ARG	Peptide
1	Q	265	GLY	Peptide
1	Q	273	ALA	Peptide,Mainchain
1	Q	37	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3350	0	3254	75	0
1	C	3350	0	3254	76	0
1	E	3350	0	3254	72	0
1	G	3350	0	3254	75	0
1	I	3350	0	3254	71	0
1	K	3350	0	3254	74	0
1	M	3350	0	3254	62	0
1	O	3350	0	3254	59	0
1	Q	3350	0	3254	60	0
2	B	3352	0	3229	62	0
2	D	3352	0	3229	61	0
2	F	3352	0	3229	62	0
2	H	3352	0	3229	51	0
2	J	3352	0	3229	51	0
2	L	3352	0	3229	49	0
2	N	3352	0	3229	62	0
2	P	3352	0	3229	67	0
2	R	3352	0	3229	63	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
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	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
5	B	28	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	28	0	12	2	0
5	F	28	0	12	2	0
5	H	28	0	12	2	0
5	J	28	0	12	2	0
5	L	28	0	12	2	0
5	N	28	0	12	2	0
5	P	28	0	12	2	0
5	R	28	0	12	2	0
6	B	62	0	51	4	0
6	D	62	0	51	4	0
6	F	62	0	51	4	0
6	H	62	0	51	4	0
6	J	62	0	51	4	0
6	L	62	0	51	4	0
6	N	62	0	51	4	0
6	P	62	0	51	4	0
6	R	62	0	51	4	0
7	A	4	0	0	1	0
7	C	4	0	0	1	0
7	E	4	0	0	1	0
7	G	4	0	0	1	0
7	I	4	0	0	1	0
7	K	4	0	0	1	0
7	M	4	0	0	1	0
7	O	4	0	0	1	0
7	Q	4	0	0	1	0
All	All	61461	0	59022	1050	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 9.

All (1050) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:TRP:CD1	2:N:401:ARG:HG3	1.38	1.57
2:F:401:ARG:HG3	1:K:346:TRP:CD1	1.38	1.55
2:D:401:ARG:HG3	1:G:346:TRP:CD1	1.36	1.54
1:E:346:TRP:CD1	2:R:401:ARG:HG3	1.43	1.53
1:A:346:TRP:CD1	2:P:401:ARG:HG3	1.49	1.48
2:B:401:ARG:HG3	1:I:346:TRP:CD1	1.64	1.31
2:D:401:ARG:CG	1:G:346:TRP:CD1	2.26	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:ARG:CD	1:G:346:TRP:NE1	2.08	1.17
2:F:401:ARG:CD	1:K:346:TRP:NE1	2.07	1.17
1:C:346:TRP:NE1	2:N:401:ARG:CD	2.09	1.15
2:F:401:ARG:CG	1:K:346:TRP:CD1	2.28	1.14
1:C:346:TRP:CD1	2:N:401:ARG:CG	2.31	1.14
1:E:346:TRP:NE1	2:R:401:ARG:CD	2.13	1.12
1:E:346:TRP:CD1	2:R:401:ARG:CG	2.35	1.09
1:A:346:TRP:NE1	2:P:401:ARG:CD	2.16	1.09
1:A:346:TRP:CD1	2:P:401:ARG:CG	2.41	1.04
2:D:401:ARG:HD2	1:G:346:TRP:HE1	1.22	1.04
1:C:346:TRP:HE1	2:N:401:ARG:HD2	1.19	1.03
1:E:346:TRP:HE1	2:R:401:ARG:HD2	1.22	1.03
2:F:401:ARG:HD2	1:K:346:TRP:HE1	1.19	1.01
1:A:346:TRP:HE1	2:P:401:ARG:HD2	1.24	1.01
1:A:346:TRP:NE1	2:P:401:ARG:HD2	1.76	0.98
2:D:401:ARG:CG	1:G:346:TRP:NE1	2.28	0.96
1:C:346:TRP:NE1	2:N:401:ARG:HG3	1.79	0.96
1:C:346:TRP:NE1	2:N:401:ARG:CG	2.29	0.96
2:D:401:ARG:CD	1:G:346:TRP:HE1	1.74	0.96
2:D:401:ARG:HG3	1:G:346:TRP:NE1	1.82	0.94
1:E:346:TRP:NE1	2:R:401:ARG:HG3	1.83	0.93
2:B:401:ARG:CD	1:I:346:TRP:NE1	2.34	0.90
2:F:401:ARG:HG3	1:K:346:TRP:NE1	1.86	0.90
1:E:346:TRP:NE1	2:R:401:ARG:HD2	1.80	0.90
2:F:401:ARG:CG	1:K:346:TRP:NE1	2.32	0.90
2:L:228:ASN:HD21	5:L:501:GDP:HN1	1.22	0.87
2:F:228:ASN:HD21	5:F:501:GDP:HN1	1.22	0.87
1:E:346:TRP:NE1	2:R:401:ARG:CG	2.34	0.87
2:R:228:ASN:HD21	5:R:501:GDP:HN1	1.22	0.87
2:B:401:ARG:CG	1:I:346:TRP:CD1	2.56	0.87
2:F:401:ARG:HD3	1:K:346:TRP:CE2	2.10	0.87
1:C:346:TRP:CE2	2:N:401:ARG:HD3	2.10	0.86
2:N:228:ASN:HD21	5:N:501:GDP:HN1	1.22	0.86
2:D:228:ASN:HD21	5:D:501:GDP:HN1	1.22	0.86
2:B:228:ASN:HD21	5:B:501:GDP:HN1	1.22	0.86
2:H:228:ASN:HD21	5:H:501:GDP:HN1	1.22	0.86
2:J:228:ASN:HD21	5:J:501:GDP:HN1	1.22	0.86
1:A:346:TRP:CE2	2:P:401:ARG:HD3	2.10	0.86
1:E:346:TRP:CE2	2:R:401:ARG:HD3	2.10	0.85
2:P:228:ASN:HD21	5:P:501:GDP:HN1	1.22	0.85
2:D:401:ARG:HD3	1:G:346:TRP:NE1	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:TRP:NE1	2:P:401:ARG:HG3	1.90	0.85
1:C:346:TRP:NE1	2:N:401:ARG:HD2	1.81	0.83
2:D:401:ARG:HD3	1:G:346:TRP:CE2	2.14	0.82
2:B:401:ARG:HD2	1:I:346:TRP:HE1	1.44	0.81
1:A:346:TRP:NE1	2:P:401:ARG:CG	2.41	0.81
2:B:401:ARG:HG3	1:I:346:TRP:NE1	1.96	0.80
2:F:401:ARG:HD3	1:K:346:TRP:NE1	1.94	0.80
2:F:401:ARG:HD2	1:K:346:TRP:NE1	1.82	0.80
1:Q:266:HIS:O	1:Q:266:HIS:CD2	2.35	0.80
1:E:266:HIS:O	1:E:266:HIS:CD2	2.35	0.80
1:I:266:HIS:O	1:I:266:HIS:CD2	2.35	0.79
1:K:266:HIS:O	1:K:266:HIS:CD2	2.35	0.79
1:M:266:HIS:CD2	1:M:266:HIS:O	2.35	0.79
1:C:266:HIS:CD2	1:C:266:HIS:O	2.35	0.79
1:A:266:HIS:CD2	1:A:266:HIS:O	2.35	0.79
1:G:266:HIS:O	1:G:266:HIS:CD2	2.35	0.79
1:O:266:HIS:CD2	1:O:266:HIS:O	2.35	0.79
1:A:346:TRP:CE2	2:P:401:ARG:CD	2.65	0.79
1:G:49:PHE:CG	1:G:49:PHE:O	2.31	0.79
1:K:49:PHE:O	1:K:49:PHE:CG	2.31	0.79
1:C:49:PHE:CG	1:C:49:PHE:O	2.31	0.78
1:E:49:PHE:CG	1:E:49:PHE:O	2.31	0.78
1:M:49:PHE:O	1:M:49:PHE:CG	2.31	0.78
1:Q:49:PHE:CG	1:Q:49:PHE:O	2.31	0.78
2:F:401:ARG:CD	1:K:346:TRP:HE1	1.80	0.78
1:E:346:TRP:CE2	2:R:401:ARG:CD	2.68	0.77
1:A:346:TRP:CG	2:P:401:ARG:HG3	2.15	0.76
2:B:401:ARG:HD2	1:I:346:TRP:NE1	1.99	0.76
2:D:401:ARG:HG3	1:G:346:TRP:HD1	1.39	0.75
2:F:401:ARG:HG3	1:K:346:TRP:HD1	1.46	0.75
1:G:147:SER:OG	1:G:148:GLY:N	2.18	0.75
1:C:147:SER:OG	1:C:148:GLY:N	2.18	0.75
1:M:147:SER:OG	1:M:148:GLY:N	2.18	0.75
1:E:147:SER:OG	1:E:148:GLY:N	2.18	0.74
1:K:147:SER:OG	1:K:148:GLY:N	2.18	0.74
1:Q:147:SER:OG	1:Q:148:GLY:N	2.18	0.74
1:E:262:TYR:HD1	1:E:265:GLY:HA2	1.54	0.73
1:E:346:TRP:CG	2:R:401:ARG:HG3	2.19	0.73
1:I:49:PHE:CG	1:I:49:PHE:O	2.31	0.73
1:K:262:TYR:HD1	1:K:265:GLY:HA2	1.54	0.73
1:Q:262:TYR:HD1	1:Q:265:GLY:HA2	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:TYR:HD1	1:C:265:GLY:HA2	1.54	0.73
1:M:262:TYR:HD1	1:M:265:GLY:HA2	1.54	0.73
1:G:262:TYR:HD1	1:G:265:GLY:HA2	1.54	0.73
1:A:49:PHE:O	1:A:49:PHE:CG	2.31	0.73
1:C:346:TRP:NE1	2:N:401:ARG:HD3	2.02	0.72
1:O:49:PHE:CG	1:O:49:PHE:O	2.31	0.72
2:B:401:ARG:CG	1:I:346:TRP:NE1	2.52	0.72
1:C:346:TRP:CE2	2:N:401:ARG:CD	2.70	0.72
1:A:339:ARG:O	1:A:339:ARG:HG3	1.90	0.72
1:G:49:PHE:CD1	1:G:49:PHE:C	2.59	0.72
1:I:339:ARG:O	1:I:339:ARG:HG3	1.90	0.72
1:O:262:TYR:HD1	1:O:265:GLY:HA2	1.54	0.72
1:O:339:ARG:O	1:O:339:ARG:HG3	1.90	0.72
1:A:262:TYR:HD1	1:A:265:GLY:HA2	1.54	0.72
1:I:262:TYR:HD1	1:I:265:GLY:HA2	1.54	0.72
1:E:339:ARG:HG3	1:E:339:ARG:O	1.89	0.71
1:K:339:ARG:O	1:K:339:ARG:HG3	1.90	0.71
1:C:49:PHE:CD1	1:C:49:PHE:C	2.59	0.71
1:I:147:SER:OG	1:I:148:GLY:N	2.18	0.71
1:Q:339:ARG:HG3	1:Q:339:ARG:O	1.89	0.71
1:A:147:SER:OG	1:A:148:GLY:N	2.18	0.71
1:A:342:GLN:HG3	1:A:342:GLN:O	1.90	0.71
1:M:49:PHE:CD1	1:M:49:PHE:C	2.59	0.71
1:O:342:GLN:O	1:O:342:GLN:HG3	1.90	0.71
1:I:342:GLN:O	1:I:342:GLN:HG3	1.90	0.70
1:O:147:SER:OG	1:O:148:GLY:N	2.18	0.70
1:C:339:ARG:O	1:C:339:ARG:HG3	1.90	0.70
1:E:49:PHE:CD1	1:E:49:PHE:C	2.59	0.70
1:G:339:ARG:HG3	1:G:339:ARG:O	1.90	0.70
1:K:49:PHE:CD1	1:K:49:PHE:C	2.59	0.70
1:K:342:GLN:HG3	1:K:342:GLN:O	1.89	0.70
1:M:342:GLN:HG3	1:M:342:GLN:O	1.90	0.70
1:M:339:ARG:O	1:M:339:ARG:HG3	1.90	0.70
1:Q:49:PHE:CD1	1:Q:49:PHE:C	2.59	0.70
1:E:342:GLN:O	1:E:342:GLN:HG3	1.90	0.70
1:C:342:GLN:HG3	1:C:342:GLN:O	1.90	0.70
1:Q:342:GLN:O	1:Q:342:GLN:HG3	1.90	0.69
1:G:342:GLN:O	1:G:342:GLN:HG3	1.90	0.69
1:C:346:TRP:CG	2:N:401:ARG:HG3	2.21	0.69
1:I:49:PHE:CD1	1:I:49:PHE:C	2.59	0.68
1:A:49:PHE:CD1	1:A:49:PHE:C	2.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:49:PHE:CD1	1:O:49:PHE:C	2.59	0.67
1:A:346:TRP:CZ2	2:P:401:ARG:HD3	2.30	0.66
1:I:2:ARG:HA	1:I:243:ARG:HH12	1.62	0.65
1:A:2:ARG:HA	1:A:243:ARG:HH12	1.62	0.65
1:K:185:TYR:OH	1:K:405:VAL:HG23	1.97	0.65
1:O:2:ARG:HA	1:O:243:ARG:HH12	1.62	0.65
1:Q:185:TYR:OH	1:Q:405:VAL:HG23	1.97	0.65
1:E:185:TYR:OH	1:E:405:VAL:HG23	1.97	0.65
1:A:90:GLU:HG3	1:A:121:ARG:HD2	1.79	0.65
1:M:90:GLU:HG3	1:M:121:ARG:HD2	1.79	0.65
1:Q:2:ARG:HA	1:Q:243:ARG:HH12	1.62	0.65
1:Q:90:GLU:HG3	1:Q:121:ARG:HD2	1.79	0.65
1:C:2:ARG:HA	1:C:243:ARG:HH12	1.62	0.65
1:C:90:GLU:HG3	1:C:121:ARG:HD2	1.79	0.65
1:E:90:GLU:HG3	1:E:121:ARG:HD2	1.79	0.65
1:G:2:ARG:HA	1:G:243:ARG:HH12	1.62	0.65
1:I:90:GLU:HG3	1:I:121:ARG:HD2	1.79	0.65
1:K:90:GLU:HG3	1:K:121:ARG:HD2	1.79	0.65
1:O:90:GLU:HG3	1:O:121:ARG:HD2	1.79	0.65
1:E:2:ARG:HA	1:E:243:ARG:HH12	1.62	0.65
1:A:185:TYR:OH	1:A:405:VAL:HG23	1.97	0.65
1:G:90:GLU:HG3	1:G:121:ARG:HD2	1.79	0.65
1:I:185:TYR:OH	1:I:405:VAL:HG23	1.97	0.65
1:M:2:ARG:HA	1:M:243:ARG:HH12	1.62	0.65
1:O:185:TYR:OH	1:O:405:VAL:HG23	1.97	0.65
1:E:346:TRP:CZ2	2:R:401:ARG:HD3	2.31	0.64
1:K:2:ARG:HA	1:K:243:ARG:HH12	1.62	0.64
2:B:401:ARG:HD3	1:I:346:TRP:CE2	2.32	0.64
1:G:185:TYR:OH	1:G:405:VAL:HG23	1.97	0.64
1:C:185:TYR:OH	1:C:405:VAL:HG23	1.97	0.64
1:M:185:TYR:OH	1:M:405:VAL:HG23	1.97	0.64
1:C:346:TRP:CZ2	2:N:401:ARG:HD3	2.32	0.63
6:D:502:TA1:H261	6:D:502:TA1:H463	1.80	0.63
6:H:502:TA1:H463	6:H:502:TA1:H261	1.80	0.63
6:N:502:TA1:H463	6:N:502:TA1:H261	1.80	0.63
2:R:85:GLN:H	2:R:85:GLN:CD	2.06	0.63
2:J:85:GLN:H	2:J:85:GLN:CD	2.06	0.63
6:L:502:TA1:H463	6:L:502:TA1:H261	1.80	0.63
2:B:85:GLN:CD	2:B:85:GLN:H	2.06	0.63
6:F:502:TA1:H261	6:F:502:TA1:H463	1.80	0.63
6:R:502:TA1:H463	6:R:502:TA1:H261	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:85:GLN:CD	2:F:85:GLN:H	2.06	0.63
2:N:85:GLN:CD	2:N:85:GLN:H	2.06	0.63
2:L:85:GLN:CD	2:L:85:GLN:H	2.06	0.63
2:P:85:GLN:CD	2:P:85:GLN:H	2.06	0.63
2:D:85:GLN:CD	2:D:85:GLN:H	2.06	0.62
2:H:85:GLN:H	2:H:85:GLN:CD	2.06	0.62
2:F:2:ARG:NH1	2:F:251:ASP:OD2	2.32	0.62
2:L:2:ARG:NH1	2:L:251:ASP:OD2	2.32	0.62
2:R:2:ARG:NH1	2:R:251:ASP:OD2	2.32	0.61
2:F:276:THR:CG2	6:F:502:TA1:H162	2.30	0.61
2:L:276:THR:CG2	6:L:502:TA1:H162	2.30	0.61
2:R:276:THR:CG2	6:R:502:TA1:H162	2.30	0.61
2:H:2:ARG:NH1	2:H:251:ASP:OD2	2.32	0.61
6:J:502:TA1:H463	6:J:502:TA1:H261	1.80	0.61
6:P:502:TA1:H261	6:P:502:TA1:H463	1.80	0.61
6:B:502:TA1:H463	6:B:502:TA1:H261	1.80	0.61
2:F:401:ARG:CD	1:K:346:TRP:CE2	2.74	0.61
2:D:2:ARG:NH1	2:D:251:ASP:OD2	2.32	0.61
2:F:401:ARG:HG3	1:K:346:TRP:CG	2.23	0.61
2:N:2:ARG:NH1	2:N:251:ASP:OD2	2.32	0.61
2:B:276:THR:CG2	6:B:502:TA1:H162	2.30	0.60
2:J:276:THR:CG2	6:J:502:TA1:H162	2.30	0.60
2:N:47:GLU:HG2	2:N:47:GLU:O	2.00	0.60
2:D:47:GLU:HG2	2:D:47:GLU:O	2.00	0.60
2:H:47:GLU:O	2:H:47:GLU:HG2	2.00	0.60
2:P:276:THR:CG2	6:P:502:TA1:H162	2.30	0.60
2:H:276:THR:CG2	6:H:502:TA1:H162	2.30	0.60
2:B:47:GLU:O	2:B:47:GLU:HG2	2.00	0.60
2:D:276:THR:CG2	6:D:502:TA1:H162	2.30	0.60
2:J:47:GLU:O	2:J:47:GLU:HG2	2.00	0.60
2:L:47:GLU:O	2:L:47:GLU:HG2	2.00	0.60
2:N:276:THR:CG2	6:N:502:TA1:H162	2.30	0.60
2:P:47:GLU:O	2:P:47:GLU:HG2	2.00	0.60
2:F:47:GLU:O	2:F:47:GLU:HG2	2.00	0.60
2:R:47:GLU:O	2:R:47:GLU:HG2	2.00	0.60
1:K:49:PHE:O	1:K:49:PHE:CD1	2.54	0.59
1:G:223:THR:O	1:G:227:LEU:HG	2.03	0.59
1:M:223:THR:O	1:M:227:LEU:HG	2.03	0.59
1:C:223:THR:O	1:C:227:LEU:HG	2.03	0.59
1:M:49:PHE:O	1:M:49:PHE:CD1	2.54	0.59
1:A:223:THR:O	1:A:227:LEU:HG	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:PHE:O	1:C:49:PHE:CD1	2.55	0.59
1:I:49:PHE:O	1:I:49:PHE:CD1	2.54	0.59
1:I:223:THR:O	1:I:227:LEU:HG	2.03	0.59
1:O:223:THR:O	1:O:227:LEU:HG	2.03	0.59
1:A:49:PHE:O	1:A:49:PHE:CD1	2.55	0.59
1:G:49:PHE:O	1:G:49:PHE:CD1	2.55	0.59
1:O:49:PHE:O	1:O:49:PHE:CD1	2.55	0.59
1:Q:223:THR:O	1:Q:227:LEU:HG	2.03	0.58
1:E:223:THR:O	1:E:227:LEU:HG	2.03	0.58
2:J:2:ARG:NH1	2:J:251:ASP:OD2	2.32	0.58
1:K:223:THR:O	1:K:227:LEU:HG	2.03	0.58
2:B:2:ARG:NH1	2:B:251:ASP:OD2	2.32	0.58
1:Q:313:MET:SD	1:Q:344:VAL:HG21	2.44	0.58
2:P:2:ARG:NH1	2:P:251:ASP:OD2	2.32	0.58
1:E:313:MET:SD	1:E:344:VAL:HG21	2.44	0.58
1:K:313:MET:SD	1:K:344:VAL:HG21	2.44	0.58
1:Q:49:PHE:O	1:Q:49:PHE:CD1	2.55	0.57
1:E:49:PHE:O	1:E:49:PHE:CD1	2.54	0.57
1:O:313:MET:SD	1:O:344:VAL:HG21	2.44	0.57
1:G:313:MET:SD	1:G:344:VAL:HG21	2.44	0.57
1:A:313:MET:SD	1:A:344:VAL:HG21	2.44	0.57
1:C:313:MET:SD	1:C:344:VAL:HG21	2.44	0.57
1:O:71:GLU:HG2	2:P:2:ARG:HH21	1.69	0.57
1:I:71:GLU:HG2	2:J:2:ARG:HH21	1.69	0.57
1:I:313:MET:SD	1:I:344:VAL:HG21	2.44	0.57
1:A:71:GLU:HG2	2:B:2:ARG:HH21	1.69	0.57
1:C:71:GLU:HG2	2:D:2:ARG:HH21	1.69	0.57
1:K:71:GLU:HG2	2:L:2:ARG:HH21	1.69	0.57
1:M:313:MET:SD	1:M:344:VAL:HG21	2.44	0.57
1:E:71:GLU:HG2	2:F:2:ARG:HH21	1.69	0.56
1:G:71:GLU:HG2	2:H:2:ARG:HH21	1.69	0.56
2:N:228:ASN:ND2	5:N:501:GDP:HN1	1.99	0.56
2:H:228:ASN:ND2	5:H:501:GDP:HN1	1.99	0.56
1:M:71:GLU:HG2	2:N:2:ARG:HH21	1.69	0.56
1:Q:71:GLU:HG2	2:R:2:ARG:HH21	1.69	0.56
2:D:228:ASN:ND2	5:D:501:GDP:HN1	1.99	0.56
2:R:228:ASN:ND2	5:R:501:GDP:HN1	1.99	0.56
2:B:401:ARG:CD	1:I:346:TRP:CE2	2.88	0.56
1:C:266:HIS:O	1:C:266:HIS:HD2	1.88	0.56
2:F:228:ASN:ND2	5:F:501:GDP:HN1	1.99	0.56
1:G:266:HIS:O	1:G:266:HIS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:228:ASN:ND2	5:L:501:GDP:HN1	1.99	0.56
1:M:266:HIS:O	1:M:266:HIS:HD2	1.88	0.56
1:A:435:VAL:HG12	1:A:435:VAL:O	2.06	0.56
1:O:435:VAL:HG12	1:O:435:VAL:O	2.06	0.56
1:I:435:VAL:HG12	1:I:435:VAL:O	2.06	0.56
2:F:401:ARG:HD3	1:K:346:TRP:CZ2	2.40	0.55
1:K:435:VAL:HG12	1:K:435:VAL:O	2.06	0.55
2:P:228:ASN:ND2	5:P:501:GDP:HN1	1.99	0.55
2:B:228:ASN:ND2	5:B:501:GDP:HN1	1.99	0.55
1:E:435:VAL:HG12	1:E:435:VAL:O	2.06	0.55
1:Q:435:VAL:HG12	1:Q:435:VAL:O	2.06	0.55
1:M:435:VAL:HG12	1:M:435:VAL:O	2.06	0.55
2:J:228:ASN:ND2	5:J:501:GDP:HN1	1.99	0.55
1:C:435:VAL:HG12	1:C:435:VAL:O	2.06	0.55
1:I:266:HIS:O	1:I:266:HIS:HD2	1.88	0.55
1:G:435:VAL:HG12	1:G:435:VAL:O	2.06	0.54
1:A:266:HIS:O	1:A:266:HIS:HD2	1.88	0.54
1:O:266:HIS:O	1:O:266:HIS:HD2	1.88	0.54
2:D:401:ARG:HD2	1:G:346:TRP:NE1	1.91	0.53
1:A:349:THR:HG23	1:A:349:THR:O	2.09	0.53
1:C:349:THR:O	1:C:349:THR:HG23	2.09	0.53
1:I:349:THR:HG23	1:I:349:THR:O	2.09	0.53
1:M:349:THR:O	1:M:349:THR:HG23	2.09	0.53
1:O:349:THR:O	1:O:349:THR:HG23	2.09	0.53
1:G:349:THR:HG23	1:G:349:THR:O	2.09	0.53
2:B:127:GLU:OE2	2:D:338:LYS:NZ	2.42	0.53
1:K:349:THR:HG23	1:K:349:THR:O	2.09	0.53
1:E:349:THR:HG23	1:E:349:THR:O	2.09	0.52
1:Q:349:THR:HG23	1:Q:349:THR:O	2.09	0.52
1:M:249:ASN:OD1	1:M:249:ASN:C	2.52	0.52
1:C:249:ASN:OD1	1:C:249:ASN:C	2.52	0.52
1:G:249:ASN:OD1	1:G:249:ASN:C	2.52	0.52
2:N:12:CYS:SG	2:N:13:GLY:N	2.82	0.52
7:C:603:HOH:O	2:D:254:LYS:NZ	2.43	0.52
7:G:603:HOH:O	2:H:254:LYS:NZ	2.43	0.52
2:D:12:CYS:SG	2:D:13:GLY:N	2.83	0.52
7:M:603:HOH:O	2:N:254:LYS:NZ	2.43	0.52
2:P:183:GLU:N	2:P:184:PRO:HD2	2.25	0.52
2:P:338:LYS:NZ	2:R:127:GLU:OE2	2.42	0.52
2:B:183:GLU:N	2:B:184:PRO:HD2	2.25	0.52
2:H:12:CYS:SG	2:H:13:GLY:N	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:183:GLU:N	2:J:184:PRO:HD2	2.25	0.52
2:L:183:GLU:N	2:L:184:PRO:HD2	2.24	0.52
2:N:183:GLU:N	2:N:184:PRO:HD2	2.25	0.52
2:R:12:CYS:SG	2:R:13:GLY:N	2.83	0.52
2:D:183:GLU:N	2:D:184:PRO:HD2	2.25	0.51
7:E:603:HOH:O	2:F:254:LYS:NZ	2.43	0.51
2:F:12:CYS:SG	2:F:13:GLY:N	2.83	0.51
2:H:183:GLU:N	2:H:184:PRO:HD2	2.24	0.51
7:Q:603:HOH:O	2:R:254:LYS:NZ	2.43	0.51
2:J:12:CYS:SG	2:J:13:GLY:N	2.83	0.51
2:L:12:CYS:SG	2:L:13:GLY:N	2.83	0.51
2:P:266:HIS:CD2	2:P:266:HIS:N	2.79	0.51
2:D:266:HIS:N	2:D:266:HIS:CD2	2.79	0.51
2:D:401:ARG:HD3	1:G:346:TRP:CZ2	2.45	0.51
2:F:183:GLU:N	2:F:184:PRO:HD2	2.25	0.51
2:H:266:HIS:N	2:H:266:HIS:CD2	2.79	0.51
7:K:603:HOH:O	2:L:254:LYS:NZ	2.43	0.51
2:R:183:GLU:N	2:R:184:PRO:HD2	2.24	0.51
2:B:12:CYS:SG	2:B:13:GLY:N	2.83	0.51
2:F:47:GLU:O	2:F:47:GLU:CG	2.58	0.51
2:L:47:GLU:O	2:L:47:GLU:CG	2.58	0.51
2:N:266:HIS:N	2:N:266:HIS:CD2	2.79	0.51
2:R:47:GLU:O	2:R:47:GLU:CG	2.58	0.51
7:A:603:HOH:O	2:B:254:LYS:NZ	2.43	0.51
7:I:603:HOH:O	2:J:254:LYS:NZ	2.43	0.51
2:J:47:GLU:O	2:J:47:GLU:CG	2.58	0.51
2:P:12:CYS:SG	2:P:13:GLY:N	2.83	0.51
1:A:224:TYR:HD1	1:A:227:LEU:HD12	1.76	0.51
2:B:47:GLU:O	2:B:47:GLU:CG	2.58	0.51
1:I:224:TYR:HD1	1:I:227:LEU:HD12	1.76	0.51
1:E:224:TYR:HD1	1:E:227:LEU:HD12	1.76	0.51
2:J:381:SER:OG	2:J:382:THR:N	2.43	0.51
1:K:224:TYR:HD1	1:K:227:LEU:HD12	1.75	0.51
1:O:224:TYR:HD1	1:O:227:LEU:HD12	1.76	0.51
2:P:47:GLU:O	2:P:47:GLU:CG	2.58	0.51
2:P:381:SER:OG	2:P:382:THR:N	2.43	0.51
1:Q:224:TYR:HD1	1:Q:227:LEU:HD12	1.76	0.51
2:B:381:SER:OG	2:B:382:THR:N	2.43	0.51
7:O:603:HOH:O	2:P:254:LYS:NZ	2.43	0.51
2:H:47:GLU:O	2:H:47:GLU:CG	2.58	0.51
2:N:47:GLU:O	2:N:47:GLU:CG	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:TYR:HD1	1:C:227:LEU:HD12	1.75	0.50
2:D:47:GLU:O	2:D:47:GLU:CG	2.58	0.50
1:K:183:GLU:N	1:K:184:PRO:HD2	2.26	0.50
2:L:266:HIS:CD2	2:L:266:HIS:N	2.79	0.50
1:M:224:TYR:HD1	1:M:227:LEU:HD12	1.75	0.50
1:Q:249:ASN:OD1	1:Q:249:ASN:C	2.52	0.50
1:E:183:GLU:N	1:E:184:PRO:HD2	2.26	0.50
2:F:266:HIS:CD2	2:F:266:HIS:N	2.79	0.50
2:F:381:SER:OG	2:F:382:THR:N	2.43	0.50
1:I:183:GLU:N	1:I:184:PRO:HD2	2.26	0.50
1:K:266:HIS:O	1:K:266:HIS:HD2	1.88	0.50
1:Q:183:GLU:N	1:Q:184:PRO:HD2	2.26	0.50
1:C:183:GLU:N	1:C:184:PRO:HD2	2.26	0.50
1:E:249:ASN:OD1	1:E:249:ASN:C	2.52	0.50
2:L:381:SER:OG	2:L:382:THR:N	2.43	0.50
2:R:266:HIS:CD2	2:R:266:HIS:N	2.79	0.50
2:R:381:SER:OG	2:R:382:THR:N	2.43	0.50
1:A:183:GLU:N	1:A:184:PRO:HD2	2.26	0.50
1:A:352:LYS:NZ	2:P:179:ASP:OD2	2.44	0.50
1:G:183:GLU:N	1:G:184:PRO:HD2	2.26	0.50
1:O:183:GLU:N	1:O:184:PRO:HD2	2.26	0.50
1:G:224:TYR:HD1	1:G:227:LEU:HD12	1.76	0.50
1:K:249:ASN:C	1:K:249:ASN:OD1	2.52	0.50
1:M:183:GLU:N	1:M:184:PRO:HD2	2.26	0.50
2:N:381:SER:OG	2:N:382:THR:N	2.43	0.50
1:Q:2:ARG:HA	1:Q:243:ARG:NH1	2.27	0.50
2:D:381:SER:OG	2:D:382:THR:N	2.43	0.50
1:E:2:ARG:HA	1:E:243:ARG:NH1	2.27	0.50
1:E:266:HIS:O	1:E:266:HIS:HD2	1.88	0.50
1:C:304:LYS:HD2	1:C:304:LYS:C	2.37	0.50
1:G:304:LYS:C	1:G:304:LYS:HD2	2.37	0.50
1:M:304:LYS:HD2	1:M:304:LYS:C	2.37	0.50
1:K:2:ARG:HA	1:K:243:ARG:NH1	2.27	0.49
2:N:338:LYS:NZ	2:P:127:GLU:OE2	2.44	0.49
1:O:2:ARG:HA	1:O:243:ARG:NH1	2.27	0.49
2:H:381:SER:OG	2:H:382:THR:N	2.43	0.49
1:I:143:GLY:O	1:I:147:SER:OG	2.20	0.49
1:Q:266:HIS:O	1:Q:266:HIS:HD2	1.88	0.49
1:A:2:ARG:HA	1:A:243:ARG:NH1	2.27	0.49
1:E:304:LYS:C	1:E:304:LYS:HD2	2.37	0.49
1:Q:304:LYS:C	1:Q:304:LYS:HD2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2:ARG:HA	1:I:243:ARG:NH1	2.27	0.49
1:K:304:LYS:HD2	1:K:304:LYS:C	2.37	0.49
1:K:100:ALA:HA	2:L:254:LYS:HG2	1.95	0.49
1:Q:100:ALA:HA	2:R:254:LYS:HG2	1.95	0.49
1:A:143:GLY:O	1:A:147:SER:OG	2.20	0.49
1:E:100:ALA:HA	2:F:254:LYS:HG2	1.95	0.49
1:I:100:ALA:HA	2:J:254:LYS:HG2	1.95	0.49
1:M:2:ARG:HA	1:M:243:ARG:NH1	2.27	0.49
1:O:100:ALA:HA	2:P:254:LYS:HG2	1.95	0.49
1:Q:266:HIS:O	1:Q:266:HIS:CG	2.62	0.49
1:A:100:ALA:HA	2:B:254:LYS:HG2	1.95	0.49
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.95	0.49
1:C:2:ARG:HA	1:C:243:ARG:NH1	2.27	0.49
1:M:100:ALA:HA	2:N:254:LYS:HG2	1.95	0.49
1:C:100:ALA:HA	2:D:254:LYS:HG2	1.95	0.49
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.95	0.49
1:G:100:ALA:HA	2:H:254:LYS:HG2	1.95	0.49
1:I:278:ALA:HA	1:I:369:ALA:HB2	1.95	0.49
1:M:278:ALA:HA	1:M:369:ALA:HB2	1.95	0.49
1:O:278:ALA:HA	1:O:369:ALA:HB2	1.95	0.49
1:A:267:PHE:N	1:A:268:PRO:HD3	2.28	0.48
1:E:266:HIS:O	1:E:266:HIS:CG	2.62	0.48
1:G:278:ALA:HA	1:G:369:ALA:HB2	1.95	0.48
2:H:266:HIS:CD2	2:H:266:HIS:H	2.31	0.48
1:I:304:LYS:HD2	1:I:304:LYS:C	2.37	0.48
2:J:266:HIS:H	2:J:266:HIS:CD2	2.31	0.48
1:M:267:PHE:N	1:M:268:PRO:HD3	2.28	0.48
1:O:143:GLY:O	1:O:147:SER:OG	2.20	0.48
1:O:267:PHE:N	1:O:268:PRO:HD3	2.28	0.48
2:B:266:HIS:H	2:B:266:HIS:CD2	2.31	0.48
2:D:266:HIS:CD2	2:D:266:HIS:H	2.31	0.48
1:I:267:PHE:N	1:I:268:PRO:HD3	2.28	0.48
2:J:266:HIS:CD2	2:J:266:HIS:N	2.79	0.48
1:A:304:LYS:HD2	1:A:304:LYS:C	2.37	0.48
1:C:267:PHE:N	1:C:268:PRO:HD3	2.28	0.48
1:G:2:ARG:HA	1:G:243:ARG:NH1	2.27	0.48
1:K:266:HIS:O	1:K:266:HIS:CG	2.62	0.48
1:A:435:VAL:O	1:A:435:VAL:CG1	2.60	0.48
1:G:267:PHE:N	1:G:268:PRO:HD3	2.28	0.48
1:I:435:VAL:O	1:I:435:VAL:CG1	2.60	0.48
1:M:435:VAL:O	1:M:435:VAL:CG1	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:266:HIS:CD2	2:N:266:HIS:H	2.31	0.48
1:O:435:VAL:O	1:O:435:VAL:CG1	2.60	0.48
2:P:266:HIS:CD2	2:P:266:HIS:H	2.31	0.48
2:B:266:HIS:CD2	2:B:266:HIS:N	2.79	0.48
1:K:278:ALA:HA	1:K:369:ALA:HB2	1.95	0.48
1:C:435:VAL:O	1:C:435:VAL:CG1	2.60	0.48
1:E:278:ALA:HA	1:E:369:ALA:HB2	1.95	0.48
2:F:266:HIS:CD2	2:F:266:HIS:H	2.31	0.48
2:L:266:HIS:CD2	2:L:266:HIS:H	2.31	0.48
1:O:304:LYS:C	1:O:304:LYS:HD2	2.37	0.48
1:Q:278:ALA:HA	1:Q:369:ALA:HB2	1.95	0.48
1:G:435:VAL:O	1:G:435:VAL:CG1	2.60	0.48
2:R:266:HIS:CD2	2:R:266:HIS:H	2.31	0.48
2:J:388:PHE:N	2:J:388:PHE:CD1	2.81	0.48
1:O:76:ASP:HA	1:O:79:ARG:HG2	1.96	0.48
1:Q:308:ARG:CZ	1:Q:308:ARG:HB3	2.44	0.48
1:A:76:ASP:HA	1:A:79:ARG:HG2	1.96	0.48
1:E:308:ARG:CZ	1:E:308:ARG:HB3	2.44	0.48
1:K:267:PHE:N	1:K:268:PRO:HD3	2.28	0.48
1:O:249:ASN:OD1	1:O:249:ASN:C	2.52	0.48
2:B:388:PHE:N	2:B:388:PHE:CD1	2.81	0.47
1:E:267:PHE:N	1:E:268:PRO:HD3	2.28	0.47
1:I:76:ASP:HA	1:I:79:ARG:HG2	1.96	0.47
1:K:308:ARG:CZ	1:K:308:ARG:HB3	2.44	0.47
1:A:181:VAL:HG12	1:A:181:VAL:O	2.14	0.47
1:A:249:ASN:C	1:A:249:ASN:OD1	2.52	0.47
1:E:312:TYR:CD1	1:E:312:TYR:N	2.82	0.47
1:I:181:VAL:HG12	1:I:181:VAL:O	2.14	0.47
1:G:144:GLY:O	1:G:148:GLY:N	2.47	0.47
1:O:181:VAL:HG12	1:O:181:VAL:O	2.14	0.47
2:P:388:PHE:N	2:P:388:PHE:CD1	2.81	0.47
1:Q:267:PHE:N	1:Q:268:PRO:HD3	2.28	0.47
1:Q:312:TYR:CD1	1:Q:312:TYR:N	2.82	0.47
1:C:312:TYR:N	1:C:312:TYR:CD1	2.82	0.47
1:K:312:TYR:N	1:K:312:TYR:CD1	2.82	0.47
1:M:312:TYR:N	1:M:312:TYR:CD1	2.82	0.47
1:O:266:HIS:O	1:O:266:HIS:CG	2.62	0.47
1:G:76:ASP:HA	1:G:79:ARG:HG2	1.96	0.47
2:L:318:VAL:O	2:L:375:ALA:HA	2.15	0.47
2:B:401:ARG:HD3	1:I:346:TRP:CZ2	2.49	0.47
2:F:318:VAL:O	2:F:375:ALA:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:TYR:CD1	1:G:312:TYR:N	2.81	0.47
1:I:249:ASN:C	1:I:249:ASN:OD1	2.52	0.47
1:O:144:GLY:O	1:O:148:GLY:N	2.47	0.47
1:A:144:GLY:O	1:A:148:GLY:N	2.47	0.47
1:C:76:ASP:HA	1:C:79:ARG:HG2	1.96	0.47
1:C:144:GLY:O	1:C:148:GLY:N	2.47	0.47
1:I:308:ARG:HB3	1:I:308:ARG:CZ	2.44	0.47
2:J:318:VAL:O	2:J:375:ALA:HA	2.15	0.47
1:M:36:MET:O	1:M:36:MET:HG3	2.15	0.47
1:M:76:ASP:HA	1:M:79:ARG:HG2	1.96	0.47
1:M:144:GLY:O	1:M:148:GLY:N	2.47	0.47
2:R:318:VAL:O	2:R:375:ALA:HA	2.15	0.47
1:A:266:HIS:O	1:A:266:HIS:CG	2.62	0.47
2:B:318:VAL:O	2:B:375:ALA:HA	2.15	0.47
1:C:36:MET:O	1:C:36:MET:HG3	2.15	0.47
1:G:36:MET:HG3	1:G:36:MET:O	2.15	0.47
2:H:318:VAL:O	2:H:375:ALA:HA	2.15	0.47
1:I:312:TYR:CD1	1:I:312:TYR:N	2.82	0.47
1:Q:435:VAL:O	1:Q:435:VAL:CG1	2.60	0.47
2:R:85:GLN:CD	2:R:85:GLN:N	2.72	0.47
1:A:308:ARG:HB3	1:A:308:ARG:CZ	2.44	0.47
1:A:312:TYR:N	1:A:312:TYR:CD1	2.82	0.47
1:E:435:VAL:O	1:E:435:VAL:CG1	2.60	0.47
2:H:85:GLN:CD	2:H:85:GLN:N	2.72	0.47
1:O:312:TYR:CD1	1:O:312:TYR:N	2.81	0.47
2:P:318:VAL:O	2:P:375:ALA:HA	2.15	0.47
1:I:266:HIS:O	1:I:266:HIS:CG	2.62	0.47
1:K:144:GLY:O	1:K:148:GLY:N	2.47	0.47
2:L:85:GLN:CD	2:L:85:GLN:N	2.72	0.47
1:M:308:ARG:CZ	1:M:308:ARG:HB3	2.44	0.47
1:O:308:ARG:HB3	1:O:308:ARG:CZ	2.44	0.47
1:Q:144:GLY:O	1:Q:148:GLY:N	2.47	0.47
2:D:85:GLN:CD	2:D:85:GLN:N	2.72	0.46
2:D:318:VAL:O	2:D:375:ALA:HA	2.15	0.46
1:E:144:GLY:O	1:E:148:GLY:N	2.47	0.46
2:F:85:GLN:CD	2:F:85:GLN:N	2.72	0.46
1:K:435:VAL:O	1:K:435:VAL:CG1	2.60	0.46
1:C:308:ARG:CZ	1:C:308:ARG:HB3	2.44	0.46
1:E:214:ARG:NH1	2:F:330:GLU:OE2	2.49	0.46
2:J:297:ASP:CG	2:J:299:LYS:HZ3	2.23	0.46
1:K:214:ARG:NH1	2:L:330:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:85:GLN:CD	2:N:85:GLN:N	2.72	0.46
2:N:318:VAL:O	2:N:375:ALA:HA	2.15	0.46
1:Q:214:ARG:NH1	2:R:330:GLU:OE2	2.49	0.46
1:G:308:ARG:HB3	1:G:308:ARG:CZ	2.44	0.46
1:O:36:MET:O	1:O:36:MET:HG3	2.15	0.46
1:C:214:ARG:NH1	2:D:330:GLU:OE2	2.49	0.46
1:G:214:ARG:NH1	2:H:330:GLU:OE2	2.49	0.46
1:I:144:GLY:O	1:I:148:GLY:N	2.47	0.46
1:M:214:ARG:NH1	2:N:330:GLU:OE2	2.49	0.46
6:R:502:TA1:H463	6:R:502:TA1:C26	2.46	0.46
1:A:270:ALA:HA	1:A:377:MET:O	2.16	0.46
1:E:76:ASP:HA	1:E:79:ARG:HG2	1.96	0.46
6:F:502:TA1:H463	6:F:502:TA1:C26	2.46	0.46
1:I:270:ALA:HA	1:I:377:MET:O	2.16	0.46
6:L:502:TA1:H463	6:L:502:TA1:C26	2.46	0.46
1:M:36:MET:SD	1:M:61:HIS:HB2	2.56	0.46
1:M:181:VAL:HG12	1:M:181:VAL:O	2.14	0.46
1:Q:76:ASP:HA	1:Q:79:ARG:HG2	1.96	0.46
1:A:36:MET:O	1:A:36:MET:HG3	2.15	0.46
1:E:36:MET:HG3	1:E:36:MET:O	2.15	0.46
2:J:85:GLN:CD	2:J:85:GLN:N	2.72	0.46
1:K:36:MET:O	1:K:36:MET:HG3	2.15	0.46
2:L:276:THR:OG1	2:L:280:SER:HB2	2.15	0.46
1:O:270:ALA:HA	1:O:377:MET:O	2.16	0.46
2:P:85:GLN:CD	2:P:85:GLN:N	2.72	0.46
2:B:85:GLN:CD	2:B:85:GLN:N	2.72	0.46
1:C:36:MET:SD	1:C:61:HIS:HB2	2.56	0.46
1:C:181:VAL:HG12	1:C:181:VAL:O	2.14	0.46
2:F:276:THR:OG1	2:F:280:SER:HB2	2.15	0.46
2:F:276:THR:HG22	6:F:502:TA1:H162	1.98	0.46
1:G:181:VAL:O	1:G:181:VAL:HG12	2.14	0.46
1:I:36:MET:O	1:I:36:MET:HG3	2.15	0.46
2:P:306:ASP:HA	2:P:307:PRO:HD2	1.81	0.46
2:R:276:THR:OG1	2:R:280:SER:HB2	2.15	0.46
1:G:36:MET:SD	1:G:61:HIS:HB2	2.56	0.46
2:J:276:THR:OG1	2:J:280:SER:HB2	2.15	0.46
1:K:76:ASP:HA	1:K:79:ARG:HG2	1.96	0.46
2:N:177:VAL:O	2:N:177:VAL:HG12	2.16	0.46
2:N:398:MET:HB3	2:N:398:MET:HE3	1.66	0.46
1:Q:36:MET:HG3	1:Q:36:MET:O	2.15	0.46
1:Q:358:GLU:HA	1:Q:359:PRO:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:276:THR:HG22	6:R:502:TA1:H162	1.98	0.46
2:R:398:MET:HB3	2:R:398:MET:HE3	1.66	0.46
2:B:276:THR:OG1	2:B:280:SER:HB2	2.15	0.46
1:G:205:ASP:HB3	1:G:303:VAL:HA	1.98	0.46
2:H:177:VAL:O	2:H:177:VAL:HG12	2.16	0.46
2:J:306:ASP:HA	2:J:307:PRO:HD2	1.81	0.46
1:K:260:VAL:HA	1:K:261:PRO:HD2	1.66	0.46
2:P:276:THR:OG1	2:P:280:SER:HB2	2.15	0.46
2:B:306:ASP:HA	2:B:307:PRO:HD2	1.81	0.46
2:D:177:VAL:O	2:D:177:VAL:HG12	2.16	0.45
2:F:398:MET:HB3	2:F:398:MET:HE3	1.66	0.45
1:G:301:GLN:O	1:G:302:MET:HB2	2.16	0.45
2:H:276:THR:OG1	2:H:280:SER:HB2	2.15	0.45
1:M:205:ASP:HB3	1:M:303:VAL:HA	1.99	0.45
2:P:276:THR:HG22	6:P:502:TA1:H162	1.98	0.45
1:A:36:MET:SD	1:A:61:HIS:HB2	2.56	0.45
1:C:205:ASP:HB3	1:C:303:VAL:HA	1.99	0.45
1:C:270:ALA:HA	1:C:377:MET:O	2.16	0.45
2:D:276:THR:OG1	2:D:280:SER:HB2	2.16	0.45
1:G:270:ALA:HA	1:G:377:MET:O	2.16	0.45
2:L:388:PHE:N	2:L:388:PHE:CD1	2.81	0.45
1:M:270:ALA:HA	1:M:377:MET:O	2.16	0.45
2:N:276:THR:OG1	2:N:280:SER:HB2	2.16	0.45
1:O:36:MET:SD	1:O:61:HIS:HB2	2.56	0.45
1:E:270:ALA:HA	1:E:377:MET:O	2.16	0.45
2:J:177:VAL:O	2:J:177:VAL:HG12	2.16	0.45
2:J:316:ALA:HB3	2:J:378:ILE:HB	1.99	0.45
1:K:270:ALA:HA	1:K:377:MET:O	2.16	0.45
1:M:301:GLN:O	1:M:302:MET:HB2	2.16	0.45
1:Q:270:ALA:HA	1:Q:377:MET:O	2.16	0.45
2:B:177:VAL:O	2:B:177:VAL:HG12	2.16	0.45
1:C:301:GLN:O	1:C:302:MET:HB2	2.16	0.45
1:E:260:VAL:HA	1:E:261:PRO:HD2	1.66	0.45
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.99	0.45
1:C:345:ASP:HB2	1:C:439:SER:HB2	1.98	0.45
2:D:398:MET:HB3	2:D:398:MET:HE3	1.66	0.45
2:F:388:PHE:N	2:F:388:PHE:CD1	2.81	0.45
1:G:345:ASP:HB2	1:G:439:SER:HB2	1.98	0.45
1:I:36:MET:SD	1:I:61:HIS:HB2	2.56	0.45
1:M:345:ASP:HB2	1:M:439:SER:HB2	1.98	0.45
2:P:177:VAL:O	2:P:177:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:205:ASP:HB3	1:K:303:VAL:HA	1.98	0.45
2:L:398:MET:HB3	2:L:398:MET:HE3	1.66	0.45
1:M:224:TYR:HA	1:M:227:LEU:HD12	1.98	0.45
1:O:345:ASP:HB2	1:O:439:SER:HB2	1.98	0.45
2:P:316:ALA:HB3	2:P:378:ILE:HB	1.99	0.45
1:A:224:TYR:HA	1:A:227:LEU:HD12	1.98	0.45
1:A:345:ASP:HB2	1:A:439:SER:HB2	1.98	0.45
1:E:301:GLN:O	1:E:302:MET:HB2	2.16	0.45
1:I:214:ARG:NH1	2:J:330:GLU:OE2	2.49	0.45
1:K:260:VAL:HG13	1:K:265:GLY:HA3	1.99	0.45
1:K:301:GLN:O	1:K:302:MET:HB2	2.16	0.45
1:M:266:HIS:O	1:M:266:HIS:CG	2.62	0.45
1:O:214:ARG:NH1	2:P:330:GLU:OE2	2.49	0.45
1:O:224:TYR:HA	1:O:227:LEU:HD12	1.98	0.45
1:Q:36:MET:SD	1:Q:61:HIS:HB2	2.56	0.45
1:Q:301:GLN:O	1:Q:302:MET:HB2	2.16	0.45
1:A:214:ARG:NH1	2:B:330:GLU:OE2	2.49	0.45
1:A:260:VAL:HG13	1:A:265:GLY:HA3	1.99	0.45
1:C:224:TYR:HA	1:C:227:LEU:HD12	1.98	0.45
1:E:205:ASP:HB3	1:E:303:VAL:HA	1.99	0.45
1:I:205:ASP:HB3	1:I:303:VAL:HA	1.98	0.45
1:I:224:TYR:HA	1:I:227:LEU:HD12	1.98	0.45
1:I:260:VAL:HG13	1:I:265:GLY:HA3	1.99	0.45
1:K:36:MET:SD	1:K:61:HIS:HB2	2.56	0.45
1:Q:205:ASP:HB3	1:Q:303:VAL:HA	1.99	0.45
2:R:177:VAL:HG12	2:R:177:VAL:O	2.16	0.45
2:R:388:PHE:N	2:R:388:PHE:CD1	2.81	0.45
2:D:97:SER:OG	2:D:98:GLY:N	2.50	0.45
1:E:36:MET:SD	1:E:61:HIS:HB2	2.56	0.45
1:E:260:VAL:HG13	1:E:265:GLY:HA3	1.99	0.45
1:G:260:VAL:HG13	1:G:265:GLY:HA3	1.99	0.45
1:I:345:ASP:HB2	1:I:439:SER:HB2	1.98	0.45
1:O:260:VAL:HG13	1:O:265:GLY:HA3	1.99	0.45
1:Q:260:VAL:HA	1:Q:261:PRO:HD2	1.66	0.45
1:Q:260:VAL:HG13	1:Q:265:GLY:HA3	1.99	0.45
1:C:260:VAL:HG13	1:C:265:GLY:HA3	1.99	0.45
1:E:181:VAL:HG12	1:E:181:VAL:O	2.14	0.45
2:F:177:VAL:HG12	2:F:177:VAL:O	2.16	0.45
1:G:224:TYR:HA	1:G:227:LEU:HD12	1.98	0.45
2:H:97:SER:OG	2:H:98:GLY:N	2.50	0.45
1:I:301:GLN:O	1:I:302:MET:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:260:VAL:HG13	1:M:265:GLY:HA3	1.99	0.45
2:N:97:SER:OG	2:N:98:GLY:N	2.50	0.45
1:O:205:ASP:HB3	1:O:303:VAL:HA	1.99	0.45
1:Q:181:VAL:HG12	1:Q:181:VAL:O	2.14	0.45
1:A:205:ASP:HB3	1:A:303:VAL:HA	1.99	0.44
2:F:305:CYS:SG	2:F:384:ILE:HA	2.58	0.44
1:K:181:VAL:HG12	1:K:181:VAL:O	2.14	0.44
2:L:305:CYS:SG	2:L:384:ILE:HA	2.58	0.44
1:Q:224:TYR:HA	1:Q:227:LEU:HD12	1.98	0.44
1:A:257:THR:O	2:P:404:PHE:CD2	2.71	0.44
1:A:301:GLN:O	1:A:302:MET:HB2	2.16	0.44
1:C:266:HIS:O	1:C:266:HIS:CG	2.62	0.44
2:H:202:TYR:N	2:H:202:TYR:CD1	2.85	0.44
2:H:398:MET:HB3	2:H:398:MET:HE3	1.66	0.44
1:K:224:TYR:HA	1:K:227:LEU:HD12	1.98	0.44
1:O:301:GLN:O	1:O:302:MET:HB2	2.16	0.44
2:R:305:CYS:SG	2:R:384:ILE:HA	2.58	0.44
2:B:105:LYS:O	2:B:110:GLU:N	2.51	0.44
2:D:202:TYR:CD1	2:D:202:TYR:N	2.85	0.44
1:E:224:TYR:HA	1:E:227:LEU:HD12	1.98	0.44
2:F:313:LEU:HD23	2:F:344:VAL:HG11	2.00	0.44
2:H:49:ILE:CG2	2:H:53:TYR:HB2	2.47	0.44
2:H:388:PHE:N	2:H:388:PHE:CD1	2.81	0.44
1:K:345:ASP:HB2	1:K:439:SER:HB2	1.98	0.44
2:L:177:VAL:O	2:L:177:VAL:HG12	2.16	0.44
2:L:313:LEU:HD23	2:L:344:VAL:HG11	1.99	0.44
2:N:49:ILE:CG2	2:N:53:TYR:HB2	2.47	0.44
2:N:202:TYR:CD1	2:N:202:TYR:N	2.85	0.44
2:R:313:LEU:HD23	2:R:344:VAL:HG11	1.99	0.44
1:G:143:GLY:O	1:G:147:SER:OG	2.20	0.44
2:H:105:LYS:HG2	2:H:411:GLU:CD	2.43	0.44
2:J:105:LYS:O	2:J:110:GLU:N	2.51	0.44
2:J:305:CYS:SG	2:J:384:ILE:HA	2.57	0.44
1:K:62:VAL:HA	1:K:63:PRO:HD3	1.84	0.44
2:N:105:LYS:O	2:N:110:GLU:N	2.51	0.44
2:N:105:LYS:HG2	2:N:411:GLU:CD	2.43	0.44
2:N:305:CYS:SG	2:N:384:ILE:HA	2.58	0.44
2:P:105:LYS:O	2:P:110:GLU:N	2.51	0.44
2:P:105:LYS:HG2	2:P:411:GLU:CD	2.43	0.44
1:Q:345:ASP:HB2	1:Q:439:SER:HB2	1.98	0.44
2:B:105:LYS:HG2	2:B:411:GLU:CD	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:ILE:CG2	2:D:53:TYR:HB2	2.48	0.44
2:D:105:LYS:O	2:D:110:GLU:N	2.51	0.44
2:D:105:LYS:HG2	2:D:411:GLU:CD	2.43	0.44
2:D:248:LEU:HB2	2:D:355:VAL:H	1.83	0.44
2:H:248:LEU:HB2	2:H:355:VAL:H	1.83	0.44
2:H:276:THR:HG22	6:H:502:TA1:H162	1.98	0.44
2:J:105:LYS:HG2	2:J:411:GLU:CD	2.43	0.44
1:O:172:TYR:HA	1:O:173:PRO:HD3	1.87	0.44
1:E:345:ASP:HB2	1:E:439:SER:HB2	1.98	0.44
1:G:266:HIS:O	1:G:266:HIS:CG	2.62	0.44
2:H:105:LYS:O	2:H:110:GLU:N	2.51	0.44
2:J:202:TYR:N	2:J:202:TYR:CD1	2.85	0.44
2:L:260:VAL:HA	2:L:261:PRO:HD2	1.83	0.44
2:N:248:LEU:HB2	2:N:355:VAL:H	1.83	0.44
2:B:202:TYR:N	2:B:202:TYR:CD1	2.85	0.44
2:B:305:CYS:SG	2:B:384:ILE:HA	2.58	0.44
2:D:305:CYS:SG	2:D:384:ILE:HA	2.58	0.44
2:D:388:PHE:N	2:D:388:PHE:CD1	2.81	0.44
2:F:49:ILE:CG2	2:F:53:TYR:HB2	2.47	0.44
1:G:62:VAL:HA	1:G:63:PRO:HD3	1.84	0.44
2:H:260:VAL:HA	2:H:261:PRO:HD2	1.83	0.44
1:I:172:TYR:HA	1:I:173:PRO:HD3	1.87	0.44
2:J:49:ILE:CG2	2:J:53:TYR:HB2	2.47	0.44
2:L:49:ILE:CG2	2:L:53:TYR:HB2	2.48	0.44
6:N:502:TA1:H463	6:N:502:TA1:C26	2.46	0.44
2:P:49:ILE:CG2	2:P:53:TYR:HB2	2.47	0.44
2:R:49:ILE:CG2	2:R:53:TYR:HB2	2.47	0.44
2:B:49:ILE:CG2	2:B:53:TYR:HB2	2.48	0.44
1:C:143:GLY:O	1:C:147:SER:OG	2.20	0.44
6:D:502:TA1:H463	6:D:502:TA1:C26	2.46	0.44
2:H:305:CYS:SG	2:H:384:ILE:HA	2.57	0.44
2:J:313:LEU:HD23	2:J:344:VAL:HG11	2.00	0.44
2:P:202:TYR:N	2:P:202:TYR:CD1	2.85	0.44
2:P:248:LEU:HB2	2:P:355:VAL:H	1.83	0.44
2:P:305:CYS:SG	2:P:384:ILE:HA	2.58	0.44
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.88	0.44
2:B:248:LEU:HB2	2:B:355:VAL:H	1.83	0.44
2:D:276:THR:HG22	6:D:502:TA1:H162	1.98	0.44
2:J:248:LEU:HB2	2:J:355:VAL:H	1.83	0.44
2:R:316:ALA:HB3	2:R:378:ILE:HB	1.99	0.44
2:B:313:LEU:HD23	2:B:344:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:260:VAL:HA	2:D:261:PRO:HD2	1.83	0.43
1:E:62:VAL:HA	1:E:63:PRO:HD3	1.84	0.43
2:F:105:LYS:HG2	2:F:411:GLU:CD	2.43	0.43
2:F:316:ALA:HB3	2:F:378:ILE:HB	1.99	0.43
1:I:260:VAL:HA	1:I:261:PRO:HD2	1.66	0.43
2:L:105:LYS:HG2	2:L:411:GLU:CD	2.43	0.43
2:L:316:ALA:HB3	2:L:378:ILE:HB	1.99	0.43
2:N:313:LEU:HD23	2:N:344:VAL:HG11	1.99	0.43
2:N:388:PHE:N	2:N:388:PHE:CD1	2.81	0.43
2:P:313:LEU:HD23	2:P:344:VAL:HG11	2.00	0.43
2:R:105:LYS:HG2	2:R:411:GLU:CD	2.43	0.43
1:I:62:VAL:HA	1:I:63:PRO:HD3	1.84	0.43
2:L:105:LYS:O	2:L:110:GLU:N	2.51	0.43
1:M:121:ARG:HA	1:M:121:ARG:HD3	1.84	0.43
2:D:313:LEU:HD23	2:D:344:VAL:HG11	2.00	0.43
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.99	0.43
2:F:105:LYS:O	2:F:110:GLU:N	2.51	0.43
2:F:260:VAL:HA	2:F:261:PRO:HD2	1.83	0.43
6:H:502:TA1:H463	6:H:502:TA1:C26	2.46	0.43
2:N:276:THR:HG22	6:N:502:TA1:H162	1.98	0.43
2:N:316:ALA:HB3	2:N:378:ILE:HB	1.99	0.43
2:H:316:ALA:HB3	2:H:378:ILE:HB	1.99	0.43
1:I:433:GLU:O	1:I:437:VAL:N	2.50	0.43
2:J:260:VAL:HA	2:J:261:PRO:HD2	1.83	0.43
2:R:105:LYS:O	2:R:110:GLU:N	2.51	0.43
1:A:433:GLU:O	1:A:437:VAL:N	2.50	0.43
2:B:88:ARG:HA	2:B:89:PRO:HD3	1.88	0.43
1:C:62:VAL:HA	1:C:63:PRO:HD3	1.84	0.43
1:G:260:VAL:HA	1:G:261:PRO:HD2	1.66	0.43
2:H:313:LEU:HD23	2:H:344:VAL:HG11	2.00	0.43
2:J:276:THR:HG22	6:J:502:TA1:H162	1.98	0.43
1:O:286:LEU:HB3	1:O:291:ILE:HG13	2.01	0.43
2:P:88:ARG:HA	2:P:89:PRO:HD3	1.88	0.43
1:A:62:VAL:HA	1:A:63:PRO:HD3	1.84	0.43
1:A:260:VAL:HA	1:A:261:PRO:HD2	1.66	0.43
1:C:121:ARG:HA	1:C:121:ARG:HD3	1.84	0.43
2:D:404:PHE:CE1	1:G:261:PRO:HB3	2.54	0.43
1:E:200:CYS:SG	1:E:268:PRO:HG2	2.59	0.43
2:L:205:ASP:OD1	2:L:205:ASP:C	2.61	0.43
1:O:433:GLU:O	1:O:437:VAL:N	2.50	0.43
2:R:260:VAL:HA	2:R:261:PRO:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLY:HA3	1:A:356:ASN:HA	2.00	0.43
2:B:260:VAL:HA	2:B:261:PRO:HD2	1.83	0.43
2:B:276:THR:HG22	6:B:502:TA1:H162	1.98	0.43
2:F:202:TYR:CD1	2:F:202:TYR:N	2.85	0.43
2:F:205:ASP:OD1	2:F:205:ASP:C	2.61	0.43
1:I:246:GLY:HA3	1:I:356:ASN:HA	2.00	0.43
2:J:88:ARG:HA	2:J:89:PRO:HD3	1.88	0.43
1:K:433:GLU:O	1:K:437:VAL:N	2.50	0.43
2:L:202:TYR:N	2:L:202:TYR:CD1	2.85	0.43
1:M:246:GLY:HA3	1:M:356:ASN:HA	2.00	0.43
2:N:260:VAL:HA	2:N:261:PRO:HD2	1.83	0.43
1:O:246:GLY:HA3	1:O:356:ASN:HA	2.00	0.43
1:Q:62:VAL:HA	1:Q:63:PRO:HD3	1.84	0.43
1:Q:200:CYS:SG	1:Q:268:PRO:HG2	2.59	0.43
1:Q:286:LEU:HB3	1:Q:291:ILE:HG13	2.01	0.43
1:A:286:LEU:HB3	1:A:291:ILE:HG13	2.01	0.43
2:B:62:VAL:HA	2:B:63:PRO:HD3	1.91	0.43
1:C:286:LEU:HB3	1:C:291:ILE:HG13	2.01	0.43
1:E:433:GLU:O	1:E:437:VAL:N	2.50	0.43
1:G:246:GLY:HA3	1:G:356:ASN:HA	2.00	0.43
2:J:205:ASP:OD1	2:J:205:ASP:C	2.61	0.43
1:K:200:CYS:SG	1:K:268:PRO:HG2	2.59	0.43
1:K:286:LEU:HB3	1:K:291:ILE:HG13	2.01	0.43
2:L:276:THR:HG22	6:L:502:TA1:H162	1.98	0.43
1:M:286:LEU:HB3	1:M:291:ILE:HG13	2.01	0.43
2:N:62:VAL:HA	2:N:63:PRO:HD3	1.91	0.43
2:P:332:MET:SD	2:P:332:MET:C	3.02	0.43
1:Q:433:GLU:O	1:Q:437:VAL:N	2.50	0.43
2:R:202:TYR:N	2:R:202:TYR:CD1	2.85	0.43
1:A:346:TRP:CE2	2:P:401:ARG:CG	3.00	0.43
2:B:205:ASP:OD1	2:B:205:ASP:C	2.61	0.43
2:B:332:MET:SD	2:B:332:MET:C	3.02	0.43
1:C:246:GLY:HA3	1:C:356:ASN:HA	2.00	0.43
1:E:286:LEU:HB3	1:E:291:ILE:HG13	2.01	0.43
2:F:332:MET:SD	2:F:332:MET:C	3.02	0.43
1:G:395:PHE:CD2	1:G:395:PHE:C	2.96	0.43
2:H:205:ASP:C	2:H:205:ASP:OD1	2.61	0.43
1:I:286:LEU:HB3	1:I:291:ILE:HG13	2.01	0.43
2:R:205:ASP:C	2:R:205:ASP:OD1	2.61	0.43
2:R:332:MET:SD	2:R:332:MET:C	3.02	0.43
1:C:260:VAL:HA	1:C:261:PRO:HD2	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:205:ASP:C	2:D:205:ASP:OD1	2.61	0.43
1:G:286:LEU:HB3	1:G:291:ILE:HG13	2.01	0.43
2:J:332:MET:SD	2:J:332:MET:C	3.02	0.43
2:L:332:MET:SD	2:L:332:MET:C	3.02	0.43
1:M:172:TYR:HA	1:M:173:PRO:HD3	1.87	0.43
2:P:97:SER:OG	2:P:98:GLY:N	2.50	0.43
2:R:62:VAL:HA	2:R:63:PRO:HD3	1.91	0.43
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.87	0.42
1:C:395:PHE:CD2	1:C:395:PHE:C	2.96	0.42
1:E:308:ARG:CZ	1:E:308:ARG:CB	2.97	0.42
1:E:395:PHE:CD2	1:E:395:PHE:C	2.96	0.42
1:G:172:TYR:HA	1:G:173:PRO:HD3	1.88	0.42
1:I:273:ALA:O	1:I:291:ILE:HG23	2.19	0.42
1:K:308:ARG:CZ	1:K:308:ARG:CB	2.97	0.42
1:K:395:PHE:CD2	1:K:395:PHE:C	2.96	0.42
1:M:62:VAL:HA	1:M:63:PRO:HD3	1.84	0.42
2:N:332:MET:C	2:N:332:MET:SD	3.02	0.42
1:O:260:VAL:HA	1:O:261:PRO:HD2	1.66	0.42
1:A:273:ALA:O	1:A:291:ILE:HG23	2.19	0.42
2:B:97:SER:OG	2:B:98:GLY:N	2.50	0.42
2:B:182:VAL:HB	2:B:185:TYR:HB2	2.01	0.42
1:I:200:CYS:SG	1:I:268:PRO:HG2	2.59	0.42
2:J:97:SER:OG	2:J:98:GLY:N	2.50	0.42
2:J:182:VAL:HB	2:J:185:TYR:HB2	2.01	0.42
1:M:273:ALA:O	1:M:291:ILE:HG23	2.19	0.42
2:N:205:ASP:OD1	2:N:205:ASP:C	2.61	0.42
2:P:205:ASP:C	2:P:205:ASP:OD1	2.61	0.42
1:Q:308:ARG:CZ	1:Q:308:ARG:CB	2.97	0.42
1:Q:315:CYS:HB3	1:Q:351:PHE:CD2	2.53	0.42
1:Q:395:PHE:CD2	1:Q:395:PHE:C	2.96	0.42
2:D:332:MET:SD	2:D:332:MET:C	3.02	0.42
1:E:218:ASP:OD1	1:E:280:LYS:NZ	2.52	0.42
1:E:315:CYS:HB3	1:E:351:PHE:CD2	2.53	0.42
1:G:121:ARG:HA	1:G:121:ARG:HD3	1.85	0.42
2:H:182:VAL:HB	2:H:185:TYR:HB2	2.01	0.42
1:K:218:ASP:OD1	1:K:280:LYS:NZ	2.52	0.42
1:K:315:CYS:HB3	1:K:351:PHE:CD2	2.53	0.42
1:M:395:PHE:CD2	1:M:395:PHE:C	2.96	0.42
2:N:182:VAL:HB	2:N:185:TYR:HB2	2.01	0.42
1:O:273:ALA:O	1:O:291:ILE:HG23	2.19	0.42
2:P:62:VAL:HA	2:P:63:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:260:VAL:HA	2:P:261:PRO:HD2	1.83	0.42
1:Q:218:ASP:OD1	1:Q:280:LYS:NZ	2.52	0.42
1:A:200:CYS:SG	1:A:268:PRO:HG2	2.59	0.42
1:C:273:ALA:O	1:C:291:ILE:HG23	2.19	0.42
1:C:315:CYS:HB3	1:C:351:PHE:CD2	2.53	0.42
2:D:182:VAL:HB	2:D:185:TYR:HB2	2.01	0.42
1:G:273:ALA:O	1:G:291:ILE:HG23	2.19	0.42
1:G:315:CYS:HB3	1:G:351:PHE:CD2	2.53	0.42
2:J:331:GLN:OE1	2:J:331:GLN:HA	2.20	0.42
1:O:62:VAL:HA	1:O:63:PRO:HD3	1.84	0.42
2:P:182:VAL:HB	2:P:185:TYR:HB2	2.01	0.42
2:R:105:LYS:HA	2:R:109:THR:OG1	2.20	0.42
2:B:331:GLN:OE1	2:B:331:GLN:HA	2.20	0.42
2:F:105:LYS:HA	2:F:109:THR:OG1	2.20	0.42
1:I:308:ARG:CZ	1:I:308:ARG:CB	2.97	0.42
1:I:402:ARG:HA	1:I:402:ARG:HD3	1.81	0.42
2:L:105:LYS:HA	2:L:109:THR:OG1	2.20	0.42
1:M:315:CYS:HB3	1:M:351:PHE:CD2	2.53	0.42
1:O:200:CYS:SG	1:O:268:PRO:HG2	2.59	0.42
2:P:331:GLN:HA	2:P:331:GLN:OE1	2.20	0.42
2:R:182:VAL:HB	2:R:185:TYR:HB2	2.01	0.42
2:R:248:LEU:HB2	2:R:355:VAL:H	1.83	0.42
1:A:308:ARG:CZ	1:A:308:ARG:CB	2.97	0.42
1:C:200:CYS:SG	1:C:268:PRO:HG2	2.59	0.42
2:F:182:VAL:HB	2:F:185:TYR:HB2	2.01	0.42
2:F:248:LEU:HB2	2:F:355:VAL:H	1.83	0.42
1:G:433:GLU:O	1:G:437:VAL:N	2.50	0.42
2:H:332:MET:SD	2:H:332:MET:C	3.02	0.42
1:K:246:GLY:HA3	1:K:356:ASN:HA	2.00	0.42
2:L:182:VAL:HB	2:L:185:TYR:HB2	2.01	0.42
1:M:200:CYS:SG	1:M:268:PRO:HG2	2.59	0.42
2:P:288:VAL:N	2:P:289:PRO:CD	2.82	0.42
1:A:218:ASP:OD1	1:A:280:LYS:NZ	2.52	0.42
1:A:402:ARG:HA	1:A:402:ARG:HD3	1.82	0.42
2:B:179:ASP:OD1	1:I:352:LYS:NZ	2.52	0.42
2:B:288:VAL:N	2:B:289:PRO:CD	2.82	0.42
1:C:402:ARG:HA	1:C:402:ARG:HD3	1.82	0.42
1:E:246:GLY:HA3	1:E:356:ASN:HA	2.00	0.42
2:H:105:LYS:HA	2:H:109:THR:OG1	2.20	0.42
1:I:218:ASP:OD1	1:I:280:LYS:NZ	2.52	0.42
1:I:315:CYS:HB3	1:I:351:PHE:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:288:VAL:N	2:J:289:PRO:CD	2.82	0.42
1:M:402:ARG:HA	1:M:402:ARG:HD3	1.81	0.42
1:O:308:ARG:CZ	1:O:308:ARG:CB	2.97	0.42
1:C:433:GLU:O	1:C:437:VAL:N	2.50	0.42
1:G:200:CYS:SG	1:G:268:PRO:HG2	2.59	0.42
1:G:308:ARG:CZ	1:G:308:ARG:CB	2.97	0.42
2:H:288:VAL:N	2:H:289:PRO:CD	2.82	0.42
2:L:248:LEU:HB2	2:L:355:VAL:H	1.83	0.42
1:M:260:VAL:HA	1:M:261:PRO:HD2	1.66	0.42
1:M:433:GLU:O	1:M:437:VAL:N	2.50	0.42
1:O:218:ASP:OD1	1:O:280:LYS:NZ	2.52	0.42
6:P:502:TA1:H463	6:P:502:TA1:C26	2.46	0.42
1:Q:246:GLY:HA3	1:Q:356:ASN:HA	2.00	0.42
1:A:352:LYS:NZ	2:P:179:ASP:OD1	2.48	0.42
2:D:105:LYS:HA	2:D:109:THR:OG1	2.20	0.42
2:D:288:VAL:N	2:D:289:PRO:CD	2.82	0.42
1:G:402:ARG:HA	1:G:402:ARG:HD3	1.82	0.42
1:K:402:ARG:HA	1:K:402:ARG:HD3	1.81	0.42
2:L:262:PHE:HA	2:L:263:PRO:HD3	1.90	0.42
1:A:315:CYS:HB3	1:A:351:PHE:CD2	2.54	0.42
6:B:502:TA1:H463	6:B:502:TA1:C26	2.46	0.42
1:C:218:ASP:OD1	1:C:280:LYS:NZ	2.52	0.42
1:C:308:ARG:CZ	1:C:308:ARG:CB	2.97	0.42
1:E:402:ARG:HA	1:E:402:ARG:HD3	1.82	0.42
1:G:218:ASP:OD1	1:G:280:LYS:NZ	2.52	0.42
2:L:19:LYS:HA	2:L:19:LYS:HD2	1.90	0.42
1:M:218:ASP:OD1	1:M:280:LYS:NZ	2.52	0.42
1:M:308:ARG:CZ	1:M:308:ARG:CB	2.97	0.42
2:N:40:SER:OG	2:N:41:ASP:N	2.53	0.42
2:N:105:LYS:HA	2:N:109:THR:OG1	2.20	0.42
2:N:288:VAL:N	2:N:289:PRO:CD	2.82	0.42
1:O:315:CYS:HB3	1:O:351:PHE:CD2	2.54	0.42
1:Q:35:GLN:HE21	1:Q:37:PRO:HG3	1.85	0.42
2:B:401:ARG:HG3	1:I:346:TRP:CG	2.38	0.41
2:F:168:THR:O	2:F:201:THR:HA	2.20	0.41
2:F:262:PHE:HA	2:F:263:PRO:HD3	1.90	0.41
2:L:168:THR:O	2:L:201:THR:HA	2.20	0.41
1:O:402:ARG:HA	1:O:402:ARG:HD3	1.82	0.41
2:R:168:THR:O	2:R:201:THR:HA	2.20	0.41
1:C:217:LEU:HD23	1:C:217:LEU:HA	1.85	0.41
2:D:40:SER:OG	2:D:41:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:331:GLN:OE1	2:D:331:GLN:HA	2.20	0.41
1:E:35:GLN:HE21	1:E:37:PRO:HG3	1.85	0.41
2:H:40:SER:OG	2:H:41:ASP:N	2.53	0.41
2:H:331:GLN:HA	2:H:331:GLN:OE1	2.20	0.41
1:K:35:GLN:HE21	1:K:37:PRO:HG3	1.85	0.41
1:Q:402:ARG:HA	1:Q:402:ARG:HD3	1.81	0.41
1:A:35:GLN:HE21	1:A:37:PRO:HG3	1.85	0.41
1:I:35:GLN:HE21	1:I:37:PRO:HG3	1.85	0.41
6:J:502:TA1:H463	6:J:502:TA1:C26	2.46	0.41
2:L:288:VAL:N	2:L:289:PRO:CD	2.82	0.41
2:N:331:GLN:OE1	2:N:331:GLN:HA	2.20	0.41
2:P:104:ALA:O	2:P:108:TYR:HB3	2.21	0.41
1:A:352:LYS:HB2	2:P:179:ASP:O	2.20	0.41
2:B:104:ALA:O	2:B:108:TYR:HB3	2.21	0.41
2:F:104:ALA:O	2:F:108:TYR:HB3	2.21	0.41
2:L:104:ALA:O	2:L:108:TYR:HB3	2.21	0.41
1:O:35:GLN:HE21	1:O:37:PRO:HG3	1.85	0.41
2:R:262:PHE:HA	2:R:263:PRO:HD3	1.90	0.41
2:F:270:PRO:HA	2:F:377:PHE:O	2.21	0.41
2:F:288:VAL:N	2:F:289:PRO:CD	2.82	0.41
1:G:217:LEU:HD23	1:G:217:LEU:HA	1.85	0.41
2:J:104:ALA:O	2:J:108:TYR:HB3	2.21	0.41
2:J:168:THR:O	2:J:201:THR:HA	2.20	0.41
2:L:270:PRO:HA	2:L:377:PHE:O	2.21	0.41
2:L:331:GLN:OE1	2:L:331:GLN:HA	2.20	0.41
2:R:104:ALA:O	2:R:108:TYR:HB3	2.21	0.41
2:R:270:PRO:HA	2:R:377:PHE:O	2.21	0.41
2:F:331:GLN:OE1	2:F:331:GLN:HA	2.20	0.41
1:G:35:GLN:HE21	1:G:37:PRO:HG3	1.85	0.41
2:R:288:VAL:N	2:R:289:PRO:CD	2.82	0.41
2:B:168:THR:O	2:B:201:THR:HA	2.20	0.41
1:C:273:ALA:HB3	1:C:295:CYS:SG	2.61	0.41
1:G:273:ALA:HB3	1:G:295:CYS:SG	2.61	0.41
1:I:222:PRO:HG2	2:J:326:LYS:HB2	2.03	0.41
1:I:339:ARG:O	1:I:339:ARG:CG	2.64	0.41
2:J:27:GLU:HA	2:J:369:ARG:NE	2.36	0.41
1:M:273:ALA:HB3	1:M:295:CYS:SG	2.61	0.41
2:P:105:LYS:HA	2:P:109:THR:OG1	2.20	0.41
2:P:168:THR:O	2:P:201:THR:HA	2.20	0.41
2:R:40:SER:OG	2:R:41:ASP:N	2.53	0.41
1:A:222:PRO:HG2	2:B:326:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:HB3	1:A:295:CYS:SG	2.61	0.41
1:A:339:ARG:O	1:A:339:ARG:CG	2.64	0.41
1:C:35:GLN:HE21	1:C:37:PRO:HG3	1.85	0.41
2:F:40:SER:OG	2:F:41:ASP:N	2.53	0.41
1:I:273:ALA:HB3	1:I:295:CYS:SG	2.61	0.41
2:J:270:PRO:HA	2:J:377:PHE:O	2.20	0.41
1:O:222:PRO:HG2	2:P:326:LYS:HB2	2.03	0.41
1:O:273:ALA:HB3	1:O:295:CYS:SG	2.61	0.41
2:B:27:GLU:HA	2:B:369:ARG:NE	2.36	0.41
2:B:105:LYS:HA	2:B:109:THR:OG1	2.20	0.41
2:B:270:PRO:HA	2:B:377:PHE:O	2.21	0.41
1:C:222:PRO:HG2	2:D:326:LYS:HB2	2.03	0.41
1:E:222:PRO:HG2	2:F:326:LYS:HB2	2.03	0.41
1:E:273:ALA:O	1:E:291:ILE:HG23	2.19	0.41
1:E:346:TRP:CE2	2:R:401:ARG:CG	3.00	0.41
2:F:27:GLU:HA	2:F:369:ARG:NE	2.36	0.41
2:J:262:PHE:HA	2:J:263:PRO:HD3	1.90	0.41
2:J:398:MET:HE3	2:J:398:MET:HB3	1.66	0.41
1:K:143:GLY:O	1:K:147:SER:OG	2.20	0.41
1:K:222:PRO:HG2	2:L:326:LYS:HB2	2.03	0.41
1:M:35:GLN:HE21	1:M:37:PRO:HG3	1.85	0.41
1:M:222:PRO:HG2	2:N:326:LYS:HB2	2.03	0.41
2:P:27:GLU:HA	2:P:369:ARG:NE	2.36	0.41
2:P:270:PRO:HA	2:P:377:PHE:O	2.21	0.41
1:Q:222:PRO:HG2	2:R:326:LYS:HB2	2.03	0.41
1:Q:273:ALA:O	1:Q:291:ILE:HG23	2.19	0.41
2:R:27:GLU:HA	2:R:369:ARG:NE	2.36	0.41
2:R:331:GLN:OE1	2:R:331:GLN:HA	2.20	0.41
1:C:358:GLU:HA	1:C:359:PRO:HD3	1.81	0.41
2:D:347:ILE:HB	2:D:350:ASN:OD1	2.21	0.41
2:F:185:TYR:OH	2:F:399:PHE:HA	2.21	0.41
1:G:222:PRO:HG2	2:H:326:LYS:HB2	2.03	0.41
2:H:104:ALA:O	2:H:108:TYR:HB3	2.21	0.41
2:H:347:ILE:HB	2:H:350:ASN:OD1	2.21	0.41
2:J:105:LYS:HA	2:J:109:THR:OG1	2.20	0.41
1:K:273:ALA:O	1:K:291:ILE:HG23	2.19	0.41
2:N:168:THR:O	2:N:201:THR:HA	2.20	0.41
2:N:347:ILE:HB	2:N:350:ASN:OD1	2.21	0.41
1:O:339:ARG:O	1:O:339:ARG:CG	2.64	0.41
1:Q:273:ALA:HB3	1:Q:295:CYS:SG	2.61	0.41
2:D:104:ALA:O	2:D:108:TYR:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:ALA:HB3	1:E:295:CYS:SG	2.61	0.40
2:F:97:SER:OG	2:F:98:GLY:N	2.50	0.40
2:H:168:THR:O	2:H:201:THR:HA	2.20	0.40
2:L:27:GLU:HA	2:L:369:ARG:NE	2.36	0.40
2:L:97:SER:OG	2:L:98:GLY:N	2.50	0.40
1:O:217:LEU:HD23	1:O:217:LEU:HA	1.85	0.40
2:R:97:SER:OG	2:R:98:GLY:N	2.50	0.40
2:R:185:TYR:OH	2:R:399:PHE:HA	2.22	0.40
2:B:262:PHE:HA	2:B:263:PRO:HD3	1.90	0.40
2:B:347:ILE:HB	2:B:350:ASN:OD1	2.21	0.40
2:D:168:THR:O	2:D:201:THR:HA	2.20	0.40
2:D:185:TYR:OH	2:D:399:PHE:HA	2.22	0.40
2:H:185:TYR:OH	2:H:399:PHE:HA	2.22	0.40
1:I:395:PHE:CD2	1:I:395:PHE:C	2.96	0.40
2:J:40:SER:OG	2:J:41:ASP:N	2.53	0.40
2:L:183:GLU:N	2:L:184:PRO:CD	2.84	0.40
2:L:185:TYR:OH	2:L:399:PHE:HA	2.22	0.40
2:R:183:GLU:N	2:R:184:PRO:CD	2.84	0.40
1:C:138:PHE:CD1	1:C:138:PHE:N	2.90	0.40
2:D:183:GLU:N	2:D:184:PRO:CD	2.84	0.40
1:E:138:PHE:CD1	1:E:138:PHE:N	2.90	0.40
1:E:143:GLY:O	1:E:147:SER:OG	2.20	0.40
2:F:183:GLU:N	2:F:184:PRO:CD	2.84	0.40
2:H:183:GLU:N	2:H:184:PRO:CD	2.84	0.40
1:K:138:PHE:CD1	1:K:138:PHE:N	2.90	0.40
1:K:273:ALA:HB3	1:K:295:CYS:SG	2.61	0.40
1:M:138:PHE:CD1	1:M:138:PHE:N	2.90	0.40
2:N:104:ALA:O	2:N:108:TYR:HB3	2.21	0.40
2:N:183:GLU:N	2:N:184:PRO:CD	2.84	0.40
2:N:185:TYR:OH	2:N:399:PHE:HA	2.22	0.40
2:P:347:ILE:HB	2:P:350:ASN:OD1	2.21	0.40
1:Q:36:MET:HA	1:Q:37:PRO:HD3	1.42	0.40
2:B:40:SER:OG	2:B:41:ASP:N	2.53	0.40
1:E:183:GLU:N	1:E:184:PRO:CD	2.84	0.40
1:E:352:LYS:NZ	2:R:179:ASP:OD2	2.52	0.40
1:G:138:PHE:CD1	1:G:138:PHE:N	2.90	0.40
2:H:140:SER:O	2:H:147:SER:HB2	2.22	0.40
2:H:270:PRO:HA	2:H:377:PHE:O	2.21	0.40
2:H:338:LYS:NZ	2:J:127:GLU:OE2	2.54	0.40
2:J:347:ILE:HB	2:J:350:ASN:OD1	2.21	0.40
1:K:356:ASN:C	1:K:356:ASN:OD1	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:40:SER:OG	2:L:41:ASP:N	2.53	0.40
2:P:19:LYS:HA	2:P:19:LYS:HD2	1.90	0.40
1:Q:183:GLU:N	1:Q:184:PRO:CD	2.84	0.40
1:A:395:PHE:CD2	1:A:395:PHE:C	2.96	0.40
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.04	0.40
1:C:339:ARG:O	1:C:339:ARG:CG	2.64	0.40
2:D:140:SER:O	2:D:147:SER:HB2	2.22	0.40
1:G:339:ARG:O	1:G:339:ARG:CG	2.64	0.40
2:H:214:PHE:O	2:H:218:LYS:HA	2.22	0.40
2:H:262:PHE:HA	2:H:263:PRO:HD3	1.90	0.40
1:K:183:GLU:N	1:K:184:PRO:CD	2.84	0.40
1:M:180:ALA:HB3	1:M:183:GLU:HG3	2.04	0.40
1:M:356:ASN:OD1	1:M:356:ASN:C	2.63	0.40
1:M:358:GLU:HA	1:M:359:PRO:HD3	1.81	0.40
2:N:140:SER:O	2:N:147:SER:HB2	2.22	0.40
2:N:214:PHE:O	2:N:218:LYS:HA	2.22	0.40
2:P:262:PHE:HA	2:P:263:PRO:HD3	1.90	0.40
1:Q:138:PHE:CD1	1:Q:138:PHE:N	2.90	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%)	401 (95%)	19 (4%)	4 (1%)	14	50
1	C	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	14	50
1	E	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	14	50
1	G	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	14	50
1	I	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	14	50
1	K	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	14	50
1	O	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	14	50
1	Q	424/439 (97%)	401 (95%)	19 (4%)	4 (1%)	14	50
2	B	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	24	64
2	D	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	24	64
2	F	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	24	64
2	H	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	24	64
2	J	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	24	64
2	L	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	24	64
2	N	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	24	64
2	P	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	24	64
2	R	424/427 (99%)	409 (96%)	13 (3%)	2 (0%)	24	64
All	All	7632/7794 (98%)	7290 (96%)	288 (4%)	54 (1%)	20	56

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ASP
1	A	274	PRO
1	A	342	GLN
2	B	50	ASN
1	C	98	ASP
1	C	274	PRO
1	C	342	GLN
2	D	50	ASN
1	E	98	ASP
1	E	274	PRO
1	E	342	GLN
2	F	50	ASN
1	G	98	ASP
1	G	274	PRO
1	G	342	GLN
2	H	50	ASN
1	I	98	ASP
1	I	274	PRO
1	I	342	GLN
2	J	50	ASN
1	K	98	ASP

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Mol	Chain	Res	Type
1	K	274	PRO
1	K	342	GLN
2	L	50	ASN
1	M	98	ASP
1	M	274	PRO
1	M	342	GLN
2	N	50	ASN
1	O	98	ASP
1	O	274	PRO
1	O	342	GLN
2	P	50	ASN
1	Q	98	ASP
1	Q	274	PRO
1	Q	342	GLN
2	R	50	ASN
1	A	348	PRO
1	C	348	PRO
1	E	348	PRO
1	G	348	PRO
1	I	348	PRO
1	K	348	PRO
1	M	348	PRO
1	O	348	PRO
1	Q	348	PRO
2	B	73	GLY
2	D	73	GLY
2	F	73	GLY
2	H	73	GLY
2	J	73	GLY
2	L	73	GLY
2	N	73	GLY
2	P	73	GLY
2	R	73	GLY

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%)	360 (100%)	0	100	100
1	C	360/368 (98%)	360 (100%)	0	100	100
1	E	360/368 (98%)	360 (100%)	0	100	100
1	G	360/368 (98%)	360 (100%)	0	100	100
1	I	360/368 (98%)	360 (100%)	0	100	100
1	K	360/368 (98%)	360 (100%)	0	100	100
1	M	360/368 (98%)	360 (100%)	0	100	100
1	O	360/368 (98%)	360 (100%)	0	100	100
1	Q	360/368 (98%)	360 (100%)	0	100	100
2	B	367/368 (100%)	367 (100%)	0	100	100
2	D	367/368 (100%)	367 (100%)	0	100	100
2	F	367/368 (100%)	367 (100%)	0	100	100
2	H	367/368 (100%)	367 (100%)	0	100	100
2	J	367/368 (100%)	367 (100%)	0	100	100
2	L	367/368 (100%)	367 (100%)	0	100	100
2	N	367/368 (100%)	367 (100%)	0	100	100
2	P	367/368 (100%)	367 (100%)	0	100	100
2	R	367/368 (100%)	367 (100%)	0	100	100
All	All	6543/6624 (99%)	6543 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	35	GLN
1	A	102	ASN
2	B	96	GLN
2	B	102	ASN
1	C	31	GLN
1	C	35	GLN
1	C	102	ASN
2	D	96	GLN
1	E	31	GLN
1	E	35	GLN

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Mol	Chain	Res	Type
1	E	102	ASN
1	G	31	GLN
1	G	35	GLN
1	G	102	ASN
2	H	96	GLN
1	I	31	GLN
1	I	35	GLN
1	I	102	ASN
2	J	96	GLN
1	K	31	GLN
1	K	35	GLN
1	K	102	ASN
2	L	37	HIS
2	L	96	GLN
1	M	31	GLN
1	M	35	GLN
1	M	102	ASN
2	N	96	GLN
1	O	31	GLN
1	O	35	GLN
1	O	102	ASN
2	P	96	GLN
2	P	102	ASN
1	Q	31	GLN
1	Q	35	GLN
1	Q	102	ASN
2	R	96	GLN
2	R	102	ASN
2	R	281	GLN
2	R	282	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 9 are monoatomic - leaving 27 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
6	TA1	J	502	-	68,68,68	2.20	26 (38%)	105,105,105	1.49	13 (12%)
3	GTP	Q	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	E	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
6	TA1	D	502	-	68,68,68	2.20	26 (38%)	105,105,105	1.49	13 (12%)
5	GDP	F	501	-	29,30,30	2.97	12 (41%)	45,47,47	3.49	18 (40%)
3	GTP	G	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
6	TA1	H	502	-	68,68,68	2.20	26 (38%)	105,105,105	1.49	13 (12%)
3	GTP	I	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
6	TA1	L	502	-	68,68,68	2.20	26 (38%)	105,105,105	1.49	13 (12%)
6	TA1	F	502	-	68,68,68	2.20	26 (38%)	105,105,105	1.49	13 (12%)
5	GDP	L	501	-	29,30,30	2.96	12 (41%)	45,47,47	3.49	18 (40%)
3	GTP	A	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
6	TA1	N	502	-	68,68,68	2.20	26 (38%)	105,105,105	1.49	13 (12%)
5	GDP	B	501	-	29,30,30	2.96	13 (44%)	45,47,47	3.49	18 (40%)
6	TA1	R	502	-	68,68,68	2.20	26 (38%)	105,105,105	1.49	13 (12%)
3	GTP	O	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	C	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
3	GTP	M	501	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
6	TA1	B	502	-	68,68,68	2.21	26 (38%)	105,105,105	1.49	13 (12%)
5	GDP	D	501	-	29,30,30	2.96	12 (41%)	45,47,47	3.49	17 (37%)
5	GDP	P	501	-	29,30,30	2.97	12 (41%)	45,47,47	3.49	17 (37%)
5	GDP	H	501	-	29,30,30	2.96	12 (41%)	45,47,47	3.49	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	TA1	P	502	-	68,68,68	2.20	26 (38%)	105,105,105	1.49	12 (11%)
5	GDP	N	501	-	29,30,30	2.96	11 (37%)	45,47,47	3.49	18 (40%)
3	GTP	K	501	4	33,34,34	1.88	3 (9%)	50,54,54	0.91	3 (6%)
5	GDP	R	501	-	29,30,30	2.97	12 (41%)	45,47,47	3.48	17 (37%)
5	GDP	J	501	-	29,30,30	2.95	13 (44%)	45,47,47	3.49	17 (37%)

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
6	TA1	J	502	-	-	9/41/127/127	0/7/7/7
3	GTP	Q	501	4	-	4/22/38/38	0/3/3/3
3	GTP	E	501	4	-	4/22/38/38	0/3/3/3
6	TA1	D	502	-	-	9/41/127/127	0/7/7/7
5	GDP	F	501	-	-	4/16/32/32	0/3/3/3
3	GTP	G	501	4	-	4/22/38/38	0/3/3/3
6	TA1	H	502	-	-	9/41/127/127	0/7/7/7
3	GTP	I	501	4	-	4/22/38/38	0/3/3/3
6	TA1	L	502	-	-	9/41/127/127	0/7/7/7
6	TA1	F	502	-	-	9/41/127/127	0/7/7/7
5	GDP	L	501	-	-	4/16/32/32	0/3/3/3
3	GTP	A	501	4	-	4/22/38/38	0/3/3/3
6	TA1	N	502	-	-	9/41/127/127	0/7/7/7
5	GDP	B	501	-	-	4/16/32/32	0/3/3/3
6	TA1	R	502	-	-	9/41/127/127	0/7/7/7
3	GTP	O	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
6	TA1	B	502	-	-	9/41/127/127	0/7/7/7
5	GDP	D	501	-	-	4/16/32/32	0/3/3/3
5	GDP	P	501	-	-	4/16/32/32	0/3/3/3
5	GDP	H	501	-	-	4/16/32/32	0/3/3/3
6	TA1	P	502	-	-	9/41/127/127	0/7/7/7
5	GDP	N	501	-	-	4/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	K	501	4	-	4/22/38/38	0/3/3/3
5	GDP	R	501	-	-	4/16/32/32	0/3/3/3
5	GDP	J	501	-	-	4/16/32/32	0/3/3/3

All (370) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	501	GDP	PA-O3A	7.63	1.67	1.59
5	H	501	GDP	PA-O3A	7.58	1.67	1.59
5	P	501	GDP	PA-O3A	7.58	1.67	1.59
5	N	501	GDP	PA-O3A	7.57	1.67	1.59
5	B	501	GDP	PA-O3A	7.57	1.67	1.59
5	L	501	GDP	PA-O3A	7.57	1.67	1.59
5	D	501	GDP	PA-O3A	7.55	1.67	1.59
5	F	501	GDP	PA-O3A	7.55	1.67	1.59
5	J	501	GDP	PA-O3A	7.47	1.67	1.59
6	F	502	TA1	C08-C09	6.54	1.50	1.38
6	P	502	TA1	C08-C09	6.51	1.50	1.38
6	H	502	TA1	C08-C09	6.51	1.50	1.38
6	D	502	TA1	C08-C09	6.51	1.50	1.38
6	N	502	TA1	C08-C09	6.49	1.50	1.38
6	B	502	TA1	C08-C09	6.49	1.50	1.38
6	R	502	TA1	C08-C09	6.48	1.50	1.38
6	L	502	TA1	C08-C09	6.47	1.50	1.38
6	J	502	TA1	C08-C09	6.46	1.50	1.38
3	O	501	GTP	PA-O3A	-6.16	1.52	1.59
3	G	501	GTP	PA-O3A	-6.16	1.52	1.59
3	C	501	GTP	PA-O3A	-6.11	1.52	1.59
3	I	501	GTP	PA-O3A	-6.11	1.52	1.59
3	A	501	GTP	PA-O3A	-6.10	1.52	1.59
3	M	501	GTP	PA-O3A	-6.08	1.52	1.59
3	K	501	GTP	PA-O3A	-6.07	1.52	1.59
3	Q	501	GTP	PA-O3A	-6.07	1.52	1.59
5	H	501	GDP	O6-C6	6.07	1.35	1.23
5	F	501	GDP	O6-C6	6.06	1.35	1.23
5	P	501	GDP	O6-C6	6.05	1.35	1.23
5	N	501	GDP	O6-C6	6.05	1.35	1.23
5	D	501	GDP	O6-C6	6.03	1.35	1.23
3	E	501	GTP	PA-O3A	-6.02	1.53	1.59
5	L	501	GDP	O6-C6	6.02	1.35	1.23
5	J	501	GDP	O6-C6	6.01	1.35	1.23
5	R	501	GDP	O6-C6	6.01	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	GDP	O6-C6	6.00	1.34	1.23
5	J	501	GDP	C8-N9	5.82	1.50	1.37
5	R	501	GDP	C8-N9	5.81	1.50	1.37
5	L	501	GDP	C8-N9	5.80	1.50	1.37
5	D	501	GDP	C8-N9	5.79	1.50	1.37
5	B	501	GDP	C8-N9	5.79	1.50	1.37
5	P	501	GDP	C8-N9	5.79	1.50	1.37
5	H	501	GDP	C8-N9	5.78	1.50	1.37
5	F	501	GDP	C8-N9	5.78	1.50	1.37
3	E	501	GTP	PB-O3A	-5.76	1.53	1.59
5	N	501	GDP	C8-N9	5.76	1.50	1.37
3	A	501	GTP	PB-O3A	-5.75	1.53	1.59
3	K	501	GTP	PB-O3A	-5.75	1.53	1.59
3	Q	501	GTP	PB-O3A	-5.73	1.53	1.59
3	C	501	GTP	PB-O3A	-5.72	1.53	1.59
3	I	501	GTP	PB-O3A	-5.71	1.53	1.59
3	M	501	GTP	PB-O3A	-5.71	1.53	1.59
3	O	501	GTP	PB-O3A	-5.69	1.53	1.59
6	B	502	TA1	C07-C06	-5.69	1.25	1.38
6	F	502	TA1	C07-C06	-5.68	1.25	1.38
6	N	502	TA1	C07-C06	-5.68	1.25	1.38
3	G	501	GTP	PB-O3A	-5.67	1.53	1.59
6	H	502	TA1	C07-C06	-5.67	1.25	1.38
6	J	502	TA1	C07-C06	-5.67	1.25	1.38
6	P	502	TA1	C07-C06	-5.67	1.25	1.38
6	R	502	TA1	C07-C06	-5.67	1.25	1.38
6	D	502	TA1	C07-C06	-5.66	1.25	1.38
6	L	502	TA1	C07-C06	-5.63	1.25	1.38
6	B	502	TA1	C18-C10	5.43	1.69	1.57
6	J	502	TA1	C18-C10	5.41	1.69	1.57
6	R	502	TA1	C18-C10	5.41	1.69	1.57
6	N	502	TA1	C18-C10	5.41	1.69	1.57
6	H	502	TA1	C18-C10	5.40	1.69	1.57
3	Q	501	GTP	PB-O3B	5.40	1.65	1.59
6	D	502	TA1	C18-C10	5.39	1.69	1.57
6	P	502	TA1	C18-C10	5.38	1.69	1.57
6	L	502	TA1	C18-C10	5.36	1.69	1.57
6	F	502	TA1	C18-C10	5.36	1.69	1.57
3	E	501	GTP	PB-O3B	5.36	1.65	1.59
3	C	501	GTP	PB-O3B	5.35	1.65	1.59
3	O	501	GTP	PB-O3B	5.34	1.65	1.59
3	M	501	GTP	PB-O3B	5.34	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GTP	PB-O3B	5.32	1.65	1.59
3	G	501	GTP	PB-O3B	5.29	1.65	1.59
3	I	501	GTP	PB-O3B	5.29	1.65	1.59
3	K	501	GTP	PB-O3B	5.25	1.65	1.59
6	L	502	TA1	C09-C04	4.90	1.46	1.39
6	F	502	TA1	C09-C04	4.87	1.46	1.39
6	B	502	TA1	C09-C04	4.85	1.46	1.39
6	J	502	TA1	C09-C04	4.84	1.46	1.39
6	D	502	TA1	C09-C04	4.84	1.46	1.39
6	N	502	TA1	C09-C04	4.84	1.46	1.39
6	P	502	TA1	C09-C04	4.84	1.46	1.39
6	H	502	TA1	C09-C04	4.83	1.46	1.39
6	R	502	TA1	C09-C04	4.83	1.46	1.39
5	F	501	GDP	C2-N1	4.73	1.49	1.37
5	N	501	GDP	C2-N1	4.72	1.49	1.37
5	B	501	GDP	C2-N1	4.72	1.49	1.37
5	D	501	GDP	C2-N1	4.71	1.49	1.37
5	L	501	GDP	C2-N1	4.71	1.49	1.37
5	H	501	GDP	C2-N1	4.71	1.49	1.37
5	J	501	GDP	C2-N1	4.70	1.49	1.37
5	R	501	GDP	C2-N1	4.70	1.49	1.37
5	P	501	GDP	C2-N1	4.70	1.49	1.37
5	J	501	GDP	PB-O1B	4.32	1.63	1.50
5	L	501	GDP	PB-O1B	4.31	1.63	1.50
5	P	501	GDP	PB-O1B	4.31	1.63	1.50
5	F	501	GDP	PB-O1B	4.31	1.63	1.50
5	H	501	GDP	PB-O1B	4.30	1.63	1.50
5	R	501	GDP	PB-O1B	4.30	1.63	1.50
5	D	501	GDP	PB-O1B	4.30	1.63	1.50
5	N	501	GDP	PB-O1B	4.30	1.63	1.50
5	B	501	GDP	PB-O1B	4.29	1.63	1.50
6	L	502	TA1	C45-C24	4.27	1.61	1.54
6	J	502	TA1	C45-C24	4.26	1.61	1.54
6	F	502	TA1	C45-C24	4.24	1.61	1.54
6	B	502	TA1	C45-C24	4.24	1.61	1.54
6	D	502	TA1	C45-C24	4.23	1.61	1.54
6	N	502	TA1	C45-C24	4.23	1.61	1.54
6	R	502	TA1	C45-C24	4.23	1.61	1.54
6	H	502	TA1	C45-C24	4.23	1.61	1.54
6	P	502	TA1	C45-C24	4.19	1.61	1.54
5	F	501	GDP	PB-O2B	-3.94	1.40	1.54
5	L	501	GDP	PB-O2B	-3.93	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	501	GDP	PB-O2B	-3.93	1.40	1.54
5	R	501	GDP	PB-O2B	-3.93	1.40	1.54
5	D	501	GDP	PB-O2B	-3.93	1.40	1.54
5	N	501	GDP	PB-O2B	-3.93	1.40	1.54
5	B	501	GDP	PB-O2B	-3.92	1.40	1.54
5	H	501	GDP	PB-O2B	-3.92	1.40	1.54
5	J	501	GDP	PB-O2B	-3.92	1.40	1.54
6	H	502	TA1	C36-C31	3.79	1.45	1.39
6	L	502	TA1	C36-C31	3.78	1.45	1.39
6	P	502	TA1	C36-C31	3.78	1.45	1.39
6	F	502	TA1	C36-C31	3.78	1.45	1.39
6	D	502	TA1	C36-C31	3.77	1.45	1.39
6	B	502	TA1	C36-C31	3.77	1.45	1.39
6	J	502	TA1	C36-C31	3.75	1.45	1.39
6	N	502	TA1	C36-C31	3.74	1.45	1.39
6	R	502	TA1	C36-C31	3.73	1.45	1.39
6	L	502	TA1	O02-C03	3.53	1.41	1.34
6	B	502	TA1	O02-C03	3.52	1.41	1.34
6	R	502	TA1	O02-C03	3.51	1.41	1.34
6	N	502	TA1	O02-C03	3.51	1.41	1.34
6	J	502	TA1	O02-C03	3.51	1.41	1.34
6	D	502	TA1	O02-C03	3.50	1.41	1.34
6	H	502	TA1	O02-C03	3.48	1.41	1.34
6	P	502	TA1	O02-C03	3.47	1.41	1.34
6	J	502	TA1	C25-C24	3.46	1.39	1.34
6	F	502	TA1	O02-C03	3.46	1.41	1.34
6	P	502	TA1	C25-C24	3.45	1.39	1.34
5	R	501	GDP	O4'-C1'	3.45	1.50	1.42
6	L	502	TA1	C25-C24	3.43	1.39	1.34
6	D	502	TA1	C25-C24	3.43	1.39	1.34
5	L	501	GDP	O4'-C1'	3.42	1.49	1.42
5	F	501	GDP	O4'-C1'	3.42	1.49	1.42
6	H	502	TA1	C25-C24	3.41	1.39	1.34
5	P	501	GDP	O4'-C1'	3.41	1.49	1.42
5	H	501	GDP	O4'-C1'	3.41	1.49	1.42
5	J	501	GDP	O4'-C1'	3.41	1.49	1.42
6	N	502	TA1	C25-C24	3.41	1.39	1.34
5	D	501	GDP	O4'-C1'	3.40	1.49	1.42
6	F	502	TA1	C25-C24	3.40	1.39	1.34
6	R	502	TA1	C25-C24	3.40	1.39	1.34
5	B	501	GDP	O4'-C1'	3.40	1.49	1.42
5	N	501	GDP	O4'-C1'	3.40	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	502	TA1	C25-C24	3.39	1.39	1.34
6	F	502	TA1	C46-C45	3.33	1.60	1.53
6	L	502	TA1	C46-C45	3.33	1.60	1.53
6	P	502	TA1	C46-C45	3.33	1.60	1.53
6	B	502	TA1	C46-C45	3.32	1.60	1.53
6	J	502	TA1	C46-C45	3.32	1.60	1.53
6	H	502	TA1	C46-C45	3.31	1.60	1.53
6	D	502	TA1	C46-C45	3.31	1.60	1.53
6	N	502	TA1	C46-C45	3.30	1.60	1.53
6	R	502	TA1	C46-C45	3.28	1.60	1.53
6	J	502	TA1	C43-C01	3.22	1.60	1.54
6	B	502	TA1	C43-C01	3.22	1.60	1.54
6	L	502	TA1	C43-C01	3.21	1.60	1.54
6	H	502	TA1	C43-C01	3.20	1.60	1.54
6	D	502	TA1	C43-C01	3.20	1.60	1.54
6	P	502	TA1	C43-C01	3.20	1.60	1.54
6	N	502	TA1	C43-C01	3.19	1.60	1.54
6	R	502	TA1	C43-C01	3.16	1.60	1.54
6	F	502	TA1	C43-C01	3.16	1.60	1.54
6	R	502	TA1	C11-C10	3.13	1.61	1.54
5	J	501	GDP	C8-N7	3.12	1.41	1.32
5	P	501	GDP	C8-N7	3.12	1.41	1.32
5	F	501	GDP	C8-N7	3.12	1.41	1.32
6	P	502	TA1	C11-C10	3.12	1.61	1.54
6	B	502	TA1	C11-C10	3.11	1.61	1.54
6	H	502	TA1	C11-C10	3.10	1.61	1.54
6	N	502	TA1	C11-C10	3.10	1.61	1.54
6	F	502	TA1	C11-C10	3.10	1.61	1.54
6	D	502	TA1	C11-C10	3.10	1.61	1.54
5	N	501	GDP	C8-N7	3.10	1.41	1.32
6	L	502	TA1	C11-C10	3.09	1.61	1.54
5	D	501	GDP	C8-N7	3.09	1.41	1.32
6	J	502	TA1	C11-C10	3.09	1.61	1.54
5	B	501	GDP	C8-N7	3.09	1.41	1.32
5	L	501	GDP	C8-N7	3.09	1.41	1.32
5	R	501	GDP	C8-N7	3.08	1.41	1.32
5	H	501	GDP	C8-N7	3.08	1.41	1.32
5	N	501	GDP	C5-N7	-2.92	1.33	1.39
5	F	501	GDP	C5-N7	-2.91	1.33	1.39
5	L	501	GDP	C5-N7	-2.91	1.33	1.39
5	P	501	GDP	C5-N7	-2.91	1.33	1.39
6	P	502	TA1	C43-C26	2.90	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	GDP	C5-N7	-2.90	1.33	1.39
5	H	501	GDP	C5-N7	-2.89	1.33	1.39
5	J	501	GDP	C5-N7	-2.89	1.33	1.39
5	R	501	GDP	C5-N7	-2.89	1.33	1.39
6	F	502	TA1	C43-C26	2.87	1.58	1.52
6	D	502	TA1	C43-C26	2.87	1.58	1.52
6	R	502	TA1	C43-C26	2.87	1.58	1.52
5	B	501	GDP	C5-N7	-2.87	1.33	1.39
6	J	502	TA1	C43-C26	2.86	1.58	1.52
6	H	502	TA1	C43-C26	2.85	1.58	1.52
6	L	502	TA1	C43-C26	2.85	1.58	1.52
6	N	502	TA1	C43-C26	2.84	1.58	1.52
6	B	502	TA1	C43-C26	2.84	1.58	1.52
5	P	501	GDP	C5-C4	2.73	1.46	1.38
5	F	501	GDP	C5-C4	2.73	1.46	1.38
5	N	501	GDP	C5-C4	2.73	1.46	1.38
5	J	501	GDP	C5-C4	2.71	1.46	1.38
5	R	501	GDP	C5-C4	2.71	1.46	1.38
5	B	501	GDP	C5-C4	2.71	1.46	1.38
5	D	501	GDP	C5-C4	2.71	1.46	1.38
5	H	501	GDP	C5-C4	2.70	1.46	1.38
5	L	501	GDP	C5-C4	2.70	1.46	1.38
6	B	502	TA1	C26-C25	2.63	1.56	1.51
6	R	502	TA1	C26-C25	2.61	1.56	1.51
6	L	502	TA1	C26-C25	2.60	1.56	1.51
6	N	502	TA1	C26-C25	2.60	1.56	1.51
6	F	502	TA1	C26-C25	2.59	1.56	1.51
6	N	502	TA1	C01-C45	2.58	1.66	1.56
6	R	502	TA1	C01-C45	2.57	1.66	1.56
6	P	502	TA1	C26-C25	2.57	1.56	1.51
6	D	502	TA1	C26-C25	2.57	1.56	1.51
6	H	502	TA1	C26-C25	2.57	1.56	1.51
6	B	502	TA1	C01-C45	2.56	1.66	1.56
6	J	502	TA1	C26-C25	2.56	1.56	1.51
6	D	502	TA1	C01-C45	2.56	1.66	1.56
6	L	502	TA1	C01-C45	2.55	1.66	1.56
6	L	502	TA1	C18-C20	2.55	1.62	1.55
6	P	502	TA1	C01-C45	2.55	1.66	1.56
6	P	502	TA1	C18-C20	2.55	1.62	1.55
6	H	502	TA1	C01-C45	2.55	1.66	1.56
6	F	502	TA1	C18-C20	2.55	1.62	1.55
6	J	502	TA1	C01-C45	2.55	1.66	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	502	TA1	C01-C45	2.55	1.66	1.56
6	J	502	TA1	C18-C20	2.54	1.62	1.55
6	B	502	TA1	C18-C20	2.54	1.62	1.55
6	N	502	TA1	C18-C20	2.53	1.62	1.55
6	D	502	TA1	C18-C20	2.53	1.62	1.55
6	H	502	TA1	C18-C20	2.52	1.62	1.55
6	R	502	TA1	C18-C20	2.52	1.62	1.55
6	P	502	TA1	C04-C03	-2.50	1.44	1.50
6	R	502	TA1	C04-C03	-2.49	1.44	1.50
6	J	502	TA1	C04-C03	-2.48	1.44	1.50
6	D	502	TA1	C04-C03	-2.47	1.44	1.50
6	F	502	TA1	C04-C03	-2.47	1.44	1.50
6	B	502	TA1	C04-C03	-2.47	1.44	1.50
6	H	502	TA1	C04-C03	-2.47	1.44	1.50
6	N	502	TA1	C04-C03	-2.46	1.44	1.50
6	L	502	TA1	C04-C03	-2.45	1.44	1.50
6	N	502	TA1	C41-C42	2.45	1.43	1.38
5	N	501	GDP	C2-N3	-2.44	1.27	1.33
6	L	502	TA1	C41-C42	2.43	1.43	1.38
5	H	501	GDP	C2-N3	-2.43	1.27	1.33
5	J	501	GDP	C2-N3	-2.41	1.27	1.33
6	R	502	TA1	C41-C42	2.41	1.43	1.38
5	D	501	GDP	C2-N3	-2.41	1.27	1.33
5	R	501	GDP	C2-N3	-2.41	1.27	1.33
6	F	502	TA1	C41-C42	2.40	1.43	1.38
5	B	501	GDP	C2-N3	-2.40	1.27	1.33
6	D	502	TA1	C41-C42	2.40	1.43	1.38
5	P	501	GDP	C2-N3	-2.40	1.27	1.33
6	H	502	TA1	C41-C42	2.40	1.43	1.38
5	F	501	GDP	C2-N3	-2.39	1.27	1.33
6	B	502	TA1	C41-C42	2.39	1.43	1.38
6	J	502	TA1	C41-C42	2.38	1.43	1.38
5	L	501	GDP	C2-N3	-2.37	1.27	1.33
6	P	502	TA1	C41-C42	2.37	1.43	1.38
6	J	502	TA1	C16-C15	2.33	1.57	1.52
6	P	502	TA1	C16-C15	2.32	1.56	1.52
6	B	502	TA1	C16-C15	2.32	1.56	1.52
6	N	502	TA1	C16-C15	2.32	1.56	1.52
6	F	502	TA1	C16-C15	2.31	1.56	1.52
6	D	502	TA1	C16-C15	2.31	1.56	1.52
6	R	502	TA1	C16-C15	2.31	1.56	1.52
6	H	502	TA1	C16-C15	2.30	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	502	TA1	C16-C15	2.30	1.56	1.52
6	B	502	TA1	C06-C05	2.16	1.42	1.38
6	R	502	TA1	C10-C02	2.15	1.62	1.57
6	J	502	TA1	C37-C29	2.14	1.54	1.52
6	R	502	TA1	C37-C29	2.14	1.54	1.52
6	L	502	TA1	C10-C02	2.14	1.62	1.57
6	P	502	TA1	O09-C21	2.14	1.49	1.44
6	F	502	TA1	O09-C21	2.14	1.49	1.44
6	P	502	TA1	C37-C29	2.13	1.54	1.52
6	F	502	TA1	C37-C29	2.13	1.54	1.52
6	H	502	TA1	C37-C29	2.13	1.54	1.52
6	H	502	TA1	O09-C21	2.12	1.49	1.44
6	D	502	TA1	C37-C29	2.12	1.54	1.52
6	H	502	TA1	C08-C07	2.12	1.42	1.38
6	D	502	TA1	C10-C02	2.12	1.62	1.57
6	H	502	TA1	C10-C02	2.12	1.62	1.57
6	J	502	TA1	C08-C07	2.12	1.42	1.38
6	L	502	TA1	O09-C21	2.12	1.49	1.44
6	N	502	TA1	C10-C02	2.12	1.62	1.57
6	J	502	TA1	C10-C02	2.11	1.62	1.57
6	P	502	TA1	C10-C02	2.11	1.62	1.57
6	D	502	TA1	O09-C21	2.11	1.49	1.44
6	J	502	TA1	C06-C05	2.11	1.42	1.38
6	F	502	TA1	C06-C05	2.10	1.42	1.38
6	R	502	TA1	C08-C07	2.10	1.42	1.38
6	B	502	TA1	C37-C29	2.10	1.54	1.52
6	J	502	TA1	O09-C21	2.10	1.49	1.44
6	B	502	TA1	C10-C02	2.10	1.62	1.57
6	D	502	TA1	C06-C05	2.10	1.42	1.38
6	B	502	TA1	C08-C07	2.10	1.42	1.38
6	L	502	TA1	C06-C05	2.10	1.42	1.38
6	B	502	TA1	C33-C32	2.10	1.42	1.38
6	B	502	TA1	C39-C38	2.10	1.42	1.38
6	H	502	TA1	C33-C32	2.10	1.42	1.38
6	F	502	TA1	C10-C02	2.10	1.62	1.57
6	R	502	TA1	O09-C21	2.09	1.49	1.44
6	N	502	TA1	O09-C21	2.09	1.49	1.44
6	B	502	TA1	O09-C21	2.09	1.49	1.44
6	D	502	TA1	C33-C32	2.09	1.42	1.38
6	D	502	TA1	C08-C07	2.09	1.42	1.38
6	L	502	TA1	C08-C07	2.09	1.42	1.38
6	H	502	TA1	C06-C05	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	502	TA1	C37-C29	2.08	1.54	1.52
6	F	502	TA1	C08-C07	2.08	1.42	1.38
6	N	502	TA1	C06-C05	2.08	1.42	1.38
6	R	502	TA1	C33-C32	2.08	1.42	1.38
6	L	502	TA1	C37-C29	2.08	1.54	1.52
6	F	502	TA1	C33-C32	2.08	1.42	1.38
6	L	502	TA1	C39-C38	2.07	1.42	1.38
6	P	502	TA1	C06-C05	2.07	1.42	1.38
6	L	502	TA1	C33-C32	2.07	1.42	1.38
6	P	502	TA1	C39-C38	2.07	1.42	1.38
6	R	502	TA1	C06-C05	2.07	1.42	1.38
6	P	502	TA1	C33-C32	2.07	1.42	1.38
6	D	502	TA1	C39-C38	2.07	1.42	1.38
6	H	502	TA1	C39-C38	2.07	1.42	1.38
6	N	502	TA1	C08-C07	2.07	1.42	1.38
6	J	502	TA1	C33-C32	2.06	1.42	1.38
6	P	502	TA1	C08-C07	2.06	1.42	1.38
6	N	502	TA1	C34-C33	2.05	1.42	1.38
6	J	502	TA1	C39-C38	2.05	1.42	1.38
6	R	502	TA1	C39-C38	2.04	1.42	1.38
6	F	502	TA1	C39-C38	2.04	1.42	1.38
6	N	502	TA1	C33-C32	2.04	1.42	1.38
6	N	502	TA1	C39-C38	2.04	1.42	1.38
6	P	502	TA1	C34-C33	2.04	1.42	1.38
6	F	502	TA1	C34-C33	2.04	1.42	1.38
6	L	502	TA1	C34-C33	2.03	1.42	1.38
6	R	502	TA1	C34-C33	2.03	1.42	1.38
6	J	502	TA1	C34-C33	2.03	1.42	1.38
5	P	501	GDP	O3'-C3'	2.03	1.48	1.43
6	D	502	TA1	C34-C33	2.02	1.42	1.38
5	F	501	GDP	C5'-C4'	-2.02	1.45	1.51
6	B	502	TA1	C34-C33	2.02	1.42	1.38
5	H	501	GDP	O3'-C3'	2.01	1.47	1.43
5	J	501	GDP	C5'-C4'	-2.01	1.45	1.51
5	L	501	GDP	C5'-C4'	-2.01	1.45	1.51
5	J	501	GDP	O3'-C3'	2.01	1.47	1.43
5	R	501	GDP	O3'-C3'	2.01	1.47	1.43
5	B	501	GDP	C5'-C4'	-2.01	1.45	1.51
6	H	502	TA1	C34-C33	2.01	1.42	1.38
5	B	501	GDP	O3'-C3'	2.01	1.47	1.43
5	D	501	GDP	O3'-C3'	2.01	1.47	1.43

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	501	GDP	N9-C8-N7	-10.76	93.45	113.40
5	F	501	GDP	N9-C8-N7	-10.75	93.46	113.40
5	R	501	GDP	N9-C8-N7	-10.75	93.47	113.40
5	L	501	GDP	N9-C8-N7	-10.75	93.47	113.40
5	P	501	GDP	N9-C8-N7	-10.74	93.48	113.40
5	B	501	GDP	N9-C8-N7	-10.74	93.48	113.40
5	D	501	GDP	N9-C8-N7	-10.74	93.48	113.40
5	N	501	GDP	N9-C8-N7	-10.74	93.49	113.40
5	H	501	GDP	N9-C8-N7	-10.73	93.51	113.40
5	L	501	GDP	C8-N7-C5	9.22	120.68	104.26
5	F	501	GDP	C8-N7-C5	9.21	120.66	104.26
5	N	501	GDP	C8-N7-C5	9.21	120.66	104.26
5	H	501	GDP	C8-N7-C5	9.20	120.66	104.26
5	D	501	GDP	C8-N7-C5	9.20	120.65	104.26
5	R	501	GDP	C8-N7-C5	9.20	120.65	104.26
5	B	501	GDP	C8-N7-C5	9.20	120.64	104.26
5	P	501	GDP	C8-N7-C5	9.19	120.62	104.26
5	J	501	GDP	C8-N7-C5	9.18	120.62	104.26
5	N	501	GDP	C6-C5-N7	8.65	146.03	130.29
5	F	501	GDP	C6-C5-N7	8.65	146.03	130.29
5	H	501	GDP	C6-C5-N7	8.65	146.03	130.29
5	L	501	GDP	C6-C5-N7	8.64	146.02	130.29
5	P	501	GDP	C6-C5-N7	8.64	146.01	130.29
5	B	501	GDP	C6-C5-N7	8.64	146.01	130.29
5	D	501	GDP	C6-C5-N7	8.63	146.00	130.29
5	J	501	GDP	C6-C5-N7	8.61	145.97	130.29
5	R	501	GDP	C6-C5-N7	8.61	145.96	130.29
5	N	501	GDP	C6-C5-C4	-6.29	109.37	118.83
5	F	501	GDP	C6-C5-C4	-6.28	109.38	118.83
5	J	501	GDP	N2-C2-N3	6.28	131.92	119.67
5	P	501	GDP	C6-C5-C4	-6.27	109.40	118.83
5	H	501	GDP	N2-C2-N3	6.27	131.91	119.67
5	J	501	GDP	C6-C5-C4	-6.27	109.40	118.83
5	B	501	GDP	N2-C2-N3	6.27	131.91	119.67
5	D	501	GDP	C6-C5-C4	-6.27	109.40	118.83
5	B	501	GDP	C6-C5-C4	-6.27	109.40	118.83
5	F	501	GDP	N2-C2-N3	6.27	131.90	119.67
5	L	501	GDP	C6-C5-C4	-6.26	109.41	118.83
5	L	501	GDP	N2-C2-N3	6.26	131.89	119.67
5	N	501	GDP	N2-C2-N3	6.26	131.89	119.67
5	D	501	GDP	N2-C2-N3	6.26	131.88	119.67
5	P	501	GDP	N2-C2-N3	6.25	131.88	119.67
5	H	501	GDP	C6-C5-C4	-6.25	109.42	118.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	501	GDP	N2-C2-N3	6.25	131.86	119.67
5	R	501	GDP	C6-C5-C4	-6.24	109.44	118.83
5	J	501	GDP	C8-N9-C4	5.93	117.14	106.03
5	F	501	GDP	C8-N9-C4	5.92	117.12	106.03
5	P	501	GDP	C8-N9-C4	5.92	117.12	106.03
5	N	501	GDP	C8-N9-C4	5.91	117.11	106.03
5	B	501	GDP	C8-N9-C4	5.91	117.11	106.03
5	R	501	GDP	C8-N9-C4	5.91	117.10	106.03
5	D	501	GDP	C8-N9-C4	5.90	117.08	106.03
5	L	501	GDP	C8-N9-C4	5.88	117.05	106.03
5	H	501	GDP	C8-N9-C4	5.88	117.05	106.03
6	L	502	TA1	C08-C09-C04	-5.85	114.61	120.36
6	F	502	TA1	C07-C06-C05	5.84	127.45	120.24
6	H	502	TA1	C07-C06-C05	5.84	127.44	120.24
6	F	502	TA1	C08-C09-C04	-5.84	114.63	120.36
6	R	502	TA1	C07-C06-C05	5.83	127.43	120.24
6	J	502	TA1	C07-C06-C05	5.82	127.42	120.24
6	B	502	TA1	C07-C06-C05	5.82	127.42	120.24
6	B	502	TA1	C08-C09-C04	-5.82	114.65	120.36
6	D	502	TA1	C08-C09-C04	-5.81	114.65	120.36
6	D	502	TA1	C07-C06-C05	5.81	127.41	120.24
6	L	502	TA1	C07-C06-C05	5.80	127.40	120.24
6	R	502	TA1	C08-C09-C04	-5.80	114.66	120.36
6	N	502	TA1	C08-C09-C04	-5.80	114.66	120.36
6	N	502	TA1	C07-C06-C05	5.80	127.39	120.24
6	P	502	TA1	C08-C09-C04	-5.80	114.67	120.36
6	J	502	TA1	C08-C09-C04	-5.79	114.67	120.36
6	H	502	TA1	C08-C09-C04	-5.78	114.68	120.36
6	P	502	TA1	C07-C06-C05	5.78	127.37	120.24
5	N	501	GDP	C5-C6-N1	4.53	124.79	113.25
5	F	501	GDP	C5-C6-N1	4.53	124.78	113.25
5	P	501	GDP	C5-C6-N1	4.52	124.75	113.25
5	L	501	GDP	C5-C6-N1	4.52	124.75	113.25
5	H	501	GDP	C5-C6-N1	4.52	124.75	113.25
5	D	501	GDP	C5-C6-N1	4.51	124.74	113.25
5	B	501	GDP	C5-C6-N1	4.51	124.74	113.25
5	J	501	GDP	C5-C6-N1	4.51	124.74	113.25
5	R	501	GDP	C5-C6-N1	4.50	124.69	113.25
5	J	501	GDP	N2-C2-N1	-4.24	107.81	116.76
5	N	501	GDP	N2-C2-N1	-4.23	107.82	116.76
5	H	501	GDP	N2-C2-N1	-4.23	107.83	116.76
5	R	501	GDP	N2-C2-N1	-4.22	107.86	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GDP	N2-C2-N1	-4.22	107.86	116.76
5	B	501	GDP	N2-C2-N1	-4.22	107.86	116.76
5	P	501	GDP	N2-C2-N1	-4.21	107.87	116.76
5	L	501	GDP	N2-C2-N1	-4.20	107.89	116.76
5	F	501	GDP	N2-C2-N1	-4.20	107.89	116.76
5	L	501	GDP	C2-N3-C4	4.08	119.33	112.30
5	P	501	GDP	C2-N3-C4	4.08	119.33	112.30
5	H	501	GDP	C2-N3-C4	4.08	119.33	112.30
5	F	501	GDP	C2-N3-C4	4.08	119.33	112.30
6	L	502	TA1	C09-C04-C03	-4.08	111.41	120.40
5	J	501	GDP	C2-N3-C4	4.08	119.32	112.30
5	R	501	GDP	C2-N3-C4	4.07	119.32	112.30
5	B	501	GDP	C2-N3-C4	4.07	119.31	112.30
5	D	501	GDP	C2-N3-C4	4.07	119.31	112.30
5	N	501	GDP	C2-N3-C4	4.07	119.31	112.30
6	B	502	TA1	C09-C04-C03	-4.07	111.43	120.40
6	F	502	TA1	C09-C04-C03	-4.06	111.45	120.40
6	N	502	TA1	C09-C04-C03	-4.06	111.45	120.40
6	D	502	TA1	C09-C04-C03	-4.05	111.46	120.40
6	J	502	TA1	C09-C04-C03	-4.05	111.46	120.40
6	H	502	TA1	C09-C04-C03	-4.05	111.47	120.40
6	R	502	TA1	C09-C04-C03	-4.05	111.47	120.40
6	P	502	TA1	C09-C04-C03	-4.02	111.53	120.40
5	P	501	GDP	O6-C6-C5	-4.02	115.93	126.53
5	L	501	GDP	O6-C6-C5	-4.01	115.94	126.53
5	F	501	GDP	O6-C6-C5	-4.01	115.95	126.53
5	N	501	GDP	O6-C6-C5	-4.01	115.95	126.53
5	D	501	GDP	O6-C6-C5	-4.01	115.96	126.53
5	B	501	GDP	O6-C6-C5	-4.01	115.96	126.53
5	H	501	GDP	O6-C6-C5	-4.01	115.96	126.53
5	R	501	GDP	O6-C6-C5	-3.99	116.00	126.53
5	J	501	GDP	O6-C6-C5	-3.99	116.00	126.53
5	H	501	GDP	C4-C5-N7	-3.86	104.55	110.67
5	L	501	GDP	C4-C5-N7	-3.85	104.57	110.67
5	B	501	GDP	C4-C5-N7	-3.84	104.59	110.67
5	P	501	GDP	C4-C5-N7	-3.84	104.59	110.67
5	N	501	GDP	C4-C5-N7	-3.83	104.60	110.67
5	D	501	GDP	C4-C5-N7	-3.83	104.60	110.67
5	F	501	GDP	C4-C5-N7	-3.83	104.60	110.67
5	R	501	GDP	C4-C5-N7	-3.83	104.60	110.67
5	J	501	GDP	C4-C5-N7	-3.81	104.64	110.67
5	N	501	GDP	C2-N1-C6	-3.79	118.24	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	501	GDP	C2-N1-C6	-3.77	118.27	125.11
5	J	501	GDP	C2-N1-C6	-3.77	118.27	125.11
5	D	501	GDP	C2-N1-C6	-3.77	118.28	125.11
5	R	501	GDP	C2-N1-C6	-3.76	118.29	125.11
5	B	501	GDP	C2-N1-C6	-3.76	118.29	125.11
5	P	501	GDP	C2-N1-C6	-3.76	118.30	125.11
5	L	501	GDP	C2-N1-C6	-3.76	118.30	125.11
5	F	501	GDP	C2-N1-C6	-3.75	118.31	125.11
6	L	502	TA1	C05-C04-C03	3.66	128.47	120.40
6	N	502	TA1	C05-C04-C03	3.65	128.45	120.40
6	F	502	TA1	C05-C04-C03	3.65	128.45	120.40
6	B	502	TA1	C05-C04-C03	3.65	128.44	120.40
6	H	502	TA1	C05-C04-C03	3.64	128.43	120.40
6	J	502	TA1	C05-C04-C03	3.64	128.43	120.40
6	D	502	TA1	C05-C04-C03	3.64	128.43	120.40
6	R	502	TA1	C05-C04-C03	3.64	128.43	120.40
6	P	502	TA1	C05-C04-C03	3.63	128.40	120.40
5	R	501	GDP	C2'-C3'-C4'	3.53	109.44	102.61
5	L	501	GDP	C2'-C3'-C4'	3.53	109.43	102.61
5	F	501	GDP	C2'-C3'-C4'	3.53	109.43	102.61
5	B	501	GDP	C2'-C3'-C4'	3.53	109.42	102.61
5	N	501	GDP	C2'-C3'-C4'	3.53	109.42	102.61
5	D	501	GDP	C2'-C3'-C4'	3.52	109.42	102.61
5	H	501	GDP	C2'-C3'-C4'	3.52	109.41	102.61
5	J	501	GDP	C2'-C3'-C4'	3.52	109.41	102.61
5	P	501	GDP	C2'-C3'-C4'	3.52	109.40	102.61
6	N	502	TA1	C17-C18-C20	3.25	109.87	102.58
6	R	502	TA1	C17-C18-C20	3.24	109.85	102.58
6	H	502	TA1	C17-C18-C20	3.24	109.84	102.58
6	D	502	TA1	C17-C18-C20	3.23	109.83	102.58
6	B	502	TA1	C17-C18-C20	3.23	109.83	102.58
6	J	502	TA1	C17-C18-C20	3.22	109.81	102.58
6	F	502	TA1	C17-C18-C20	3.22	109.81	102.58
6	P	502	TA1	C17-C18-C20	3.21	109.80	102.58
6	L	502	TA1	C17-C18-C20	3.21	109.79	102.58
6	B	502	TA1	O04-C11-C14	-2.98	101.81	108.13
6	F	502	TA1	O04-C11-C14	-2.97	101.83	108.13
6	H	502	TA1	O04-C11-C14	-2.97	101.84	108.13
6	P	502	TA1	O04-C11-C14	-2.97	101.84	108.13
6	N	502	TA1	O04-C11-C14	-2.97	101.84	108.13
6	D	502	TA1	O04-C11-C14	-2.96	101.84	108.13
6	J	502	TA1	O04-C11-C14	-2.96	101.85	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	502	TA1	O04-C11-C14	-2.96	101.85	108.13
6	R	502	TA1	O04-C11-C14	-2.95	101.86	108.13
6	R	502	TA1	C45-C01-C02	2.90	115.12	111.93
6	B	502	TA1	C45-C01-C02	2.90	115.12	111.93
6	J	502	TA1	C45-C01-C02	2.89	115.11	111.93
6	D	502	TA1	C45-C01-C02	2.89	115.11	111.93
6	H	502	TA1	C45-C01-C02	2.87	115.09	111.93
6	P	502	TA1	C45-C01-C02	2.87	115.09	111.93
6	N	502	TA1	C45-C01-C02	2.87	115.08	111.93
6	F	502	TA1	C45-C01-C02	2.86	115.07	111.93
6	L	502	TA1	C45-C01-C02	2.85	115.06	111.93
5	J	501	GDP	C1'-N9-C8	-2.68	119.11	126.73
5	B	501	GDP	C1'-N9-C8	-2.67	119.14	126.73
5	P	501	GDP	C1'-N9-C8	-2.67	119.15	126.73
5	H	501	GDP	C1'-N9-C8	-2.66	119.17	126.73
5	D	501	GDP	C1'-N9-C8	-2.66	119.18	126.73
5	F	501	GDP	C1'-N9-C8	-2.66	119.19	126.73
5	R	501	GDP	C1'-N9-C8	-2.65	119.19	126.73
5	L	501	GDP	C1'-N9-C8	-2.65	119.21	126.73
3	K	501	GTP	O2G-PG-O3B	2.65	113.51	104.64
5	N	501	GDP	C1'-N9-C8	-2.64	119.22	126.73
3	A	501	GTP	O2G-PG-O3B	2.64	113.49	104.64
3	O	501	GTP	O2G-PG-O3B	2.64	113.48	104.64
3	G	501	GTP	O2G-PG-O3B	2.64	113.48	104.64
3	C	501	GTP	O2G-PG-O3B	2.63	113.45	104.64
3	M	501	GTP	O2G-PG-O3B	2.63	113.45	104.64
3	I	501	GTP	O2G-PG-O3B	2.63	113.45	104.64
3	E	501	GTP	O2G-PG-O3B	2.62	113.43	104.64
3	Q	501	GTP	O2G-PG-O3B	2.62	113.43	104.64
6	N	502	TA1	O01-C01-C43	2.52	113.49	107.04
6	L	502	TA1	O01-C01-C43	2.52	113.48	107.04
6	R	502	TA1	O01-C01-C43	2.51	113.46	107.04
6	F	502	TA1	O01-C01-C43	2.51	113.45	107.04
6	D	502	TA1	O01-C01-C43	2.50	113.43	107.04
6	P	502	TA1	O01-C01-C43	2.50	113.43	107.04
6	H	502	TA1	O01-C01-C43	2.50	113.42	107.04
6	B	502	TA1	O01-C01-C43	2.49	113.41	107.04
6	J	502	TA1	O01-C01-C43	2.49	113.41	107.04
5	R	501	GDP	O2'-C2'-C3'	2.36	119.40	111.82
5	B	501	GDP	O2'-C2'-C3'	2.36	119.38	111.82
5	L	501	GDP	O2'-C2'-C3'	2.36	119.38	111.82
5	F	501	GDP	O2'-C2'-C3'	2.36	119.37	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	501	GDP	O2'-C2'-C3'	2.36	119.37	111.82
5	J	501	GDP	O2'-C2'-C3'	2.36	119.37	111.82
5	D	501	GDP	O2'-C2'-C3'	2.35	119.36	111.82
5	N	501	GDP	O2'-C2'-C3'	2.35	119.34	111.82
5	H	501	GDP	O2'-C2'-C3'	2.34	119.33	111.82
6	B	502	TA1	C06-C05-C04	-2.34	118.06	120.36
6	F	502	TA1	C06-C05-C04	-2.32	118.08	120.36
6	H	502	TA1	C06-C05-C04	-2.32	118.08	120.36
6	J	502	TA1	C06-C05-C04	-2.32	118.09	120.36
6	D	502	TA1	C06-C05-C04	-2.32	118.09	120.36
6	R	502	TA1	C06-C05-C04	-2.31	118.09	120.36
6	N	502	TA1	C06-C05-C04	-2.31	118.10	120.36
6	P	502	TA1	C06-C05-C04	-2.29	118.11	120.36
6	L	502	TA1	C06-C05-C04	-2.28	118.12	120.36
6	L	502	TA1	C14-C11-C15	-2.25	83.06	85.38
6	H	502	TA1	C14-C11-C15	-2.23	83.08	85.38
6	D	502	TA1	C14-C11-C15	-2.23	83.08	85.38
6	R	502	TA1	C14-C11-C15	-2.22	83.08	85.38
6	J	502	TA1	C14-C11-C15	-2.22	83.08	85.38
6	N	502	TA1	C14-C11-C15	-2.22	83.09	85.38
6	H	502	TA1	C10-C18-C17	-2.22	102.33	106.55
6	F	502	TA1	C14-C11-C15	-2.22	83.09	85.38
6	R	502	TA1	C10-C18-C17	-2.22	102.34	106.55
6	N	502	TA1	C10-C18-C17	-2.21	102.34	106.55
6	P	502	TA1	C14-C11-C15	-2.20	83.10	85.38
5	P	501	GDP	O3B-PB-O2B	2.20	116.07	107.80
6	D	502	TA1	C10-C18-C17	-2.20	102.37	106.55
6	B	502	TA1	C10-C18-C17	-2.20	102.37	106.55
5	N	501	GDP	O3B-PB-O2B	2.20	116.06	107.80
5	D	501	GDP	O3B-PB-O2B	2.20	116.05	107.80
5	H	501	GDP	O3B-PB-O2B	2.20	116.05	107.80
6	J	502	TA1	C10-C18-C17	-2.20	102.38	106.55
5	L	501	GDP	O3B-PB-O2B	2.20	116.04	107.80
5	R	501	GDP	O3B-PB-O2B	2.19	116.03	107.80
6	B	502	TA1	C14-C11-C15	-2.19	83.11	85.38
5	J	501	GDP	O3B-PB-O2B	2.19	116.02	107.80
6	L	502	TA1	C10-C18-C17	-2.19	102.39	106.55
5	F	501	GDP	O3B-PB-O2B	2.19	116.00	107.80
6	F	502	TA1	C10-C18-C17	-2.18	102.40	106.55
5	B	501	GDP	O3B-PB-O2B	2.18	115.98	107.80
6	P	502	TA1	C10-C18-C17	-2.17	102.42	106.55
6	J	502	TA1	O06-C15-C11	2.17	92.95	90.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	502	TA1	O06-C15-C11	2.17	92.95	90.58
6	B	502	TA1	O06-C15-C11	2.15	92.93	90.58
6	D	502	TA1	O06-C15-C11	2.15	92.93	90.58
6	H	502	TA1	O06-C15-C11	2.15	92.93	90.58
6	L	502	TA1	O06-C15-C11	2.14	92.92	90.58
6	R	502	TA1	O06-C15-C11	2.14	92.92	90.58
6	N	502	TA1	O06-C15-C11	2.14	92.92	90.58
6	P	502	TA1	O06-C15-C11	2.14	92.92	90.58
3	O	501	GTP	O5'-C5'-C4'	2.09	116.11	108.99
3	G	501	GTP	O5'-C5'-C4'	2.09	116.11	108.99
3	Q	501	GTP	O5'-C5'-C4'	2.09	116.10	108.99
5	B	501	GDP	C4'-O4'-C1'	2.09	114.07	109.47
3	M	501	GTP	O5'-C5'-C4'	2.08	116.09	108.99
3	I	501	GTP	O5'-C5'-C4'	2.08	116.09	108.99
3	K	501	GTP	O5'-C5'-C4'	2.08	116.09	108.99
3	C	501	GTP	O5'-C5'-C4'	2.08	116.08	108.99
3	A	501	GTP	O5'-C5'-C4'	2.07	116.06	108.99
3	E	501	GTP	O5'-C5'-C4'	2.07	116.06	108.99
5	L	501	GDP	C4'-O4'-C1'	2.07	114.04	109.47
5	N	501	GDP	C4'-O4'-C1'	2.07	114.04	109.47
5	D	501	GDP	C4'-O4'-C1'	2.07	114.03	109.47
5	R	501	GDP	C4'-O4'-C1'	2.07	114.03	109.47
5	F	501	GDP	C4'-O4'-C1'	2.07	114.03	109.47
5	H	501	GDP	C4'-O4'-C1'	2.06	114.02	109.47
5	P	501	GDP	C4'-O4'-C1'	2.06	114.02	109.47
5	J	501	GDP	C4'-O4'-C1'	2.06	114.01	109.47
3	M	501	GTP	O3G-PG-O3B	2.04	111.48	104.64
3	G	501	GTP	O3G-PG-O3B	2.03	111.46	104.64
3	Q	501	GTP	O3G-PG-O3B	2.03	111.45	104.64
3	E	501	GTP	O3G-PG-O3B	2.03	111.45	104.64
6	N	502	TA1	C21-O09-C22	2.03	120.13	115.95
3	C	501	GTP	O3G-PG-O3B	2.02	111.43	104.64
6	R	502	TA1	C21-O09-C22	2.02	120.12	115.95
3	A	501	GTP	O3G-PG-O3B	2.02	111.41	104.64
3	K	501	GTP	O3G-PG-O3B	2.02	111.41	104.64
3	I	501	GTP	O3G-PG-O3B	2.02	111.40	104.64
6	L	502	TA1	C21-O09-C22	2.02	120.11	115.95
3	O	501	GTP	O3G-PG-O3B	2.02	111.40	104.64
6	B	502	TA1	C21-O09-C22	2.01	120.10	115.95
6	H	502	TA1	C21-O09-C22	2.01	120.10	115.95
5	N	501	GDP	O4'-C4'-C3'	-2.01	101.16	105.15
6	D	502	TA1	C21-O09-C22	2.01	120.09	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	501	GDP	O4'-C4'-C3'	-2.01	101.17	105.15
5	F	501	GDP	O4'-C4'-C3'	-2.00	101.17	105.15
6	J	502	TA1	C21-O09-C22	2.00	120.08	115.95
6	F	502	TA1	C21-O09-C22	2.00	120.08	115.95
5	B	501	GDP	O4'-C4'-C3'	-2.00	101.18	105.15

There are no chirality outliers.

All (153) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	GDP	PA-O3A-PB-O2B
5	B	501	GDP	C5'-O5'-PA-O3A
5	B	501	GDP	C5'-O5'-PA-O2A
5	D	501	GDP	PA-O3A-PB-O2B
5	D	501	GDP	C5'-O5'-PA-O3A
5	D	501	GDP	C5'-O5'-PA-O2A
5	F	501	GDP	PA-O3A-PB-O2B
5	F	501	GDP	C5'-O5'-PA-O3A
5	F	501	GDP	C5'-O5'-PA-O2A
5	H	501	GDP	PA-O3A-PB-O2B
5	H	501	GDP	C5'-O5'-PA-O3A
5	H	501	GDP	C5'-O5'-PA-O2A
5	J	501	GDP	PA-O3A-PB-O2B
5	J	501	GDP	C5'-O5'-PA-O3A
5	J	501	GDP	C5'-O5'-PA-O2A
5	L	501	GDP	PA-O3A-PB-O2B
5	L	501	GDP	C5'-O5'-PA-O3A
5	L	501	GDP	C5'-O5'-PA-O2A
5	N	501	GDP	PA-O3A-PB-O2B
5	N	501	GDP	C5'-O5'-PA-O3A
5	N	501	GDP	C5'-O5'-PA-O2A
5	P	501	GDP	PA-O3A-PB-O2B
5	P	501	GDP	C5'-O5'-PA-O3A
5	P	501	GDP	C5'-O5'-PA-O2A
5	R	501	GDP	PA-O3A-PB-O2B
5	R	501	GDP	C5'-O5'-PA-O3A
5	R	501	GDP	C5'-O5'-PA-O2A
6	B	502	TA1	O02-C03-C04-C09
6	D	502	TA1	O02-C03-C04-C09
6	F	502	TA1	O02-C03-C04-C09
6	H	502	TA1	O02-C03-C04-C09
6	J	502	TA1	O02-C03-C04-C09

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Mol	Chain	Res	Type	Atoms
6	L	502	TA1	O02-C03-C04-C09
6	N	502	TA1	O02-C03-C04-C09
6	P	502	TA1	O02-C03-C04-C09
6	R	502	TA1	O02-C03-C04-C09
6	B	502	TA1	O02-C03-C04-C05
6	D	502	TA1	O02-C03-C04-C05
6	F	502	TA1	O02-C03-C04-C05
6	H	502	TA1	O02-C03-C04-C05
6	J	502	TA1	O02-C03-C04-C05
6	L	502	TA1	O02-C03-C04-C05
6	N	502	TA1	O02-C03-C04-C05
6	P	502	TA1	O02-C03-C04-C05
6	R	502	TA1	O02-C03-C04-C05
6	B	502	TA1	O03-C03-C04-C05
6	D	502	TA1	O03-C03-C04-C05
6	F	502	TA1	O03-C03-C04-C05
6	H	502	TA1	O03-C03-C04-C05
6	J	502	TA1	O03-C03-C04-C05
6	L	502	TA1	O03-C03-C04-C05
6	N	502	TA1	O03-C03-C04-C05
6	R	502	TA1	O03-C03-C04-C05
6	P	502	TA1	O03-C03-C04-C05
6	B	502	TA1	O03-C03-C04-C09
6	D	502	TA1	O03-C03-C04-C09
6	F	502	TA1	O03-C03-C04-C09
6	H	502	TA1	O03-C03-C04-C09
6	J	502	TA1	O03-C03-C04-C09
6	L	502	TA1	O03-C03-C04-C09
6	N	502	TA1	O03-C03-C04-C09
6	P	502	TA1	O03-C03-C04-C09
6	R	502	TA1	O03-C03-C04-C09
6	B	502	TA1	N01-C30-C31-C36
6	D	502	TA1	N01-C30-C31-C36
6	F	502	TA1	N01-C30-C31-C36
6	H	502	TA1	N01-C30-C31-C36
6	L	502	TA1	N01-C30-C31-C36
6	N	502	TA1	N01-C30-C31-C36
6	P	502	TA1	N01-C30-C31-C36
6	R	502	TA1	N01-C30-C31-C36
6	J	502	TA1	N01-C30-C31-C36
6	L	502	TA1	O14-C30-C31-C36
6	N	502	TA1	O14-C30-C31-C36

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Mol	Chain	Res	Type	Atoms
6	B	502	TA1	O14-C30-C31-C36
6	D	502	TA1	O14-C30-C31-C36
6	F	502	TA1	O14-C30-C31-C36
6	H	502	TA1	O14-C30-C31-C36
6	J	502	TA1	O14-C30-C31-C36
6	P	502	TA1	O14-C30-C31-C36
6	R	502	TA1	O14-C30-C31-C36
6	B	502	TA1	N01-C30-C31-C32
6	D	502	TA1	N01-C30-C31-C32
6	F	502	TA1	N01-C30-C31-C32
6	H	502	TA1	N01-C30-C31-C32
6	J	502	TA1	N01-C30-C31-C32
6	N	502	TA1	N01-C30-C31-C32
6	P	502	TA1	N01-C30-C31-C32
6	R	502	TA1	N01-C30-C31-C32
6	L	502	TA1	N01-C30-C31-C32
6	B	502	TA1	O14-C30-C31-C32
6	D	502	TA1	O14-C30-C31-C32
6	F	502	TA1	O14-C30-C31-C32
6	H	502	TA1	O14-C30-C31-C32
6	J	502	TA1	O14-C30-C31-C32
6	L	502	TA1	O14-C30-C31-C32
6	N	502	TA1	O14-C30-C31-C32
6	P	502	TA1	O14-C30-C31-C32
6	R	502	TA1	O14-C30-C31-C32
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'
3	O	501	GTP	C3'-C4'-C5'-O5'
3	Q	501	GTP	C3'-C4'-C5'-O5'
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	K	501	GTP	O4'-C4'-C5'-O5'
3	M	501	GTP	O4'-C4'-C5'-O5'
3	O	501	GTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	Q	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
5	B	501	GDP	PA-O3A-PB-O3B
5	D	501	GDP	PA-O3A-PB-O3B
5	F	501	GDP	PA-O3A-PB-O3B
5	H	501	GDP	PA-O3A-PB-O3B
5	J	501	GDP	PA-O3A-PB-O3B
5	L	501	GDP	PA-O3A-PB-O3B
5	N	501	GDP	PA-O3A-PB-O3B
5	P	501	GDP	PA-O3A-PB-O3B
5	R	501	GDP	PA-O3A-PB-O3B
6	B	502	TA1	C15-C11-O04-C12
6	D	502	TA1	C15-C11-O04-C12
6	F	502	TA1	C15-C11-O04-C12
6	H	502	TA1	C15-C11-O04-C12
6	J	502	TA1	C15-C11-O04-C12
6	L	502	TA1	C15-C11-O04-C12
6	N	502	TA1	C15-C11-O04-C12
6	P	502	TA1	C15-C11-O04-C12
6	R	502	TA1	C15-C11-O04-C12
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

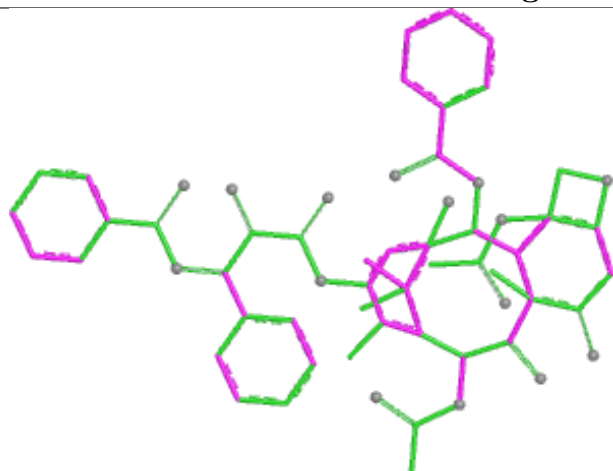
There are no ring outliers.

18 monomers are involved in 54 short contacts:

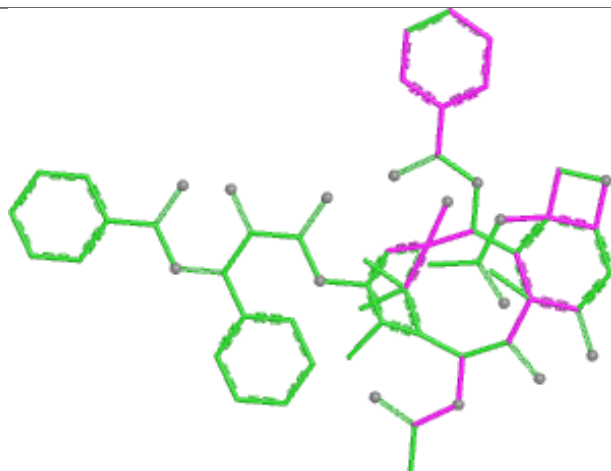
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	502	TA1	4	0
6	D	502	TA1	4	0
5	F	501	GDP	2	0
6	H	502	TA1	4	0
6	L	502	TA1	4	0
6	F	502	TA1	4	0
5	L	501	GDP	2	0
6	N	502	TA1	4	0
5	B	501	GDP	2	0
6	R	502	TA1	4	0
6	B	502	TA1	4	0
5	D	501	GDP	2	0
5	P	501	GDP	2	0
5	H	501	GDP	2	0
6	P	502	TA1	4	0
5	N	501	GDP	2	0
5	R	501	GDP	2	0
5	J	501	GDP	2	0

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

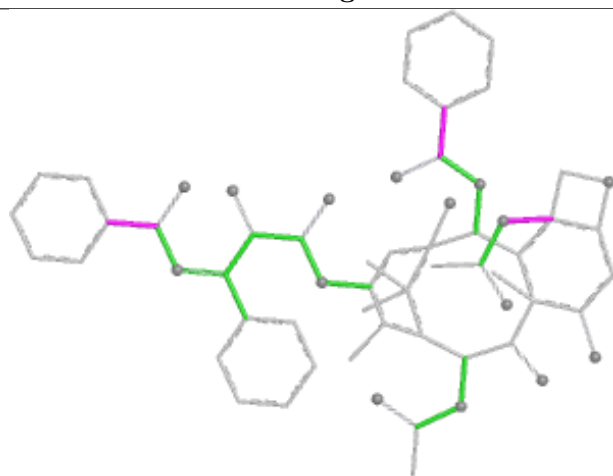
Ligand TA1 J 502



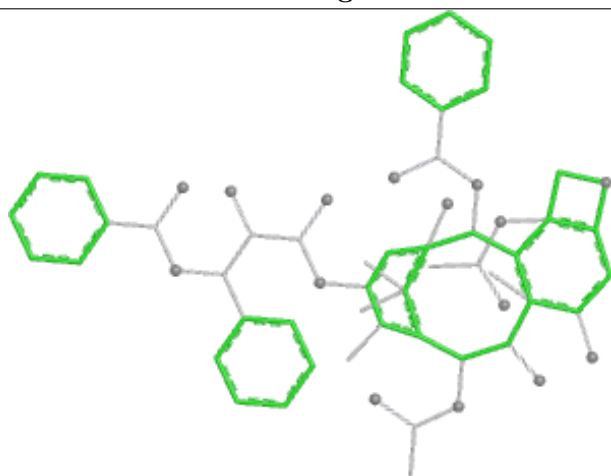
Bond lengths



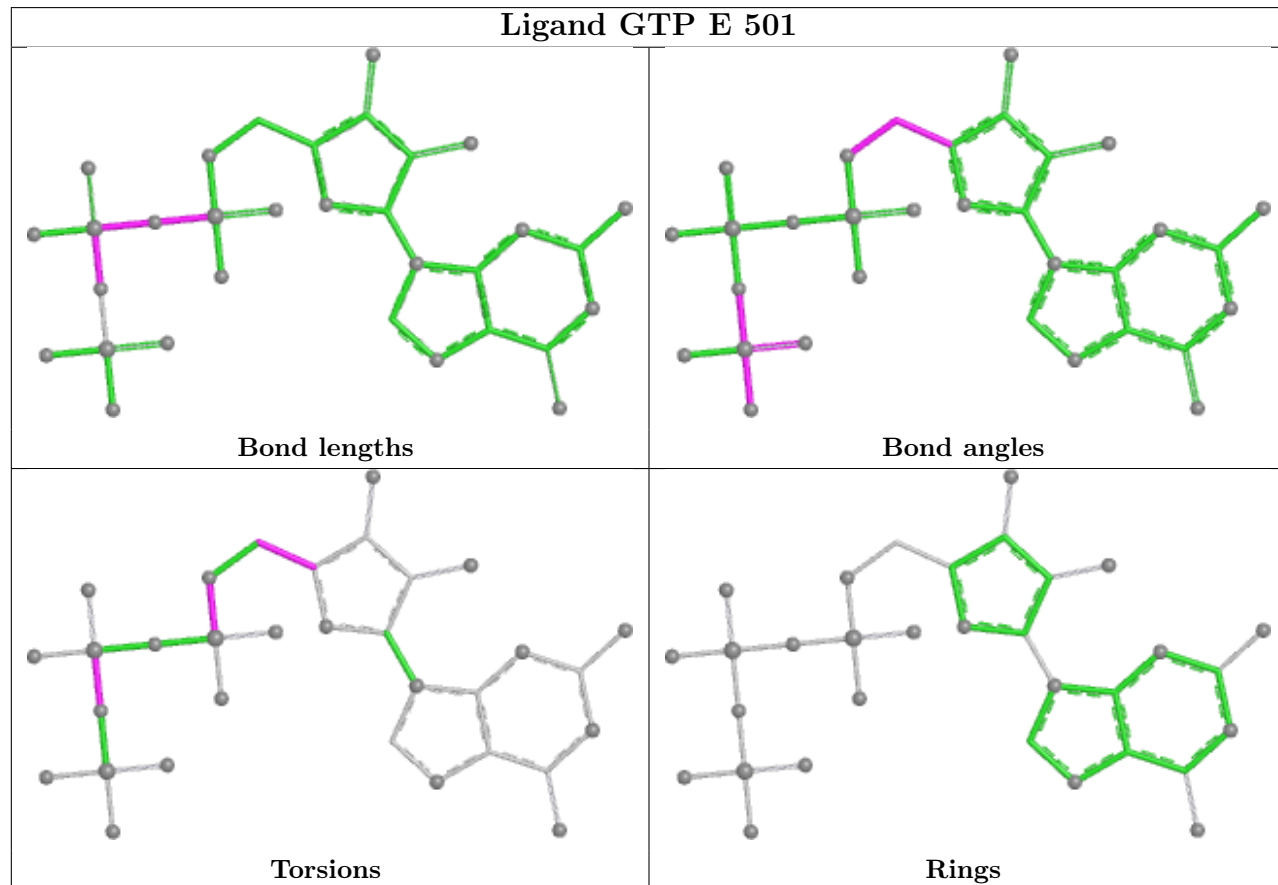
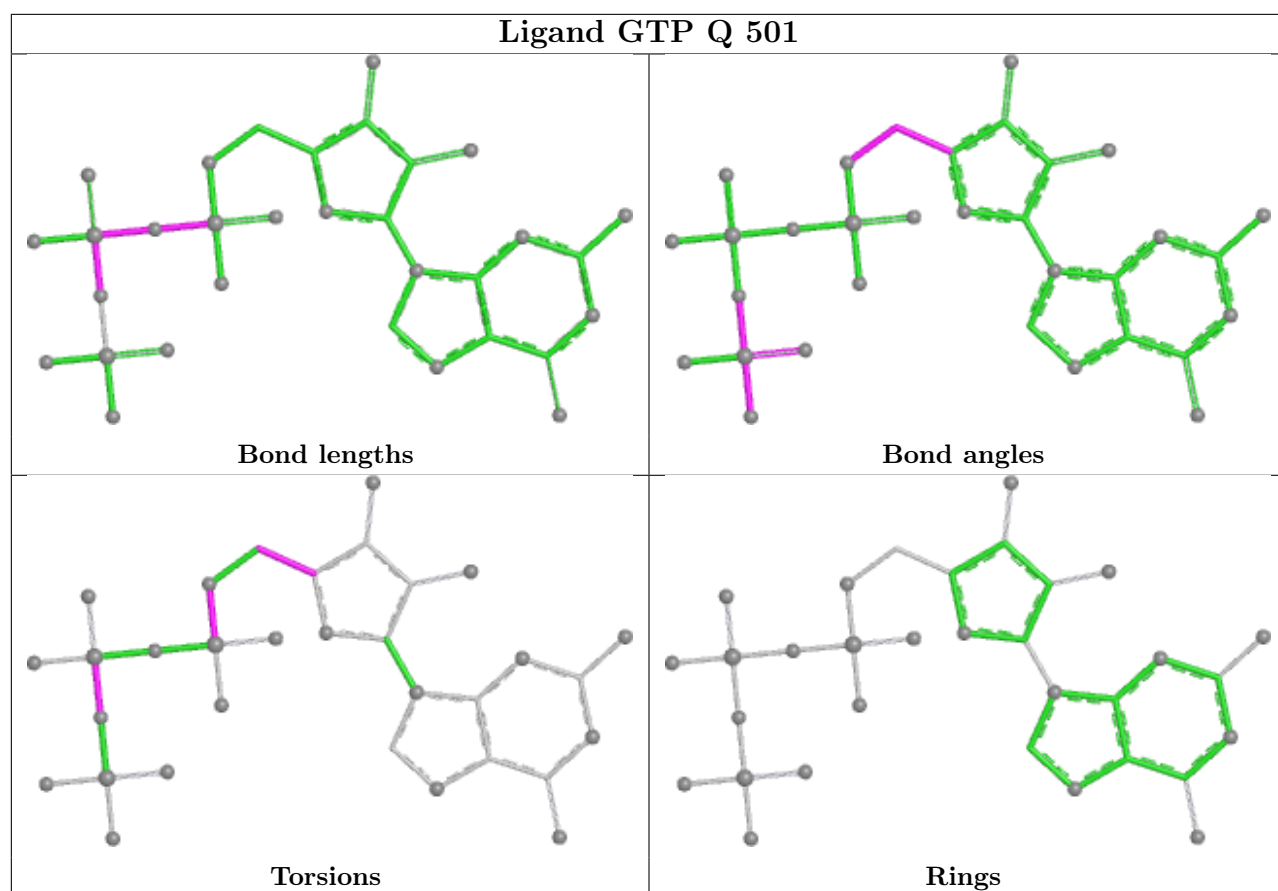
Bond angles



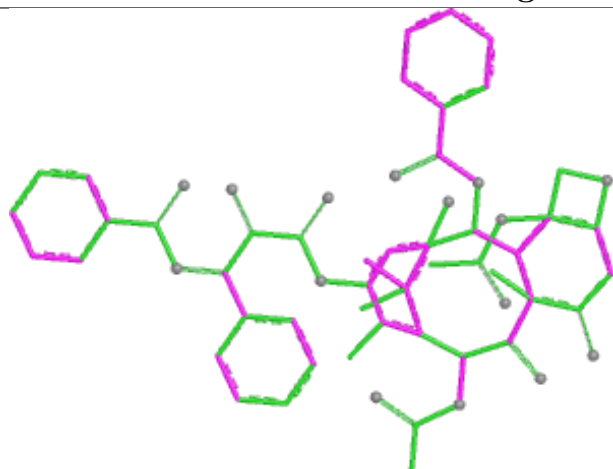
Torsions



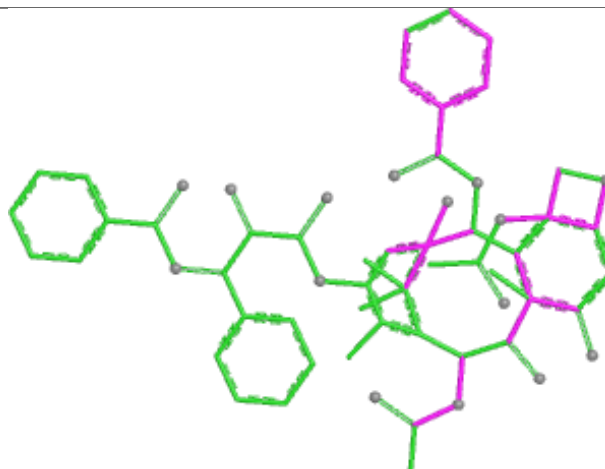
Rings



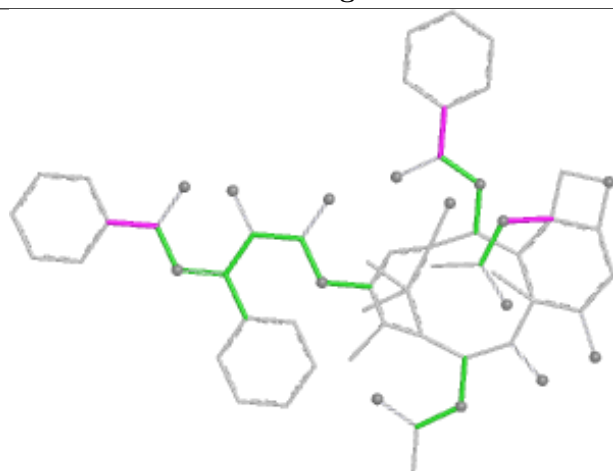
Ligand TA1 D 502



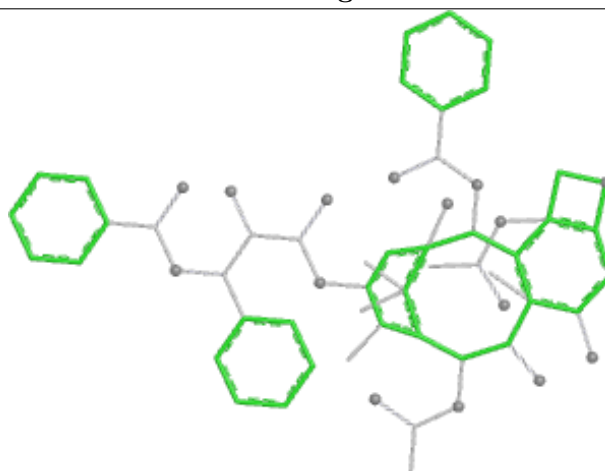
Bond lengths



Bond angles

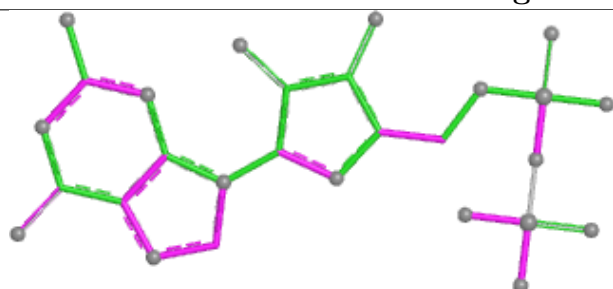


Torsions

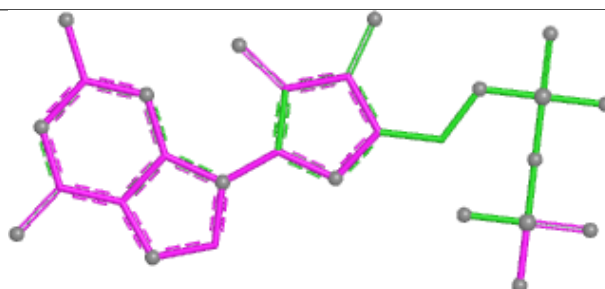


Rings

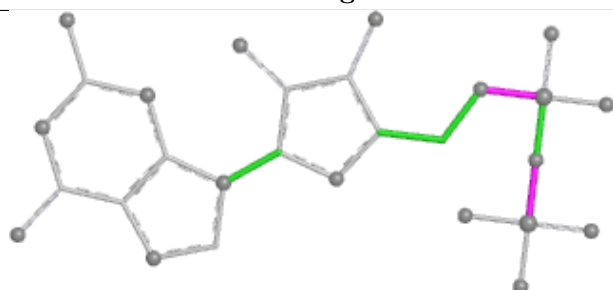
Ligand GDP F 501



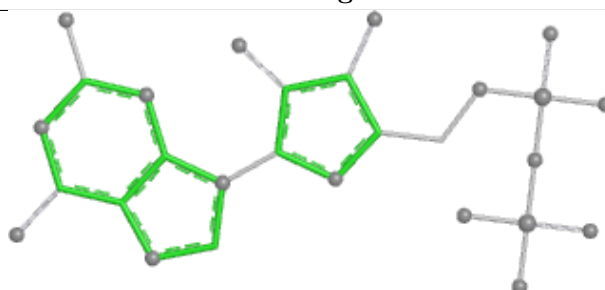
Bond lengths



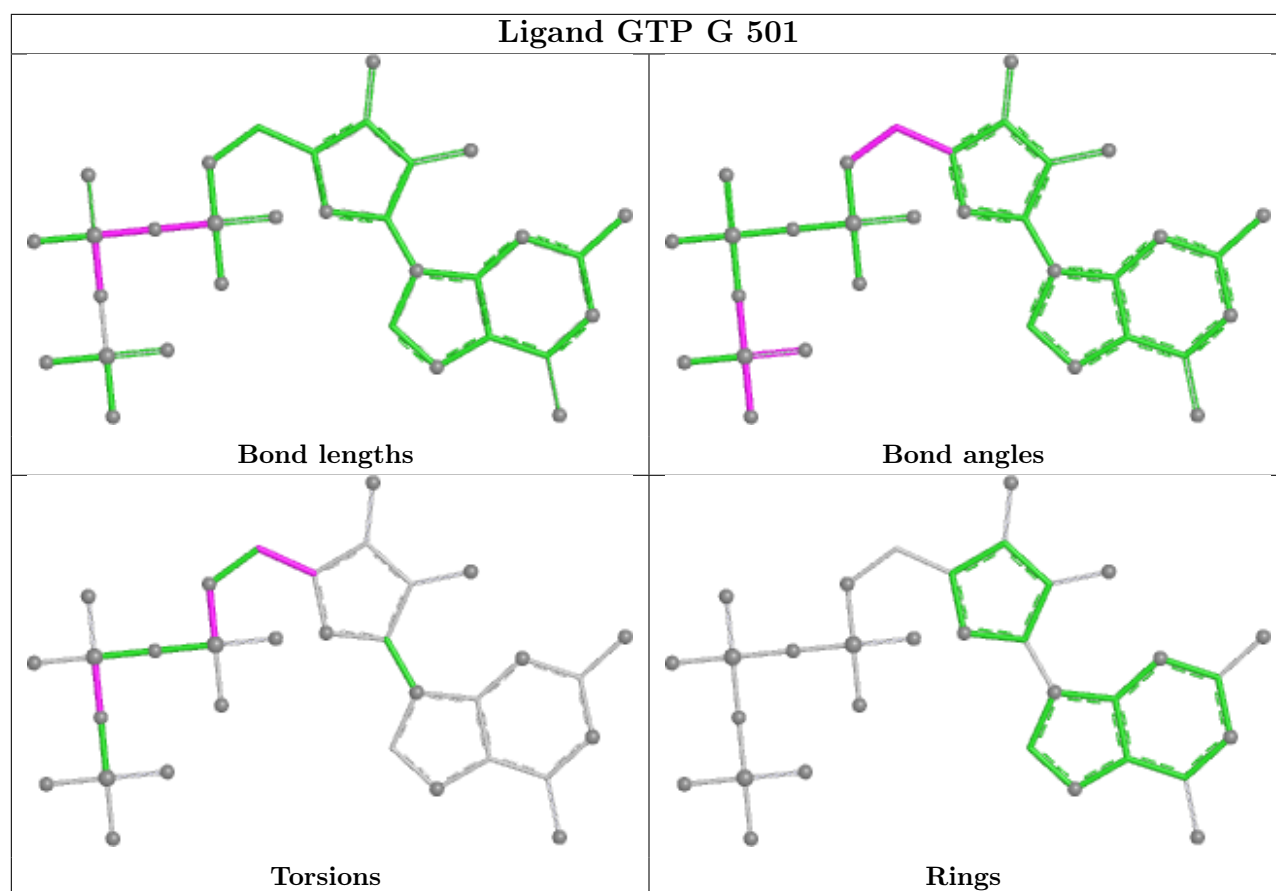
Bond angles



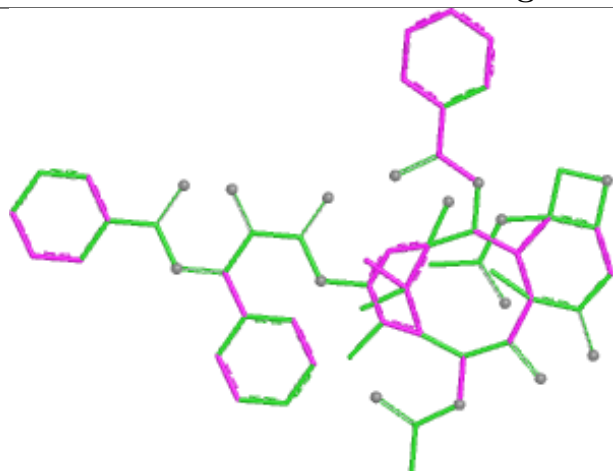
Torsions



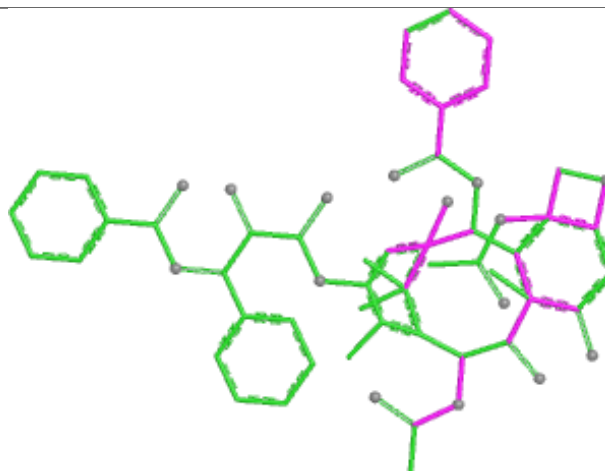
Rings



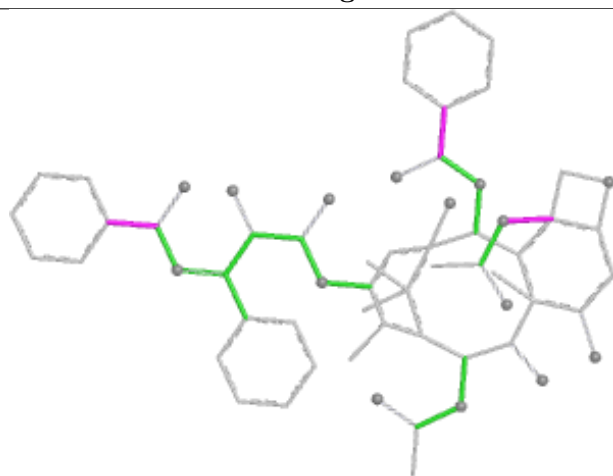
Ligand TA1 H 502



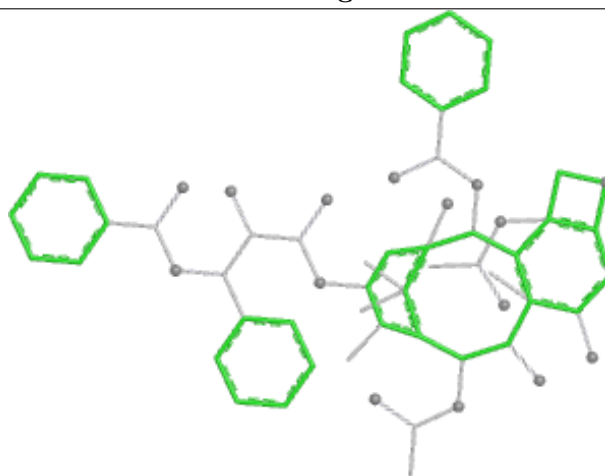
Bond lengths



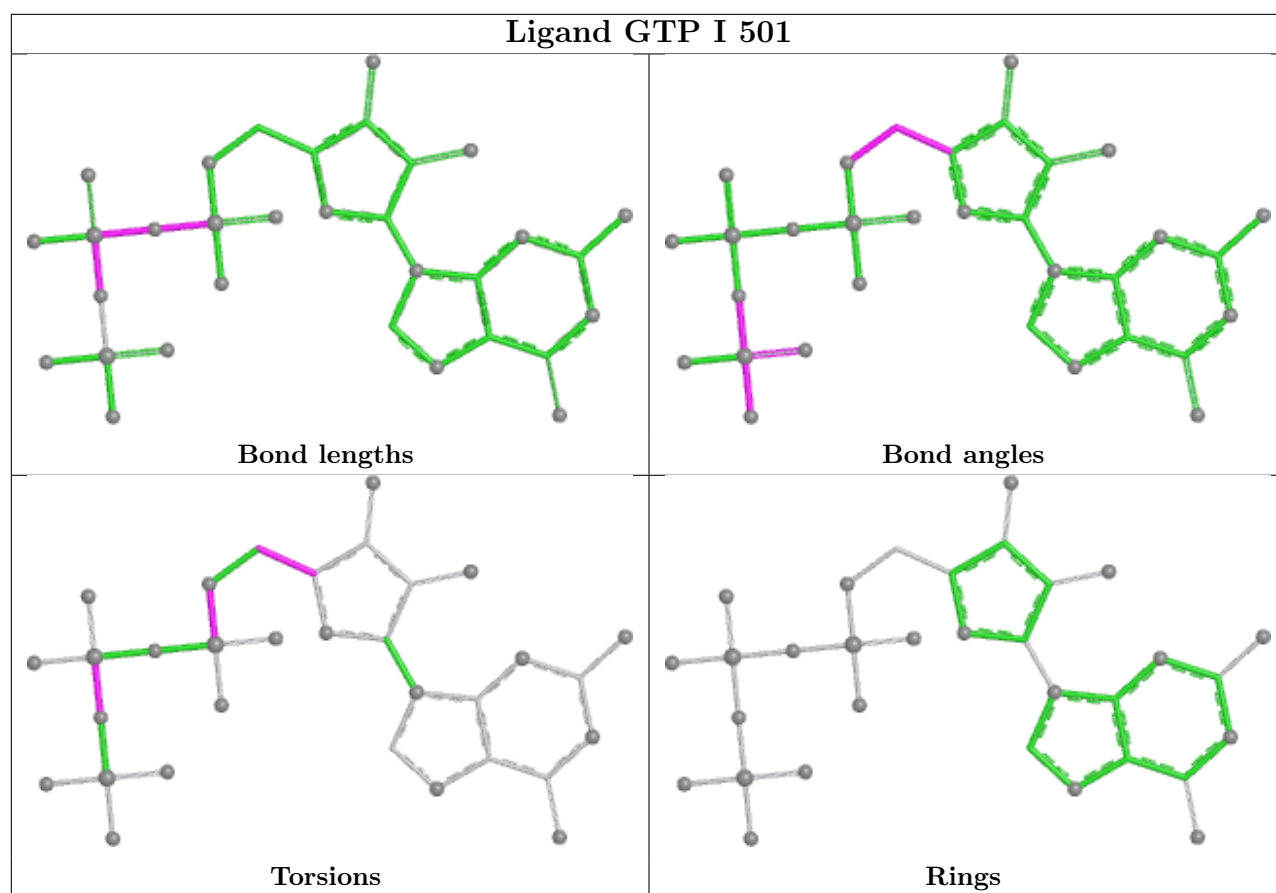
Bond angles

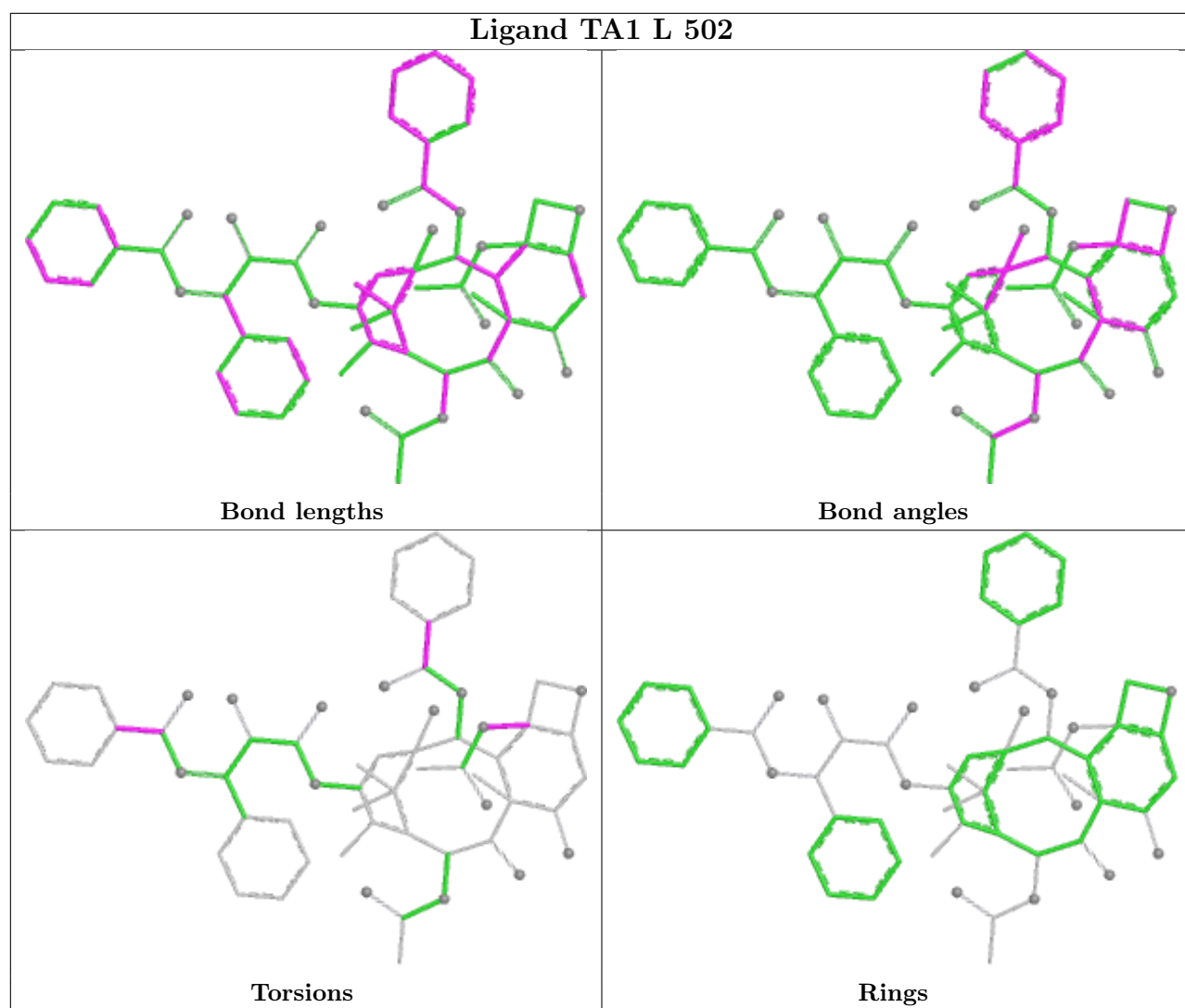


Torsions

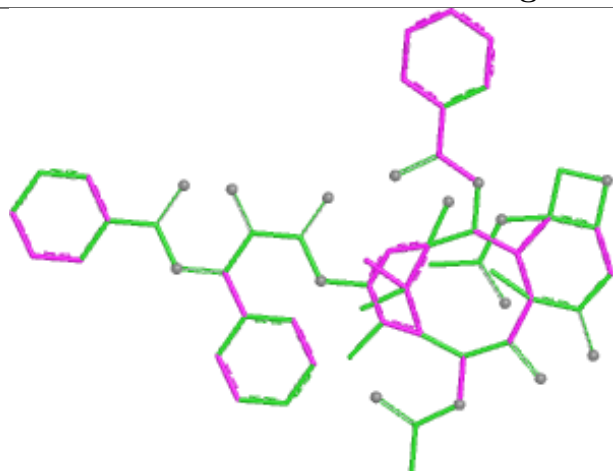


Rings

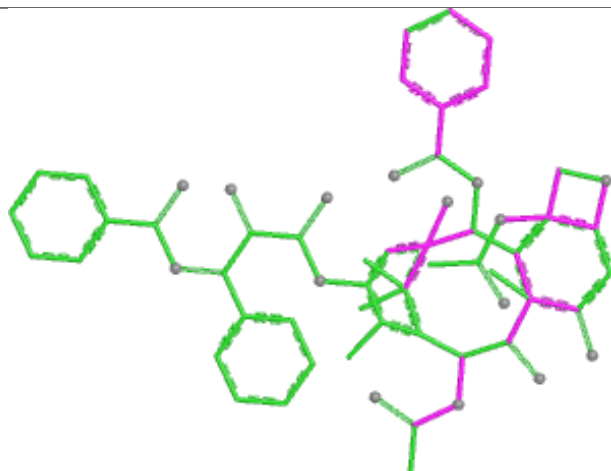




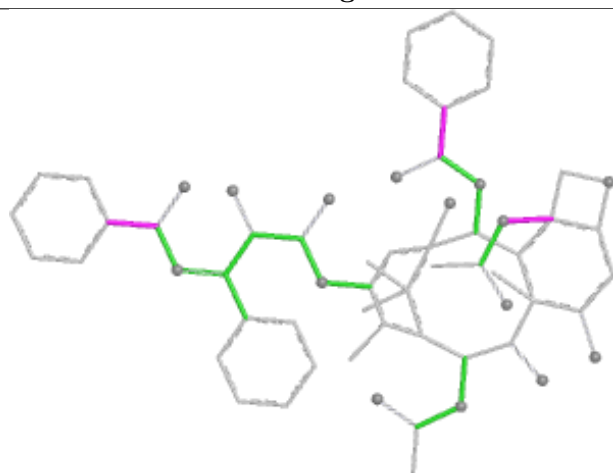
Ligand TA1 F 502



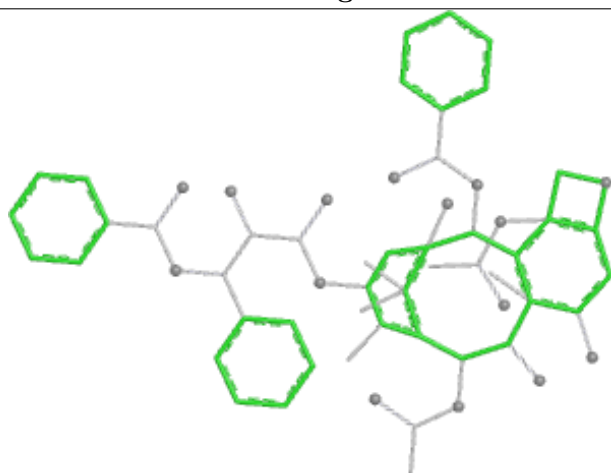
Bond lengths



Bond angles

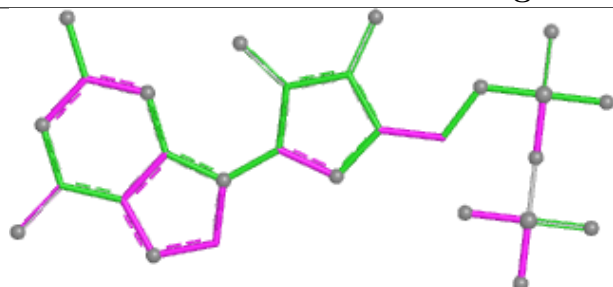


Torsions

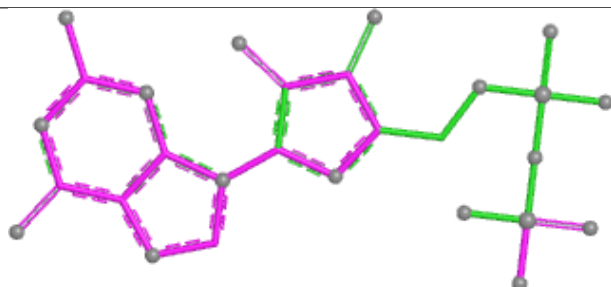


Rings

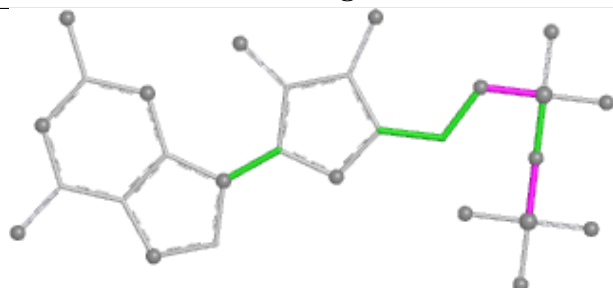
Ligand GDP L 501



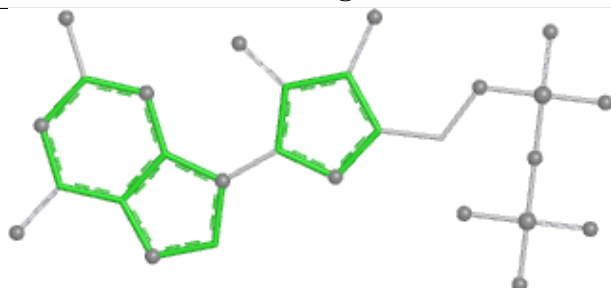
Bond lengths



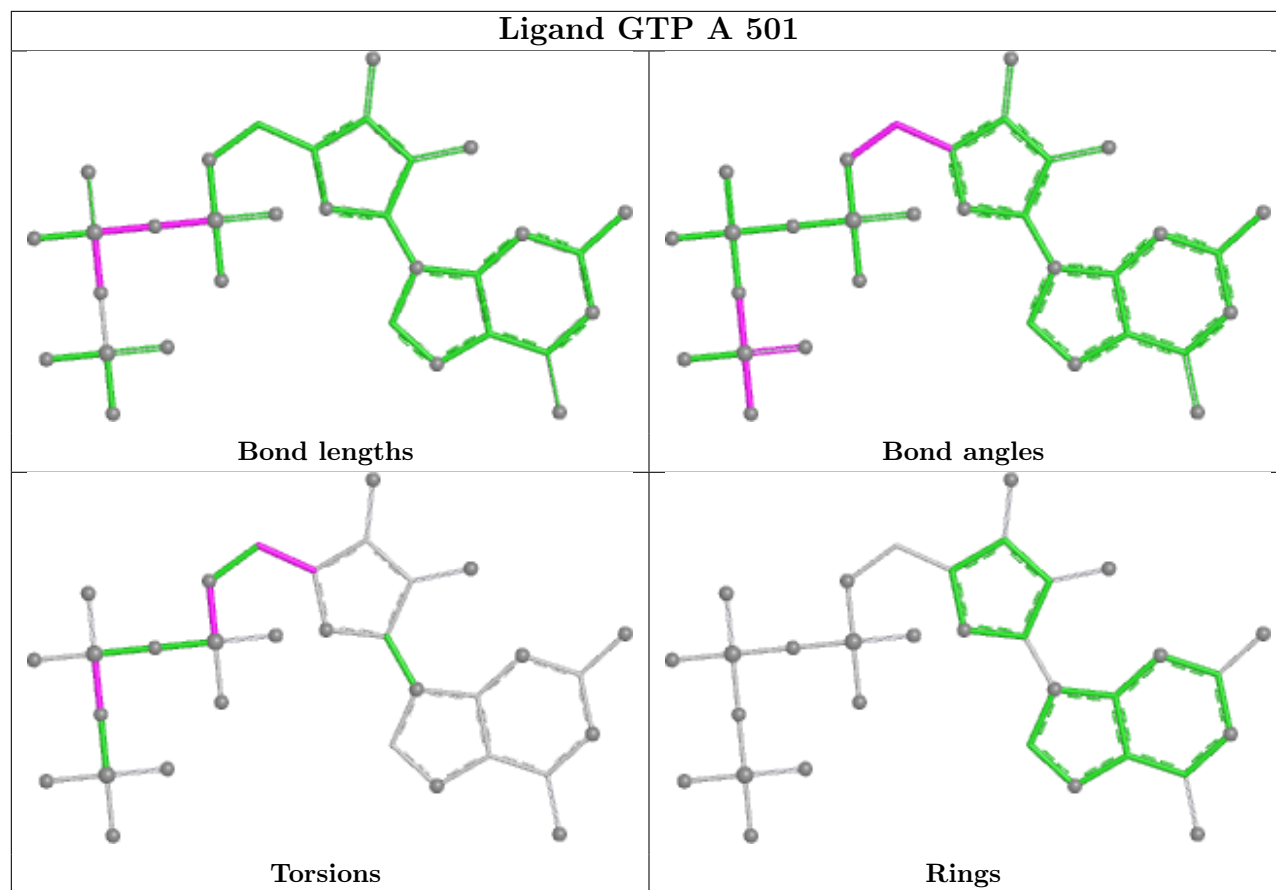
Bond angles



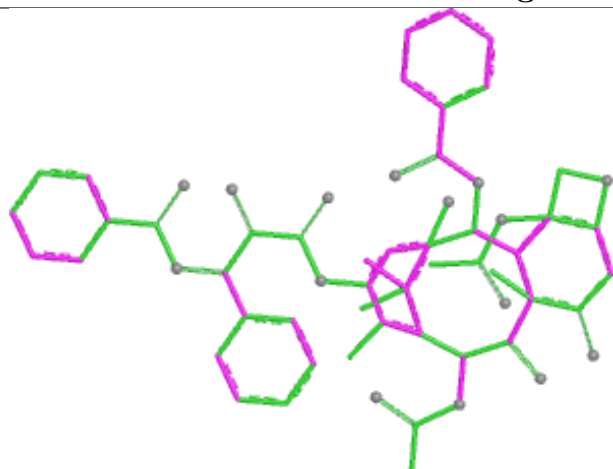
Torsions



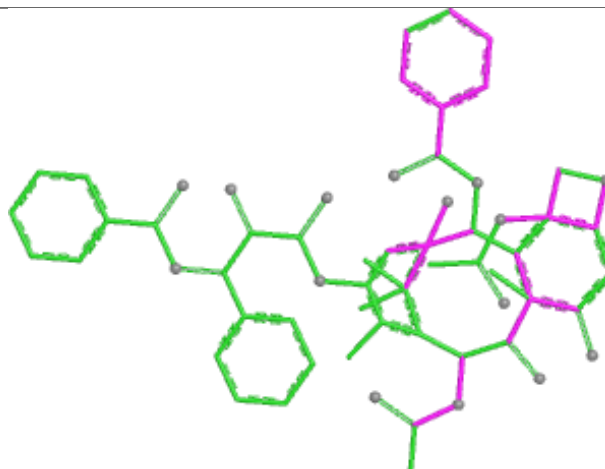
Rings



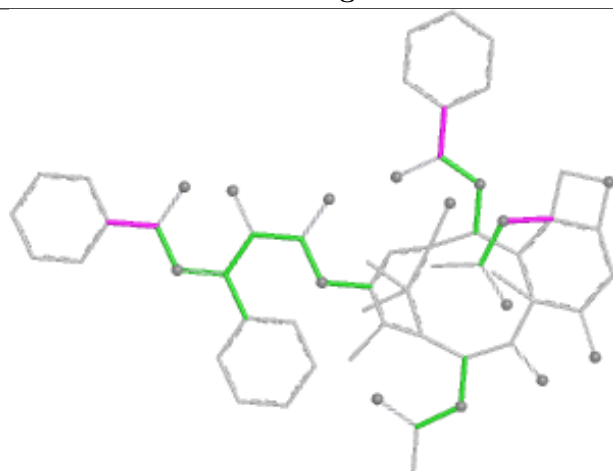
Ligand TA1 N 502



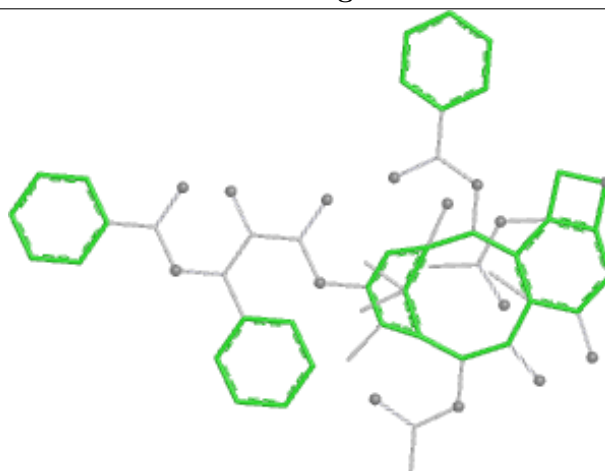
Bond lengths



Bond angles

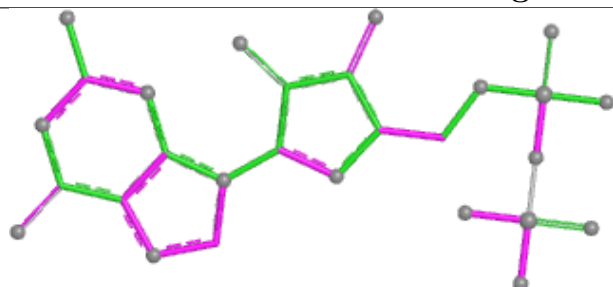


Torsions

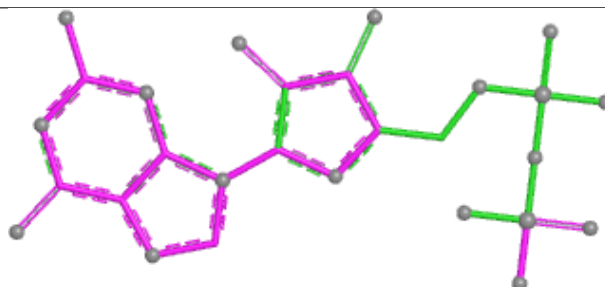


Rings

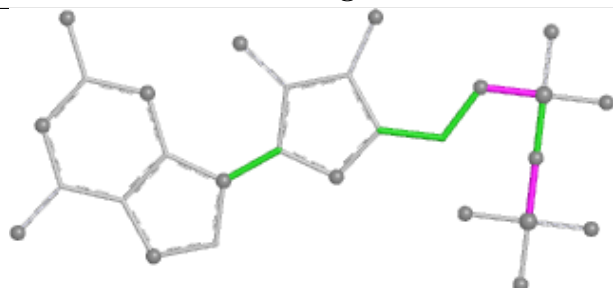
Ligand GDP B 501



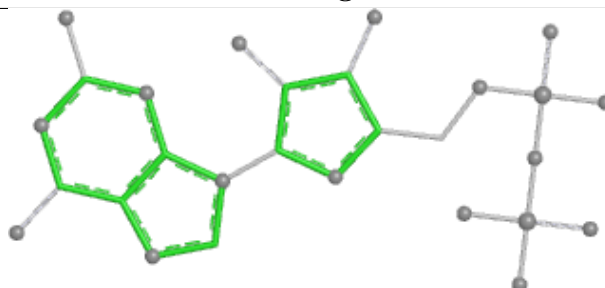
Bond lengths



Bond angles

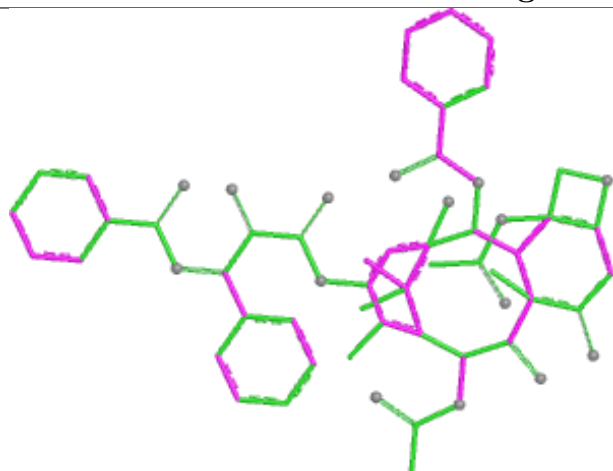


Torsions

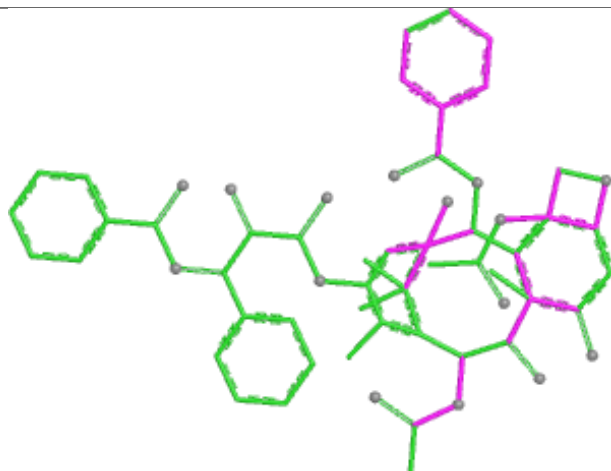


Rings

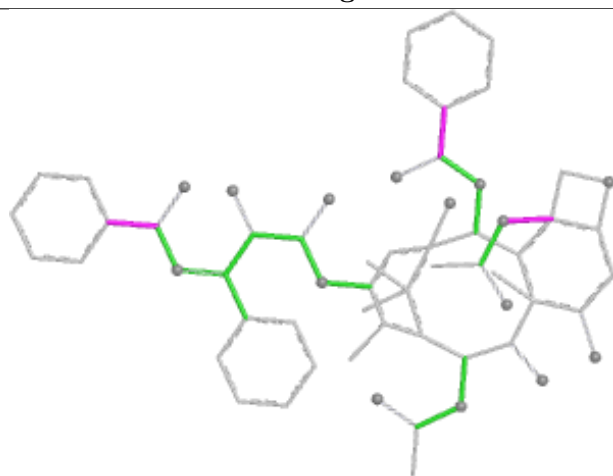
Ligand TA1 R 502



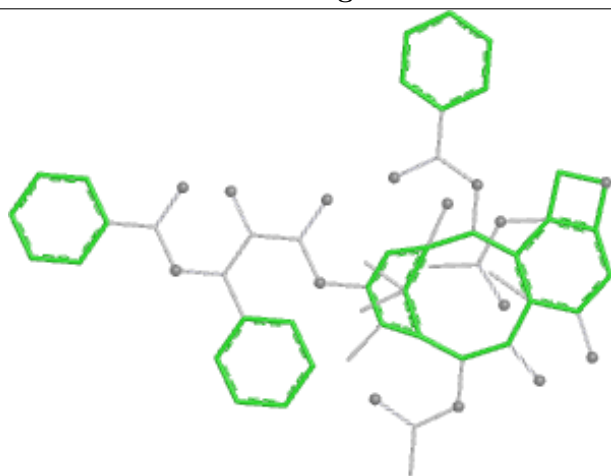
Bond lengths



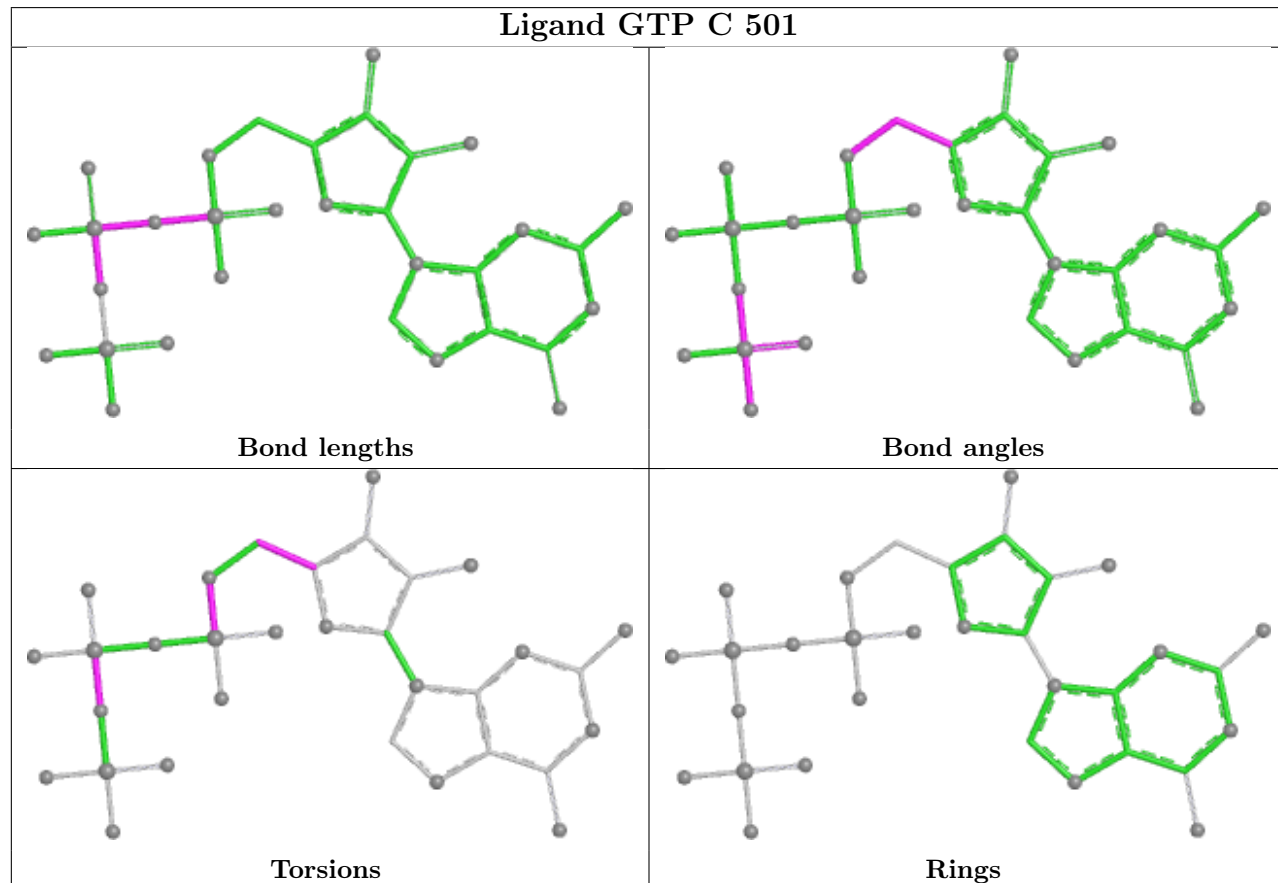
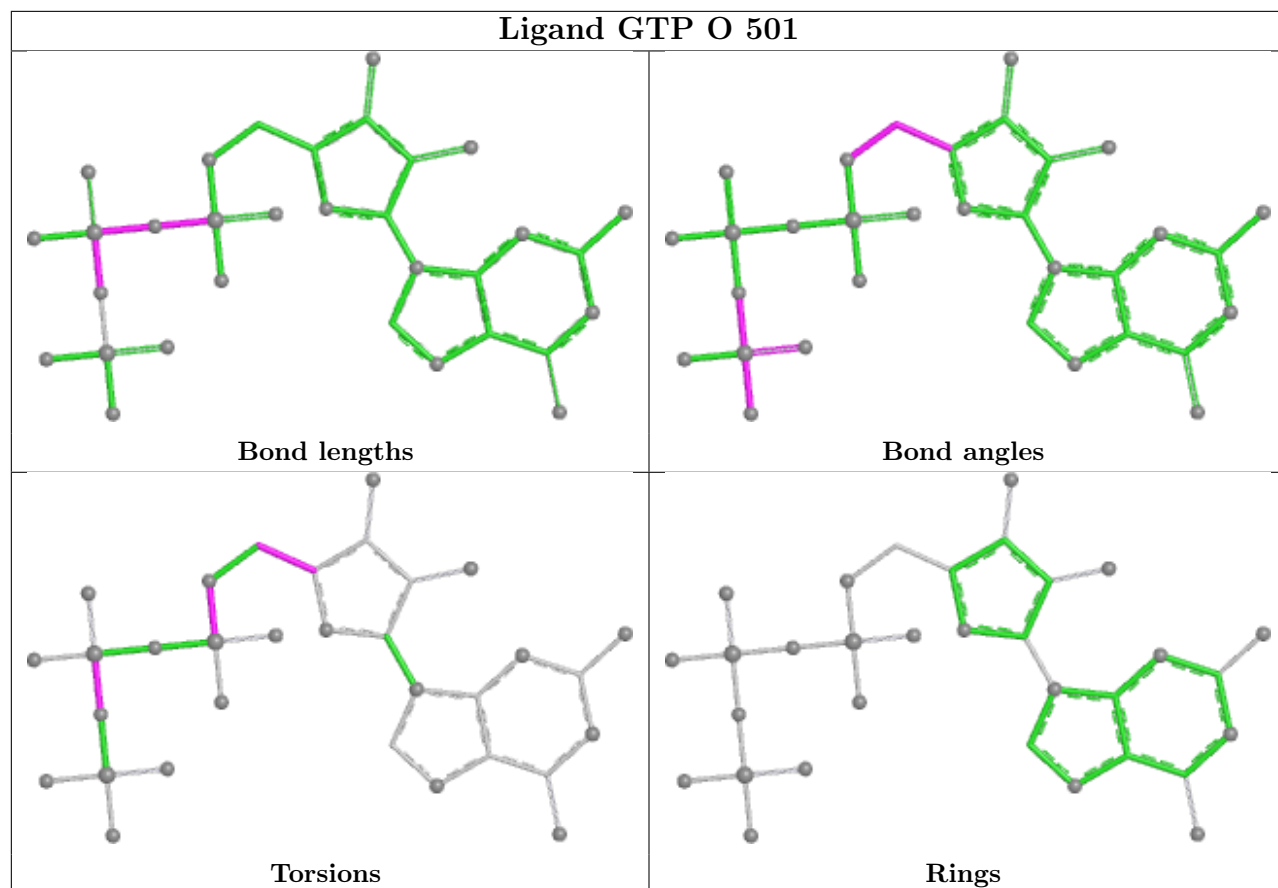
Bond angles

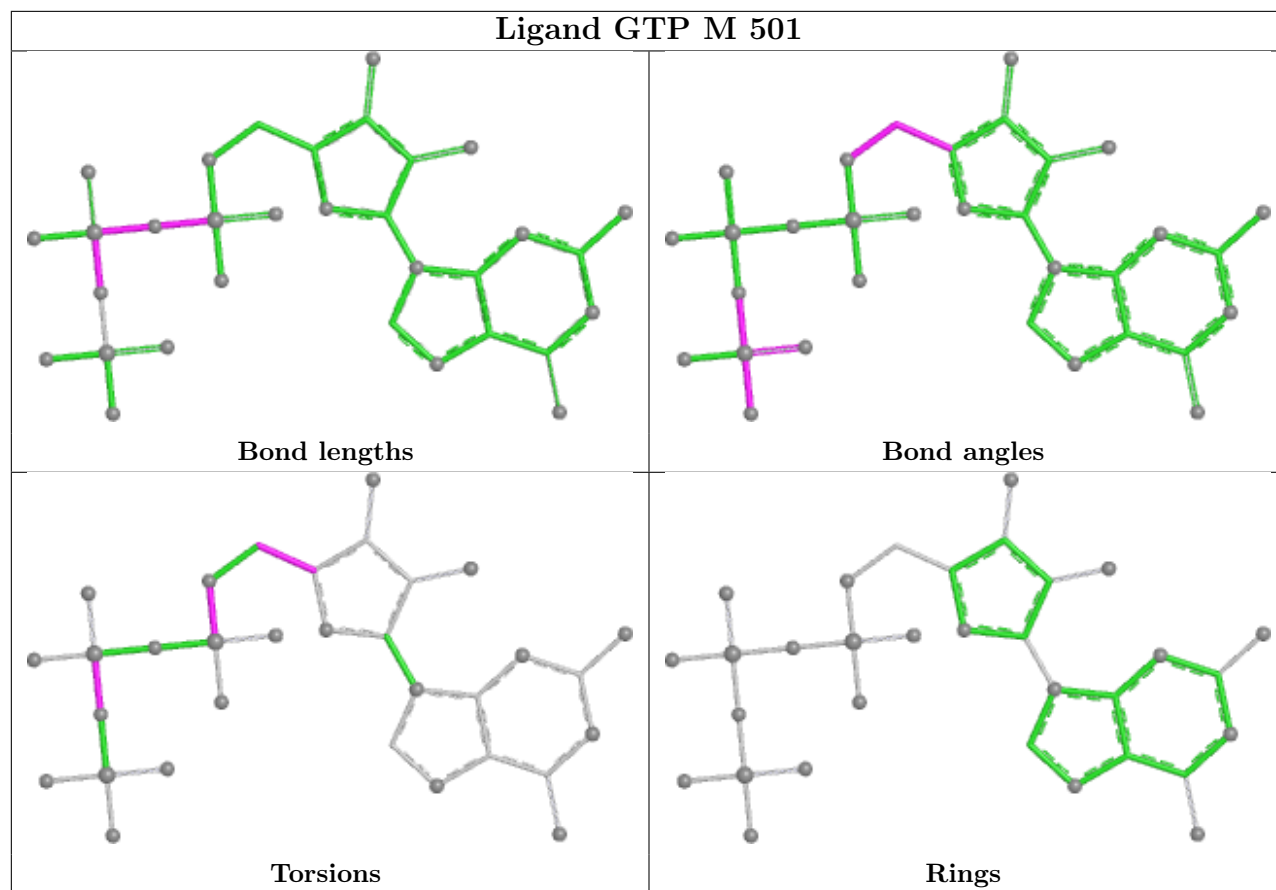


Torsions

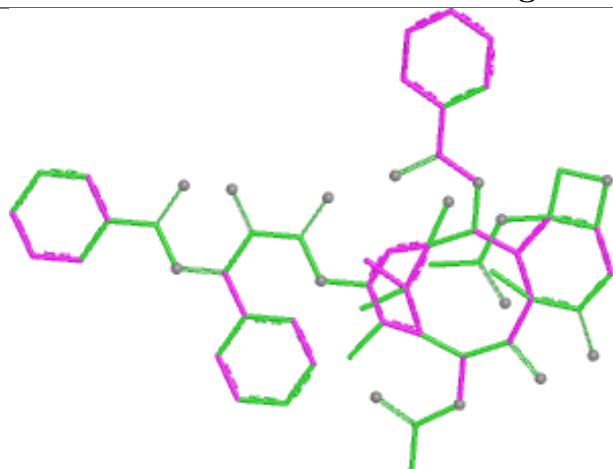


Rings

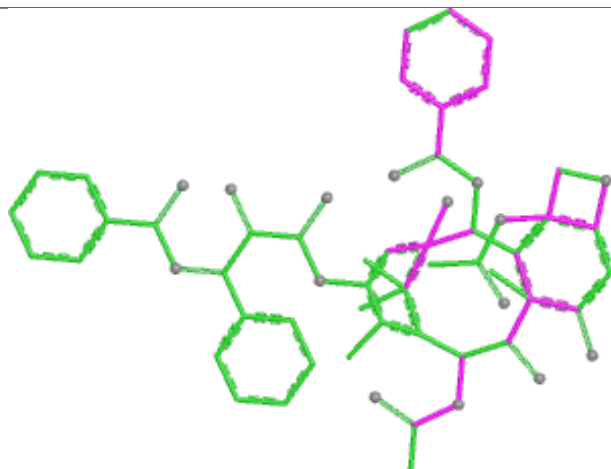




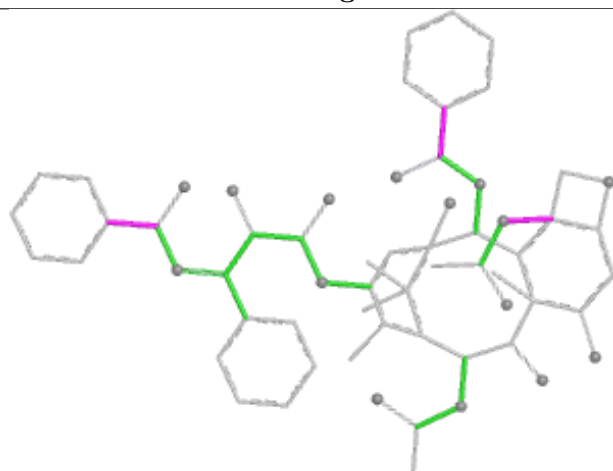
Ligand TA1 B 502



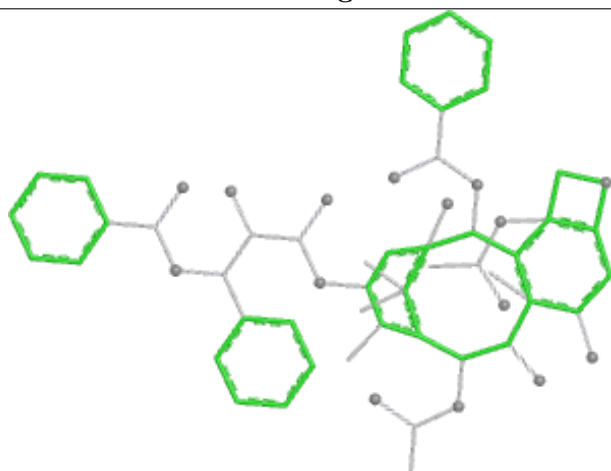
Bond lengths



Bond angles

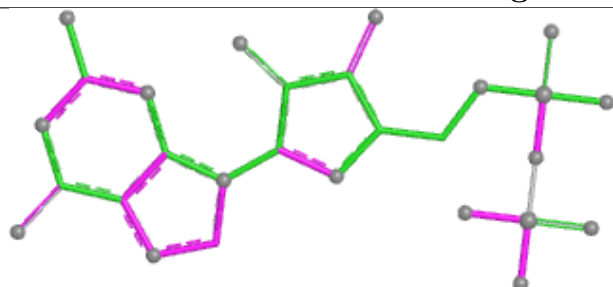


Torsions

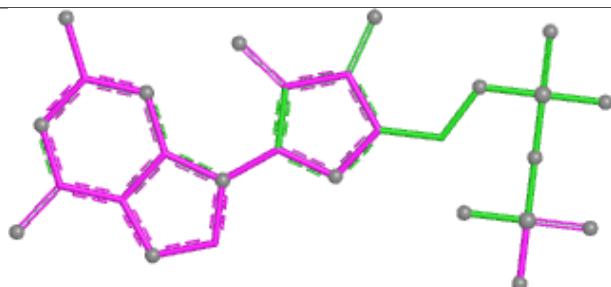


Rings

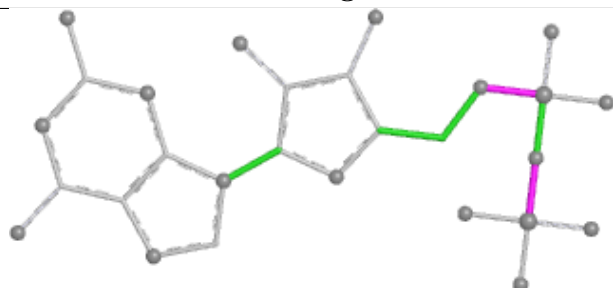
Ligand GDP D 501



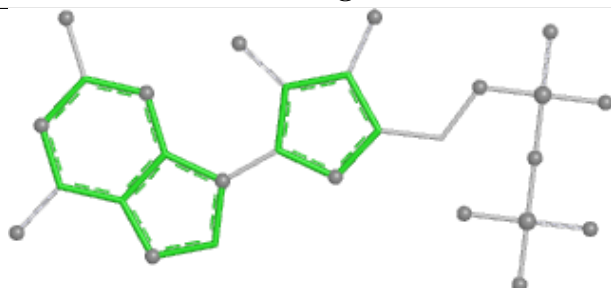
Bond lengths



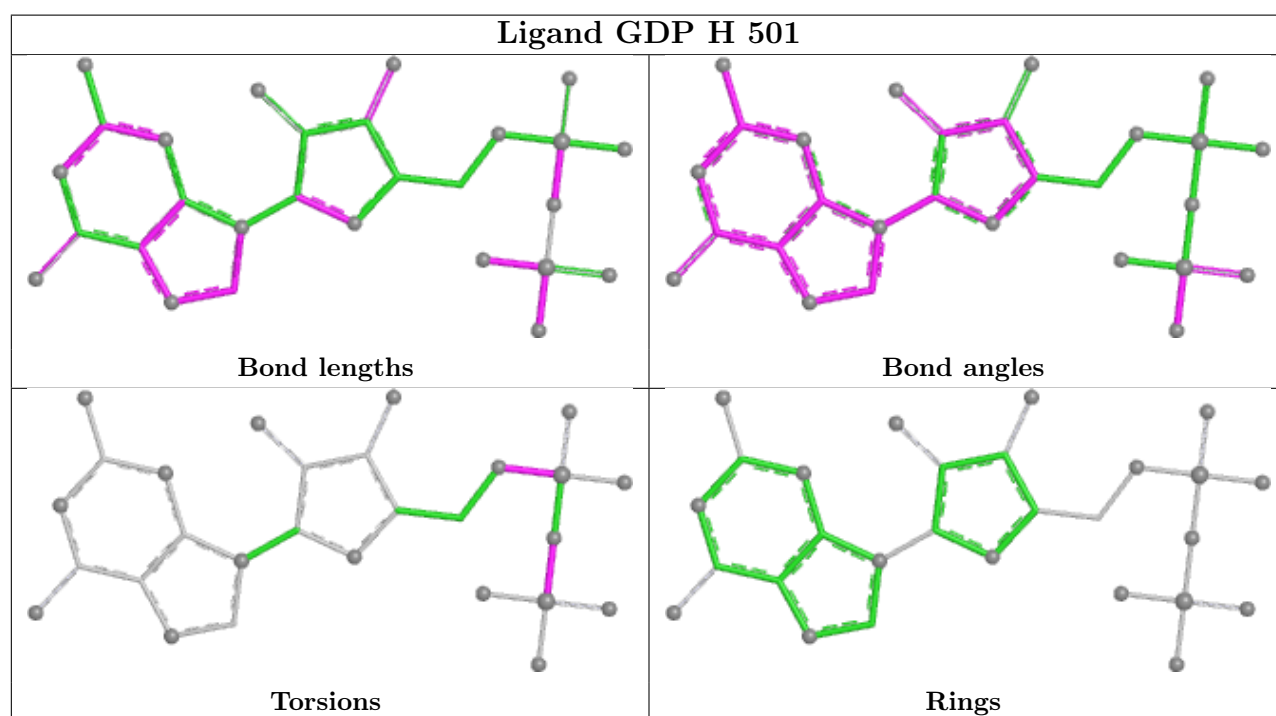
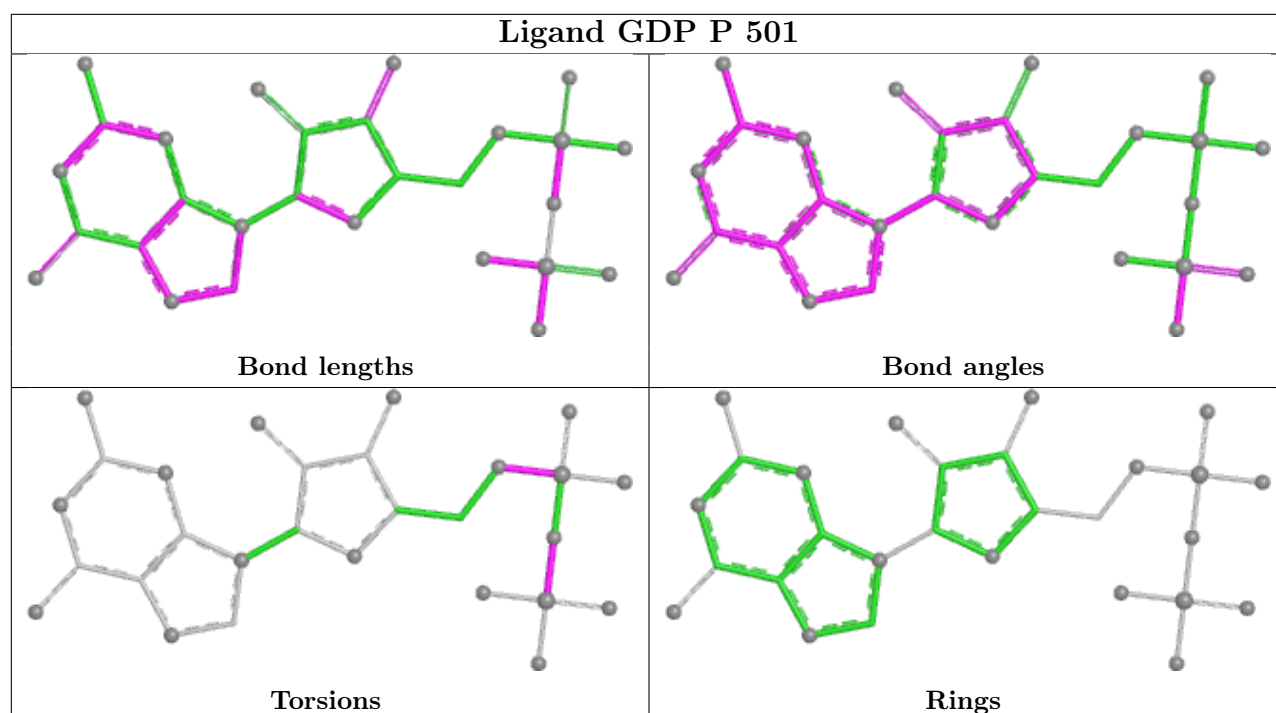
Bond angles



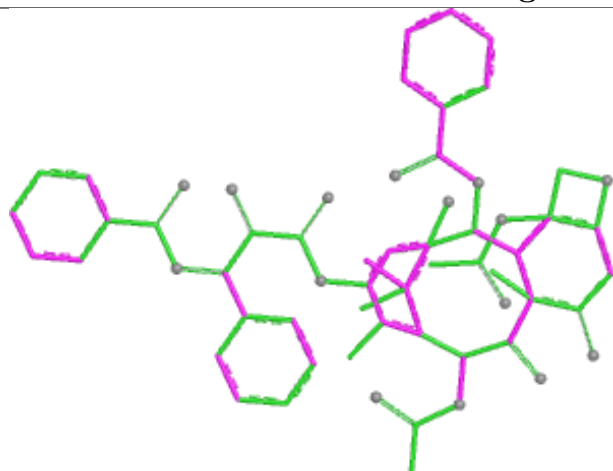
Torsions



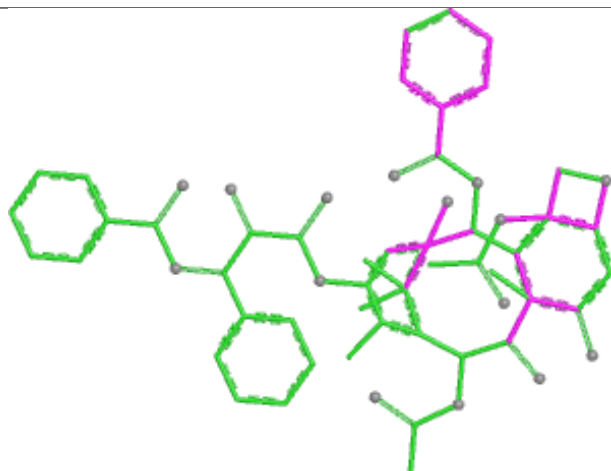
Rings



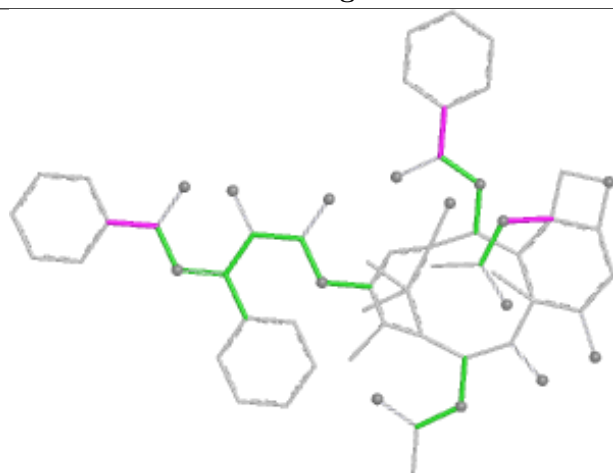
Ligand TA1 P 502



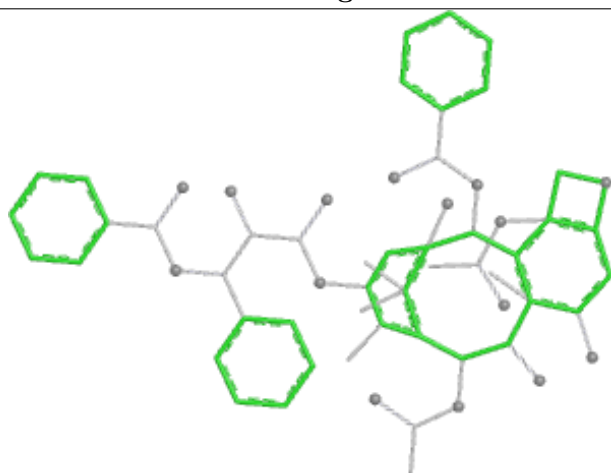
Bond lengths



Bond angles

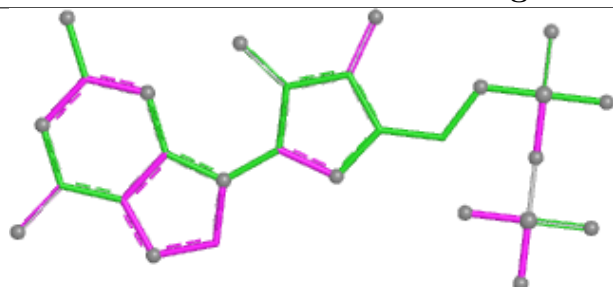


Torsions

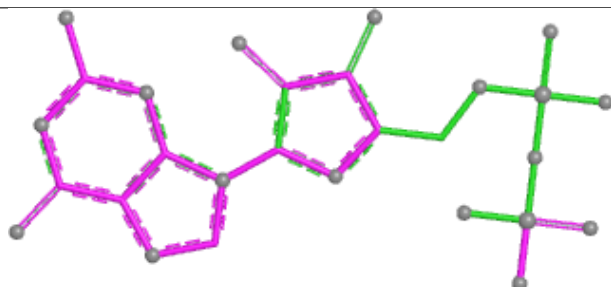


Rings

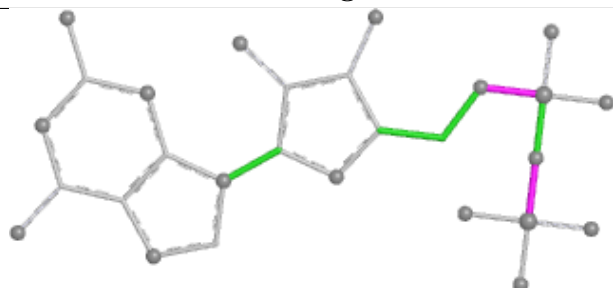
Ligand GDP N 501



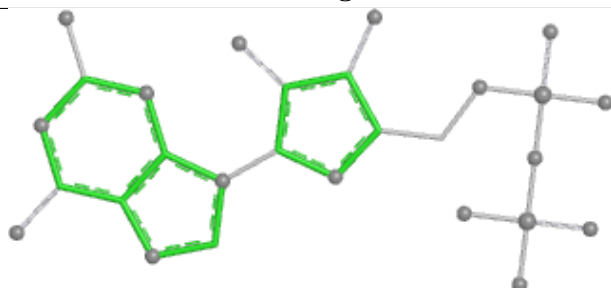
Bond lengths



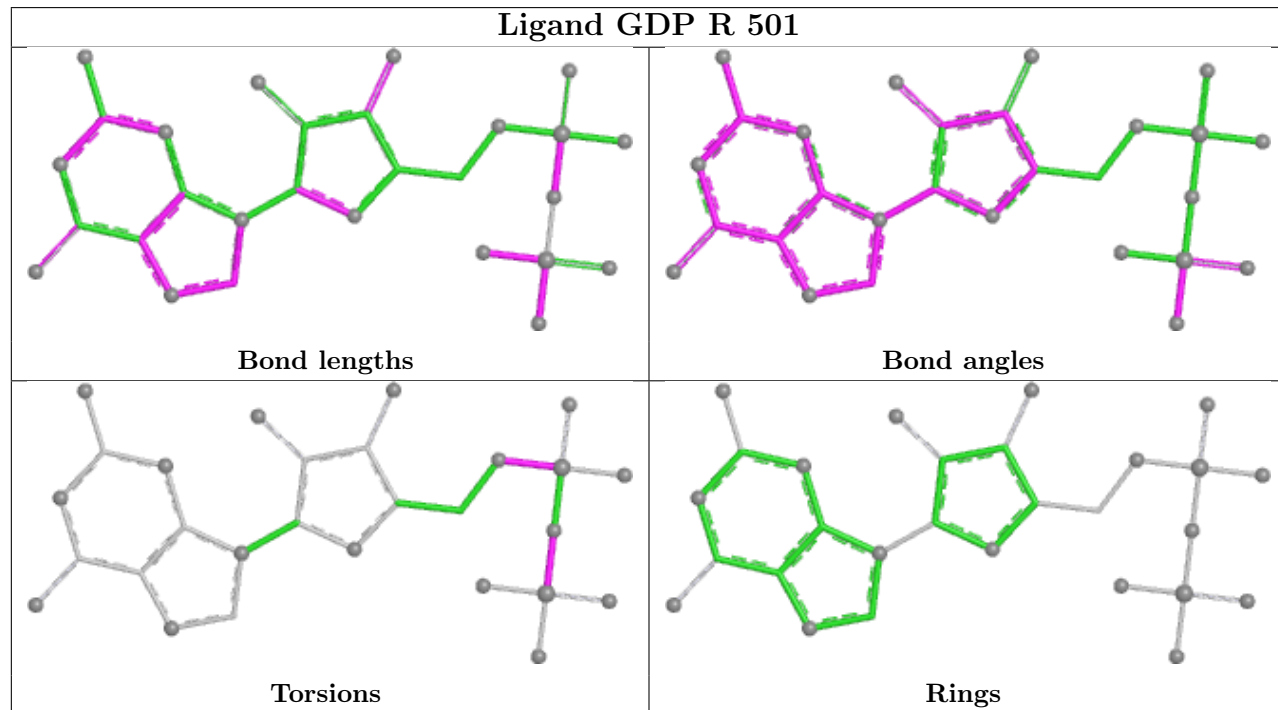
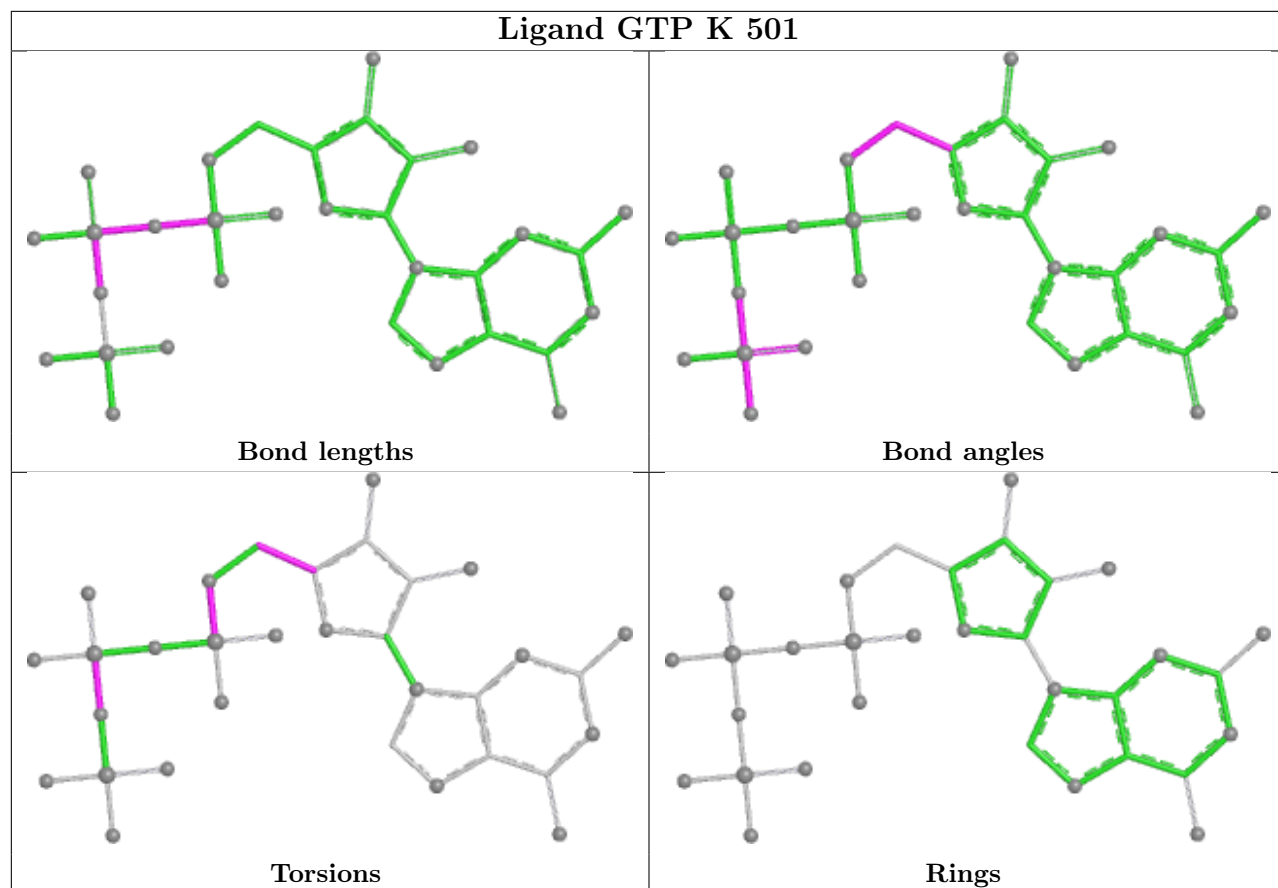
Bond angles

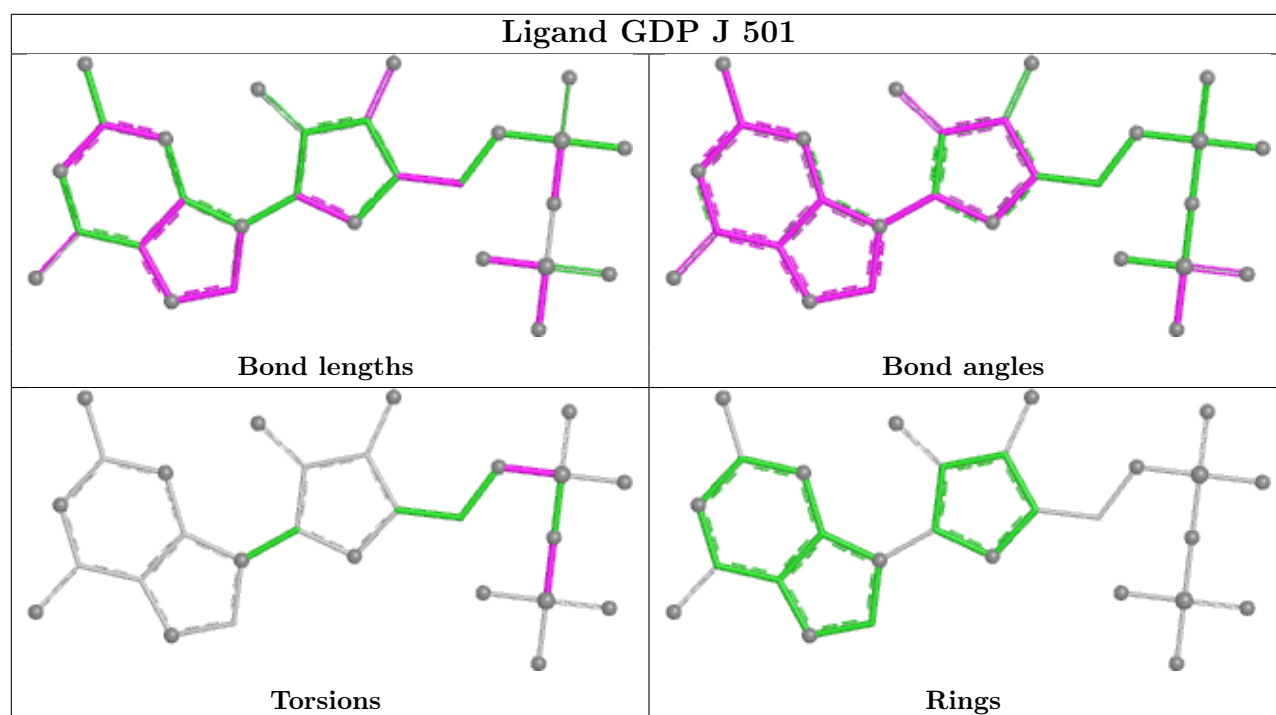


Torsions



Rings





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.

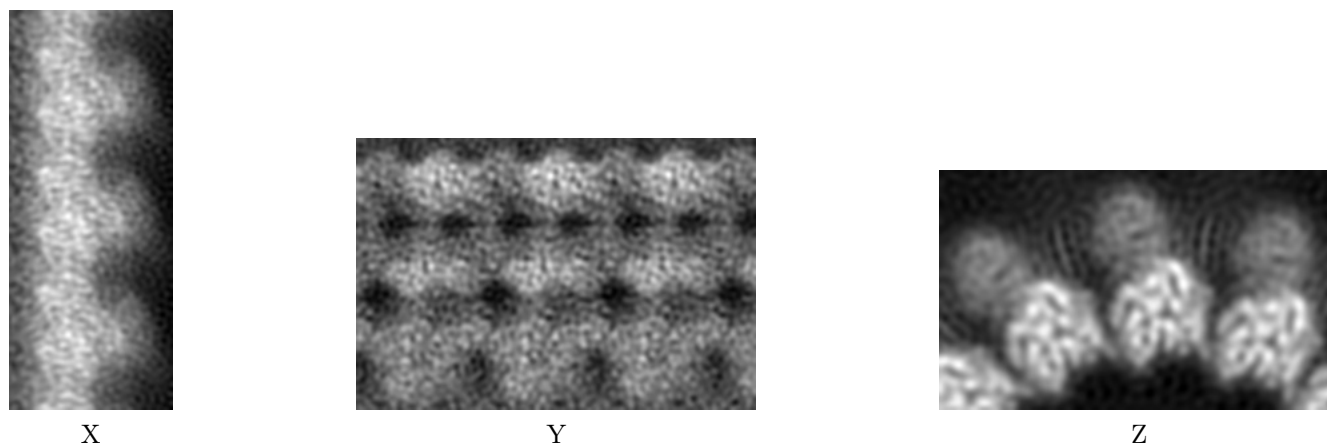
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5897. 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](#)

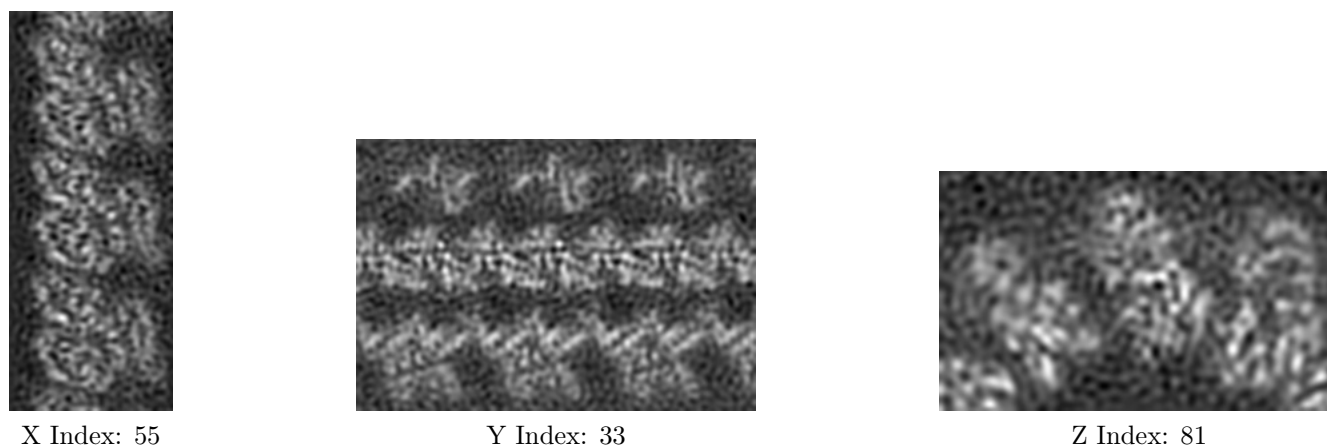
6.1.1 Primary map



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

6.2 Central slices [i](#)

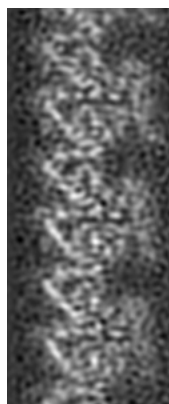
6.2.1 Primary map



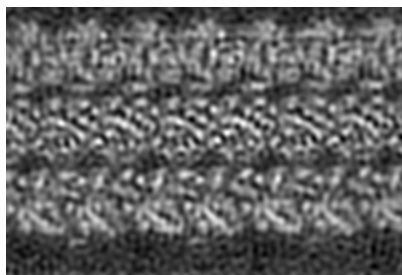
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

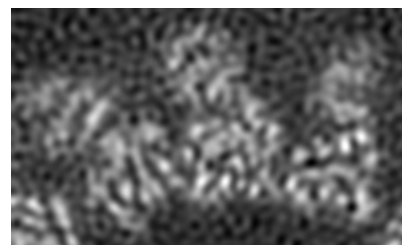
6.3.1 Primary map



X Index: 58



Y Index: 22

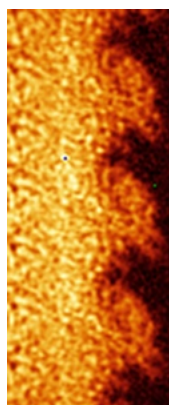


Z Index: 72

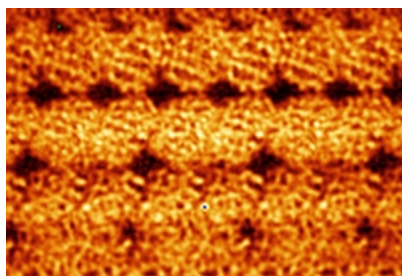
The images above show the largest variance slices of the map in three orthogonal directions.

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

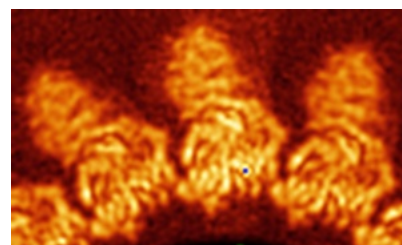
6.4.1 Primary map



X



Y

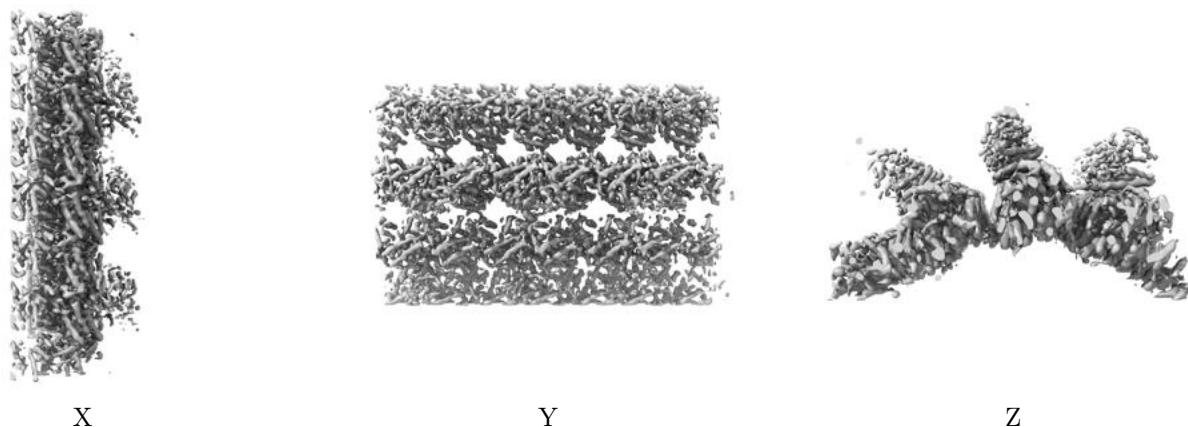


Z

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.

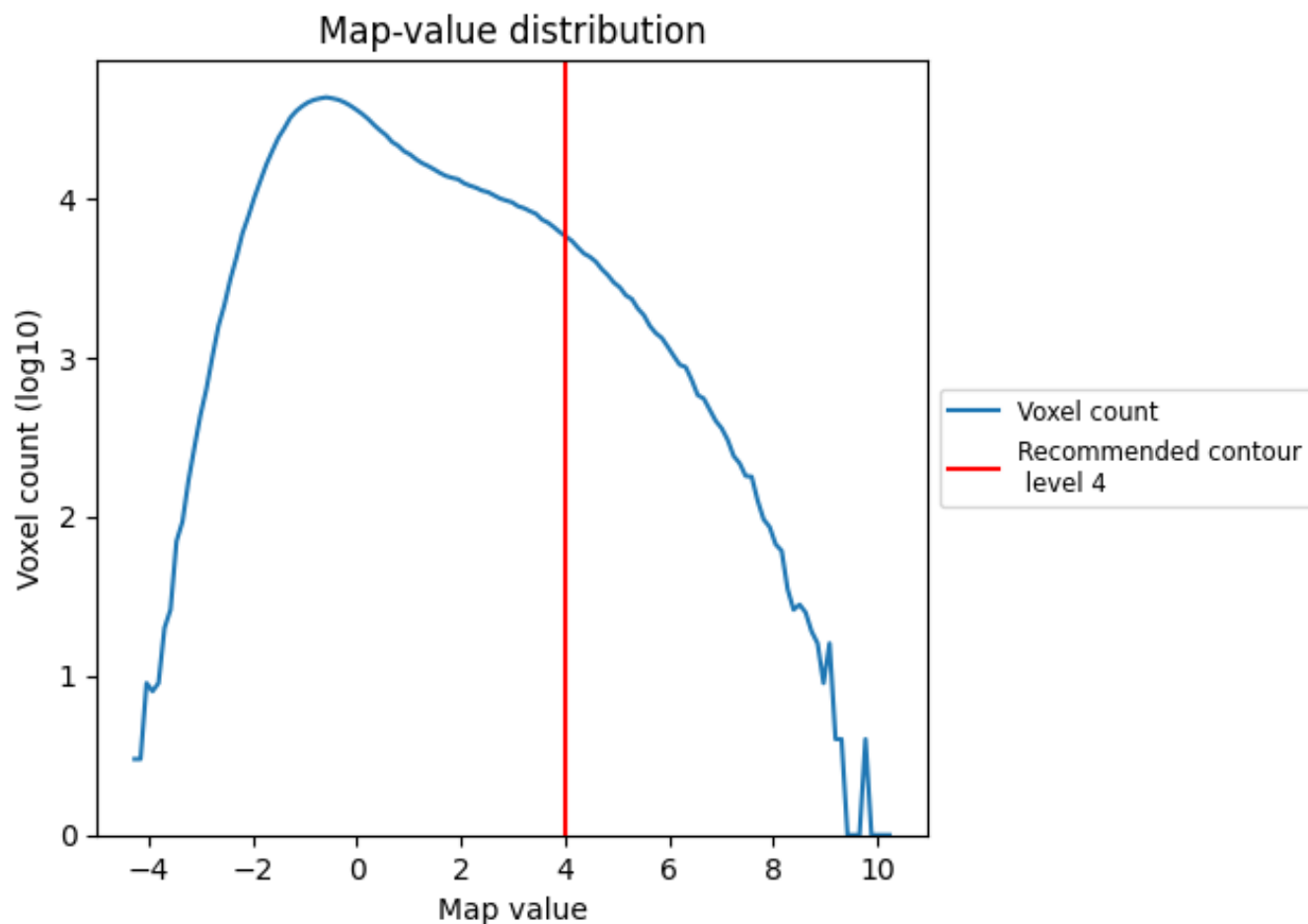
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

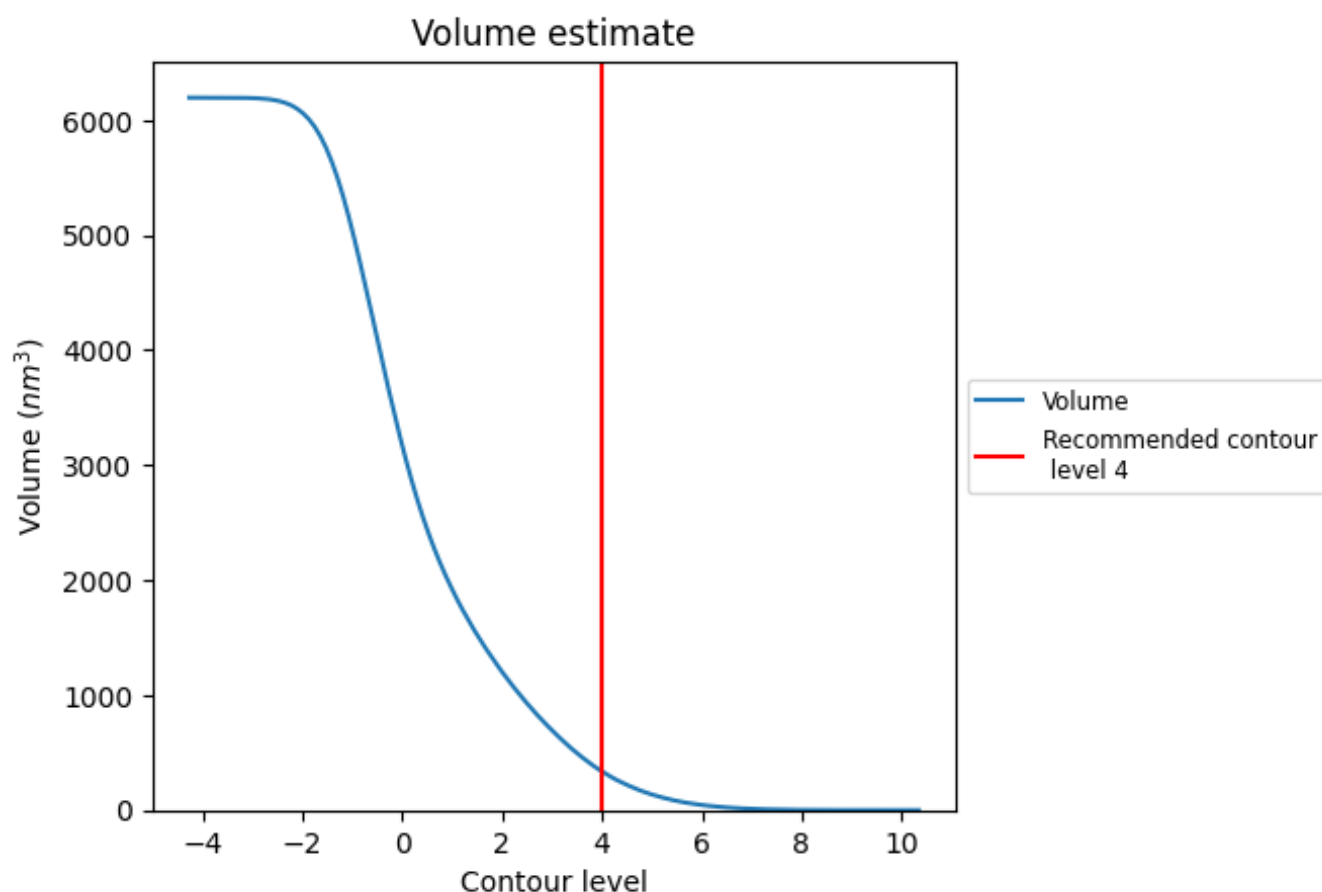
This section contains the results of statistical analysis of the map.

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 336 nm³; this corresponds to an approximate mass of 304 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.

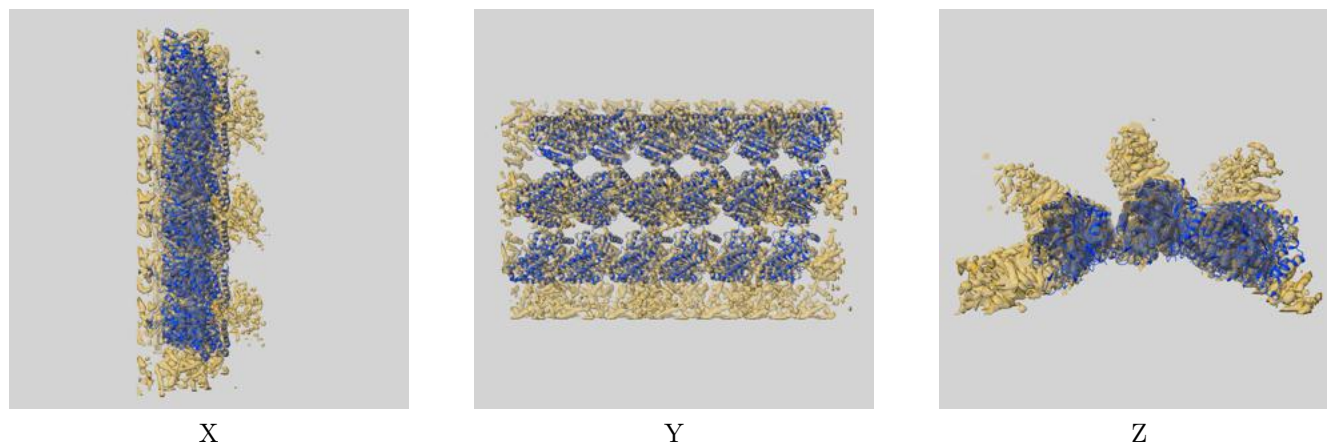
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

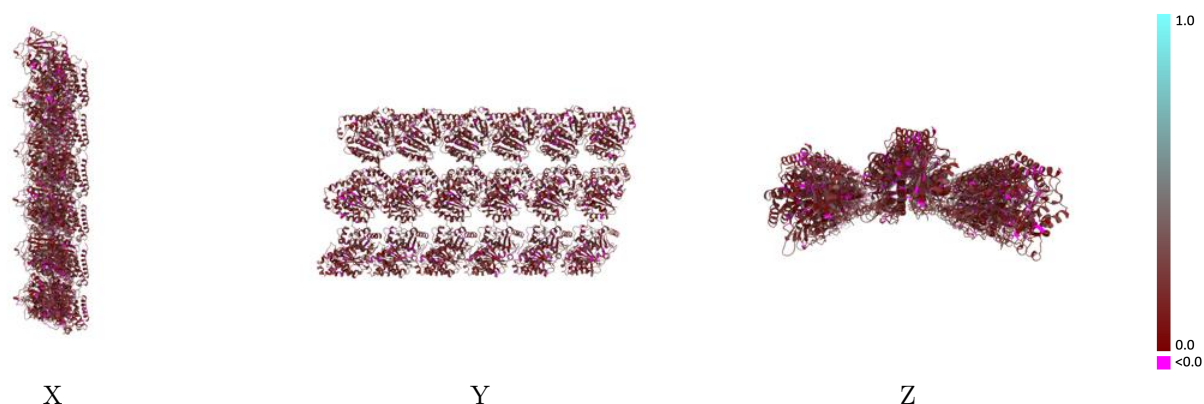
This section contains information regarding the fit between EMDB map EMD-5897 and PDB model 3J6G. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



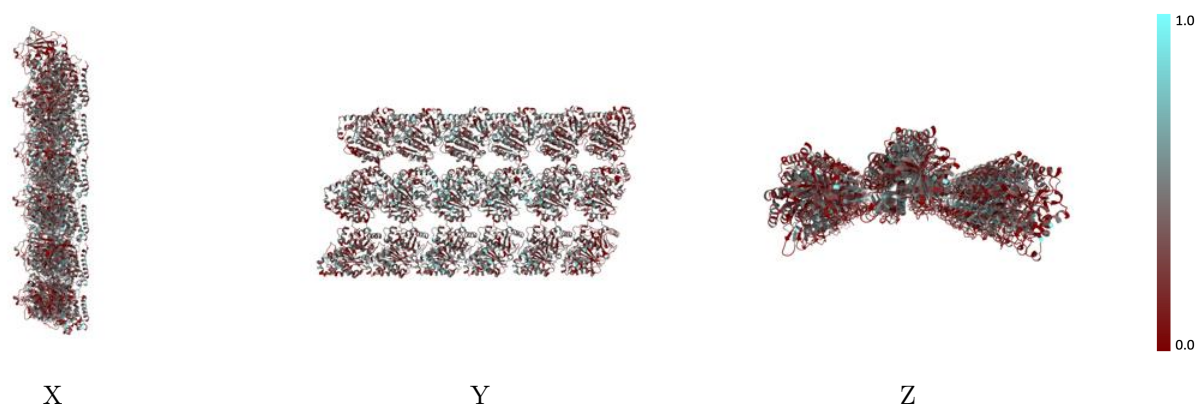
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



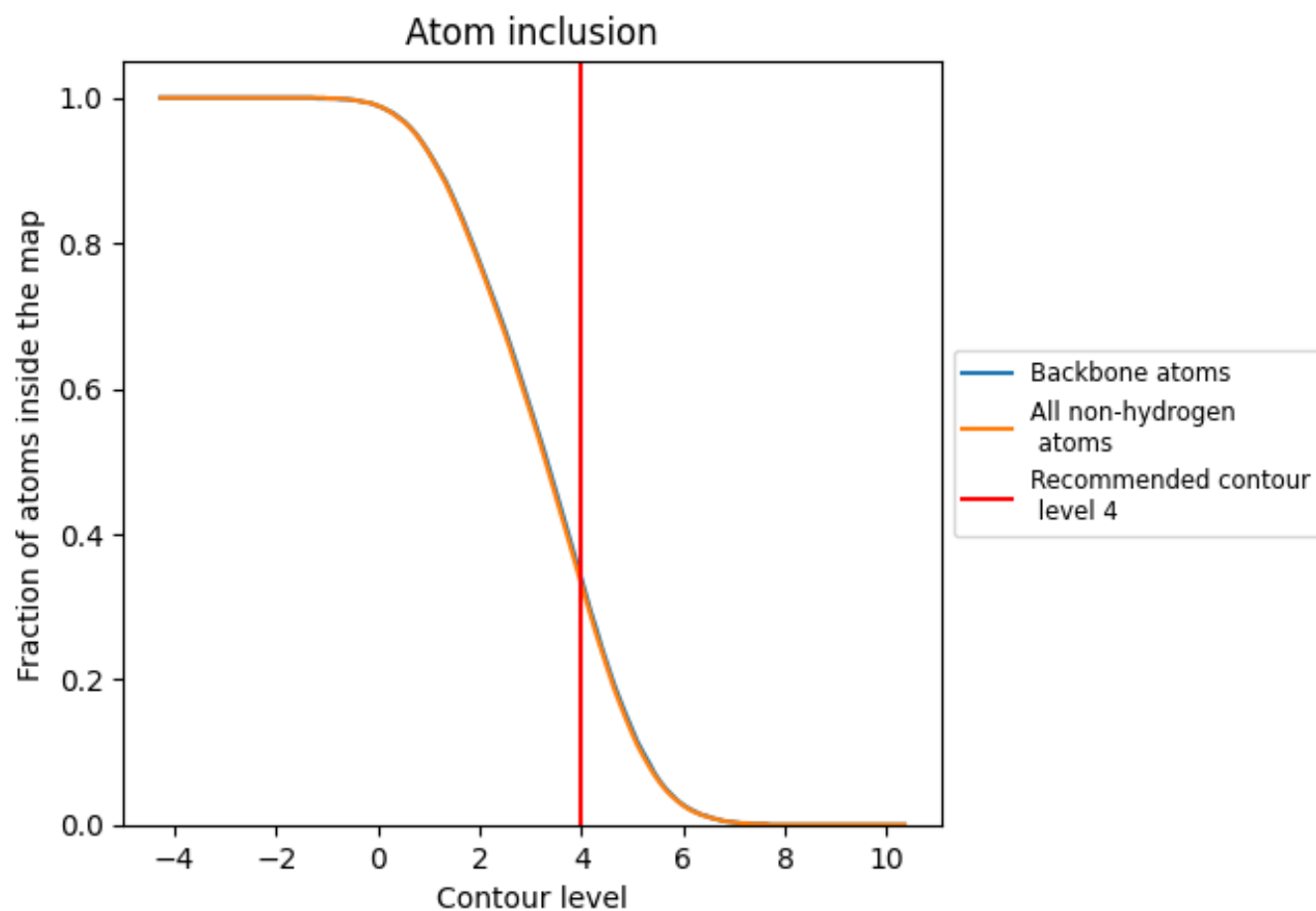
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 33% 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	 0.3300	 0.1940
A	 0.3910	 0.2000
B	 0.3990	 0.1980
C	 0.3570	 0.1970
D	 0.3620	 0.1960
E	 0.3590	 0.2000
F	 0.3690	 0.2000
G	 0.3380	 0.1910
H	 0.2870	 0.1910
I	 0.3760	 0.1910
J	 0.3300	 0.1920
K	 0.3400	 0.1920
L	 0.2850	 0.1910
M	 0.2540	 0.1880
N	 0.3250	 0.1940
O	 0.3070	 0.1910
P	 0.3660	 0.1960
Q	 0.2630	 0.1860
R	 0.3240	 0.1940

