



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 04:13 AM EDT

PDB ID : 5OCW
Title : Structure of Mycobacterium tuberculosis tryptophan synthase in space group F222
Authors : Futterer, K.; Abrahams, K.; Cox, J.A.G.; Besra, G.S.
Deposited on : 2017-07-03
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

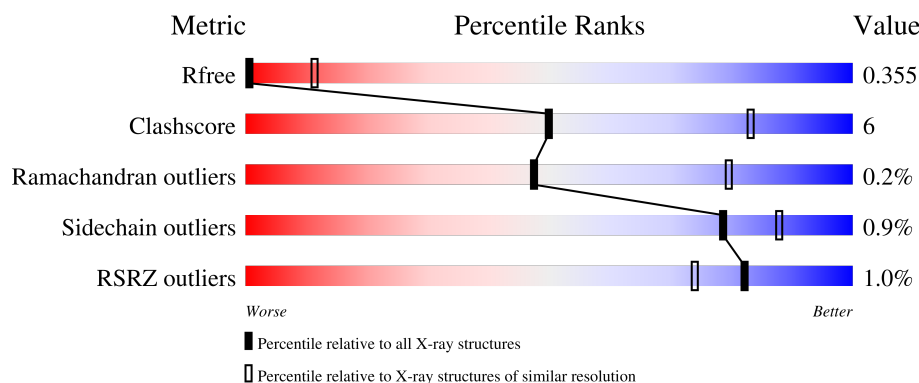
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	290	<div> <div>77%</div> <div>10%</div> <div>•</div> <div>11%</div> </div>
1	C	290	<div> <div>76%</div> <div>9%</div> <div>•</div> <div>14%</div> </div>
1	E	290	<div>4%</div> <div> <div>76%</div> <div>9%</div> <div>14%</div> </div>
1	G	290	<div> <div>75%</div> <div>10%</div> <div>•</div> <div>14%</div> </div>
1	I	290	<div>2%</div> <div> <div>75%</div> <div>9%</div> <div>•</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	290	
1	M	290	
1	O	290	
1	Q	290	
1	S	290	
1	U	290	
1	W	290	
2	B	442	
2	D	442	
2	F	442	
2	H	442	
2	J	442	
2	L	442	
2	N	442	
2	P	442	
2	R	442	
2	T	442	
2	V	442	
2	X	442	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	P1T	D	501	-	-	-	X
3	P1T	P	501	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 57878 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	1	0
			1852	1159	335	353	5			
1	C	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			
1	E	249	Total	C	N	O	S	0	1	0
			1814	1137	327	345	5			
1	G	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			
1	I	249	Total	C	N	O	S	0	1	0
			1814	1137	327	345	5			
1	K	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			
1	M	249	Total	C	N	O	S	0	1	0
			1814	1137	327	345	5			
1	O	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			
1	Q	249	Total	C	N	O	S	0	1	0
			1814	1137	327	345	5			
1	S	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			
1	U	249	Total	C	N	O	S	0	1	0
			1814	1137	327	345	5			
1	W	248	Total	C	N	O	S	0	0	0
			1799	1129	322	343	5			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WFY1
A	-18	GLY	-	expression tag	UNP P9WFY1
A	-17	SER	-	expression tag	UNP P9WFY1
A	-16	SER	-	expression tag	UNP P9WFY1
A	-15	HIS	-	expression tag	UNP P9WFY1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P9WIFY1
A	-13	HIS	-	expression tag	UNP P9WIFY1
A	-12	HIS	-	expression tag	UNP P9WIFY1
A	-11	HIS	-	expression tag	UNP P9WIFY1
A	-10	HIS	-	expression tag	UNP P9WIFY1
A	-9	SER	-	expression tag	UNP P9WIFY1
A	-8	SER	-	expression tag	UNP P9WIFY1
A	-7	GLY	-	expression tag	UNP P9WIFY1
A	-6	LEU	-	expression tag	UNP P9WIFY1
A	-5	VAL	-	expression tag	UNP P9WIFY1
A	-4	PRO	-	expression tag	UNP P9WIFY1
A	-3	ARG	-	expression tag	UNP P9WIFY1
A	-2	GLY	-	expression tag	UNP P9WIFY1
A	-1	SER	-	expression tag	UNP P9WIFY1
A	0	HIS	-	expression tag	UNP P9WIFY1
C	-19	MET	-	initiating methionine	UNP P9WIFY1
C	-18	GLY	-	expression tag	UNP P9WIFY1
C	-17	SER	-	expression tag	UNP P9WIFY1
C	-16	SER	-	expression tag	UNP P9WIFY1
C	-15	HIS	-	expression tag	UNP P9WIFY1
C	-14	HIS	-	expression tag	UNP P9WIFY1
C	-13	HIS	-	expression tag	UNP P9WIFY1
C	-12	HIS	-	expression tag	UNP P9WIFY1
C	-11	HIS	-	expression tag	UNP P9WIFY1
C	-10	HIS	-	expression tag	UNP P9WIFY1
C	-9	SER	-	expression tag	UNP P9WIFY1
C	-8	SER	-	expression tag	UNP P9WIFY1
C	-7	GLY	-	expression tag	UNP P9WIFY1
C	-6	LEU	-	expression tag	UNP P9WIFY1
C	-5	VAL	-	expression tag	UNP P9WIFY1
C	-4	PRO	-	expression tag	UNP P9WIFY1
C	-3	ARG	-	expression tag	UNP P9WIFY1
C	-2	GLY	-	expression tag	UNP P9WIFY1
C	-1	SER	-	expression tag	UNP P9WIFY1
C	0	HIS	-	expression tag	UNP P9WIFY1
E	-19	MET	-	initiating methionine	UNP P9WIFY1
E	-18	GLY	-	expression tag	UNP P9WIFY1
E	-17	SER	-	expression tag	UNP P9WIFY1
E	-16	SER	-	expression tag	UNP P9WIFY1
E	-15	HIS	-	expression tag	UNP P9WIFY1
E	-14	HIS	-	expression tag	UNP P9WIFY1
E	-13	HIS	-	expression tag	UNP P9WIFY1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	HIS	-	expression tag	UNP P9WIFY1
E	-11	HIS	-	expression tag	UNP P9WIFY1
E	-10	HIS	-	expression tag	UNP P9WIFY1
E	-9	SER	-	expression tag	UNP P9WIFY1
E	-8	SER	-	expression tag	UNP P9WIFY1
E	-7	GLY	-	expression tag	UNP P9WIFY1
E	-6	LEU	-	expression tag	UNP P9WIFY1
E	-5	VAL	-	expression tag	UNP P9WIFY1
E	-4	PRO	-	expression tag	UNP P9WIFY1
E	-3	ARG	-	expression tag	UNP P9WIFY1
E	-2	GLY	-	expression tag	UNP P9WIFY1
E	-1	SER	-	expression tag	UNP P9WIFY1
E	0	HIS	-	expression tag	UNP P9WIFY1
G	-19	MET	-	initiating methionine	UNP P9WIFY1
G	-18	GLY	-	expression tag	UNP P9WIFY1
G	-17	SER	-	expression tag	UNP P9WIFY1
G	-16	SER	-	expression tag	UNP P9WIFY1
G	-15	HIS	-	expression tag	UNP P9WIFY1
G	-14	HIS	-	expression tag	UNP P9WIFY1
G	-13	HIS	-	expression tag	UNP P9WIFY1
G	-12	HIS	-	expression tag	UNP P9WIFY1
G	-11	HIS	-	expression tag	UNP P9WIFY1
G	-10	HIS	-	expression tag	UNP P9WIFY1
G	-9	SER	-	expression tag	UNP P9WIFY1
G	-8	SER	-	expression tag	UNP P9WIFY1
G	-7	GLY	-	expression tag	UNP P9WIFY1
G	-6	LEU	-	expression tag	UNP P9WIFY1
G	-5	VAL	-	expression tag	UNP P9WIFY1
G	-4	PRO	-	expression tag	UNP P9WIFY1
G	-3	ARG	-	expression tag	UNP P9WIFY1
G	-2	GLY	-	expression tag	UNP P9WIFY1
G	-1	SER	-	expression tag	UNP P9WIFY1
G	0	HIS	-	expression tag	UNP P9WIFY1
I	-19	MET	-	initiating methionine	UNP P9WIFY1
I	-18	GLY	-	expression tag	UNP P9WIFY1
I	-17	SER	-	expression tag	UNP P9WIFY1
I	-16	SER	-	expression tag	UNP P9WIFY1
I	-15	HIS	-	expression tag	UNP P9WIFY1
I	-14	HIS	-	expression tag	UNP P9WIFY1
I	-13	HIS	-	expression tag	UNP P9WIFY1
I	-12	HIS	-	expression tag	UNP P9WIFY1
I	-11	HIS	-	expression tag	UNP P9WIFY1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-10	HIS	-	expression tag	UNP P9WIFY1
I	-9	SER	-	expression tag	UNP P9WIFY1
I	-8	SER	-	expression tag	UNP P9WIFY1
I	-7	GLY	-	expression tag	UNP P9WIFY1
I	-6	LEU	-	expression tag	UNP P9WIFY1
I	-5	VAL	-	expression tag	UNP P9WIFY1
I	-4	PRO	-	expression tag	UNP P9WIFY1
I	-3	ARG	-	expression tag	UNP P9WIFY1
I	-2	GLY	-	expression tag	UNP P9WIFY1
I	-1	SER	-	expression tag	UNP P9WIFY1
I	0	HIS	-	expression tag	UNP P9WIFY1
K	-19	MET	-	initiating methionine	UNP P9WIFY1
K	-18	GLY	-	expression tag	UNP P9WIFY1
K	-17	SER	-	expression tag	UNP P9WIFY1
K	-16	SER	-	expression tag	UNP P9WIFY1
K	-15	HIS	-	expression tag	UNP P9WIFY1
K	-14	HIS	-	expression tag	UNP P9WIFY1
K	-13	HIS	-	expression tag	UNP P9WIFY1
K	-12	HIS	-	expression tag	UNP P9WIFY1
K	-11	HIS	-	expression tag	UNP P9WIFY1
K	-10	HIS	-	expression tag	UNP P9WIFY1
K	-9	SER	-	expression tag	UNP P9WIFY1
K	-8	SER	-	expression tag	UNP P9WIFY1
K	-7	GLY	-	expression tag	UNP P9WIFY1
K	-6	LEU	-	expression tag	UNP P9WIFY1
K	-5	VAL	-	expression tag	UNP P9WIFY1
K	-4	PRO	-	expression tag	UNP P9WIFY1
K	-3	ARG	-	expression tag	UNP P9WIFY1
K	-2	GLY	-	expression tag	UNP P9WIFY1
K	-1	SER	-	expression tag	UNP P9WIFY1
K	0	HIS	-	expression tag	UNP P9WIFY1
M	-19	MET	-	initiating methionine	UNP P9WIFY1
M	-18	GLY	-	expression tag	UNP P9WIFY1
M	-17	SER	-	expression tag	UNP P9WIFY1
M	-16	SER	-	expression tag	UNP P9WIFY1
M	-15	HIS	-	expression tag	UNP P9WIFY1
M	-14	HIS	-	expression tag	UNP P9WIFY1
M	-13	HIS	-	expression tag	UNP P9WIFY1
M	-12	HIS	-	expression tag	UNP P9WIFY1
M	-11	HIS	-	expression tag	UNP P9WIFY1
M	-10	HIS	-	expression tag	UNP P9WIFY1
M	-9	SER	-	expression tag	UNP P9WIFY1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-8	SER	-	expression tag	UNP P9WIFY1
M	-7	GLY	-	expression tag	UNP P9WIFY1
M	-6	LEU	-	expression tag	UNP P9WIFY1
M	-5	VAL	-	expression tag	UNP P9WIFY1
M	-4	PRO	-	expression tag	UNP P9WIFY1
M	-3	ARG	-	expression tag	UNP P9WIFY1
M	-2	GLY	-	expression tag	UNP P9WIFY1
M	-1	SER	-	expression tag	UNP P9WIFY1
M	0	HIS	-	expression tag	UNP P9WIFY1
O	-19	MET	-	initiating methionine	UNP P9WIFY1
O	-18	GLY	-	expression tag	UNP P9WIFY1
O	-17	SER	-	expression tag	UNP P9WIFY1
O	-16	SER	-	expression tag	UNP P9WIFY1
O	-15	HIS	-	expression tag	UNP P9WIFY1
O	-14	HIS	-	expression tag	UNP P9WIFY1
O	-13	HIS	-	expression tag	UNP P9WIFY1
O	-12	HIS	-	expression tag	UNP P9WIFY1
O	-11	HIS	-	expression tag	UNP P9WIFY1
O	-10	HIS	-	expression tag	UNP P9WIFY1
O	-9	SER	-	expression tag	UNP P9WIFY1
O	-8	SER	-	expression tag	UNP P9WIFY1
O	-7	GLY	-	expression tag	UNP P9WIFY1
O	-6	LEU	-	expression tag	UNP P9WIFY1
O	-5	VAL	-	expression tag	UNP P9WIFY1
O	-4	PRO	-	expression tag	UNP P9WIFY1
O	-3	ARG	-	expression tag	UNP P9WIFY1
O	-2	GLY	-	expression tag	UNP P9WIFY1
O	-1	SER	-	expression tag	UNP P9WIFY1
O	0	HIS	-	expression tag	UNP P9WIFY1
Q	-19	MET	-	initiating methionine	UNP P9WIFY1
Q	-18	GLY	-	expression tag	UNP P9WIFY1
Q	-17	SER	-	expression tag	UNP P9WIFY1
Q	-16	SER	-	expression tag	UNP P9WIFY1
Q	-15	HIS	-	expression tag	UNP P9WIFY1
Q	-14	HIS	-	expression tag	UNP P9WIFY1
Q	-13	HIS	-	expression tag	UNP P9WIFY1
Q	-12	HIS	-	expression tag	UNP P9WIFY1
Q	-11	HIS	-	expression tag	UNP P9WIFY1
Q	-10	HIS	-	expression tag	UNP P9WIFY1
Q	-9	SER	-	expression tag	UNP P9WIFY1
Q	-8	SER	-	expression tag	UNP P9WIFY1
Q	-7	GLY	-	expression tag	UNP P9WIFY1

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-6	LEU	-	expression tag	UNP P9WIFY1
Q	-5	VAL	-	expression tag	UNP P9WIFY1
Q	-4	PRO	-	expression tag	UNP P9WIFY1
Q	-3	ARG	-	expression tag	UNP P9WIFY1
Q	-2	GLY	-	expression tag	UNP P9WIFY1
Q	-1	SER	-	expression tag	UNP P9WIFY1
Q	0	HIS	-	expression tag	UNP P9WIFY1
S	-19	MET	-	initiating methionine	UNP P9WIFY1
S	-18	GLY	-	expression tag	UNP P9WIFY1
S	-17	SER	-	expression tag	UNP P9WIFY1
S	-16	SER	-	expression tag	UNP P9WIFY1
S	-15	HIS	-	expression tag	UNP P9WIFY1
S	-14	HIS	-	expression tag	UNP P9WIFY1
S	-13	HIS	-	expression tag	UNP P9WIFY1
S	-12	HIS	-	expression tag	UNP P9WIFY1
S	-11	HIS	-	expression tag	UNP P9WIFY1
S	-10	HIS	-	expression tag	UNP P9WIFY1
S	-9	SER	-	expression tag	UNP P9WIFY1
S	-8	SER	-	expression tag	UNP P9WIFY1
S	-7	GLY	-	expression tag	UNP P9WIFY1
S	-6	LEU	-	expression tag	UNP P9WIFY1
S	-5	VAL	-	expression tag	UNP P9WIFY1
S	-4	PRO	-	expression tag	UNP P9WIFY1
S	-3	ARG	-	expression tag	UNP P9WIFY1
S	-2	GLY	-	expression tag	UNP P9WIFY1
S	-1	SER	-	expression tag	UNP P9WIFY1
S	0	HIS	-	expression tag	UNP P9WIFY1
U	-19	MET	-	initiating methionine	UNP P9WIFY1
U	-18	GLY	-	expression tag	UNP P9WIFY1
U	-17	SER	-	expression tag	UNP P9WIFY1
U	-16	SER	-	expression tag	UNP P9WIFY1
U	-15	HIS	-	expression tag	UNP P9WIFY1
U	-14	HIS	-	expression tag	UNP P9WIFY1
U	-13	HIS	-	expression tag	UNP P9WIFY1
U	-12	HIS	-	expression tag	UNP P9WIFY1
U	-11	HIS	-	expression tag	UNP P9WIFY1
U	-10	HIS	-	expression tag	UNP P9WIFY1
U	-9	SER	-	expression tag	UNP P9WIFY1
U	-8	SER	-	expression tag	UNP P9WIFY1
U	-7	GLY	-	expression tag	UNP P9WIFY1
U	-6	LEU	-	expression tag	UNP P9WIFY1
U	-5	VAL	-	expression tag	UNP P9WIFY1

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-4	PRO	-	expression tag	UNP P9WIFY1
U	-3	ARG	-	expression tag	UNP P9WIFY1
U	-2	GLY	-	expression tag	UNP P9WIFY1
U	-1	SER	-	expression tag	UNP P9WIFY1
U	0	HIS	-	expression tag	UNP P9WIFY1
W	-19	MET	-	initiating methionine	UNP P9WIFY1
W	-18	GLY	-	expression tag	UNP P9WIFY1
W	-17	SER	-	expression tag	UNP P9WIFY1
W	-16	SER	-	expression tag	UNP P9WIFY1
W	-15	HIS	-	expression tag	UNP P9WIFY1
W	-14	HIS	-	expression tag	UNP P9WIFY1
W	-13	HIS	-	expression tag	UNP P9WIFY1
W	-12	HIS	-	expression tag	UNP P9WIFY1
W	-11	HIS	-	expression tag	UNP P9WIFY1
W	-10	HIS	-	expression tag	UNP P9WIFY1
W	-9	SER	-	expression tag	UNP P9WIFY1
W	-8	SER	-	expression tag	UNP P9WIFY1
W	-7	GLY	-	expression tag	UNP P9WIFY1
W	-6	LEU	-	expression tag	UNP P9WIFY1
W	-5	VAL	-	expression tag	UNP P9WIFY1
W	-4	PRO	-	expression tag	UNP P9WIFY1
W	-3	ARG	-	expression tag	UNP P9WIFY1
W	-2	GLY	-	expression tag	UNP P9WIFY1
W	-1	SER	-	expression tag	UNP P9WIFY1
W	0	HIS	-	expression tag	UNP P9WIFY1

- Molecule 2 is a protein called Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			
2	D	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			
2	F	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			
2	H	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			
2	J	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			
2	L	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			
2	N	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			
2	R	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			
2	T	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			
2	V	399	Total	C	N	O	S	0	3	0
			3002	1874	547	567	14			
2	X	399	Total	C	N	O	S	0	1	0
			2983	1863	542	565	13			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-31	MET	-	initiating methionine	UNP P9WFX9
B	-30	GLY	-	expression tag	UNP P9WFX9
B	-29	SER	-	expression tag	UNP P9WFX9
B	-28	SER	-	expression tag	UNP P9WFX9
B	-27	HIS	-	expression tag	UNP P9WFX9
B	-26	HIS	-	expression tag	UNP P9WFX9
B	-25	HIS	-	expression tag	UNP P9WFX9
B	-24	HIS	-	expression tag	UNP P9WFX9
B	-23	HIS	-	expression tag	UNP P9WFX9
B	-22	HIS	-	expression tag	UNP P9WFX9
B	-21	SER	-	expression tag	UNP P9WFX9
B	-20	SER	-	expression tag	UNP P9WFX9
B	-19	GLY	-	expression tag	UNP P9WFX9
B	-18	LEU	-	expression tag	UNP P9WFX9
B	-17	VAL	-	expression tag	UNP P9WFX9
B	-16	PRO	-	expression tag	UNP P9WFX9
B	-15	ARG	-	expression tag	UNP P9WFX9
B	-14	GLY	-	expression tag	UNP P9WFX9
B	-13	SER	-	expression tag	UNP P9WFX9
B	-12	HIS	-	expression tag	UNP P9WFX9
D	-31	MET	-	initiating methionine	UNP P9WFX9
D	-30	GLY	-	expression tag	UNP P9WFX9
D	-29	SER	-	expression tag	UNP P9WFX9
D	-28	SER	-	expression tag	UNP P9WFX9
D	-27	HIS	-	expression tag	UNP P9WFX9
D	-26	HIS	-	expression tag	UNP P9WFX9
D	-25	HIS	-	expression tag	UNP P9WFX9
D	-24	HIS	-	expression tag	UNP P9WFX9
D	-23	HIS	-	expression tag	UNP P9WFX9

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Chain	Residue	Modelled	Actual	Comment	Reference
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D	-21	SER	-	expression tag	UNP P9WFX9
D	-20	SER	-	expression tag	UNP P9WFX9
D	-19	GLY	-	expression tag	UNP P9WFX9
D	-18	LEU	-	expression tag	UNP P9WFX9
D	-17	VAL	-	expression tag	UNP P9WFX9
D	-16	PRO	-	expression tag	UNP P9WFX9
D	-15	ARG	-	expression tag	UNP P9WFX9
D	-14	GLY	-	expression tag	UNP P9WFX9
D	-13	SER	-	expression tag	UNP P9WFX9
D	-12	HIS	-	expression tag	UNP P9WFX9
F	-31	MET	-	initiating methionine	UNP P9WFX9
F	-30	GLY	-	expression tag	UNP P9WFX9
F	-29	SER	-	expression tag	UNP P9WFX9
F	-28	SER	-	expression tag	UNP P9WFX9
F	-27	HIS	-	expression tag	UNP P9WFX9
F	-26	HIS	-	expression tag	UNP P9WFX9
F	-25	HIS	-	expression tag	UNP P9WFX9
F	-24	HIS	-	expression tag	UNP P9WFX9
F	-23	HIS	-	expression tag	UNP P9WFX9
F	-22	HIS	-	expression tag	UNP P9WFX9
F	-21	SER	-	expression tag	UNP P9WFX9
F	-20	SER	-	expression tag	UNP P9WFX9
F	-19	GLY	-	expression tag	UNP P9WFX9
F	-18	LEU	-	expression tag	UNP P9WFX9
F	-17	VAL	-	expression tag	UNP P9WFX9
F	-16	PRO	-	expression tag	UNP P9WFX9
F	-15	ARG	-	expression tag	UNP P9WFX9
F	-14	GLY	-	expression tag	UNP P9WFX9
F	-13	SER	-	expression tag	UNP P9WFX9
F	-12	HIS	-	expression tag	UNP P9WFX9
H	-31	MET	-	initiating methionine	UNP P9WFX9
H	-30	GLY	-	expression tag	UNP P9WFX9
H	-29	SER	-	expression tag	UNP P9WFX9
H	-28	SER	-	expression tag	UNP P9WFX9
H	-27	HIS	-	expression tag	UNP P9WFX9
H	-26	HIS	-	expression tag	UNP P9WFX9
H	-25	HIS	-	expression tag	UNP P9WFX9
H	-24	HIS	-	expression tag	UNP P9WFX9
H	-23	HIS	-	expression tag	UNP P9WFX9
H	-22	HIS	-	expression tag	UNP P9WFX9
H	-21	SER	-	expression tag	UNP P9WFX9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-20	SER	-	expression tag	UNP P9WFX9
H	-19	GLY	-	expression tag	UNP P9WFX9
H	-18	LEU	-	expression tag	UNP P9WFX9
H	-17	VAL	-	expression tag	UNP P9WFX9
H	-16	PRO	-	expression tag	UNP P9WFX9
H	-15	ARG	-	expression tag	UNP P9WFX9
H	-14	GLY	-	expression tag	UNP P9WFX9
H	-13	SER	-	expression tag	UNP P9WFX9
H	-12	HIS	-	expression tag	UNP P9WFX9
J	-31	MET	-	initiating methionine	UNP P9WFX9
J	-30	GLY	-	expression tag	UNP P9WFX9
J	-29	SER	-	expression tag	UNP P9WFX9
J	-28	SER	-	expression tag	UNP P9WFX9
J	-27	HIS	-	expression tag	UNP P9WFX9
J	-26	HIS	-	expression tag	UNP P9WFX9
J	-25	HIS	-	expression tag	UNP P9WFX9
J	-24	HIS	-	expression tag	UNP P9WFX9
J	-23	HIS	-	expression tag	UNP P9WFX9
J	-22	HIS	-	expression tag	UNP P9WFX9
J	-21	SER	-	expression tag	UNP P9WFX9
J	-20	SER	-	expression tag	UNP P9WFX9
J	-19	GLY	-	expression tag	UNP P9WFX9
J	-18	LEU	-	expression tag	UNP P9WFX9
J	-17	VAL	-	expression tag	UNP P9WFX9
J	-16	PRO	-	expression tag	UNP P9WFX9
J	-15	ARG	-	expression tag	UNP P9WFX9
J	-14	GLY	-	expression tag	UNP P9WFX9
J	-13	SER	-	expression tag	UNP P9WFX9
J	-12	HIS	-	expression tag	UNP P9WFX9
L	-31	MET	-	initiating methionine	UNP P9WFX9
L	-30	GLY	-	expression tag	UNP P9WFX9
L	-29	SER	-	expression tag	UNP P9WFX9
L	-28	SER	-	expression tag	UNP P9WFX9
L	-27	HIS	-	expression tag	UNP P9WFX9
L	-26	HIS	-	expression tag	UNP P9WFX9
L	-25	HIS	-	expression tag	UNP P9WFX9
L	-24	HIS	-	expression tag	UNP P9WFX9
L	-23	HIS	-	expression tag	UNP P9WFX9
L	-22	HIS	-	expression tag	UNP P9WFX9
L	-21	SER	-	expression tag	UNP P9WFX9
L	-20	SER	-	expression tag	UNP P9WFX9
L	-19	GLY	-	expression tag	UNP P9WFX9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-18	LEU	-	expression tag	UNP P9WFX9
L	-17	VAL	-	expression tag	UNP P9WFX9
L	-16	PRO	-	expression tag	UNP P9WFX9
L	-15	ARG	-	expression tag	UNP P9WFX9
L	-14	GLY	-	expression tag	UNP P9WFX9
L	-13	SER	-	expression tag	UNP P9WFX9
L	-12	HIS	-	expression tag	UNP P9WFX9
N	-31	MET	-	initiating methionine	UNP P9WFX9
N	-30	GLY	-	expression tag	UNP P9WFX9
N	-29	SER	-	expression tag	UNP P9WFX9
N	-28	SER	-	expression tag	UNP P9WFX9
N	-27	HIS	-	expression tag	UNP P9WFX9
N	-26	HIS	-	expression tag	UNP P9WFX9
N	-25	HIS	-	expression tag	UNP P9WFX9
N	-24	HIS	-	expression tag	UNP P9WFX9
N	-23	HIS	-	expression tag	UNP P9WFX9
N	-22	HIS	-	expression tag	UNP P9WFX9
N	-21	SER	-	expression tag	UNP P9WFX9
N	-20	SER	-	expression tag	UNP P9WFX9
N	-19	GLY	-	expression tag	UNP P9WFX9
N	-18	LEU	-	expression tag	UNP P9WFX9
N	-17	VAL	-	expression tag	UNP P9WFX9
N	-16	PRO	-	expression tag	UNP P9WFX9
N	-15	ARG	-	expression tag	UNP P9WFX9
N	-14	GLY	-	expression tag	UNP P9WFX9
N	-13	SER	-	expression tag	UNP P9WFX9
N	-12	HIS	-	expression tag	UNP P9WFX9
P	-31	MET	-	initiating methionine	UNP P9WFX9
P	-30	GLY	-	expression tag	UNP P9WFX9
P	-29	SER	-	expression tag	UNP P9WFX9
P	-28	SER	-	expression tag	UNP P9WFX9
P	-27	HIS	-	expression tag	UNP P9WFX9
P	-26	HIS	-	expression tag	UNP P9WFX9
P	-25	HIS	-	expression tag	UNP P9WFX9
P	-24	HIS	-	expression tag	UNP P9WFX9
P	-23	HIS	-	expression tag	UNP P9WFX9
P	-22	HIS	-	expression tag	UNP P9WFX9
P	-21	SER	-	expression tag	UNP P9WFX9
P	-20	SER	-	expression tag	UNP P9WFX9
P	-19	GLY	-	expression tag	UNP P9WFX9
P	-18	LEU	-	expression tag	UNP P9WFX9
P	-17	VAL	-	expression tag	UNP P9WFX9

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-16	PRO	-	expression tag	UNP P9WFX9
P	-15	ARG	-	expression tag	UNP P9WFX9
P	-14	GLY	-	expression tag	UNP P9WFX9
P	-13	SER	-	expression tag	UNP P9WFX9
P	-12	HIS	-	expression tag	UNP P9WFX9
R	-31	MET	-	initiating methionine	UNP P9WFX9
R	-30	GLY	-	expression tag	UNP P9WFX9
R	-29	SER	-	expression tag	UNP P9WFX9
R	-28	SER	-	expression tag	UNP P9WFX9
R	-27	HIS	-	expression tag	UNP P9WFX9
R	-26	HIS	-	expression tag	UNP P9WFX9
R	-25	HIS	-	expression tag	UNP P9WFX9
R	-24	HIS	-	expression tag	UNP P9WFX9
R	-23	HIS	-	expression tag	UNP P9WFX9
R	-22	HIS	-	expression tag	UNP P9WFX9
R	-21	SER	-	expression tag	UNP P9WFX9
R	-20	SER	-	expression tag	UNP P9WFX9
R	-19	GLY	-	expression tag	UNP P9WFX9
R	-18	LEU	-	expression tag	UNP P9WFX9
R	-17	VAL	-	expression tag	UNP P9WFX9
R	-16	PRO	-	expression tag	UNP P9WFX9
R	-15	ARG	-	expression tag	UNP P9WFX9
R	-14	GLY	-	expression tag	UNP P9WFX9
R	-13	SER	-	expression tag	UNP P9WFX9
R	-12	HIS	-	expression tag	UNP P9WFX9
T	-31	MET	-	initiating methionine	UNP P9WFX9
T	-30	GLY	-	expression tag	UNP P9WFX9
T	-29	SER	-	expression tag	UNP P9WFX9
T	-28	SER	-	expression tag	UNP P9WFX9
T	-27	HIS	-	expression tag	UNP P9WFX9
T	-26	HIS	-	expression tag	UNP P9WFX9
T	-25	HIS	-	expression tag	UNP P9WFX9
T	-24	HIS	-	expression tag	UNP P9WFX9
T	-23	HIS	-	expression tag	UNP P9WFX9
T	-22	HIS	-	expression tag	UNP P9WFX9
T	-21	SER	-	expression tag	UNP P9WFX9
T	-20	SER	-	expression tag	UNP P9WFX9
T	-19	GLY	-	expression tag	UNP P9WFX9
T	-18	LEU	-	expression tag	UNP P9WFX9
T	-17	VAL	-	expression tag	UNP P9WFX9
T	-16	PRO	-	expression tag	UNP P9WFX9
T	-15	ARG	-	expression tag	UNP P9WFX9

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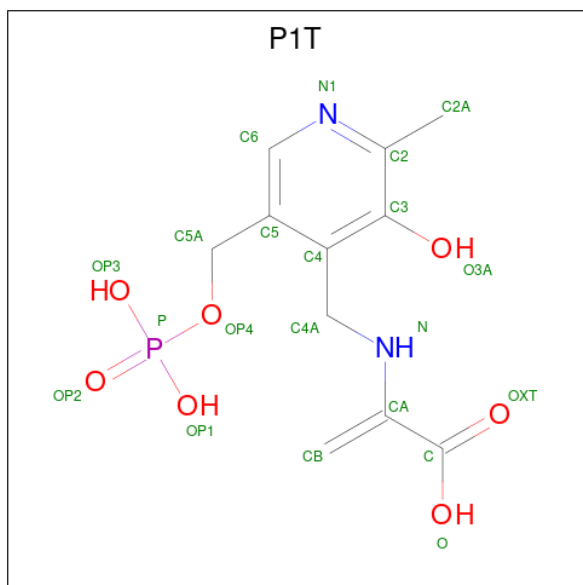
Chain	Residue	Modelled	Actual	Comment	Reference
T	-14	GLY	-	expression tag	UNP P9WFX9
T	-13	SER	-	expression tag	UNP P9WFX9
T	-12	HIS	-	expression tag	UNP P9WFX9
V	-31	MET	-	initiating methionine	UNP P9WFX9
V	-30	GLY	-	expression tag	UNP P9WFX9
V	-29	SER	-	expression tag	UNP P9WFX9
V	-28	SER	-	expression tag	UNP P9WFX9
V	-27	HIS	-	expression tag	UNP P9WFX9
V	-26	HIS	-	expression tag	UNP P9WFX9
V	-25	HIS	-	expression tag	UNP P9WFX9
V	-24	HIS	-	expression tag	UNP P9WFX9
V	-23	HIS	-	expression tag	UNP P9WFX9
V	-22	HIS	-	expression tag	UNP P9WFX9
V	-21	SER	-	expression tag	UNP P9WFX9
V	-20	SER	-	expression tag	UNP P9WFX9
V	-19	GLY	-	expression tag	UNP P9WFX9
V	-18	LEU	-	expression tag	UNP P9WFX9
V	-17	VAL	-	expression tag	UNP P9WFX9
V	-16	PRO	-	expression tag	UNP P9WFX9
V	-15	ARG	-	expression tag	UNP P9WFX9
V	-14	GLY	-	expression tag	UNP P9WFX9
V	-13	SER	-	expression tag	UNP P9WFX9
V	-12	HIS	-	expression tag	UNP P9WFX9
X	-31	MET	-	initiating methionine	UNP P9WFX9
X	-30	GLY	-	expression tag	UNP P9WFX9
X	-29	SER	-	expression tag	UNP P9WFX9
X	-28	SER	-	expression tag	UNP P9WFX9
X	-27	HIS	-	expression tag	UNP P9WFX9
X	-26	HIS	-	expression tag	UNP P9WFX9
X	-25	HIS	-	expression tag	UNP P9WFX9
X	-24	HIS	-	expression tag	UNP P9WFX9
X	-23	HIS	-	expression tag	UNP P9WFX9
X	-22	HIS	-	expression tag	UNP P9WFX9
X	-21	SER	-	expression tag	UNP P9WFX9
X	-20	SER	-	expression tag	UNP P9WFX9
X	-19	GLY	-	expression tag	UNP P9WFX9
X	-18	LEU	-	expression tag	UNP P9WFX9
X	-17	VAL	-	expression tag	UNP P9WFX9
X	-16	PRO	-	expression tag	UNP P9WFX9
X	-15	ARG	-	expression tag	UNP P9WFX9
X	-14	GLY	-	expression tag	UNP P9WFX9
X	-13	SER	-	expression tag	UNP P9WFX9

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-12	HIS	-	expression tag	UNP P9WFX9

- Molecule 3 is 2-[(3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL)METHYL)AMINO]ACRYLIC ACID (three-letter code: P1T) (formula: $C_{11}H_{15}N_2O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	D	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	F	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	H	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	J	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	L	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	N	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	P	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	R	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	T	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

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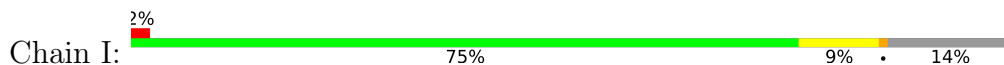
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	V	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
3	X	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 1: Tryptophan synthase alpha chain

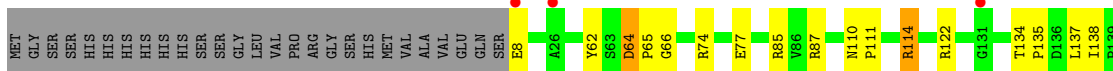
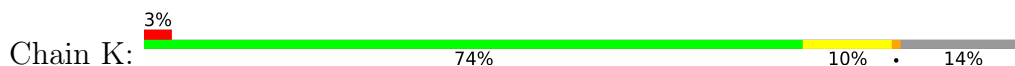




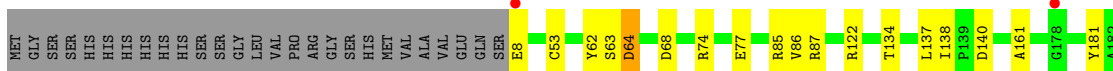
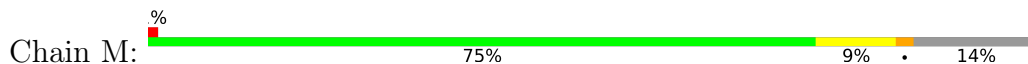
- Molecule 1: Tryptophan synthase alpha chain



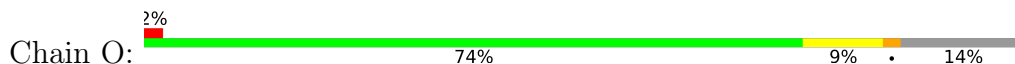
- Molecule 1: Tryptophan synthase alpha chain



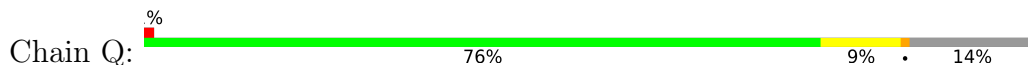
- Molecule 1: Tryptophan synthase alpha chain

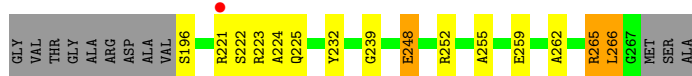
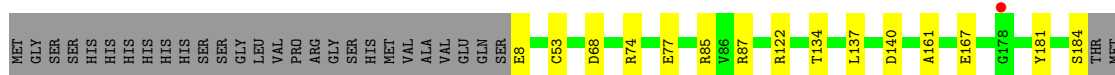


- Molecule 1: Tryptophan synthase alpha chain

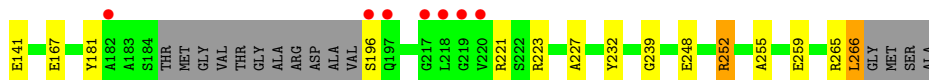
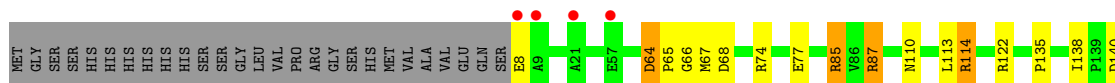
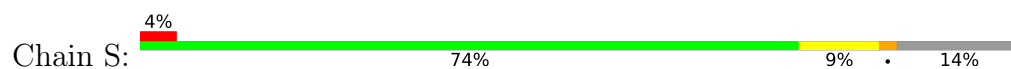


- Molecule 1: Tryptophan synthase alpha chain

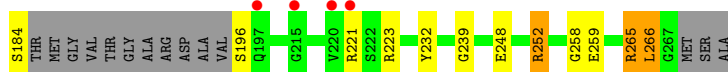
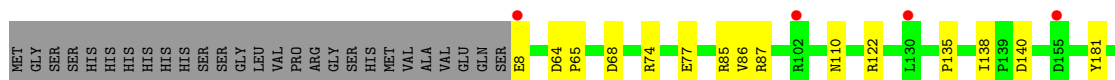
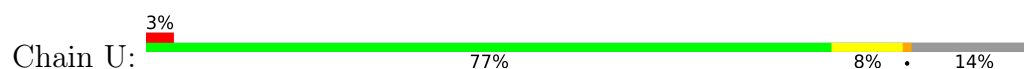




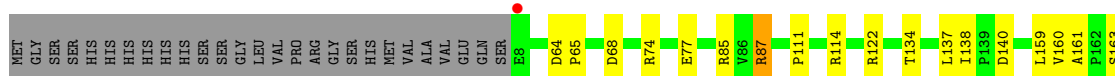
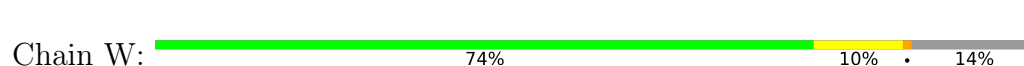
• Molecule 1: Tryptophan synthase alpha chain



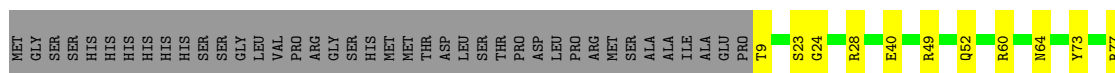
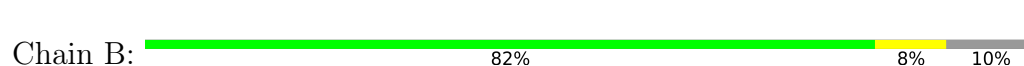
• Molecule 1: Tryptophan synthase alpha chain




• Molecule 1: Tryptophan synthase alpha chain

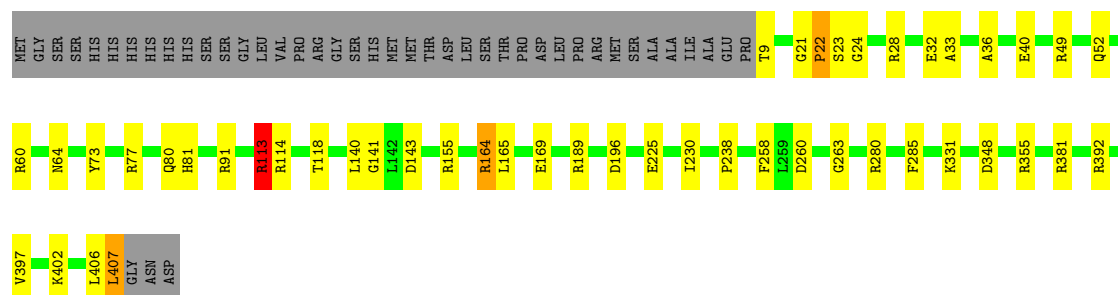


• Molecule 2: Tryptophan synthase beta chain




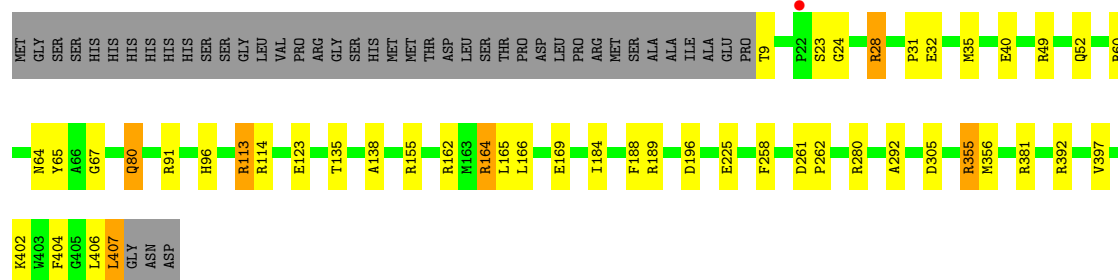
- Molecule 2: Tryptophan synthase beta chain

Chain D:  79% 10% 10%




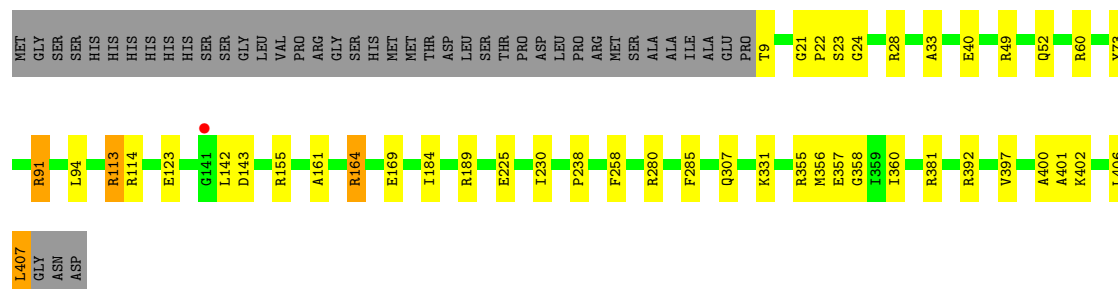
- Molecule 2: Tryptophan synthase beta chain

Chain F:  79% 10% 10%




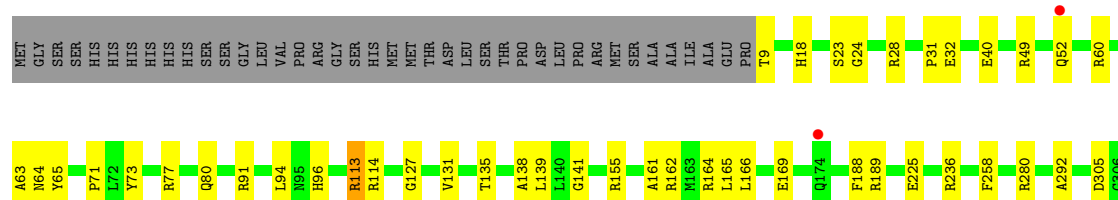
- Molecule 2: Tryptophan synthase beta chain

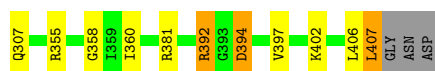
Chain H:  80% 10% 10%



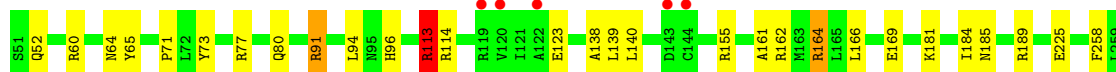
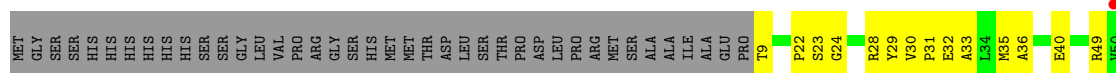
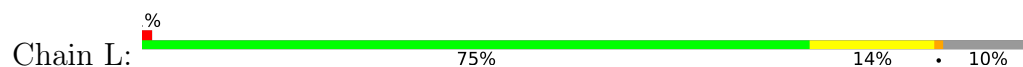
- Molecule 2: Tryptophan synthase beta chain

Chain J:  78% 12% 10%

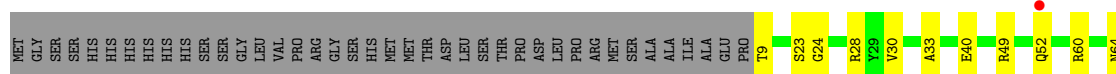
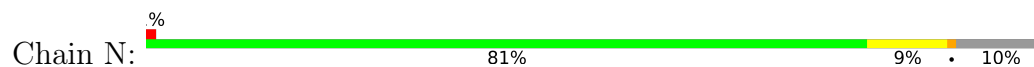




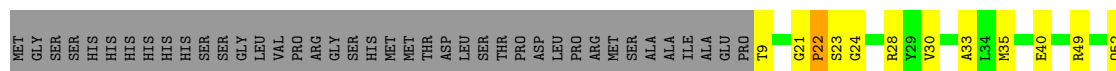
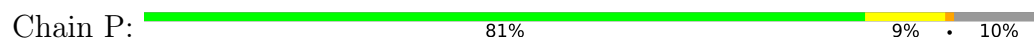
• Molecule 2: Tryptophan synthase beta chain



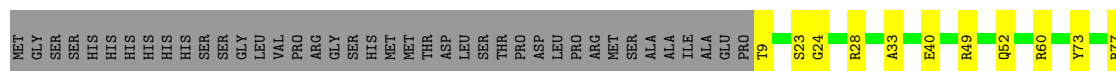
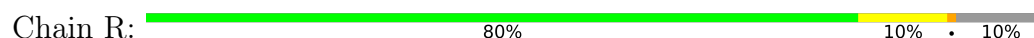
• Molecule 2: Tryptophan synthase beta chain

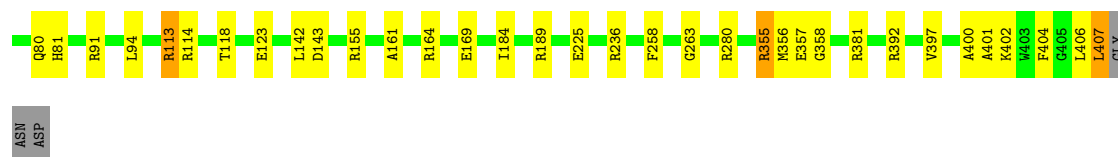


• Molecule 2: Tryptophan synthase beta chain



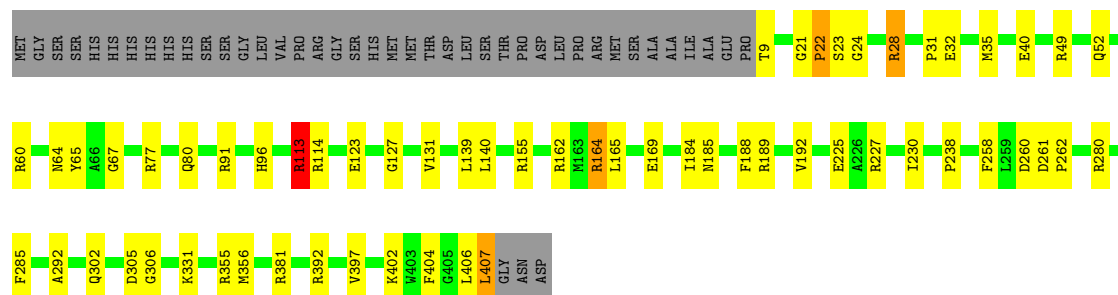
• Molecule 2: Tryptophan synthase beta chain





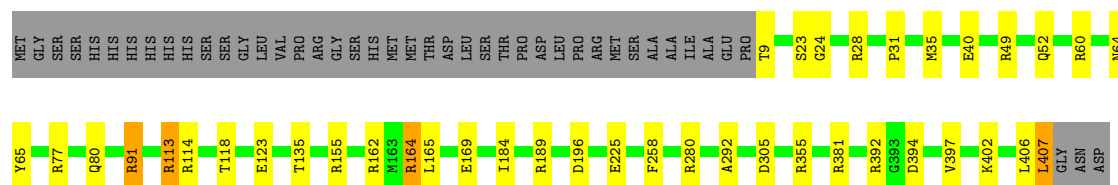
- Molecule 2: Tryptophan synthase beta chain

Chain T: 76% 13% 10%



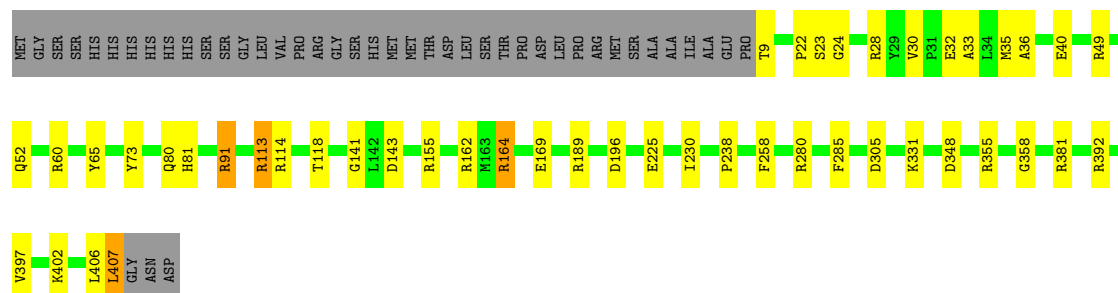
- Molecule 2: Tryptophan synthase beta chain

Chain V: 81% 8% 10%



- Molecule 2: Tryptophan synthase beta chain

Chain X: 80% 10% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	426.05Å 432.11Å 434.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 4.00 49.80 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.80-4.00) 95.1 (49.80-4.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.358 , 0.368 0.346 , 0.355	Depositor DCC
R_{free} test set	8243 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	171.2	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , -9.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.108 for -h,l,k 0.036 for l,-k,h 0.060 for -k,-h,-l 0.029 for -k,-l,h 0.029 for l,-h,-k	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	57878	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P1T

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	1.37	29/1881 (1.5%)	1.54	34/2566 (1.3%)
1	C	1.32	25/1828 (1.4%)	1.42	29/2495 (1.2%)
1	E	1.33	24/1843 (1.3%)	1.52	30/2514 (1.2%)
1	G	1.33	30/1828 (1.6%)	1.43	29/2495 (1.2%)
1	I	1.36	26/1843 (1.4%)	1.55	34/2514 (1.4%)
1	K	1.34	27/1828 (1.5%)	1.43	31/2495 (1.2%)
1	M	1.37	27/1843 (1.5%)	1.55	34/2514 (1.4%)
1	O	1.33	25/1828 (1.4%)	1.43	30/2495 (1.2%)
1	Q	1.37	28/1843 (1.5%)	1.54	34/2514 (1.4%)
1	S	1.37	27/1827 (1.5%)	1.46	33/2492 (1.3%)
1	U	1.36	28/1843 (1.5%)	1.55	34/2514 (1.4%)
1	W	1.32	24/1828 (1.3%)	1.43	30/2495 (1.2%)
2	B	1.27	42/3062 (1.4%)	1.24	40/4148 (1.0%)
2	D	1.24	40/3043 (1.3%)	1.26	37/4123 (0.9%)
2	F	1.29	40/3062 (1.3%)	1.22	39/4148 (0.9%)
2	H	1.22	40/3043 (1.3%)	1.30	35/4123 (0.8%)
2	J	1.28	42/3062 (1.4%)	1.23	39/4148 (0.9%)
2	L	1.25	42/3043 (1.4%)	1.27	37/4123 (0.9%)
2	N	1.28	41/3062 (1.3%)	1.24	39/4148 (0.9%)
2	P	1.25	43/3043 (1.4%)	1.27	35/4123 (0.8%)
2	R	1.28	42/3062 (1.4%)	1.23	36/4148 (0.9%)
2	T	1.25	42/3043 (1.4%)	1.27	37/4123 (0.9%)
2	V	1.27	42/3062 (1.4%)	1.24	40/4148 (1.0%)
2	X	1.24	42/3043 (1.4%)	1.27	38/4123 (0.9%)
All	All	1.29	818/58693 (1.4%)	1.35	834/79729 (1.0%)

All (818) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	24	GLY	N-CA	-17.82	1.19	1.46
2	B	24	GLY	N-CA	-17.53	1.19	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	221	ARG	CZ-NH2	-17.50	1.10	1.33
2	J	24	GLY	N-CA	-17.49	1.19	1.46
1	Q	221	ARG	CZ-NH2	-17.47	1.10	1.33
2	F	23	SER	CA-CB	-17.40	1.26	1.52
1	U	221	ARG	CZ-NH2	-17.36	1.10	1.33
1	I	221	ARG	CZ-NH2	-17.32	1.10	1.33
2	R	24	GLY	N-CA	-17.30	1.20	1.46
2	N	24	GLY	N-CA	-17.26	1.20	1.46
2	F	24	GLY	N-CA	-17.24	1.20	1.46
1	A	221	ARG	CZ-NH2	-17.24	1.10	1.33
1	E	221	ARG	CZ-NH2	-17.20	1.10	1.33
1	S	252	ARG	CZ-NH1	-16.37	1.11	1.33
1	M	232	TYR	CE1-CZ	-16.34	1.17	1.38
1	Q	232	TYR	CE1-CZ	-16.30	1.17	1.38
1	S	232	TYR	CE1-CZ	-16.08	1.17	1.38
1	I	232	TYR	CE1-CZ	-16.07	1.17	1.38
1	A	232	TYR	CE1-CZ	-15.95	1.17	1.38
1	U	232	TYR	CE1-CZ	-15.95	1.17	1.38
1	G	232	TYR	CE1-CZ	-15.94	1.17	1.38
1	E	232	TYR	CE1-CZ	-15.92	1.17	1.38
1	C	232	TYR	CE1-CZ	-15.87	1.18	1.38
1	W	232	TYR	CE1-CZ	-15.71	1.18	1.38
1	K	232	TYR	CE1-CZ	-15.71	1.18	1.38
1	O	232	TYR	CE1-CZ	-15.70	1.18	1.38
2	B	280	ARG	CZ-NH2	-15.61	1.12	1.33
2	V	280	ARG	CZ-NH2	-15.55	1.12	1.33
2	P	24	GLY	N-CA	-15.54	1.22	1.46
1	O	252	ARG	CZ-NH1	-15.52	1.12	1.33
2	L	24	GLY	N-CA	-15.50	1.22	1.46
2	F	280	ARG	CZ-NH2	-15.47	1.12	1.33
2	N	280	ARG	CZ-NH2	-15.47	1.12	1.33
2	J	280	ARG	CZ-NH2	-15.47	1.12	1.33
2	T	24	GLY	N-CA	-15.41	1.23	1.46
2	P	280	ARG	CZ-NH2	-15.39	1.13	1.33
2	R	280	ARG	CZ-NH2	-15.39	1.13	1.33
2	T	280	ARG	CZ-NH2	-15.39	1.13	1.33
1	K	252	ARG	CZ-NH1	-15.39	1.13	1.33
2	L	280	ARG	CZ-NH2	-15.26	1.13	1.33
2	H	280	ARG	CZ-NH2	-15.25	1.13	1.33
1	C	252	ARG	CZ-NH1	-15.23	1.13	1.33
1	I	252	ARG	CZ-NH1	-15.22	1.13	1.33
2	L	113	ARG	CZ-NH2	-15.19	1.13	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	252	ARG	CZ-NH1	-15.16	1.13	1.33
2	X	24	GLY	N-CA	-15.14	1.23	1.46
2	X	280	ARG	CZ-NH2	-15.13	1.13	1.33
1	K	221	ARG	CZ-NH2	-15.12	1.13	1.33
1	G	221	ARG	CZ-NH2	-15.12	1.13	1.33
1	M	252	ARG	CZ-NH1	-15.11	1.13	1.33
1	W	252	ARG	CZ-NH1	-15.10	1.13	1.33
2	D	280	ARG	CZ-NH2	-15.07	1.13	1.33
1	S	221	ARG	CZ-NH2	-15.05	1.13	1.33
1	U	252	ARG	CZ-NH1	-14.97	1.13	1.33
1	Q	252	ARG	CZ-NH1	-14.93	1.13	1.33
1	O	221	ARG	CZ-NH2	-14.93	1.13	1.33
2	D	24	GLY	N-CA	-14.87	1.23	1.46
2	T	113	ARG	CZ-NH2	-14.85	1.13	1.33
1	G	252	ARG	CZ-NH1	-14.77	1.13	1.33
2	H	24	GLY	N-CA	-14.71	1.24	1.46
2	P	113	ARG	CZ-NH2	-14.69	1.14	1.33
1	W	221	ARG	CZ-NH2	-14.65	1.14	1.33
1	A	252	ARG	CZ-NH1	-14.55	1.14	1.33
1	G	232	TYR	CG-CD2	-14.27	1.20	1.39
1	C	221	ARG	CZ-NH2	-14.24	1.14	1.33
1	S	232	TYR	CG-CD2	-14.23	1.20	1.39
2	X	113	ARG	CZ-NH2	-14.06	1.14	1.33
2	D	113	ARG	CZ-NH2	-13.96	1.15	1.33
1	C	232	TYR	CG-CD2	-13.92	1.21	1.39
2	J	381	ARG	CZ-NH1	-13.86	1.15	1.33
2	R	381	ARG	CZ-NH1	-13.81	1.15	1.33
2	V	381	ARG	CZ-NH1	-13.80	1.15	1.33
2	N	381	ARG	CZ-NH1	-13.79	1.15	1.33
1	K	232	TYR	CG-CD2	-13.75	1.21	1.39
2	B	381	ARG	CZ-NH1	-13.73	1.15	1.33
1	W	232	TYR	CG-CD2	-13.72	1.21	1.39
1	M	232	TYR	CG-CD2	-13.68	1.21	1.39
2	F	113	ARG	CZ-NH1	-13.66	1.15	1.33
1	O	232	TYR	CG-CD2	-13.66	1.21	1.39
1	Q	232	TYR	CG-CD2	-13.54	1.21	1.39
1	I	232	TYR	CG-CD2	-13.52	1.21	1.39
1	A	232	TYR	CG-CD2	-13.51	1.21	1.39
1	U	232	TYR	CG-CD2	-13.43	1.21	1.39
1	E	232	TYR	CG-CD2	-13.31	1.21	1.39
2	X	49	ARG	CZ-NH2	-13.31	1.15	1.33
1	M	232	TYR	CG-CD1	-13.23	1.22	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	49	ARG	CZ-NH2	-13.22	1.15	1.33
1	A	232	TYR	CG-CD1	-13.21	1.22	1.39
2	J	9	THR	CB-CG2	-13.21	1.08	1.52
2	T	49	ARG	CZ-NH2	-13.17	1.16	1.33
2	P	49	ARG	CZ-NH2	-13.07	1.16	1.33
2	N	392	ARG	CZ-NH1	-13.01	1.16	1.33
2	V	9	THR	CB-CG2	-13.01	1.09	1.52
2	F	49	ARG	CZ-NH2	-12.98	1.16	1.33
2	D	49	ARG	CZ-NH2	-12.97	1.16	1.33
1	I	232	TYR	CG-CD1	-12.97	1.22	1.39
1	Q	232	TYR	CG-CD1	-12.97	1.22	1.39
2	J	49	ARG	CZ-NH2	-12.94	1.16	1.33
2	V	49	ARG	CZ-NH2	-12.91	1.16	1.33
1	U	232	TYR	CG-CD1	-12.88	1.22	1.39
2	H	49	ARG	CZ-NH2	-12.84	1.16	1.33
1	C	232	TYR	CG-CD1	-12.76	1.22	1.39
2	N	49	ARG	CZ-NH2	-12.74	1.16	1.33
1	E	232	TYR	CG-CD1	-12.73	1.22	1.39
2	B	49	ARG	CZ-NH2	-12.71	1.16	1.33
2	L	169	GLU	CD-OE1	-12.71	1.11	1.25
1	G	232	TYR	CG-CD1	-12.65	1.22	1.39
2	J	392	ARG	CZ-NH1	-12.65	1.16	1.33
2	R	9	THR	CB-CG2	-12.64	1.10	1.52
2	R	49	ARG	CZ-NH2	-12.64	1.16	1.33
2	P	23	SER	CA-CB	-12.63	1.34	1.52
2	R	392	ARG	CZ-NH1	-12.62	1.16	1.33
2	F	392	ARG	CZ-NH1	-12.60	1.16	1.33
2	F	9	THR	CB-CG2	-12.57	1.10	1.52
2	F	258	PHE	CG-CD1	-12.56	1.20	1.38
2	N	9	THR	CB-CG2	-12.54	1.10	1.52
2	V	392	ARG	CZ-NH1	-12.48	1.16	1.33
2	R	258	PHE	CG-CD1	-12.48	1.20	1.38
2	P	169	GLU	CD-OE1	-12.47	1.11	1.25
2	T	23	SER	CA-CB	-12.45	1.34	1.52
1	W	232	TYR	CG-CD1	-12.45	1.23	1.39
1	S	232	TYR	CG-CD1	-12.44	1.23	1.39
2	N	258	PHE	CG-CD1	-12.42	1.20	1.38
2	B	392	ARG	CZ-NH1	-12.42	1.17	1.33
2	B	9	THR	CB-CG2	-12.38	1.11	1.52
2	B	258	PHE	CG-CD1	-12.37	1.20	1.38
1	K	232	TYR	CG-CD1	-12.35	1.23	1.39
1	O	232	TYR	CG-CD1	-12.30	1.23	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	169	GLU	CD-OE1	-12.30	1.12	1.25
2	J	113	ARG	CZ-NH2	-12.27	1.17	1.33
2	J	258	PHE	CG-CD1	-12.27	1.20	1.38
2	L	23	SER	CA-CB	-12.26	1.34	1.52
2	F	113	ARG	CZ-NH2	-12.25	1.17	1.33
2	N	28	ARG	CZ-NH2	-12.23	1.17	1.33
1	M	232	TYR	CE2-CZ	-12.21	1.22	1.38
2	R	113	ARG	CZ-NH2	-12.20	1.17	1.33
2	X	169	GLU	CD-OE1	-12.15	1.12	1.25
2	V	113	ARG	CZ-NH2	-12.13	1.17	1.33
2	J	28	ARG	CZ-NH2	-12.13	1.17	1.33
2	H	381	ARG	CZ-NH1	-12.09	1.17	1.33
2	R	28	ARG	CZ-NH2	-12.07	1.17	1.33
2	N	113	ARG	CZ-NH2	-12.06	1.17	1.33
2	P	113	ARG	CZ-NH1	-12.06	1.17	1.33
2	B	28	ARG	CZ-NH2	-12.05	1.17	1.33
1	A	232	TYR	CE2-CZ	-12.03	1.23	1.38
2	L	113	ARG	CZ-NH1	-12.00	1.17	1.33
2	L	381	ARG	CZ-NH1	-11.99	1.17	1.33
2	B	113	ARG	CZ-NH2	-11.97	1.17	1.33
2	V	258	PHE	CG-CD1	-11.97	1.20	1.38
2	V	28	ARG	CZ-NH2	-11.95	1.17	1.33
2	X	258	PHE	CG-CD2	-11.94	1.20	1.38
2	D	169	GLU	CD-OE1	-11.94	1.12	1.25
2	F	28	ARG	CZ-NH2	-11.92	1.17	1.33
2	T	392	ARG	CZ-NH1	-11.88	1.17	1.33
2	P	381	ARG	CZ-NH1	-11.84	1.17	1.33
1	I	232	TYR	CE2-CZ	-11.84	1.23	1.38
2	D	258	PHE	CG-CD2	-11.84	1.21	1.38
2	H	392	ARG	CZ-NH1	-11.82	1.17	1.33
2	D	258	PHE	CG-CD1	-11.80	1.21	1.38
1	G	232	TYR	CE2-CZ	-11.78	1.23	1.38
2	T	381	ARG	CZ-NH1	-11.78	1.17	1.33
2	D	91	ARG	CZ-NH1	-11.77	1.17	1.33
2	X	113	ARG	CZ-NH1	-11.76	1.17	1.33
2	X	258	PHE	CG-CD1	-11.74	1.21	1.38
2	H	28	ARG	CZ-NH2	-11.72	1.17	1.33
2	H	258	PHE	CG-CD1	-11.71	1.21	1.38
2	D	28	ARG	CZ-NH2	-11.71	1.17	1.33
2	X	381	ARG	CZ-NH1	-11.69	1.17	1.33
1	G	265	ARG	CZ-NH2	-11.67	1.17	1.33
2	X	91	ARG	CZ-NH1	-11.66	1.17	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	392	ARG	CZ-NH1	-11.66	1.17	1.33
2	R	155	ARG	CZ-NH1	-11.64	1.18	1.33
2	D	381	ARG	CZ-NH1	-11.63	1.18	1.33
1	U	232	TYR	CE2-CZ	-11.61	1.23	1.38
2	H	258	PHE	CG-CD2	-11.60	1.21	1.38
2	V	23	SER	CA-CB	-11.60	1.35	1.52
1	Q	232	TYR	CE2-CZ	-11.60	1.23	1.38
2	D	113	ARG	CZ-NH1	-11.59	1.18	1.33
2	T	258	PHE	CG-CD2	-11.59	1.21	1.38
2	X	28	ARG	CZ-NH2	-11.59	1.18	1.33
2	L	28	ARG	CZ-NH2	-11.56	1.18	1.33
1	K	265	ARG	CZ-NH2	-11.56	1.18	1.33
2	T	258	PHE	CG-CD1	-11.55	1.21	1.38
2	F	155	ARG	CZ-NH1	-11.54	1.18	1.33
2	L	258	PHE	CG-CD1	-11.53	1.21	1.38
2	V	155	ARG	CZ-NH1	-11.53	1.18	1.33
2	T	91	ARG	CZ-NH1	-11.53	1.18	1.33
1	C	232	TYR	CE2-CZ	-11.51	1.23	1.38
1	O	265	ARG	CZ-NH2	-11.49	1.18	1.33
2	F	91	ARG	CZ-NH2	-11.49	1.18	1.33
2	N	155	ARG	CZ-NH1	-11.48	1.18	1.33
1	E	232	TYR	CE2-CZ	-11.48	1.23	1.38
2	J	23	SER	CA-CB	-11.47	1.35	1.52
2	P	392	ARG	CZ-NH1	-11.46	1.18	1.33
2	T	28	ARG	CZ-NH2	-11.45	1.18	1.33
2	P	258	PHE	CG-CD2	-11.45	1.21	1.38
2	R	258	PHE	CG-CD2	-11.44	1.21	1.38
2	X	155	ARG	CZ-NH2	-11.43	1.18	1.33
2	R	155	ARG	CZ-NH2	-11.42	1.18	1.33
2	X	392	ARG	CZ-NH1	-11.42	1.18	1.33
1	W	232	TYR	CE2-CZ	-11.42	1.23	1.38
2	H	91	ARG	CZ-NH1	-11.41	1.18	1.33
2	H	155	ARG	CZ-NH2	-11.41	1.18	1.33
2	L	28	ARG	CZ-NH1	-11.40	1.18	1.33
1	C	265	ARG	CZ-NH2	-11.40	1.18	1.33
2	F	258	PHE	CG-CD2	-11.40	1.21	1.38
2	J	155	ARG	CZ-NH1	-11.39	1.18	1.33
1	O	85	ARG	CZ-NH1	-11.38	1.18	1.33
2	P	91	ARG	CZ-NH1	-11.38	1.18	1.33
1	S	265	ARG	CZ-NH2	-11.38	1.18	1.33
2	P	258	PHE	CG-CD1	-11.37	1.21	1.38
1	U	265	ARG	CZ-NH2	-11.36	1.18	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	265	ARG	CZ-NH2	-11.36	1.18	1.33
2	L	91	ARG	CZ-NH1	-11.35	1.18	1.33
2	L	258	PHE	CG-CD2	-11.33	1.21	1.38
2	B	91	ARG	CZ-NH2	-11.33	1.18	1.33
2	B	258	PHE	CG-CD2	-11.32	1.21	1.38
2	J	155	ARG	CZ-NH2	-11.32	1.18	1.33
2	P	28	ARG	CZ-NH2	-11.32	1.18	1.33
1	U	265	ARG	CZ-NH1	-11.31	1.18	1.33
1	I	265	ARG	CZ-NH1	-11.31	1.18	1.33
1	C	85	ARG	CZ-NH1	-11.30	1.18	1.33
2	F	155	ARG	CZ-NH2	-11.29	1.18	1.33
1	E	85	ARG	CZ-NH1	-11.29	1.18	1.33
1	G	85	ARG	CZ-NH1	-11.28	1.18	1.33
2	N	91	ARG	CZ-NH2	-11.28	1.18	1.33
2	R	91	ARG	CZ-NH2	-11.28	1.18	1.33
2	B	155	ARG	CZ-NH1	-11.27	1.18	1.33
2	L	114	ARG	CZ-NH2	-11.27	1.18	1.33
2	D	392	ARG	CZ-NH1	-11.27	1.18	1.33
1	Q	265	ARG	CZ-NH2	-11.27	1.18	1.33
2	T	114	ARG	CZ-NH2	-11.26	1.18	1.33
2	H	28	ARG	CZ-NH1	-11.26	1.18	1.33
1	K	85	ARG	CZ-NH1	-11.25	1.18	1.33
1	S	232	TYR	CE2-CZ	-11.25	1.24	1.38
1	Q	265	ARG	CZ-NH1	-11.23	1.18	1.33
2	H	91	ARG	CZ-NH2	-11.22	1.18	1.33
1	M	265	ARG	CZ-NH1	-11.22	1.18	1.33
2	X	155	ARG	CZ-NH1	-11.22	1.18	1.33
1	W	85	ARG	CZ-NH1	-11.21	1.18	1.33
1	S	85	ARG	CZ-NH1	-11.21	1.18	1.33
2	V	155	ARG	CZ-NH2	-11.21	1.18	1.33
2	D	155	ARG	CZ-NH1	-11.20	1.18	1.33
2	L	91	ARG	CZ-NH2	-11.20	1.18	1.33
2	P	114	ARG	CZ-NH2	-11.19	1.18	1.33
2	T	28	ARG	CZ-NH1	-11.19	1.18	1.33
1	A	265	ARG	CZ-NH1	-11.19	1.18	1.33
2	L	155	ARG	CZ-NH2	-11.18	1.18	1.33
2	D	23	SER	CA-CB	-11.18	1.36	1.52
2	N	155	ARG	CZ-NH2	-11.18	1.18	1.33
2	R	91	ARG	CZ-NH1	-11.17	1.18	1.33
2	D	155	ARG	CZ-NH2	-11.17	1.18	1.33
2	H	114	ARG	CZ-NH2	-11.16	1.18	1.33
2	T	91	ARG	CZ-NH2	-11.16	1.18	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	265	ARG	CZ-NH2	-11.15	1.18	1.33
2	T	155	ARG	CZ-NH1	-11.15	1.18	1.33
1	I	265	ARG	CZ-NH2	-11.15	1.18	1.33
2	J	258	PHE	CG-CD2	-11.15	1.22	1.38
1	O	232	TYR	CE2-CZ	-11.15	1.24	1.38
2	X	91	ARG	CZ-NH2	-11.15	1.18	1.33
2	T	113	ARG	CZ-NH1	-11.14	1.18	1.33
2	T	155	ARG	CZ-NH2	-11.14	1.18	1.33
2	L	155	ARG	CZ-NH1	-11.13	1.18	1.33
1	M	265	ARG	CZ-NH2	-11.13	1.18	1.33
1	K	232	TYR	CE2-CZ	-11.12	1.24	1.38
1	E	265	ARG	CZ-NH1	-11.12	1.18	1.33
2	V	91	ARG	CZ-NH2	-11.11	1.18	1.33
2	J	114	ARG	CZ-NH2	-11.11	1.18	1.33
1	A	265	ARG	CZ-NH2	-11.08	1.18	1.33
2	P	91	ARG	CZ-NH2	-11.06	1.18	1.33
2	F	91	ARG	CZ-NH1	-11.05	1.18	1.33
2	R	114	ARG	CZ-NH2	-11.05	1.18	1.33
2	N	23	SER	CA-CB	-11.05	1.36	1.52
2	P	155	ARG	CZ-NH2	-11.04	1.18	1.33
2	J	91	ARG	CZ-NH1	-11.04	1.18	1.33
2	N	258	PHE	CG-CD2	-11.04	1.22	1.38
2	V	258	PHE	CG-CD2	-11.04	1.22	1.38
2	N	114	ARG	CZ-NH2	-11.04	1.18	1.33
2	H	155	ARG	CZ-NH1	-11.03	1.18	1.33
1	O	265	ARG	CZ-NH1	-11.03	1.18	1.33
1	I	85	ARG	CZ-NH1	-11.02	1.18	1.33
2	X	114	ARG	CZ-NH2	-11.01	1.18	1.33
1	Q	85	ARG	CZ-NH1	-11.01	1.18	1.33
2	B	91	ARG	CZ-NH1	-11.00	1.18	1.33
2	B	155	ARG	CZ-NH2	-11.00	1.18	1.33
2	D	28	ARG	CZ-NH1	-10.99	1.18	1.33
2	J	91	ARG	CZ-NH2	-10.98	1.18	1.33
2	D	114	ARG	CZ-NH2	-10.98	1.18	1.33
2	P	28	ARG	CZ-NH1	-10.98	1.18	1.33
1	K	265	ARG	CZ-NH1	-10.98	1.18	1.33
1	W	265	ARG	CZ-NH1	-10.97	1.18	1.33
2	V	114	ARG	CZ-NH2	-10.96	1.18	1.33
2	J	28	ARG	CZ-NH1	-10.96	1.18	1.33
2	V	91	ARG	CZ-NH1	-10.95	1.18	1.33
2	B	23	SER	CA-CB	-10.94	1.36	1.52
1	S	8	GLU	CD-OE1	-10.94	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	28	ARG	CZ-NH1	-10.93	1.18	1.33
2	N	91	ARG	CZ-NH1	-10.92	1.18	1.33
2	D	91	ARG	CZ-NH2	-10.90	1.18	1.33
1	G	265	ARG	CZ-NH1	-10.86	1.19	1.33
2	N	28	ARG	CZ-NH1	-10.86	1.19	1.33
2	F	114	ARG	CZ-NH2	-10.84	1.19	1.33
1	A	85	ARG	CZ-NH1	-10.84	1.19	1.33
1	U	85	ARG	CZ-NH1	-10.84	1.19	1.33
1	C	265	ARG	CZ-NH1	-10.83	1.19	1.33
2	X	23	SER	CA-CB	-10.83	1.36	1.52
2	N	114	ARG	CZ-NH1	-10.82	1.19	1.33
2	P	155	ARG	CZ-NH1	-10.81	1.19	1.33
2	J	114	ARG	CZ-NH1	-10.80	1.19	1.33
2	B	114	ARG	CZ-NH2	-10.79	1.19	1.33
2	B	28	ARG	CZ-NH1	-10.79	1.19	1.33
2	V	114	ARG	CZ-NH1	-10.76	1.19	1.33
1	M	85	ARG	CZ-NH1	-10.72	1.19	1.33
2	V	28	ARG	CZ-NH1	-10.72	1.19	1.33
1	W	122	ARG	CZ-NH2	-10.70	1.19	1.33
2	R	28	ARG	CZ-NH1	-10.69	1.19	1.33
2	F	114	ARG	CZ-NH1	-10.68	1.19	1.33
1	G	122	ARG	CZ-NH1	-10.65	1.19	1.33
1	A	85	ARG	CZ-NH2	-10.64	1.19	1.33
1	K	122	ARG	CZ-NH1	-10.63	1.19	1.33
1	Q	85	ARG	CZ-NH2	-10.63	1.19	1.33
1	K	85	ARG	CZ-NH2	-10.60	1.19	1.33
1	S	85	ARG	CZ-NH2	-10.59	1.19	1.33
1	W	122	ARG	CZ-NH1	-10.58	1.19	1.33
1	C	122	ARG	CZ-NH1	-10.57	1.19	1.33
1	O	85	ARG	CZ-NH2	-10.54	1.19	1.33
1	U	85	ARG	CZ-NH2	-10.54	1.19	1.33
1	S	265	ARG	CZ-NH1	-10.53	1.19	1.33
1	K	122	ARG	CZ-NH2	-10.53	1.19	1.33
1	I	85	ARG	CZ-NH2	-10.53	1.19	1.33
1	G	122	ARG	CZ-NH2	-10.53	1.19	1.33
1	A	122	ARG	CZ-NH2	-10.52	1.19	1.33
2	B	114	ARG	CZ-NH1	-10.52	1.19	1.33
1	C	122	ARG	CZ-NH2	-10.52	1.19	1.33
1	C	85	ARG	CZ-NH2	-10.52	1.19	1.33
1	O	122	ARG	CZ-NH1	-10.52	1.19	1.33
2	R	114	ARG	CZ-NH1	-10.52	1.19	1.33
2	F	28	ARG	CZ-NH1	-10.51	1.19	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	122	ARG	CZ-NH2	-10.51	1.19	1.33
1	I	122	ARG	CZ-NH2	-10.50	1.19	1.33
1	M	85	ARG	CZ-NH2	-10.50	1.19	1.33
2	H	113	ARG	CZ-NH2	-10.48	1.19	1.33
1	O	122	ARG	CZ-NH2	-10.46	1.19	1.33
1	Q	122	ARG	CZ-NH2	-10.45	1.19	1.33
2	J	169	GLU	CG-CD	-10.44	1.36	1.51
1	M	122	ARG	CZ-NH2	-10.44	1.19	1.33
1	U	122	ARG	CZ-NH2	-10.43	1.19	1.33
1	G	85	ARG	CZ-NH2	-10.42	1.19	1.33
1	S	122	ARG	CZ-NH1	-10.40	1.19	1.33
1	W	85	ARG	CZ-NH2	-10.39	1.19	1.33
2	H	392	ARG	CZ-NH2	-10.37	1.19	1.33
2	V	169	GLU	CG-CD	-10.34	1.36	1.51
1	E	85	ARG	CZ-NH2	-10.33	1.19	1.33
2	D	392	ARG	CZ-NH2	-10.31	1.19	1.33
2	X	392	ARG	CZ-NH2	-10.31	1.19	1.33
2	H	113	ARG	CZ-NH1	-10.24	1.19	1.33
1	E	122	ARG	CZ-NH2	-10.23	1.19	1.33
2	T	392	ARG	CZ-NH2	-10.19	1.19	1.33
2	P	392	ARG	CZ-NH2	-10.19	1.19	1.33
2	N	169	GLU	CG-CD	-10.18	1.36	1.51
1	O	87	ARG	CZ-NH2	-10.15	1.19	1.33
1	E	122	ARG	CZ-NH1	-10.13	1.19	1.33
2	B	169	GLU	CG-CD	-10.07	1.36	1.51
2	F	381	ARG	CZ-NH1	-10.07	1.20	1.33
2	L	392	ARG	CZ-NH2	-10.06	1.20	1.33
2	R	23	SER	CA-CB	-10.02	1.38	1.52
2	R	169	GLU	CG-CD	-9.98	1.36	1.51
1	Q	122	ARG	CZ-NH1	-9.97	1.20	1.33
1	C	87	ARG	CZ-NH2	-9.97	1.20	1.33
1	I	122	ARG	CZ-NH1	-9.95	1.20	1.33
2	H	164	ARG	CZ-NH1	-9.95	1.20	1.33
2	H	114	ARG	CZ-NH1	-9.94	1.20	1.33
1	M	122	ARG	CZ-NH1	-9.94	1.20	1.33
1	W	87	ARG	CZ-NH2	-9.92	1.20	1.33
1	A	122	ARG	CZ-NH1	-9.91	1.20	1.33
1	U	122	ARG	CZ-NH1	-9.88	1.20	1.33
1	K	87	ARG	CZ-NH2	-9.88	1.20	1.33
1	Q	196	SER	CB-OG	-9.76	1.29	1.42
2	D	114	ARG	CZ-NH1	-9.71	1.20	1.33
2	L	114	ARG	CZ-NH1	-9.65	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	392	ARG	CZ-NH2	-9.63	1.20	1.33
2	R	392	ARG	CZ-NH2	-9.62	1.20	1.33
2	N	392	ARG	CZ-NH2	-9.61	1.20	1.33
2	J	392	ARG	CZ-NH2	-9.54	1.20	1.33
2	X	114	ARG	CZ-NH1	-9.54	1.20	1.33
2	T	114	ARG	CZ-NH1	-9.53	1.20	1.33
2	V	49	ARG	CZ-NH1	-9.53	1.20	1.33
1	S	87	ARG	CZ-NH2	-9.53	1.20	1.33
2	N	49	ARG	CZ-NH1	-9.52	1.20	1.33
1	A	196	SER	CA-CB	-9.50	1.38	1.52
2	H	169	GLU	CG-CD	-9.50	1.37	1.51
2	V	392	ARG	CZ-NH2	-9.48	1.20	1.33
2	R	49	ARG	CZ-NH1	-9.48	1.20	1.33
1	I	196	SER	CB-OG	-9.46	1.29	1.42
2	B	392	ARG	CZ-NH2	-9.44	1.20	1.33
1	E	266	LEU	CB-CG	-9.43	1.25	1.52
2	J	49	ARG	CZ-NH1	-9.37	1.20	1.33
2	P	114	ARG	CZ-NH1	-9.34	1.21	1.33
1	U	196	SER	CA-CB	-9.34	1.39	1.52
2	R	164	ARG	CZ-NH1	-9.29	1.21	1.33
2	B	49	ARG	CZ-NH1	-9.29	1.21	1.33
2	F	49	ARG	CZ-NH1	-9.29	1.21	1.33
1	M	196	SER	CB-OG	-9.28	1.30	1.42
2	J	60	ARG	CD-NE	-9.28	1.30	1.46
1	I	196	SER	CA-CB	-9.27	1.39	1.52
1	Q	196	SER	CA-CB	-9.26	1.39	1.52
2	V	164	ARG	CZ-NH1	-9.24	1.21	1.33
1	A	196	SER	CB-OG	-9.23	1.30	1.42
2	N	60	ARG	CD-NE	-9.22	1.30	1.46
1	U	196	SER	CB-OG	-9.15	1.30	1.42
2	R	60	ARG	CD-NE	-9.05	1.31	1.46
2	F	169	GLU	CD-OE1	-9.03	1.15	1.25
2	B	164	ARG	CZ-NH1	-9.02	1.21	1.33
1	M	196	SER	CA-CB	-8.97	1.39	1.52
2	N	9	THR	N-CA	-8.95	1.28	1.46
2	V	60	ARG	CD-NE	-8.93	1.31	1.46
1	E	196	SER	CA-CB	-8.88	1.39	1.52
2	F	9	THR	N-CA	-8.87	1.28	1.46
2	B	60	ARG	CD-NE	-8.78	1.31	1.46
2	N	164	ARG	CZ-NH1	-8.76	1.21	1.33
2	X	60	ARG	CD-NE	-8.75	1.31	1.46
2	T	60	ARG	CD-NE	-8.75	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	167	GLU	CD-OE2	-8.74	1.16	1.25
2	L	60	ARG	CD-NE	-8.70	1.31	1.46
2	T	49	ARG	CZ-NH1	-8.70	1.21	1.33
2	F	60	ARG	CD-NE	-8.65	1.31	1.46
2	J	9	THR	N-CA	-8.65	1.29	1.46
2	J	164	ARG	CZ-NH1	-8.63	1.21	1.33
2	R	9	THR	N-CA	-8.63	1.29	1.46
2	H	169	GLU	CD-OE1	-8.62	1.16	1.25
2	P	60	ARG	CD-NE	-8.62	1.31	1.46
2	H	49	ARG	CZ-NH1	-8.62	1.21	1.33
2	V	9	THR	N-CA	-8.62	1.29	1.46
2	D	60	ARG	CD-NE	-8.61	1.31	1.46
2	R	169	GLU	CD-OE1	-8.58	1.16	1.25
2	X	49	ARG	CZ-NH1	-8.58	1.22	1.33
1	I	8	GLU	CG-CD	-8.55	1.39	1.51
2	B	9	THR	N-CA	-8.54	1.29	1.46
1	Q	87	ARG	CG-CD	-8.53	1.30	1.51
2	L	113	ARG	NE-CZ	-8.44	1.22	1.33
2	R	113	ARG	CD-NE	-8.42	1.32	1.46
1	U	87	ARG	CB-CG	-8.41	1.29	1.52
2	P	113	ARG	NE-CZ	-8.41	1.22	1.33
2	V	113	ARG	CD-NE	-8.41	1.32	1.46
2	D	49	ARG	CZ-NH1	-8.41	1.22	1.33
1	Q	87	ARG	CB-CG	-8.40	1.29	1.52
1	U	87	ARG	CG-CD	-8.40	1.30	1.51
2	T	113	ARG	NE-CZ	-8.39	1.22	1.33
1	G	196	SER	CA-CB	-8.37	1.40	1.52
2	J	113	ARG	CD-NE	-8.35	1.32	1.46
1	S	196	SER	CA-CB	-8.35	1.40	1.52
2	B	113	ARG	CD-NE	-8.34	1.32	1.46
1	M	87	ARG	CB-CG	-8.32	1.30	1.52
2	N	113	ARG	CD-NE	-8.31	1.32	1.46
2	L	49	ARG	CZ-NH1	-8.29	1.22	1.33
1	K	196	SER	CA-CB	-8.29	1.40	1.52
1	A	87	ARG	CB-CG	-8.27	1.30	1.52
1	I	87	ARG	CB-CG	-8.27	1.30	1.52
2	P	49	ARG	CZ-NH1	-8.26	1.22	1.33
1	A	87	ARG	CG-CD	-8.21	1.31	1.51
1	W	196	SER	CA-CB	-8.21	1.40	1.52
1	Q	8	GLU	CG-CD	-8.17	1.39	1.51
2	X	113	ARG	NE-CZ	-8.16	1.22	1.33
1	E	87	ARG	CB-CG	-8.14	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	196	SER	CA-CB	-8.13	1.40	1.52
2	H	60	ARG	CD-NE	-8.04	1.32	1.46
2	V	169	GLU	CD-OE1	-8.03	1.16	1.25
1	M	8	GLU	CG-CD	-8.01	1.40	1.51
1	M	87	ARG	CG-CD	-7.99	1.31	1.51
2	D	258	PHE	CE2-CZ	-7.97	1.22	1.37
2	F	258	PHE	CE2-CZ	-7.94	1.22	1.37
2	D	113	ARG	NE-CZ	-7.94	1.22	1.33
2	R	258	PHE	CE2-CZ	-7.93	1.22	1.37
1	I	87	ARG	CG-CD	-7.86	1.32	1.51
2	H	113	ARG	NE-CZ	-7.84	1.22	1.33
2	F	113	ARG	CD-NE	-7.84	1.33	1.46
2	X	22	PRO	N-CA	-7.83	1.33	1.47
2	D	258	PHE	CE1-CZ	-7.77	1.22	1.37
1	C	196	SER	CA-CB	-7.77	1.41	1.52
2	X	258	PHE	CE2-CZ	-7.75	1.22	1.37
2	H	258	PHE	CE2-CZ	-7.75	1.22	1.37
1	O	87	ARG	CD-NE	-7.74	1.33	1.46
2	B	169	GLU	CD-OE1	-7.72	1.17	1.25
2	B	258	PHE	CE2-CZ	-7.71	1.22	1.37
1	Q	87	ARG	NE-CZ	-7.70	1.23	1.33
2	X	258	PHE	CE1-CZ	-7.69	1.22	1.37
2	T	258	PHE	CE2-CZ	-7.67	1.22	1.37
2	L	258	PHE	CE2-CZ	-7.67	1.22	1.37
2	H	23	SER	CA-CB	-7.66	1.41	1.52
2	B	258	PHE	CE1-CZ	-7.65	1.22	1.37
1	A	8	GLU	CG-CD	-7.63	1.40	1.51
2	P	258	PHE	CE2-CZ	-7.61	1.22	1.37
2	J	258	PHE	CE2-CZ	-7.59	1.23	1.37
2	R	258	PHE	CE1-CZ	-7.57	1.23	1.37
1	W	87	ARG	CD-NE	-7.56	1.33	1.46
2	H	258	PHE	CE1-CZ	-7.55	1.23	1.37
2	N	258	PHE	CE2-CZ	-7.55	1.23	1.37
2	V	258	PHE	CE2-CZ	-7.52	1.23	1.37
2	H	113	ARG	CD-NE	-7.51	1.33	1.46
1	U	8	GLU	CG-CD	-7.50	1.40	1.51
2	T	258	PHE	CE1-CZ	-7.49	1.23	1.37
2	F	23	SER	CA-C	-7.49	1.33	1.52
1	I	87	ARG	NE-CZ	-7.47	1.23	1.33
2	L	22	PRO	N-CA	-7.47	1.34	1.47
2	F	258	PHE	CE1-CZ	-7.47	1.23	1.37
1	K	87	ARG	CD-NE	-7.46	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	381	ARG	CZ-NH2	-7.45	1.23	1.33
2	P	22	PRO	N-CA	-7.45	1.34	1.47
1	C	87	ARG	CD-NE	-7.43	1.33	1.46
2	T	113	ARG	CD-NE	-7.43	1.33	1.46
2	N	381	ARG	CZ-NH2	-7.42	1.23	1.33
2	B	169	GLU	CD-OE2	-7.39	1.17	1.25
2	X	113	ARG	CD-NE	-7.38	1.33	1.46
2	J	9	THR	CA-CB	-7.38	1.34	1.53
2	D	22	PRO	N-CA	-7.36	1.34	1.47
1	S	87	ARG	CD-NE	-7.36	1.33	1.46
2	B	381	ARG	CZ-NH2	-7.35	1.23	1.33
2	N	258	PHE	CE1-CZ	-7.33	1.23	1.37
2	L	113	ARG	CD-NE	-7.33	1.33	1.46
2	T	169	GLU	CG-CD	-7.30	1.41	1.51
2	P	258	PHE	CE1-CZ	-7.28	1.23	1.37
2	V	381	ARG	CZ-NH2	-7.26	1.23	1.33
2	J	258	PHE	CE1-CZ	-7.25	1.23	1.37
2	P	113	ARG	CD-NE	-7.25	1.34	1.46
2	L	258	PHE	CE1-CZ	-7.24	1.23	1.37
2	N	9	THR	CA-CB	-7.24	1.34	1.53
1	M	87	ARG	NE-CZ	-7.22	1.23	1.33
2	V	258	PHE	CE1-CZ	-7.22	1.23	1.37
2	B	113	ARG	NE-CZ	-7.22	1.23	1.33
1	K	196	SER	CB-OG	-7.21	1.32	1.42
2	R	113	ARG	CZ-NH1	-7.21	1.23	1.33
2	H	9	THR	CA-CB	-7.18	1.34	1.53
2	N	113	ARG	NE-CZ	-7.18	1.23	1.33
2	R	9	THR	CA-CB	-7.17	1.34	1.53
2	T	22	PRO	N-CA	-7.15	1.35	1.47
2	R	113	ARG	NE-CZ	-7.15	1.23	1.33
2	V	9	THR	CA-CB	-7.14	1.34	1.53
2	J	169	GLU	CD-OE2	-7.14	1.17	1.25
1	U	87	ARG	NE-CZ	-7.12	1.23	1.33
2	B	113	ARG	CZ-NH1	-7.11	1.23	1.33
2	D	113	ARG	CD-NE	-7.10	1.34	1.46
2	J	113	ARG	NE-CZ	-7.09	1.23	1.33
1	E	196	SER	N-CA	-7.08	1.32	1.46
2	F	9	THR	CA-CB	-7.07	1.34	1.53
2	L	9	THR	CA-CB	-7.07	1.34	1.53
2	B	9	THR	CA-CB	-7.03	1.35	1.53
1	A	87	ARG	NE-CZ	-7.01	1.24	1.33
1	I	266	LEU	CB-CG	-6.99	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	9	THR	CB-CG2	-6.99	1.29	1.52
2	V	113	ARG	NE-CZ	-6.98	1.24	1.33
1	Q	266	LEU	CB-CG	-6.97	1.32	1.52
2	N	113	ARG	CZ-NH1	-6.97	1.24	1.33
1	U	221	ARG	CD-NE	-6.95	1.34	1.46
1	A	221	ARG	CD-NE	-6.95	1.34	1.46
1	O	196	SER	CB-OG	-6.95	1.33	1.42
2	L	169	GLU	CB-CG	-6.93	1.39	1.52
2	D	169	GLU	CG-CD	-6.90	1.41	1.51
1	I	221	ARG	CD-NE	-6.90	1.34	1.46
1	M	221	ARG	CD-NE	-6.88	1.34	1.46
2	L	9	THR	CB-CG2	-6.88	1.29	1.52
1	I	196	SER	N-CA	-6.87	1.32	1.46
1	E	221	ARG	CD-NE	-6.87	1.34	1.46
2	T	9	THR	CB-CG2	-6.86	1.29	1.52
1	A	196	SER	N-CA	-6.86	1.32	1.46
1	U	196	SER	N-CA	-6.86	1.32	1.46
2	F	113	ARG	NE-CZ	-6.85	1.24	1.33
2	X	9	THR	CA-CB	-6.84	1.35	1.53
2	T	9	THR	CA-CB	-6.82	1.35	1.53
1	S	196	SER	CB-OG	-6.81	1.33	1.42
1	Q	221	ARG	CD-NE	-6.80	1.34	1.46
1	G	196	SER	CB-OG	-6.80	1.33	1.42
1	W	196	SER	CB-OG	-6.80	1.33	1.42
2	H	9	THR	N-CA	-6.79	1.32	1.46
2	P	9	THR	N-CA	-6.79	1.32	1.46
2	D	9	THR	CB-CG2	-6.78	1.29	1.52
2	V	113	ARG	CZ-NH1	-6.77	1.24	1.33
2	N	169	GLU	CD-OE2	-6.77	1.18	1.25
2	P	9	THR	CA-CB	-6.74	1.35	1.53
2	D	9	THR	CA-CB	-6.72	1.35	1.53
2	P	169	GLU	CB-CG	-6.72	1.39	1.52
1	M	266	LEU	CB-CG	-6.72	1.33	1.52
2	T	164	ARG	CZ-NH1	-6.72	1.24	1.33
1	G	196	SER	N-CA	-6.70	1.32	1.46
2	X	9	THR	N-CA	-6.69	1.32	1.46
2	T	9	THR	N-CA	-6.68	1.32	1.46
2	J	169	GLU	CB-CG	-6.68	1.39	1.52
2	V	169	GLU	CB-CG	-6.64	1.39	1.52
2	F	52	GLN	CG-CD	-6.64	1.35	1.51
2	L	9	THR	N-CA	-6.64	1.33	1.46
2	X	169	GLU	CG-CD	-6.61	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	113	ARG	CZ-NH1	-6.60	1.24	1.33
2	L	164	ARG	CZ-NH1	-6.60	1.24	1.33
2	T	169	GLU	CB-CG	-6.58	1.39	1.52
2	D	169	GLU	CB-CG	-6.58	1.39	1.52
2	N	169	GLU	CD-OE1	-6.58	1.18	1.25
1	G	8	GLU	CB-CG	-6.57	1.39	1.52
2	J	169	GLU	CD-OE1	-6.57	1.18	1.25
2	D	9	THR	N-CA	-6.55	1.33	1.46
2	X	169	GLU	CB-CG	-6.55	1.39	1.52
1	G	167	GLU	CD-OE1	6.55	1.32	1.25
2	R	23	SER	CA-C	-6.52	1.35	1.52
1	S	248	GLU	CD-OE2	-6.51	1.18	1.25
2	L	169	GLU	CG-CD	-6.51	1.42	1.51
2	T	23	SER	CA-C	-6.49	1.36	1.52
2	F	225	GLU	CD-OE1	-6.49	1.18	1.25
1	S	196	SER	N-CA	-6.48	1.33	1.46
1	Q	8	GLU	CD-OE2	-6.47	1.18	1.25
2	N	169	GLU	CB-CG	-6.46	1.39	1.52
1	K	196	SER	N-CA	-6.46	1.33	1.46
2	H	9	THR	CB-CG2	-6.45	1.31	1.52
2	N	52	GLN	CG-CD	-6.45	1.36	1.51
1	Q	196	SER	N-CA	-6.44	1.33	1.46
2	P	164	ARG	CZ-NH1	-6.42	1.24	1.33
2	X	9	THR	CB-CG2	-6.42	1.31	1.52
2	D	164	ARG	CZ-NH1	-6.41	1.24	1.33
2	X	164	ARG	CZ-NH1	-6.41	1.24	1.33
1	O	196	SER	N-CA	-6.40	1.33	1.46
1	W	196	SER	N-CA	-6.39	1.33	1.46
2	R	52	GLN	CG-CD	-6.38	1.36	1.51
2	V	23	SER	CA-C	-6.38	1.36	1.52
2	B	52	GLN	CG-CD	-6.36	1.36	1.51
2	B	225	GLU	CD-OE1	-6.35	1.18	1.25
2	J	52	GLN	CG-CD	-6.32	1.36	1.51
1	M	196	SER	N-CA	-6.31	1.33	1.46
2	F	169	GLU	CB-CG	-6.31	1.40	1.52
2	N	23	SER	CA-C	-6.30	1.36	1.52
2	H	169	GLU	CB-CG	-6.29	1.40	1.52
2	R	169	GLU	CB-CG	-6.28	1.40	1.52
1	C	196	SER	CB-OG	-6.28	1.34	1.42
1	M	77	GLU	CD-OE2	-6.27	1.18	1.25
1	A	266	LEU	CB-CG	-6.25	1.34	1.52
2	P	169	GLU	CG-CD	-6.23	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	52	GLN	CG-CD	-6.23	1.36	1.51
2	B	169	GLU	CB-CG	-6.22	1.40	1.52
2	B	381	ARG	CD-NE	-6.21	1.35	1.46
2	B	23	SER	CA-C	-6.20	1.36	1.52
2	H	169	GLU	CD-OE2	-6.19	1.18	1.25
1	C	196	SER	N-CA	-6.19	1.33	1.46
1	G	266	LEU	CA-C	-6.19	1.36	1.52
2	H	225	GLU	CD-OE2	-6.18	1.18	1.25
2	X	225	GLU	CD-OE2	-6.17	1.18	1.25
2	T	225	GLU	CD-OE2	-6.15	1.18	1.25
2	R	381	ARG	CZ-NH2	-6.13	1.25	1.33
2	J	381	ARG	CD-NE	-6.11	1.36	1.46
2	T	225	GLU	CD-OE1	-6.11	1.19	1.25
2	N	381	ARG	CD-NE	-6.09	1.36	1.46
2	J	23	SER	CA-C	-6.09	1.37	1.52
1	S	8	GLU	CB-CG	-6.09	1.40	1.52
1	S	248	GLU	CD-OE1	-6.08	1.19	1.25
1	A	248	GLU	CD-OE2	-6.08	1.19	1.25
1	U	266	LEU	CB-CG	-6.08	1.34	1.52
1	G	87	ARG	CZ-NH2	-6.07	1.25	1.33
2	D	225	GLU	CD-OE2	-6.07	1.19	1.25
2	H	225	GLU	CD-OE1	-6.06	1.19	1.25
2	P	225	GLU	CD-OE2	-6.05	1.19	1.25
2	H	23	SER	N-CA	-6.01	1.34	1.46
2	V	381	ARG	CD-NE	-6.00	1.36	1.46
1	E	248	GLU	CD-OE2	-5.98	1.19	1.25
1	U	77	GLU	CD-OE2	-5.98	1.19	1.25
1	U	248	GLU	CD-OE1	-5.98	1.19	1.25
2	V	40	GLU	CD-OE1	-5.98	1.19	1.25
1	G	74	ARG	CG-CD	-5.98	1.37	1.51
2	N	225	GLU	CD-OE1	-5.96	1.19	1.25
1	M	248	GLU	CD-OE1	-5.96	1.19	1.25
2	X	225	GLU	CD-OE1	-5.96	1.19	1.25
1	U	248	GLU	CD-OE2	-5.95	1.19	1.25
1	E	77	GLU	CD-OE2	-5.95	1.19	1.25
2	R	225	GLU	CD-OE1	-5.95	1.19	1.25
1	K	248	GLU	CD-OE2	-5.94	1.19	1.25
2	T	52	GLN	CG-CD	-5.94	1.37	1.51
1	Q	77	GLU	CD-OE2	-5.93	1.19	1.25
2	F	40	GLU	CD-OE1	-5.92	1.19	1.25
2	L	22	PRO	C-O	-5.92	1.11	1.23
1	I	248	GLU	CD-OE2	-5.92	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	22	PRO	C-O	-5.91	1.11	1.23
2	J	225	GLU	CD-OE1	-5.90	1.19	1.25
2	V	225	GLU	CD-OE1	-5.88	1.19	1.25
2	R	381	ARG	CD-NE	-5.88	1.36	1.46
2	V	169	GLU	CD-OE2	-5.88	1.19	1.25
1	W	248	GLU	CD-OE1	-5.87	1.19	1.25
2	F	225	GLU	CD-OE2	-5.86	1.19	1.25
1	Q	87	ARG	CZ-NH1	-5.86	1.25	1.33
2	L	225	GLU	CD-OE2	-5.86	1.19	1.25
2	D	225	GLU	CD-OE1	-5.85	1.19	1.25
2	V	40	GLU	CD-OE2	-5.85	1.19	1.25
1	W	248	GLU	CD-OE2	-5.85	1.19	1.25
2	P	225	GLU	CD-OE1	-5.84	1.19	1.25
2	X	52	GLN	CG-CD	-5.84	1.37	1.51
1	I	77	GLU	CD-OE2	-5.84	1.19	1.25
2	J	40	GLU	CD-OE2	-5.84	1.19	1.25
1	O	74	ARG	CG-CD	-5.84	1.37	1.51
2	F	164	ARG	CZ-NH1	-5.83	1.25	1.33
2	L	52	GLN	CG-CD	-5.83	1.37	1.51
1	C	248	GLU	CD-OE1	-5.82	1.19	1.25
1	E	248	GLU	CD-OE1	-5.81	1.19	1.25
2	D	52	GLN	CG-CD	-5.80	1.37	1.51
1	O	248	GLU	CD-OE2	-5.80	1.19	1.25
1	M	266	LEU	CA-CB	-5.80	1.40	1.53
1	G	248	GLU	CD-OE2	-5.80	1.19	1.25
1	O	248	GLU	CD-OE1	-5.80	1.19	1.25
2	F	40	GLU	CD-OE2	-5.79	1.19	1.25
1	E	87	ARG	CG-CD	-5.78	1.37	1.51
1	W	74	ARG	CZ-NH1	-5.78	1.25	1.33
2	P	52	GLN	CG-CD	-5.77	1.37	1.51
1	G	87	ARG	CG-CD	-5.77	1.37	1.51
1	Q	248	GLU	CD-OE1	-5.77	1.19	1.25
1	K	74	ARG	CZ-NH2	-5.77	1.25	1.33
1	Q	248	GLU	CD-OE2	-5.77	1.19	1.25
2	H	40	GLU	CD-OE1	-5.76	1.19	1.25
1	G	248	GLU	CD-OE1	-5.75	1.19	1.25
2	V	225	GLU	CD-OE2	-5.75	1.19	1.25
1	K	74	ARG	CG-CD	-5.75	1.37	1.51
2	P	23	SER	CA-C	-5.73	1.38	1.52
2	R	40	GLU	CD-OE2	-5.73	1.19	1.25
1	I	266	LEU	CA-CB	-5.73	1.40	1.53
1	S	74	ARG	CG-CD	-5.73	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	40	GLU	CD-OE2	-5.72	1.19	1.25
2	J	225	GLU	CD-OE2	-5.72	1.19	1.25
2	L	225	GLU	CD-OE1	-5.72	1.19	1.25
1	A	184	SER	CB-OG	-5.72	1.34	1.42
2	P	40	GLU	CD-OE1	-5.71	1.19	1.25
2	R	404	PHE	C-N	5.71	1.43	1.33
2	L	40	GLU	CD-OE1	-5.71	1.19	1.25
2	J	40	GLU	CD-OE1	-5.70	1.19	1.25
1	C	223	ARG	CD-NE	-5.70	1.36	1.46
2	B	40	GLU	CD-OE2	-5.68	1.19	1.25
1	A	248	GLU	CD-OE1	-5.67	1.19	1.25
1	I	248	GLU	CD-OE1	-5.67	1.19	1.25
1	A	266	LEU	CA-CB	-5.65	1.40	1.53
1	K	248	GLU	CD-OE1	-5.65	1.19	1.25
2	X	40	GLU	CD-OE1	-5.64	1.19	1.25
2	J	23	SER	CB-OG	-5.63	1.34	1.42
2	B	225	GLU	CD-OE2	-5.62	1.19	1.25
1	U	266	LEU	CA-CB	-5.62	1.40	1.53
1	W	74	ARG	CG-CD	-5.62	1.37	1.51
1	A	77	GLU	CD-OE2	-5.62	1.19	1.25
1	C	248	GLU	CD-OE2	-5.62	1.19	1.25
2	L	23	SER	CA-C	-5.62	1.38	1.52
1	S	74	ARG	CZ-NH1	-5.62	1.25	1.33
2	H	40	GLU	CD-OE2	-5.61	1.19	1.25
2	B	40	GLU	CD-OE1	-5.61	1.19	1.25
1	M	248	GLU	CD-OE2	-5.61	1.19	1.25
2	N	40	GLU	CD-OE2	-5.61	1.19	1.25
2	P	40	GLU	CD-OE2	-5.58	1.19	1.25
1	A	184	SER	CA-CB	-5.57	1.44	1.52
2	F	407	LEU	C-O	5.57	1.33	1.23
2	T	22	PRO	C-O	-5.56	1.12	1.23
1	O	74	ARG	CZ-NH2	-5.56	1.25	1.33
1	C	74	ARG	CG-CD	-5.56	1.38	1.51
2	R	40	GLU	CD-OE1	-5.55	1.19	1.25
2	N	225	GLU	CD-OE2	-5.55	1.19	1.25
2	H	381	ARG	CD-NE	-5.54	1.37	1.46
2	L	40	GLU	CD-OE2	-5.51	1.19	1.25
2	T	40	GLU	CD-OE2	-5.49	1.19	1.25
1	W	223	ARG	CD-NE	-5.48	1.37	1.46
1	M	77	GLU	CD-OE1	-5.45	1.19	1.25
1	G	167	GLU	CG-CD	-5.44	1.43	1.51
2	N	40	GLU	CD-OE1	-5.44	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	225	GLU	CD-OE2	-5.43	1.19	1.25
2	H	52	GLN	CG-CD	-5.40	1.38	1.51
2	F	381	ARG	CD-NE	-5.39	1.37	1.46
2	X	23	SER	CA-C	-5.38	1.39	1.52
1	Q	223	ARG	CD-NE	-5.37	1.37	1.46
1	C	74	ARG	CZ-NH1	-5.37	1.26	1.33
2	T	381	ARG	CD-NE	-5.36	1.37	1.46
2	T	40	GLU	CD-OE1	-5.36	1.19	1.25
1	C	77	GLU	CD-OE2	-5.35	1.19	1.25
1	S	77	GLU	CD-OE2	-5.35	1.19	1.25
2	D	40	GLU	CD-OE2	-5.34	1.19	1.25
1	G	77	GLU	CD-OE1	-5.31	1.19	1.25
1	G	77	GLU	CD-OE2	-5.29	1.19	1.25
1	E	223	ARG	CD-NE	-5.29	1.37	1.46
2	D	40	GLU	CD-OE1	-5.29	1.19	1.25
1	U	8	GLU	CD-OE2	-5.29	1.19	1.25
1	E	87	ARG	CZ-NH1	-5.28	1.26	1.33
1	K	77	GLU	CD-OE2	-5.28	1.19	1.25
1	O	74	ARG	CZ-NH1	-5.27	1.26	1.33
1	M	223	ARG	CD-NE	-5.26	1.37	1.46
1	C	77	GLU	CD-OE1	-5.26	1.19	1.25
1	E	196	SER	CB-OG	-5.23	1.35	1.42
2	P	381	ARG	CD-NE	-5.23	1.37	1.46
1	K	223	ARG	CD-NE	-5.23	1.37	1.46
1	S	223	ARG	CD-NE	-5.23	1.37	1.46
2	L	381	ARG	CD-NE	-5.22	1.37	1.46
1	K	74	ARG	CZ-NH1	-5.20	1.26	1.33
2	D	23	SER	CA-C	-5.20	1.39	1.52
2	P	22	PRO	C-N	-5.17	1.22	1.34
2	L	22	PRO	C-N	-5.17	1.22	1.34
1	G	8	GLU	CA-CB	-5.17	1.42	1.53
1	G	87	ARG	NE-CZ	-5.15	1.26	1.33
2	D	381	ARG	CD-NE	-5.14	1.37	1.46
1	O	87	ARG	CB-CG	-5.14	1.38	1.52
1	K	87	ARG	CB-CG	-5.14	1.38	1.52
1	C	87	ARG	CB-CG	-5.14	1.38	1.52
1	A	223	ARG	CD-NE	-5.13	1.37	1.46
2	T	52	GLN	CD-NE2	-5.13	1.20	1.32
2	B	196	ASP	CB-CG	-5.13	1.41	1.51
2	X	381	ARG	CD-NE	-5.13	1.37	1.46
2	P	52	GLN	CD-NE2	-5.13	1.20	1.32
2	F	196	ASP	CB-CG	-5.12	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	223	ARG	CD-NE	-5.12	1.37	1.46
1	W	87	ARG	CB-CG	-5.12	1.38	1.52
1	U	77	GLU	CD-OE1	-5.11	1.20	1.25
1	G	87	ARG	CB-CG	-5.11	1.38	1.52
1	K	77	GLU	CD-OE1	-5.09	1.20	1.25
1	O	8	GLU	CA-CB	-5.09	1.42	1.53
2	X	22	PRO	C-N	-5.09	1.22	1.34
1	I	87	ARG	CZ-NH1	-5.08	1.26	1.33
1	S	167	GLU	CB-CG	-5.08	1.42	1.52
1	S	87	ARG	CB-CG	-5.07	1.38	1.52
2	R	169	GLU	CD-OE2	-5.06	1.20	1.25
1	U	223	ARG	CD-NE	-5.06	1.37	1.46
1	K	8	GLU	CA-CB	-5.02	1.43	1.53
2	V	196	ASP	CB-CG	-5.02	1.41	1.51
2	X	22	PRO	C-O	-5.02	1.13	1.23
1	Q	266	LEU	CA-CB	-5.01	1.42	1.53
1	W	77	GLU	CD-OE2	-5.00	1.20	1.25
1	A	77	GLU	CD-OE1	-5.00	1.20	1.25

All (834) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	221	ARG	NE-CZ-NH1	28.37	134.49	120.30
1	M	221	ARG	NE-CZ-NH1	28.25	134.43	120.30
1	Q	221	ARG	NE-CZ-NH1	28.08	134.34	120.30
1	I	221	ARG	NE-CZ-NH1	28.03	134.32	120.30
1	A	221	ARG	NE-CZ-NH1	28.02	134.31	120.30
1	U	221	ARG	NE-CZ-NH1	27.97	134.28	120.30
1	E	221	ARG	NE-CZ-NH2	-26.07	107.27	120.30
1	M	221	ARG	NE-CZ-NH2	-25.75	107.43	120.30
1	U	221	ARG	NE-CZ-NH2	-25.63	107.48	120.30
1	I	221	ARG	NE-CZ-NH2	-25.45	107.58	120.30
1	A	221	ARG	NE-CZ-NH2	-25.41	107.59	120.30
1	Q	221	ARG	NE-CZ-NH2	-25.37	107.61	120.30
2	H	164	ARG	NE-CZ-NH2	24.85	132.72	120.30
1	G	221	ARG	NE-CZ-NH1	24.78	132.69	120.30
1	S	221	ARG	NE-CZ-NH1	24.64	132.62	120.30
1	W	221	ARG	NE-CZ-NH1	24.37	132.49	120.30
1	K	221	ARG	NE-CZ-NH1	24.22	132.41	120.30
1	O	221	ARG	NE-CZ-NH1	23.84	132.22	120.30
1	C	221	ARG	NE-CZ-NH1	23.70	132.15	120.30
1	G	221	ARG	NE-CZ-NH2	-22.14	109.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	221	ARG	NE-CZ-NH2	-21.96	109.32	120.30
1	S	221	ARG	NE-CZ-NH2	-21.94	109.33	120.30
1	O	221	ARG	NE-CZ-NH2	-21.67	109.46	120.30
2	P	49	ARG	NE-CZ-NH1	21.27	130.94	120.30
1	W	221	ARG	NE-CZ-NH2	-21.16	109.72	120.30
2	L	49	ARG	NE-CZ-NH1	21.11	130.85	120.30
2	X	49	ARG	NE-CZ-NH1	21.05	130.82	120.30
1	C	221	ARG	NE-CZ-NH2	-21.02	109.79	120.30
2	H	49	ARG	NE-CZ-NH1	21.02	130.81	120.30
2	D	49	ARG	NE-CZ-NH1	20.97	130.78	120.30
2	T	49	ARG	NE-CZ-NH1	20.66	130.63	120.30
1	S	252	ARG	NE-CZ-NH2	19.68	130.14	120.30
2	B	392	ARG	NE-CZ-NH2	19.47	130.04	120.30
2	N	392	ARG	NE-CZ-NH2	19.22	129.91	120.30
2	R	392	ARG	NE-CZ-NH2	19.13	129.87	120.30
2	V	392	ARG	NE-CZ-NH2	19.04	129.82	120.30
2	J	392	ARG	NE-CZ-NH2	18.98	129.79	120.30
2	N	49	ARG	NE-CZ-NH1	18.95	129.78	120.30
2	N	280	ARG	NE-CZ-NH1	18.95	129.77	120.30
2	V	49	ARG	NE-CZ-NH1	18.91	129.75	120.30
2	B	49	ARG	NE-CZ-NH1	18.78	129.69	120.30
2	T	280	ARG	NE-CZ-NH1	18.75	129.68	120.30
2	J	49	ARG	NE-CZ-NH1	18.72	129.66	120.30
2	F	392	ARG	NE-CZ-NH2	18.71	129.66	120.30
2	H	280	ARG	NE-CZ-NH1	18.62	129.61	120.30
2	B	280	ARG	NE-CZ-NH1	18.57	129.59	120.30
2	R	49	ARG	NE-CZ-NH1	18.57	129.58	120.30
2	P	280	ARG	NE-CZ-NH1	18.47	129.53	120.30
2	L	280	ARG	NE-CZ-NH1	18.45	129.53	120.30
2	V	280	ARG	NE-CZ-NH1	18.38	129.49	120.30
2	J	280	ARG	NE-CZ-NH1	18.37	129.48	120.30
2	X	280	ARG	NE-CZ-NH1	18.35	129.47	120.30
2	R	280	ARG	NE-CZ-NH1	18.29	129.44	120.30
2	F	49	ARG	NE-CZ-NH1	18.11	129.35	120.30
2	F	280	ARG	NE-CZ-NH1	18.11	129.35	120.30
2	D	280	ARG	NE-CZ-NH1	18.08	129.34	120.30
1	E	252	ARG	NE-CZ-NH2	17.69	129.15	120.30
2	L	114	ARG	NE-CZ-NH1	17.39	129.00	120.30
1	O	252	ARG	NE-CZ-NH2	17.34	128.97	120.30
1	M	252	ARG	NE-CZ-NH2	17.29	128.95	120.30
2	P	114	ARG	NE-CZ-NH1	17.26	128.93	120.30
1	U	252	ARG	NE-CZ-NH2	17.26	128.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	114	ARG	NE-CZ-NH1	17.23	128.91	120.30
2	T	114	ARG	NE-CZ-NH1	17.18	128.89	120.30
1	K	252	ARG	NE-CZ-NH2	17.16	128.88	120.30
2	X	114	ARG	NE-CZ-NH1	17.16	128.88	120.30
1	C	252	ARG	NE-CZ-NH2	17.14	128.87	120.30
1	W	252	ARG	NE-CZ-NH2	17.14	128.87	120.30
2	H	114	ARG	NE-CZ-NH1	17.07	128.83	120.30
1	A	252	ARG	NE-CZ-NH2	17.04	128.82	120.30
1	I	252	ARG	NE-CZ-NH2	17.00	128.80	120.30
1	Q	252	ARG	NE-CZ-NH2	16.99	128.80	120.30
1	E	122	ARG	NE-CZ-NH1	16.93	128.76	120.30
1	I	122	ARG	NE-CZ-NH1	16.85	128.73	120.30
1	A	122	ARG	NE-CZ-NH1	16.84	128.72	120.30
1	Q	122	ARG	NE-CZ-NH1	16.80	128.70	120.30
1	U	122	ARG	NE-CZ-NH1	16.72	128.66	120.30
1	C	85	ARG	NE-CZ-NH2	16.70	128.65	120.30
1	M	122	ARG	NE-CZ-NH1	16.70	128.65	120.30
1	G	252	ARG	NE-CZ-NH2	16.57	128.58	120.30
1	W	85	ARG	NE-CZ-NH2	16.43	128.51	120.30
1	K	85	ARG	NE-CZ-NH2	16.41	128.50	120.30
1	O	85	ARG	NE-CZ-NH2	16.41	128.50	120.30
1	G	85	ARG	NE-CZ-NH2	16.33	128.46	120.30
1	S	85	ARG	NE-CZ-NH2	16.27	128.44	120.30
1	E	87	ARG	NE-CZ-NH1	-16.14	112.23	120.30
1	G	265	ARG	NE-CZ-NH1	15.75	128.18	120.30
2	B	28	ARG	NE-CZ-NH1	15.60	128.10	120.30
1	O	265	ARG	NE-CZ-NH1	15.60	128.10	120.30
2	R	28	ARG	NE-CZ-NH1	15.51	128.06	120.30
1	C	265	ARG	NE-CZ-NH1	15.44	128.02	120.30
2	V	28	ARG	NE-CZ-NH1	15.41	128.01	120.30
2	F	28	ARG	NE-CZ-NH1	15.33	127.97	120.30
1	S	265	ARG	NE-CZ-NH1	15.31	127.96	120.30
1	M	265	ARG	NE-CZ-NH2	15.30	127.95	120.30
2	J	28	ARG	NE-CZ-NH1	15.29	127.94	120.30
1	K	265	ARG	NE-CZ-NH1	15.24	127.92	120.30
2	N	28	ARG	NE-CZ-NH1	15.23	127.92	120.30
1	Q	87	ARG	NE-CZ-NH1	-15.23	112.69	120.30
1	W	265	ARG	NE-CZ-NH1	15.18	127.89	120.30
1	A	265	ARG	NE-CZ-NH2	14.94	127.77	120.30
1	Q	265	ARG	NE-CZ-NH2	14.76	127.68	120.30
1	U	265	ARG	NE-CZ-NH2	14.67	127.63	120.30
1	I	265	ARG	NE-CZ-NH2	14.64	127.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	91	ARG	NE-CZ-NH1	14.60	127.60	120.30
2	D	91	ARG	NE-CZ-NH2	14.55	127.58	120.30
2	X	91	ARG	NE-CZ-NH2	14.53	127.57	120.30
2	L	392	ARG	NE-CZ-NH2	14.53	127.56	120.30
1	E	265	ARG	NE-CZ-NH2	14.52	127.56	120.30
2	T	91	ARG	NE-CZ-NH2	14.50	127.55	120.30
2	H	392	ARG	NE-CZ-NH2	14.48	127.54	120.30
1	U	223	ARG	NE-CZ-NH2	-14.41	113.09	120.30
1	A	223	ARG	NE-CZ-NH2	-14.33	113.13	120.30
2	P	91	ARG	NE-CZ-NH2	14.33	127.46	120.30
2	L	155	ARG	NE-CZ-NH2	14.32	127.46	120.30
2	P	155	ARG	NE-CZ-NH2	14.24	127.42	120.30
2	T	155	ARG	NE-CZ-NH2	14.24	127.42	120.30
2	L	91	ARG	NE-CZ-NH2	14.20	127.40	120.30
1	U	85	ARG	NE-CZ-NH1	14.16	127.38	120.30
2	X	392	ARG	NE-CZ-NH2	14.15	127.38	120.30
2	P	392	ARG	NE-CZ-NH2	14.15	127.38	120.30
2	D	392	ARG	NE-CZ-NH2	14.14	127.37	120.30
1	M	85	ARG	NE-CZ-NH1	14.14	127.37	120.30
2	D	155	ARG	NE-CZ-NH2	14.12	127.36	120.30
1	E	223	ARG	NE-CZ-NH2	-14.10	113.25	120.30
2	F	155	ARG	NE-CZ-NH1	14.09	127.34	120.30
2	T	392	ARG	NE-CZ-NH2	14.06	127.33	120.30
2	X	155	ARG	NE-CZ-NH2	14.03	127.32	120.30
1	G	122	ARG	NE-CZ-NH2	14.03	127.31	120.30
1	A	85	ARG	NE-CZ-NH1	14.02	127.31	120.30
2	R	91	ARG	NE-CZ-NH1	14.02	127.31	120.30
1	W	122	ARG	NE-CZ-NH2	13.99	127.30	120.30
1	I	223	ARG	NE-CZ-NH2	-13.94	113.33	120.30
1	I	85	ARG	NE-CZ-NH1	13.94	127.27	120.30
2	V	164	ARG	NE-CZ-NH1	-13.93	113.33	120.30
2	T	164	ARG	NE-CZ-NH1	-13.91	113.35	120.30
2	J	155	ARG	NE-CZ-NH1	13.88	127.24	120.30
1	E	85	ARG	NE-CZ-NH1	13.88	127.24	120.30
2	H	155	ARG	NE-CZ-NH2	13.87	127.23	120.30
1	Q	85	ARG	NE-CZ-NH1	13.87	127.23	120.30
2	H	91	ARG	NE-CZ-NH2	13.86	127.23	120.30
2	V	91	ARG	NE-CZ-NH1	13.83	127.21	120.30
2	J	91	ARG	NE-CZ-NH1	13.80	127.20	120.30
2	H	28	ARG	NE-CZ-NH1	13.78	127.19	120.30
2	F	114	ARG	NE-CZ-NH2	13.76	127.18	120.30
2	B	164	ARG	NE-CZ-NH1	-13.71	113.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	91	ARG	NE-CZ-NH1	13.70	127.15	120.30
1	M	223	ARG	NE-CZ-NH2	-13.69	113.45	120.30
2	V	155	ARG	NE-CZ-NH1	13.68	127.14	120.30
2	X	164	ARG	NE-CZ-NH1	-13.68	113.46	120.30
2	H	164	ARG	NE-CZ-NH1	-13.67	113.47	120.30
1	K	122	ARG	NE-CZ-NH2	13.66	127.13	120.30
2	R	155	ARG	NE-CZ-NH1	13.65	127.12	120.30
2	T	164	ARG	NE-CZ-NH2	13.65	127.12	120.30
1	S	122	ARG	NE-CZ-NH2	13.60	127.10	120.30
2	P	28	ARG	NE-CZ-NH1	13.55	127.08	120.30
1	O	122	ARG	NE-CZ-NH2	13.54	127.07	120.30
1	C	122	ARG	NE-CZ-NH2	13.49	127.05	120.30
2	T	407	LEU	CB-CG-CD1	-13.46	88.11	111.00
2	R	114	ARG	NE-CZ-NH2	13.45	127.02	120.30
2	X	164	ARG	NE-CZ-NH2	13.44	127.02	120.30
2	P	407	LEU	CB-CG-CD1	-13.43	88.17	111.00
2	B	91	ARG	NE-CZ-NH1	13.43	127.01	120.30
2	B	114	ARG	NE-CZ-NH2	13.37	126.98	120.30
2	N	155	ARG	NE-CZ-NH1	13.37	126.98	120.30
2	B	155	ARG	NE-CZ-NH1	13.37	126.98	120.30
2	L	28	ARG	NE-CZ-NH2	13.36	126.98	120.30
2	V	114	ARG	NE-CZ-NH2	13.35	126.98	120.30
2	T	28	ARG	NE-CZ-NH1	13.33	126.97	120.30
2	X	407	LEU	CB-CG-CD1	-13.31	88.37	111.00
2	D	164	ARG	NE-CZ-NH1	-13.31	113.65	120.30
2	N	114	ARG	NE-CZ-NH2	13.31	126.95	120.30
2	H	28	ARG	NE-CZ-NH2	13.27	126.94	120.30
2	R	164	ARG	NE-CZ-NH1	-13.27	113.67	120.30
1	C	87	ARG	NE-CZ-NH2	-13.22	113.69	120.30
2	P	28	ARG	NE-CZ-NH2	13.21	126.91	120.30
1	O	87	ARG	NE-CZ-NH2	-13.21	113.70	120.30
2	L	407	LEU	CB-CG-CD1	-13.20	88.56	111.00
2	X	28	ARG	NE-CZ-NH1	13.18	126.89	120.30
2	J	114	ARG	NE-CZ-NH2	13.15	126.88	120.30
2	D	28	ARG	NE-CZ-NH1	13.14	126.87	120.30
2	X	28	ARG	NE-CZ-NH2	13.11	126.86	120.30
1	I	87	ARG	NE-CZ-NH1	-13.09	113.76	120.30
2	L	28	ARG	NE-CZ-NH1	13.09	126.84	120.30
2	D	407	LEU	CB-CG-CD1	-12.93	89.01	111.00
2	D	164	ARG	NE-CZ-NH2	12.93	126.76	120.30
1	W	87	ARG	NE-CZ-NH2	-12.92	113.84	120.30
2	D	28	ARG	NE-CZ-NH2	12.88	126.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	87	ARG	NE-CZ-NH2	-12.85	113.88	120.30
2	T	28	ARG	NE-CZ-NH2	12.80	126.70	120.30
2	L	164	ARG	NE-CZ-NH1	-12.80	113.90	120.30
1	S	87	ARG	NE-CZ-NH2	-12.76	113.92	120.30
2	L	164	ARG	NE-CZ-NH2	12.75	126.67	120.30
2	P	164	ARG	NE-CZ-NH1	-12.74	113.93	120.30
2	P	164	ARG	NE-CZ-NH2	12.68	126.64	120.30
1	M	87	ARG	NE-CZ-NH1	-12.61	113.99	120.30
2	J	164	ARG	NE-CZ-NH1	-12.59	114.00	120.30
1	S	223	ARG	NE-CZ-NH1	-12.47	114.06	120.30
1	M	265	ARG	NH1-CZ-NH2	-12.47	105.69	119.40
1	I	265	ARG	NE-CZ-NH1	12.45	126.52	120.30
1	E	265	ARG	NE-CZ-NH1	12.43	126.52	120.30
2	N	164	ARG	NE-CZ-NH1	-12.42	114.09	120.30
2	F	407	LEU	CB-CG-CD1	-12.40	89.93	111.00
1	U	87	ARG	NE-CZ-NH1	-12.38	114.11	120.30
1	U	265	ARG	NE-CZ-NH1	12.35	126.47	120.30
1	I	265	ARG	NH1-CZ-NH2	-12.31	105.86	119.40
2	H	28	ARG	NH1-CZ-NH2	-12.31	105.86	119.40
1	Q	265	ARG	NE-CZ-NH1	12.31	126.45	120.30
1	A	87	ARG	NE-CZ-NH1	-12.30	114.15	120.30
1	Q	265	ARG	NH1-CZ-NH2	-12.30	105.87	119.40
1	U	265	ARG	NH1-CZ-NH2	-12.28	105.89	119.40
1	A	265	ARG	NH1-CZ-NH2	-12.28	105.89	119.40
1	E	265	ARG	NH1-CZ-NH2	-12.25	105.92	119.40
1	G	265	ARG	NH1-CZ-NH2	-12.22	105.96	119.40
1	W	223	ARG	NE-CZ-NH1	-12.20	114.20	120.30
2	P	28	ARG	NH1-CZ-NH2	-12.18	106.00	119.40
2	R	164	ARG	NE-CZ-NH2	12.14	126.37	120.30
1	O	265	ARG	NH1-CZ-NH2	-12.13	106.06	119.40
1	M	265	ARG	NE-CZ-NH1	12.13	126.36	120.30
1	K	265	ARG	NH1-CZ-NH2	-12.07	106.12	119.40
2	N	155	ARG	NE-CZ-NH2	12.07	126.34	120.30
1	A	265	ARG	NE-CZ-NH1	12.07	126.33	120.30
2	R	28	ARG	NH1-CZ-NH2	-12.04	106.15	119.40
2	L	28	ARG	NH1-CZ-NH2	-12.04	106.16	119.40
1	W	265	ARG	NH1-CZ-NH2	-12.03	106.17	119.40
1	S	265	ARG	NH1-CZ-NH2	-12.02	106.18	119.40
2	V	164	ARG	NE-CZ-NH2	12.02	126.31	120.30
2	H	49	ARG	NH1-CZ-NH2	-12.01	106.19	119.40
2	V	155	ARG	NE-CZ-NH2	12.01	126.31	120.30
2	J	155	ARG	NE-CZ-NH2	11.98	126.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	ARG	NH1-CZ-NH2	-11.97	106.23	119.40
1	E	85	ARG	NE-CZ-NH2	11.97	126.29	120.30
2	V	28	ARG	NH1-CZ-NH2	-11.96	106.24	119.40
2	B	155	ARG	NE-CZ-NH2	11.96	126.28	120.30
2	X	28	ARG	NH1-CZ-NH2	-11.96	106.25	119.40
1	C	223	ARG	NE-CZ-NH1	-11.90	114.35	120.30
2	T	28	ARG	NH1-CZ-NH2	-11.89	106.33	119.40
2	J	114	ARG	NE-CZ-NH1	11.88	126.24	120.30
2	R	114	ARG	NE-CZ-NH1	11.87	126.23	120.30
2	J	28	ARG	NH1-CZ-NH2	-11.86	106.35	119.40
2	R	155	ARG	NE-CZ-NH2	11.84	126.22	120.30
2	D	28	ARG	NH1-CZ-NH2	-11.84	106.38	119.40
2	N	28	ARG	NH1-CZ-NH2	-11.84	106.38	119.40
2	B	114	ARG	NE-CZ-NH1	11.83	126.22	120.30
2	L	49	ARG	NH1-CZ-NH2	-11.83	106.38	119.40
2	L	91	ARG	NH1-CZ-NH2	-11.83	106.38	119.40
2	L	91	ARG	NE-CZ-NH1	11.83	126.22	120.30
2	B	28	ARG	NH1-CZ-NH2	-11.83	106.39	119.40
2	L	155	ARG	NH1-CZ-NH2	-11.81	106.41	119.40
2	P	49	ARG	NH1-CZ-NH2	-11.80	106.42	119.40
2	X	91	ARG	NH1-CZ-NH2	-11.80	106.42	119.40
1	E	122	ARG	NH1-CZ-NH2	-11.79	106.43	119.40
2	X	49	ARG	NH1-CZ-NH2	-11.79	106.43	119.40
2	P	91	ARG	NH1-CZ-NH2	-11.79	106.44	119.40
2	N	392	ARG	NH1-CZ-NH2	-11.78	106.44	119.40
2	L	392	ARG	NH1-CZ-NH2	-11.77	106.45	119.40
1	A	122	ARG	NH1-CZ-NH2	-11.77	106.45	119.40
1	I	122	ARG	NH1-CZ-NH2	-11.77	106.45	119.40
2	J	155	ARG	NH1-CZ-NH2	-11.76	106.47	119.40
1	E	85	ARG	NH1-CZ-NH2	-11.75	106.47	119.40
2	T	155	ARG	NH1-CZ-NH2	-11.74	106.48	119.40
2	T	49	ARG	NH1-CZ-NH2	-11.73	106.49	119.40
1	G	87	ARG	NE-CZ-NH2	-11.73	114.44	120.30
2	N	114	ARG	NE-CZ-NH1	11.73	126.16	120.30
1	Q	122	ARG	NH1-CZ-NH2	-11.72	106.51	119.40
1	S	85	ARG	NH1-CZ-NH2	-11.72	106.51	119.40
2	B	392	ARG	NH1-CZ-NH2	-11.71	106.52	119.40
2	F	28	ARG	NH1-CZ-NH2	-11.71	106.52	119.40
1	U	122	ARG	NH1-CZ-NH2	-11.70	106.53	119.40
1	C	85	ARG	NH1-CZ-NH2	-11.69	106.54	119.40
2	V	155	ARG	NH1-CZ-NH2	-11.68	106.55	119.40
1	W	85	ARG	NH1-CZ-NH2	-11.68	106.55	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	155	ARG	NH1-CZ-NH2	-11.67	106.56	119.40
2	T	91	ARG	NH1-CZ-NH2	-11.67	106.57	119.40
2	L	155	ARG	NE-CZ-NH1	11.66	126.13	120.30
2	B	164	ARG	NE-CZ-NH2	11.65	126.12	120.30
2	D	155	ARG	NH1-CZ-NH2	-11.65	106.59	119.40
2	V	114	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	M	122	ARG	NH1-CZ-NH2	-11.64	106.59	119.40
2	P	392	ARG	NH1-CZ-NH2	-11.64	106.60	119.40
2	H	392	ARG	NH1-CZ-NH2	-11.63	106.61	119.40
1	K	85	ARG	NH1-CZ-NH2	-11.63	106.61	119.40
2	H	155	ARG	NE-CZ-NH1	11.62	126.11	120.30
2	F	155	ARG	NH1-CZ-NH2	-11.62	106.62	119.40
2	D	49	ARG	NH1-CZ-NH2	-11.62	106.62	119.40
1	O	85	ARG	NH1-CZ-NH2	-11.60	106.64	119.40
2	H	155	ARG	NH1-CZ-NH2	-11.59	106.65	119.40
2	R	155	ARG	NH1-CZ-NH2	-11.59	106.65	119.40
2	T	155	ARG	NE-CZ-NH1	11.59	126.09	120.30
2	P	91	ARG	NE-CZ-NH1	11.58	126.09	120.30
2	H	91	ARG	NE-CZ-NH1	11.57	126.09	120.30
2	N	155	ARG	NH1-CZ-NH2	-11.56	106.68	119.40
2	H	91	ARG	NH1-CZ-NH2	-11.56	106.68	119.40
2	D	91	ARG	NH1-CZ-NH2	-11.56	106.69	119.40
2	X	392	ARG	NH1-CZ-NH2	-11.55	106.69	119.40
2	B	155	ARG	NH1-CZ-NH2	-11.51	106.74	119.40
2	X	155	ARG	NH1-CZ-NH2	-11.51	106.74	119.40
2	R	114	ARG	NH1-CZ-NH2	-11.51	106.74	119.40
2	D	155	ARG	NE-CZ-NH1	11.50	126.05	120.30
2	B	91	ARG	NE-CZ-NH2	11.49	126.04	120.30
2	R	60	ARG	NE-CZ-NH1	11.48	126.04	120.30
2	F	155	ARG	NE-CZ-NH2	11.48	126.04	120.30
2	R	392	ARG	NH1-CZ-NH2	-11.47	106.78	119.40
2	D	392	ARG	NH1-CZ-NH2	-11.47	106.78	119.40
2	B	114	ARG	NH1-CZ-NH2	-11.46	106.80	119.40
2	F	114	ARG	NH1-CZ-NH2	-11.45	106.81	119.40
2	P	392	ARG	NE-CZ-NH1	11.44	126.02	120.30
2	F	114	ARG	NE-CZ-NH1	11.43	126.02	120.30
2	P	155	ARG	NE-CZ-NH1	11.43	126.01	120.30
2	T	392	ARG	NH1-CZ-NH2	-11.42	106.83	119.40
2	X	91	ARG	NE-CZ-NH1	11.42	126.01	120.30
2	L	114	ARG	NH1-CZ-NH2	-11.42	106.84	119.40
2	F	91	ARG	NH1-CZ-NH2	-11.39	106.87	119.40
1	G	85	ARG	NH1-CZ-NH2	-11.39	106.87	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	392	ARG	NH1-CZ-NH2	-11.38	106.88	119.40
2	N	114	ARG	NH1-CZ-NH2	-11.38	106.88	119.40
2	J	114	ARG	NH1-CZ-NH2	-11.38	106.89	119.40
2	H	114	ARG	NH1-CZ-NH2	-11.37	106.89	119.40
2	V	114	ARG	NH1-CZ-NH2	-11.36	106.90	119.40
2	T	114	ARG	NH1-CZ-NH2	-11.34	106.92	119.40
1	Q	87	ARG	CG-CD-NE	-11.34	87.98	111.80
2	L	392	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	I	85	ARG	NH1-CZ-NH2	-11.33	106.93	119.40
2	D	114	ARG	NH1-CZ-NH2	-11.33	106.94	119.40
2	B	91	ARG	NH1-CZ-NH2	-11.33	106.94	119.40
2	P	114	ARG	NH1-CZ-NH2	-11.32	106.94	119.40
1	K	265	ARG	NE-CZ-NH2	11.32	125.96	120.30
2	V	392	ARG	NH1-CZ-NH2	-11.30	106.97	119.40
2	X	155	ARG	NE-CZ-NH1	11.29	125.94	120.30
1	W	265	ARG	NE-CZ-NH2	11.29	125.94	120.30
2	X	114	ARG	NH1-CZ-NH2	-11.27	107.00	119.40
1	Q	223	ARG	NE-CZ-NH2	-11.26	114.67	120.30
2	F	392	ARG	NH1-CZ-NH2	-11.26	107.02	119.40
1	M	85	ARG	NH1-CZ-NH2	-11.24	107.03	119.40
2	X	392	ARG	NE-CZ-NH1	11.24	125.92	120.30
1	U	85	ARG	NH1-CZ-NH2	-11.23	107.05	119.40
2	J	91	ARG	NH1-CZ-NH2	-11.23	107.05	119.40
2	N	91	ARG	NH1-CZ-NH2	-11.20	107.08	119.40
2	T	91	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	U	87	ARG	CG-CD-NE	-11.15	88.38	111.80
1	I	87	ARG	CG-CD-NE	-11.15	88.39	111.80
1	A	87	ARG	CG-CD-NE	-11.14	88.41	111.80
1	M	87	ARG	CG-CD-NE	-11.13	88.43	111.80
1	G	265	ARG	NE-CZ-NH2	11.12	125.86	120.30
1	S	265	ARG	NE-CZ-NH2	11.11	125.86	120.30
2	R	91	ARG	NH1-CZ-NH2	-11.11	107.17	119.40
2	V	91	ARG	NH1-CZ-NH2	-11.11	107.18	119.40
1	A	85	ARG	NH1-CZ-NH2	-11.10	107.19	119.40
2	D	392	ARG	NE-CZ-NH1	11.10	125.85	120.30
2	H	392	ARG	NE-CZ-NH1	11.09	125.84	120.30
1	O	265	ARG	NE-CZ-NH2	11.08	125.84	120.30
2	T	392	ARG	NE-CZ-NH1	11.06	125.83	120.30
2	H	60	ARG	NE-CZ-NH1	-11.03	114.78	120.30
1	Q	85	ARG	NH1-CZ-NH2	-11.02	107.28	119.40
2	J	164	ARG	NE-CZ-NH2	11.00	125.80	120.30
1	I	85	ARG	NE-CZ-NH2	10.99	125.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	164	ARG	NE-CZ-NH2	10.98	125.79	120.30
2	R	28	ARG	NE-CZ-NH2	10.96	125.78	120.30
2	N	91	ARG	NE-CZ-NH2	10.93	125.76	120.30
2	H	407	LEU	CB-CG-CD1	-10.90	92.47	111.00
1	C	265	ARG	NE-CZ-NH2	10.89	125.75	120.30
2	J	91	ARG	NE-CZ-NH2	10.89	125.75	120.30
2	V	28	ARG	NE-CZ-NH2	10.89	125.74	120.30
2	D	91	ARG	NE-CZ-NH1	10.87	125.73	120.30
2	V	49	ARG	NH1-CZ-NH2	-10.84	107.47	119.40
1	W	122	ARG	NH1-CZ-NH2	-10.84	107.48	119.40
2	P	113	ARG	NE-CZ-NH1	-10.81	114.89	120.30
2	N	28	ARG	NE-CZ-NH2	10.80	125.70	120.30
2	T	60	ARG	NE-CZ-NH1	-10.80	114.90	120.30
2	J	28	ARG	NE-CZ-NH2	10.78	125.69	120.30
2	J	49	ARG	NH1-CZ-NH2	-10.76	107.56	119.40
2	R	49	ARG	NH1-CZ-NH2	-10.75	107.57	119.40
1	S	122	ARG	NH1-CZ-NH2	-10.73	107.59	119.40
2	L	113	ARG	NE-CZ-NH1	-10.71	114.94	120.30
2	N	49	ARG	NH1-CZ-NH2	-10.70	107.63	119.40
1	K	122	ARG	NH1-CZ-NH2	-10.69	107.64	119.40
1	G	122	ARG	NH1-CZ-NH2	-10.67	107.66	119.40
1	O	223	ARG	NE-CZ-NH1	-10.67	114.97	120.30
2	B	60	ARG	NE-CZ-NH2	-10.65	114.98	120.30
1	O	122	ARG	NH1-CZ-NH2	-10.62	107.72	119.40
2	B	49	ARG	NH1-CZ-NH2	-10.61	107.73	119.40
2	V	91	ARG	NE-CZ-NH2	10.60	125.60	120.30
1	M	85	ARG	NE-CZ-NH2	10.60	125.60	120.30
1	I	266	LEU	CB-CG-CD1	-10.57	93.03	111.00
1	U	85	ARG	NE-CZ-NH2	10.54	125.57	120.30
2	F	49	ARG	NH1-CZ-NH2	-10.54	107.81	119.40
1	K	223	ARG	NE-CZ-NH1	-10.53	115.03	120.30
1	M	266	LEU	CB-CG-CD1	-10.51	93.13	111.00
1	C	122	ARG	NH1-CZ-NH2	-10.49	107.86	119.40
2	V	60	ARG	NE-CZ-NH2	-10.48	115.06	120.30
2	F	91	ARG	NE-CZ-NH2	10.47	125.54	120.30
2	N	9	THR	N-CA-CB	-10.46	90.43	110.30
2	N	60	ARG	NE-CZ-NH2	-10.45	115.07	120.30
2	R	91	ARG	NE-CZ-NH2	10.43	125.52	120.30
2	F	28	ARG	NE-CZ-NH2	10.41	125.50	120.30
2	B	28	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	A	85	ARG	NE-CZ-NH2	10.39	125.50	120.30
1	U	266	LEU	CB-CG-CD1	-10.37	93.37	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	85	ARG	NE-CZ-NH2	10.37	125.48	120.30
2	J	9	THR	N-CA-CB	-10.33	90.67	110.30
2	V	9	THR	N-CA-CB	-10.23	90.86	110.30
1	A	74	ARG	NE-CZ-NH1	10.19	125.39	120.30
2	B	9	THR	N-CA-CB	-10.17	90.97	110.30
1	U	74	ARG	NE-CZ-NH1	10.17	125.39	120.30
2	R	9	THR	N-CA-CB	-10.16	91.00	110.30
2	F	9	THR	N-CA-CB	-10.11	91.10	110.30
2	H	9	THR	CA-CB-CG2	-10.08	98.29	112.40
1	Q	266	LEU	CB-CG-CD1	-10.06	93.90	111.00
2	F	60	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	S	122	ARG	NE-CZ-NH1	10.01	125.31	120.30
2	X	113	ARG	NE-CZ-NH1	-9.99	115.31	120.30
1	Q	87	ARG	NH1-CZ-NH2	9.98	130.38	119.40
2	D	113	ARG	NE-CZ-NH1	-9.98	115.31	120.30
2	J	60	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	K	122	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	W	122	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	G	223	ARG	NE-CZ-NH1	-9.82	115.39	120.30
1	O	122	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	A	266	LEU	CB-CG-CD1	-9.81	94.32	111.00
2	J	60	ARG	NE-CZ-NH1	9.77	125.19	120.30
2	N	60	ARG	NE-CZ-NH1	9.77	125.18	120.30
2	P	60	ARG	NE-CZ-NH1	-9.76	115.42	120.30
2	V	60	ARG	NE-CZ-NH1	9.76	125.18	120.30
2	D	9	THR	CA-CB-CG2	-9.64	98.91	112.40
1	C	122	ARG	NE-CZ-NH1	9.60	125.10	120.30
2	X	9	THR	CA-CB-CG2	-9.54	99.04	112.40
2	P	9	THR	CA-CB-CG2	-9.50	99.10	112.40
1	S	85	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	G	122	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	G	266	LEU	CB-CG-CD2	-9.39	95.03	111.00
2	T	113	ARG	NE-CZ-NH1	-9.35	115.63	120.30
1	W	85	ARG	NE-CZ-NH1	9.25	124.92	120.30
2	L	60	ARG	NE-CZ-NH1	-9.20	115.70	120.30
2	F	407	LEU	CB-CG-CD2	-9.18	95.40	111.00
1	I	87	ARG	NH1-CZ-NH2	9.17	129.49	119.40
1	K	85	ARG	NE-CZ-NH1	9.16	124.88	120.30
2	B	60	ARG	NE-CZ-NH1	9.13	124.87	120.30
2	D	60	ARG	NE-CZ-NH1	-9.11	115.75	120.30
1	O	85	ARG	NE-CZ-NH1	9.10	124.85	120.30
2	F	164	ARG	NE-CZ-NH1	-9.06	115.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	87	ARG	NH1-CZ-NH2	9.06	129.37	119.40
2	L	9	THR	CA-CB-CG2	-9.06	99.72	112.40
1	A	122	ARG	NE-CZ-NH2	9.05	124.82	120.30
1	I	122	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	E	223	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	U	122	ARG	NE-CZ-NH2	9.03	124.81	120.30
1	E	122	ARG	NE-CZ-NH2	9.02	124.81	120.30
2	F	164	ARG	NE-CZ-NH2	9.00	124.80	120.30
1	C	85	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	Q	122	ARG	NE-CZ-NH2	8.98	124.79	120.30
1	M	122	ARG	NE-CZ-NH2	8.91	124.76	120.30
1	I	223	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	U	87	ARG	NH1-CZ-NH2	8.75	129.03	119.40
1	A	87	ARG	NH1-CZ-NH2	8.73	129.00	119.40
1	G	85	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	M	74	ARG	NE-CZ-NH2	-8.70	115.95	120.30
2	T	9	THR	CA-CB-CG2	-8.69	100.23	112.40
1	I	74	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	A	223	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	U	223	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	I	74	ARG	NE-CZ-NH2	-8.49	116.05	120.30
2	X	225	GLU	OE1-CD-OE2	-8.41	113.21	123.30
2	T	381	ARG	NE-CZ-NH2	8.35	124.47	120.30
2	F	225	GLU	OE1-CD-OE2	-8.34	113.29	123.30
2	L	113	ARG	NE-CZ-NH2	8.31	124.46	120.30
1	M	223	ARG	NE-CZ-NH1	8.31	124.46	120.30
2	H	225	GLU	OE1-CD-OE2	-8.19	113.47	123.30
1	M	77	GLU	OE1-CD-OE2	-8.10	113.58	123.30
1	M	74	ARG	NE-CZ-NH1	8.07	124.33	120.30
2	N	225	GLU	OE1-CD-OE2	-8.02	113.67	123.30
1	Q	74	ARG	NE-CZ-NH1	7.99	124.29	120.30
2	X	60	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	W	266	LEU	CB-CG-CD2	-7.95	97.49	111.00
2	L	225	GLU	OE1-CD-OE2	-7.94	113.77	123.30
2	P	113	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	A	74	ARG	NE-CZ-NH2	-7.92	116.34	120.30
2	H	114	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	C	266	LEU	CB-CG-CD2	-7.91	97.56	111.00
2	T	113	ARG	NE-CZ-NH2	7.87	124.24	120.30
2	B	225	GLU	OE1-CD-OE2	-7.86	113.87	123.30
2	D	225	GLU	OE1-CD-OE2	-7.79	113.95	123.30
2	J	225	GLU	OE1-CD-OE2	-7.79	113.95	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	40	GLU	OE1-CD-OE2	-7.76	113.99	123.30
2	V	225	GLU	OE1-CD-OE2	-7.74	114.01	123.30
1	S	248	GLU	OE1-CD-OE2	-7.74	114.02	123.30
2	R	225	GLU	OE1-CD-OE2	-7.73	114.02	123.30
2	T	114	ARG	NE-CZ-NH2	7.72	124.16	120.30
2	L	114	ARG	NE-CZ-NH2	7.65	124.13	120.30
2	D	114	ARG	NE-CZ-NH2	7.65	124.12	120.30
2	F	60	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	Q	74	ARG	NE-CZ-NH2	-7.61	116.49	120.30
2	T	225	GLU	OE1-CD-OE2	-7.60	114.18	123.30
2	P	114	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	K	248	GLU	OE1-CD-OE2	-7.59	114.19	123.30
2	P	225	GLU	OE1-CD-OE2	-7.58	114.21	123.30
2	X	114	ARG	NE-CZ-NH2	7.58	124.09	120.30
2	N	164	ARG	CD-NE-CZ	-7.55	113.03	123.60
1	E	87	ARG	CG-CD-NE	-7.53	95.99	111.80
1	U	248	GLU	OE1-CD-OE2	-7.50	114.30	123.30
2	L	9	THR	N-CA-CB	-7.48	96.08	110.30
2	H	40	GLU	OE1-CD-OE2	-7.46	114.34	123.30
1	A	77	GLU	OE1-CD-OE2	-7.46	114.35	123.30
2	R	60	ARG	NE-CZ-NH2	-7.43	116.58	120.30
2	X	9	THR	N-CA-CB	-7.42	96.21	110.30
1	Q	77	GLU	OE1-CD-OE2	-7.39	114.43	123.30
2	F	402	LYS	CD-CE-NZ	7.39	128.69	111.70
2	D	9	THR	N-CA-CB	-7.38	96.28	110.30
2	T	9	THR	N-CA-CB	-7.38	96.28	110.30
2	X	113	ARG	NE-CZ-NH2	7.37	123.98	120.30
1	E	248	GLU	OE1-CD-OE2	-7.36	114.47	123.30
1	I	248	GLU	OE1-CD-OE2	-7.36	114.47	123.30
1	O	248	GLU	OE1-CD-OE2	-7.36	114.47	123.30
2	D	40	GLU	OE1-CD-OE2	-7.36	114.47	123.30
1	G	77	GLU	OE1-CD-OE2	-7.36	114.47	123.30
1	M	87	ARG	NE-CZ-NH2	-7.36	116.62	120.30
2	J	164	ARG	CD-NE-CZ	-7.35	113.31	123.60
2	P	9	THR	N-CA-CB	-7.35	96.34	110.30
1	U	74	ARG	NE-CZ-NH2	-7.35	116.63	120.30
2	N	402	LYS	CD-CE-NZ	7.35	128.59	111.70
1	O	87	ARG	NH1-CZ-NH2	7.34	127.48	119.40
2	R	164	ARG	CD-NE-CZ	-7.31	113.36	123.60
2	J	402	LYS	CD-CE-NZ	7.31	128.51	111.70
2	H	9	THR	N-CA-CB	-7.30	96.43	110.30
1	I	77	GLU	OE1-CD-OE2	-7.30	114.54	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	GLU	OE1-CD-OE2	-7.28	114.57	123.30
1	E	77	GLU	OE1-CD-OE2	-7.27	114.58	123.30
1	U	266	LEU	CA-CB-CG	-7.27	98.58	115.30
2	X	40	GLU	OE1-CD-OE2	-7.27	114.58	123.30
2	V	402	LYS	CD-CE-NZ	7.26	128.40	111.70
1	W	77	GLU	OE1-CD-OE2	-7.25	114.60	123.30
2	B	402	LYS	CD-CE-NZ	7.25	128.37	111.70
1	C	87	ARG	NH1-CZ-NH2	7.22	127.34	119.40
1	K	87	ARG	NH1-CZ-NH2	7.21	127.33	119.40
2	X	23	SER	CB-CA-C	-7.17	96.47	110.10
2	B	40	GLU	OE1-CD-OE2	-7.17	114.70	123.30
1	O	266	LEU	CB-CG-CD2	-7.16	98.83	111.00
1	U	266	LEU	CB-CA-C	-7.16	96.60	110.20
1	W	87	ARG	NH1-CZ-NH2	7.15	127.26	119.40
1	G	87	ARG	NH1-CZ-NH2	7.14	127.25	119.40
1	I	87	ARG	NE-CZ-NH2	-7.13	116.74	120.30
2	B	164	ARG	CD-NE-CZ	-7.12	113.63	123.60
1	W	248	GLU	OE1-CD-OE2	-7.11	114.76	123.30
1	I	266	LEU	CA-CB-CG	-7.11	98.94	115.30
2	V	164	ARG	CD-NE-CZ	-7.11	113.65	123.60
2	V	40	GLU	OE1-CD-OE2	-7.10	114.78	123.30
2	B	381	ARG	NE-CZ-NH1	7.08	123.84	120.30
2	R	402	LYS	CD-CE-NZ	7.08	127.99	111.70
2	X	381	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	C	77	GLU	OE1-CD-OE2	-7.04	114.86	123.30
2	L	40	GLU	OE1-CD-OE2	-7.01	114.89	123.30
1	Q	266	LEU	CA-CB-CG	-7.00	99.19	115.30
1	M	266	LEU	CB-CA-C	-7.00	96.90	110.20
1	S	87	ARG	NH1-CZ-NH2	6.99	127.09	119.40
1	M	266	LEU	CA-CB-CG	-6.98	99.25	115.30
2	F	40	GLU	OE1-CD-OE2	-6.97	114.94	123.30
1	S	266	LEU	CB-CG-CD2	-6.97	99.15	111.00
2	P	40	GLU	OE1-CD-OE2	-6.96	114.95	123.30
2	J	40	GLU	OE1-CD-OE2	-6.94	114.97	123.30
1	M	248	GLU	OE1-CD-OE2	-6.93	114.98	123.30
1	U	77	GLU	OE1-CD-OE2	-6.93	114.98	123.30
1	A	87	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	266	LEU	CA-CB-CG	-6.90	99.42	115.30
2	T	40	GLU	OE1-CD-OE2	-6.90	115.02	123.30
1	U	87	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	K	266	LEU	CB-CG-CD2	-6.88	99.30	111.00
1	Q	266	LEU	CB-CA-C	-6.86	97.16	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	402	LYS	CD-CE-NZ	6.83	127.41	111.70
1	G	248	GLU	OE1-CD-OE2	-6.83	115.11	123.30
2	D	23	SER	CB-CA-C	-6.83	97.13	110.10
2	L	402	LYS	CD-CE-NZ	6.82	127.39	111.70
1	I	266	LEU	CB-CA-C	-6.82	97.25	110.20
1	Q	87	ARG	NE-CZ-NH2	-6.79	116.91	120.30
2	P	402	LYS	CD-CE-NZ	6.78	127.30	111.70
2	T	402	LYS	CD-CE-NZ	6.78	127.29	111.70
1	A	266	LEU	CB-CA-C	-6.75	97.37	110.20
2	D	113	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	G	266	LEU	CA-CB-CG	-6.75	99.78	115.30
1	Q	248	GLU	OE1-CD-OE2	-6.74	115.21	123.30
2	N	40	GLU	OE1-CD-OE2	-6.72	115.23	123.30
2	V	381	ARG	NE-CZ-NH1	6.71	123.66	120.30
2	N	392	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	H	402	LYS	CD-CE-NZ	6.68	127.07	111.70
2	D	402	LYS	CD-CE-NZ	6.67	127.04	111.70
2	R	407	LEU	CB-CG-CD1	-6.63	99.74	111.00
1	M	232	TYR	CB-CG-CD1	6.62	124.97	121.00
1	E	266	LEU	CB-CA-C	-6.59	97.68	110.20
1	G	232	TYR	CB-CG-CD1	6.59	124.95	121.00
1	S	74	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	K	77	GLU	OE1-CD-OE2	-6.58	115.41	123.30
1	S	77	GLU	OE1-CD-OE2	-6.54	115.45	123.30
1	U	232	TYR	CB-CG-CD1	6.52	124.91	121.00
1	S	252	ARG	NE-CZ-NH1	-6.51	117.04	120.30
2	D	381	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	C	248	GLU	OE1-CD-OE2	-6.48	115.52	123.30
2	J	381	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	C	232	TYR	CB-CG-CD1	6.44	124.87	121.00
1	A	232	TYR	CB-CG-CD1	6.40	124.84	121.00
1	M	232	TYR	CD1-CG-CD2	-6.40	110.86	117.90
1	I	232	TYR	CB-CG-CD1	6.34	124.80	121.00
1	W	232	TYR	CB-CG-CD1	6.33	124.80	121.00
2	T	23	SER	CB-CA-C	-6.32	98.09	110.10
2	N	280	ARG	NH1-CZ-NH2	-6.31	112.46	119.40
1	O	232	TYR	CB-CG-CD1	6.30	124.78	121.00
1	O	252	ARG	NE-CZ-NH1	-6.30	117.15	120.30
2	B	407	LEU	CB-CG-CD1	-6.29	100.31	111.00
2	N	381	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	Q	232	TYR	CB-CG-CD1	6.29	124.77	121.00
1	U	232	TYR	CD1-CG-CD2	-6.28	110.99	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	77	GLU	OE1-CD-OE2	-6.28	115.77	123.30
2	B	392	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	K	232	TYR	CB-CG-CD1	6.26	124.76	121.00
1	Q	232	TYR	CD1-CG-CD2	-6.25	111.03	117.90
1	E	252	ARG	NH1-CZ-NH2	-6.22	112.55	119.40
2	H	280	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	L	23	SER	CB-CA-C	-6.20	98.31	110.10
1	A	232	TYR	CD1-CG-CD2	-6.20	111.08	117.90
1	I	232	TYR	CD1-CG-CD2	-6.20	111.08	117.90
1	Q	232	TYR	CD1-CE1-CZ	6.18	125.37	119.80
1	M	223	ARG	CD-NE-CZ	6.18	132.25	123.60
1	E	232	TYR	CB-CG-CD1	6.17	124.70	121.00
1	S	232	TYR	CB-CG-CD1	6.15	124.69	121.00
1	E	232	TYR	CD1-CG-CD2	-6.13	111.15	117.90
1	M	232	TYR	CD1-CE1-CZ	6.11	125.30	119.80
2	R	392	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	232	TYR	CD1-CE1-CZ	6.09	125.28	119.80
1	I	223	ARG	CD-NE-CZ	6.07	132.09	123.60
2	J	407	LEU	CB-CG-CD1	-6.06	100.70	111.00
2	J	392	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	U	232	TYR	CD1-CE1-CZ	6.05	125.25	119.80
2	R	280	ARG	NH1-CZ-NH2	-6.05	112.75	119.40
2	V	23	SER	CA-C-N	-6.04	104.11	116.20
2	F	392	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	J	280	ARG	NH1-CZ-NH2	-6.04	112.76	119.40
2	B	23	SER	CA-C-N	-6.02	104.17	116.20
1	E	232	TYR	CD1-CE1-CZ	6.02	125.22	119.80
1	K	266	LEU	CA-CB-CG	-6.01	101.48	115.30
1	S	252	ARG	NH1-CZ-NH2	-6.00	112.80	119.40
1	G	232	TYR	CD1-CG-CD2	-6.00	111.30	117.90
1	I	232	TYR	CD1-CE1-CZ	5.98	125.18	119.80
2	P	23	SER	CB-CA-C	-5.97	98.75	110.10
1	U	223	ARG	CD-NE-CZ	5.97	131.95	123.60
2	F	280	ARG	NH1-CZ-NH2	-5.96	112.85	119.40
1	O	232	TYR	CD1-CG-CD2	-5.95	111.36	117.90
2	N	407	LEU	CB-CG-CD1	-5.94	100.89	111.00
1	W	232	TYR	CD1-CG-CD2	-5.94	111.36	117.90
1	C	232	TYR	CD1-CG-CD2	-5.94	111.36	117.90
2	P	280	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	L	381	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	O	64	ASP	CB-CG-OD1	5.92	123.63	118.30
2	B	280	ARG	NH1-CZ-NH2	-5.91	112.90	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	252	ARG	NH1-CZ-NH2	-5.91	112.90	119.40
1	G	74	ARG	CG-CD-NE	-5.90	99.40	111.80
1	O	266	LEU	CA-CB-CG	-5.90	101.72	115.30
1	M	252	ARG	NH1-CZ-NH2	-5.90	112.91	119.40
2	N	9	THR	N-CA-C	5.90	126.93	111.00
1	A	223	ARG	CD-NE-CZ	5.90	131.86	123.60
2	B	23	SER	C-N-CA	-5.89	109.92	122.30
2	V	23	SER	C-N-CA	-5.88	109.94	122.30
2	T	280	ARG	NE-CZ-NH2	-5.87	117.36	120.30
2	V	280	ARG	NH1-CZ-NH2	-5.86	112.95	119.40
1	I	252	ARG	NH1-CZ-NH2	-5.86	112.95	119.40
2	J	23	SER	C-N-CA	-5.86	110.00	122.30
2	T	280	ARG	NH1-CZ-NH2	-5.86	112.96	119.40
2	L	280	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	K	232	TYR	CD1-CG-CD2	-5.85	111.47	117.90
1	U	252	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
2	X	280	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
1	C	232	TYR	CD1-CE1-CZ	5.82	125.04	119.80
2	J	23	SER	CA-C-N	-5.82	104.57	116.20
2	V	392	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	N	23	SER	C-N-CA	-5.81	110.09	122.30
2	F	23	SER	C-N-CA	-5.80	110.13	122.30
2	V	407	LEU	CB-CG-CD1	-5.79	101.15	111.00
1	G	252	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	S	232	TYR	CD1-CG-CD2	-5.78	111.54	117.90
1	C	266	LEU	CA-CB-CG	-5.77	102.03	115.30
1	Q	223	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	G	266	LEU	CB-CA-C	-5.75	99.28	110.20
1	E	87	ARG	NH1-CZ-NH2	5.74	125.71	119.40
2	L	280	ARG	NH1-CZ-NH2	-5.73	113.10	119.40
1	S	266	LEU	CA-CB-CG	-5.72	102.14	115.30
2	V	9	THR	N-CA-C	5.72	126.45	111.00
1	A	252	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
2	D	280	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
2	R	23	SER	C-N-CA	-5.71	110.30	122.30
2	P	280	ARG	NH1-CZ-NH2	-5.70	113.14	119.40
1	G	232	TYR	CD1-CE1-CZ	5.68	124.91	119.80
1	O	232	TYR	CD1-CE1-CZ	5.68	124.91	119.80
2	J	113	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	W	232	TYR	CD1-CE1-CZ	5.67	124.90	119.80
1	K	232	TYR	CD1-CE1-CZ	5.66	124.89	119.80
1	C	64	ASP	CB-CG-OD1	5.66	123.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	258	PHE	CB-CG-CD2	5.65	124.76	120.80
2	J	9	THR	N-CA-C	5.64	126.23	111.00
2	B	258	PHE	CB-CG-CD2	5.64	124.75	120.80
2	H	280	ARG	NH1-CZ-NH2	-5.64	113.20	119.40
1	W	266	LEU	CA-CB-CG	-5.64	102.33	115.30
1	K	114	ARG	NE-CZ-NH1	-5.60	117.50	120.30
2	N	23	SER	CA-C-N	-5.59	105.01	116.20
2	B	280	ARG	CD-NE-CZ	5.59	131.42	123.60
1	K	64	ASP	CB-CG-OD1	5.59	123.33	118.30
1	M	232	TYR	CZ-CE2-CD2	5.58	124.83	119.80
1	G	232	TYR	CZ-CE2-CD2	5.58	124.82	119.80
2	B	280	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	S	64	ASP	CB-CG-OD1	5.57	123.31	118.30
1	W	64	ASP	CB-CG-OD1	5.57	123.31	118.30
1	K	266	LEU	N-CA-CB	-5.56	99.28	110.40
1	W	252	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	M	232	TYR	CE1-CZ-CE2	-5.53	110.95	119.80
2	X	280	ARG	NE-CZ-NH2	-5.53	117.53	120.30
2	F	23	SER	CA-C-N	-5.52	105.15	116.20
2	N	258	PHE	CB-CG-CD2	5.52	124.66	120.80
1	S	223	ARG	NE-CZ-NH2	5.52	123.06	120.30
2	R	258	PHE	CB-CG-CD2	5.52	124.66	120.80
2	N	280	ARG	CD-NE-CZ	5.51	131.32	123.60
2	V	113	ARG	NE-CZ-NH2	5.51	123.06	120.30
2	B	9	THR	N-CA-C	5.51	125.87	111.00
2	H	23	SER	CB-CA-C	-5.51	99.64	110.10
2	V	280	ARG	CD-NE-CZ	5.51	131.31	123.60
2	D	280	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	252	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	Q	232	TYR	CE1-CZ-CE2	-5.50	111.00	119.80
1	S	232	TYR	CD1-CE1-CZ	5.49	124.75	119.80
2	B	9	THR	CA-CB-CG2	-5.49	104.71	112.40
1	U	232	TYR	CE1-CZ-CE2	-5.49	111.01	119.80
2	J	280	ARG	CD-NE-CZ	5.49	131.28	123.60
2	V	280	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	232	TYR	CE1-CZ-CE2	-5.48	111.03	119.80
1	K	252	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	C	114	ARG	NE-CZ-NH1	-5.47	117.57	120.30
1	E	223	ARG	CD-NE-CZ	5.47	131.25	123.60
2	V	258	PHE	CB-CG-CD2	5.46	124.62	120.80
2	P	381	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	R	381	ARG	NE-CZ-NH1	5.45	123.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	64	ASP	CB-CG-OD1	5.44	123.20	118.30
1	W	74	ARG	NE-CZ-NH2	5.44	123.02	120.30
2	F	258	PHE	CE1-CZ-CE2	-5.44	110.21	120.00
2	F	280	ARG	CD-NE-CZ	5.43	131.21	123.60
1	O	266	LEU	N-CA-CB	-5.43	99.53	110.40
1	G	232	TYR	CE1-CZ-CE2	-5.43	111.11	119.80
1	O	114	ARG	NE-CZ-NH1	-5.43	117.59	120.30
2	R	280	ARG	CD-NE-CZ	5.42	131.19	123.60
1	K	232	TYR	CZ-CE2-CD2	5.42	124.68	119.80
1	A	232	TYR	CZ-CE2-CD2	5.42	124.68	119.80
1	U	232	TYR	CZ-CE2-CD2	5.42	124.68	119.80
2	H	49	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	S	232	TYR	CZ-CE2-CD2	5.41	124.67	119.80
1	O	232	TYR	CZ-CE2-CD2	5.39	124.66	119.80
1	S	266	LEU	N-CA-CB	-5.39	99.62	110.40
2	P	164	ARG	CD-NE-CZ	5.39	131.15	123.60
1	Q	232	TYR	CZ-CE2-CD2	5.39	124.65	119.80
1	C	232	TYR	CE1-CZ-CE2	-5.39	111.18	119.80
1	I	232	TYR	CE1-CZ-CE2	-5.39	111.18	119.80
2	R	9	THR	N-CA-C	5.37	125.51	111.00
2	B	258	PHE	CE1-CZ-CE2	-5.37	110.34	120.00
2	H	23	SER	CA-C-N	-5.36	105.48	116.20
2	N	258	PHE	CE1-CZ-CE2	-5.36	110.36	120.00
1	S	114	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	I	232	TYR	CZ-CE2-CD2	5.36	124.62	119.80
1	E	232	TYR	CE1-CZ-CE2	-5.35	111.24	119.80
2	J	258	PHE	CB-CG-CD2	5.34	124.54	120.80
1	K	232	TYR	CE1-CZ-CE2	-5.34	111.26	119.80
1	O	232	TYR	CE1-CZ-CE2	-5.33	111.27	119.80
1	W	232	TYR	CZ-CE2-CD2	5.32	124.59	119.80
1	C	266	LEU	N-CA-CB	-5.31	99.77	110.40
1	K	252	ARG	NH1-CZ-NH2	-5.31	113.55	119.40
2	N	9	THR	CA-CB-CG2	-5.31	104.96	112.40
1	C	232	TYR	CZ-CE2-CD2	5.31	124.58	119.80
1	W	266	LEU	N-CA-CB	-5.30	99.80	110.40
1	C	252	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
1	Q	223	ARG	CD-NE-CZ	5.29	131.01	123.60
1	O	74	ARG	NE-CZ-NH2	5.29	122.95	120.30
2	R	258	PHE	CE1-CZ-CE2	-5.29	110.47	120.00
2	D	258	PHE	CE1-CZ-CE2	-5.29	110.48	120.00
2	D	280	ARG	CD-NE-CZ	5.29	131.00	123.60
1	K	74	ARG	NE-CZ-NH2	5.29	122.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	232	TYR	CE1-CZ-CE2	-5.28	111.35	119.80
2	T	280	ARG	CD-NE-CZ	5.28	130.99	123.60
1	W	252	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
1	Q	167	GLU	OE1-CD-OE2	5.27	129.62	123.30
1	S	232	TYR	CE1-CZ-CE2	-5.27	111.37	119.80
1	Q	232	TYR	CB-CG-CD2	5.27	124.16	121.00
2	V	258	PHE	CE1-CZ-CE2	-5.26	110.53	120.00
2	L	280	ARG	CD-NE-CZ	5.26	130.96	123.60
2	X	258	PHE	CE1-CZ-CE2	-5.26	110.54	120.00
1	A	64	ASP	CB-CG-OD1	5.25	123.02	118.30
1	U	64	ASP	CB-CG-OD1	5.25	123.02	118.30
2	X	280	ARG	CD-NE-CZ	5.24	130.94	123.60
2	D	164	ARG	CD-NE-CZ	5.23	130.93	123.60
1	E	232	TYR	CZ-CE2-CD2	5.23	124.50	119.80
1	M	232	TYR	CB-CG-CD2	5.22	124.13	121.00
2	B	381	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
1	W	114	ARG	NE-CZ-NH1	-5.22	117.69	120.30
2	F	9	THR	N-CA-C	5.21	125.08	111.00
2	J	258	PHE	CE1-CZ-CE2	-5.20	110.64	120.00
2	V	9	THR	CA-CB-CG2	-5.19	105.13	112.40
2	V	381	ARG	NH1-CZ-NH2	-5.18	113.71	119.40
1	E	232	TYR	CB-CG-CD2	5.17	124.11	121.00
2	H	164	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
2	T	49	ARG	NE-CZ-NH2	5.15	122.88	120.30
2	X	164	ARG	CD-NE-CZ	5.15	130.81	123.60
2	T	258	PHE	CE1-CZ-CE2	-5.15	110.74	120.00
2	L	164	ARG	CD-NE-CZ	5.14	130.79	123.60
2	P	280	ARG	CD-NE-CZ	5.13	130.78	123.60
2	H	280	ARG	CD-NE-CZ	5.13	130.78	123.60
2	H	258	PHE	CE1-CZ-CE2	-5.12	110.78	120.00
1	I	232	TYR	CB-CG-CD2	5.12	124.07	121.00
2	N	113	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	G	64	ASP	CB-CG-OD1	5.11	122.90	118.30
2	D	258	PHE	CD1-CG-CD2	-5.11	111.66	118.30
1	M	64	ASP	CB-CG-OD1	5.10	122.89	118.30
2	L	258	PHE	CE1-CZ-CE2	-5.09	110.83	120.00
2	R	49	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	E	74	ARG	NE-CZ-NH1	-5.09	117.76	120.30
2	L	164	ARG	CG-CD-NE	-5.09	101.12	111.80
1	U	232	TYR	CB-CG-CD2	5.08	124.05	121.00
1	A	232	TYR	CB-CG-CD2	5.08	124.05	121.00
2	J	280	ARG	NE-CZ-NH2	-5.08	117.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	49	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	K	74	ARG	CG-CD-NE	-5.06	101.17	111.80
2	N	280	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	J	9	THR	CA-CB-CG2	-5.05	105.32	112.40
2	T	164	ARG	CG-CD-NE	-5.05	101.19	111.80
2	B	258	PHE	CD1-CG-CD2	-5.04	111.75	118.30
2	F	9	THR	CA-CB-CG2	-5.03	105.36	112.40
1	I	64	ASP	CB-CG-OD1	5.03	122.83	118.30
1	O	252	ARG	NH1-CZ-NH2	-5.02	113.87	119.40
2	F	258	PHE	CD1-CG-CD2	-5.02	111.77	118.30
1	S	8	GLU	CA-CB-CG	-5.02	102.36	113.40
1	G	167	GLU	OE1-CD-OE2	5.01	129.32	123.30
2	X	164	ARG	CG-CD-NE	-5.01	101.28	111.80
2	F	280	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	S	74	ARG	CG-CD-NE	-5.00	101.29	111.80
2	X	258	PHE	CD1-CG-CD2	-5.00	111.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1852	0	1855	50	0
1	C	1799	0	1819	10	22
1	E	1814	0	1834	16	2
1	G	1799	0	1816	57	0
1	I	1814	0	1834	32	0
1	K	1799	0	1819	63	3
1	M	1814	0	1834	40	0
1	O	1799	0	1819	20	14
1	Q	1814	0	1829	32	0
1	S	1799	0	1818	37	3
1	U	1814	0	1834	23	0
1	W	1799	0	1819	18	22
2	B	3002	0	2929	28	9

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2983	0	2908	47	13
2	F	3002	0	2926	78	4
2	H	2983	0	2908	54	2
2	J	3002	0	2929	102	3
2	L	2983	0	2908	152	0
2	N	3002	0	2929	26	13
2	P	2983	0	2908	41	5
2	R	3002	0	2929	72	3
2	T	2983	0	2906	113	0
2	V	3002	0	2929	27	10
2	X	2983	0	2908	43	12
3	B	21	0	11	0	0
3	D	21	0	11	0	0
3	F	21	0	11	0	0
3	H	21	0	11	0	0
3	J	21	0	11	0	0
3	L	21	0	11	0	0
3	N	21	0	11	0	0
3	P	21	0	11	0	0
3	R	21	0	11	0	0
3	T	21	0	11	0	0
3	V	21	0	11	0	0
3	X	21	0	11	0	0
All	All	57878	0	57079	663	70

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (663) 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:A:69:GLY:HA3	1:A:188:VAL:CB	1.25	1.67
2:L:80:GLN:HE22	1:U:259:GLU:CG	1.03	1.59
1:G:228:GLN:NE2	2:R:118:THR:CB	1.69	1.53
2:L:80:GLN:NE2	1:U:259:GLU:HG2	1.26	1.47
1:G:262:ALA:HB2	2:T:80:GLN:NE2	1.30	1.47
1:G:262:ALA:CB	2:T:80:GLN:HE22	1.29	1.44
2:L:80:GLN:NE2	1:U:259:GLU:CG	1.74	1.43
2:B:118:THR:HG23	1:M:228:GLN:NE2	1.39	1.37
2:B:118:THR:CG2	1:M:228:GLN:NE2	1.94	1.29
1:A:69:GLY:CA	1:A:188:VAL:CB	2.10	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLY:CA	1:A:219:GLY:HA3	1.61	1.28
2:L:80:GLN:OE1	1:U:259:GLU:N	1.66	1.25
1:G:228:GLN:OE1	2:R:118:THR:HG21	1.06	1.24
2:B:118:THR:HG21	1:M:228:GLN:CD	1.59	1.23
2:D:81:HIS:CE1	1:M:255:ALA:HA	1.74	1.22
1:G:228:GLN:CG	2:R:118:THR:CG2	2.17	1.21
1:G:228:GLN:CG	2:R:118:THR:HG22	1.72	1.19
1:K:114:ARG:HG2	2:L:306:GLY:N	1.62	1.14
1:S:65:PRO:O	2:T:189[A]:ARG:NH2	1.81	1.12
1:G:255:ALA:HB1	2:T:355:ARG:NH2	1.64	1.12
1:A:190:GLY:CA	1:A:219:GLY:CA	2.27	1.11
1:A:189:THR:CB	1:A:240:SER:OG	1.97	1.11
2:B:239:ASP:OD1	2:L:262:PRO:HG3	1.46	1.11
1:K:138:ILE:HG23	2:L:30:VAL:O	1.51	1.11
1:A:191:ALA:N	1:A:219:GLY:HA3	1.67	1.10
2:L:80:GLN:NE2	1:U:259:GLU:HG3	1.55	1.10
1:K:110:ASN:ND2	2:L:306:GLY:O	1.85	1.09
2:J:236:ARG:CD	2:T:261:ASP:OD1	2.03	1.06
1:I:255:ALA:HA	2:X:81:HIS:HE1	1.20	1.06
1:A:190:GLY:C	1:A:219:GLY:HA3	1.75	1.06
1:A:190:GLY:N	1:A:219:GLY:CA	2.18	1.05
1:S:64:ASP:OD2	2:T:185:ASN:ND2	1.87	1.05
1:I:255:ALA:HA	2:X:81:HIS:CE1	1.91	1.05
1:K:64:ASP:OD2	2:L:181:LYS:NZ	1.89	1.04
1:G:223:ARG:HH12	2:T:77:ARG:HD2	1.21	1.04
1:A:190:GLY:HA3	1:A:219:GLY:N	1.72	1.03
1:K:114:ARG:NE	2:L:303:ASP:O	1.89	1.03
1:G:259:GLU:OE2	2:T:355:ARG:HB3	1.56	1.03
2:L:356:MET:SD	1:U:259:GLU:OE2	2.19	1.01
1:A:259:GLU:HG3	2:P:80:GLN:HE22	1.25	1.01
2:D:81:HIS:HE1	1:M:255:ALA:HA	1.07	1.00
1:A:259:GLU:CG	2:P:80:GLN:HE22	1.73	1.00
2:J:162:ARG:HG3	2:L:397:VAL:HG21	1.41	1.00
1:G:228:GLN:CD	2:R:118:THR:CB	2.15	0.99
2:F:355:ARG:HB3	1:Q:259:GLU:OE2	1.63	0.99
2:L:80:GLN:OE1	1:U:258:GLY:C	2.01	0.98
1:G:259:GLU:HG2	2:T:356:MET:CE	1.93	0.98
2:F:355:ARG:NH2	1:Q:255:ALA:HB1	1.79	0.97
2:D:355:ARG:NH2	1:M:252:ARG:HE	1.60	0.97
2:B:118:THR:CG2	1:M:228:GLN:CD	2.29	0.97
1:G:259:GLU:HG2	2:T:356:MET:HE1	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:135:THR:HG23	2:L:358:GLY:O	1.63	0.96
1:K:65:PRO:O	2:L:189[A]:ARG:NH2	1.99	0.95
1:K:168:ARG:CD	2:L:35:MET:HB3	1.96	0.95
2:L:355:ARG:HH21	1:U:252:ARG:NE	1.63	0.95
2:D:260:ASP:O	2:R:236:ARG:HD2	1.67	0.95
2:F:355:ARG:CG	1:Q:259:GLU:OE2	2.13	0.95
1:A:189:THR:CB	1:A:240:SER:CB	2.44	0.95
2:F:355:ARG:HE	1:Q:259:GLU:CD	1.71	0.94
2:J:236:ARG:HD3	2:T:261:ASP:OD1	1.66	0.94
2:L:355:ARG:NH2	1:U:252:ARG:NE	2.16	0.93
1:K:168:ARG:NH2	2:L:35:MET:HG3	1.83	0.93
1:G:68:ASP:O	2:H:189[A]:ARG:NH2	2.02	0.93
1:A:69:GLY:H	1:A:188:VAL:HA	1.34	0.92
2:J:236:ARG:HD2	2:T:261:ASP:OD1	1.67	0.92
1:Q:68:ASP:O	2:R:189:ARG:NH2	2.03	0.92
1:K:65:PRO:O	2:L:189[B]:ARG:NH2	2.01	0.91
2:R:357:GLU:O	2:T:65:TYR:CE1	2.23	0.91
2:D:260:ASP:HB3	2:R:236:ARG:NE	1.86	0.91
1:K:168:ARG:CZ	2:L:35:MET:HG3	2.01	0.91
2:F:356:MET:CE	1:Q:259:GLU:HG2	2.01	0.90
1:K:168:ARG:NE	2:L:35:MET:CB	2.35	0.90
1:K:66:GLY:O	2:L:189[A]:ARG:CZ	2.20	0.89
2:D:81:HIS:HE1	1:M:255:ALA:CA	1.85	0.89
2:D:81:HIS:CE1	1:M:255:ALA:CA	2.55	0.89
2:F:355:ARG:CB	1:Q:259:GLU:OE2	2.21	0.89
2:J:64:ASN:HA	2:L:71:PRO:HB2	1.55	0.88
1:K:114:ARG:HG3	2:L:304:GLU:O	1.72	0.88
1:G:228:GLN:CG	2:R:118:THR:HG21	1.93	0.88
2:D:355:ARG:CZ	1:M:252:ARG:NE	2.37	0.88
1:G:255:ALA:HB1	2:T:355:ARG:HH22	1.39	0.87
2:L:355:ARG:NH2	1:U:252:ARG:CD	2.38	0.87
1:G:228:GLN:NE2	2:R:118:THR:CA	2.37	0.87
1:A:190:GLY:N	1:A:219:GLY:HA2	1.89	0.86
2:F:65:TYR:CE1	2:H:357:GLU:O	2.29	0.86
1:A:190:GLY:HA3	1:A:219:GLY:CA	2.01	0.86
2:D:355:ARG:NH2	1:M:252:ARG:NE	2.24	0.85
1:K:168:ARG:NE	2:L:35:MET:HB3	1.92	0.85
1:I:68:ASP:O	2:J:189:ARG:NH2	2.09	0.84
2:F:406:LEU:HD22	2:H:164:ARG:NH2	1.91	0.84
1:K:114:ARG:HG2	2:L:305:ASP:C	1.97	0.84
2:J:236:ARG:NH2	2:T:262:PRO:HD3	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:ARG:NH1	2:T:77:ARG:HD2	1.83	0.84
1:I:228:GLN:NE2	2:V:118:THR:HG23	1.93	0.83
2:J:406:LEU:HD22	2:L:164:ARG:NH2	1.93	0.83
1:A:191:ALA:H	1:A:219:GLY:HA3	1.39	0.83
1:I:228:GLN:NE2	2:V:118:THR:CG2	2.43	0.81
1:G:259:GLU:OE2	2:T:355:ARG:CB	2.28	0.81
1:G:262:ALA:HB2	2:T:80:GLN:CD	1.98	0.81
2:R:357:GLU:O	2:T:65:TYR:HE1	1.62	0.81
1:S:64:ASP:CG	2:T:185:ASN:HD21	1.84	0.81
1:W:68:ASP:O	2:X:189[A]:ARG:NH2	2.13	0.80
1:A:259:GLU:HG3	2:P:80:GLN:NE2	1.96	0.80
1:A:190:GLY:CA	1:A:219:GLY:N	2.44	0.80
2:J:236:ARG:NH1	2:T:262:PRO:HD2	1.96	0.80
1:G:248:GLU:OE1	2:T:404:PHE:O	2.00	0.79
2:J:236:ARG:HB3	2:T:227:ARG:HH22	1.47	0.79
2:F:164:ARG:C	2:H:406:LEU:HD13	2.03	0.79
1:G:228:GLN:OE1	2:R:118:THR:CG2	1.81	0.78
1:G:68:ASP:O	2:H:189[A]:ARG:NH1	2.17	0.78
1:S:114:ARG:HG2	2:T:306:GLY:CA	2.13	0.78
2:L:80:GLN:CD	1:U:259:GLU:HG3	2.02	0.78
1:I:252:ARG:HE	2:X:355:ARG:NH2	1.80	0.78
2:J:162:ARG:CG	2:L:397:VAL:HG21	2.12	0.78
2:F:64:ASN:O	2:H:73:TYR:HB2	1.84	0.77
1:A:69:GLY:HA3	1:A:188:VAL:CA	2.13	0.77
2:B:118:THR:HG23	1:M:228:GLN:HE21	1.48	0.77
1:G:68:ASP:O	2:H:189[A]:ARG:CZ	2.33	0.77
2:J:138:ALA:HB1	2:L:354:CYS:O	1.84	0.77
1:A:191:ALA:H	1:A:219:GLY:CA	1.96	0.77
2:D:348:ASP:OD2	1:M:251:PRO:HG2	1.84	0.77
1:A:69:GLY:N	1:A:188:VAL:HA	2.00	0.77
1:A:190:GLY:H	1:A:219:GLY:CA	1.97	0.76
1:G:259:GLU:CD	2:T:355:ARG:HE	1.88	0.76
1:A:189:THR:CB	1:A:240:SER:HB2	2.16	0.76
1:I:255:ALA:CA	2:X:81:HIS:HE1	1.96	0.76
1:A:190:GLY:HA3	1:A:218:LEU:C	2.06	0.76
2:J:166:LEU:HD21	2:L:360:ILE:HG13	1.65	0.76
1:I:255:ALA:CA	2:X:81:HIS:CE1	2.69	0.76
1:E:138:ILE:HD13	2:F:35:MET:SD	2.26	0.76
2:B:118:THR:HG21	1:M:228:GLN:OE1	1.85	0.75
2:D:355:ARG:NE	1:M:252:ARG:CZ	2.49	0.75
1:A:190:GLY:HA3	1:A:219:GLY:HA3	1.61	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:355:ARG:NE	1:Q:259:GLU:OE2	2.19	0.75
2:F:65:TYR:HE1	2:H:357:GLU:O	1.68	0.75
1:K:114:ARG:CG	2:L:306:GLY:N	2.47	0.75
1:G:228:GLN:NE2	2:R:118:THR:HG22	1.17	0.75
1:G:228:GLN:OE1	2:R:118:THR:CB	2.28	0.75
2:H:143:ASP:OD1	1:Q:222:SER:OG	2.05	0.74
1:K:111:PRO:HA	2:L:305:ASP:O	1.87	0.74
1:K:141:GLU:HB3	2:L:29:TYR:CE2	2.22	0.74
2:F:356:MET:HE1	1:Q:259:GLU:HG2	1.70	0.74
2:B:239:ASP:OD1	2:L:262:PRO:CG	2.31	0.74
2:B:118:THR:HG23	1:M:228:GLN:HE22	1.50	0.74
1:C:68:ASP:O	2:D:189[A]:ARG:NH2	2.20	0.74
2:F:356:MET:HE3	1:Q:259:GLU:HG2	1.68	0.74
1:S:114:ARG:NH2	2:T:302:GLN:HG3	2.03	0.74
2:L:80:GLN:OE1	1:U:259:GLU:CA	2.36	0.73
1:W:161:ALA:CB	2:X:33:ALA:HA	2.19	0.73
2:J:236:ARG:HB3	2:T:227:ARG:NH2	2.03	0.73
2:R:401:ALA:N	2:T:165:LEU:HD21	2.03	0.73
2:D:355:ARG:HE	1:M:252:ARG:NH2	1.86	0.73
1:G:262:ALA:HB2	2:T:80:GLN:HE22	0.59	0.73
1:S:141:GLU:HG3	2:T:28:ARG:O	1.87	0.73
2:F:80:GLN:OE1	1:Q:262:ALA:HB2	1.89	0.73
2:F:355:ARG:CZ	1:Q:255:ALA:HB1	2.17	0.72
1:A:69:GLY:CA	1:A:188:VAL:CA	2.68	0.72
1:S:135:PRO:O	2:T:31:PRO:HB3	1.90	0.72
2:R:73:TYR:HB2	2:T:64:ASN:O	1.89	0.72
2:J:397:VAL:HG21	2:L:162:ARG:HG3	1.71	0.72
1:S:138:ILE:HD13	2:T:35:MET:HG3	1.72	0.72
2:R:401:ALA:HA	2:T:165:LEU:HD21	1.71	0.71
1:G:228:GLN:CD	2:R:118:THR:HG22	1.17	0.71
2:F:355:ARG:CD	1:Q:259:GLU:OE2	2.39	0.71
1:G:228:GLN:CD	2:R:118:THR:HG21	0.52	0.71
2:J:64:ASN:HA	2:L:71:PRO:CB	2.21	0.71
1:A:69:GLY:N	1:A:188:VAL:CA	2.54	0.70
1:A:252:ARG:HD2	2:P:355:ARG:NH2	2.05	0.70
2:J:135:THR:O	2:L:358:GLY:HA3	1.91	0.70
1:O:68:ASP:O	2:P:189[A]:ARG:NH2	2.24	0.70
1:G:228:GLN:CD	2:R:118:THR:CG2	0.90	0.70
1:G:259:GLU:HG2	2:T:356:MET:HE3	1.73	0.70
1:S:138:ILE:HD13	2:T:35:MET:CG	2.21	0.70
2:J:73:TYR:OH	2:L:139:LEU:HD11	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:355:ARG:HG2	1:Q:259:GLU:OE2	1.91	0.69
2:F:355:ARG:NE	1:Q:259:GLU:CD	2.43	0.69
1:G:223:ARG:HD3	2:T:77:ARG:HH22	1.57	0.69
2:F:165:LEU:HD21	2:H:401:ALA:N	2.07	0.69
2:D:355:ARG:CZ	1:M:252:ARG:CZ	2.70	0.69
1:K:138:ILE:CG2	2:L:30:VAL:O	2.38	0.69
1:G:225:GLN:OE1	2:R:143:ASP:OD2	2.11	0.68
1:O:65:PRO:O	2:P:189[A]:ARG:NH2	2.26	0.68
1:A:191:ALA:N	1:A:219:GLY:CA	2.49	0.68
1:S:66:GLY:O	2:T:189[B]:ARG:HG2	1.92	0.68
1:C:68:ASP:O	2:D:189[A]:ARG:NH1	2.26	0.68
1:S:66:GLY:O	2:T:189[A]:ARG:HG2	1.94	0.68
2:F:407:LEU:N	2:F:407:LEU:HD12	2.00	0.68
1:S:68:ASP:O	2:T:189[A]:ARG:NH1	2.26	0.68
2:J:139:LEU:HD11	2:L:73:TYR:OH	1.94	0.68
2:R:401:ALA:CA	2:T:165:LEU:HD21	2.23	0.68
2:J:138:ALA:HB3	2:L:358:GLY:HA2	1.76	0.68
2:N:135:THR:HG23	2:P:358:GLY:O	1.95	0.67
2:D:260:ASP:O	2:R:236:ARG:CD	2.41	0.67
2:L:355:ARG:NH2	1:U:252:ARG:HD2	2.09	0.67
2:B:118:THR:CG2	1:M:228:GLN:HE22	2.02	0.67
2:V:406:LEU:HD22	2:X:164:ARG:NH2	2.09	0.67
2:J:236:ARG:NH2	2:T:260:ASP:O	2.27	0.67
1:S:113:LEU:CD1	2:T:292:ALA:HB2	2.24	0.67
2:J:166:LEU:HG	2:L:360:ILE:HD11	1.76	0.66
2:R:73:TYR:HD1	2:T:64:ASN:HB3	1.60	0.66
1:K:114:ARG:CG	2:L:305:ASP:C	2.63	0.66
2:H:406:LEU:O	2:H:407:LEU:HG	1.95	0.66
2:J:392:ARG:NH2	2:L:392:ARG:NH1	2.44	0.66
2:J:397:VAL:CG1	2:L:161:ALA:CB	2.73	0.66
1:A:184:SER:OG	1:A:218:LEU:HD12	1.96	0.66
1:G:262:ALA:CB	2:T:80:GLN:NE2	2.13	0.66
1:I:252:ARG:NE	2:X:355:ARG:CZ	2.59	0.66
2:J:161:ALA:CB	2:L:397:VAL:CG1	2.74	0.66
1:O:114:ARG:HG2	2:P:306:GLY:N	2.11	0.66
2:L:80:GLN:HE22	1:U:259:GLU:HG2	0.49	0.65
2:J:166:LEU:CD1	2:L:360:ILE:HD11	2.26	0.65
1:G:223:ARG:HH12	2:T:77:ARG:CD	2.04	0.65
2:T:406:LEU:O	2:T:407:LEU:HG	1.97	0.65
2:J:65:TYR:O	2:L:91:ARG:NH2	2.29	0.65
2:L:406:LEU:O	2:L:407:LEU:HG	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:65:PRO:O	2:P:189[B]:ARG:NH2	2.31	0.64
1:G:259:GLU:OE2	2:T:355:ARG:NE	2.28	0.64
1:I:228:GLN:CD	2:V:118:THR:HG21	2.18	0.64
2:D:260:ASP:O	2:R:236:ARG:NH1	2.31	0.64
1:K:161:ALA:HB2	2:L:33:ALA:HB2	1.79	0.64
1:O:68:ASP:O	2:P:189[A]:ARG:NH1	2.30	0.64
2:F:165:LEU:HD21	2:H:400:ALA:C	2.19	0.63
2:J:397:VAL:HG11	2:L:161:ALA:HB3	1.80	0.63
2:P:406:LEU:O	2:P:407:LEU:HG	1.98	0.63
2:X:406:LEU:O	2:X:407:LEU:HG	1.98	0.63
2:J:161:ALA:CB	2:L:397:VAL:HG12	2.28	0.63
1:I:252:ARG:NE	2:X:355:ARG:NH2	2.45	0.63
1:S:138:ILE:HD13	2:T:35:MET:SD	2.38	0.63
2:F:355:ARG:HH22	1:Q:255:ALA:HB1	1.59	0.63
1:G:222:SER:OG	2:R:143:ASP:OD1	2.15	0.63
1:K:114:ARG:HB2	2:L:306:GLY:HA3	1.81	0.63
1:I:251:PRO:HG2	2:X:348:ASP:OD2	1.98	0.63
1:A:190:GLY:H	1:A:219:GLY:N	1.97	0.63
1:G:224:ALA:CB	2:R:142:LEU:HA	2.29	0.63
2:J:138:ALA:HB3	2:L:358:GLY:CA	2.28	0.62
1:G:262:ALA:HB1	2:T:80:GLN:HE22	1.54	0.62
1:W:68:ASP:O	2:X:189[A]:ARG:CZ	2.47	0.62
1:G:228:GLN:HE21	2:R:118:THR:CG2	1.31	0.62
1:A:265:ARG:C	1:A:266:LEU:HG	2.17	0.62
1:A:190:GLY:N	1:A:219:GLY:HA3	1.98	0.62
1:K:66:GLY:O	2:L:189[B]:ARG:HG2	2.00	0.62
2:F:164:ARG:O	2:H:406:LEU:HD13	1.99	0.62
2:J:161:ALA:HB1	2:L:397:VAL:HG12	1.80	0.62
2:H:406:LEU:C	2:H:407:LEU:HG	2.20	0.62
2:J:392:ARG:CZ	2:L:392:ARG:CZ	2.77	0.62
1:W:161:ALA:HB3	2:X:33:ALA:HA	1.81	0.62
1:A:190:GLY:N	1:A:219:GLY:N	2.48	0.61
2:F:162:ARG:CG	2:H:397:VAL:HG21	2.30	0.61
2:D:355:ARG:NE	1:M:252:ARG:NH2	2.48	0.61
2:F:407:LEU:N	2:F:407:LEU:CD1	2.63	0.61
1:I:228:GLN:NE2	2:V:118:THR:HG21	2.15	0.61
2:D:406:LEU:O	2:D:407:LEU:HG	2.00	0.61
2:J:63:ALA:O	2:L:71:PRO:HB3	1.99	0.61
1:I:85:ARG:HA	2:J:305:ASP:OD2	1.99	0.61
1:O:68:ASP:O	2:P:189[A]:ARG:CZ	2.49	0.61
1:W:68:ASP:O	2:X:189[A]:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:71:PRO:HB2	2:L:64:ASN:HA	1.82	0.61
2:J:397:VAL:CG1	2:L:161:ALA:HB3	2.30	0.61
1:K:168:ARG:CZ	2:L:35:MET:CG	2.77	0.61
1:U:265:ARG:C	1:U:266:LEU:HG	2.17	0.61
2:N:113:ARG:HG3	2:N:113:ARG:HH11	1.66	0.61
2:J:166:LEU:CG	2:L:360:ILE:HD11	2.31	0.60
2:R:406:LEU:HD13	2:T:164:ARG:C	2.22	0.60
2:V:113:ARG:HG3	2:V:113:ARG:HH11	1.67	0.60
1:E:135:PRO:O	2:F:31:PRO:HB3	2.01	0.60
2:J:161:ALA:HB3	2:L:397:VAL:CG1	2.31	0.60
1:A:189:THR:CB	1:A:240:SER:H	2.13	0.60
2:J:139:LEU:HA	2:L:357:GLU:HA	1.84	0.60
2:J:166:LEU:HD21	2:L:360:ILE:CG1	2.31	0.60
2:N:162:ARG:HG3	2:P:397:VAL:HG21	1.83	0.60
1:K:114:ARG:HG2	2:L:306:GLY:H	1.61	0.60
2:J:236:ARG:HH12	2:T:262:PRO:HD2	1.66	0.60
1:K:168:ARG:CD	2:L:35:MET:CB	2.73	0.60
2:F:80:GLN:OE1	1:Q:262:ALA:CB	2.49	0.59
2:P:406:LEU:C	2:P:407:LEU:HG	2.22	0.59
1:A:184:SER:OG	1:A:218:LEU:CD1	2.50	0.59
2:J:64:ASN:CA	2:L:71:PRO:HB2	2.29	0.59
2:J:138:ALA:CB	2:L:354:CYS:O	2.50	0.59
1:K:114:ARG:CG	2:L:304:GLU:O	2.49	0.59
1:M:68:ASP:O	2:N:189:ARG:NH2	2.35	0.59
2:F:164:ARG:NH1	2:H:406:LEU:C	2.56	0.59
1:M:265:ARG:C	1:M:266:LEU:HG	2.18	0.59
1:I:265:ARG:C	1:I:266:LEU:HG	2.18	0.59
1:K:66:GLY:O	2:L:189[B]:ARG:NE	2.36	0.59
2:B:118:THR:HG21	1:M:228:GLN:NE2	1.81	0.59
2:F:135:THR:HG23	2:H:358:GLY:O	2.02	0.59
1:S:113:LEU:HD12	2:T:292:ALA:CB	2.32	0.59
2:F:162:ARG:HG3	2:H:397:VAL:HG21	1.84	0.59
1:G:255:ALA:HB1	2:T:355:ARG:CZ	2.31	0.59
2:L:406:LEU:C	2:L:407:LEU:HG	2.23	0.59
1:S:110:ASN:HB2	2:T:292:ALA:O	2.03	0.59
2:B:113:ARG:HG3	2:B:113:ARG:HH11	1.66	0.58
2:J:113:ARG:HG3	2:J:113:ARG:HH11	1.67	0.58
2:R:358:GLY:HA3	2:T:65:TYR:OH	2.03	0.58
2:R:113:ARG:HH11	2:R:113:ARG:HG3	1.68	0.58
2:J:397:VAL:CG1	2:L:161:ALA:HB1	2.34	0.58
2:R:400:ALA:C	2:T:165:LEU:HD21	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:406:LEU:C	2:T:407:LEU:HG	2.23	0.58
1:S:113:LEU:HD12	2:T:292:ALA:HB3	1.84	0.58
1:K:168:ARG:NH1	2:L:35:MET:CE	2.66	0.58
1:O:161:ALA:CB	2:P:33:ALA:HA	2.34	0.58
1:S:114:ARG:HG2	2:T:306:GLY:N	2.18	0.58
2:F:397:VAL:CG1	2:H:161:ALA:HB3	2.33	0.57
1:K:114:ARG:HH21	2:L:303:ASP:C	2.07	0.57
2:X:406:LEU:C	2:X:407:LEU:HG	2.23	0.57
2:H:143:ASP:OD2	1:Q:225:GLN:CG	2.52	0.57
1:I:135:PRO:O	2:J:31:PRO:HA	2.03	0.57
2:L:80:GLN:CD	1:U:259:GLU:CG	2.57	0.57
1:S:66:GLY:HA3	2:T:188:PHE:CE1	2.40	0.57
1:U:68:ASP:O	2:V:189:ARG:NH2	2.31	0.57
2:J:94:LEU:HD22	2:L:96:HIS:HA	1.87	0.57
1:Q:265:ARG:C	1:Q:266:LEU:HG	2.23	0.57
2:F:397:VAL:HG11	2:H:161:ALA:HB3	1.87	0.57
1:I:67:MET:SD	2:J:31:PRO:HG3	2.44	0.57
1:A:68:ASP:O	2:B:189:ARG:NH2	2.32	0.57
1:O:138:ILE:HG23	2:P:30:VAL:O	2.05	0.57
2:R:357:GLU:O	2:T:65:TYR:CZ	2.58	0.57
1:C:68:ASP:O	2:D:189[A]:ARG:CZ	2.52	0.56
2:D:260:ASP:O	2:R:236:ARG:CZ	2.53	0.56
1:E:141:GLU:HG3	2:F:28:ARG:O	2.05	0.56
2:J:162:ARG:HG3	2:L:397:VAL:CG2	2.26	0.56
2:J:360:ILE:HD11	2:L:166:LEU:HG	1.87	0.56
1:C:161:ALA:CB	2:D:33:ALA:HA	2.34	0.56
2:R:73:TYR:HD1	2:T:64:ASN:CB	2.19	0.56
2:J:94:LEU:CD2	2:L:96:HIS:HA	2.36	0.56
2:J:236:ARG:CZ	2:T:262:PRO:HD3	2.35	0.56
2:L:355:ARG:HH21	1:U:252:ARG:CZ	2.16	0.56
1:I:228:GLN:HE22	2:V:118:THR:HG23	1.71	0.56
1:E:66:GLY:HA3	2:F:188:PHE:CE1	2.41	0.56
1:K:114:ARG:HB3	2:L:305:ASP:O	2.05	0.56
2:D:406:LEU:C	2:D:407:LEU:HG	2.25	0.56
2:F:64:ASN:HB3	2:H:73:TYR:HD1	1.70	0.56
1:G:225:GLN:HG3	2:R:143:ASP:OD2	2.06	0.56
2:D:80:GLN:OE1	1:M:258:GLY:O	2.25	0.55
2:J:166:LEU:HD11	2:L:360:ILE:HD11	1.87	0.55
2:N:161:ALA:HB3	2:P:397:VAL:CG1	2.37	0.55
1:A:190:GLY:H	1:A:219:GLY:HA2	1.61	0.55
2:B:407:LEU:HD12	2:B:407:LEU:N	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:236:ARG:NH1	2:T:262:PRO:CD	2.68	0.55
2:H:143:ASP:OD2	1:Q:225:GLN:HG3	2.07	0.55
1:K:168:ARG:HB3	2:L:32:GLU:OE2	2.07	0.55
2:R:407:LEU:CD1	2:R:407:LEU:N	2.68	0.55
2:F:65:TYR:CZ	2:H:357:GLU:O	2.59	0.55
2:F:165:LEU:HD21	2:H:401:ALA:HA	1.87	0.55
2:F:397:VAL:CG1	2:H:161:ALA:CB	2.84	0.55
2:F:65:TYR:HH	2:H:358:GLY:HA3	1.71	0.55
2:J:358:GLY:CA	2:L:138:ALA:HB3	2.35	0.55
2:J:96:HIS:HB2	2:L:94:LEU:HD21	1.88	0.55
2:J:161:ALA:HB1	2:L:397:VAL:CG1	2.37	0.55
1:K:66:GLY:O	2:L:189[A]:ARG:NH1	2.39	0.55
2:V:165:LEU:HD12	2:X:397:VAL:HG13	1.88	0.55
2:H:142:LEU:HA	1:Q:224:ALA:HB1	1.90	0.54
1:K:168:ARG:HD2	2:L:35:MET:HB3	1.85	0.54
2:N:407:LEU:HD12	2:N:407:LEU:N	2.20	0.54
2:R:407:LEU:N	2:R:407:LEU:HD12	2.16	0.54
2:F:165:LEU:HD21	2:H:401:ALA:CA	2.36	0.54
1:K:114:ARG:HB2	2:L:306:GLY:CA	2.37	0.54
1:W:138:ILE:HG23	2:X:30:VAL:O	2.08	0.54
1:E:65:PRO:O	2:F:189:ARG:NH1	2.40	0.54
1:G:223:ARG:HD3	2:T:77:ARG:NH2	2.20	0.54
1:K:168:ARG:NH1	2:L:35:MET:HE2	2.22	0.54
2:H:142:LEU:HA	1:Q:224:ALA:CB	2.38	0.54
2:J:94:LEU:HD22	2:L:96:HIS:CA	2.37	0.54
1:G:228:GLN:HE21	2:R:118:THR:HG23	0.86	0.54
2:N:406:LEU:HD22	2:P:164:ARG:NH2	2.22	0.54
2:V:64:ASN:O	2:X:73:TYR:HB2	2.08	0.54
1:K:114:ARG:CB	2:L:305:ASP:C	2.77	0.53
2:N:139:LEU:HD11	2:P:73:TYR:OH	2.09	0.53
1:G:161:ALA:CB	2:H:33:ALA:HA	2.39	0.53
1:I:252:ARG:CZ	2:X:355:ARG:NE	2.71	0.53
1:S:113:LEU:CD1	2:T:292:ALA:CB	2.86	0.53
2:J:236:ARG:CZ	2:T:260:ASP:O	2.57	0.53
2:J:236:ARG:HH22	2:T:262:PRO:HD3	1.70	0.53
1:K:114:ARG:HB3	2:L:305:ASP:C	2.29	0.53
1:K:161:ALA:HB3	2:L:33:ALA:HA	1.90	0.53
1:W:163:SER:O	2:X:36:ALA:HB2	2.08	0.53
2:B:64:ASN:O	2:D:73:TYR:HB2	2.09	0.53
2:D:80:GLN:OE1	1:M:258:GLY:C	2.46	0.53
1:S:114:ARG:HH21	2:T:302:GLN:HG3	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:HIS:CE1	1:M:255:ALA:CB	2.92	0.53
1:A:255:ALA:O	2:P:80:GLN:OE1	2.26	0.52
2:J:65:TYR:O	2:L:94:LEU:HD11	2.08	0.52
2:R:406:LEU:CD1	2:T:165:LEU:HA	2.39	0.52
1:I:258:GLY:O	2:X:80:GLN:OE1	2.26	0.52
1:M:62:TYR:HA	2:N:307:GLN:OE1	2.09	0.52
2:R:406:LEU:HD12	2:T:165:LEU:HD23	1.90	0.52
2:J:71:PRO:HB2	2:L:64:ASN:O	2.10	0.52
2:R:406:LEU:O	2:R:407:LEU:HB2	2.10	0.52
2:J:71:PRO:CB	2:L:64:ASN:HA	2.39	0.52
2:F:165:LEU:HA	2:H:406:LEU:CD1	2.40	0.52
1:I:252:ARG:NH2	2:X:355:ARG:HE	2.08	0.52
2:N:161:ALA:CB	2:P:397:VAL:CG1	2.88	0.52
2:N:407:LEU:N	2:N:407:LEU:CD1	2.73	0.51
2:B:407:LEU:N	2:B:407:LEU:CD1	2.71	0.51
2:B:113:ARG:HG3	2:B:113:ARG:NH1	2.25	0.51
2:D:260:ASP:HB3	2:R:236:ARG:CD	2.41	0.51
2:J:96:HIS:HB2	2:L:94:LEU:CD2	2.41	0.51
2:V:165:LEU:CD1	2:X:397:VAL:HG13	2.41	0.51
1:G:227:ALA:CB	1:G:266:LEU:HD12	2.40	0.51
2:N:113:ARG:HG3	2:N:113:ARG:NH1	2.25	0.51
1:S:138:ILE:HG22	2:T:32:GLU:HB2	1.93	0.51
2:F:138:ALA:O	2:H:355:ARG:O	2.28	0.50
2:V:113:ARG:HG3	2:V:113:ARG:NH1	2.26	0.50
1:E:159:LEU:O	2:F:32:GLU:HG2	2.12	0.50
1:K:168:ARG:NE	2:L:35:MET:HB2	2.23	0.50
1:A:252:ARG:CD	2:P:355:ARG:NH2	2.73	0.50
2:F:65:TYR:OH	2:H:357:GLU:O	2.29	0.50
2:J:407:LEU:CD1	2:J:407:LEU:N	2.72	0.50
2:R:113:ARG:HG3	2:R:113:ARG:NH1	2.26	0.50
1:W:65:PRO:O	2:X:189[B]:ARG:NH2	2.45	0.50
1:E:85:ARG:HE	2:F:305:ASP:CG	2.14	0.50
2:J:113:ARG:HG3	2:J:113:ARG:NH1	2.26	0.50
2:R:94:LEU:HD13	2:T:67:GLY:HA3	1.94	0.50
1:O:111:PRO:HA	2:P:305:ASP:O	2.11	0.50
2:B:73:TYR:HB2	2:D:64:ASN:O	2.12	0.50
1:E:85:ARG:NH2	2:F:305:ASP:OD1	2.42	0.50
2:V:406:LEU:O	2:V:407:LEU:HB2	2.11	0.50
1:K:168:ARG:NE	2:L:35:MET:CG	2.74	0.50
1:O:161:ALA:HB3	2:P:33:ALA:HA	1.93	0.50
1:U:110:ASN:HB2	2:V:292:ALA:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:LEU:O	2:B:407:LEU:HB2	2.12	0.50
1:A:69:GLY:HA2	1:A:188:VAL:CB	2.32	0.49
2:J:165:LEU:HD21	2:L:400:ALA:C	2.32	0.49
2:J:406:LEU:O	2:J:407:LEU:HB2	2.11	0.49
1:G:225:GLN:CG	2:R:143:ASP:OD2	2.60	0.49
1:I:258:GLY:C	2:X:80:GLN:OE1	2.51	0.49
2:J:165:LEU:HD21	2:L:401:ALA:N	2.27	0.49
2:V:407:LEU:HD12	2:V:407:LEU:N	2.21	0.49
2:F:65:TYR:O	2:H:91:ARG:NH2	2.34	0.49
1:G:259:GLU:CG	2:T:356:MET:HE1	2.30	0.49
2:V:135:THR:HG23	2:X:358:GLY:O	2.12	0.49
1:E:138:ILE:HD13	2:F:35:MET:CG	2.43	0.49
2:J:65:TYR:CE1	2:L:359:ILE:HD11	2.48	0.49
2:J:236:ARG:CZ	2:T:262:PRO:CD	2.90	0.49
2:N:406:LEU:O	2:N:407:LEU:HB2	2.12	0.49
1:C:163:SER:O	2:D:36:ALA:HB2	2.13	0.49
2:R:357:GLU:O	2:T:65:TYR:OH	2.31	0.49
2:J:407:LEU:N	2:J:407:LEU:HD12	2.19	0.49
2:D:348:ASP:OD2	1:M:251:PRO:CG	2.59	0.49
2:J:161:ALA:HB3	2:L:397:VAL:HG11	1.93	0.49
1:K:66:GLY:O	2:L:189[A]:ARG:HG2	2.12	0.49
1:K:168:ARG:NE	2:L:35:MET:HG3	2.25	0.49
1:A:259:GLU:CG	2:P:80:GLN:NE2	2.56	0.49
2:D:355:ARG:NH2	1:M:252:ARG:CZ	2.75	0.49
1:G:259:GLU:OE2	2:T:355:ARG:CD	2.61	0.49
2:J:392:ARG:NH2	2:L:392:ARG:CZ	2.76	0.49
2:D:260:ASP:HB3	2:R:236:ARG:HE	1.72	0.48
2:J:64:ASN:O	2:L:71:PRO:HB2	2.13	0.48
1:M:161:ALA:CB	2:N:33:ALA:HA	2.43	0.48
1:I:85:ARG:HE	2:J:305:ASP:CG	2.17	0.48
2:F:162:ARG:HG3	2:H:397:VAL:HG11	1.96	0.48
1:W:168:ARG:NE	2:X:35:MET:HB3	2.29	0.48
2:F:404:PHE:O	1:Q:248:GLU:OE2	2.31	0.48
1:K:66:GLY:O	2:L:189[B]:ARG:CG	2.61	0.48
2:V:162:ARG:HG3	2:X:397:VAL:HG21	1.95	0.48
2:R:397:VAL:HG21	2:T:162:ARG:CG	2.43	0.48
2:R:401:ALA:HA	2:T:165:LEU:CD2	2.42	0.48
2:D:77:ARG:NH1	1:M:223:ARG:HE	2.11	0.48
1:K:168:ARG:NH1	2:L:35:MET:HE3	2.28	0.48
1:Q:161:ALA:CB	2:R:33:ALA:HA	2.44	0.48
2:R:358:GLY:CA	2:T:65:TYR:OH	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:86:VAL:N	2:V:305:ASP:OD2	2.39	0.48
2:F:65:TYR:HH	2:H:358:GLY:CA	2.27	0.48
1:W:65:PRO:O	2:X:189[A]:ARG:NH2	2.46	0.48
1:I:66:GLY:C	2:J:188:PHE:HE1	2.17	0.48
2:V:407:LEU:N	2:V:407:LEU:CD1	2.72	0.48
2:V:397:VAL:HG21	2:X:162:ARG:HG3	1.96	0.47
2:F:406:LEU:O	2:F:407:LEU:HB2	2.14	0.47
2:H:142:LEU:CA	1:Q:224:ALA:CB	2.92	0.47
1:K:66:GLY:C	2:L:189[A]:ARG:CZ	2.81	0.47
2:R:161:ALA:HB3	2:T:397:VAL:HG11	1.96	0.47
2:J:166:LEU:HA	2:L:354:CYS:HB3	1.96	0.47
1:K:114:ARG:CZ	2:L:303:ASP:O	2.59	0.47
1:S:67:MET:SD	2:T:192:VAL:HG11	2.54	0.47
1:S:110:ASN:OD1	2:T:292:ALA:N	2.45	0.47
2:F:166:LEU:HD11	2:H:360:ILE:HD11	1.97	0.47
2:F:164:ARG:HB3	2:H:406:LEU:HB3	1.95	0.47
2:R:407:LEU:HD12	2:R:407:LEU:HA	1.67	0.47
2:F:356:MET:HE1	1:Q:259:GLU:CG	2.41	0.47
1:I:255:ALA:CB	2:X:81:HIS:CE1	2.97	0.47
1:K:64:ASP:HB3	2:L:185:ASN:HD21	1.80	0.47
2:R:358:GLY:O	2:T:96:HIS:NE2	2.37	0.47
2:J:360:ILE:HG13	2:L:166:LEU:HD21	1.96	0.46
1:E:135:PRO:O	2:F:31:PRO:CB	2.63	0.46
2:F:355:ARG:NH2	1:Q:255:ALA:CB	2.66	0.46
1:S:227:ALA:CB	1:S:266:LEU:HD12	2.45	0.46
1:M:161:ALA:HB3	2:N:33:ALA:HA	1.97	0.46
1:O:168:ARG:NE	2:P:35:MET:HB3	2.30	0.46
1:E:138:ILE:HG21	2:F:35:MET:HG3	1.98	0.46
2:N:161:ALA:HB3	2:P:397:VAL:HG11	1.98	0.46
1:K:62:TYR:HD1	2:L:307:GLN:OE1	1.98	0.46
2:P:21:GLY:HA3	2:P:22:PRO:HD3	1.69	0.46
2:F:65:TYR:OH	2:H:358:GLY:HA3	2.16	0.46
1:I:159:LEU:O	2:J:32:GLU:HG2	2.16	0.46
1:K:114:ARG:HG2	2:L:305:ASP:CA	2.45	0.46
1:O:114:ARG:HG3	2:P:304:GLU:O	2.15	0.46
1:S:227:ALA:HB2	1:S:266:LEU:HD12	1.98	0.46
1:C:266:LEU:HA	1:C:266:LEU:HD23	1.79	0.46
2:J:397:VAL:HG12	2:L:161:ALA:HB1	1.98	0.46
1:S:65:PRO:HD2	2:T:189[B]:ARG:HH22	1.81	0.46
2:J:139:LEU:HD12	2:L:357:GLU:OE1	2.15	0.45
1:K:114:ARG:CG	2:L:304:GLU:C	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:ALA:HB1	2:H:355:ARG:HA	1.99	0.45
1:O:266:LEU:HA	1:O:266:LEU:HD23	1.80	0.45
2:B:406:LEU:HD22	2:D:164:ARG:NH2	2.32	0.45
1:S:66:GLY:HA3	2:T:188:PHE:HE1	1.81	0.45
2:J:96:HIS:CA	2:L:94:LEU:HD22	2.47	0.45
2:R:397:VAL:HG13	2:T:165:LEU:HD12	1.98	0.45
2:R:406:LEU:HD13	2:T:164:ARG:O	2.16	0.45
2:F:113:ARG:HH11	2:F:113:ARG:HG3	1.82	0.45
1:G:228:GLN:NE2	2:R:118:THR:N	2.65	0.45
1:W:168:ARG:CD	2:X:35:MET:HB3	2.47	0.45
1:C:227:ALA:CB	1:C:266:LEU:HD12	2.47	0.45
1:E:110:ASN:OD1	2:F:292:ALA:N	2.44	0.45
1:E:135:PRO:O	2:F:31:PRO:HA	2.17	0.45
2:R:161:ALA:CB	2:T:397:VAL:CG1	2.95	0.45
1:A:191:ALA:N	1:A:219:GLY:O	2.51	0.44
2:N:407:LEU:HD12	2:N:407:LEU:HA	1.67	0.44
2:B:165:LEU:CD1	2:D:397:VAL:HG13	2.48	0.44
1:C:227:ALA:HB2	1:C:266:LEU:HD12	2.00	0.44
1:I:252:ARG:CZ	2:X:355:ARG:CZ	2.96	0.44
1:U:138:ILE:HD13	2:V:35:MET:SD	2.58	0.44
1:G:227:ALA:HB1	1:G:266:LEU:HD12	1.99	0.44
2:L:285:PHE:CD1	2:L:331:LYS:HD2	2.53	0.44
1:M:138:ILE:HG23	2:N:30:VAL:O	2.18	0.44
2:P:285:PHE:CD1	2:P:331:LYS:HD2	2.53	0.44
1:A:191:ALA:H	1:A:219:GLY:C	2.20	0.44
1:O:168:ARG:CD	2:P:35:MET:HB3	2.47	0.44
1:E:138:ILE:CD1	2:F:35:MET:SD	3.03	0.44
1:A:252:ARG:HD2	2:P:355:ARG:HH21	1.82	0.44
2:J:139:LEU:CD1	2:L:357:GLU:OE1	2.65	0.44
2:J:141:GLY:CA	2:L:77:ARG:NH2	2.81	0.44
1:K:168:ARG:HE	2:L:35:MET:CB	2.25	0.44
2:T:21:GLY:HA3	2:T:22:PRO:HD3	1.70	0.44
1:W:227:ALA:CB	1:W:266:LEU:HD12	2.47	0.44
2:V:65:TYR:O	2:X:91:ARG:NH2	2.49	0.44
2:V:91:ARG:NH1	2:X:65:TYR:O	2.48	0.44
2:B:236:ARG:CZ	2:L:260:ASP:O	2.66	0.44
2:F:96:HIS:NE2	2:H:358:GLY:O	2.41	0.44
2:R:397:VAL:HG11	2:T:162:ARG:HG3	1.99	0.44
2:J:141:GLY:HA2	2:L:77:ARG:NH2	2.33	0.43
1:M:64:ASP:OD2	2:N:308:THR:HB	2.18	0.43
2:R:161:ALA:HB1	2:T:397:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:GLY:HA3	2:D:22:PRO:HD3	1.69	0.43
2:R:406:LEU:HD22	2:T:164:ARG:NH2	2.33	0.43
1:S:85:ARG:HH11	2:T:305:ASP:CG	2.21	0.43
1:W:111:PRO:HA	2:X:305:ASP:O	2.18	0.43
2:F:67:GLY:HA3	2:H:94:LEU:HD13	2.00	0.43
1:G:223:ARG:NH1	2:T:77:ARG:CD	2.66	0.43
1:G:225:GLN:CD	2:R:143:ASP:OD2	2.56	0.43
1:I:110:ASN:OD1	2:J:292:ALA:N	2.46	0.43
2:T:285:PHE:CD1	2:T:331:LYS:HD2	2.54	0.43
1:I:66:GLY:HA3	2:J:188:PHE:CE1	2.54	0.43
2:J:397:VAL:HG12	2:L:161:ALA:CB	2.46	0.43
2:N:64:ASN:O	2:P:73:TYR:HB2	2.18	0.43
1:A:189:THR:CA	1:A:240:SER:OG	2.65	0.43
2:L:113:ARG:NH2	2:L:140:LEU:O	2.49	0.43
2:B:113:ARG:HH11	2:B:113:ARG:CG	2.27	0.43
1:E:138:ILE:HG21	2:F:35:MET:CG	2.49	0.43
2:H:21:GLY:HA3	2:H:22:PRO:HD3	1.78	0.43
2:J:65:TYR:HE1	2:L:359:ILE:HD11	1.83	0.43
2:J:236:ARG:CZ	2:T:261:ASP:HA	2.48	0.43
1:K:168:ARG:HE	2:L:35:MET:HB2	1.82	0.43
1:U:65:PRO:O	2:V:189:ARG:NH1	2.52	0.43
2:D:113:ARG:NH2	2:D:140:LEU:O	2.48	0.42
2:D:230:ILE:HG21	2:D:238:PRO:HD3	2.01	0.42
1:K:227:ALA:CB	1:K:266:LEU:HD12	2.49	0.42
1:C:160:VAL:HA	2:D:32:GLU:HG2	2.01	0.42
2:J:165:LEU:HD11	2:L:397:VAL:HA	2.01	0.42
1:M:86:VAL:N	2:N:305:ASP:OD2	2.49	0.42
1:S:114:ARG:HG2	2:T:306:GLY:HA3	1.95	0.42
2:J:358:GLY:HA3	2:L:138:ALA:HB3	1.99	0.42
2:J:394:ASP:OD2	2:L:162:ARG:NH1	2.52	0.42
1:K:165:THR:HG23	2:L:36:ALA:CB	2.49	0.42
1:M:68:ASP:O	2:N:189:ARG:NH1	2.49	0.42
2:N:65:TYR:O	2:P:91:ARG:NH2	2.52	0.42
1:W:87:ARG:HE	1:W:87:ARG:HB3	1.43	0.42
1:W:160:VAL:HA	2:X:32:GLU:HG2	2.02	0.42
1:W:227:ALA:HB2	1:W:266:LEU:HD12	2.01	0.42
2:J:236:ARG:NE	2:T:260:ASP:O	2.52	0.42
1:S:64:ASP:HB3	2:T:185:ASN:ND2	2.34	0.42
1:S:87:ARG:HE	1:S:87:ARG:HB3	1.40	0.42
2:V:164:ARG:HH11	2:V:164:ARG:HD3	1.36	0.42
1:K:135:PRO:O	2:L:31:PRO:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:168:ARG:NH2	2:P:35:MET:HG3	2.35	0.42
1:S:138:ILE:CD1	2:T:35:MET:SD	3.06	0.42
1:O:66:GLY:O	2:P:189[B]:ARG:HG2	2.20	0.42
1:A:65:PRO:O	2:B:189:ARG:NH1	2.52	0.42
1:O:110:ASN:ND2	2:P:306:GLY:O	2.48	0.42
1:O:227:ALA:CB	1:O:266:LEU:HD12	2.50	0.42
1:A:252:ARG:CD	2:P:355:ARG:HH21	2.32	0.42
2:F:164:ARG:HH12	2:H:407:LEU:N	2.18	0.42
2:H:285:PHE:CD1	2:H:331:LYS:HD2	2.55	0.42
1:K:66:GLY:O	2:L:189[A]:ARG:CG	2.68	0.42
1:K:266:LEU:HA	1:K:266:LEU:HD23	1.79	0.42
2:X:285:PHE:CD1	2:X:331:LYS:HD2	2.55	0.42
1:G:65:PRO:O	2:H:189[B]:ARG:NH2	2.53	0.42
1:I:80:LEU:HD21	2:J:307:GLN:NE2	2.34	0.42
2:J:96:HIS:CB	2:L:94:LEU:HD21	2.49	0.42
1:K:114:ARG:CB	2:L:306:GLY:N	2.83	0.42
1:K:141:GLU:OE1	2:L:29:TYR:CZ	2.73	0.42
2:X:196:ASP:OD1	2:X:196:ASP:N	2.53	0.42
2:B:165:LEU:HD12	2:D:397:VAL:HG13	2.02	0.41
1:S:135:PRO:O	2:T:31:PRO:CB	2.64	0.41
2:H:230:ILE:HG21	2:H:238:PRO:HD3	2.02	0.41
1:O:227:ALA:HB2	1:O:266:LEU:HD12	2.02	0.41
1:A:259:GLU:HG3	2:P:80:GLN:CD	2.40	0.41
2:B:123:GLU:HG3	2:B:184:ILE:HG12	2.02	0.41
1:M:63:SER:OG	2:N:308:THR:N	2.47	0.41
2:T:113:ARG:HA	2:T:113:ARG:HD3	1.91	0.41
2:N:123:GLU:HG3	2:N:184:ILE:HG12	2.03	0.41
1:O:64:ASP:OD2	2:P:181:LYS:NZ	2.29	0.41
2:T:230:ILE:HG21	2:T:238:PRO:HD3	2.03	0.41
2:B:397:VAL:HG13	2:D:165:LEU:HD12	2.02	0.41
2:D:285:PHE:CD1	2:D:331:LYS:HD2	2.56	0.41
2:D:355:ARG:HH21	1:M:252:ARG:HH21	1.68	0.41
2:F:164:ARG:HH11	2:F:164:ARG:HD3	1.54	0.41
2:R:123:GLU:HG3	2:R:184:ILE:HG12	2.03	0.41
2:F:355:ARG:CD	1:Q:259:GLU:CD	2.87	0.41
2:H:123:GLU:HG3	2:H:184:ILE:CG1	2.51	0.41
2:N:164:ARG:HH11	2:N:164:ARG:HD3	1.37	0.41
2:D:77:ARG:NH1	1:M:223:ARG:HH21	2.18	0.41
1:G:62:TYR:HA	2:H:307:GLN:OE1	2.21	0.41
1:G:228:GLN:NE2	2:R:118:THR:CG2	0.55	0.41
2:R:77:ARG:NE	2:T:139:LEU:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:397:VAL:O	2:T:165:LEU:HD11	2.20	0.41
2:T:113:ARG:NH2	2:T:140:LEU:O	2.49	0.41
2:B:123:GLU:HG3	2:B:184:ILE:CG1	2.51	0.41
2:D:263:GLY:CA	2:R:263:GLY:HA3	2.51	0.41
2:F:123:GLU:HG3	2:F:184:ILE:HG12	2.02	0.41
1:G:228:GLN:HG3	2:R:118:THR:HG22	1.84	0.41
1:I:141:GLU:OE1	2:J:18:HIS:NE2	2.49	0.41
1:I:252:ARG:NH2	2:X:355:ARG:NE	2.69	0.41
2:J:64:ASN:C	2:L:71:PRO:HB2	2.40	0.41
2:J:94:LEU:HD11	2:L:65:TYR:O	2.21	0.41
1:K:161:ALA:HB2	2:L:33:ALA:CB	2.49	0.41
1:K:227:ALA:HB2	1:K:266:LEU:HD12	2.02	0.41
1:Q:134:THR:HB	1:Q:137:LEU:HB3	2.03	0.41
2:T:123:GLU:HG3	2:T:184:ILE:CG1	2.51	0.41
1:U:135:PRO:O	2:V:31:PRO:HB3	2.21	0.41
2:V:123:GLU:HG3	2:V:184:ILE:HG12	2.02	0.41
2:H:123:GLU:HG3	2:H:184:ILE:HG12	2.03	0.41
2:P:113:ARG:NH2	2:P:140:LEU:O	2.50	0.41
1:W:134:THR:HB	1:W:137:LEU:HB3	2.03	0.41
2:X:230:ILE:HG21	2:X:238:PRO:HD3	2.03	0.40
2:D:260:ASP:O	2:R:236:ARG:NE	2.54	0.40
2:F:64:ASN:CB	2:H:73:TYR:HD1	2.33	0.40
2:F:356:MET:CE	1:Q:259:GLU:CG	2.86	0.40
1:Q:68:ASP:O	2:R:189:ARG:CZ	2.68	0.40
1:C:134:THR:HB	1:C:137:LEU:HB3	2.03	0.40
2:F:113:ARG:HG3	2:F:113:ARG:NH1	2.36	0.40
2:J:127:GLY:O	2:J:131:VAL:HG23	2.21	0.40
1:S:114:ARG:HG2	2:T:306:GLY:HA2	2.01	0.40
2:F:165:LEU:HD11	2:H:397:VAL:O	2.21	0.40
1:K:134:THR:HB	1:K:137:LEU:HB3	2.04	0.40
2:L:123:GLU:HG3	2:L:184:ILE:HG12	2.04	0.40
2:T:127:GLY:O	2:T:131:VAL:HG23	2.21	0.40
1:A:173:VAL:HG11	1:A:210:SER:HB3	2.04	0.40
1:E:173:VAL:HG11	1:E:210:SER:HB3	2.04	0.40
1:M:134:THR:HB	1:M:137:LEU:HB3	2.04	0.40
1:S:64:ASP:CB	2:T:185:ASN:ND2	2.85	0.40
1:S:110:ASN:CB	2:T:292:ALA:O	2.69	0.40
1:W:159:LEU:O	2:X:32:GLU:HB3	2.22	0.40

All (70) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:GLN:NE2	2:D:118:THR:CG2[2_555]	0.66	1.54
1:W:228:GLN:NE2	2:X:118:THR:CG2[3_555]	0.68	1.52
1:O:228:GLN:NE2	2:P:118:THR:CG2[2_555]	0.69	1.51
2:B:77:ARG:CZ	1:C:223:ARG:NH2[2_555]	0.73	1.47
1:C:228:GLN:CD	2:D:118:THR:CG2[2_555]	0.76	1.44
2:N:77:ARG:NH1	1:O:223:ARG:NH2[2_555]	0.77	1.43
2:N:77:ARG:CZ	1:O:223:ARG:NH2[2_555]	0.81	1.39
2:B:77:ARG:NH1	1:C:223:ARG:NH1[2_555]	0.83	1.37
2:V:77:ARG:NH1	1:W:223:ARG:NH1[3_555]	0.95	1.25
1:W:228:GLN:CD	2:X:118:THR:CG2[3_555]	0.95	1.25
2:V:77:ARG:CZ	1:W:223:ARG:NH2[3_555]	0.97	1.23
2:B:77:ARG:NH1	1:C:223:ARG:CZ[2_555]	1.03	1.17
2:N:77:ARG:NH1	1:O:223:ARG:CZ[2_555]	1.06	1.14
2:B:77:ARG:NH2	1:C:223:ARG:NH2[2_555]	1.10	1.10
2:V:77:ARG:NH1	1:W:223:ARG:CZ[3_555]	1.11	1.09
1:W:228:GLN:NE2	2:X:118:THR:CB[3_555]	1.32	0.88
2:V:77:ARG:CZ	1:W:223:ARG:CZ[3_555]	1.38	0.82
2:B:77:ARG:CZ	1:C:223:ARG:CZ[2_555]	1.48	0.72
2:V:77:ARG:NE	1:W:223:ARG:NH2[3_555]	1.49	0.71
2:V:77:ARG:NH2	1:W:223:ARG:NH2[3_555]	1.49	0.71
1:C:228:GLN:NE2	2:D:118:THR:CB[2_555]	1.51	0.69
1:W:224:ALA:CB	2:X:141:GLY:O[3_555]	1.52	0.68
2:J:77:ARG:NH1	1:K:223:ARG:NH2[3_555]	1.57	0.63
2:N:77:ARG:NH2	1:O:223:ARG:NH2[2_555]	1.60	0.60
1:C:224:ALA:CB	2:D:141:GLY:O[2_555]	1.65	0.55
2:N:77:ARG:NH1	1:O:223:ARG:NH1[2_555]	1.66	0.54
2:B:77:ARG:NH1	1:C:223:ARG:NH2[2_555]	1.67	0.53
2:B:77:ARG:NE	1:C:223:ARG:NH2[2_555]	1.70	0.50
2:F:262:PRO:CG	2:N:239:ASP:OD1[11_554]	1.73	0.47
1:O:228:GLN:CD	2:P:118:THR:CG2[2_555]	1.73	0.47
1:C:228:GLN:OE1	2:D:118:THR:CG2[2_555]	1.77	0.43
1:W:228:GLN:CD	2:X:118:THR:CB[3_555]	1.80	0.40
2:R:355:ARG:NH2	1:S:252:ARG:NH1[4_555]	1.82	0.38
1:O:228:GLN:NE2	2:P:118:THR:CB[2_555]	1.84	0.36
2:N:404:PHE:O	1:O:248:GLU:OE1[2_555]	1.86	0.34
2:B:77:ARG:NH2	1:C:223:ARG:CZ[2_555]	1.90	0.30
1:C:228:GLN:CD	2:D:118:THR:CB[2_555]	1.90	0.30
2:V:77:ARG:NH1	1:W:223:ARG:NH2[3_555]	1.91	0.29
1:W:228:GLN:OE1	2:X:118:THR:CG2[3_555]	1.92	0.28
2:F:261:ASP:OD1	2:N:236:ARG:CD[11_554]	1.95	0.25
1:W:228:GLN:NE2	2:X:118:THR:CA[3_555]	1.95	0.25
2:F:262:PRO:CG	2:N:239:ASP:CG[11_554]	1.96	0.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:77:ARG:NH2	1:W:223:ARG:CZ[3_555]	1.99	0.21
1:W:228:GLN:OE1	2:X:118:THR:CB[3_555]	1.99	0.21
1:W:196:SER:OG	2:X:196:ASP:OD2[3_555]	2.00	0.20
1:C:228:GLN:CG	2:D:118:THR:CG2[2_555]	2.01	0.19
2:J:77:ARG:CZ	1:K:223:ARG:NH2[3_555]	2.01	0.19
1:E:259:GLU:OE2	2:H:356:MET:SD[4_555]	2.02	0.18
2:J:77:ARG:NH2	1:K:223:ARG:NH2[3_555]	2.03	0.17
2:R:356:MET:SD	1:S:259:GLU:OE2[4_555]	2.03	0.17
1:C:228:GLN:OE1	2:D:118:THR:CB[2_555]	2.04	0.16
2:F:262:PRO:CG	2:N:239:ASP:OD2[11_554]	2.04	0.16
2:N:77:ARG:NE	1:O:223:ARG:NH2[2_555]	2.04	0.16
2:V:77:ARG:NH1	1:W:223:ARG:NE[3_555]	2.05	0.15
1:W:228:GLN:CG	2:X:118:THR:CG2[3_555]	2.06	0.14
1:C:196:SER:OG	2:D:196:ASP:OD2[2_555]	2.07	0.13
1:C:222:SER:OG	2:D:143:ASP:OD1[2_555]	2.07	0.13
2:V:77:ARG:CZ	1:W:223:ARG:NH1[3_555]	2.08	0.12
2:N:355:ARG:NH2	1:O:255:ALA:CB[2_555]	2.10	0.10
2:R:81:HIS:NE2	1:S:255:ALA:CB[4_555]	2.10	0.10
1:O:224:ALA:CB	2:P:141:GLY:O[2_555]	2.11	0.09
1:W:224:ALA:CA	2:X:141:GLY:O[3_555]	2.11	0.09
1:C:225:GLN:OE1	2:D:143:ASP:OD2[2_555]	2.12	0.08
1:C:228:GLN:NE2	2:D:118:THR:CA[2_555]	2.12	0.08
2:N:77:ARG:CZ	1:O:223:ARG:CZ[2_555]	2.12	0.08
1:W:222:SER:OG	2:X:143:ASP:OD1[3_555]	2.13	0.07
2:B:77:ARG:CZ	1:C:223:ARG:NH1[2_555]	2.14	0.06
1:C:224:ALA:CA	2:D:141:GLY:O[2_555]	2.16	0.04
1:O:222:SER:OG	2:P:143:ASP:OD1[2_555]	2.17	0.03
1:E:259:GLU:OE2	2:H:356:MET:CE[4_555]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	254/290 (88%)	246 (97%)	4 (2%)	4 (2%)	9	44
1	C	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	34	71
1	E	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	34	71
1	G	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	34	71
1	I	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	34	71
1	K	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	34	71
1	M	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	34	71
1	O	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	34	71
1	Q	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	34	71
1	S	242/290 (83%)	239 (99%)	2 (1%)	1 (0%)	34	71
1	U	246/290 (85%)	242 (98%)	3 (1%)	1 (0%)	34	71
1	W	244/290 (84%)	241 (99%)	2 (1%)	1 (0%)	34	71
2	B	400/442 (90%)	392 (98%)	8 (2%)	0	100	100
2	D	398/442 (90%)	387 (97%)	11 (3%)	0	100	100
2	F	400/442 (90%)	392 (98%)	8 (2%)	0	100	100
2	H	398/442 (90%)	387 (97%)	11 (3%)	0	100	100
2	J	400/442 (90%)	393 (98%)	7 (2%)	0	100	100
2	L	398/442 (90%)	387 (97%)	11 (3%)	0	100	100
2	N	400/442 (90%)	392 (98%)	8 (2%)	0	100	100
2	P	398/442 (90%)	387 (97%)	11 (3%)	0	100	100
2	R	400/442 (90%)	393 (98%)	7 (2%)	0	100	100
2	T	398/442 (90%)	387 (97%)	11 (3%)	0	100	100
2	V	400/442 (90%)	392 (98%)	8 (2%)	0	100	100
2	X	398/442 (90%)	387 (97%)	11 (3%)	0	100	100
All	All	7734/8784 (88%)	7576 (98%)	143 (2%)	15 (0%)	47	79

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	THR
1	A	188	VAL
1	A	191	ALA
1	C	239	GLY
1	G	239	GLY
1	K	239	GLY

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Mol	Chain	Res	Type
1	O	239	GLY
1	S	239	GLY
1	W	239	GLY
1	M	239	GLY
1	A	239	GLY
1	E	239	GLY
1	I	239	GLY
1	Q	239	GLY
1	U	239	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 X-ray entries followed by that with respect to entries of similar resolution.

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	180/211 (85%)	177 (98%)	3 (2%)	60	78
1	C	179/211 (85%)	177 (99%)	2 (1%)	73	85
1	E	180/211 (85%)	177 (98%)	3 (2%)	60	78
1	G	179/211 (85%)	177 (99%)	2 (1%)	73	85
1	I	180/211 (85%)	177 (98%)	3 (2%)	60	78
1	K	179/211 (85%)	177 (99%)	2 (1%)	73	85
1	M	180/211 (85%)	176 (98%)	4 (2%)	52	71
1	O	179/211 (85%)	177 (99%)	2 (1%)	73	85
1	Q	180/211 (85%)	176 (98%)	4 (2%)	52	71
1	S	179/211 (85%)	177 (99%)	2 (1%)	73	85
1	U	180/211 (85%)	177 (98%)	3 (2%)	60	78
1	W	179/211 (85%)	177 (99%)	2 (1%)	73	85
2	B	298/331 (90%)	295 (99%)	3 (1%)	76	86
2	D	296/331 (89%)	295 (100%)	1 (0%)	92	95
2	F	298/331 (90%)	296 (99%)	2 (1%)	84	90
2	H	296/331 (89%)	295 (100%)	1 (0%)	92	95
2	J	298/331 (90%)	295 (99%)	3 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	296/331 (89%)	295 (100%)	1 (0%)	92	95
2	N	298/331 (90%)	295 (99%)	3 (1%)	76	86
2	P	296/331 (89%)	295 (100%)	1 (0%)	92	95
2	R	298/331 (90%)	296 (99%)	2 (1%)	84	90
2	T	296/331 (89%)	295 (100%)	1 (0%)	92	95
2	V	298/331 (90%)	295 (99%)	3 (1%)	76	86
2	X	296/331 (89%)	295 (100%)	1 (0%)	92	95
All	All	5718/6504 (88%)	5664 (99%)	54 (1%)	78	88

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ASP
1	A	181	TYR
1	A	184	SER
2	B	80	GLN
2	B	355	ARG
2	B	394	ASP
1	C	140	ASP
1	C	181	TYR
2	D	113	ARG
1	E	140	ASP
1	E	181	TYR
1	E	184	SER
2	F	80	GLN
2	F	355	ARG
1	G	140	ASP
1	G	181	TYR
2	H	113	ARG
1	I	140	ASP
1	I	181	TYR
1	I	184	SER
2	J	80	GLN
2	J	355	ARG
2	J	394	ASP
1	K	140	ASP
1	K	181	TYR
2	L	113	ARG
1	M	53	CYS
1	M	140	ASP

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Mol	Chain	Res	Type
1	M	181	TYR
1	M	184	SER
2	N	80	GLN
2	N	355	ARG
2	N	394	ASP
1	O	140	ASP
1	O	181	TYR
2	P	113	ARG
1	Q	53	CYS
1	Q	140	ASP
1	Q	181	TYR
1	Q	184	SER
2	R	80	GLN
2	R	355	ARG
1	S	140	ASP
1	S	181	TYR
2	T	113	ARG
1	U	140	ASP
1	U	181	TYR
1	U	184	SER
2	V	80	GLN
2	V	355	ARG
2	V	394	ASP
1	W	140	ASP
1	W	181	TYR
2	X	113	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	81	HIS
1	I	228	GLN
2	L	81	HIS
1	M	228	GLN
2	P	80	GLN
2	P	81	HIS
2	T	80	GLN
2	T	81	HIS
2	X	81	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	P1T	B	501	-	20,21,21	2.53	4 (20%)	28,30,30	1.36	4 (14%)
3	P1T	N	501	-	20,21,21	2.58	4 (20%)	28,30,30	1.39	3 (10%)
3	P1T	X	501	-	20,21,21	2.54	4 (20%)	28,30,30	1.40	4 (14%)
3	P1T	T	501	-	20,21,21	2.49	4 (20%)	28,30,30	1.45	4 (14%)
3	P1T	D	501	-	20,21,21	2.54	5 (25%)	28,30,30	1.42	3 (10%)
3	P1T	V	501	-	20,21,21	2.60	4 (20%)	28,30,30	1.36	3 (10%)
3	P1T	H	501	-	20,21,21	2.53	4 (20%)	28,30,30	1.33	3 (10%)
3	P1T	F	501	-	20,21,21	2.54	4 (20%)	28,30,30	1.38	4 (14%)
3	P1T	P	501	-	20,21,21	2.56	4 (20%)	28,30,30	1.38	3 (10%)
3	P1T	R	501	-	20,21,21	2.58	4 (20%)	28,30,30	1.33	4 (14%)
3	P1T	L	501	-	20,21,21	2.68	4 (20%)	28,30,30	1.41	4 (14%)
3	P1T	J	501	-	20,21,21	2.61	4 (20%)	28,30,30	1.33	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P1T	B	501	-	-	3/14/15/15	0/1/1/1
3	P1T	N	501	-	-	3/14/15/15	0/1/1/1
3	P1T	X	501	-	-	3/14/15/15	0/1/1/1
3	P1T	T	501	-	-	3/14/15/15	0/1/1/1
3	P1T	D	501	-	-	3/14/15/15	0/1/1/1
3	P1T	V	501	-	-	3/14/15/15	0/1/1/1
3	P1T	H	501	-	-	3/14/15/15	0/1/1/1
3	P1T	F	501	-	-	3/14/15/15	0/1/1/1
3	P1T	P	501	-	-	3/14/15/15	0/1/1/1
3	P1T	R	501	-	-	3/14/15/15	0/1/1/1
3	P1T	L	501	-	-	3/14/15/15	0/1/1/1
3	P1T	J	501	-	-	3/14/15/15	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	501	P1T	C3-C2	8.06	1.49	1.40
3	R	501	P1T	C3-C2	7.80	1.48	1.40
3	V	501	P1T	C3-C2	7.69	1.48	1.40
3	F	501	P1T	C3-C2	7.52	1.48	1.40
3	P	501	P1T	C3-C2	7.50	1.48	1.40
3	J	501	P1T	C3-C2	7.50	1.48	1.40
3	H	501	P1T	C3-C2	7.47	1.48	1.40
3	N	501	P1T	C3-C2	7.37	1.48	1.40
3	X	501	P1T	C3-C2	7.33	1.48	1.40
3	B	501	P1T	C3-C2	7.23	1.48	1.40
3	D	501	P1T	C3-C2	7.19	1.48	1.40
3	T	501	P1T	C3-C2	6.97	1.47	1.40
3	J	501	P1T	C5-C4	5.81	1.48	1.40
3	L	501	P1T	C5-C4	5.65	1.48	1.40
3	N	501	P1T	C5-C4	5.64	1.48	1.40
3	T	501	P1T	C5-C4	5.62	1.48	1.40
3	V	501	P1T	C5-C4	5.62	1.48	1.40
3	X	501	P1T	C5-C4	5.52	1.48	1.40
3	R	501	P1T	C5-C4	5.51	1.48	1.40
3	P	501	P1T	C5-C4	5.51	1.48	1.40
3	N	501	P1T	C3-C4	5.46	1.48	1.40
3	D	501	P1T	C5-C4	5.43	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	P1T	C5-C4	5.42	1.48	1.40
3	J	501	P1T	C3-C4	5.38	1.48	1.40
3	D	501	P1T	C3-C4	5.37	1.48	1.40
3	F	501	P1T	C5-C4	5.36	1.48	1.40
3	B	501	P1T	C3-C4	5.32	1.48	1.40
3	H	501	P1T	C5-C4	5.27	1.47	1.40
3	L	501	P1T	C3-C4	5.27	1.48	1.40
3	X	501	P1T	C3-C4	5.26	1.48	1.40
3	V	501	P1T	C3-C4	5.24	1.48	1.40
3	H	501	P1T	C3-C4	5.07	1.47	1.40
3	T	501	P1T	C3-C4	5.04	1.47	1.40
3	R	501	P1T	C3-C4	5.04	1.47	1.40
3	F	501	P1T	C3-C4	5.02	1.47	1.40
3	P	501	P1T	C3-C4	4.94	1.47	1.40
3	P	501	P1T	CA-C	-3.18	1.45	1.49
3	H	501	P1T	CA-C	-3.00	1.45	1.49
3	D	501	P1T	CA-C	-2.94	1.45	1.49
3	B	501	P1T	CA-C	-2.94	1.45	1.49
3	L	501	P1T	CA-C	-2.89	1.45	1.49
3	F	501	P1T	CA-C	-2.86	1.45	1.49
3	T	501	P1T	CA-C	-2.84	1.45	1.49
3	V	501	P1T	CA-C	-2.81	1.45	1.49
3	J	501	P1T	CA-C	-2.71	1.45	1.49
3	N	501	P1T	CA-C	-2.67	1.45	1.49
3	X	501	P1T	CA-C	-2.61	1.46	1.49
3	R	501	P1T	CA-C	-2.61	1.46	1.49
3	D	501	P1T	O-C	-2.03	1.24	1.30

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	P1T	C4A-C4-C3	3.72	124.03	120.04
3	N	501	P1T	C4A-C4-C3	3.41	123.69	120.04
3	X	501	P1T	C4A-C4-C3	3.36	123.64	120.04
3	V	501	P1T	C4A-C4-C3	3.33	123.61	120.04
3	P	501	P1T	C4A-C4-C3	3.32	123.59	120.04
3	B	501	P1T	C4A-C4-C3	3.30	123.57	120.04
3	L	501	P1T	C4A-C4-C3	3.17	123.44	120.04
3	T	501	P1T	C4A-C4-C3	3.14	123.41	120.04
3	R	501	P1T	C4A-C4-C3	3.12	123.38	120.04
3	F	501	P1T	C4A-C4-C3	3.10	123.36	120.04
3	J	501	P1T	C4A-C4-C3	3.07	123.33	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	501	P1T	C4A-C4-C3	3.01	123.27	120.04
3	T	501	P1T	C6-N1-C2	2.74	124.24	119.17
3	B	501	P1T	C6-N1-C2	2.72	124.20	119.17
3	X	501	P1T	C6-N1-C2	2.64	124.06	119.17
3	J	501	P1T	C6-N1-C2	2.63	124.04	119.17
3	H	501	P1T	C6-N1-C2	2.63	124.04	119.17
3	L	501	P1T	C6-N1-C2	2.59	123.96	119.17
3	N	501	P1T	C6-N1-C2	2.58	123.94	119.17
3	D	501	P1T	C6-N1-C2	2.54	123.86	119.17
3	F	501	P1T	O-C-CA	2.53	119.61	114.14
3	T	501	P1T	O-C-CA	2.52	119.59	114.14
3	V	501	P1T	C6-N1-C2	2.50	123.81	119.17
3	R	501	P1T	C6-N1-C2	2.46	123.72	119.17
3	F	501	P1T	C6-N1-C2	2.44	123.69	119.17
3	D	501	P1T	O-C-CA	2.44	119.41	114.14
3	X	501	P1T	O-C-CA	2.41	119.35	114.14
3	P	501	P1T	O3A-C3-C2	2.40	122.73	117.49
3	L	501	P1T	O3A-C3-C2	2.37	122.66	117.49
3	P	501	P1T	C6-N1-C2	2.35	123.51	119.17
3	F	501	P1T	O3A-C3-C2	2.34	122.60	117.49
3	R	501	P1T	O3A-C3-C2	2.34	122.58	117.49
3	N	501	P1T	O-C-CA	2.31	119.15	114.14
3	L	501	P1T	O-C-CA	2.27	119.05	114.14
3	H	501	P1T	O3A-C3-C2	2.26	122.42	117.49
3	B	501	P1T	O-C-CA	2.24	118.98	114.14
3	V	501	P1T	O3A-C3-C2	2.21	122.32	117.49
3	R	501	P1T	O-C-CA	2.14	118.77	114.14
3	J	501	P1T	O3A-C3-C2	2.13	122.13	117.49
3	X	501	P1T	C4-C4A-N	2.10	115.51	111.22
3	T	501	P1T	O3A-C3-C2	2.08	122.02	117.49
3	B	501	P1T	O3A-C3-C2	2.00	121.85	117.49

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	P1T	C5-C4-C4A-N
3	D	501	P1T	C5-C4-C4A-N
3	F	501	P1T	C5-C4-C4A-N
3	H	501	P1T	C5-C4-C4A-N
3	J	501	P1T	C5-C4-C4A-N
3	L	501	P1T	C5-C4-C4A-N

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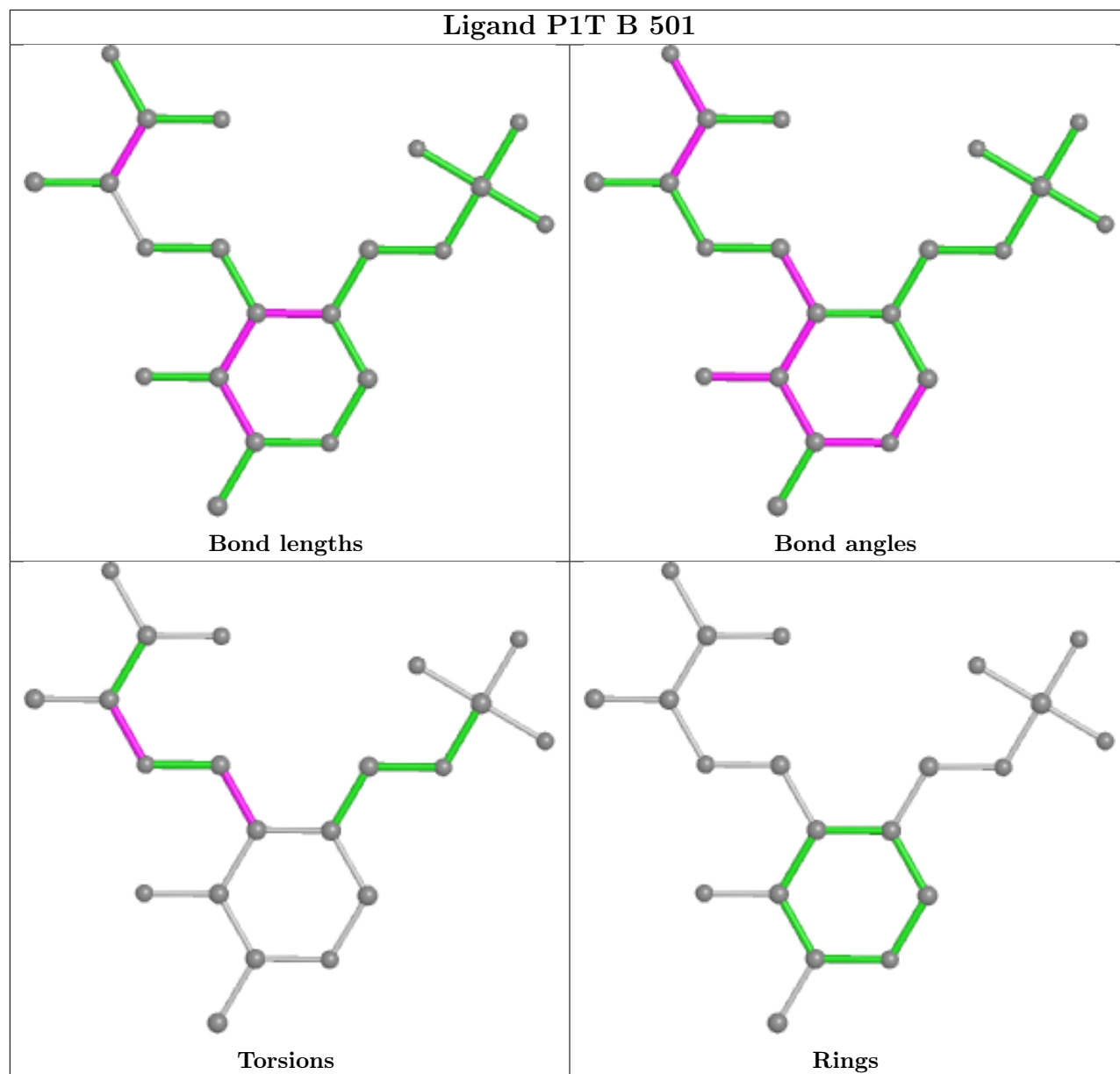
Mol	Chain	Res	Type	Atoms
3	N	501	P1T	C5-C4-C4A-N
3	P	501	P1T	C5-C4-C4A-N
3	R	501	P1T	C5-C4-C4A-N
3	T	501	P1T	C5-C4-C4A-N
3	V	501	P1T	C5-C4-C4A-N
3	X	501	P1T	C5-C4-C4A-N
3	B	501	P1T	C-CA-N-C4A
3	D	501	P1T	C-CA-N-C4A
3	F	501	P1T	C-CA-N-C4A
3	H	501	P1T	C-CA-N-C4A
3	J	501	P1T	C-CA-N-C4A
3	L	501	P1T	C-CA-N-C4A
3	N	501	P1T	C-CA-N-C4A
3	P	501	P1T	C-CA-N-C4A
3	R	501	P1T	C-CA-N-C4A
3	T	501	P1T	C-CA-N-C4A
3	V	501	P1T	C-CA-N-C4A
3	X	501	P1T	C-CA-N-C4A
3	B	501	P1T	C3-C4-C4A-N
3	D	501	P1T	C3-C4-C4A-N
3	F	501	P1T	C3-C4-C4A-N
3	H	501	P1T	C3-C4-C4A-N
3	J	501	P1T	C3-C4-C4A-N
3	L	501	P1T	C3-C4-C4A-N
3	V	501	P1T	C3-C4-C4A-N
3	X	501	P1T	C3-C4-C4A-N
3	N	501	P1T	C3-C4-C4A-N
3	P	501	P1T	C3-C4-C4A-N
3	R	501	P1T	C3-C4-C4A-N
3	T	501	P1T	C3-C4-C4A-N

There are no ring outliers.

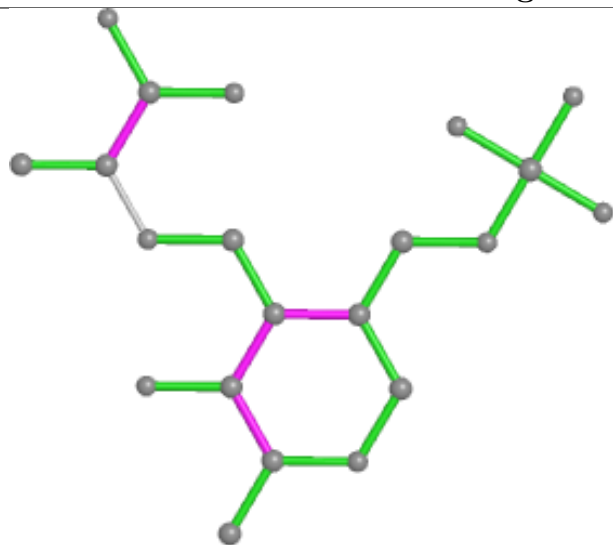
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

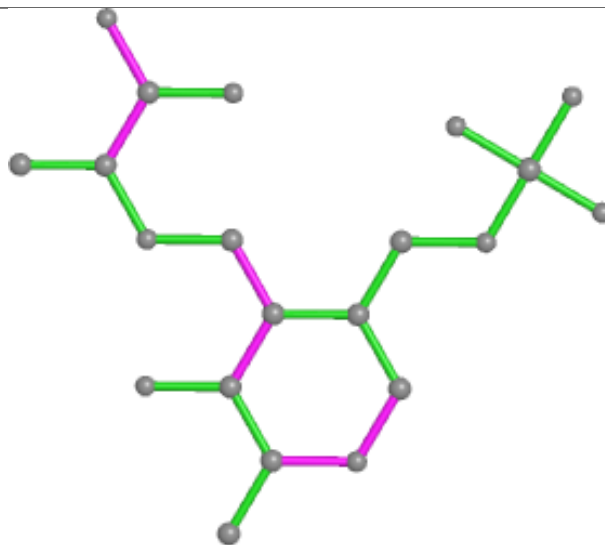
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



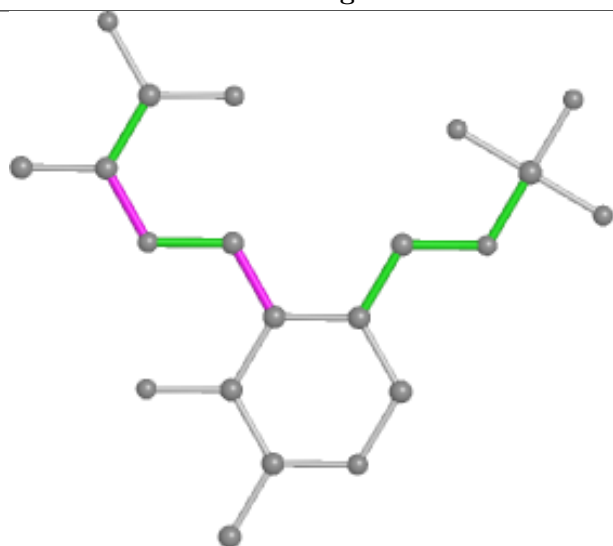
Ligand P1T N 501



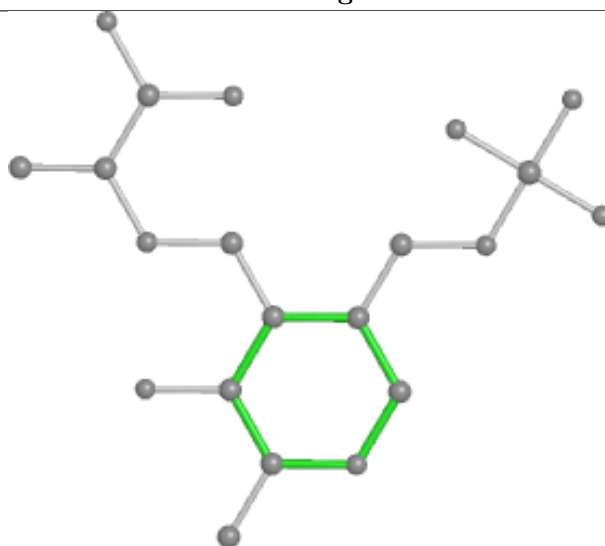
Bond lengths



Bond angles

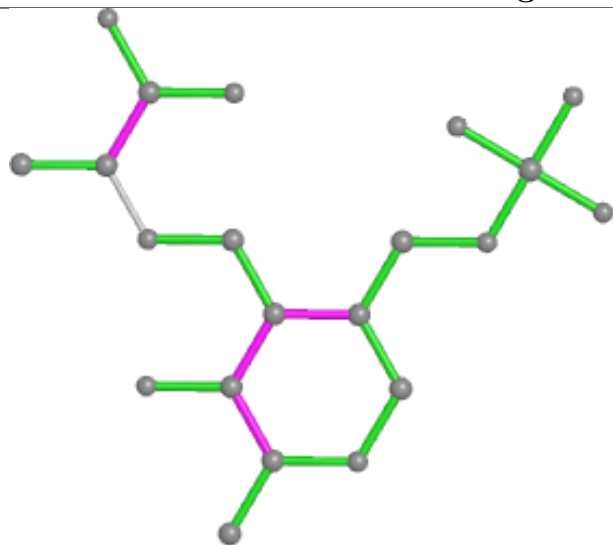


Torsions

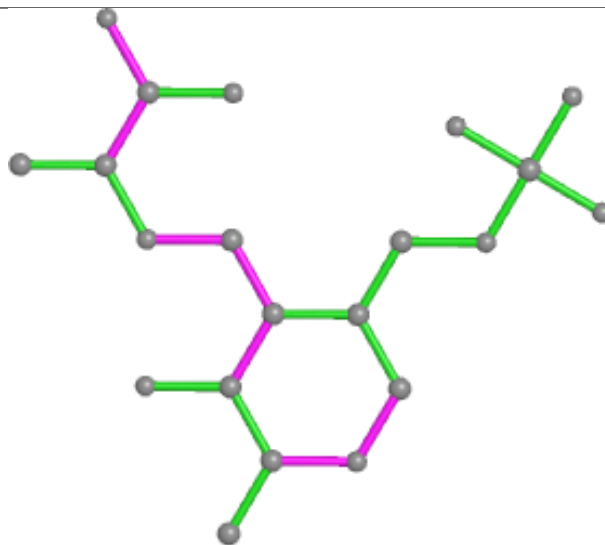


Rings

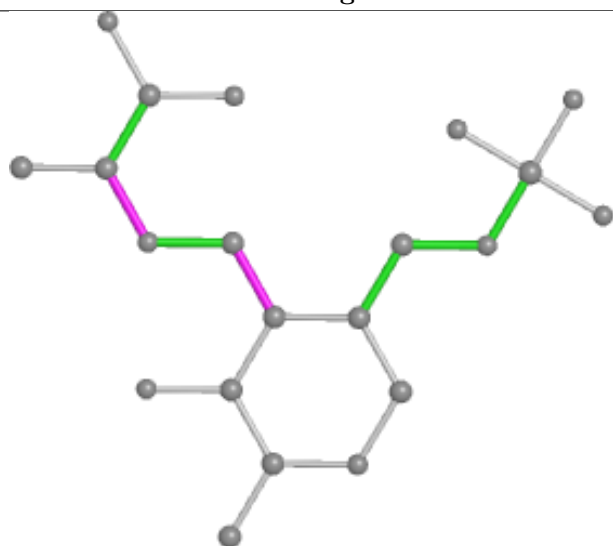
Ligand P1T X 501



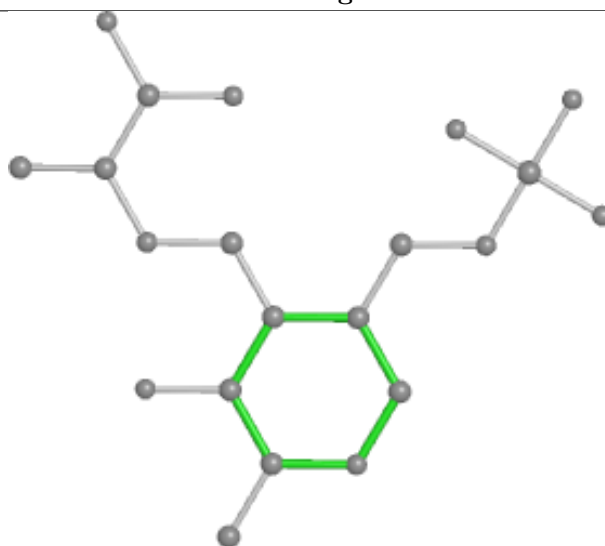
Bond lengths



Bond angles

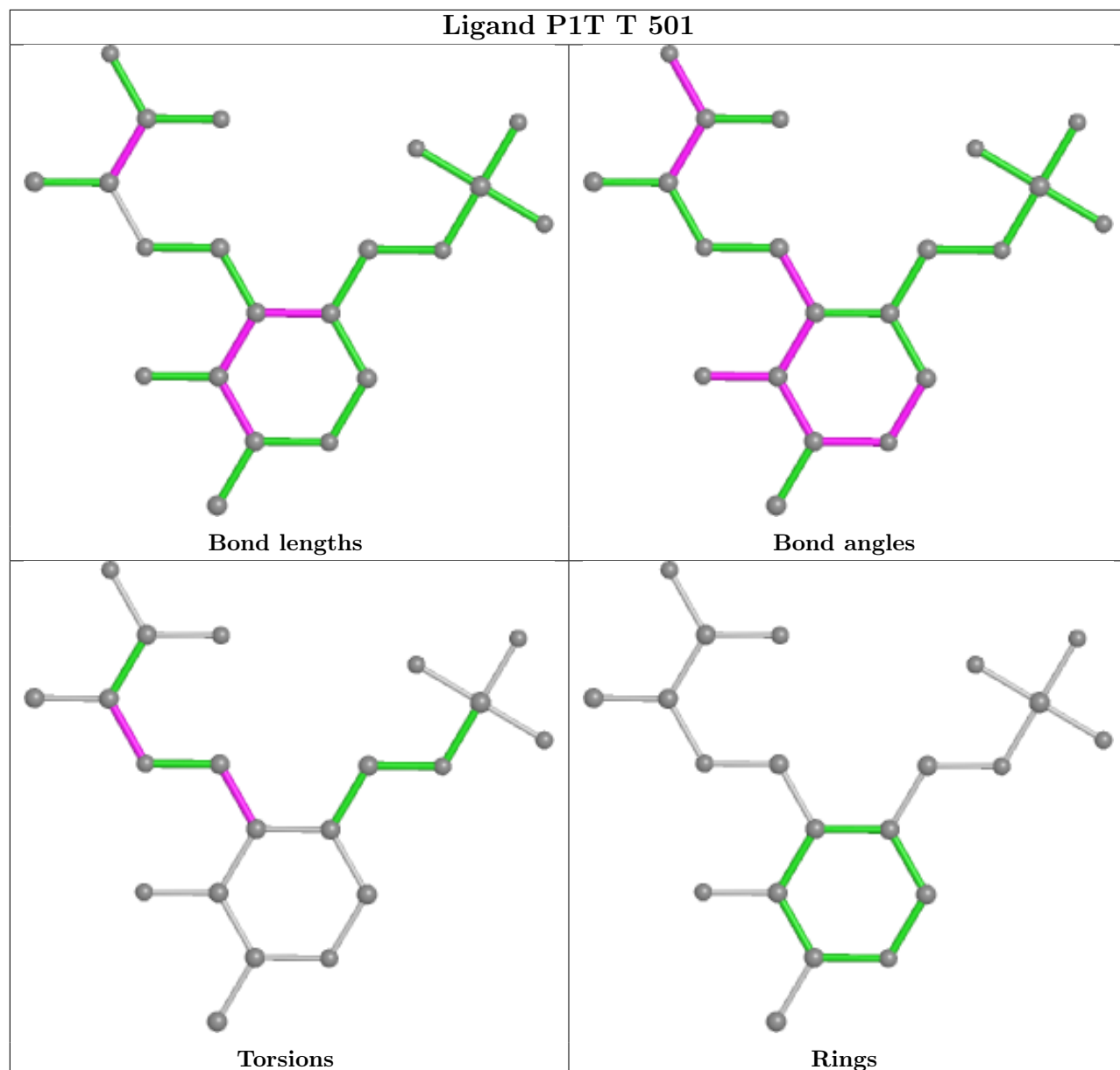


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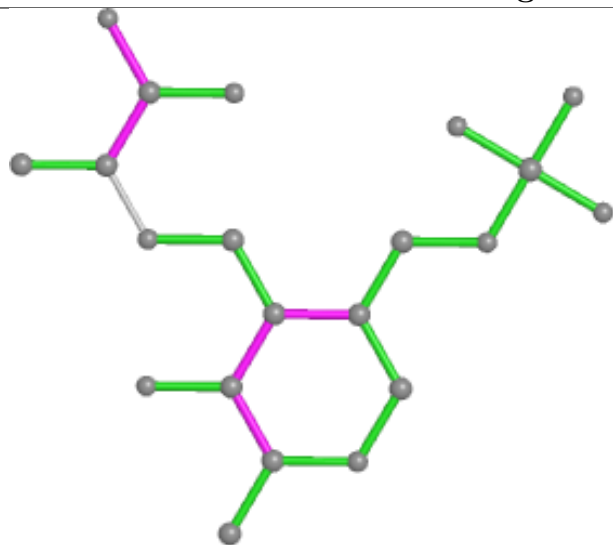


Rings

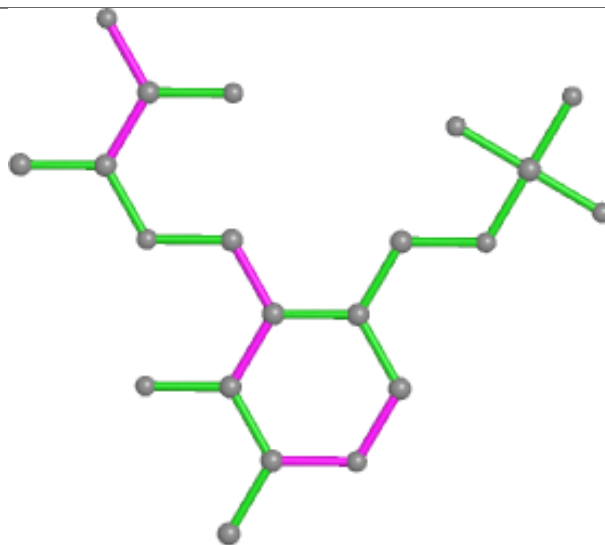
Ligand P1T T 501



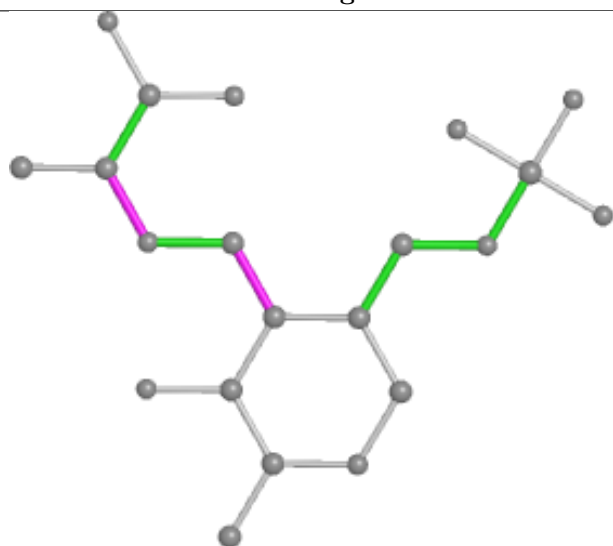
Ligand P1T D 501



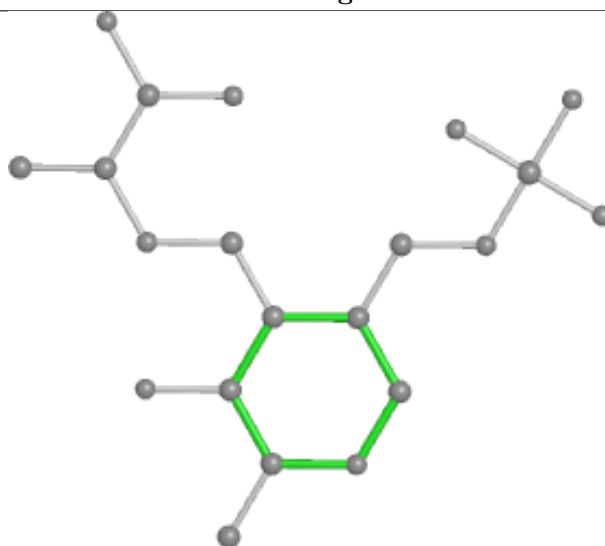
Bond lengths



Bond angles

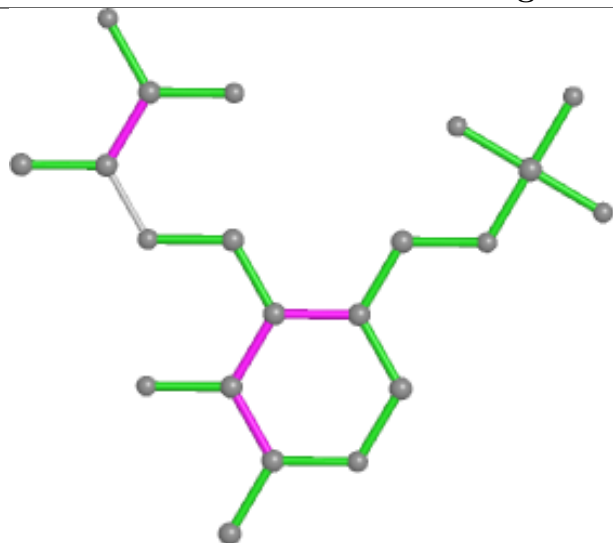


Torsions

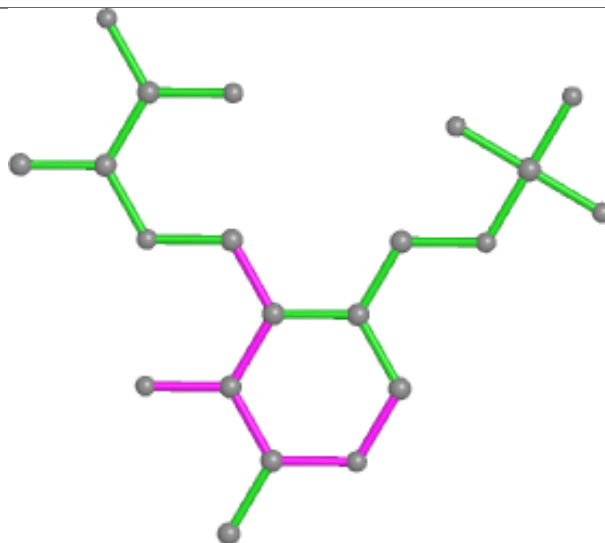


Rings

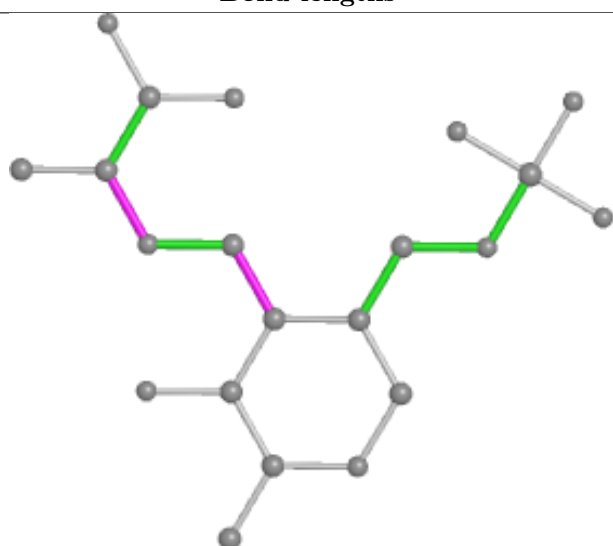
Ligand P1T V 501



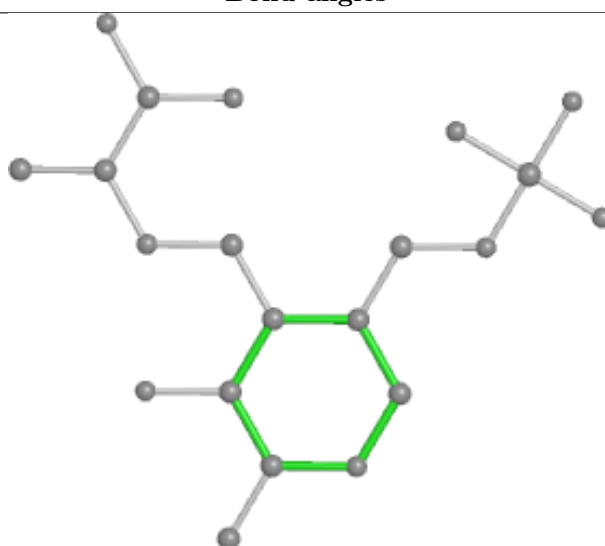
Bond lengths



Bond angles

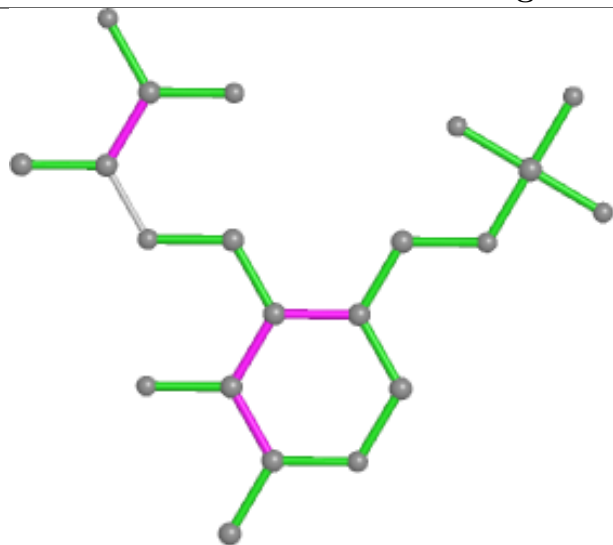


Torsions

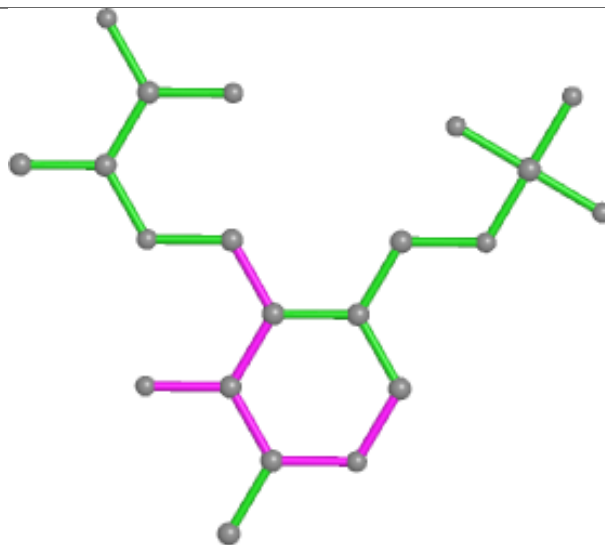


Rings

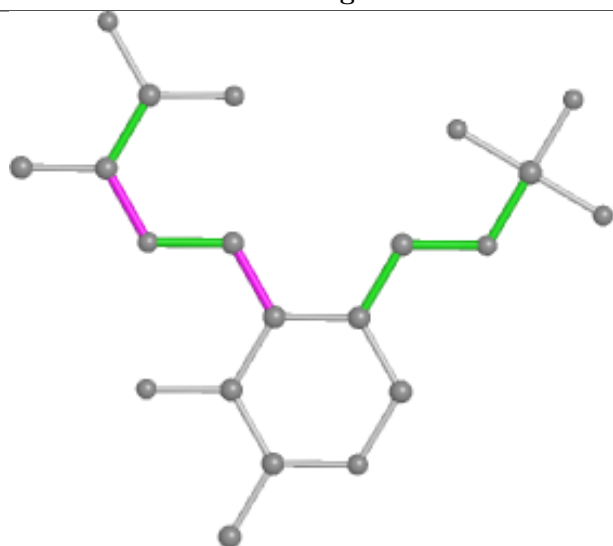
Ligand P1T H 501



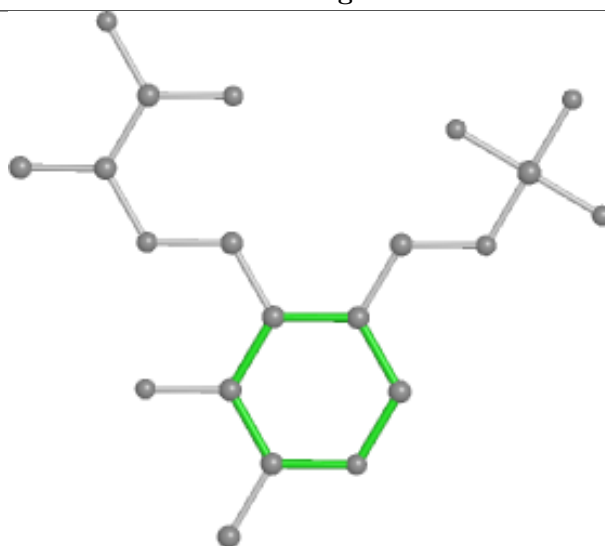
Bond lengths



Bond angles

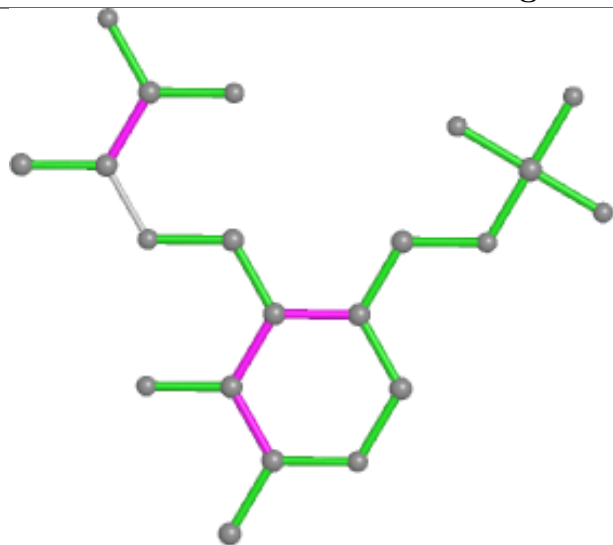


Torsions

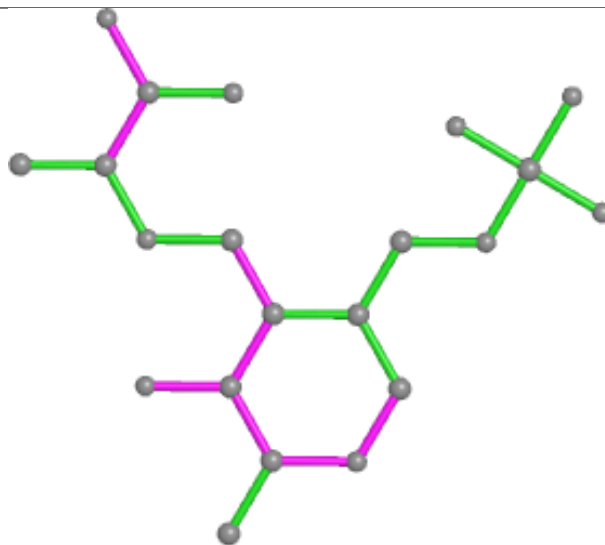


Rings

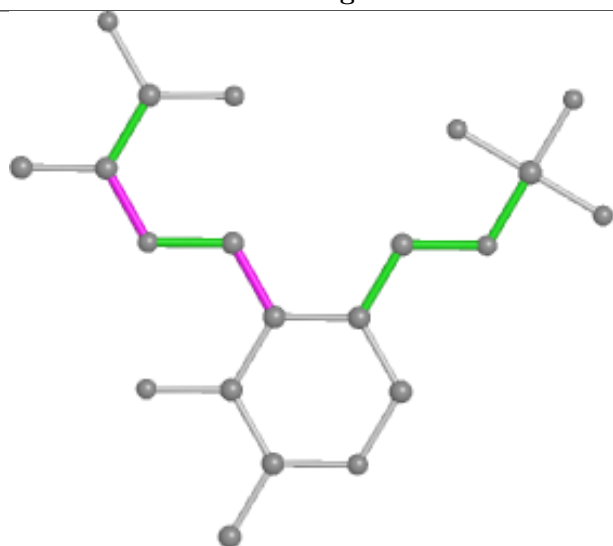
Ligand P1T F 501



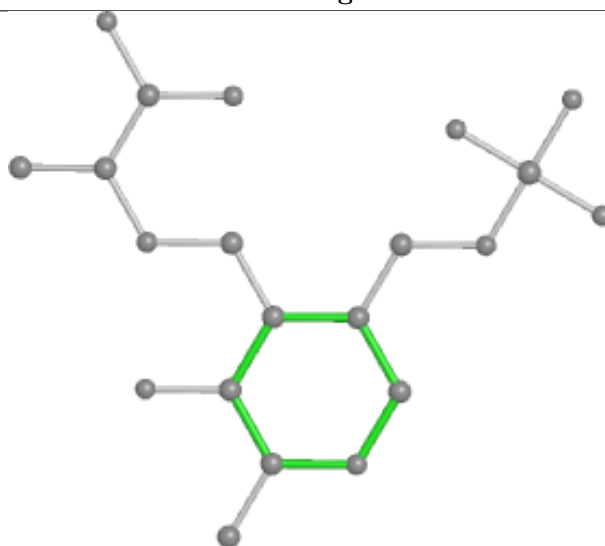
Bond lengths



Bond angles

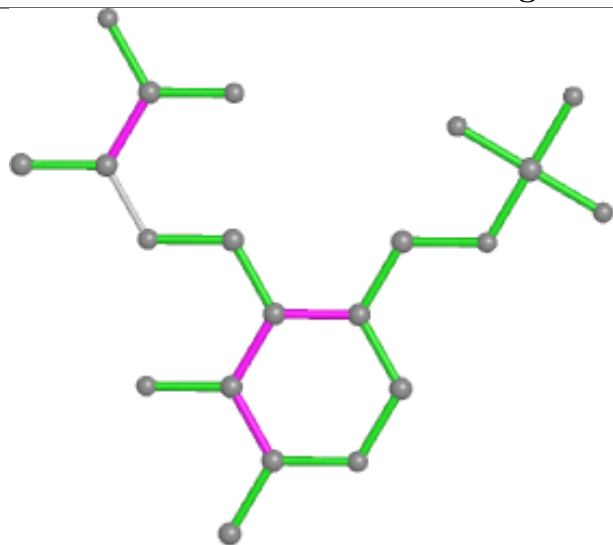


Torsions

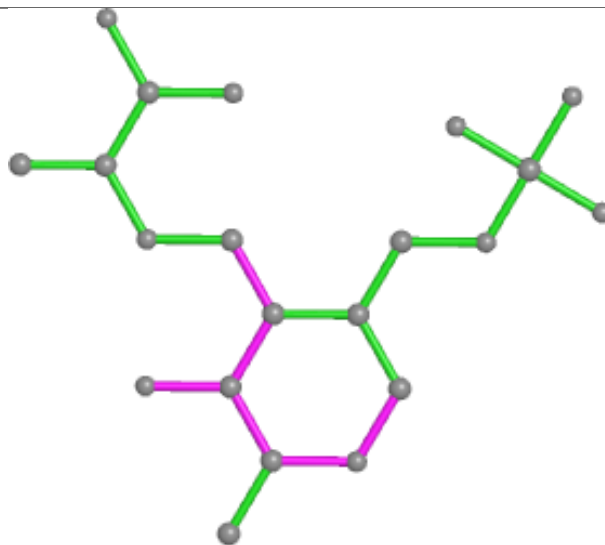


Rings

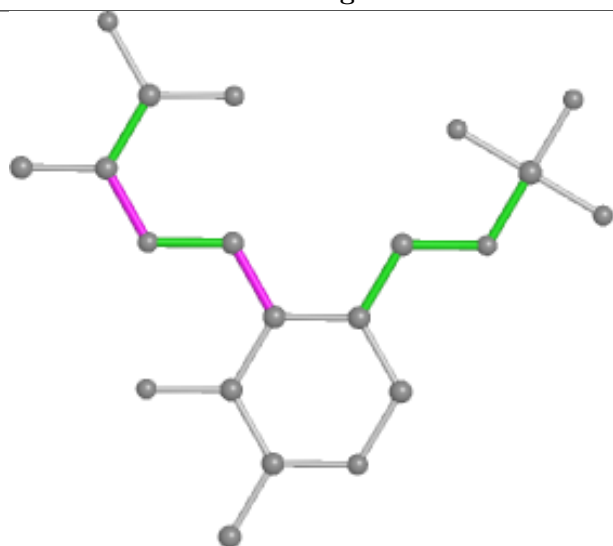
Ligand P1T P 501



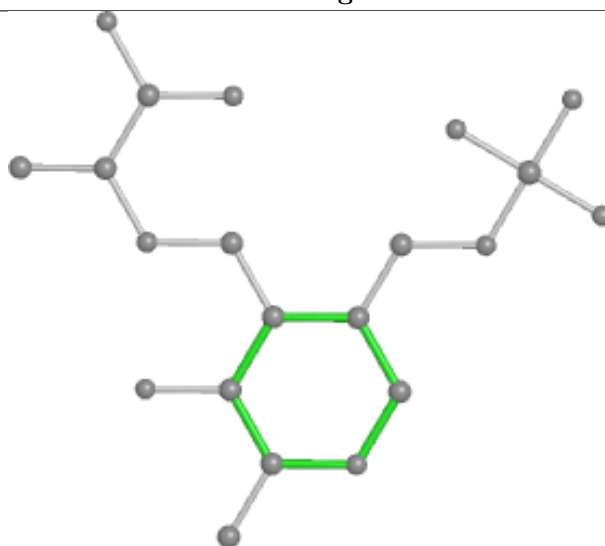
Bond lengths



Bond angles

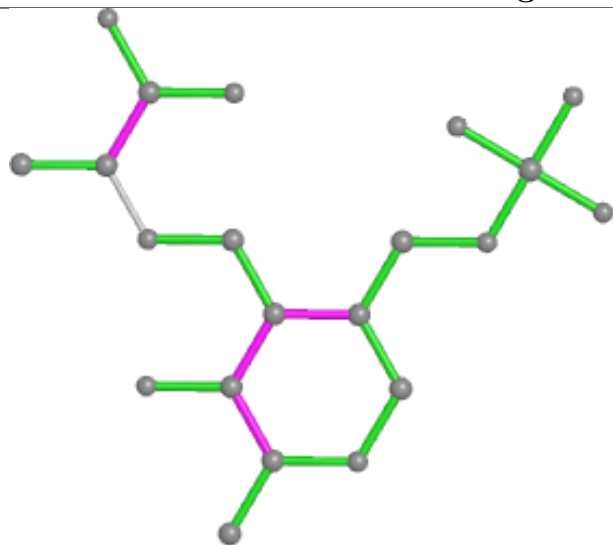


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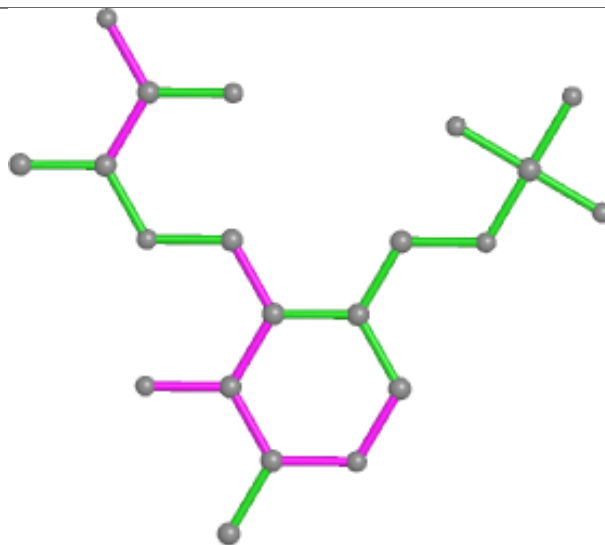


Rings

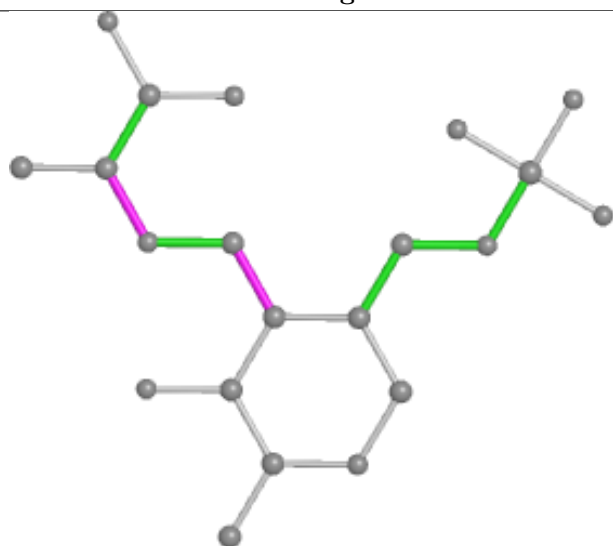
Ligand P1T R 501



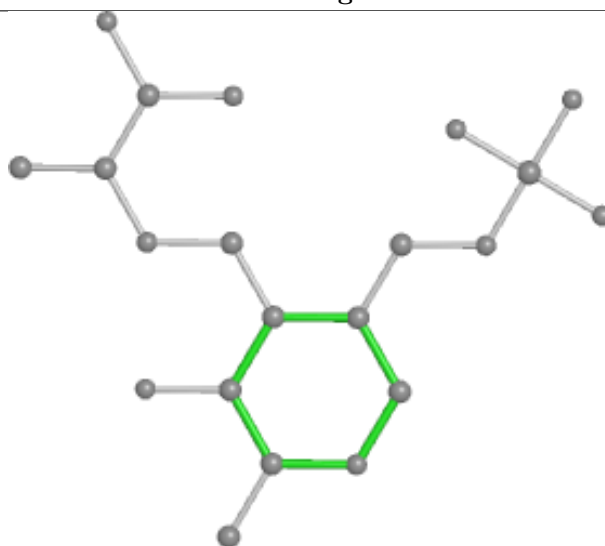
Bond lengths



Bond angles

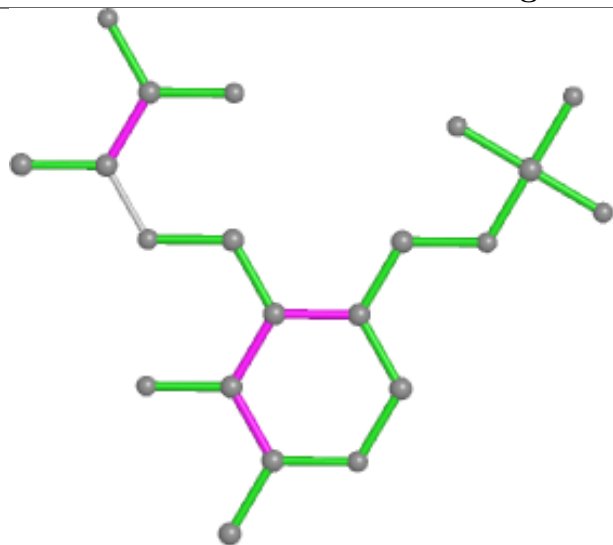


Torsions

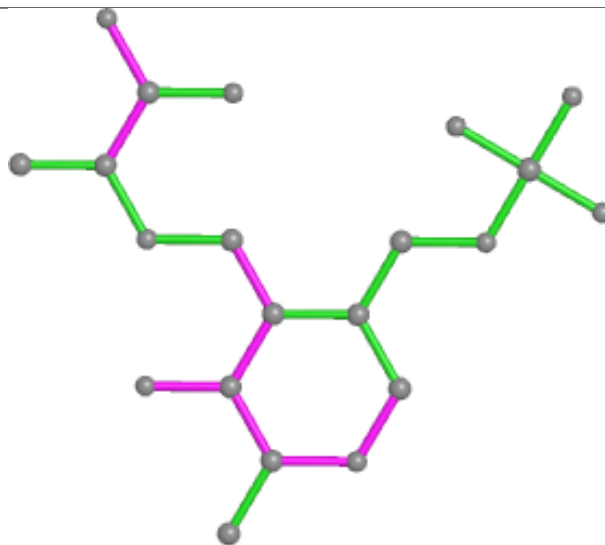


Rings

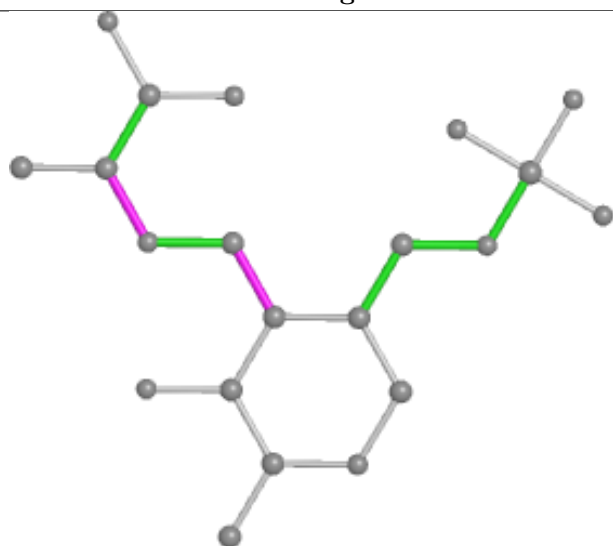
Ligand P1T L 501



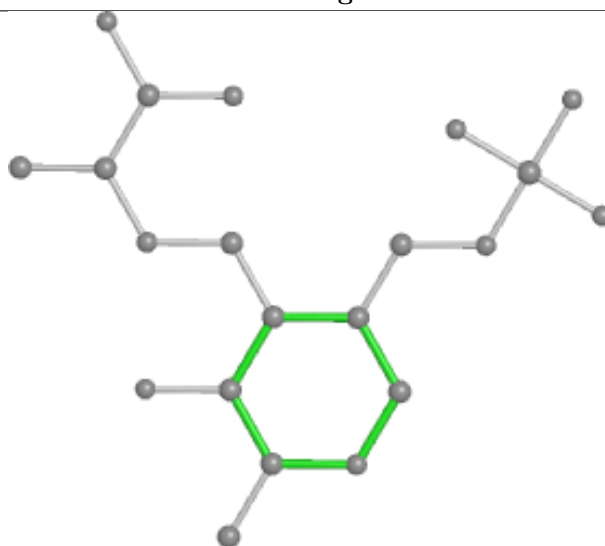
Bond lengths



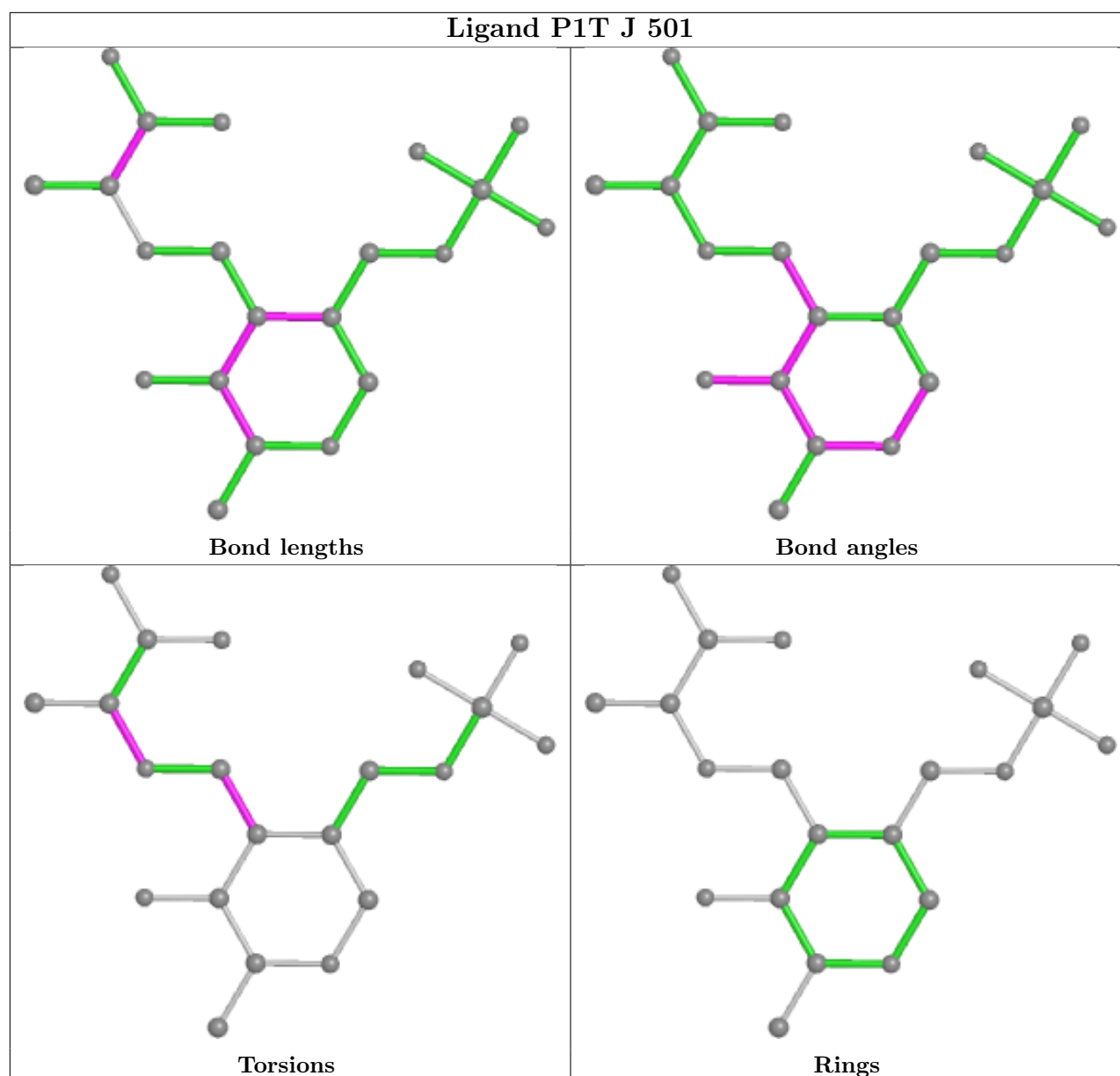
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	9:ALA	C	10:SER	N	3.34

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	257/290 (88%)	-0.37	1 (0%) 92 87	94, 142, 184, 206	0
1	C	248/290 (85%)	-0.49	1 (0%) 92 87	58, 86, 106, 117	0
1	E	249/290 (85%)	0.08	12 (4%) 30 25	132, 176, 211, 238	0
1	G	248/290 (85%)	-0.22	1 (0%) 92 87	111, 138, 159, 173	0
1	I	249/290 (85%)	-0.25	5 (2%) 65 56	130, 169, 200, 211	0
1	K	248/290 (85%)	0.02	10 (4%) 38 30	149, 199, 236, 255	0
1	M	249/290 (85%)	-0.24	4 (1%) 72 62	112, 127, 142, 156	0
1	O	248/290 (85%)	-0.22	6 (2%) 59 49	122, 144, 161, 171	0
1	Q	249/290 (85%)	-0.17	2 (0%) 86 79	109, 135, 156, 170	0
1	S	248/290 (85%)	0.16	11 (4%) 34 28	118, 148, 178, 188	0
1	U	249/290 (85%)	0.04	8 (3%) 47 37	146, 214, 264, 302	0
1	W	248/290 (85%)	-0.41	1 (0%) 92 87	88, 117, 145, 162	0
2	B	399/442 (90%)	-0.58	0 100 100	53, 79, 101, 123	0
2	D	399/442 (90%)	-0.57	0 100 100	49, 61, 81, 91	0
2	F	399/442 (90%)	-0.41	1 (0%) 94 90	98, 113, 137, 149	0
2	H	399/442 (90%)	-0.42	1 (0%) 94 90	97, 108, 119, 126	0
2	J	399/442 (90%)	-0.32	2 (0%) 91 85	125, 156, 188, 200	0
2	L	399/442 (90%)	-0.09	6 (1%) 73 64	126, 165, 198, 208	0
2	N	399/442 (90%)	-0.35	3 (0%) 86 79	109, 118, 137, 149	0
2	P	399/442 (90%)	-0.34	1 (0%) 94 90	110, 125, 140, 147	0
2	R	399/442 (90%)	-0.40	0 100 100	89, 101, 111, 123	0
2	T	399/442 (90%)	-0.34	0 100 100	89, 103, 118, 135	0
2	V	399/442 (90%)	-0.46	0 100 100	91, 123, 162, 180	0
2	X	399/442 (90%)	-0.48	0 100 100	83, 97, 121, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7778/8784 (88%)	-0.31	76 (0%) 82 74	49, 122, 198, 302	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	218	LEU	7.6
1	S	217	GLY	5.5
1	E	218	LEU	5.3
1	E	217	GLY	4.7
1	E	57	GLU	4.7
1	K	209	VAL	4.4
1	C	8	GLU	4.3
1	S	9	ALA	4.3
1	E	8	GLU	4.3
1	U	102	ARG	4.2
1	U	197	GLN	4.0
2	L	120	VAL	4.0
1	O	8	GLU	3.9
1	M	183	ALA	3.8
2	L	144	CYS	3.8
1	E	220	VAL	3.5
1	S	8	GLU	3.5
1	K	210	SER	3.4
1	K	8	GLU	3.4
1	E	219	GLY	3.4
1	K	208	ALA	3.3
1	U	221	ARG	3.2
1	S	220	VAL	3.2
1	S	219	GLY	3.1
2	L	122	ALA	3.1
1	S	196	SER	3.1
1	E	197	GLN	3.0
2	L	119	ARG	3.0
1	I	183	ALA	2.9
2	L	143	ASP	2.9
1	W	8	GLU	2.9
2	N	52	GLN	2.8
1	K	183	ALA	2.8
1	I	218	LEU	2.8
1	O	209	VAL	2.8
1	U	8	GLU	2.7
1	O	183	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	S	57	GLU	2.7
1	O	208	ALA	2.7
1	I	217	GLY	2.6
1	U	155	ASP	2.6
1	I	184	SER	2.5
1	Q	221	ARG	2.5
1	S	182	ALA	2.5
1	E	129	GLY	2.5
2	N	240	ALA	2.4
2	J	52	GLN	2.4
1	U	215	GLY	2.4
1	S	197	GLN	2.3
2	J	174	GLN	2.3
1	A	102	ARG	2.3
1	U	220	VAL	2.3
2	L	50	VAL	2.3
1	E	216	VAL	2.3
2	H	141	GLY	2.2
1	S	21	ALA	2.2
1	K	26	ALA	2.2
1	K	257	THR	2.2
1	I	182	ALA	2.2
2	N	387	VAL	2.1
1	K	213	PRO	2.1
2	F	22	PRO	2.1
1	K	175	ALA	2.1
1	O	218	LEU	2.1
1	M	178	GLY	2.1
1	E	180	VAL	2.1
1	M	221	ARG	2.1
1	K	131	GLY	2.1
1	E	182	ALA	2.1
1	G	178	GLY	2.0
2	P	81	HIS	2.0
1	U	130	LEU	2.0
1	O	136	ASP	2.0
1	M	8	GLU	2.0
1	E	221	ARG	2.0
1	Q	178	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

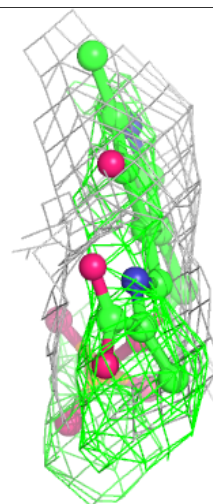
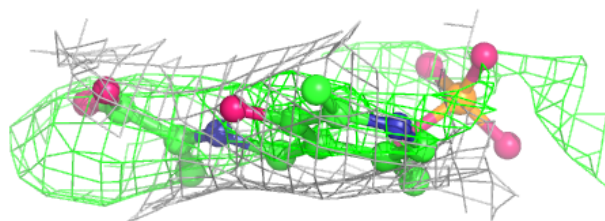
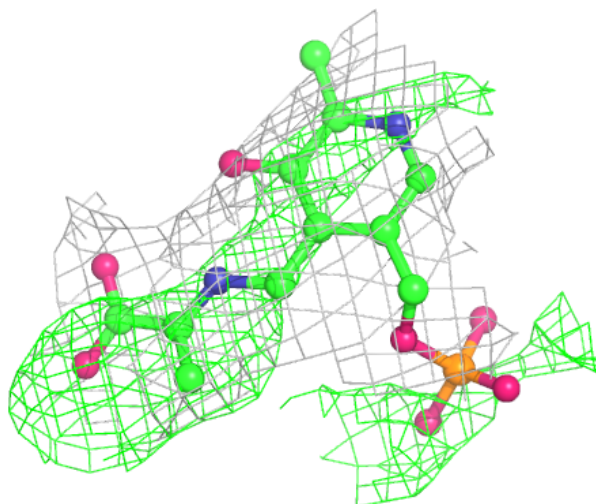
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	P1T	P	501	21/21	0.76	0.45	175,175,175,175	0
3	P1T	D	501	21/21	0.79	0.45	175,175,175,175	0
3	P1T	L	501	21/21	0.81	0.32	175,175,175,175	0
3	P1T	B	501	21/21	0.86	0.41	175,175,175,175	0
3	P1T	T	501	21/21	0.86	0.36	175,175,175,175	0
3	P1T	N	501	21/21	0.87	0.30	175,175,175,175	0
3	P1T	F	501	21/21	0.88	0.34	175,175,175,175	0
3	P1T	J	501	21/21	0.88	0.30	175,175,175,175	0
3	P1T	X	501	21/21	0.88	0.36	175,175,175,175	0
3	P1T	V	501	21/21	0.90	0.30	175,175,175,175	0
3	P1T	R	501	21/21	0.91	0.32	175,175,175,175	0
3	P1T	H	501	21/21	0.91	0.30	175,175,175,175	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

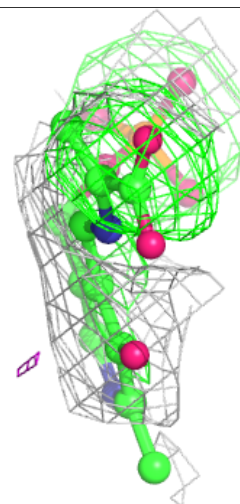
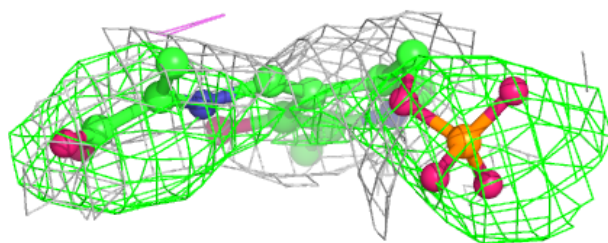
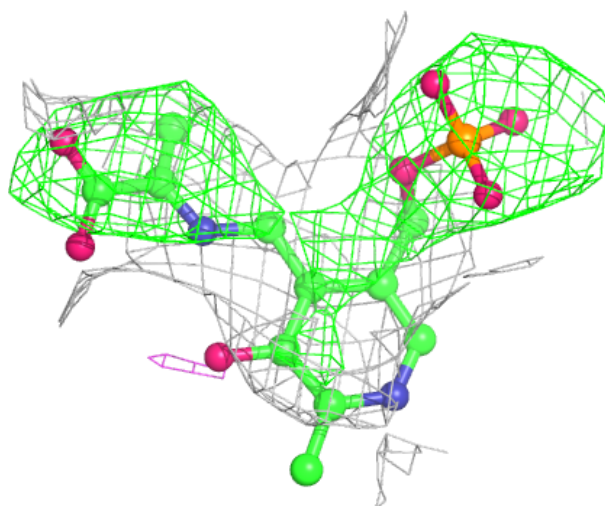
Electron density around P1T P 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



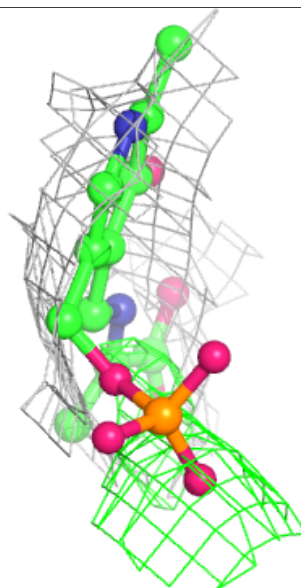
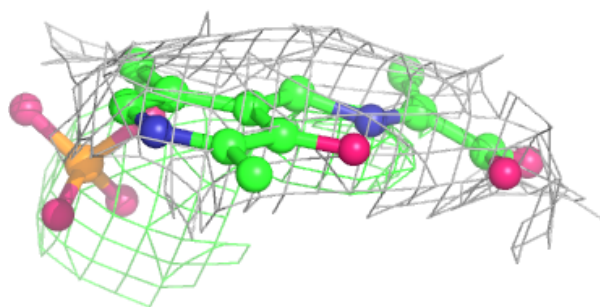
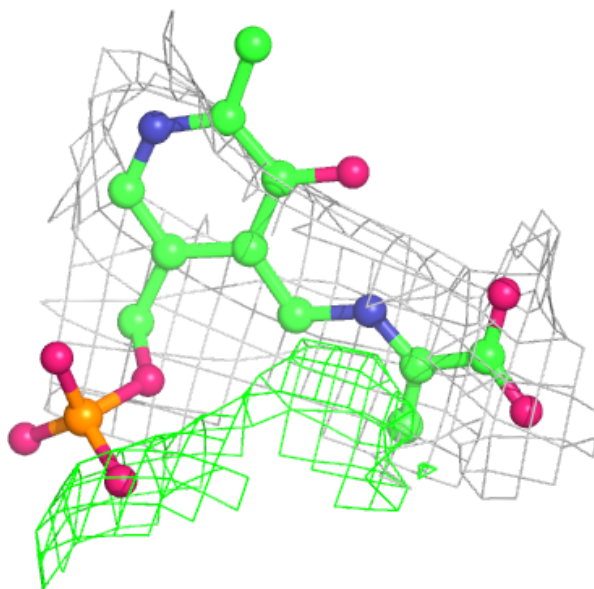
Electron density around P1T D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



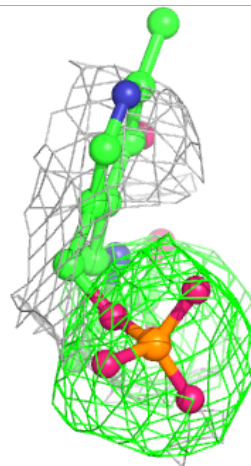
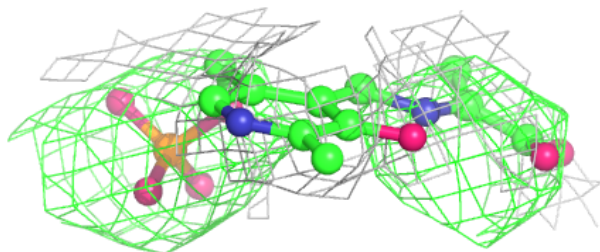
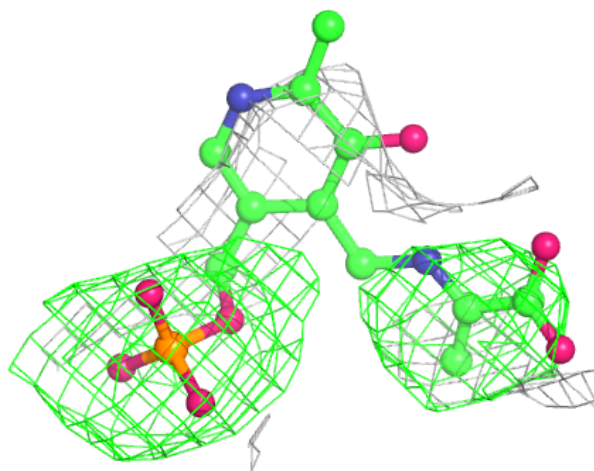
Electron density around P1T L 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



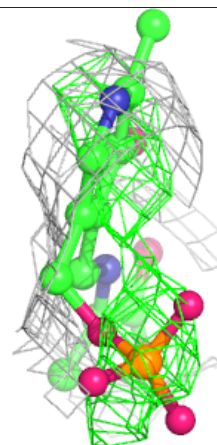
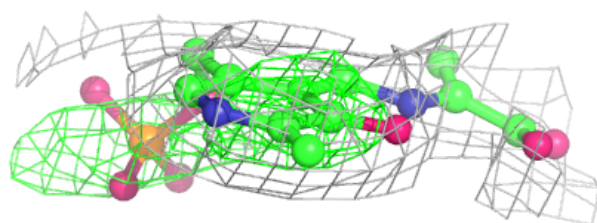
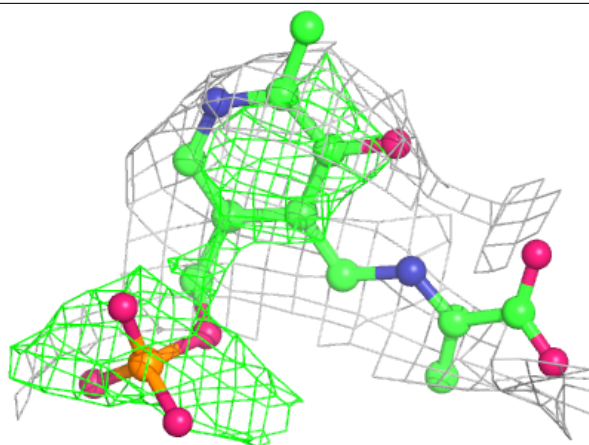
Electron density around P1T B 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



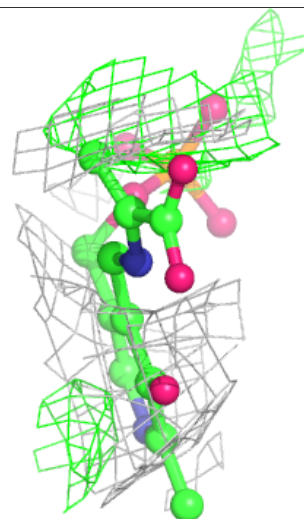
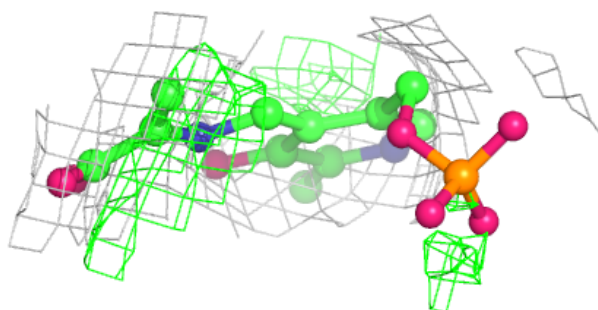
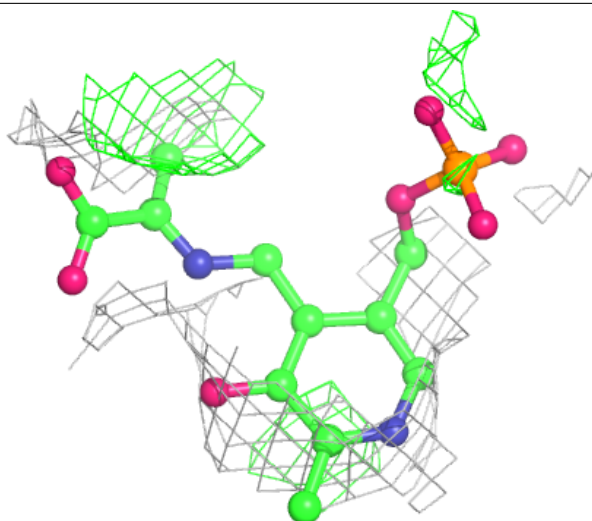
Electron density around P1T T 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



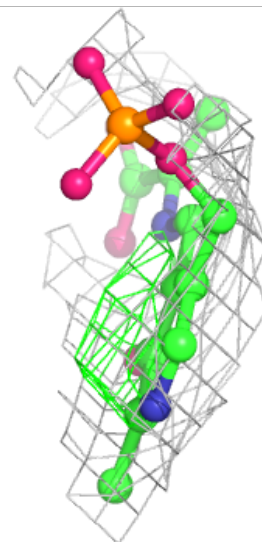
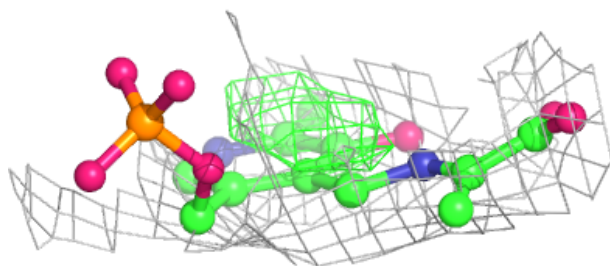
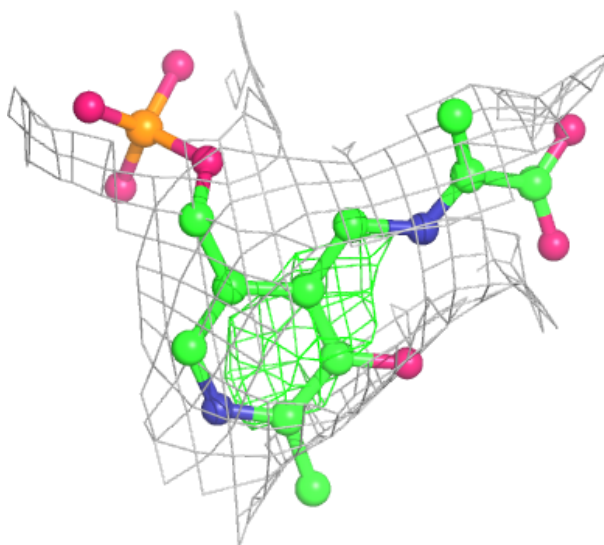
Electron density around P1T N 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



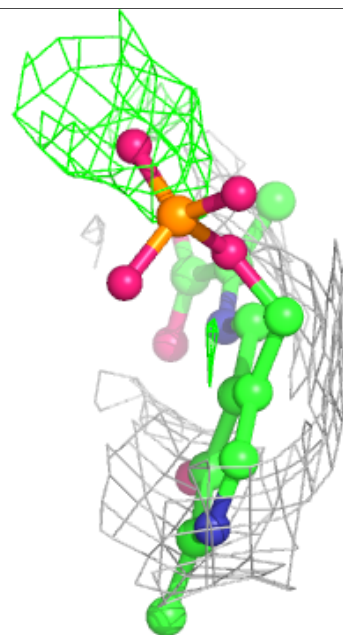
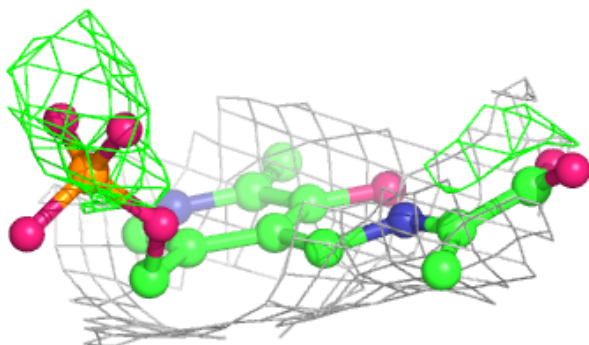
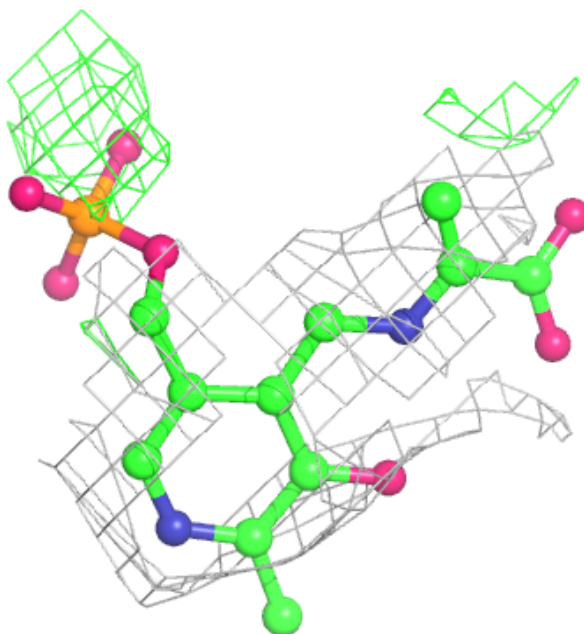
Electron density around P1T F 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



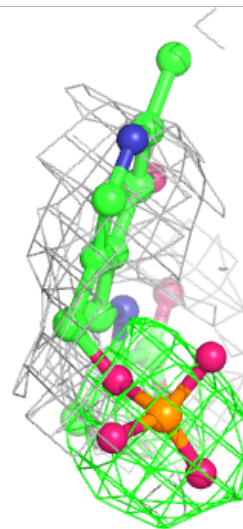
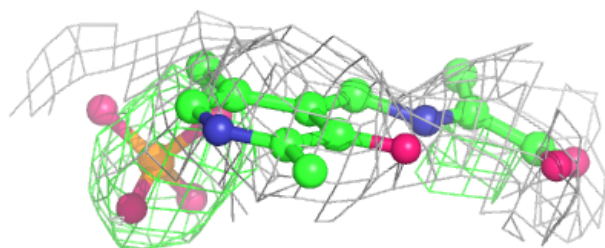
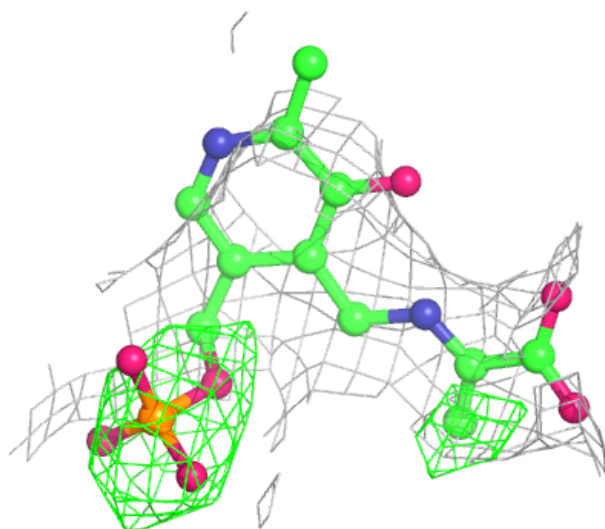
Electron density around P1T J 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



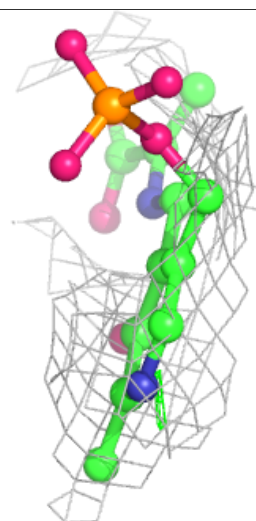
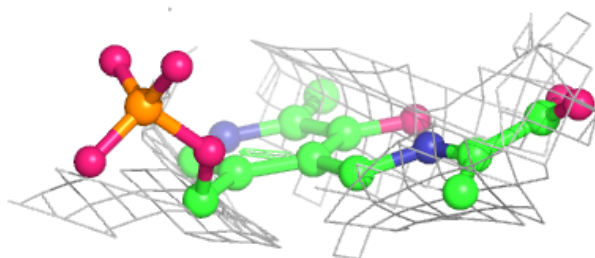
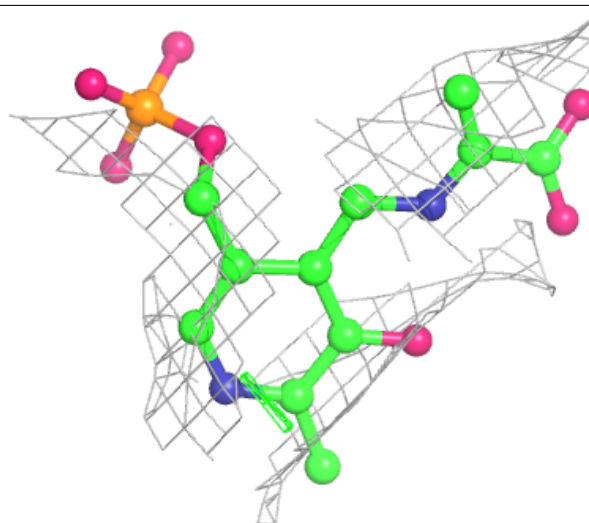
Electron density around P1T X 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



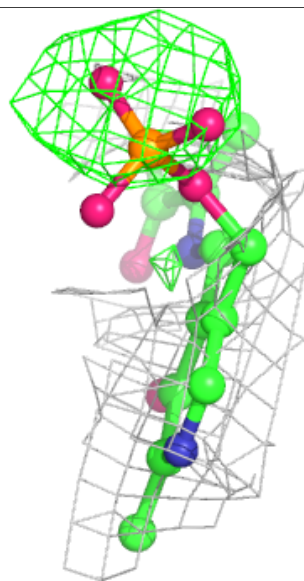
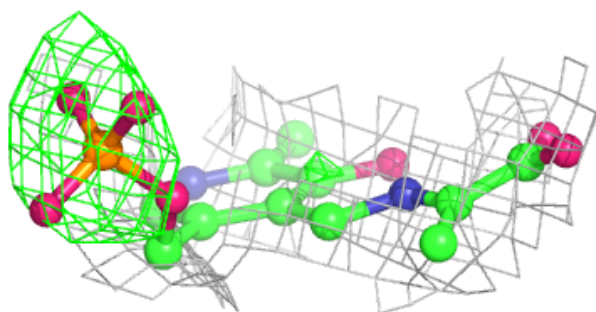
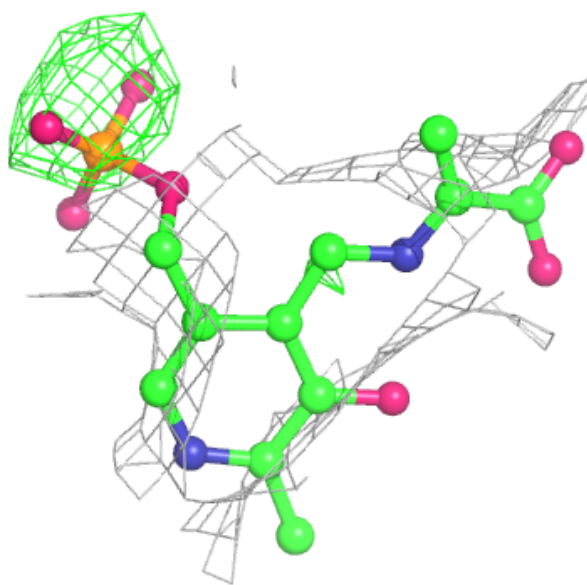
Electron density around P1T V 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



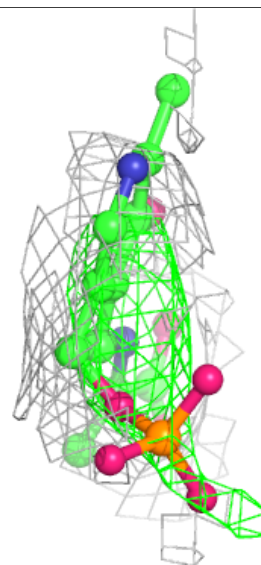
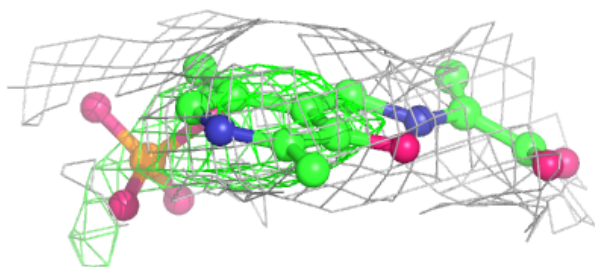
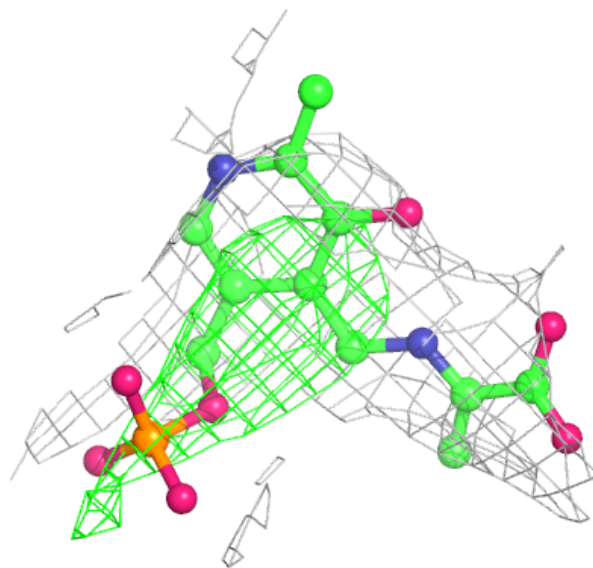
Electron density around P1T R 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P1T H 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.