



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:42 am GMT

PDB ID : 3J6F
EMDB ID: : EMD-5896
Title : Minimized average structure of GDP-bound dynamic microtubules
Authors : Alushin, G.M.; Lander, G.C.; Kellogg, E.H.; Zhang, R.; Baker, D.; Nogales, E.
Deposited on : 2014-02-19
Resolution : 4.90 Å(reported)
Based on PDB ID : 1JFF

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

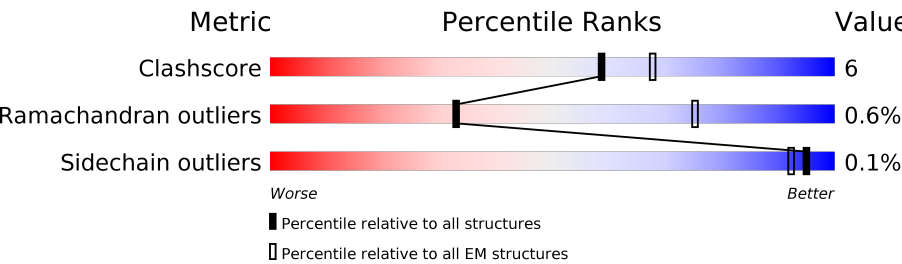
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.90 Å.

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












Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	439	79% 17% . .
1	C	439	78% 18% . .
1	E	439	79% 17% . .
1	G	439	78% 17% . .
1	I	439	79% 17% . .
1	K	439	79% 17% . .
1	M	439	79% 16% . .
1	O	439	79% 16% . .
1	Q	439	79% 17% . .

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Mol	Chain	Length	Quality of chain
2	B	427	 85% 13% •
2	D	427	 84% 13% •
2	F	427	 85% 13% •
2	H	427	 85% 13% •
2	J	427	 85% 13% •
2	L	427	 85% 13% •
2	N	427	 84% 13% •
2	P	427	 83% 14% •
2	R	427	 83% 15% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 60903 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Tubulin alpha-1A chain.

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

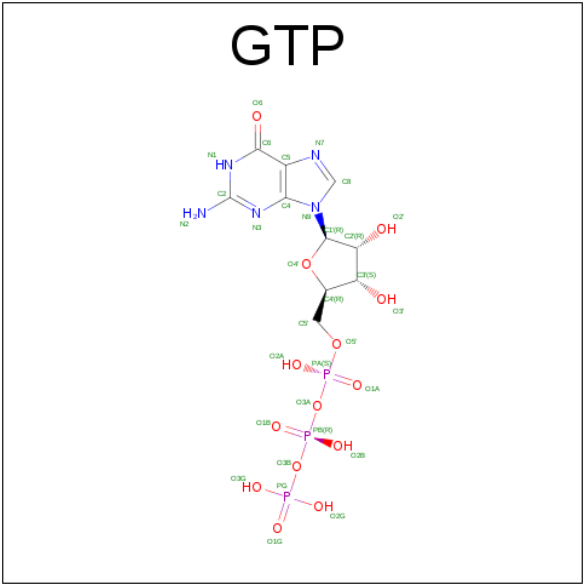
There are 9 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Tubulin beta chain.

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

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



- Molecule 6 is water.

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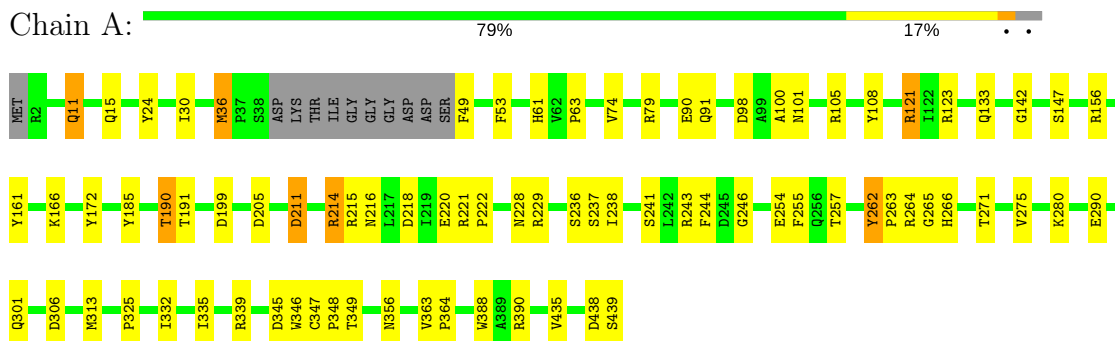
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Mol	Chain	Residues	Atoms		AltConf
6	G	4	Total 4	O 4	0
6	I	4	Total 4	O 4	0
6	K	4	Total 4	O 4	0
6	M	4	Total 4	O 4	0
6	O	4	Total 4	O 4	0
6	Q	4	Total 4	O 4	0

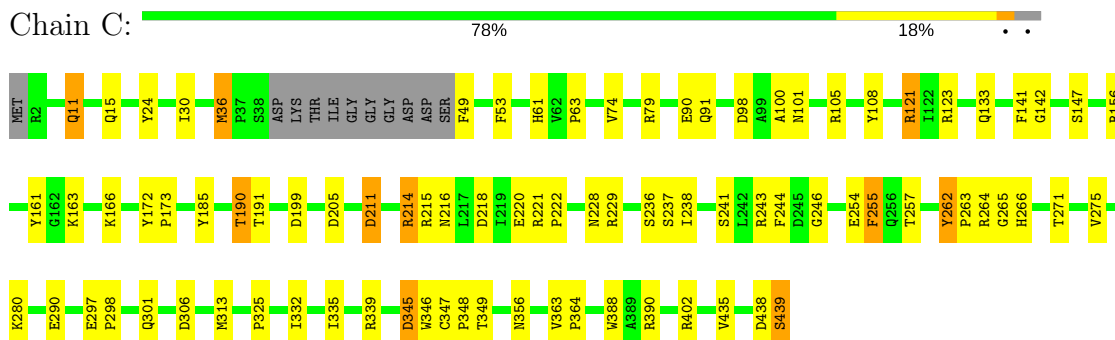
3 Residue-property plots

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

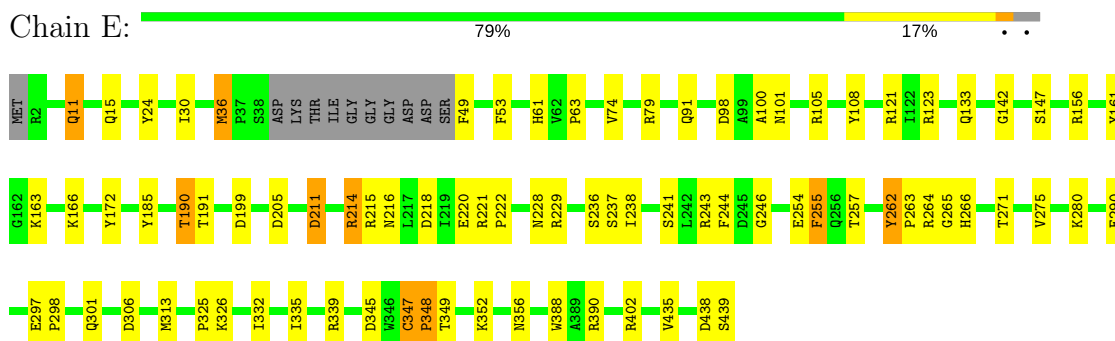
- Molecule 1: Tubulin alpha-1A chain



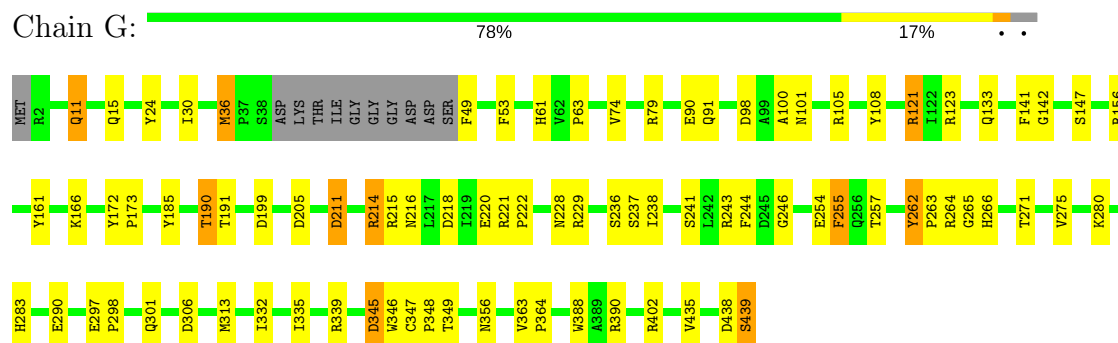
- Molecule 1: Tubulin alpha-1A chain



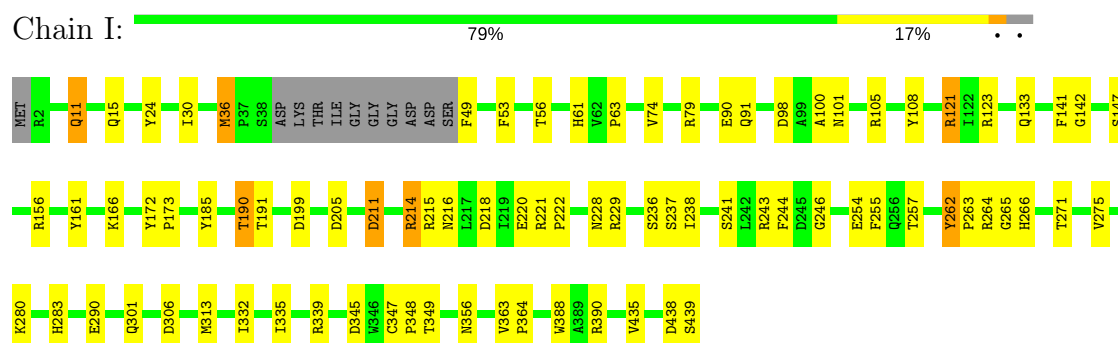
- Molecule 1: Tubulin alpha-1A chain



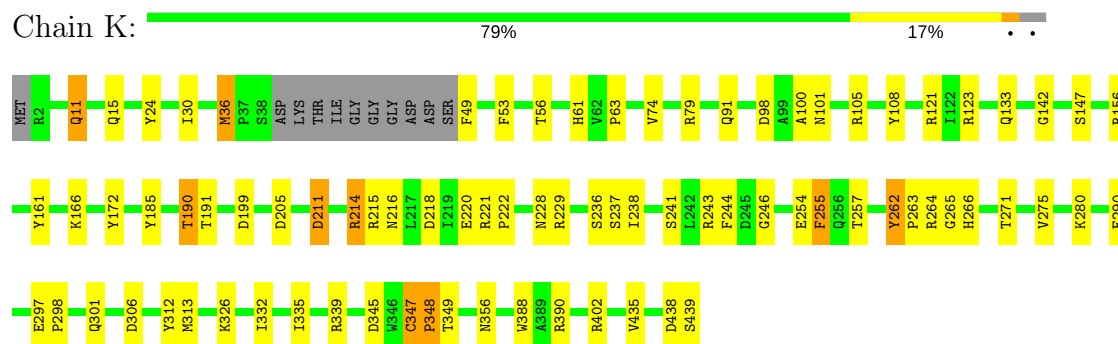
- Molecule 1: Tubulin alpha-1A chain



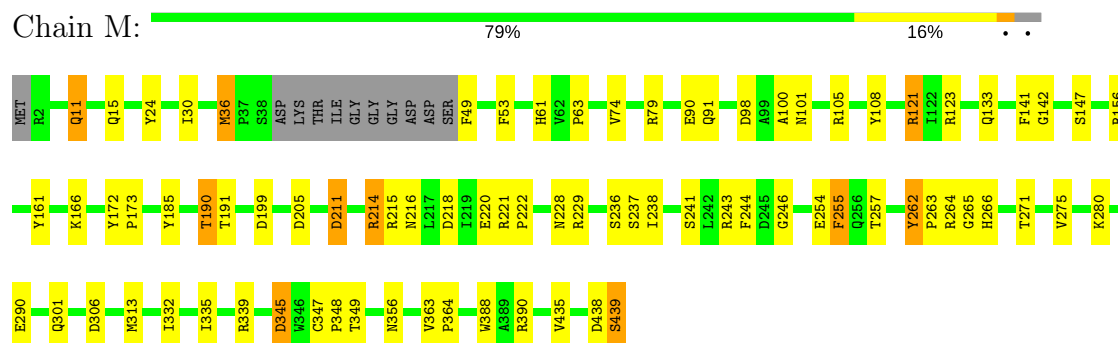
- Molecule 1: Tubulin alpha-1A chain



- Molecule 1: Tubulin alpha-1A chain



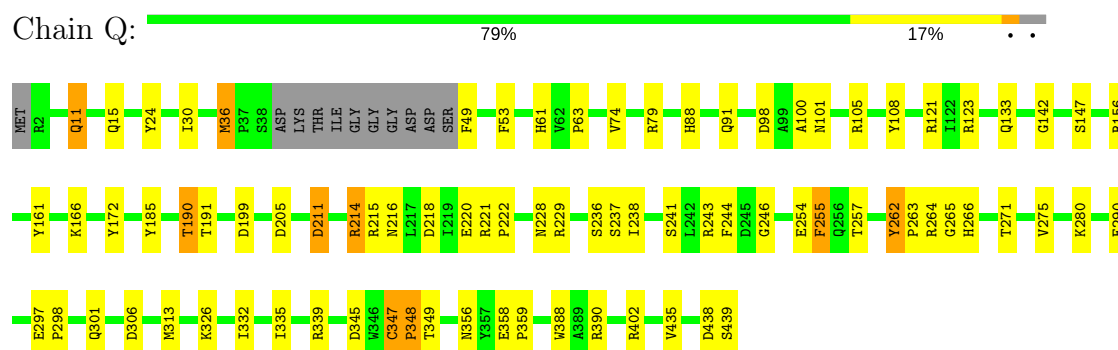
- Molecule 1: Tubulin alpha-1A chain



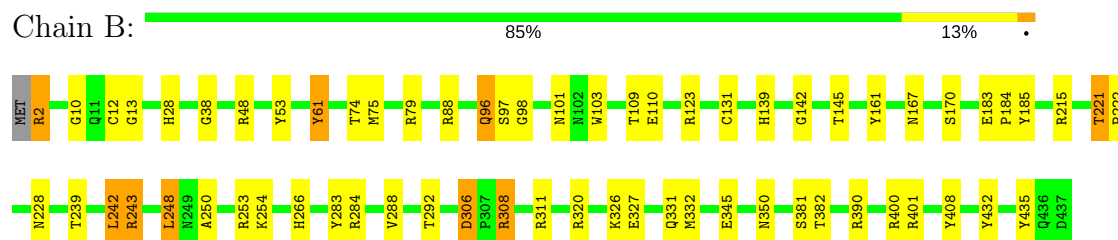
- Molecule 1: Tubulin alpha-1A chain



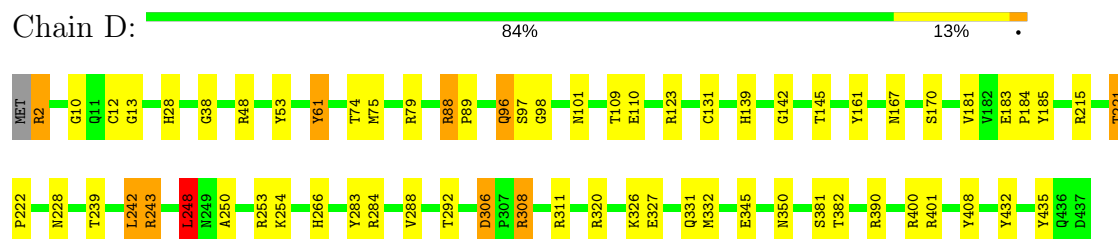
- Molecule 1: Tubulin alpha-1A chain



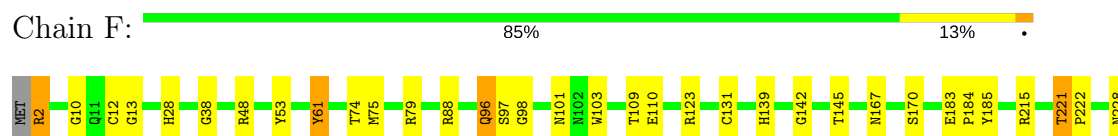
- Molecule 2: Tubulin beta chain



- Molecule 2: Tubulin beta chain



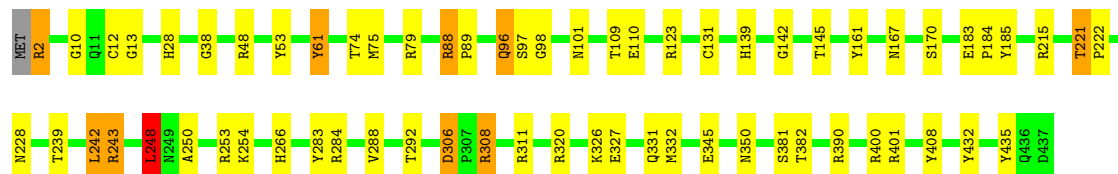
- Molecule 2: Tubulin beta chain





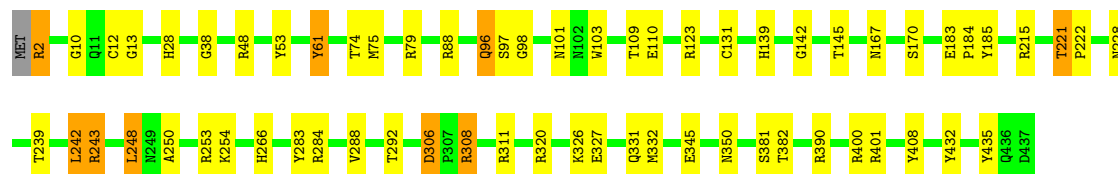
• Molecule 2: Tubulin beta chain

Chain H: 85% 13%



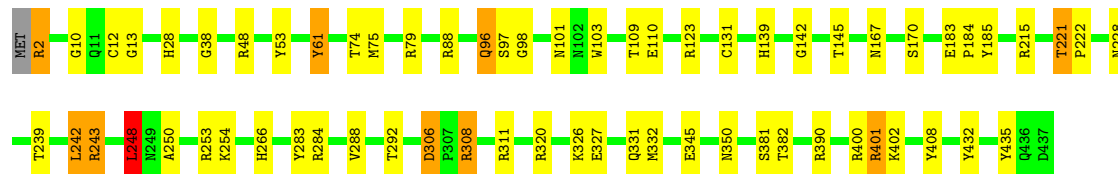
• Molecule 2: Tubulin beta chain

Chain J: 85% 13%



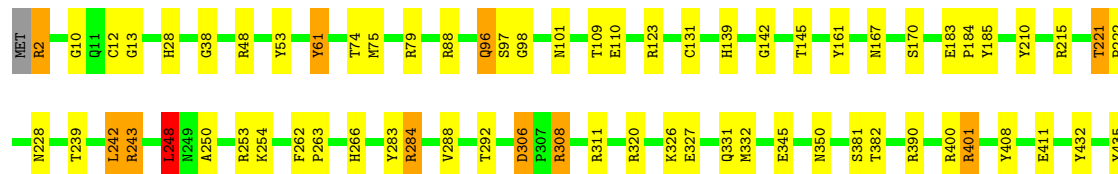
• Molecule 2: Tubulin beta chain

Chain L: 85% 13%



• Molecule 2: Tubulin beta chain

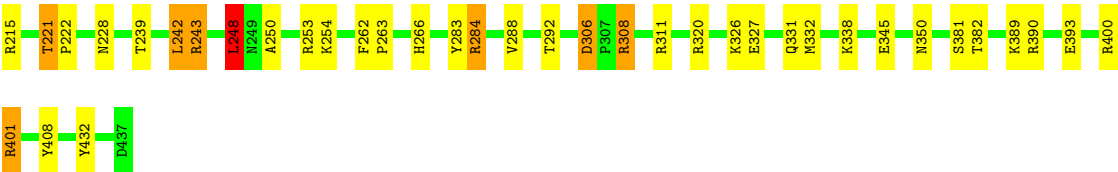
Chain N: 84% 13%



• Molecule 2: Tubulin beta chain

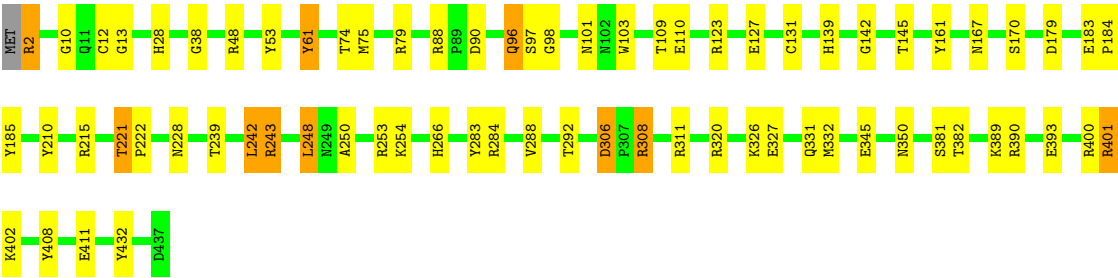
Chain P: 83% 14%





• Molecule 2: Tubulin beta chain

Chain R: 83% 15%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	54445	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	ctftilt	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25.0	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	72000	Depositor
Image detector	KODAK SO-163 film	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	C	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	E	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	G	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	I	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	K	1.14	10/3427 (0.3%)	1.44	45/4651 (1.0%)
1	M	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	O	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
1	Q	1.14	10/3427 (0.3%)	1.44	44/4651 (0.9%)
2	B	1.05	5/3427 (0.1%)	1.56	48/4642 (1.0%)
2	D	1.05	5/3427 (0.1%)	1.56	49/4642 (1.1%)
2	F	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
2	H	1.05	5/3427 (0.1%)	1.56	48/4642 (1.0%)
2	J	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
2	L	1.05	5/3427 (0.1%)	1.56	48/4642 (1.0%)
2	N	1.05	5/3427 (0.1%)	1.56	48/4642 (1.0%)
2	P	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
2	R	1.05	5/3427 (0.1%)	1.56	47/4642 (1.0%)
All	All	1.09	135/61686 (0.2%)	1.50	826/83637 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
2	N	0	1
2	P	0	1
2	R	0	1
All	All	0	9

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	265	GLY	CA-C	-15.06	1.27	1.51
1	M	265	GLY	CA-C	-15.03	1.27	1.51
1	E	265	GLY	CA-C	-15.01	1.27	1.51
1	I	265	GLY	CA-C	-15.01	1.27	1.51
1	G	265	GLY	CA-C	-15.00	1.27	1.51
1	C	265	GLY	CA-C	-14.99	1.27	1.51
1	A	265	GLY	CA-C	-14.98	1.27	1.51
1	K	265	GLY	CA-C	-14.96	1.27	1.51
1	O	265	GLY	CA-C	-14.94	1.27	1.51
2	J	250	ALA	N-CA	-12.84	1.20	1.46
2	N	250	ALA	N-CA	-12.83	1.20	1.46
2	H	250	ALA	N-CA	-12.82	1.20	1.46
2	D	250	ALA	N-CA	-12.82	1.20	1.46
2	B	250	ALA	N-CA	-12.81	1.20	1.46
2	F	250	ALA	N-CA	-12.81	1.20	1.46
2	L	250	ALA	N-CA	-12.81	1.20	1.46
2	R	250	ALA	N-CA	-12.81	1.20	1.46
2	P	250	ALA	N-CA	-12.80	1.20	1.46
1	E	266	HIS	N-CA	-11.03	1.24	1.46
1	I	266	HIS	N-CA	-11.01	1.24	1.46
1	M	266	HIS	N-CA	-11.01	1.24	1.46
1	Q	266	HIS	N-CA	-11.00	1.24	1.46
1	A	266	HIS	N-CA	-10.99	1.24	1.46
1	C	266	HIS	N-CA	-10.98	1.24	1.46
1	O	266	HIS	N-CA	-10.98	1.24	1.46
1	G	266	HIS	N-CA	-10.97	1.24	1.46
1	K	266	HIS	N-CA	-10.97	1.24	1.46
1	G	265	GLY	N-CA	-8.67	1.33	1.46
1	I	265	GLY	N-CA	-8.65	1.33	1.46
1	M	265	GLY	N-CA	-8.65	1.33	1.46
1	A	265	GLY	N-CA	-8.64	1.33	1.46
1	K	265	GLY	N-CA	-8.64	1.33	1.46
1	C	265	GLY	N-CA	-8.64	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	265	GLY	N-CA	-8.63	1.33	1.46
1	E	265	GLY	N-CA	-8.61	1.33	1.46
1	Q	265	GLY	N-CA	-8.61	1.33	1.46
1	G	348	PRO	N-CA	-8.08	1.33	1.47
1	I	348	PRO	N-CA	-8.08	1.33	1.47
1	C	348	PRO	N-CA	-8.08	1.33	1.47
1	K	348	PRO	N-CA	-8.06	1.33	1.47
1	A	348	PRO	N-CA	-8.04	1.33	1.47
1	M	348	PRO	N-CA	-8.04	1.33	1.47
1	E	348	PRO	N-CA	-8.03	1.33	1.47
1	Q	348	PRO	N-CA	-8.02	1.33	1.47
1	O	348	PRO	N-CA	-8.00	1.33	1.47
1	I	264	ARG	CA-C	-7.61	1.33	1.52
1	E	264	ARG	CA-C	-7.60	1.33	1.52
1	A	264	ARG	CA-C	-7.60	1.33	1.52
1	G	264	ARG	CA-C	-7.60	1.33	1.52
1	O	264	ARG	CA-C	-7.59	1.33	1.52
1	M	264	ARG	CA-C	-7.59	1.33	1.52
1	K	264	ARG	CA-C	-7.59	1.33	1.52
1	Q	264	ARG	CA-C	-7.58	1.33	1.52
1	C	264	ARG	CA-C	-7.58	1.33	1.52
1	E	439	SER	N-CA	-7.33	1.31	1.46
1	K	439	SER	N-CA	-7.33	1.31	1.46
1	M	439	SER	N-CA	-7.32	1.31	1.46
1	I	439	SER	N-CA	-7.31	1.31	1.46
1	G	439	SER	N-CA	-7.30	1.31	1.46
1	C	439	SER	N-CA	-7.30	1.31	1.46
1	A	439	SER	N-CA	-7.29	1.31	1.46
1	Q	439	SER	N-CA	-7.29	1.31	1.46
1	O	439	SER	N-CA	-7.28	1.31	1.46
1	C	438	ASP	CA-C	-7.12	1.34	1.52
1	Q	438	ASP	CA-C	-7.11	1.34	1.52
1	E	438	ASP	CA-C	-7.11	1.34	1.52
1	O	438	ASP	CA-C	-7.10	1.34	1.52
1	K	438	ASP	CA-C	-7.10	1.34	1.52
1	G	438	ASP	CA-C	-7.09	1.34	1.52
1	A	438	ASP	CA-C	-7.09	1.34	1.52
1	I	438	ASP	CA-C	-7.09	1.34	1.52
1	M	438	ASP	CA-C	-7.09	1.34	1.52
1	Q	348	PRO	CA-C	-7.06	1.38	1.52
1	K	348	PRO	CA-C	-7.05	1.38	1.52
1	I	348	PRO	CA-C	-7.04	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	348	PRO	CA-C	-7.03	1.38	1.52
1	G	348	PRO	CA-C	-7.03	1.38	1.52
1	A	348	PRO	CA-C	-7.02	1.38	1.52
1	O	348	PRO	CA-C	-7.01	1.38	1.52
1	M	348	PRO	CA-C	-7.00	1.38	1.52
1	E	348	PRO	CA-C	-6.99	1.38	1.52
2	H	96	GLN	CA-C	-6.68	1.35	1.52
2	F	96	GLN	CA-C	-6.67	1.35	1.52
2	D	96	GLN	CA-C	-6.67	1.35	1.52
2	P	96	GLN	CA-C	-6.67	1.35	1.52
2	F	38	GLY	CA-C	-6.67	1.41	1.51
2	H	38	GLY	CA-C	-6.67	1.41	1.51
2	N	96	GLN	CA-C	-6.66	1.35	1.52
2	B	96	GLN	CA-C	-6.66	1.35	1.52
2	L	96	GLN	CA-C	-6.65	1.35	1.52
2	J	96	GLN	CA-C	-6.64	1.35	1.52
2	J	38	GLY	CA-C	-6.63	1.41	1.51
2	D	38	GLY	CA-C	-6.63	1.41	1.51
2	R	38	GLY	CA-C	-6.63	1.41	1.51
2	R	96	GLN	CA-C	-6.63	1.35	1.52
2	B	38	GLY	CA-C	-6.62	1.41	1.51
2	L	38	GLY	CA-C	-6.62	1.41	1.51
2	P	38	GLY	CA-C	-6.61	1.41	1.51
2	N	38	GLY	CA-C	-6.60	1.41	1.51
1	O	347	CYS	N-CA	-6.21	1.33	1.46
1	I	347	CYS	N-CA	-6.18	1.33	1.46
1	E	347	CYS	N-CA	-6.17	1.34	1.46
1	A	347	CYS	N-CA	-6.17	1.34	1.46
1	C	347	CYS	N-CA	-6.16	1.34	1.46
1	K	347	CYS	N-CA	-6.16	1.34	1.46
1	M	347	CYS	N-CA	-6.16	1.34	1.46
1	G	347	CYS	N-CA	-6.15	1.34	1.46
1	Q	347	CYS	N-CA	-6.14	1.34	1.46
2	F	97	SER	N-CA	-5.71	1.34	1.46
2	R	97	SER	N-CA	-5.70	1.34	1.46
2	N	242	LEU	N-CA	-5.68	1.34	1.46
2	P	97	SER	N-CA	-5.67	1.34	1.46
2	N	97	SER	N-CA	-5.67	1.35	1.46
2	H	97	SER	N-CA	-5.67	1.35	1.46
2	D	97	SER	N-CA	-5.67	1.35	1.46
2	H	242	LEU	N-CA	-5.67	1.35	1.46
2	B	97	SER	N-CA	-5.66	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	242	LEU	N-CA	-5.66	1.35	1.46
2	P	242	LEU	N-CA	-5.66	1.35	1.46
2	B	242	LEU	N-CA	-5.66	1.35	1.46
2	J	97	SER	N-CA	-5.66	1.35	1.46
2	L	97	SER	N-CA	-5.66	1.35	1.46
2	F	242	LEU	N-CA	-5.66	1.35	1.46
2	R	242	LEU	N-CA	-5.65	1.35	1.46
2	D	242	LEU	N-CA	-5.63	1.35	1.46
2	J	242	LEU	N-CA	-5.61	1.35	1.46
1	Q	49	PHE	N-CA	-5.14	1.36	1.46
1	K	49	PHE	N-CA	-5.14	1.36	1.46
1	E	49	PHE	N-CA	-5.12	1.36	1.46
1	M	49	PHE	N-CA	-5.11	1.36	1.46
1	O	49	PHE	N-CA	-5.10	1.36	1.46
1	A	49	PHE	N-CA	-5.10	1.36	1.46
1	G	49	PHE	N-CA	-5.09	1.36	1.46
1	C	49	PHE	N-CA	-5.09	1.36	1.46
1	I	49	PHE	N-CA	-5.06	1.36	1.46

All (826) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	48	ARG	NE-CZ-NH1	20.40	130.50	120.30
2	P	48	ARG	NE-CZ-NH1	20.32	130.46	120.30
2	J	48	ARG	NE-CZ-NH1	20.31	130.45	120.30
2	H	48	ARG	NE-CZ-NH1	20.30	130.45	120.30
2	B	48	ARG	NE-CZ-NH1	20.29	130.44	120.30
2	L	48	ARG	NE-CZ-NH1	20.26	130.43	120.30
2	N	48	ARG	NE-CZ-NH1	20.26	130.43	120.30
2	D	48	ARG	NE-CZ-NH1	20.25	130.43	120.30
2	F	48	ARG	NE-CZ-NH1	20.20	130.40	120.30
2	H	2	ARG	NE-CZ-NH1	17.75	129.17	120.30
2	R	2	ARG	NE-CZ-NH1	17.72	129.16	120.30
2	B	2	ARG	NE-CZ-NH1	17.67	129.14	120.30
2	D	2	ARG	NE-CZ-NH1	17.63	129.11	120.30
2	L	2	ARG	NE-CZ-NH1	17.62	129.11	120.30
2	F	2	ARG	NE-CZ-NH1	17.61	129.10	120.30
2	P	2	ARG	NE-CZ-NH1	17.60	129.10	120.30
2	N	2	ARG	NE-CZ-NH1	17.60	129.10	120.30
2	J	2	ARG	NE-CZ-NH1	17.58	129.09	120.30
2	P	308	ARG	NE-CZ-NH2	-17.31	111.65	120.30
2	F	308	ARG	NE-CZ-NH2	-17.25	111.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	308	ARG	NE-CZ-NH2	-17.24	111.68	120.30
2	L	308	ARG	NE-CZ-NH2	-17.20	111.70	120.30
2	L	88	ARG	NE-CZ-NH1	17.17	128.89	120.30
2	B	308	ARG	NE-CZ-NH2	-17.17	111.71	120.30
2	R	308	ARG	NE-CZ-NH2	-17.16	111.72	120.30
2	D	308	ARG	NE-CZ-NH2	-17.16	111.72	120.30
2	N	308	ARG	NE-CZ-NH2	-17.09	111.75	120.30
2	H	308	ARG	NE-CZ-NH2	-17.09	111.75	120.30
2	N	88	ARG	NE-CZ-NH1	17.09	128.84	120.30
2	J	88	ARG	NE-CZ-NH1	17.07	128.84	120.30
2	B	88	ARG	NE-CZ-NH1	17.05	128.82	120.30
2	D	88	ARG	NE-CZ-NH1	17.05	128.82	120.30
2	H	88	ARG	NE-CZ-NH1	17.03	128.81	120.30
2	R	88	ARG	NE-CZ-NH1	16.99	128.80	120.30
2	P	88	ARG	NE-CZ-NH1	16.99	128.79	120.30
2	F	88	ARG	NE-CZ-NH1	16.91	128.75	120.30
2	R	48	ARG	NE-CZ-NH2	-14.40	113.10	120.30
2	J	48	ARG	NE-CZ-NH2	-14.34	113.13	120.30
2	L	48	ARG	NE-CZ-NH2	-14.34	113.13	120.30
2	B	48	ARG	NE-CZ-NH2	-14.33	113.14	120.30
2	P	48	ARG	NE-CZ-NH2	-14.32	113.14	120.30
2	N	48	ARG	NE-CZ-NH2	-14.29	113.16	120.30
2	D	48	ARG	NE-CZ-NH2	-14.28	113.16	120.30
2	F	48	ARG	NE-CZ-NH2	-14.27	113.16	120.30
2	H	48	ARG	NE-CZ-NH2	-14.24	113.18	120.30
2	N	88	ARG	NE-CZ-NH2	-13.71	113.44	120.30
2	L	88	ARG	NE-CZ-NH2	-13.68	113.46	120.30
2	H	88	ARG	NE-CZ-NH2	-13.63	113.49	120.30
2	J	88	ARG	NE-CZ-NH2	-13.62	113.49	120.30
2	B	88	ARG	NE-CZ-NH2	-13.61	113.49	120.30
2	R	88	ARG	NE-CZ-NH2	-13.59	113.50	120.30
2	F	88	ARG	NE-CZ-NH2	-13.54	113.53	120.30
2	P	88	ARG	NE-CZ-NH2	-13.53	113.53	120.30
2	D	88	ARG	NE-CZ-NH2	-13.53	113.54	120.30
1	K	105	ARG	NE-CZ-NH2	-13.42	113.59	120.30
1	I	105	ARG	NE-CZ-NH2	-13.40	113.60	120.30
1	E	105	ARG	NE-CZ-NH2	-13.39	113.60	120.30
1	A	105	ARG	NE-CZ-NH2	-13.38	113.61	120.30
1	M	105	ARG	NE-CZ-NH2	-13.35	113.62	120.30
1	O	105	ARG	NE-CZ-NH2	-13.35	113.63	120.30
1	G	105	ARG	NE-CZ-NH2	-13.33	113.63	120.30
1	C	105	ARG	NE-CZ-NH2	-13.31	113.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	105	ARG	NE-CZ-NH2	-13.28	113.66	120.30
2	L	400	ARG	NE-CZ-NH2	13.20	126.90	120.30
2	H	400	ARG	NE-CZ-NH2	13.19	126.89	120.30
2	F	400	ARG	NE-CZ-NH2	13.16	126.88	120.30
2	J	400	ARG	NE-CZ-NH2	13.11	126.86	120.30
2	B	400	ARG	NE-CZ-NH2	13.11	126.85	120.30
2	N	400	ARG	NE-CZ-NH2	13.09	126.85	120.30
2	R	400	ARG	NE-CZ-NH2	13.02	126.81	120.30
2	P	400	ARG	NE-CZ-NH2	13.01	126.81	120.30
2	D	400	ARG	NE-CZ-NH2	12.99	126.80	120.30
2	H	283	TYR	CB-CG-CD1	-12.60	113.44	121.00
2	N	283	TYR	CB-CG-CD1	-12.53	113.48	121.00
2	P	283	TYR	CB-CG-CD1	-12.52	113.49	121.00
2	D	283	TYR	CB-CG-CD1	-12.50	113.50	121.00
2	B	283	TYR	CB-CG-CD1	-12.50	113.50	121.00
2	J	215	ARG	NE-CZ-NH2	-12.49	114.06	120.30
2	R	283	TYR	CB-CG-CD1	-12.48	113.51	121.00
2	L	283	TYR	CB-CG-CD1	-12.47	113.52	121.00
2	L	215	ARG	NE-CZ-NH2	-12.46	114.07	120.30
2	F	283	TYR	CB-CG-CD1	-12.46	113.52	121.00
2	R	215	ARG	NE-CZ-NH2	-12.45	114.08	120.30
2	J	283	TYR	CB-CG-CD1	-12.44	113.54	121.00
2	B	215	ARG	NE-CZ-NH2	-12.40	114.10	120.30
2	F	215	ARG	NE-CZ-NH2	-12.40	114.10	120.30
2	P	215	ARG	NE-CZ-NH2	-12.39	114.11	120.30
2	H	215	ARG	NE-CZ-NH2	-12.38	114.11	120.30
2	D	215	ARG	NE-CZ-NH2	-12.30	114.15	120.30
2	N	215	ARG	NE-CZ-NH2	-12.29	114.16	120.30
1	E	123	ARG	NE-CZ-NH2	-11.83	114.38	120.30
1	O	123	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	Q	123	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	A	123	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	C	123	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	K	123	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	I	123	ARG	NE-CZ-NH2	-11.77	114.42	120.30
1	M	123	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	G	123	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	G	215	ARG	NE-CZ-NH1	11.33	125.96	120.30
1	O	215	ARG	NE-CZ-NH1	11.31	125.95	120.30
1	I	215	ARG	NE-CZ-NH1	11.27	125.94	120.30
1	Q	215	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	A	215	ARG	NE-CZ-NH1	11.26	125.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	215	ARG	NE-CZ-NH1	11.24	125.92	120.30
1	M	215	ARG	NE-CZ-NH1	11.24	125.92	120.30
1	I	214	ARG	NE-CZ-NH2	-11.23	114.69	120.30
1	C	215	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	E	215	ARG	NE-CZ-NH1	11.15	125.88	120.30
1	Q	214	ARG	NE-CZ-NH2	-11.15	114.73	120.30
1	E	214	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	M	214	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	O	214	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	A	214	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	K	214	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	C	214	ARG	NE-CZ-NH2	-11.12	114.74	120.30
2	L	284	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	G	214	ARG	NE-CZ-NH2	-11.08	114.76	120.30
2	D	284	ARG	NE-CZ-NH1	11.05	125.83	120.30
2	H	284	ARG	NE-CZ-NH1	11.04	125.82	120.30
2	B	284	ARG	NE-CZ-NH1	11.04	125.82	120.30
2	N	284	ARG	NE-CZ-NH1	11.04	125.82	120.30
2	J	284	ARG	NE-CZ-NH1	11.02	125.81	120.30
2	P	284	ARG	NE-CZ-NH1	11.02	125.81	120.30
2	R	284	ARG	NE-CZ-NH1	10.97	125.79	120.30
2	F	284	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	K	390	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	E	390	ARG	NE-CZ-NH1	10.83	125.72	120.30
1	I	390	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	K	265	GLY	CA-C-N	-10.81	93.41	117.20
1	A	265	GLY	CA-C-N	-10.80	93.43	117.20
1	O	390	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	O	265	GLY	CA-C-N	-10.80	93.43	117.20
1	C	265	GLY	CA-C-N	-10.80	93.44	117.20
1	M	265	GLY	CA-C-N	-10.79	93.45	117.20
1	E	265	GLY	CA-C-N	-10.79	93.46	117.20
1	I	265	GLY	CA-C-N	-10.79	93.46	117.20
1	G	265	GLY	CA-C-N	-10.79	93.47	117.20
1	Q	265	GLY	CA-C-N	-10.78	93.47	117.20
1	Q	390	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	M	390	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	G	390	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	A	390	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	C	390	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	C	36	MET	CG-SD-CE	10.01	116.21	100.20
1	E	36	MET	CG-SD-CE	10.00	116.20	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	36	MET	CG-SD-CE	10.00	116.19	100.20
1	I	36	MET	CG-SD-CE	9.99	116.19	100.20
1	Q	36	MET	CG-SD-CE	9.99	116.19	100.20
1	A	36	MET	CG-SD-CE	9.98	116.17	100.20
1	K	36	MET	CG-SD-CE	9.97	116.15	100.20
1	O	36	MET	CG-SD-CE	9.96	116.14	100.20
1	G	36	MET	CG-SD-CE	9.96	116.14	100.20
1	G	264	ARG	C-N-CA	-9.91	101.49	122.30
1	O	264	ARG	C-N-CA	-9.91	101.49	122.30
1	K	264	ARG	C-N-CA	-9.91	101.50	122.30
1	A	264	ARG	C-N-CA	-9.90	101.50	122.30
1	E	264	ARG	C-N-CA	-9.90	101.50	122.30
1	Q	264	ARG	C-N-CA	-9.90	101.50	122.30
1	C	264	ARG	C-N-CA	-9.90	101.51	122.30
1	M	264	ARG	C-N-CA	-9.90	101.51	122.30
1	I	264	ARG	C-N-CA	-9.88	101.56	122.30
2	L	401	ARG	NE-CZ-NH2	9.53	125.07	120.30
2	F	401	ARG	NE-CZ-NH2	9.50	125.05	120.30
2	R	401	ARG	NE-CZ-NH2	9.50	125.05	120.30
2	J	401	ARG	NE-CZ-NH2	9.49	125.05	120.30
2	B	401	ARG	NE-CZ-NH2	9.44	125.02	120.30
2	N	401	ARG	NE-CZ-NH2	9.44	125.02	120.30
2	D	401	ARG	NE-CZ-NH2	9.43	125.01	120.30
2	H	243	ARG	NE-CZ-NH1	9.41	125.00	120.30
2	J	243	ARG	NE-CZ-NH1	9.41	125.00	120.30
2	H	401	ARG	NE-CZ-NH2	9.40	125.00	120.30
2	B	243	ARG	NE-CZ-NH1	9.38	124.99	120.30
2	D	243	ARG	NE-CZ-NH1	9.38	124.99	120.30
2	F	243	ARG	NE-CZ-NH1	9.38	124.99	120.30
2	P	401	ARG	NE-CZ-NH2	9.37	124.98	120.30
2	L	243	ARG	NE-CZ-NH1	9.35	124.97	120.30
2	N	243	ARG	NE-CZ-NH1	9.32	124.96	120.30
2	R	243	ARG	NE-CZ-NH1	9.32	124.96	120.30
2	H	283	TYR	CB-CG-CD2	9.30	126.58	121.00
2	P	243	ARG	NE-CZ-NH1	9.30	124.95	120.30
2	N	283	TYR	CB-CG-CD2	9.28	126.57	121.00
2	B	283	TYR	CB-CG-CD2	9.27	126.56	121.00
2	J	283	TYR	CB-CG-CD2	9.26	126.55	121.00
2	L	283	TYR	CB-CG-CD2	9.25	126.55	121.00
2	D	283	TYR	CB-CG-CD2	9.23	126.54	121.00
2	P	283	TYR	CB-CG-CD2	9.23	126.54	121.00
2	F	283	TYR	CB-CG-CD2	9.21	126.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	283	TYR	CB-CG-CD2	9.19	126.52	121.00
1	O	265	GLY	O-C-N	9.08	137.23	122.70
1	A	265	GLY	O-C-N	9.06	137.19	122.70
1	K	265	GLY	O-C-N	9.06	137.19	122.70
1	M	265	GLY	O-C-N	9.05	137.19	122.70
1	C	265	GLY	O-C-N	9.05	137.18	122.70
1	G	265	GLY	O-C-N	9.05	137.18	122.70
1	I	265	GLY	O-C-N	9.04	137.17	122.70
1	Q	265	GLY	O-C-N	9.03	137.14	122.70
1	E	265	GLY	O-C-N	9.02	137.14	122.70
2	F	185	TYR	CB-CG-CD2	-8.99	115.61	121.00
2	R	185	TYR	CB-CG-CD2	-8.96	115.62	121.00
2	H	185	TYR	CB-CG-CD2	-8.95	115.63	121.00
2	P	185	TYR	CB-CG-CD2	-8.92	115.65	121.00
2	B	185	TYR	CB-CG-CD2	-8.92	115.65	121.00
2	L	185	TYR	CB-CG-CD2	-8.91	115.65	121.00
2	N	185	TYR	CB-CG-CD2	-8.90	115.66	121.00
2	D	185	TYR	CB-CG-CD2	-8.87	115.68	121.00
2	J	185	TYR	CB-CG-CD2	-8.85	115.69	121.00
1	Q	229	ARG	NE-CZ-NH2	8.39	124.49	120.30
1	K	229	ARG	NE-CZ-NH2	8.37	124.48	120.30
1	I	229	ARG	NE-CZ-NH2	8.35	124.48	120.30
1	A	229	ARG	NE-CZ-NH2	8.31	124.46	120.30
1	E	229	ARG	NE-CZ-NH2	8.30	124.45	120.30
1	G	229	ARG	NE-CZ-NH2	8.29	124.45	120.30
1	C	229	ARG	NE-CZ-NH2	8.27	124.43	120.30
1	M	229	ARG	NE-CZ-NH2	8.27	124.43	120.30
1	O	229	ARG	NE-CZ-NH2	8.27	124.43	120.30
1	O	262	TYR	CB-CG-CD2	-8.22	116.07	121.00
1	I	262	TYR	CB-CG-CD2	-8.20	116.08	121.00
1	G	262	TYR	CB-CG-CD2	-8.19	116.08	121.00
1	E	262	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	A	262	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	Q	262	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	K	262	TYR	CB-CG-CD2	-8.16	116.10	121.00
1	C	262	TYR	CB-CG-CD2	-8.14	116.11	121.00
2	L	123	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	K	339	ARG	NE-CZ-NH2	8.13	124.37	120.30
1	I	339	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	M	262	TYR	CB-CG-CD2	-8.12	116.13	121.00
2	N	123	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	G	339	ARG	NE-CZ-NH2	8.11	124.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	123	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	O	339	ARG	NE-CZ-NH2	8.10	124.35	120.30
2	F	123	ARG	NE-CZ-NH2	-8.08	116.26	120.30
2	H	123	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	339	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	C	339	ARG	NE-CZ-NH2	8.06	124.33	120.30
2	B	123	ARG	NE-CZ-NH2	-8.05	116.28	120.30
2	R	123	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	E	339	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	M	339	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	Q	339	ARG	NE-CZ-NH2	8.02	124.31	120.30
2	J	123	ARG	NE-CZ-NH2	-7.98	116.31	120.30
2	P	123	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	C	11	GLN	CB-CA-C	-7.96	94.48	110.40
1	Q	11	GLN	CB-CA-C	-7.95	94.50	110.40
1	K	11	GLN	CB-CA-C	-7.95	94.51	110.40
1	E	11	GLN	CB-CA-C	-7.95	94.51	110.40
1	A	11	GLN	CB-CA-C	-7.94	94.52	110.40
1	I	11	GLN	CB-CA-C	-7.94	94.53	110.40
1	O	11	GLN	CB-CA-C	-7.94	94.53	110.40
1	G	11	GLN	CB-CA-C	-7.93	94.53	110.40
1	M	11	GLN	CB-CA-C	-7.93	94.53	110.40
2	L	101	ASN	CB-CG-OD1	-7.82	105.95	121.60
2	P	101	ASN	CB-CG-OD1	-7.81	105.98	121.60
2	D	101	ASN	CB-CG-OD1	-7.80	106.00	121.60
2	B	101	ASN	CB-CG-OD1	-7.80	106.00	121.60
2	F	101	ASN	CB-CG-OD1	-7.80	106.01	121.60
2	N	101	ASN	CB-CG-OD1	-7.79	106.01	121.60
2	H	101	ASN	CB-CG-OD1	-7.79	106.02	121.60
2	J	101	ASN	CB-CG-OD1	-7.79	106.02	121.60
2	R	101	ASN	CB-CG-OD1	-7.79	106.03	121.60
2	F	311	ARG	NE-CZ-NH2	-7.72	116.44	120.30
2	D	253	ARG	NE-CZ-NH2	7.71	124.16	120.30
2	N	311	ARG	NE-CZ-NH2	-7.71	116.45	120.30
2	J	311	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	M	121	ARG	NE-CZ-NH1	-7.70	116.45	120.30
2	F	400	ARG	NE-CZ-NH1	-7.69	116.45	120.30
2	J	96	GLN	C-N-CA	-7.69	102.47	121.70
2	F	253	ARG	NE-CZ-NH2	7.69	124.14	120.30
2	L	96	GLN	C-N-CA	-7.68	102.50	121.70
2	N	96	GLN	C-N-CA	-7.68	102.50	121.70
2	B	311	ARG	NE-CZ-NH2	-7.67	116.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	253	ARG	NE-CZ-NH2	7.67	124.14	120.30
2	D	311	ARG	NE-CZ-NH2	-7.67	116.46	120.30
2	B	96	GLN	C-N-CA	-7.67	102.53	121.70
2	J	400	ARG	NE-CZ-NH1	-7.67	116.47	120.30
2	R	96	GLN	C-N-CA	-7.67	102.53	121.70
2	H	96	GLN	C-N-CA	-7.67	102.53	121.70
2	H	432	TYR	CB-CG-CD2	-7.67	116.40	121.00
2	L	311	ARG	NE-CZ-NH2	-7.67	116.47	120.30
2	J	253	ARG	NE-CZ-NH2	7.67	124.13	120.30
2	B	253	ARG	NE-CZ-NH2	7.66	124.13	120.30
2	P	96	GLN	C-N-CA	-7.66	102.54	121.70
2	D	96	GLN	C-N-CA	-7.66	102.55	121.70
2	L	400	ARG	NE-CZ-NH1	-7.66	116.47	120.30
2	F	96	GLN	C-N-CA	-7.66	102.55	121.70
2	P	253	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	I	121	ARG	NE-CZ-NH1	-7.65	116.47	120.30
2	R	253	ARG	NE-CZ-NH2	7.65	124.12	120.30
2	H	311	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	121	ARG	NE-CZ-NH1	-7.64	116.48	120.30
2	R	432	TYR	CB-CG-CD2	-7.64	116.42	121.00
2	N	400	ARG	NE-CZ-NH1	-7.63	116.48	120.30
2	P	311	ARG	NE-CZ-NH2	-7.63	116.48	120.30
2	H	253	ARG	NE-CZ-NH2	7.63	124.12	120.30
2	H	400	ARG	NE-CZ-NH1	-7.63	116.48	120.30
2	L	432	TYR	CB-CG-CD2	-7.63	116.42	121.00
1	O	121	ARG	NE-CZ-NH1	-7.63	116.49	120.30
2	P	432	TYR	CB-CG-CD2	-7.62	116.42	121.00
2	D	432	TYR	CB-CG-CD2	-7.62	116.43	121.00
2	R	311	ARG	NE-CZ-NH2	-7.62	116.49	120.30
2	L	253	ARG	NE-CZ-NH2	7.62	124.11	120.30
2	B	400	ARG	NE-CZ-NH1	-7.62	116.49	120.30
2	P	400	ARG	NE-CZ-NH1	-7.62	116.49	120.30
2	B	432	TYR	CB-CG-CD2	-7.61	116.44	121.00
2	N	432	TYR	CB-CG-CD2	-7.61	116.44	121.00
1	E	121	ARG	NE-CZ-NH1	-7.60	116.50	120.30
1	K	121	ARG	NE-CZ-NH1	-7.60	116.50	120.30
2	J	432	TYR	CB-CG-CD2	-7.59	116.44	121.00
1	C	121	ARG	NE-CZ-NH1	-7.59	116.51	120.30
1	Q	121	ARG	NE-CZ-NH1	-7.59	116.51	120.30
1	G	121	ARG	NE-CZ-NH1	-7.58	116.51	120.30
2	F	432	TYR	CB-CG-CD2	-7.57	116.46	121.00
2	D	400	ARG	NE-CZ-NH1	-7.52	116.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	308	ARG	NE-CZ-NH1	7.52	124.06	120.30
2	R	400	ARG	NE-CZ-NH1	-7.51	116.55	120.30
2	F	308	ARG	NE-CZ-NH1	7.50	124.05	120.30
2	J	308	ARG	NE-CZ-NH1	7.47	124.04	120.30
2	R	308	ARG	NE-CZ-NH1	7.45	124.02	120.30
2	L	308	ARG	NE-CZ-NH1	7.42	124.01	120.30
2	B	308	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	I	156	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	C	185	TYR	CB-CG-CD2	-7.41	116.55	121.00
1	G	185	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	O	185	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	K	185	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	Q	185	TYR	CB-CG-CD2	-7.37	116.58	121.00
2	D	308	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	M	172	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	M	185	TYR	CB-CG-CD2	-7.36	116.58	121.00
2	N	308	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	E	172	TYR	CB-CG-CD2	-7.35	116.59	121.00
1	I	185	TYR	CB-CG-CD2	-7.34	116.59	121.00
1	O	172	TYR	CB-CG-CD2	-7.34	116.59	121.00
1	C	172	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	A	156	ARG	NE-CZ-NH2	7.33	123.96	120.30
2	H	308	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	A	185	TYR	CB-CG-CD2	-7.32	116.61	121.00
1	C	156	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	M	156	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	E	185	TYR	CB-CG-CD2	-7.32	116.61	121.00
1	A	172	TYR	CB-CG-CD2	-7.31	116.61	121.00
1	Q	156	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	G	156	ARG	NE-CZ-NH2	7.29	123.95	120.30
1	K	172	TYR	CB-CG-CD2	-7.28	116.63	121.00
1	K	156	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	O	156	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	G	172	TYR	CB-CG-CD2	-7.26	116.64	121.00
1	Q	172	TYR	CB-CG-CD2	-7.26	116.64	121.00
1	E	156	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	I	172	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	I	24	TYR	CB-CG-CD1	-7.03	116.78	121.00
1	A	24	TYR	CB-CG-CD1	-6.99	116.81	121.00
1	K	24	TYR	CB-CG-CD1	-6.99	116.81	121.00
1	G	79	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	Q	24	TYR	CB-CG-CD1	-6.97	116.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	K	79	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	E	24	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	C	24	TYR	CB-CG-CD1	-6.94	116.84	121.00
1	O	24	TYR	CB-CG-CD1	-6.94	116.84	121.00
1	M	24	TYR	CB-CG-CD1	-6.93	116.84	121.00
1	A	79	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	M	79	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	O	79	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	264	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	Q	264	ARG	NE-CZ-NH1	-6.91	116.85	120.30
1	E	264	ARG	NE-CZ-NH1	-6.91	116.85	120.30
1	G	24	TYR	CB-CG-CD1	-6.90	116.86	121.00
1	O	264	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	I	264	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	I	79	ARG	NE-CZ-NH2	-6.89	116.86	120.30
2	D	2	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	L	320	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	H	320	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	E	79	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	C	264	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	G	264	ARG	NE-CZ-NH1	-6.86	116.87	120.30
2	H	2	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	K	264	ARG	NE-CZ-NH1	-6.85	116.88	120.30
2	R	320	ARG	NE-CZ-NH1	6.85	123.72	120.30
2	R	2	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	P	2	ARG	NE-CZ-NH2	-6.83	116.88	120.30
2	B	2	ARG	NE-CZ-NH2	-6.83	116.88	120.30
2	N	2	ARG	NE-CZ-NH2	-6.83	116.89	120.30
2	N	320	ARG	NE-CZ-NH1	6.83	123.72	120.30
2	B	320	ARG	NE-CZ-NH1	6.82	123.71	120.30
2	J	320	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	Q	79	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	M	264	ARG	NE-CZ-NH1	-6.80	116.90	120.30
2	J	2	ARG	NE-CZ-NH2	-6.80	116.90	120.30
2	F	2	ARG	NE-CZ-NH2	-6.79	116.90	120.30
2	L	2	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	D	320	ARG	NE-CZ-NH1	6.76	123.68	120.30
2	P	320	ARG	NE-CZ-NH1	6.75	123.67	120.30
2	F	320	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	P	79	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	M	438	ASP	CA-C-N	-6.60	102.69	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	438	ASP	CA-C-N	-6.59	102.70	117.20
2	N	79	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	A	438	ASP	CA-C-N	-6.58	102.72	117.20
1	K	244	PHE	CB-CG-CD2	-6.58	116.19	120.80
2	B	79	ARG	NE-CZ-NH1	6.58	123.59	120.30
2	J	79	ARG	NE-CZ-NH1	6.58	123.59	120.30
2	R	79	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	G	244	PHE	CB-CG-CD2	-6.57	116.20	120.80
1	I	438	ASP	CA-C-N	-6.57	102.74	117.20
1	C	438	ASP	CA-C-N	-6.57	102.74	117.20
1	O	438	ASP	CA-C-N	-6.57	102.75	117.20
1	Q	438	ASP	CA-C-N	-6.57	102.75	117.20
2	F	79	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	K	438	ASP	CA-C-N	-6.57	102.75	117.20
1	E	438	ASP	CA-C-N	-6.57	102.76	117.20
1	Q	244	PHE	CB-CG-CD2	-6.54	116.22	120.80
1	A	244	PHE	CB-CG-CD2	-6.53	116.23	120.80
2	L	79	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	H	79	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	O	244	PHE	CB-CG-CD2	-6.51	116.25	120.80
2	D	79	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	E	244	PHE	CB-CG-CD2	-6.48	116.26	120.80
1	E	105	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	C	244	PHE	CB-CG-CD2	-6.47	116.27	120.80
1	I	244	PHE	CB-CG-CD2	-6.45	116.29	120.80
1	M	244	PHE	CB-CG-CD2	-6.43	116.30	120.80
1	K	105	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	105	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	M	105	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	O	105	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	C	105	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	Q	105	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	I	105	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	G	105	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	O	142	GLY	C-N-CA	-6.25	109.18	122.30
1	A	142	GLY	C-N-CA	-6.23	109.21	122.30
1	I	142	GLY	C-N-CA	-6.23	109.22	122.30
1	C	142	GLY	C-N-CA	-6.22	109.23	122.30
1	M	142	GLY	C-N-CA	-6.22	109.23	122.30
1	G	142	GLY	C-N-CA	-6.22	109.24	122.30
1	Q	142	GLY	C-N-CA	-6.22	109.25	122.30
1	E	142	GLY	C-N-CA	-6.21	109.25	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	142	GLY	C-N-CA	-6.21	109.25	122.30
2	R	306	ASP	CB-CG-OD2	6.16	123.84	118.30
1	K	205	ASP	CB-CG-OD2	-6.14	112.78	118.30
2	J	306	ASP	CB-CG-OD2	6.13	123.82	118.30
2	R	185	TYR	CB-CA-C	-6.13	98.14	110.40
2	J	185	TYR	CB-CA-C	-6.12	98.15	110.40
2	D	185	TYR	CB-CA-C	-6.12	98.15	110.40
2	F	185	TYR	CB-CA-C	-6.12	98.15	110.40
2	H	185	TYR	CB-CA-C	-6.12	98.16	110.40
2	L	185	TYR	CB-CA-C	-6.12	98.16	110.40
2	B	306	ASP	CB-CG-OD2	6.12	123.81	118.30
2	D	306	ASP	CB-CG-OD2	6.12	123.81	118.30
1	G	205	ASP	CB-CG-OD2	-6.12	112.79	118.30
2	H	306	ASP	CB-CG-OD2	6.12	123.81	118.30
2	P	306	ASP	CB-CG-OD2	6.12	123.80	118.30
2	F	306	ASP	CB-CG-OD2	6.11	123.80	118.30
1	G	339	ARG	NH1-CZ-NH2	-6.11	112.67	119.40
2	B	185	TYR	CB-CA-C	-6.11	98.18	110.40
2	N	306	ASP	CB-CG-OD2	6.11	123.80	118.30
1	O	11	GLN	N-CA-CB	6.11	121.59	110.60
1	M	205	ASP	CB-CG-OD2	-6.10	112.81	118.30
2	L	306	ASP	CB-CG-OD2	6.10	123.79	118.30
1	G	11	GLN	N-CA-CB	6.10	121.58	110.60
1	I	11	GLN	N-CA-CB	6.10	121.58	110.60
2	P	185	TYR	CB-CA-C	-6.10	98.21	110.40
1	M	190	THR	CB-CA-C	-6.09	95.16	111.60
1	O	339	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
1	A	11	GLN	N-CA-CB	6.09	121.56	110.60
1	C	11	GLN	N-CA-CB	6.09	121.56	110.60
2	N	185	TYR	CB-CA-C	-6.08	98.23	110.40
1	K	190	THR	CB-CA-C	-6.08	95.18	111.60
1	Q	11	GLN	N-CA-CB	6.08	121.55	110.60
1	E	11	GLN	N-CA-CB	6.08	121.54	110.60
1	A	339	ARG	NH1-CZ-NH2	-6.08	112.71	119.40
1	I	190	THR	CB-CA-C	-6.08	95.19	111.60
1	O	190	THR	CB-CA-C	-6.08	95.19	111.60
1	C	205	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	I	205	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	K	11	GLN	N-CA-CB	6.08	121.54	110.60
1	E	339	ARG	NH1-CZ-NH2	-6.08	112.72	119.40
1	A	190	THR	CB-CA-C	-6.07	95.20	111.60
1	C	348	PRO	CA-N-CD	6.07	120.20	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	190	THR	CB-CA-C	-6.07	95.20	111.60
1	G	190	THR	CB-CA-C	-6.07	95.20	111.60
1	Q	190	THR	CB-CA-C	-6.07	95.20	111.60
1	C	339	ARG	NH1-CZ-NH2	-6.07	112.72	119.40
1	I	339	ARG	NH1-CZ-NH2	-6.07	112.72	119.40
1	Q	205	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	Q	348	PRO	CA-N-CD	6.07	120.20	111.70
1	M	11	GLN	N-CA-CB	6.07	121.52	110.60
1	K	339	ARG	NH1-CZ-NH2	-6.06	112.73	119.40
1	C	190	THR	CB-CA-C	-6.06	95.23	111.60
1	Q	339	ARG	NH1-CZ-NH2	-6.06	112.73	119.40
1	A	205	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	A	348	PRO	CA-N-CD	6.05	120.17	111.70
1	E	205	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	M	348	PRO	CA-N-CD	6.05	120.16	111.70
1	G	348	PRO	CA-N-CD	6.04	120.16	111.70
1	E	348	PRO	CA-N-CD	6.04	120.16	111.70
1	G	438	ASP	C-N-CA	-6.04	106.61	121.70
1	I	348	PRO	CA-N-CD	6.03	120.15	111.70
1	M	438	ASP	C-N-CA	-6.03	106.61	121.70
1	O	438	ASP	C-N-CA	-6.03	106.62	121.70
1	O	348	PRO	CA-N-CD	6.03	120.14	111.70
1	M	339	ARG	NH1-CZ-NH2	-6.03	112.77	119.40
1	A	438	ASP	C-N-CA	-6.03	106.64	121.70
1	K	348	PRO	CA-N-CD	6.03	120.14	111.70
1	Q	438	ASP	C-N-CA	-6.02	106.64	121.70
1	C	438	ASP	C-N-CA	-6.02	106.64	121.70
1	I	438	ASP	C-N-CA	-6.02	106.65	121.70
1	E	438	ASP	C-N-CA	-6.01	106.67	121.70
1	K	438	ASP	C-N-CA	-6.01	106.68	121.70
1	O	205	ASP	CB-CG-OD2	-6.00	112.90	118.30
2	H	308	ARG	CD-NE-CZ	5.99	131.99	123.60
2	N	308	ARG	CD-NE-CZ	5.98	131.98	123.60
2	J	311	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	R	308	ARG	CD-NE-CZ	5.98	131.97	123.60
2	B	61	TYR	CB-CG-CD1	-5.97	117.42	121.00
2	H	61	TYR	CB-CG-CD1	-5.97	117.42	121.00
2	L	308	ARG	CD-NE-CZ	5.97	131.95	123.60
2	L	61	TYR	CB-CG-CD1	-5.96	117.42	121.00
2	N	61	TYR	CB-CG-CD1	-5.96	117.42	121.00
2	R	61	TYR	CB-CG-CD1	-5.96	117.42	121.00
2	B	308	ARG	CD-NE-CZ	5.96	131.95	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	308	ARG	CD-NE-CZ	5.96	131.94	123.60
2	D	311	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	I	108	TYR	CB-CG-CD1	-5.95	117.43	121.00
2	F	308	ARG	CD-NE-CZ	5.94	131.92	123.60
2	D	61	TYR	CB-CG-CD1	-5.93	117.44	121.00
2	P	308	ARG	CD-NE-CZ	5.93	131.90	123.60
2	J	308	ARG	CD-NE-CZ	5.92	131.89	123.60
2	P	61	TYR	CB-CG-CD1	-5.92	117.45	121.00
2	J	253	ARG	NH1-CZ-NH2	-5.91	112.90	119.40
2	R	311	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	K	265	GLY	C-N-CA	-5.91	106.93	121.70
2	H	311	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	I	265	GLY	C-N-CA	-5.91	106.94	121.70
1	O	265	GLY	C-N-CA	-5.91	106.94	121.70
2	F	61	TYR	CB-CG-CD1	-5.90	117.46	121.00
2	B	311	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	265	GLY	C-N-CA	-5.90	106.95	121.70
1	A	265	GLY	C-N-CA	-5.90	106.95	121.70
1	G	265	GLY	C-N-CA	-5.90	106.96	121.70
1	M	265	GLY	C-N-CA	-5.90	106.96	121.70
1	M	108	TYR	CB-CG-CD1	-5.90	117.46	121.00
1	E	108	TYR	CB-CG-CD1	-5.89	117.46	121.00
2	R	253	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
1	E	265	GLY	C-N-CA	-5.89	106.98	121.70
2	L	311	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	O	108	TYR	CB-CG-CD1	-5.89	117.47	121.00
1	Q	265	GLY	C-N-CA	-5.88	106.99	121.70
1	I	214	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	P	253	ARG	NH1-CZ-NH2	-5.88	112.94	119.40
1	Q	108	TYR	CB-CG-CD1	-5.88	117.47	121.00
2	J	61	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	A	108	TYR	CB-CG-CD1	-5.86	117.48	121.00
2	B	253	ARG	NH1-CZ-NH2	-5.86	112.95	119.40
2	F	311	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	N	253	ARG	NH1-CZ-NH2	-5.86	112.95	119.40
2	H	253	ARG	NH1-CZ-NH2	-5.86	112.96	119.40
2	L	253	ARG	NH1-CZ-NH2	-5.86	112.96	119.40
2	F	253	ARG	NH1-CZ-NH2	-5.86	112.96	119.40
1	E	214	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	M	214	ARG	NE-CZ-NH1	5.85	123.22	120.30
2	N	311	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	G	108	TYR	CB-CG-CD1	-5.85	117.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	253	ARG	NH1-CZ-NH2	-5.84	112.98	119.40
2	J	292	THR	CA-CB-CG2	-5.82	104.25	112.40
1	C	108	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	G	214	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	G	438	ASP	O-C-N	5.81	131.99	122.70
2	B	292	THR	CA-CB-CG2	-5.80	104.27	112.40
2	R	292	THR	CA-CB-CG2	-5.80	104.28	112.40
1	M	438	ASP	O-C-N	5.80	131.98	122.70
2	P	311	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	D	292	THR	CA-CB-CG2	-5.80	104.29	112.40
2	H	432	TYR	CB-CG-CD1	5.80	124.48	121.00
1	M	11	GLN	CA-CB-CG	5.80	126.15	113.40
2	F	292	THR	CA-CB-CG2	-5.79	104.29	112.40
2	P	292	THR	CA-CB-CG2	-5.79	104.29	112.40
1	Q	11	GLN	CA-CB-CG	5.79	126.14	113.40
1	A	438	ASP	O-C-N	5.79	131.97	122.70
1	C	438	ASP	O-C-N	5.79	131.97	122.70
1	E	11	GLN	CA-CB-CG	5.79	126.14	113.40
1	A	11	GLN	CA-CB-CG	5.79	126.14	113.40
1	I	438	ASP	O-C-N	5.79	131.96	122.70
1	K	11	GLN	CA-CB-CG	5.79	126.13	113.40
1	O	11	GLN	CA-CB-CG	5.79	126.13	113.40
1	G	11	GLN	CA-CB-CG	5.79	126.13	113.40
1	C	11	GLN	CA-CB-CG	5.78	126.13	113.40
2	N	292	THR	CA-CB-CG2	-5.78	104.30	112.40
1	O	438	ASP	O-C-N	5.78	131.95	122.70
2	L	292	THR	CA-CB-CG2	-5.78	104.31	112.40
1	A	214	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	214	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	I	11	GLN	CA-CB-CG	5.78	126.12	113.40
1	Q	438	ASP	O-C-N	5.78	131.95	122.70
1	K	214	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	N	248	LEU	CA-C-N	-5.77	104.50	117.20
2	D	248	LEU	CA-C-N	-5.77	104.50	117.20
2	R	248	LEU	CA-C-N	-5.77	104.50	117.20
2	H	248	LEU	CA-C-N	-5.77	104.51	117.20
1	K	108	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	E	438	ASP	O-C-N	5.76	131.92	122.70
2	F	248	LEU	CA-C-N	-5.76	104.53	117.20
2	H	292	THR	CA-CB-CG2	-5.76	104.34	112.40
2	J	248	LEU	CA-C-N	-5.76	104.54	117.20
2	B	248	LEU	CA-C-N	-5.75	104.54	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	438	ASP	O-C-N	5.75	131.91	122.70
2	R	432	TYR	CB-CG-CD1	5.75	124.45	121.00
2	P	248	LEU	CA-C-N	-5.74	104.56	117.20
2	L	248	LEU	CA-C-N	-5.74	104.57	117.20
2	P	239	THR	CA-CB-CG2	-5.74	104.36	112.40
2	P	432	TYR	CB-CG-CD1	5.74	124.44	121.00
1	O	214	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	H	239	THR	CA-CB-CG2	-5.72	104.39	112.40
2	F	239	THR	CA-CB-CG2	-5.72	104.39	112.40
2	N	432	TYR	CB-CG-CD1	5.71	124.43	121.00
1	Q	214	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	J	239	THR	CA-CB-CG2	-5.71	104.40	112.40
2	B	239	THR	CA-CB-CG2	-5.71	104.41	112.40
2	L	432	TYR	CB-CG-CD1	5.70	124.42	121.00
2	B	432	TYR	CB-CG-CD1	5.70	124.42	121.00
2	L	239	THR	CA-CB-CG2	-5.69	104.43	112.40
2	R	239	THR	CA-CB-CG2	-5.69	104.44	112.40
1	M	236	SER	CB-CA-C	-5.68	99.30	110.10
2	D	432	TYR	CB-CG-CD1	5.68	124.41	121.00
1	E	236	SER	CB-CA-C	-5.68	99.31	110.10
1	G	236	SER	CB-CA-C	-5.68	99.31	110.10
2	D	239	THR	CA-CB-CG2	-5.67	104.46	112.40
2	N	239	THR	CA-CB-CG2	-5.67	104.46	112.40
1	A	236	SER	CB-CA-C	-5.67	99.33	110.10
1	I	236	SER	CB-CA-C	-5.67	99.33	110.10
1	C	236	SER	CB-CA-C	-5.67	99.33	110.10
1	K	236	SER	CB-CA-C	-5.67	99.33	110.10
1	Q	236	SER	CB-CA-C	-5.66	99.34	110.10
2	J	432	TYR	CB-CG-CD1	5.66	124.40	121.00
1	O	236	SER	CB-CA-C	-5.66	99.35	110.10
2	F	432	TYR	CB-CG-CD1	5.66	124.39	121.00
2	D	101	ASN	CA-CB-CG	-5.60	101.07	113.40
2	P	101	ASN	CA-CB-CG	-5.60	101.08	113.40
2	J	101	ASN	CA-CB-CG	-5.60	101.09	113.40
2	N	101	ASN	CA-CB-CG	-5.59	101.09	113.40
2	B	101	ASN	CA-CB-CG	-5.59	101.10	113.40
2	L	101	ASN	CA-CB-CG	-5.59	101.10	113.40
2	H	101	ASN	CA-CB-CG	-5.59	101.11	113.40
2	P	101	ASN	CB-CG-ND2	5.58	130.10	116.70
2	F	101	ASN	CA-CB-CG	-5.58	101.12	113.40
2	R	101	ASN	CA-CB-CG	-5.58	101.12	113.40
2	H	101	ASN	CB-CG-ND2	5.57	130.07	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	101	ASN	CB-CG-ND2	5.57	130.07	116.70
2	J	101	ASN	CB-CG-ND2	5.57	130.07	116.70
2	F	101	ASN	CB-CG-ND2	5.57	130.06	116.70
2	N	101	ASN	CB-CG-ND2	5.57	130.06	116.70
1	Q	306	ASP	CB-CG-OD1	5.57	123.31	118.30
2	D	101	ASN	CB-CG-ND2	5.57	130.06	116.70
2	R	101	ASN	CB-CG-ND2	5.57	130.06	116.70
1	G	306	ASP	CB-CG-OD1	5.56	123.31	118.30
2	L	101	ASN	CB-CG-ND2	5.56	130.04	116.70
1	K	306	ASP	CB-CG-OD1	5.55	123.30	118.30
1	O	306	ASP	CB-CG-OD1	5.55	123.29	118.30
1	M	306	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	306	ASP	CB-CG-OD1	5.53	123.28	118.30
1	I	306	ASP	CB-CG-OD1	5.51	123.26	118.30
2	N	401	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
1	E	306	ASP	CB-CG-OD1	5.49	123.24	118.30
2	J	401	ARG	NH1-CZ-NH2	-5.49	113.36	119.40
2	L	401	ARG	NH1-CZ-NH2	-5.49	113.36	119.40
2	F	401	ARG	NH1-CZ-NH2	-5.48	113.37	119.40
1	C	161	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	C	306	ASP	CB-CG-OD1	5.47	123.22	118.30
2	B	401	ARG	NH1-CZ-NH2	-5.47	113.39	119.40
2	D	401	ARG	NH1-CZ-NH2	-5.47	113.39	119.40
1	M	121	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	O	211	ASP	CB-CG-OD2	5.46	123.21	118.30
2	P	53	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	Q	211	ASP	CB-CG-OD2	5.46	123.21	118.30
2	R	401	ARG	NH1-CZ-NH2	-5.45	113.40	119.40
2	H	48	ARG	CD-NE-CZ	5.45	131.23	123.60
1	M	211	ASP	CB-CG-OD2	5.45	123.20	118.30
1	K	211	ASP	CB-CG-OD2	5.45	123.20	118.30
2	N	48	ARG	CD-NE-CZ	5.45	131.22	123.60
2	H	401	ARG	NH1-CZ-NH2	-5.44	113.42	119.40
1	I	161	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	Q	161	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	A	211	ASP	CB-CG-OD2	5.43	123.19	118.30
2	F	48	ARG	CD-NE-CZ	5.43	131.21	123.60
2	P	48	ARG	CD-NE-CZ	5.43	131.21	123.60
2	B	48	ARG	CD-NE-CZ	5.43	131.20	123.60
2	D	48	ARG	CD-NE-CZ	5.43	131.20	123.60
1	G	161	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	K	123	ARG	NE-CZ-NH1	5.42	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	211	ASP	CB-CG-OD2	5.42	123.18	118.30
2	P	401	ARG	NH1-CZ-NH2	-5.42	113.44	119.40
2	J	48	ARG	CD-NE-CZ	5.42	131.19	123.60
1	A	161	TYR	CB-CG-CD1	-5.42	117.75	121.00
2	L	48	ARG	CD-NE-CZ	5.42	131.19	123.60
1	M	161	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	O	161	TYR	CB-CG-CD1	-5.41	117.76	121.00
1	E	123	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	I	211	ASP	CB-CG-OD2	5.40	123.16	118.30
1	G	211	ASP	CB-CG-OD2	5.39	123.16	118.30
2	R	48	ARG	CD-NE-CZ	5.39	131.15	123.60
1	E	211	ASP	CB-CG-OD2	5.39	123.15	118.30
1	E	161	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	M	123	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	N	53	TYR	CB-CG-CD2	-5.38	117.77	121.00
2	J	53	TYR	CB-CG-CD2	-5.37	117.78	121.00
2	N	97	SER	CA-C-N	-5.37	105.46	116.20
2	B	53	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	A	123	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	E	121	ARG	NE-CZ-NH2	5.36	122.98	120.30
2	J	97	SER	CA-C-N	-5.36	105.48	116.20
2	F	97	SER	CA-C-N	-5.36	105.49	116.20
1	O	123	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	P	97	SER	CA-C-N	-5.36	105.49	116.20
2	R	53	TYR	CB-CG-CD2	-5.36	117.79	121.00
2	R	97	SER	CA-C-N	-5.35	105.50	116.20
2	F	53	TYR	CB-CG-CD2	-5.35	117.79	121.00
2	H	97	SER	CA-C-N	-5.35	105.51	116.20
2	B	97	SER	CA-C-N	-5.34	105.51	116.20
2	D	97	SER	CA-C-N	-5.34	105.51	116.20
2	H	53	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	K	161	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	G	339	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	L	97	SER	CA-C-N	-5.34	105.52	116.20
1	Q	123	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	J	253	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	121	ARG	NE-CZ-NH2	5.33	122.96	120.30
2	D	53	TYR	CB-CG-CD2	-5.33	117.81	121.00
2	N	185	TYR	CA-CB-CG	5.33	123.52	113.40
1	E	339	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	121	ARG	NE-CZ-NH2	5.32	122.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	185	TYR	CA-CB-CG	5.32	123.50	113.40
1	I	123	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	J	185	TYR	CA-CB-CG	5.31	123.50	113.40
2	B	185	TYR	CA-CB-CG	5.31	123.50	113.40
2	D	61	TYR	CA-CB-CG	-5.31	103.31	113.40
2	R	253	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	G	123	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	339	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	P	185	TYR	CA-CB-CG	5.31	123.48	113.40
2	F	215	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	H	185	TYR	CA-CB-CG	5.30	123.48	113.40
1	I	121	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	Q	339	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	R	185	TYR	CA-CB-CG	5.30	123.47	113.40
2	F	185	TYR	CA-CB-CG	5.30	123.47	113.40
2	N	61	TYR	CA-CB-CG	-5.30	103.33	113.40
1	Q	121	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	O	121	ARG	NE-CZ-NH2	5.30	122.95	120.30
2	H	61	TYR	CA-CB-CG	-5.29	103.34	113.40
1	O	339	ARG	NE-CZ-NH1	5.29	122.95	120.30
2	R	61	TYR	CA-CB-CG	-5.29	103.34	113.40
1	C	339	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	L	53	TYR	CB-CG-CD2	-5.29	117.83	121.00
2	L	185	TYR	CA-CB-CG	5.29	123.45	113.40
2	F	61	TYR	CA-CB-CG	-5.29	103.35	113.40
2	B	61	TYR	CA-CB-CG	-5.29	103.36	113.40
2	L	215	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	L	61	TYR	CA-CB-CG	-5.28	103.37	113.40
2	J	61	TYR	CA-CB-CG	-5.27	103.38	113.40
1	K	121	ARG	NE-CZ-NH2	5.27	122.94	120.30
2	L	253	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	P	253	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	R	215	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	P	61	TYR	CA-CB-CG	-5.26	103.41	113.40
2	H	253	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	J	215	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	M	339	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	P	215	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	I	339	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	B	253	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	C	98	ASP	CA-C-N	-5.22	105.70	117.20
1	K	98	ASP	CA-C-N	-5.22	105.71	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	98	ASP	CA-C-N	-5.22	105.71	117.20
1	O	98	ASP	CA-C-N	-5.22	105.71	117.20
1	A	98	ASP	CA-C-N	-5.22	105.72	117.20
2	B	215	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	N	253	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	D	215	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	G	98	ASP	CA-C-N	-5.21	105.73	117.20
1	G	121	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	I	98	ASP	CA-C-N	-5.21	105.74	117.20
1	E	98	ASP	CA-C-N	-5.21	105.74	117.20
2	N	215	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	Q	98	ASP	CA-C-N	-5.21	105.74	117.20
1	K	339	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	F	253	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	I	347	CYS	N-CA-C	5.19	125.01	111.00
2	L	306	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	K	347	CYS	N-CA-C	5.18	124.99	111.00
1	O	347	CYS	N-CA-C	5.18	124.98	111.00
2	D	306	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	A	347	CYS	N-CA-C	5.17	124.96	111.00
1	Q	347	CYS	N-CA-C	5.17	124.95	111.00
1	C	347	CYS	N-CA-C	5.16	124.94	111.00
1	E	347	CYS	N-CA-C	5.16	124.94	111.00
1	G	347	CYS	N-CA-C	5.16	124.93	111.00
2	B	306	ASP	CB-CG-OD1	-5.16	113.66	118.30
2	J	306	ASP	CB-CG-OD1	-5.16	113.66	118.30
2	R	306	ASP	CB-CG-OD1	-5.16	113.66	118.30
2	P	306	ASP	CB-CG-OD1	-5.16	113.66	118.30
2	H	215	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	F	306	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	M	347	CYS	N-CA-C	5.14	124.89	111.00
2	D	253	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	H	306	ASP	CB-CG-OD1	-5.11	113.70	118.30
2	H	161	TYR	CB-CG-CD2	-5.11	117.94	121.00
2	N	306	ASP	CB-CG-OD1	-5.10	113.71	118.30
2	R	161	TYR	CB-CG-CD2	-5.08	117.95	121.00
2	P	161	TYR	CB-CG-CD2	-5.07	117.96	121.00
2	B	161	TYR	CB-CG-CD2	-5.05	117.97	121.00
2	L	435	TYR	CB-CG-CD2	-5.04	117.97	121.00
2	F	435	TYR	CB-CG-CD2	-5.04	117.98	121.00
2	J	435	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	B	435	TYR	CB-CG-CD2	-5.02	117.99	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	312	TYR	CB-CG-CD2	-5.02	117.99	121.00
2	N	161	TYR	CB-CG-CD2	-5.02	117.99	121.00
2	D	161	TYR	CB-CG-CD2	-5.02	117.99	121.00
2	N	435	TYR	CB-CG-CD2	-5.02	117.99	121.00
2	H	435	TYR	CB-CG-CD2	-5.01	118.00	121.00
2	D	96	GLN	N-CA-C	5.00	124.51	111.00
2	D	435	TYR	CB-CG-CD2	-5.00	118.00	121.00
2	L	96	GLN	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	248	LEU	Peptide
2	D	248	LEU	Peptide
2	F	248	LEU	Peptide
2	H	248	LEU	Peptide
2	J	248	LEU	Peptide
2	L	248	LEU	Peptide
2	N	248	LEU	Peptide
2	P	248	LEU	Peptide
2	R	248	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3350	0	3254	39	0
1	C	3350	0	3254	46	0
1	E	3350	0	3254	43	0
1	G	3350	0	3254	45	0
1	I	3350	0	3254	40	0
1	K	3350	0	3254	40	0
1	M	3350	0	3254	41	0
1	O	3350	0	3254	38	0
1	Q	3350	0	3254	42	0
2	B	3352	0	3227	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3352	0	3227	36	0
2	F	3352	0	3227	35	0
2	H	3352	0	3227	35	0
2	J	3352	0	3227	34	0
2	L	3352	0	3227	36	0
2	N	3352	0	3227	40	0
2	P	3352	0	3227	44	0
2	R	3352	0	3227	42	0
3	A	32	0	12	2	0
3	C	32	0	12	2	0
3	E	32	0	12	2	0
3	G	32	0	12	2	0
3	I	32	0	12	2	0
3	K	32	0	12	2	0
3	M	32	0	12	2	0
3	O	32	0	12	2	0
3	Q	32	0	12	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
4	Q	1	0	0	0	0
5	B	28	0	12	2	0
5	D	28	0	12	2	0
5	F	28	0	12	2	0
5	H	28	0	12	2	0
5	J	28	0	12	2	0
5	L	28	0	12	2	0
5	N	28	0	12	2	0
5	P	28	0	12	2	0
5	R	28	0	12	2	0
6	A	4	0	0	0	0
6	C	4	0	0	0	0
6	E	4	0	0	0	0
6	G	4	0	0	0	0
6	I	4	0	0	0	0
6	K	4	0	0	0	0
6	M	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	O	4	0	0	0	0
6	Q	4	0	0	0	0
All	All	60903	0	58545	666	0

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

All (666) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:228:ASN:HD21	5:J:901:GDP:HN1	1.17	0.91
2:L:228:ASN:HD21	5:L:901:GDP:HN1	1.17	0.90
2:B:228:ASN:HD21	5:B:901:GDP:HN1	1.17	0.90
2:F:228:ASN:HD21	5:F:901:GDP:HN1	1.17	0.90
2:R:228:ASN:HD21	5:R:901:GDP:HN1	1.17	0.90
2:P:228:ASN:HD21	5:P:901:GDP:HN1	1.17	0.90
2:H:228:ASN:HD21	5:H:901:GDP:HN1	1.17	0.88
2:D:228:ASN:HD21	5:D:901:GDP:HN1	1.17	0.88
2:N:228:ASN:HD21	5:N:901:GDP:HN1	1.17	0.87
1:K:238:ILE:O	1:K:238:ILE:HG22	1.77	0.84
1:E:238:ILE:O	1:E:238:ILE:HG22	1.78	0.83
1:G:238:ILE:O	1:G:238:ILE:HG22	1.78	0.83
1:Q:238:ILE:O	1:Q:238:ILE:HG22	1.77	0.83
1:C:238:ILE:O	1:C:238:ILE:HG22	1.78	0.83
1:M:238:ILE:HG22	1:M:238:ILE:O	1.77	0.83
1:I:238:ILE:O	1:I:238:ILE:HG22	1.77	0.82
1:A:238:ILE:O	1:A:238:ILE:HG22	1.77	0.81
1:O:238:ILE:HG22	1:O:238:ILE:O	1.77	0.81
2:L:345:GLU:N	2:L:345:GLU:OE1	2.16	0.79
2:H:345:GLU:N	2:H:345:GLU:OE1	2.16	0.78
2:J:345:GLU:N	2:J:345:GLU:OE1	2.16	0.76
2:B:345:GLU:OE1	2:B:345:GLU:N	2.16	0.76
2:P:345:GLU:OE1	2:P:345:GLU:N	2.16	0.76
2:F:345:GLU:OE1	2:F:345:GLU:N	2.16	0.73
2:N:345:GLU:N	2:N:345:GLU:OE1	2.16	0.73
2:R:345:GLU:N	2:R:345:GLU:OE1	2.16	0.73
2:D:345:GLU:OE1	2:D:345:GLU:N	2.16	0.73
2:F:266:HIS:O	2:F:266:HIS:ND1	2.22	0.72
2:L:266:HIS:ND1	2:L:266:HIS:O	2.22	0.72
2:R:266:HIS:ND1	2:R:266:HIS:O	2.22	0.72
2:D:266:HIS:ND1	2:D:266:HIS:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:266:HIS:O	2:H:266:HIS:ND1	2.22	0.71
2:P:266:HIS:O	2:P:266:HIS:ND1	2.22	0.71
2:B:266:HIS:ND1	2:B:266:HIS:O	2.22	0.71
2:J:266:HIS:ND1	2:J:266:HIS:O	2.22	0.71
2:N:266:HIS:ND1	2:N:266:HIS:O	2.22	0.70
1:Q:238:ILE:O	1:Q:238:ILE:CG2	2.40	0.70
1:E:238:ILE:CG2	1:E:238:ILE:O	2.40	0.70
1:K:238:ILE:CG2	1:K:238:ILE:O	2.40	0.70
1:O:238:ILE:CG2	1:O:238:ILE:O	2.40	0.69
1:C:238:ILE:CG2	1:C:238:ILE:O	2.40	0.69
1:G:238:ILE:O	1:G:238:ILE:CG2	2.40	0.69
1:A:238:ILE:CG2	1:A:238:ILE:O	2.40	0.69
1:M:238:ILE:CG2	1:M:238:ILE:O	2.40	0.69
2:P:284:ARG:NH1	2:R:90:ASP:OD2	2.27	0.68
1:I:238:ILE:O	1:I:238:ILE:CG2	2.40	0.67
1:O:243:ARG:NE	1:O:243:ARG:HA	2.10	0.67
1:A:243:ARG:HA	1:A:243:ARG:NE	2.10	0.67
1:G:243:ARG:NE	1:G:243:ARG:HA	2.10	0.66
1:I:243:ARG:HA	1:I:243:ARG:NE	2.10	0.66
1:C:243:ARG:NE	1:C:243:ARG:HA	2.10	0.66
1:M:243:ARG:NE	1:M:243:ARG:HA	2.10	0.66
2:P:381:SER:OG	2:P:382:THR:N	2.29	0.66
2:B:381:SER:OG	2:B:382:THR:N	2.29	0.65
2:J:381:SER:OG	2:J:382:THR:N	2.29	0.65
1:Q:243:ARG:HA	1:Q:243:ARG:NE	2.10	0.65
1:K:243:ARG:NE	1:K:243:ARG:HA	2.10	0.65
1:E:243:ARG:NE	1:E:243:ARG:HA	2.10	0.65
2:H:381:SER:OG	2:H:382:THR:N	2.29	0.64
1:E:15:GLN:HA	1:E:15:GLN:OE1	1.98	0.64
2:D:381:SER:OG	2:D:382:THR:N	2.29	0.64
1:K:15:GLN:HA	1:K:15:GLN:OE1	1.98	0.64
2:N:381:SER:OG	2:N:382:THR:N	2.29	0.64
1:Q:15:GLN:OE1	1:Q:15:GLN:HA	1.98	0.64
1:A:15:GLN:OE1	1:A:15:GLN:HA	1.98	0.64
1:I:15:GLN:OE1	1:I:15:GLN:HA	1.98	0.64
1:O:15:GLN:OE1	1:O:15:GLN:HA	1.98	0.64
1:G:15:GLN:OE1	1:G:15:GLN:HA	1.98	0.63
1:C:15:GLN:OE1	1:C:15:GLN:HA	1.98	0.63
1:M:15:GLN:OE1	1:M:15:GLN:HA	1.98	0.63
2:R:381:SER:OG	2:R:382:THR:N	2.29	0.62
2:F:381:SER:OG	2:F:382:THR:N	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:381:SER:OG	2:L:382:THR:N	2.29	0.62
2:L:306:ASP:OD1	2:L:306:ASP:C	2.40	0.60
1:C:11:GLN:HG2	1:C:74:VAL:HG21	1.84	0.60
2:F:306:ASP:OD1	2:F:306:ASP:C	2.40	0.59
1:G:11:GLN:HG2	1:G:74:VAL:HG21	1.84	0.59
2:F:221:THR:N	2:F:222:PRO:HD3	2.17	0.59
2:L:221:THR:N	2:L:222:PRO:HD3	2.17	0.59
1:M:11:GLN:HG2	1:M:74:VAL:HG21	1.84	0.59
1:O:11:GLN:HG2	1:O:74:VAL:HG21	1.84	0.59
2:R:306:ASP:OD1	2:R:306:ASP:C	2.40	0.59
1:Q:11:GLN:HG2	1:Q:74:VAL:HG21	1.84	0.59
2:R:221:THR:N	2:R:222:PRO:HD3	2.17	0.59
1:A:11:GLN:HG2	1:A:74:VAL:HG21	1.84	0.59
2:N:284:ARG:NH1	2:P:90:ASP:OD2	2.32	0.59
2:B:221:THR:N	2:B:222:PRO:HD3	2.17	0.59
2:D:221:THR:N	2:D:222:PRO:HD3	2.17	0.59
2:H:221:THR:N	2:H:222:PRO:HD3	2.17	0.59
1:I:11:GLN:HG2	1:I:74:VAL:HG21	1.84	0.59
2:N:221:THR:N	2:N:222:PRO:HD3	2.17	0.59
2:P:221:THR:N	2:P:222:PRO:HD3	2.17	0.59
1:E:11:GLN:HG2	1:E:74:VAL:HG21	1.84	0.59
2:J:221:THR:N	2:J:222:PRO:HD3	2.17	0.59
1:K:11:GLN:HG2	1:K:74:VAL:HG21	1.84	0.59
1:I:290:GLU:OE1	1:I:290:GLU:HA	2.03	0.58
2:J:306:ASP:C	2:J:306:ASP:OD1	2.40	0.58
1:A:290:GLU:OE1	1:A:290:GLU:HA	2.03	0.58
2:B:306:ASP:OD1	2:B:306:ASP:C	2.40	0.58
1:O:290:GLU:OE1	1:O:290:GLU:HA	2.04	0.58
1:C:290:GLU:HA	1:C:290:GLU:OE1	2.03	0.58
1:M:290:GLU:HA	1:M:290:GLU:OE1	2.03	0.58
1:G:290:GLU:OE1	1:G:290:GLU:HA	2.03	0.58
2:P:306:ASP:C	2:P:306:ASP:OD1	2.40	0.58
2:D:306:ASP:OD1	2:D:306:ASP:C	2.40	0.58
1:G:262:TYR:HB3	1:G:263:PRO:HD2	1.86	0.58
2:H:306:ASP:OD1	2:H:306:ASP:C	2.40	0.58
1:M:262:TYR:HB3	1:M:263:PRO:HD2	1.86	0.58
2:N:306:ASP:OD1	2:N:306:ASP:C	2.40	0.58
1:C:262:TYR:HB3	1:C:263:PRO:HD2	1.86	0.57
1:A:262:TYR:HB3	1:A:263:PRO:HD2	1.86	0.57
1:I:262:TYR:HB3	1:I:263:PRO:HD2	1.86	0.57
1:O:262:TYR:HB3	1:O:263:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:TYR:HB3	1:E:263:PRO:HD2	1.86	0.57
1:K:262:TYR:HB3	1:K:263:PRO:HD2	1.86	0.57
1:K:290:GLU:HA	1:K:290:GLU:OE1	2.03	0.57
1:Q:262:TYR:HB3	1:Q:263:PRO:HD2	1.86	0.57
1:Q:290:GLU:OE1	1:Q:290:GLU:HA	2.03	0.57
1:E:290:GLU:HA	1:E:290:GLU:OE1	2.04	0.57
2:P:228:ASN:ND2	5:P:901:GDP:HN1	1.98	0.55
2:B:228:ASN:ND2	5:B:901:GDP:HN1	1.98	0.55
2:J:228:ASN:ND2	5:J:901:GDP:HN1	1.98	0.55
2:F:345:GLU:CD	2:F:345:GLU:H	2.10	0.53
2:L:345:GLU:H	2:L:345:GLU:CD	2.10	0.53
1:O:388:TRP:CE3	1:O:388:TRP:HA	2.44	0.53
1:A:388:TRP:HA	1:A:388:TRP:CE3	2.44	0.53
3:E:501:GTP:O1A	2:F:254:LYS:NZ	2.42	0.53
3:K:501:GTP:O1A	2:L:254:LYS:NZ	2.42	0.53
1:M:216:ASN:HB3	1:M:275:VAL:O	2.09	0.53
2:R:345:GLU:CD	2:R:345:GLU:H	2.10	0.53
2:R:228:ASN:ND2	5:R:901:GDP:HN1	1.98	0.53
1:C:216:ASN:HB3	1:C:275:VAL:O	2.09	0.53
1:G:216:ASN:HB3	1:G:275:VAL:O	2.09	0.53
1:G:388:TRP:CE3	1:G:388:TRP:HA	2.44	0.53
1:I:388:TRP:HA	1:I:388:TRP:CE3	2.44	0.53
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.44	0.53
1:E:388:TRP:CE3	1:E:388:TRP:HA	2.44	0.53
1:Q:388:TRP:CE3	1:Q:388:TRP:HA	2.44	0.53
1:K:388:TRP:HA	1:K:388:TRP:CE3	2.44	0.53
2:F:228:ASN:ND2	5:F:901:GDP:HN1	1.98	0.52
1:G:271:THR:OG1	1:G:301:GLN:NE2	2.42	0.52
2:P:306:ASP:OD1	2:P:308:ARG:HG2	2.09	0.52
2:B:306:ASP:OD1	2:B:308:ARG:HG2	2.10	0.52
1:C:271:THR:OG1	1:C:301:GLN:NE2	2.42	0.52
2:H:221:THR:H	2:H:222:PRO:HD3	1.73	0.52
2:J:306:ASP:OD1	2:J:308:ARG:HG2	2.10	0.52
1:M:388:TRP:HA	1:M:388:TRP:CE3	2.44	0.52
2:N:221:THR:H	2:N:222:PRO:HD3	1.73	0.52
2:D:221:THR:H	2:D:222:PRO:HD3	1.73	0.52
1:M:271:THR:OG1	1:M:301:GLN:NE2	2.42	0.52
1:Q:271:THR:OG1	1:Q:301:GLN:NE2	2.42	0.52
1:E:271:THR:OG1	1:E:301:GLN:NE2	2.42	0.52
2:H:221:THR:N	2:H:222:PRO:CD	2.73	0.52
2:H:306:ASP:OD1	2:H:308:ARG:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:216:ASN:HB3	1:K:275:VAL:O	2.09	0.52
2:L:221:THR:H	2:L:222:PRO:HD3	1.73	0.52
2:L:228:ASN:ND2	5:L:901:GDP:HN1	1.98	0.52
2:D:221:THR:N	2:D:222:PRO:CD	2.73	0.52
2:D:306:ASP:OD1	2:D:308:ARG:HG2	2.10	0.52
2:F:10:GLY:HA2	2:F:145:THR:OG1	2.10	0.52
1:K:271:THR:OG1	1:K:301:GLN:NE2	2.42	0.52
2:N:306:ASP:OD1	2:N:308:ARG:HG2	2.10	0.52
1:Q:216:ASN:HB3	1:Q:275:VAL:O	2.09	0.52
2:R:10:GLY:HA2	2:R:145:THR:OG1	2.10	0.52
1:E:216:ASN:HB3	1:E:275:VAL:O	2.09	0.52
2:F:221:THR:H	2:F:222:PRO:HD3	1.73	0.52
2:H:10:GLY:HA2	2:H:145:THR:OG1	2.10	0.52
2:L:10:GLY:HA2	2:L:145:THR:OG1	2.10	0.52
2:N:221:THR:N	2:N:222:PRO:CD	2.73	0.52
2:D:10:GLY:HA2	2:D:145:THR:OG1	2.10	0.52
2:N:10:GLY:HA2	2:N:145:THR:OG1	2.10	0.52
1:O:216:ASN:HB3	1:O:275:VAL:O	2.09	0.52
2:R:221:THR:N	2:R:222:PRO:CD	2.73	0.52
2:R:221:THR:H	2:R:222:PRO:HD3	1.73	0.52
1:A:216:ASN:HB3	1:A:275:VAL:O	2.09	0.51
1:I:216:ASN:HB3	1:I:275:VAL:O	2.09	0.51
2:F:390:ARG:NE	2:F:390:ARG:HA	2.26	0.51
2:J:345:GLU:H	2:J:345:GLU:CD	2.10	0.51
2:B:390:ARG:HA	2:B:390:ARG:NE	2.26	0.51
2:H:390:ARG:NE	2:H:390:ARG:HA	2.26	0.51
2:J:390:ARG:HA	2:J:390:ARG:NE	2.26	0.51
2:L:390:ARG:HA	2:L:390:ARG:NE	2.26	0.51
2:P:10:GLY:HA2	2:P:145:THR:OG1	2.10	0.51
2:P:390:ARG:NE	2:P:390:ARG:HA	2.26	0.51
2:R:390:ARG:HA	2:R:390:ARG:NE	2.26	0.51
2:B:345:GLU:CD	2:B:345:GLU:H	2.10	0.51
1:O:388:TRP:HA	1:O:388:TRP:HE3	1.74	0.51
2:B:10:GLY:HA2	2:B:145:THR:OG1	2.10	0.51
2:D:390:ARG:HA	2:D:390:ARG:NE	2.26	0.51
2:J:10:GLY:HA2	2:J:145:THR:OG1	2.10	0.51
2:P:221:THR:H	2:P:222:PRO:HD3	1.73	0.51
1:Q:388:TRP:HE3	1:Q:388:TRP:HA	1.74	0.51
1:A:271:THR:OG1	1:A:301:GLN:NE2	2.42	0.51
2:B:221:THR:H	2:B:222:PRO:HD3	1.73	0.51
1:I:271:THR:OG1	1:I:301:GLN:NE2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:237:SER:O	1:K:241:SER:OG	2.29	0.51
2:N:390:ARG:NE	2:N:390:ARG:HA	2.26	0.51
1:O:271:THR:OG1	1:O:301:GLN:NE2	2.42	0.51
2:P:345:GLU:H	2:P:345:GLU:CD	2.10	0.51
1:Q:237:SER:O	1:Q:241:SER:OG	2.29	0.51
2:R:306:ASP:OD1	2:R:308:ARG:HG2	2.09	0.51
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.74	0.51
1:E:237:SER:O	1:E:241:SER:OG	2.29	0.51
2:F:306:ASP:OD1	2:F:308:ARG:HG2	2.10	0.51
2:J:221:THR:H	2:J:222:PRO:HD3	1.73	0.51
1:K:388:TRP:HA	1:K:388:TRP:HE3	1.74	0.51
2:L:306:ASP:OD1	2:L:308:ARG:HG2	2.10	0.51
1:E:388:TRP:HE3	1:E:388:TRP:HA	1.74	0.51
2:F:221:THR:N	2:F:222:PRO:CD	2.73	0.51
1:M:388:TRP:HA	1:M:388:TRP:HE3	1.74	0.51
1:C:388:TRP:HE3	1:C:388:TRP:HA	1.74	0.51
1:I:388:TRP:HE3	1:I:388:TRP:HA	1.74	0.51
2:J:221:THR:N	2:J:222:PRO:CD	2.73	0.51
1:A:237:SER:O	1:A:241:SER:OG	2.29	0.50
2:B:221:THR:N	2:B:222:PRO:CD	2.73	0.50
1:O:237:SER:O	1:O:241:SER:OG	2.29	0.50
1:I:237:SER:O	1:I:241:SER:OG	2.29	0.50
2:L:221:THR:N	2:L:222:PRO:CD	2.73	0.50
1:K:222:PRO:HG2	2:L:326:LYS:HB2	1.92	0.50
2:P:221:THR:N	2:P:222:PRO:CD	2.73	0.50
1:G:222:PRO:HG2	2:H:326:LYS:HB2	1.92	0.50
1:G:388:TRP:HE3	1:G:388:TRP:HA	1.74	0.50
3:G:501:GTP:O1A	2:H:254:LYS:NZ	2.42	0.50
1:I:222:PRO:HG2	2:J:326:LYS:HB2	1.92	0.50
3:M:501:GTP:O1A	2:N:254:LYS:NZ	2.42	0.50
3:C:501:GTP:O1A	2:D:254:LYS:NZ	2.42	0.50
1:E:222:PRO:HG2	2:F:326:LYS:HB2	1.92	0.50
1:A:222:PRO:HG2	2:B:326:LYS:HB2	1.92	0.50
2:H:2:ARG:N	2:H:131:CYS:O	2.45	0.50
2:N:2:ARG:N	2:N:131:CYS:O	2.45	0.50
1:Q:222:PRO:HG2	2:R:326:LYS:HB2	1.92	0.50
2:B:2:ARG:N	2:B:131:CYS:O	2.45	0.50
2:D:2:ARG:N	2:D:131:CYS:O	2.45	0.50
1:C:222:PRO:HG2	2:D:326:LYS:HB2	1.92	0.50
1:G:237:SER:O	1:G:241:SER:OG	2.29	0.50
2:P:2:ARG:N	2:P:131:CYS:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:SER:O	1:C:241:SER:OG	2.29	0.50
2:F:2:ARG:N	2:F:131:CYS:O	2.45	0.50
2:J:2:ARG:N	2:J:131:CYS:O	2.45	0.50
1:M:237:SER:O	1:M:241:SER:OG	2.29	0.50
1:M:222:PRO:HG2	2:N:326:LYS:HB2	1.92	0.50
1:O:222:PRO:HG2	2:P:326:LYS:HB2	1.92	0.50
2:R:2:ARG:N	2:R:131:CYS:O	2.45	0.50
2:D:12:CYS:SG	2:D:13:GLY:N	2.85	0.49
2:H:12:CYS:SG	2:H:13:GLY:N	2.85	0.49
2:L:2:ARG:N	2:L:131:CYS:O	2.45	0.49
2:N:12:CYS:SG	2:N:13:GLY:N	2.85	0.49
2:L:12:CYS:SG	2:L:13:GLY:N	2.85	0.49
2:R:12:CYS:SG	2:R:13:GLY:N	2.85	0.49
2:P:284:ARG:NH2	2:R:90:ASP:OD2	2.44	0.49
2:F:12:CYS:SG	2:F:13:GLY:N	2.85	0.49
2:J:12:CYS:SG	2:J:13:GLY:N	2.85	0.49
3:O:501:GTP:O1A	2:P:254:LYS:NZ	2.42	0.49
3:A:501:GTP:O1A	2:B:254:LYS:NZ	2.42	0.49
3:I:501:GTP:O1A	2:J:254:LYS:NZ	2.42	0.49
2:B:12:CYS:SG	2:B:13:GLY:N	2.85	0.49
2:H:345:GLU:CD	2:H:345:GLU:H	2.10	0.49
2:P:12:CYS:SG	2:P:13:GLY:N	2.85	0.49
2:P:96:GLN:NE2	2:P:96:GLN:O	2.46	0.49
2:B:96:GLN:O	2:B:96:GLN:NE2	2.46	0.49
2:D:345:GLU:H	2:D:345:GLU:CD	2.10	0.49
2:R:96:GLN:O	2:R:96:GLN:NE2	2.46	0.49
2:F:96:GLN:NE2	2:F:96:GLN:O	2.46	0.49
2:N:345:GLU:CD	2:N:345:GLU:H	2.10	0.49
2:N:96:GLN:NE2	2:N:96:GLN:O	2.46	0.49
3:Q:501:GTP:O1A	2:R:254:LYS:NZ	2.42	0.49
2:D:96:GLN:O	2:D:96:GLN:NE2	2.46	0.48
2:J:96:GLN:NE2	2:J:96:GLN:O	2.46	0.48
2:L:96:GLN:NE2	2:L:96:GLN:O	2.46	0.48
2:H:96:GLN:NE2	2:H:96:GLN:O	2.46	0.48
1:K:220:GLU:OE1	2:L:326:LYS:NZ	2.43	0.47
1:Q:220:GLU:OE1	2:R:326:LYS:NZ	2.43	0.47
1:E:220:GLU:OE1	2:F:326:LYS:NZ	2.43	0.47
2:H:288:VAL:HB	2:H:327:GLU:HG2	1.96	0.47
2:J:288:VAL:HB	2:J:327:GLU:HG2	1.96	0.47
2:N:228:ASN:ND2	5:N:901:GDP:HN1	1.98	0.47
2:B:288:VAL:HB	2:B:327:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:288:VAL:HB	2:D:327:GLU:HG2	1.96	0.47
2:D:228:ASN:ND2	5:D:901:GDP:HN1	1.98	0.47
2:N:288:VAL:HB	2:N:327:GLU:HG2	1.96	0.47
1:M:228:ASN:HD21	3:M:501:GTP:HN1	1.63	0.47
1:M:53:PHE:HB3	1:M:61:HIS:HB3	1.97	0.47
1:O:53:PHE:HB3	1:O:61:HIS:HB3	1.97	0.47
2:P:288:VAL:HB	2:P:327:GLU:HG2	1.96	0.47
1:A:53:PHE:HB3	1:A:61:HIS:HB3	1.97	0.47
1:C:246:GLY:HA3	1:C:356:ASN:HA	1.96	0.47
1:C:53:PHE:HB3	1:C:61:HIS:HB3	1.97	0.47
2:H:228:ASN:ND2	5:H:901:GDP:HN1	1.98	0.47
1:M:246:GLY:HA3	1:M:356:ASN:HA	1.97	0.47
1:Q:53:PHE:HB3	1:Q:61:HIS:HB3	1.97	0.47
1:C:228:ASN:HD21	3:C:501:GTP:HN1	1.62	0.47
1:G:246:GLY:HA3	1:G:356:ASN:HA	1.96	0.47
1:G:53:PHE:HB3	1:G:61:HIS:HB3	1.97	0.47
1:I:53:PHE:HB3	1:I:61:HIS:HB3	1.97	0.47
1:E:53:PHE:HB3	1:E:61:HIS:HB3	1.97	0.47
1:G:228:ASN:HD21	3:G:501:GTP:HN1	1.62	0.47
1:K:53:PHE:HB3	1:K:61:HIS:HB3	1.97	0.47
2:L:288:VAL:HB	2:L:327:GLU:HG2	1.96	0.47
1:O:228:ASN:HD21	3:O:501:GTP:HN1	1.63	0.47
1:Q:228:ASN:HD21	3:Q:501:GTP:HN1	1.63	0.47
2:R:288:VAL:HB	2:R:327:GLU:HG2	1.96	0.47
1:A:228:ASN:HD21	3:A:501:GTP:HN1	1.63	0.46
1:E:325:PRO:HB2	2:R:210:TYR:OH	2.15	0.46
2:F:288:VAL:HB	2:F:327:GLU:HG2	1.96	0.46
2:N:142:GLY:HA3	2:N:183:GLU:HG3	1.97	0.46
2:P:142:GLY:HA3	2:P:183:GLU:HG3	1.97	0.46
2:B:142:GLY:HA3	2:B:183:GLU:HG3	1.97	0.46
1:E:228:ASN:HD21	3:E:501:GTP:HN1	1.63	0.46
1:Q:255:PHE:HD1	1:Q:255:PHE:HA	1.54	0.46
1:A:243:ARG:HE	1:A:243:ARG:HA	1.81	0.46
2:B:332:MET:HA	2:B:332:MET:CE	2.46	0.46
1:C:243:ARG:HE	1:C:243:ARG:HA	1.81	0.46
2:D:142:GLY:HA3	2:D:183:GLU:HG3	1.97	0.46
1:G:243:ARG:HA	1:G:243:ARG:HE	1.81	0.46
1:I:243:ARG:HE	1:I:243:ARG:HA	1.81	0.46
1:I:228:ASN:HD21	3:I:501:GTP:HN1	1.63	0.46
2:J:332:MET:CE	2:J:332:MET:HA	2.46	0.46
2:P:332:MET:CE	2:P:332:MET:HA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:GLY:HA3	2:H:183:GLU:HG3	1.97	0.46
2:J:142:GLY:HA3	2:J:183:GLU:HG3	1.97	0.46
1:K:332:ILE:HA	1:K:335:ILE:HG12	1.97	0.46
1:M:243:ARG:HA	1:M:243:ARG:HE	1.81	0.46
1:O:243:ARG:HA	1:O:243:ARG:HE	1.81	0.46
1:O:246:GLY:HA3	1:O:356:ASN:HA	1.96	0.46
1:E:255:PHE:HA	1:E:255:PHE:HD1	1.54	0.46
1:E:332:ILE:HA	1:E:335:ILE:HG12	1.97	0.46
1:K:228:ASN:HD21	3:K:501:GTP:HN1	1.63	0.46
1:Q:246:GLY:HA3	1:Q:356:ASN:HA	1.96	0.46
1:G:15:GLN:CA	1:G:15:GLN:OE1	2.61	0.46
1:I:332:ILE:HA	1:I:335:ILE:HG12	1.97	0.46
1:K:15:GLN:CA	1:K:15:GLN:OE1	2.61	0.46
1:K:246:GLY:HA3	1:K:356:ASN:HA	1.97	0.46
1:A:246:GLY:HA3	1:A:356:ASN:HA	1.97	0.46
1:E:246:GLY:HA3	1:E:356:ASN:HA	1.96	0.46
1:G:190:THR:OG1	1:G:191:THR:N	2.49	0.46
1:I:283:HIS:HA	1:K:56:THR:HG21	1.96	0.46
2:L:332:MET:CE	2:L:332:MET:HA	2.46	0.46
1:Q:332:ILE:HA	1:Q:335:ILE:HG12	1.97	0.46
1:A:332:ILE:HA	1:A:335:ILE:HG12	1.97	0.46
2:F:332:MET:HA	2:F:332:MET:CE	2.46	0.46
1:I:246:GLY:HA3	1:I:356:ASN:HA	1.96	0.46
1:K:255:PHE:HA	1:K:255:PHE:HD1	1.54	0.46
2:R:142:GLY:HA3	2:R:183:GLU:HG3	1.97	0.46
1:C:15:GLN:OE1	1:C:15:GLN:CA	2.61	0.46
1:C:190:THR:OG1	1:C:191:THR:N	2.49	0.46
2:F:142:GLY:HA3	2:F:183:GLU:HG3	1.97	0.46
1:O:332:ILE:HA	1:O:335:ILE:HG12	1.97	0.46
1:E:15:GLN:OE1	1:E:15:GLN:CA	2.61	0.45
2:R:332:MET:HA	2:R:332:MET:CE	2.46	0.45
2:H:332:MET:CE	2:H:332:MET:HA	2.46	0.45
2:L:142:GLY:HA3	2:L:183:GLU:HG3	1.97	0.45
1:M:190:THR:OG1	1:M:191:THR:N	2.49	0.45
2:N:28:HIS:NE2	2:N:243:ARG:NH1	2.65	0.45
2:N:284:ARG:NH2	2:P:90:ASP:OD2	2.49	0.45
1:A:101:ASN:HB2	2:B:254:LYS:HE3	1.99	0.45
2:D:28:HIS:NE2	2:D:243:ARG:NH1	2.65	0.45
1:E:101:ASN:HB2	2:F:254:LYS:HE3	1.98	0.45
2:H:28:HIS:NE2	2:H:243:ARG:NH1	2.65	0.45
1:I:101:ASN:HB2	2:J:254:LYS:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:190:THR:OG1	1:K:191:THR:N	2.49	0.45
1:K:101:ASN:HB2	2:L:254:LYS:HE3	1.99	0.45
1:O:220:GLU:OE1	2:P:326:LYS:NZ	2.43	0.45
2:R:28:HIS:NE2	2:R:243:ARG:NH1	2.65	0.45
1:C:101:ASN:HB2	2:D:254:LYS:HE3	1.99	0.45
1:G:101:ASN:HB2	2:H:254:LYS:HE3	1.99	0.45
1:M:101:ASN:HB2	2:N:254:LYS:HE3	1.99	0.45
1:A:220:GLU:OE1	2:B:326:LYS:NZ	2.43	0.45
2:D:332:MET:HA	2:D:332:MET:CE	2.46	0.45
1:E:190:THR:OG1	1:E:191:THR:N	2.49	0.45
2:F:28:HIS:NE2	2:F:243:ARG:NH1	2.65	0.45
2:J:331:GLN:HA	2:J:331:GLN:OE1	2.17	0.45
1:M:15:GLN:OE1	1:M:15:GLN:CA	2.61	0.45
1:O:101:ASN:HB2	2:P:254:LYS:HE3	1.99	0.45
1:I:220:GLU:OE1	2:J:326:LYS:NZ	2.43	0.45
1:Q:101:ASN:HB2	2:R:254:LYS:HE3	1.99	0.45
2:R:139:HIS:O	2:R:170:SER:HA	2.17	0.45
2:B:139:HIS:O	2:B:170:SER:HA	2.17	0.45
2:B:167:ASN:C	2:B:167:ASN:OD1	2.55	0.45
2:B:28:HIS:NE2	2:B:243:ARG:NH1	2.65	0.45
2:D:331:GLN:HA	2:D:331:GLN:OE1	2.17	0.45
2:F:139:HIS:O	2:F:170:SER:HA	2.16	0.45
2:H:331:GLN:OE1	2:H:331:GLN:HA	2.17	0.45
2:J:28:HIS:NE2	2:J:243:ARG:NH1	2.65	0.45
2:L:28:HIS:NE2	2:L:243:ARG:NH1	2.65	0.45
1:M:221:ARG:N	1:M:222:PRO:CD	2.80	0.45
1:M:313:MET:SD	1:M:435:VAL:HG11	2.57	0.45
2:N:167:ASN:C	2:N:167:ASN:OD1	2.55	0.45
2:N:331:GLN:HA	2:N:331:GLN:OE1	2.17	0.45
2:P:139:HIS:O	2:P:170:SER:HA	2.17	0.45
2:P:167:ASN:OD1	2:P:167:ASN:C	2.56	0.45
1:Q:15:GLN:CA	1:Q:15:GLN:OE1	2.61	0.45
1:C:221:ARG:N	1:C:222:PRO:CD	2.80	0.45
1:C:313:MET:SD	1:C:435:VAL:HG11	2.57	0.45
2:D:167:ASN:C	2:D:167:ASN:OD1	2.56	0.45
2:F:167:ASN:C	2:F:167:ASN:OD1	2.56	0.45
2:H:167:ASN:C	2:H:167:ASN:OD1	2.56	0.45
2:J:167:ASN:C	2:J:167:ASN:OD1	2.56	0.45
2:L:167:ASN:C	2:L:167:ASN:OD1	2.56	0.45
2:N:332:MET:HA	2:N:332:MET:CE	2.46	0.45
2:P:28:HIS:NE2	2:P:243:ARG:NH1	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:389:LYS:NZ	2:P:393:GLU:OE2	2.44	0.45
1:Q:190:THR:OG1	1:Q:191:THR:N	2.49	0.45
1:Q:313:MET:SD	1:Q:435:VAL:HG11	2.57	0.45
2:R:167:ASN:C	2:R:167:ASN:OD1	2.56	0.45
2:B:331:GLN:HA	2:B:331:GLN:OE1	2.17	0.45
2:J:139:HIS:O	2:J:170:SER:HA	2.17	0.45
1:O:313:MET:SD	1:O:435:VAL:HG11	2.57	0.45
2:P:331:GLN:OE1	2:P:331:GLN:HA	2.17	0.45
1:A:313:MET:SD	1:A:435:VAL:HG11	2.57	0.45
1:E:313:MET:SD	1:E:435:VAL:HG11	2.57	0.45
1:G:313:MET:SD	1:G:435:VAL:HG11	2.57	0.45
1:I:221:ARG:N	1:I:222:PRO:CD	2.80	0.45
1:I:313:MET:SD	1:I:435:VAL:HG11	2.57	0.45
2:L:139:HIS:O	2:L:170:SER:HA	2.17	0.45
1:M:332:ILE:HA	1:M:335:ILE:HG12	1.97	0.45
2:P:262:PHE:HA	2:P:263:PRO:HD3	1.90	0.45
1:A:221:ARG:N	1:A:222:PRO:CD	2.80	0.44
1:C:332:ILE:HA	1:C:335:ILE:HG12	1.97	0.44
1:G:332:ILE:HA	1:G:335:ILE:HG12	1.97	0.44
1:K:313:MET:SD	1:K:435:VAL:HG11	2.57	0.44
1:M:100:ALA:O	1:M:101:ASN:HB3	2.18	0.44
1:G:100:ALA:O	1:G:101:ASN:HB3	2.18	0.44
1:G:221:ARG:N	1:G:222:PRO:CD	2.80	0.44
1:G:283:HIS:HA	1:I:56:THR:HG21	2.00	0.44
2:H:61:TYR:CD1	2:H:61:TYR:N	2.86	0.44
2:L:331:GLN:OE1	2:L:331:GLN:HA	2.17	0.44
2:N:139:HIS:O	2:N:170:SER:HA	2.17	0.44
2:N:61:TYR:CD1	2:N:61:TYR:N	2.86	0.44
1:O:221:ARG:N	1:O:222:PRO:CD	2.80	0.44
1:A:100:ALA:O	1:A:101:ASN:HB3	2.18	0.44
1:C:100:ALA:O	1:C:101:ASN:HB3	2.18	0.44
2:D:139:HIS:O	2:D:170:SER:HA	2.17	0.44
2:D:61:TYR:CD1	2:D:61:TYR:N	2.86	0.44
1:O:100:ALA:O	1:O:101:ASN:HB3	2.18	0.44
2:F:331:GLN:OE1	2:F:331:GLN:HA	2.17	0.44
1:I:100:ALA:O	1:I:101:ASN:HB3	2.18	0.44
1:K:218:ASP:OD1	1:K:280:LYS:NZ	2.50	0.44
2:N:262:PHE:HA	2:N:263:PRO:HD3	1.90	0.44
1:E:100:ALA:O	1:E:101:ASN:HB3	2.18	0.44
1:K:100:ALA:O	1:K:101:ASN:HB3	2.18	0.44
2:P:61:TYR:CD1	2:P:61:TYR:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:100:ALA:O	1:Q:101:ASN:HB3	2.18	0.44
2:B:242:LEU:CD1	2:B:242:LEU:N	2.81	0.44
2:B:61:TYR:CD1	2:B:61:TYR:N	2.86	0.44
1:E:218:ASP:OD1	1:E:280:LYS:NZ	2.50	0.44
1:G:218:ASP:OD1	1:G:280:LYS:NZ	2.50	0.44
2:H:139:HIS:O	2:H:170:SER:HA	2.17	0.44
2:R:242:LEU:CD1	2:R:242:LEU:N	2.81	0.44
2:R:331:GLN:HA	2:R:331:GLN:OE1	2.17	0.44
2:F:242:LEU:CD1	2:F:242:LEU:N	2.81	0.44
2:J:242:LEU:N	2:J:242:LEU:CD1	2.81	0.44
2:J:61:TYR:CD1	2:J:61:TYR:N	2.86	0.44
2:L:74:THR:OG1	2:L:75:MET:N	2.51	0.44
2:P:242:LEU:CD1	2:P:242:LEU:N	2.81	0.44
2:F:74:THR:OG1	2:F:75:MET:N	2.51	0.44
2:H:74:THR:OG1	2:H:75:MET:N	2.51	0.44
2:L:242:LEU:N	2:L:242:LEU:CD1	2.81	0.44
1:C:325:PRO:HB2	2:N:210:TYR:OH	2.18	0.44
2:N:248:LEU:HD23	2:N:248:LEU:HA	1.80	0.44
1:Q:218:ASP:OD1	1:Q:280:LYS:NZ	2.50	0.44
1:C:218:ASP:OD1	1:C:280:LYS:NZ	2.50	0.43
2:D:74:THR:OG1	2:D:75:MET:N	2.51	0.43
2:N:74:THR:OG1	2:N:75:MET:N	2.51	0.43
2:R:74:THR:OG1	2:R:75:MET:N	2.51	0.43
1:E:30:ILE:HG12	1:E:36:MET:SD	2.58	0.43
1:I:218:ASP:OD1	1:I:280:LYS:NZ	2.50	0.43
1:K:30:ILE:HG12	1:K:36:MET:SD	2.58	0.43
1:M:218:ASP:OD1	1:M:280:LYS:NZ	2.50	0.43
1:M:63:PRO:O	1:M:91:GLN:NE2	2.50	0.43
1:Q:221:ARG:N	1:Q:222:PRO:CD	2.80	0.43
1:C:63:PRO:O	1:C:91:GLN:NE2	2.50	0.43
1:K:221:ARG:N	1:K:222:PRO:CD	2.80	0.43
1:Q:30:ILE:HG12	1:Q:36:MET:SD	2.58	0.43
1:E:221:ARG:N	1:E:222:PRO:CD	2.80	0.43
1:G:30:ILE:HG12	1:G:36:MET:SD	2.58	0.43
1:G:63:PRO:O	1:G:91:GLN:NE2	2.50	0.43
2:R:61:TYR:CD1	2:R:61:TYR:N	2.86	0.43
1:C:30:ILE:HG12	1:C:36:MET:SD	2.58	0.43
2:F:61:TYR:N	2:F:61:TYR:CD1	2.86	0.43
2:L:61:TYR:CD1	2:L:61:TYR:N	2.86	0.43
1:O:190:THR:OG1	1:O:191:THR:N	2.49	0.43
1:O:30:ILE:HG12	1:O:36:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:OD1	1:A:280:LYS:NZ	2.50	0.43
1:A:30:ILE:HG12	1:A:36:MET:SD	2.58	0.43
1:C:297:GLU:HA	1:C:298:PRO:HD3	1.89	0.43
2:D:109:THR:OG1	2:D:110:GLU:N	2.51	0.43
2:J:183:GLU:N	2:J:184:PRO:CD	2.82	0.43
2:L:248:LEU:HA	2:L:248:LEU:HD23	1.80	0.43
2:N:109:THR:OG1	2:N:110:GLU:N	2.51	0.43
2:P:109:THR:OG1	2:P:110:GLU:N	2.51	0.43
1:A:190:THR:OG1	1:A:191:THR:N	2.49	0.43
1:A:325:PRO:HB2	2:P:210:TYR:OH	2.19	0.43
2:B:109:THR:OG1	2:B:110:GLU:N	2.51	0.43
2:H:109:THR:OG1	2:H:110:GLU:N	2.51	0.43
2:J:109:THR:OG1	2:J:110:GLU:N	2.51	0.43
1:M:30:ILE:HG12	1:M:36:MET:SD	2.58	0.43
2:N:242:LEU:N	2:N:242:LEU:CD1	2.81	0.43
1:C:346:TRP:HB3	2:N:401:ARG:HG3	2.00	0.43
2:R:109:THR:OG1	2:R:110:GLU:N	2.51	0.43
2:B:183:GLU:N	2:B:184:PRO:CD	2.82	0.43
2:D:242:LEU:N	2:D:242:LEU:CD1	2.81	0.43
2:F:109:THR:OG1	2:F:110:GLU:N	2.51	0.43
1:I:190:THR:OG1	1:I:191:THR:N	2.49	0.43
1:O:218:ASP:OD1	1:O:280:LYS:NZ	2.50	0.43
2:D:248:LEU:HA	2:D:248:LEU:HD23	1.80	0.43
1:G:435:VAL:HG12	1:G:435:VAL:O	2.18	0.43
1:I:30:ILE:HG12	1:I:36:MET:SD	2.58	0.43
2:L:109:THR:OG1	2:L:110:GLU:N	2.51	0.43
2:N:183:GLU:N	2:N:184:PRO:CD	2.82	0.43
2:P:183:GLU:N	2:P:184:PRO:CD	2.82	0.43
2:D:183:GLU:N	2:D:184:PRO:CD	2.82	0.43
2:H:242:LEU:CD1	2:H:242:LEU:N	2.81	0.43
1:C:435:VAL:O	1:C:435:VAL:HG12	2.18	0.42
1:G:297:GLU:HA	1:G:298:PRO:HD3	1.89	0.42
1:O:63:PRO:O	1:O:91:GLN:NE2	2.50	0.42
2:H:183:GLU:N	2:H:184:PRO:CD	2.82	0.42
2:J:74:THR:OG1	2:J:75:MET:N	2.51	0.42
1:A:63:PRO:O	1:A:91:GLN:NE2	2.50	0.42
1:K:254:GLU:HA	1:K:257:THR:OG1	2.20	0.42
1:Q:254:GLU:HA	1:Q:257:THR:OG1	2.20	0.42
1:A:254:GLU:HA	1:A:257:THR:OG1	2.20	0.42
2:B:74:THR:OG1	2:B:75:MET:N	2.51	0.42
1:E:254:GLU:HA	1:E:257:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:183:GLU:N	2:F:184:PRO:CD	2.82	0.42
2:H:248:LEU:HA	2:H:248:LEU:HD23	1.80	0.42
1:I:254:GLU:HA	1:I:257:THR:OG1	2.20	0.42
2:L:183:GLU:N	2:L:184:PRO:CD	2.82	0.42
1:O:254:GLU:HA	1:O:257:THR:OG1	2.20	0.42
1:C:254:GLU:HA	1:C:257:THR:OG1	2.20	0.42
1:I:63:PRO:O	1:I:91:GLN:NE2	2.50	0.42
1:K:147:SER:HB2	1:K:190:THR:HG21	2.01	0.42
1:Q:347:CYS:HA	1:Q:348:PRO:HD2	1.87	0.42
2:R:183:GLU:N	2:R:184:PRO:CD	2.82	0.42
2:D:408:TYR:CD1	2:D:408:TYR:N	2.87	0.42
1:G:254:GLU:HA	1:G:257:THR:OG1	2.20	0.42
2:H:408:TYR:N	2:H:408:TYR:CD1	2.87	0.42
1:M:254:GLU:HA	1:M:257:THR:OG1	2.20	0.42
2:P:338:LYS:NZ	2:R:127:GLU:OE1	2.52	0.42
1:A:346:TRP:HB3	2:P:401:ARG:HG3	2.01	0.42
2:B:408:TYR:N	2:B:408:TYR:CD1	2.87	0.42
2:F:408:TYR:N	2:F:408:TYR:CD1	2.88	0.42
2:L:408:TYR:CD1	2:L:408:TYR:N	2.87	0.42
1:M:255:PHE:HD1	1:M:255:PHE:HA	1.54	0.42
2:N:408:TYR:N	2:N:408:TYR:CD1	2.87	0.42
2:P:408:TYR:CD1	2:P:408:TYR:N	2.87	0.42
2:P:74:THR:OG1	2:P:75:MET:N	2.51	0.42
1:Q:326:LYS:HE3	1:Q:326:LYS:HB3	1.84	0.42
2:R:408:TYR:CD1	2:R:408:TYR:N	2.87	0.42
1:E:147:SER:HB2	1:E:190:THR:HG21	2.01	0.42
2:J:408:TYR:N	2:J:408:TYR:CD1	2.88	0.42
1:Q:147:SER:HB2	1:Q:190:THR:HG21	2.01	0.42
1:Q:358:GLU:HA	1:Q:359:PRO:HD2	1.90	0.42
1:C:255:PHE:HA	1:C:255:PHE:HD1	1.54	0.42
1:E:347:CYS:HA	1:E:348:PRO:HD2	1.87	0.42
1:E:352:LYS:HD2	2:R:179:ASP:HB3	2.01	0.42
1:G:147:SER:HB2	1:G:190:THR:HG21	2.01	0.42
1:G:211:ASP:HA	1:G:214:ARG:HG2	2.02	0.42
1:I:147:SER:HB2	1:I:190:THR:HG21	2.01	0.42
1:C:211:ASP:HA	1:C:214:ARG:HG2	2.02	0.42
1:Q:63:PRO:O	1:Q:91:GLN:NE2	2.50	0.42
1:A:147:SER:HB2	1:A:190:THR:HG21	2.01	0.41
1:E:326:LYS:HE3	1:E:326:LYS:HB3	1.84	0.41
1:I:211:ASP:HA	1:I:214:ARG:HG2	2.02	0.41
1:K:147:SER:HB2	1:K:190:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:347:CYS:HA	1:K:348:PRO:HD2	1.87	0.41
1:M:211:ASP:HA	1:M:214:ARG:HG2	2.02	0.41
1:O:211:ASP:HA	1:O:214:ARG:HG2	2.02	0.41
1:A:211:ASP:HA	1:A:214:ARG:HG2	2.02	0.41
1:C:147:SER:HB2	1:C:190:THR:HG21	2.01	0.41
1:E:63:PRO:O	1:E:91:GLN:NE2	2.50	0.41
1:K:63:PRO:O	1:K:91:GLN:NE2	2.50	0.41
2:R:103:TRP:CD1	2:R:103:TRP:C	2.94	0.41
1:E:147:SER:HB2	1:E:190:THR:CG2	2.50	0.41
1:E:211:ASP:HA	1:E:214:ARG:HG2	2.02	0.41
2:F:103:TRP:CD1	2:F:103:TRP:C	2.94	0.41
1:G:147:SER:HB2	1:G:190:THR:CG2	2.50	0.41
1:G:255:PHE:HA	1:G:255:PHE:HD1	1.54	0.41
1:I:147:SER:HB2	1:I:190:THR:CG2	2.50	0.41
1:K:211:ASP:HA	1:K:214:ARG:HG2	2.02	0.41
1:Q:211:ASP:HA	1:Q:214:ARG:HG2	2.02	0.41
1:A:147:SER:HB2	1:A:190:THR:CG2	2.50	0.41
1:C:133:GLN:NE2	1:C:133:GLN:HA	2.35	0.41
1:C:147:SER:HB2	1:C:190:THR:CG2	2.50	0.41
1:G:166:LYS:NZ	1:G:199:ASP:OD2	2.49	0.41
1:G:402:ARG:HA	1:G:402:ARG:HD3	1.69	0.41
1:I:133:GLN:NE2	1:I:133:GLN:HA	2.36	0.41
1:M:133:GLN:HA	1:M:133:GLN:NE2	2.36	0.41
1:M:147:SER:HB2	1:M:190:THR:CG2	2.50	0.41
1:M:220:GLU:OE1	2:N:326:LYS:NZ	2.43	0.41
1:Q:147:SER:HB2	1:Q:190:THR:CG2	2.50	0.41
1:A:133:GLN:HA	1:A:133:GLN:NE2	2.36	0.41
1:C:166:LYS:NZ	1:C:199:ASP:OD2	2.49	0.41
1:E:133:GLN:NE2	1:E:133:GLN:HA	2.35	0.41
1:G:133:GLN:NE2	1:G:133:GLN:HA	2.36	0.41
1:K:133:GLN:HA	1:K:133:GLN:NE2	2.36	0.41
1:K:326:LYS:HB3	1:K:326:LYS:HE3	1.84	0.41
2:L:103:TRP:C	2:L:103:TRP:CD1	2.94	0.41
1:M:147:SER:HB2	1:M:190:THR:HG21	2.01	0.41
1:O:147:SER:HB2	1:O:190:THR:CG2	2.50	0.41
1:O:147:SER:HB2	1:O:190:THR:HG21	2.01	0.41
1:C:220:GLU:OE1	2:D:326:LYS:NZ	2.43	0.41
2:H:88:ARG:HA	2:H:89:PRO:HD3	1.86	0.41
1:M:166:LYS:NZ	1:M:199:ASP:OD2	2.49	0.41
1:O:133:GLN:HA	1:O:133:GLN:NE2	2.36	0.41
1:E:163:LYS:NZ	2:R:411:GLU:OE2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:TRP:CA	1:E:388:TRP:CE3	3.04	0.41
1:Q:133:GLN:HA	1:Q:133:GLN:NE2	2.36	0.41
1:A:388:TRP:CA	1:A:388:TRP:CE3	3.04	0.41
1:G:220:GLU:OE1	2:H:326:LYS:NZ	2.43	0.41
2:D:181:VAL:HG11	1:G:346:TRP:CZ3	2.56	0.41
1:G:388:TRP:CA	1:G:388:TRP:CE3	3.04	0.41
1:K:388:TRP:CA	1:K:388:TRP:CE3	3.04	0.41
2:P:103:TRP:C	2:P:103:TRP:CD1	2.94	0.41
1:Q:388:TRP:CE3	1:Q:388:TRP:CA	3.04	0.41
1:C:388:TRP:CA	1:C:388:TRP:CE3	3.04	0.41
1:G:363:VAL:HA	1:G:364:PRO:HD3	1.92	0.41
1:I:388:TRP:CA	1:I:388:TRP:CE3	3.04	0.41
1:O:388:TRP:CE3	1:O:388:TRP:CA	3.04	0.41
2:R:389:LYS:NZ	2:R:393:GLU:OE2	2.44	0.41
2:B:103:TRP:C	2:B:103:TRP:CD1	2.94	0.41
1:G:345:ASP:OD2	1:G:439:SER:OG	2.35	0.41
1:O:90:GLU:OE2	1:O:121:ARG:NH1	2.54	0.41
1:Q:297:GLU:HA	1:Q:298:PRO:HD3	1.89	0.41
1:A:166:LYS:NZ	1:A:199:ASP:OD2	2.49	0.41
1:A:90:GLU:OE2	1:A:121:ARG:NH1	2.54	0.41
1:C:363:VAL:HA	1:C:364:PRO:HD3	1.92	0.41
1:C:402:ARG:HA	1:C:402:ARG:HD3	1.69	0.41
2:D:88:ARG:HA	2:D:89:PRO:HD3	1.86	0.41
2:F:401:ARG:O	2:F:402:LYS:HB2	2.21	0.41
1:I:166:LYS:NZ	1:I:199:ASP:OD2	2.49	0.41
1:I:90:GLU:OE2	1:I:121:ARG:NH1	2.54	0.41
2:L:401:ARG:O	2:L:402:LYS:HB2	2.21	0.41
1:M:388:TRP:CA	1:M:388:TRP:CE3	3.04	0.41
1:O:166:LYS:NZ	1:O:199:ASP:OD2	2.49	0.41
1:O:283:HIS:O	1:Q:88:HIS:HD2	2.04	0.41
2:P:248:LEU:HA	2:P:248:LEU:HD23	1.80	0.41
1:C:90:GLU:OE2	1:C:121:ARG:NH1	2.54	0.40
1:E:402:ARG:HD3	1:E:402:ARG:HA	1.69	0.40
1:G:90:GLU:OE2	1:G:121:ARG:NH1	2.54	0.40
1:I:363:VAL:HA	1:I:364:PRO:HD3	1.92	0.40
1:I:435:VAL:O	1:I:435:VAL:HG12	2.18	0.40
1:O:435:VAL:O	1:O:435:VAL:HG12	2.18	0.40
1:C:345:ASP:OD2	1:C:439:SER:OG	2.35	0.40
2:J:103:TRP:CD1	2:J:103:TRP:C	2.94	0.40
1:M:90:GLU:OE2	1:M:121:ARG:NH1	2.54	0.40
1:M:363:VAL:HA	1:M:364:PRO:HD3	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:326:LYS:HE3	1:O:326:LYS:HB3	1.84	0.40
1:Q:402:ARG:HD3	1:Q:402:ARG:HA	1.69	0.40
2:R:401:ARG:O	2:R:402:LYS:HB2	2.21	0.40
1:E:166:LYS:NZ	1:E:199:ASP:OD2	2.49	0.40
1:E:297:GLU:HA	1:E:298:PRO:HD3	1.89	0.40
1:K:166:LYS:NZ	1:K:199:ASP:OD2	2.49	0.40
1:M:435:VAL:O	1:M:435:VAL:HG12	2.18	0.40
1:Q:166:LYS:NZ	1:Q:199:ASP:OD2	2.49	0.40
1:A:363:VAL:HA	1:A:364:PRO:HD3	1.92	0.40
1:C:141:PHE:HB2	1:C:173:PRO:HD3	2.04	0.40
1:E:243:ARG:HA	1:E:243:ARG:HE	1.81	0.40
1:C:163:LYS:NZ	2:N:411:GLU:OE2	2.50	0.40
1:Q:243:ARG:HE	1:Q:243:ARG:HA	1.81	0.40
1:A:435:VAL:HG12	1:A:435:VAL:O	2.18	0.40
1:G:141:PHE:HB2	1:G:173:PRO:HD3	2.04	0.40
1:I:141:PHE:HB2	1:I:173:PRO:HD3	2.04	0.40
1:K:297:GLU:HA	1:K:298:PRO:HD3	1.89	0.40
1:K:402:ARG:HA	1:K:402:ARG:HD3	1.69	0.40
1:M:141:PHE:HB2	1:M:173:PRO:HD3	2.04	0.40
1:M:345:ASP:OD2	1:M:439:SER:OG	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	C	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	E	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	G	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	K	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	M	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	O	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
1	Q	424/439 (97%)	409 (96%)	13 (3%)	2 (0%)	32	74
2	B	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	D	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	F	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	H	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	J	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	L	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	N	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	P	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
2	R	424/427 (99%)	408 (96%)	13 (3%)	3 (1%)	25	68
All	All	7632/7794 (98%)	7353 (96%)	234 (3%)	45 (1%)	33	71

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	GLY
2	D	98	GLY
2	F	98	GLY
2	H	98	GLY
2	J	98	GLY
2	L	98	GLY
2	N	98	GLY
2	P	98	GLY
2	R	98	GLY
1	A	345	ASP
1	C	345	ASP
1	E	345	ASP
1	K	345	ASP
2	B	350	ASN
2	D	350	ASN
2	F	350	ASN
1	G	345	ASP
2	H	350	ASN

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Mol	Chain	Res	Type
1	I	345	ASP
2	J	350	ASN
2	L	350	ASN
1	M	345	ASP
2	N	350	ASN
1	O	345	ASP
2	P	350	ASN
1	Q	345	ASP
2	R	350	ASN
1	A	349	THR
1	C	349	THR
1	E	349	THR
1	I	349	THR
1	M	349	THR
1	O	349	THR
1	Q	349	THR
1	G	349	THR
1	K	349	THR
2	B	221	THR
2	D	221	THR
2	F	221	THR
2	H	221	THR
2	J	221	THR
2	L	221	THR
2	N	221	THR
2	P	221	THR
2	R	221	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	C	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	E	360/368 (98%)	359 (100%)	1 (0%)	94	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	I	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	K	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	M	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	O	360/368 (98%)	359 (100%)	1 (0%)	94	96
1	Q	360/368 (98%)	359 (100%)	1 (0%)	94	96
2	B	367/368 (100%)	367 (100%)	0	100	100
2	D	367/368 (100%)	367 (100%)	0	100	100
2	F	367/368 (100%)	367 (100%)	0	100	100
2	H	367/368 (100%)	367 (100%)	0	100	100
2	J	367/368 (100%)	367 (100%)	0	100	100
2	L	367/368 (100%)	367 (100%)	0	100	100
2	N	367/368 (100%)	367 (100%)	0	100	100
2	P	367/368 (100%)	367 (100%)	0	100	100
2	R	367/368 (100%)	367 (100%)	0	100	100
All	All	6543/6624 (99%)	6534 (100%)	9 (0%)	95	97

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	PHE
1	C	255	PHE
1	E	255	PHE
1	G	255	PHE
1	I	255	PHE
1	K	255	PHE
1	M	255	PHE
1	O	255	PHE
1	Q	255	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	301	GLN
2	B	8	GLN

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Mol	Chain	Res	Type
2	B	228	ASN
2	B	249	ASN
1	C	61	HIS
1	C	301	GLN
2	D	8	GLN
2	D	228	ASN
2	D	249	ASN
1	E	61	HIS
1	E	301	GLN
2	F	8	GLN
2	F	228	ASN
2	F	249	ASN
1	G	61	HIS
1	G	301	GLN
2	H	8	GLN
2	H	11	GLN
2	H	96	GLN
2	H	228	ASN
2	H	249	ASN
1	I	61	HIS
1	I	301	GLN
2	J	8	GLN
2	J	11	GLN
2	J	96	GLN
2	J	228	ASN
2	J	249	ASN
1	K	61	HIS
1	K	301	GLN
2	L	8	GLN
2	L	11	GLN
2	L	96	GLN
2	L	228	ASN
2	L	249	ASN
1	M	61	HIS
1	M	258	ASN
1	M	301	GLN
2	N	8	GLN
2	N	96	GLN
2	N	228	ASN
2	N	249	ASN
1	O	61	HIS
1	O	301	GLN

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Mol	Chain	Res	Type
2	P	8	GLN
2	P	96	GLN
2	P	228	ASN
2	P	249	ASN
1	Q	61	HIS
1	Q	258	ASN
1	Q	301	GLN
2	R	8	GLN
2	R	96	GLN
2	R	228	ASN
2	R	249	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 9 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	A	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.15	5 (18%)
5	GDP	B	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.65	10 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GTP	C	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.15	5 (18%)
5	GDP	D	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.65	10 (38%)
3	GTP	E	501	4	27,34,34	1.52	3 (11%)	27,54,54	2.15	5 (18%)
5	GDP	F	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.65	11 (42%)
3	GTP	G	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.15	5 (18%)
5	GDP	H	901	-	25,30,30	2.71	8 (32%)	26,47,47	3.65	10 (38%)
3	GTP	I	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.15	5 (18%)
5	GDP	J	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.66	10 (38%)
3	GTP	K	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.15	4 (14%)
5	GDP	L	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.66	11 (42%)
3	GTP	M	501	4	27,34,34	1.51	3 (11%)	27,54,54	2.16	5 (18%)
5	GDP	N	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.65	10 (38%)
3	GTP	O	501	4	27,34,34	1.51	4 (14%)	27,54,54	2.15	5 (18%)
5	GDP	P	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.65	10 (38%)
3	GTP	Q	501	4	27,34,34	1.52	3 (11%)	27,54,54	2.15	5 (18%)
5	GDP	R	901	-	25,30,30	2.72	8 (32%)	26,47,47	3.64	10 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	A	501	4	-	0/18/38/38	0/3/3/3
5	GDP	B	901	-	-	0/12/32/32	0/3/3/3
3	GTP	C	501	4	-	0/18/38/38	0/3/3/3
5	GDP	D	901	-	-	0/12/32/32	0/3/3/3
3	GTP	E	501	4	-	0/18/38/38	0/3/3/3
5	GDP	F	901	-	-	0/12/32/32	0/3/3/3
3	GTP	G	501	4	-	0/18/38/38	0/3/3/3
5	GDP	H	901	-	-	0/12/32/32	0/3/3/3
3	GTP	I	501	4	-	0/18/38/38	0/3/3/3
5	GDP	J	901	-	-	0/12/32/32	0/3/3/3
3	GTP	K	501	4	-	0/18/38/38	0/3/3/3
5	GDP	L	901	-	-	0/12/32/32	0/3/3/3
3	GTP	M	501	4	-	0/18/38/38	0/3/3/3
5	GDP	N	901	-	-	0/12/32/32	0/3/3/3
3	GTP	O	501	4	-	0/18/38/38	0/3/3/3
5	GDP	P	901	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	Q	501	4	-	0/18/38/38	0/3/3/3
5	GDP	R	901	-	-	0/12/32/32	0/3/3/3

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	901	GDP	PB-O2B	-3.55	1.40	1.54
5	D	901	GDP	PB-O2B	-3.55	1.40	1.54
5	R	901	GDP	PB-O2B	-3.54	1.40	1.54
5	B	901	GDP	PB-O2B	-3.54	1.40	1.54
5	P	901	GDP	PB-O2B	-3.54	1.40	1.54
5	J	901	GDP	PB-O2B	-3.54	1.40	1.54
5	N	901	GDP	PB-O2B	-3.54	1.40	1.54
5	H	901	GDP	PB-O2B	-3.53	1.40	1.54
5	F	901	GDP	PB-O2B	-3.53	1.40	1.54
3	O	501	GTP	C8-N7	-2.01	1.30	1.34
3	C	501	GTP	O4'-C1'	2.12	1.44	1.41
3	G	501	GTP	O4'-C1'	2.13	1.44	1.41
3	M	501	GTP	O4'-C1'	2.14	1.44	1.41
3	K	501	GTP	O4'-C1'	2.14	1.44	1.41
3	O	501	GTP	O4'-C1'	2.14	1.44	1.41
3	A	501	GTP	O4'-C1'	2.15	1.44	1.41
5	H	901	GDP	O3'-C3'	2.15	1.47	1.43
5	L	901	GDP	O3'-C3'	2.15	1.47	1.43
3	I	501	GTP	O4'-C1'	2.16	1.44	1.41
5	P	901	GDP	O3'-C3'	2.16	1.47	1.43
5	N	901	GDP	O3'-C3'	2.16	1.47	1.43
5	B	901	GDP	O3'-C3'	2.17	1.47	1.43
5	F	901	GDP	O3'-C3'	2.18	1.48	1.43
5	R	901	GDP	O3'-C3'	2.18	1.48	1.43
3	E	501	GTP	O4'-C1'	2.18	1.44	1.41
5	D	901	GDP	O3'-C3'	2.18	1.48	1.43
5	J	901	GDP	O3'-C3'	2.18	1.48	1.43
3	Q	501	GTP	O4'-C1'	2.20	1.44	1.41
5	R	901	GDP	C5-C4	2.47	1.46	1.40
5	N	901	GDP	C5-C4	2.47	1.46	1.40
5	F	901	GDP	C5-C4	2.48	1.46	1.40
5	D	901	GDP	C5-C4	2.48	1.46	1.40
5	B	901	GDP	C5-C4	2.49	1.46	1.40
5	H	901	GDP	C5-C4	2.49	1.46	1.40
5	L	901	GDP	C5-C4	2.50	1.46	1.40
5	P	901	GDP	C5-C4	2.50	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	901	GDP	C5-C4	2.51	1.46	1.40
5	R	901	GDP	C8-N7	3.44	1.41	1.34
5	H	901	GDP	C8-N7	3.44	1.41	1.34
5	B	901	GDP	C8-N7	3.45	1.41	1.34
5	D	901	GDP	C8-N7	3.45	1.41	1.34
5	P	901	GDP	C8-N7	3.46	1.41	1.34
5	J	901	GDP	C8-N7	3.46	1.41	1.34
5	F	901	GDP	C8-N7	3.48	1.41	1.34
5	N	901	GDP	C8-N7	3.48	1.41	1.34
5	L	901	GDP	C8-N7	3.48	1.41	1.34
3	K	501	GTP	PG-O3B	3.81	1.66	1.60
3	G	501	GTP	PG-O3B	3.81	1.66	1.60
3	C	501	GTP	PG-O3B	3.83	1.66	1.60
3	I	501	GTP	PG-O3B	3.83	1.66	1.60
3	M	501	GTP	PG-O3B	3.83	1.66	1.60
3	Q	501	GTP	PG-O3B	3.83	1.66	1.60
3	A	501	GTP	PG-O3B	3.84	1.66	1.60
3	E	501	GTP	PG-O3B	3.84	1.66	1.60
3	O	501	GTP	PG-O3B	3.87	1.66	1.60
5	L	901	GDP	PB-O1B	3.87	1.63	1.50
5	R	901	GDP	PB-O1B	3.87	1.63	1.50
5	H	901	GDP	PB-O1B	3.87	1.63	1.50
5	N	901	GDP	PB-O1B	3.87	1.63	1.50
5	D	901	GDP	PB-O1B	3.88	1.63	1.50
5	F	901	GDP	PB-O1B	3.88	1.63	1.50
5	P	901	GDP	PB-O1B	3.88	1.64	1.50
5	B	901	GDP	PB-O1B	3.88	1.64	1.50
5	J	901	GDP	PB-O1B	3.89	1.64	1.50
5	D	901	GDP	O6-C6	4.08	1.34	1.24
5	P	901	GDP	O6-C6	4.10	1.34	1.24
5	L	901	GDP	O6-C6	4.10	1.34	1.24
5	F	901	GDP	O6-C6	4.10	1.34	1.24
5	H	901	GDP	O6-C6	4.10	1.34	1.24
5	B	901	GDP	O6-C6	4.11	1.34	1.24
5	N	901	GDP	O6-C6	4.12	1.34	1.24
5	R	901	GDP	O6-C6	4.13	1.34	1.24
5	J	901	GDP	O6-C6	4.13	1.34	1.24
3	K	501	GTP	C6-N1	4.77	1.41	1.33
3	M	501	GTP	C6-N1	4.81	1.41	1.33
3	I	501	GTP	C6-N1	4.81	1.41	1.33
3	O	501	GTP	C6-N1	4.81	1.41	1.33
3	A	501	GTP	C6-N1	4.81	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	501	GTP	C6-N1	4.82	1.41	1.33
3	E	501	GTP	C6-N1	4.82	1.41	1.33
3	Q	501	GTP	C6-N1	4.82	1.41	1.33
3	C	501	GTP	C6-N1	4.83	1.41	1.33
5	L	901	GDP	O4'-C1'	6.17	1.49	1.41
5	P	901	GDP	O4'-C1'	6.18	1.49	1.41
5	N	901	GDP	O4'-C1'	6.19	1.49	1.41
5	F	901	GDP	O4'-C1'	6.20	1.49	1.41
5	B	901	GDP	O4'-C1'	6.20	1.49	1.41
5	H	901	GDP	O4'-C1'	6.21	1.49	1.41
5	J	901	GDP	O4'-C1'	6.21	1.49	1.41
5	D	901	GDP	O4'-C1'	6.21	1.49	1.41
5	R	901	GDP	O4'-C1'	6.21	1.49	1.41
5	R	901	GDP	C2-N1	7.54	1.49	1.35
5	N	901	GDP	C2-N1	7.56	1.49	1.35
5	H	901	GDP	C2-N1	7.56	1.49	1.35
5	D	901	GDP	C2-N1	7.56	1.49	1.35
5	B	901	GDP	C2-N1	7.57	1.49	1.35
5	F	901	GDP	C2-N1	7.58	1.49	1.35
5	J	901	GDP	C2-N1	7.58	1.49	1.35
5	P	901	GDP	C2-N1	7.60	1.49	1.35
5	L	901	GDP	C2-N1	7.62	1.49	1.35

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	901	GDP	C6-C5-C4	-11.54	109.37	120.84
5	P	901	GDP	C6-C5-C4	-11.49	109.42	120.84
5	N	901	GDP	C6-C5-C4	-11.49	109.42	120.84
5	B	901	GDP	C6-C5-C4	-11.48	109.42	120.84
5	L	901	GDP	C6-C5-C4	-11.48	109.43	120.84
5	D	901	GDP	C6-C5-C4	-11.47	109.44	120.84
5	H	901	GDP	C6-C5-C4	-11.46	109.44	120.84
5	F	901	GDP	C6-C5-C4	-11.45	109.45	120.84
5	R	901	GDP	C6-C5-C4	-11.45	109.45	120.84
3	K	501	GTP	C5-C6-N1	-7.09	113.38	123.48
3	C	501	GTP	C5-C6-N1	-7.09	113.39	123.48
3	I	501	GTP	C5-C6-N1	-7.08	113.41	123.48
3	O	501	GTP	C5-C6-N1	-7.08	113.41	123.48
3	M	501	GTP	C5-C6-N1	-7.07	113.42	123.48
3	A	501	GTP	C5-C6-N1	-7.07	113.42	123.48
3	Q	501	GTP	C5-C6-N1	-7.07	113.42	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	501	GTP	C5-C6-N1	-7.06	113.43	123.48
3	E	501	GTP	C5-C6-N1	-7.05	113.44	123.48
5	D	901	GDP	N2-C2-N1	-5.88	107.84	117.24
5	N	901	GDP	N2-C2-N1	-5.87	107.86	117.24
5	L	901	GDP	N2-C2-N1	-5.87	107.86	117.24
5	P	901	GDP	N2-C2-N1	-5.86	107.86	117.24
5	B	901	GDP	N2-C2-N1	-5.86	107.88	117.24
5	R	901	GDP	N2-C2-N1	-5.85	107.89	117.24
5	F	901	GDP	N2-C2-N1	-5.83	107.91	117.24
5	H	901	GDP	N2-C2-N1	-5.83	107.92	117.24
5	J	901	GDP	N2-C2-N1	-5.83	107.92	117.24
5	J	901	GDP	C4-C5-N7	-5.07	104.51	109.41
5	R	901	GDP	C4-C5-N7	-5.06	104.52	109.41
5	P	901	GDP	C4-C5-N7	-5.06	104.53	109.41
5	B	901	GDP	C4-C5-N7	-5.05	104.53	109.41
5	H	901	GDP	C4-C5-N7	-5.05	104.53	109.41
5	D	901	GDP	C4-C5-N7	-5.03	104.55	109.41
5	N	901	GDP	C4-C5-N7	-5.01	104.57	109.41
5	F	901	GDP	C4-C5-N7	-5.01	104.57	109.41
5	L	901	GDP	C4-C5-N7	-5.00	104.58	109.41
5	L	901	GDP	N3-C2-N1	-4.97	120.20	127.46
5	J	901	GDP	N3-C2-N1	-4.95	120.23	127.46
5	H	901	GDP	N3-C2-N1	-4.95	120.23	127.46
5	R	901	GDP	N3-C2-N1	-4.95	120.24	127.46
5	B	901	GDP	N3-C2-N1	-4.94	120.24	127.46
5	D	901	GDP	N3-C2-N1	-4.94	120.24	127.46
5	F	901	GDP	N3-C2-N1	-4.94	120.25	127.46
5	N	901	GDP	N3-C2-N1	-4.94	120.25	127.46
5	P	901	GDP	N3-C2-N1	-4.93	120.26	127.46
3	K	501	GTP	N3-C2-N1	-3.19	122.80	127.46
3	Q	501	GTP	N3-C2-N1	-3.18	122.81	127.46
3	O	501	GTP	N3-C2-N1	-3.17	122.83	127.46
3	M	501	GTP	N3-C2-N1	-3.17	122.83	127.46
3	E	501	GTP	N3-C2-N1	-3.16	122.84	127.46
3	A	501	GTP	N3-C2-N1	-3.16	122.84	127.46
3	G	501	GTP	N3-C2-N1	-3.16	122.84	127.46
3	C	501	GTP	N3-C2-N1	-3.16	122.85	127.46
3	I	501	GTP	N3-C2-N1	-3.14	122.88	127.46
3	M	501	GTP	C6-C5-C4	-2.56	118.30	120.84
3	I	501	GTP	C6-C5-C4	-2.52	118.34	120.84
3	Q	501	GTP	C6-C5-C4	-2.50	118.36	120.84
3	A	501	GTP	C6-C5-C4	-2.49	118.36	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	GTP	C6-C5-C4	-2.49	118.37	120.84
3	C	501	GTP	C6-C5-C4	-2.49	118.37	120.84
3	O	501	GTP	C6-C5-C4	-2.48	118.38	120.84
3	G	501	GTP	C6-C5-C4	-2.45	118.41	120.84
3	K	501	GTP	C6-C5-C4	-2.44	118.42	120.84
5	L	901	GDP	O4'-C4'-C3'	-2.01	101.17	105.17
5	F	901	GDP	O4'-C4'-C3'	-2.01	101.18	105.17
3	M	501	GTP	O5'-C5'-C4'	2.00	116.10	109.00
3	O	501	GTP	O5'-C5'-C4'	2.01	116.12	109.00
3	E	501	GTP	O5'-C5'-C4'	2.01	116.12	109.00
3	A	501	GTP	O5'-C5'-C4'	2.01	116.13	109.00
3	I	501	GTP	O5'-C5'-C4'	2.01	116.13	109.00
3	C	501	GTP	O5'-C5'-C4'	2.01	116.14	109.00
3	Q	501	GTP	O5'-C5'-C4'	2.01	116.14	109.00
3	G	501	GTP	O5'-C5'-C4'	2.02	116.16	109.00
5	H	901	GDP	O3B-PB-O2B	2.10	116.07	107.61
5	R	901	GDP	O3B-PB-O2B	2.10	116.08	107.61
5	B	901	GDP	O3B-PB-O2B	2.10	116.09	107.61
5	L	901	GDP	O3B-PB-O2B	2.10	116.09	107.61
5	P	901	GDP	O3B-PB-O2B	2.10	116.09	107.61
5	F	901	GDP	O3B-PB-O2B	2.10	116.09	107.61
5	D	901	GDP	O3B-PB-O2B	2.10	116.10	107.61
5	J	901	GDP	O3B-PB-O2B	2.10	116.10	107.61
5	N	901	GDP	O3B-PB-O2B	2.11	116.12	107.61
5	L	901	GDP	O2'-C2'-C3'	2.32	119.25	111.83
5	D	901	GDP	O2'-C2'-C3'	2.32	119.26	111.83
5	R	901	GDP	O2'-C2'-C3'	2.32	119.26	111.83
5	N	901	GDP	O2'-C2'-C3'	2.32	119.27	111.83
5	B	901	GDP	O2'-C2'-C3'	2.32	119.28	111.83
5	H	901	GDP	O2'-C2'-C3'	2.33	119.29	111.83
5	J	901	GDP	O2'-C2'-C3'	2.33	119.29	111.83
5	F	901	GDP	O2'-C2'-C3'	2.33	119.30	111.83
5	P	901	GDP	O2'-C2'-C3'	2.34	119.31	111.83
5	R	901	GDP	C2'-C3'-C4'	3.41	109.26	102.62
5	N	901	GDP	C2'-C3'-C4'	3.42	109.28	102.62
5	D	901	GDP	C2'-C3'-C4'	3.42	109.28	102.62
5	H	901	GDP	C2'-C3'-C4'	3.43	109.29	102.62
5	B	901	GDP	C2'-C3'-C4'	3.43	109.30	102.62
5	P	901	GDP	C2'-C3'-C4'	3.43	109.31	102.62
5	F	901	GDP	C2'-C3'-C4'	3.44	109.32	102.62
5	L	901	GDP	C2'-C3'-C4'	3.44	109.33	102.62
5	J	901	GDP	C2'-C3'-C4'	3.45	109.34	102.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	901	GDP	C2-N3-C4	3.49	119.24	115.16
5	N	901	GDP	C2-N3-C4	3.53	119.28	115.16
5	J	901	GDP	C2-N3-C4	3.53	119.28	115.16
5	B	901	GDP	C2-N3-C4	3.53	119.28	115.16
5	H	901	GDP	C2-N3-C4	3.53	119.28	115.16
5	D	901	GDP	C2-N3-C4	3.53	119.28	115.16
5	R	901	GDP	C2-N3-C4	3.54	119.29	115.16
5	F	901	GDP	C2-N3-C4	3.54	119.30	115.16
5	L	901	GDP	C2-N3-C4	3.56	119.32	115.16
5	R	901	GDP	C4'-O4'-C1'	3.96	113.98	109.77
5	D	901	GDP	C4'-O4'-C1'	3.97	114.00	109.77
5	J	901	GDP	C4'-O4'-C1'	4.01	114.03	109.77
5	B	901	GDP	C4'-O4'-C1'	4.01	114.04	109.77
5	N	901	GDP	C4'-O4'-C1'	4.01	114.04	109.77
5	P	901	GDP	C4'-O4'-C1'	4.02	114.05	109.77
5	L	901	GDP	C4'-O4'-C1'	4.04	114.07	109.77
5	H	901	GDP	C4'-O4'-C1'	4.05	114.08	109.77
5	F	901	GDP	C4'-O4'-C1'	4.07	114.10	109.77
3	E	501	GTP	C6-N1-C2	5.93	124.59	116.06
3	G	501	GTP	C6-N1-C2	5.95	124.61	116.06
3	A	501	GTP	C6-N1-C2	5.95	124.62	116.06
3	I	501	GTP	C6-N1-C2	5.96	124.64	116.06
3	O	501	GTP	C6-N1-C2	5.96	124.64	116.06
3	Q	501	GTP	C6-N1-C2	5.96	124.64	116.06
3	C	501	GTP	C6-N1-C2	5.97	124.65	116.06
3	M	501	GTP	C6-N1-C2	5.98	124.66	116.06
3	K	501	GTP	C6-N1-C2	5.99	124.67	116.06
5	F	901	GDP	N2-C2-N3	7.63	131.83	117.75
5	J	901	GDP	N2-C2-N3	7.63	131.84	117.75
5	H	901	GDP	N2-C2-N3	7.63	131.84	117.75
5	R	901	GDP	N2-C2-N3	7.64	131.87	117.75
5	P	901	GDP	N2-C2-N3	7.65	131.87	117.75
5	B	901	GDP	N2-C2-N3	7.65	131.88	117.75
5	N	901	GDP	N2-C2-N3	7.66	131.88	117.75
5	D	901	GDP	N2-C2-N3	7.67	131.91	117.75
5	L	901	GDP	N2-C2-N3	7.68	131.93	117.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GTP	2	0
5	B	901	GDP	2	0
3	C	501	GTP	2	0
5	D	901	GDP	2	0
3	E	501	GTP	2	0
5	F	901	GDP	2	0
3	G	501	GTP	2	0
5	H	901	GDP	2	0
3	I	501	GTP	2	0
5	J	901	GDP	2	0
3	K	501	GTP	2	0
5	L	901	GDP	2	0
3	M	501	GTP	2	0
5	N	901	GDP	2	0
3	O	501	GTP	2	0
5	P	901	GDP	2	0
3	Q	501	GTP	2	0
5	R	901	GDP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.