



Full wwPDB EM Validation Report ⓘ

Jul 23, 2026 – 06:35 pm BST

PDB ID : 9R6C / pdb_00009r6c
EMDB ID : EMD-53610
Title : CPS secretion pathway Wza-Wzc (Conf 5)
Authors : Yuan, B.; Heinz, D.W.
Deposited on : 2025-05-11
Resolution : 6.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

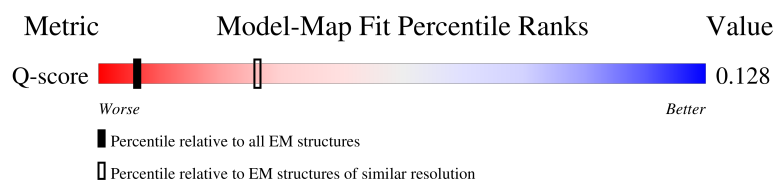
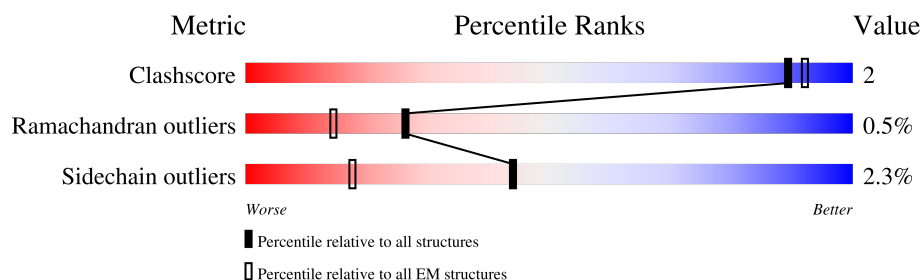
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 Å.

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



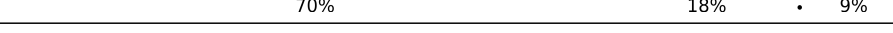
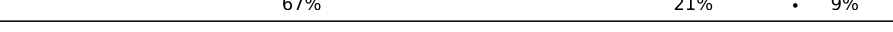
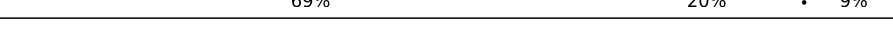
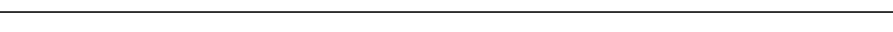
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	523 (6.20 - 7.20)

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

Mol	Chain	Length	Quality of chain
1	A	394	 81% 10% 9%
1	B	394	 84% 7% 9%
1	C	394	 78% 12% 9%
1	D	394	 85% 6% 9%

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Mol	Chain	Length	Quality of chain
1	E	394	 84% 7% 9%
1	F	394	 82% 8% 9%
1	G	394	 83% 8% 9%
1	H	394	 80% 10% 9%
1	a	394	 80% 9% 9%
1	b	394	 84% 7% 9%
1	c	394	 81% 9% 9%
1	d	394	 84% 7% 9%
1	e	394	 82% 9% 9%
1	f	394	 80% 11% 9%
1	g	394	 80% 10% 9%
1	h	394	 82% 7% 9%
2	I	738	 70% 18% 9%
2	J	738	 67% 21% 9%
2	K	738	 80% 9% 9%
2	L	738	 69% 20% 9%
2	M	738	 72% 17% 9%
2	N	738	 72% 17% 9%
2	O	738	 72% 15% 9%
2	P	738	 71% 18% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 172976 atoms, of which 86752 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 Putative polysaccharide export protein Wza.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	B	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	C	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	D	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	E	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	F	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	G	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	H	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	a	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	b	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	c	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	d	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	e	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	f	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	g	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	h	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	GLU	-	expression tag	UNP P0A930
A	381	ASN	-	expression tag	UNP P0A930
A	382	LEU	-	expression tag	UNP P0A930
A	383	TYR	-	expression tag	UNP P0A930
A	384	PHE	-	expression tag	UNP P0A930
A	385	GLN	-	expression tag	UNP P0A930
A	386	SER	-	expression tag	UNP P0A930
A	387	TRP	-	expression tag	UNP P0A930
A	388	SER	-	expression tag	UNP P0A930
A	389	HIS	-	expression tag	UNP P0A930
A	390	PRO	-	expression tag	UNP P0A930
A	391	GLN	-	expression tag	UNP P0A930
A	392	PHE	-	expression tag	UNP P0A930
A	393	GLU	-	expression tag	UNP P0A930
A	394	LYS	-	expression tag	UNP P0A930
B	380	GLU	-	expression tag	UNP P0A930
B	381	ASN	-	expression tag	UNP P0A930
B	382	LEU	-	expression tag	UNP P0A930
B	383	TYR	-	expression tag	UNP P0A930
B	384	PHE	-	expression tag	UNP P0A930
B	385	GLN	-	expression tag	UNP P0A930
B	386	SER	-	expression tag	UNP P0A930
B	387	TRP	-	expression tag	UNP P0A930
B	388	SER	-	expression tag	UNP P0A930
B	389	HIS	-	expression tag	UNP P0A930
B	390	PRO	-	expression tag	UNP P0A930
B	391	GLN	-	expression tag	UNP P0A930
B	392	PHE	-	expression tag	UNP P0A930
B	393	GLU	-	expression tag	UNP P0A930
B	394	LYS	-	expression tag	UNP P0A930
C	380	GLU	-	expression tag	UNP P0A930
C	381	ASN	-	expression tag	UNP P0A930
C	382	LEU	-	expression tag	UNP P0A930
C	383	TYR	-	expression tag	UNP P0A930
C	384	PHE	-	expression tag	UNP P0A930
C	385	GLN	-	expression tag	UNP P0A930
C	386	SER	-	expression tag	UNP P0A930
C	387	TRP	-	expression tag	UNP P0A930
C	388	SER	-	expression tag	UNP P0A930
C	389	HIS	-	expression tag	UNP P0A930
C	390	PRO	-	expression tag	UNP P0A930
C	391	GLN	-	expression tag	UNP P0A930
C	392	PHE	-	expression tag	UNP P0A930

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Chain	Residue	Modelled	Actual	Comment	Reference
C	393	GLU	-	expression tag	UNP P0A930
C	394	LYS	-	expression tag	UNP P0A930
D	380	GLU	-	expression tag	UNP P0A930
D	381	ASN	-	expression tag	UNP P0A930
D	382	LEU	-	expression tag	UNP P0A930
D	383	TYR	-	expression tag	UNP P0A930
D	384	PHE	-	expression tag	UNP P0A930
D	385	GLN	-	expression tag	UNP P0A930
D	386	SER	-	expression tag	UNP P0A930
D	387	TRP	-	expression tag	UNP P0A930
D	388	SER	-	expression tag	UNP P0A930
D	389	HIS	-	expression tag	UNP P0A930
D	390	PRO	-	expression tag	UNP P0A930
D	391	GLN	-	expression tag	UNP P0A930
D	392	PHE	-	expression tag	UNP P0A930
D	393	GLU	-	expression tag	UNP P0A930
D	394	LYS	-	expression tag	UNP P0A930
E	380	GLU	-	expression tag	UNP P0A930
E	381	ASN	-	expression tag	UNP P0A930
E	382	LEU	-	expression tag	UNP P0A930
E	383	TYR	-	expression tag	UNP P0A930
E	384	PHE	-	expression tag	UNP P0A930
E	385	GLN	-	expression tag	UNP P0A930
E	386	SER	-	expression tag	UNP P0A930
E	387	TRP	-	expression tag	UNP P0A930
E	388	SER	-	expression tag	UNP P0A930
E	389	HIS	-	expression tag	UNP P0A930
E	390	PRO	-	expression tag	UNP P0A930
E	391	GLN	-	expression tag	UNP P0A930
E	392	PHE	-	expression tag	UNP P0A930
E	393	GLU	-	expression tag	UNP P0A930
E	394	LYS	-	expression tag	UNP P0A930
F	380	GLU	-	expression tag	UNP P0A930
F	381	ASN	-	expression tag	UNP P0A930
F	382	LEU	-	expression tag	UNP P0A930
F	383	TYR	-	expression tag	UNP P0A930
F	384	PHE	-	expression tag	UNP P0A930
F	385	GLN	-	expression tag	UNP P0A930
F	386	SER	-	expression tag	UNP P0A930
F	387	TRP	-	expression tag	UNP P0A930
F	388	SER	-	expression tag	UNP P0A930
F	389	HIS	-	expression tag	UNP P0A930

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Chain	Residue	Modelled	Actual	Comment	Reference
F	390	PRO	-	expression tag	UNP P0A930
F	391	GLN	-	expression tag	UNP P0A930
F	392	PHE	-	expression tag	UNP P0A930
F	393	GLU	-	expression tag	UNP P0A930
F	394	LYS	-	expression tag	UNP P0A930
G	380	GLU	-	expression tag	UNP P0A930
G	381	ASN	-	expression tag	UNP P0A930
G	382	LEU	-	expression tag	UNP P0A930
G	383	TYR	-	expression tag	UNP P0A930
G	384	PHE	-	expression tag	UNP P0A930
G	385	GLN	-	expression tag	UNP P0A930
G	386	SER	-	expression tag	UNP P0A930
G	387	TRP	-	expression tag	UNP P0A930
G	388	SER	-	expression tag	UNP P0A930
G	389	HIS	-	expression tag	UNP P0A930
G	390	PRO	-	expression tag	UNP P0A930
G	391	GLN	-	expression tag	UNP P0A930
G	392	PHE	-	expression tag	UNP P0A930
G	393	GLU	-	expression tag	UNP P0A930
G	394	LYS	-	expression tag	UNP P0A930
H	380	GLU	-	expression tag	UNP P0A930
H	381	ASN	-	expression tag	UNP P0A930
H	382	LEU	-	expression tag	UNP P0A930
H	383	TYR	-	expression tag	UNP P0A930
H	384	PHE	-	expression tag	UNP P0A930
H	385	GLN	-	expression tag	UNP P0A930
H	386	SER	-	expression tag	UNP P0A930
H	387	TRP	-	expression tag	UNP P0A930
H	388	SER	-	expression tag	UNP P0A930
H	389	HIS	-	expression tag	UNP P0A930
H	390	PRO	-	expression tag	UNP P0A930
H	391	GLN	-	expression tag	UNP P0A930
H	392	PHE	-	expression tag	UNP P0A930
H	393	GLU	-	expression tag	UNP P0A930
H	394	LYS	-	expression tag	UNP P0A930
a	380	GLU	-	expression tag	UNP P0A930
a	381	ASN	-	expression tag	UNP P0A930
a	382	LEU	-	expression tag	UNP P0A930
a	383	TYR	-	expression tag	UNP P0A930
a	384	PHE	-	expression tag	UNP P0A930
a	385	GLN	-	expression tag	UNP P0A930
a	386	SER	-	expression tag	UNP P0A930

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Chain	Residue	Modelled	Actual	Comment	Reference
a	387	TRP	-	expression tag	UNP P0A930
a	388	SER	-	expression tag	UNP P0A930
a	389	HIS	-	expression tag	UNP P0A930
a	390	PRO	-	expression tag	UNP P0A930
a	391	GLN	-	expression tag	UNP P0A930
a	392	PHE	-	expression tag	UNP P0A930
a	393	GLU	-	expression tag	UNP P0A930
a	394	LYS	-	expression tag	UNP P0A930
b	380	GLU	-	expression tag	UNP P0A930
b	381	ASN	-	expression tag	UNP P0A930
b	382	LEU	-	expression tag	UNP P0A930
b	383	TYR	-	expression tag	UNP P0A930
b	384	PHE	-	expression tag	UNP P0A930
b	385	GLN	-	expression tag	UNP P0A930
b	386	SER	-	expression tag	UNP P0A930
b	387	TRP	-	expression tag	UNP P0A930
b	388	SER	-	expression tag	UNP P0A930
b	389	HIS	-	expression tag	UNP P0A930
b	390	PRO	-	expression tag	UNP P0A930
b	391	GLN	-	expression tag	UNP P0A930
b	392	PHE	-	expression tag	UNP P0A930
b	393	GLU	-	expression tag	UNP P0A930
b	394	LYS	-	expression tag	UNP P0A930
c	380	GLU	-	expression tag	UNP P0A930
c	381	ASN	-	expression tag	UNP P0A930
c	382	LEU	-	expression tag	UNP P0A930
c	383	TYR	-	expression tag	UNP P0A930
c	384	PHE	-	expression tag	UNP P0A930
c	385	GLN	-	expression tag	UNP P0A930
c	386	SER	-	expression tag	UNP P0A930
c	387	TRP	-	expression tag	UNP P0A930
c	388	SER	-	expression tag	UNP P0A930
c	389	HIS	-	expression tag	UNP P0A930
c	390	PRO	-	expression tag	UNP P0A930
c	391	GLN	-	expression tag	UNP P0A930
c	392	PHE	-	expression tag	UNP P0A930
c	393	GLU	-	expression tag	UNP P0A930
c	394	LYS	-	expression tag	UNP P0A930
d	380	GLU	-	expression tag	UNP P0A930
d	381	ASN	-	expression tag	UNP P0A930
d	382	LEU	-	expression tag	UNP P0A930
d	383	TYR	-	expression tag	UNP P0A930

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Chain	Residue	Modelled	Actual	Comment	Reference
d	384	PHE	-	expression tag	UNP P0A930
d	385	GLN	-	expression tag	UNP P0A930
d	386	SER	-	expression tag	UNP P0A930
d	387	TRP	-	expression tag	UNP P0A930
d	388	SER	-	expression tag	UNP P0A930
d	389	HIS	-	expression tag	UNP P0A930
d	390	PRO	-	expression tag	UNP P0A930
d	391	GLN	-	expression tag	UNP P0A930
d	392	PHE	-	expression tag	UNP P0A930
d	393	GLU	-	expression tag	UNP P0A930
d	394	LYS	-	expression tag	UNP P0A930
e	380	GLU	-	expression tag	UNP P0A930
e	381	ASN	-	expression tag	UNP P0A930
e	382	LEU	-	expression tag	UNP P0A930
e	383	TYR	-	expression tag	UNP P0A930
e	384	PHE	-	expression tag	UNP P0A930
e	385	GLN	-	expression tag	UNP P0A930
e	386	SER	-	expression tag	UNP P0A930
e	387	TRP	-	expression tag	UNP P0A930
e	388	SER	-	expression tag	UNP P0A930
e	389	HIS	-	expression tag	UNP P0A930
e	390	PRO	-	expression tag	UNP P0A930
e	391	GLN	-	expression tag	UNP P0A930
e	392	PHE	-	expression tag	UNP P0A930
e	393	GLU	-	expression tag	UNP P0A930
e	394	LYS	-	expression tag	UNP P0A930
f	380	GLU	-	expression tag	UNP P0A930
f	381	ASN	-	expression tag	UNP P0A930
f	382	LEU	-	expression tag	UNP P0A930
f	383	TYR	-	expression tag	UNP P0A930
f	384	PHE	-	expression tag	UNP P0A930
f	385	GLN	-	expression tag	UNP P0A930
f	386	SER	-	expression tag	UNP P0A930
f	387	TRP	-	expression tag	UNP P0A930
f	388	SER	-	expression tag	UNP P0A930
f	389	HIS	-	expression tag	UNP P0A930
f	390	PRO	-	expression tag	UNP P0A930
f	391	GLN	-	expression tag	UNP P0A930
f	392	PHE	-	expression tag	UNP P0A930
f	393	GLU	-	expression tag	UNP P0A930
f	394	LYS	-	expression tag	UNP P0A930
g	380	GLU	-	expression tag	UNP P0A930

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Chain	Residue	Modelled	Actual	Comment	Reference
g	381	ASN	-	expression tag	UNP P0A930
g	382	LEU	-	expression tag	UNP P0A930
g	383	TYR	-	expression tag	UNP P0A930
g	384	PHE	-	expression tag	UNP P0A930
g	385	GLN	-	expression tag	UNP P0A930
g	386	SER	-	expression tag	UNP P0A930
g	387	TRP	-	expression tag	UNP P0A930
g	388	SER	-	expression tag	UNP P0A930
g	389	HIS	-	expression tag	UNP P0A930
g	390	PRO	-	expression tag	UNP P0A930
g	391	GLN	-	expression tag	UNP P0A930
g	392	PHE	-	expression tag	UNP P0A930
g	393	GLU	-	expression tag	UNP P0A930
g	394	LYS	-	expression tag	UNP P0A930
h	380	GLU	-	expression tag	UNP P0A930
h	381	ASN	-	expression tag	UNP P0A930
h	382	LEU	-	expression tag	UNP P0A930
h	383	TYR	-	expression tag	UNP P0A930
h	384	PHE	-	expression tag	UNP P0A930
h	385	GLN	-	expression tag	UNP P0A930
h	386	SER	-	expression tag	UNP P0A930
h	387	TRP	-	expression tag	UNP P0A930
h	388	SER	-	expression tag	UNP P0A930
h	389	HIS	-	expression tag	UNP P0A930
h	390	PRO	-	expression tag	UNP P0A930
h	391	GLN	-	expression tag	UNP P0A930
h	392	PHE	-	expression tag	UNP P0A930
h	393	GLU	-	expression tag	UNP P0A930
h	394	LYS	-	expression tag	UNP P0A930

- Molecule 2 is a protein called Tyrosine-protein kinase wzc.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	I	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		
2	J	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		
2	K	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		
2	L	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		
2	M	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	N	668	Total 10487	C 3278	H 5302	N 892	O 995	S 20	0	0
2	O	668	Total 10487	C 3278	H 5302	N 892	O 995	S 20	0	0
2	P	668	Total 10487	C 3278	H 5302	N 892	O 995	S 20	0	0

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	540	MET	LYS	engineered mutation	UNP P76387
I	721	SER	-	expression tag	UNP P76387
I	722	SER	-	expression tag	UNP P76387
I	723	GLY	-	expression tag	UNP P76387
I	724	GLU	-	expression tag	UNP P76387
I	725	ASN	-	expression tag	UNP P76387
I	726	LEU	-	expression tag	UNP P76387
I	727	TYR	-	expression tag	UNP P76387
I	728	PHE	-	expression tag	UNP P76387
I	729	GLN	-	expression tag	UNP P76387
I	730	GLY	-	expression tag	UNP P76387
I	731	TRP	-	expression tag	UNP P76387
I	732	SER	-	expression tag	UNP P76387
I	733	HIS	-	expression tag	UNP P76387
I	734	PRO	-	expression tag	UNP P76387
I	735	GLN	-	expression tag	UNP P76387
I	736	PHE	-	expression tag	UNP P76387
I	737	GLU	-	expression tag	UNP P76387
I	738	LYS	-	expression tag	UNP P76387
J	540	MET	LYS	engineered mutation	UNP P76387
J	721	SER	-	expression tag	UNP P76387
J	722	SER	-	expression tag	UNP P76387
J	723	GLY	-	expression tag	UNP P76387
J	724	GLU	-	expression tag	UNP P76387
J	725	ASN	-	expression tag	UNP P76387
J	726	LEU	-	expression tag	UNP P76387
J	727	TYR	-	expression tag	UNP P76387
J	728	PHE	-	expression tag	UNP P76387
J	729	GLN	-	expression tag	UNP P76387
J	730	GLY	-	expression tag	UNP P76387
J	731	TRP	-	expression tag	UNP P76387
J	732	SER	-	expression tag	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
J	733	HIS	-	expression tag	UNP P76387
J	734	PRO	-	expression tag	UNP P76387
J	735	GLN	-	expression tag	UNP P76387
J	736	PHE	-	expression tag	UNP P76387
J	737	GLU	-	expression tag	UNP P76387
J	738	LYS	-	expression tag	UNP P76387
K	540	MET	LYS	engineered mutation	UNP P76387
K	721	SER	-	expression tag	UNP P76387
K	722	SER	-	expression tag	UNP P76387
K	723	GLY	-	expression tag	UNP P76387
K	724	GLU	-	expression tag	UNP P76387
K	725	ASN	-	expression tag	UNP P76387
K	726	LEU	-	expression tag	UNP P76387
K	727	TYR	-	expression tag	UNP P76387
K	728	PHE	-	expression tag	UNP P76387
K	729	GLN	-	expression tag	UNP P76387
K	730	GLY	-	expression tag	UNP P76387
K	731	TRP	-	expression tag	UNP P76387
K	732	SER	-	expression tag	UNP P76387
K	733	HIS	-	expression tag	UNP P76387
K	734	PRO	-	expression tag	UNP P76387
K	735	GLN	-	expression tag	UNP P76387
K	736	PHE	-	expression tag	UNP P76387
K	737	GLU	-	expression tag	UNP P76387
K	738	LYS	-	expression tag	UNP P76387
L	540	MET	LYS	engineered mutation	UNP P76387
L	721	SER	-	expression tag	UNP P76387
L	722	SER	-	expression tag	UNP P76387
L	723	GLY	-	expression tag	UNP P76387
L	724	GLU	-	expression tag	UNP P76387
L	725	ASN	-	expression tag	UNP P76387
L	726	LEU	-	expression tag	UNP P76387
L	727	TYR	-	expression tag	UNP P76387
L	728	PHE	-	expression tag	UNP P76387
L	729	GLN	-	expression tag	UNP P76387
L	730	GLY	-	expression tag	UNP P76387
L	731	TRP	-	expression tag	UNP P76387
L	732	SER	-	expression tag	UNP P76387
L	733	HIS	-	expression tag	UNP P76387
L	734	PRO	-	expression tag	UNP P76387
L	735	GLN	-	expression tag	UNP P76387
L	736	PHE	-	expression tag	UNP P76387

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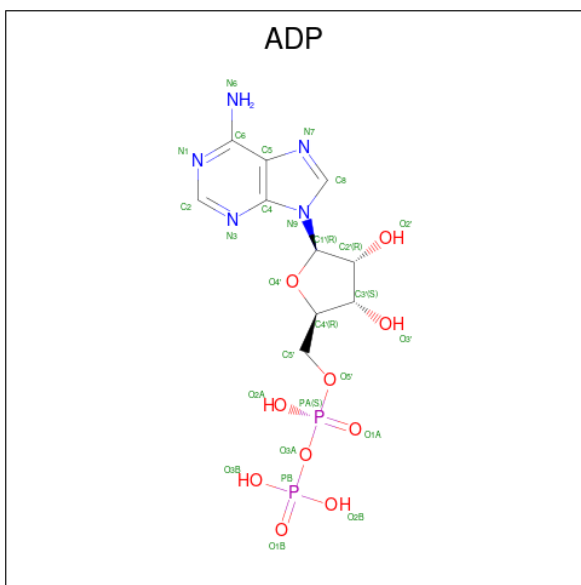
Chain	Residue	Modelled	Actual	Comment	Reference
L	737	GLU	-	expression tag	UNP P76387
L	738	LYS	-	expression tag	UNP P76387
M	540	MET	LYS	engineered mutation	UNP P76387
M	721	SER	-	expression tag	UNP P76387
M	722	SER	-	expression tag	UNP P76387
M	723	GLY	-	expression tag	UNP P76387
M	724	GLU	-	expression tag	UNP P76387
M	725	ASN	-	expression tag	UNP P76387
M	726	LEU	-	expression tag	UNP P76387
M	727	TYR	-	expression tag	UNP P76387
M	728	PHE	-	expression tag	UNP P76387
M	729	GLN	-	expression tag	UNP P76387
M	730	GLY	-	expression tag	UNP P76387
M	731	TRP	-	expression tag	UNP P76387
M	732	SER	-	expression tag	UNP P76387
M	733	HIS	-	expression tag	UNP P76387
M	734	PRO	-	expression tag	UNP P76387
M	735	GLN	-	expression tag	UNP P76387
M	736	PHE	-	expression tag	UNP P76387
M	737	GLU	-	expression tag	UNP P76387
M	738	LYS	-	expression tag	UNP P76387
N	540	MET	LYS	engineered mutation	UNP P76387
N	721	SER	-	expression tag	UNP P76387
N	722	SER	-	expression tag	UNP P76387
N	723	GLY	-	expression tag	UNP P76387
N	724	GLU	-	expression tag	UNP P76387
N	725	ASN	-	expression tag	UNP P76387
N	726	LEU	-	expression tag	UNP P76387
N	727	TYR	-	expression tag	UNP P76387
N	728	PHE	-	expression tag	UNP P76387
N	729	GLN	-	expression tag	UNP P76387
N	730	GLY	-	expression tag	UNP P76387
N	731	TRP	-	expression tag	UNP P76387
N	732	SER	-	expression tag	UNP P76387
N	733	HIS	-	expression tag	UNP P76387
N	734	PRO	-	expression tag	UNP P76387
N	735	GLN	-	expression tag	UNP P76387
N	736	PHE	-	expression tag	UNP P76387
N	737	GLU	-	expression tag	UNP P76387
N	738	LYS	-	expression tag	UNP P76387
O	540	MET	LYS	engineered mutation	UNP P76387
O	721	SER	-	expression tag	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
O	722	SER	-	expression tag	UNP P76387
O	723	GLY	-	expression tag	UNP P76387
O	724	GLU	-	expression tag	UNP P76387
O	725	ASN	-	expression tag	UNP P76387
O	726	LEU	-	expression tag	UNP P76387
O	727	TYR	-	expression tag	UNP P76387
O	728	PHE	-	expression tag	UNP P76387
O	729	GLN	-	expression tag	UNP P76387
O	730	GLY	-	expression tag	UNP P76387
O	731	TRP	-	expression tag	UNP P76387
O	732	SER	-	expression tag	UNP P76387
O	733	HIS	-	expression tag	UNP P76387
O	734	PRO	-	expression tag	UNP P76387
O	735	GLN	-	expression tag	UNP P76387
O	736	PHE	-	expression tag	UNP P76387
O	737	GLU	-	expression tag	UNP P76387
O	738	LYS	-	expression tag	UNP P76387
P	540	MET	LYS	engineered mutation	UNP P76387
P	721	SER	-	expression tag	UNP P76387
P	722	SER	-	expression tag	UNP P76387
P	723	GLY	-	expression tag	UNP P76387
P	724	GLU	-	expression tag	UNP P76387
P	725	ASN	-	expression tag	UNP P76387
P	726	LEU	-	expression tag	UNP P76387
P	727	TYR	-	expression tag	UNP P76387
P	728	PHE	-	expression tag	UNP P76387
P	729	GLN	-	expression tag	UNP P76387
P	730	GLY	-	expression tag	UNP P76387
P	731	TRP	-	expression tag	UNP P76387
P	732	SER	-	expression tag	UNP P76387
P	733	HIS	-	expression tag	UNP P76387
P	734	PRO	-	expression tag	UNP P76387
P	735	GLN	-	expression tag	UNP P76387
P	736	PHE	-	expression tag	UNP P76387
P	737	GLU	-	expression tag	UNP P76387
P	738	LYS	-	expression tag	UNP P76387

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



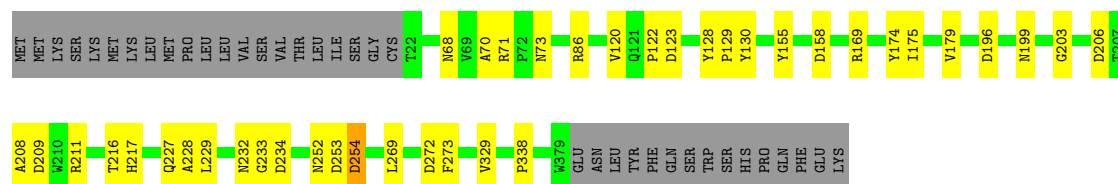
Mol	Chain	Residues	Atoms						AltConf
3	I	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	J	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	K	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	L	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	M	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	N	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	O	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	P	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

3 Residue-property plots

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

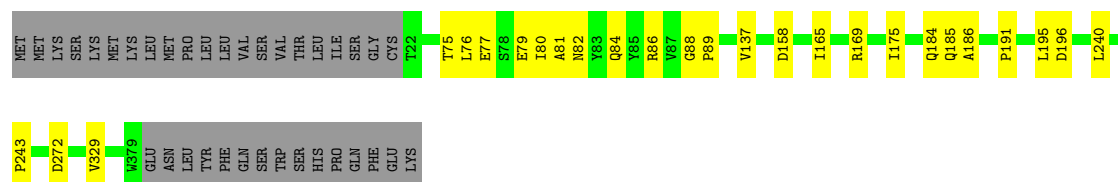
- Molecule 1: Putative polysaccharide export protein Wza

Chain A: 



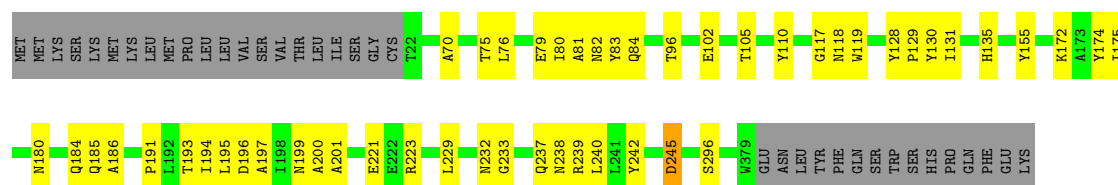
- Molecule 1: Putative polysaccharide export protein Wza

Chain B: 



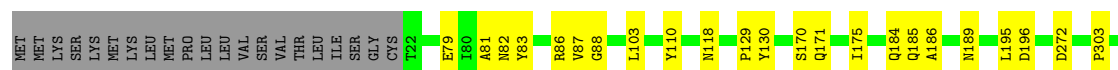
- Molecule 1: Putative polysaccharide export protein Wza

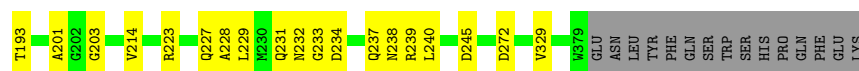
Chain C: 



- Molecule 1: Putative polysaccharide export protein Wza

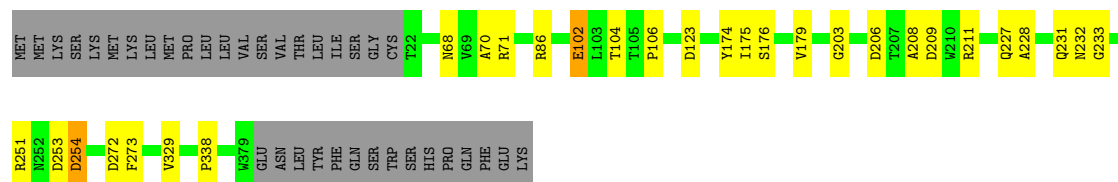
Chain D: 





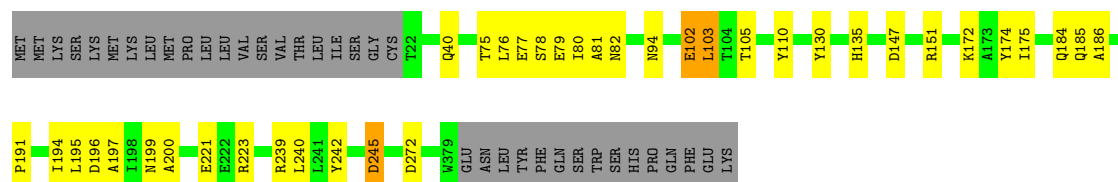
- Molecule 1: Putative polysaccharide export protein Wza

Chain b: 84% 7% 9%



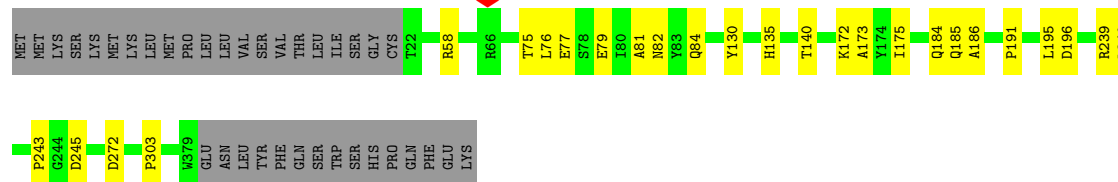
- Molecule 1: Putative polysaccharide export protein Wza

Chain c: 81% 9% 9%



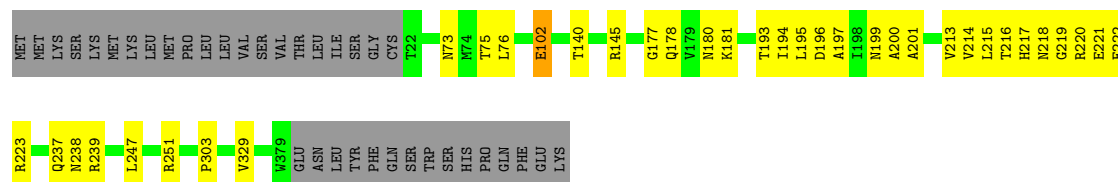
- Molecule 1: Putative polysaccharide export protein Wza

Chain d: 84% 7% 9%



- Molecule 1: Putative polysaccharide export protein Wza

Chain e: 82% 9% 9%

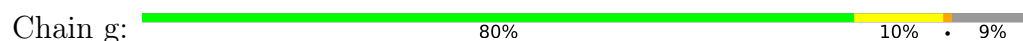


- Molecule 1: Putative polysaccharide export protein Wza

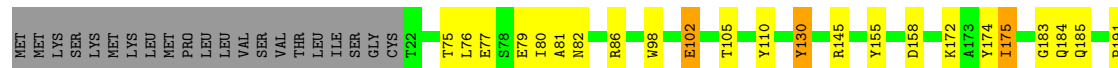
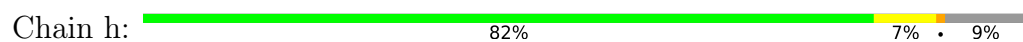
Chain f: 80% 11% 9%



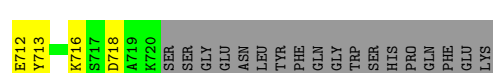
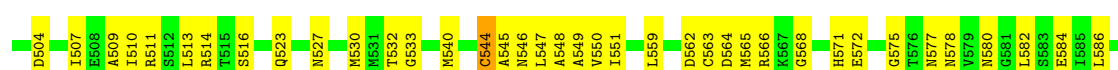
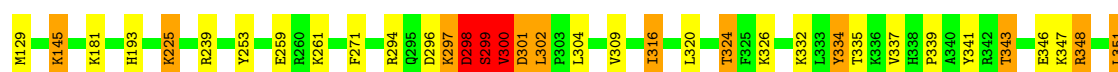
• Molecule 1: Putative polysaccharide export protein Wza



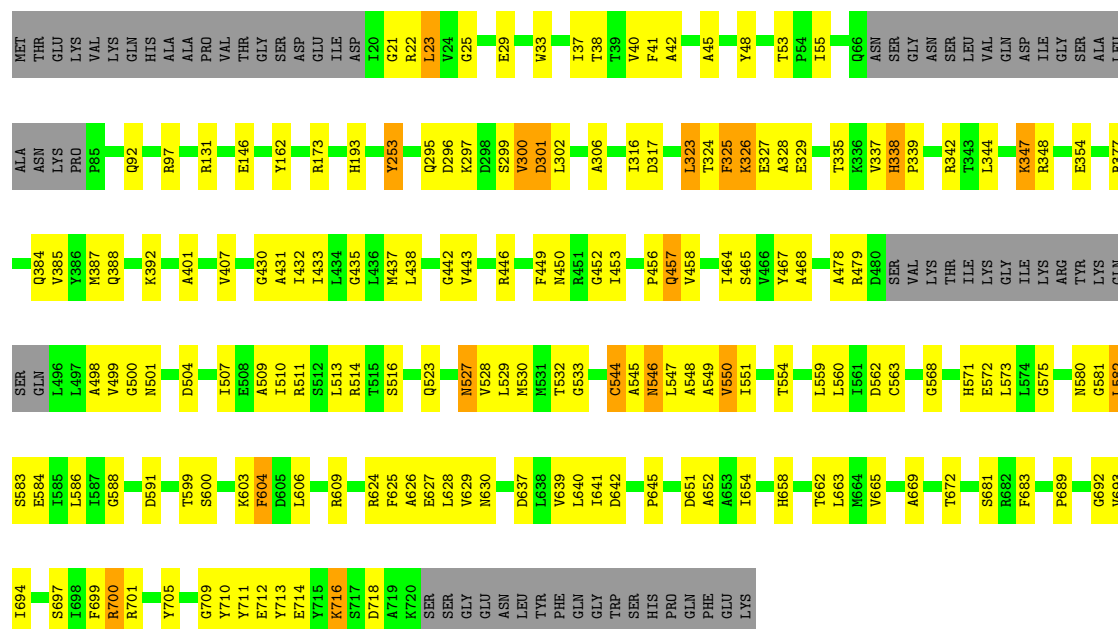
• Molecule 1: Putative polysaccharide export protein Wza



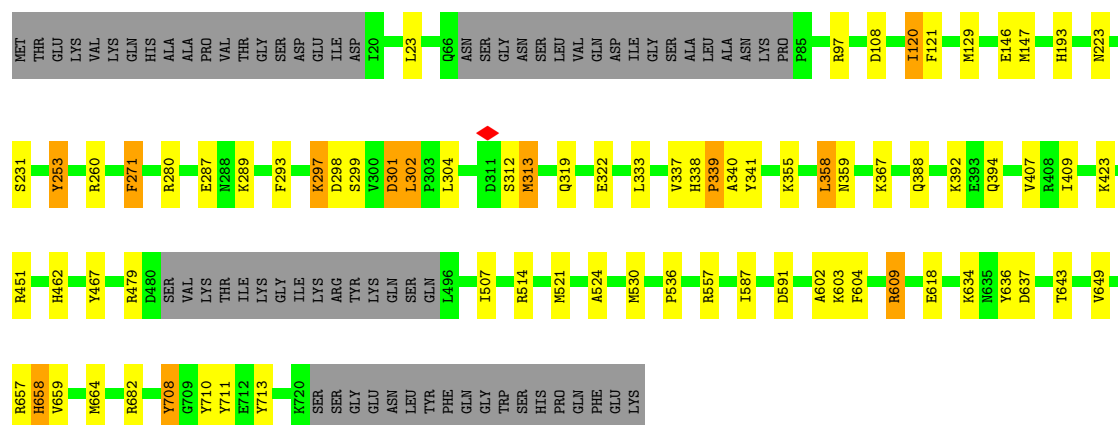
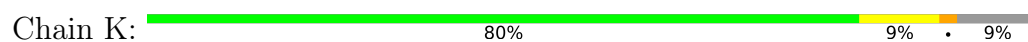
• Molecule 2: Tyrosine-protein kinase wzc



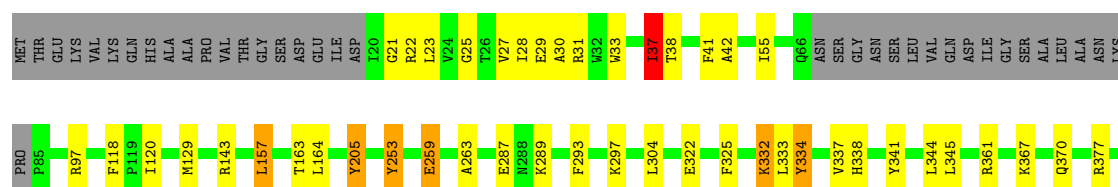
- Molecule 2: Tyrosine-protein kinase wzc

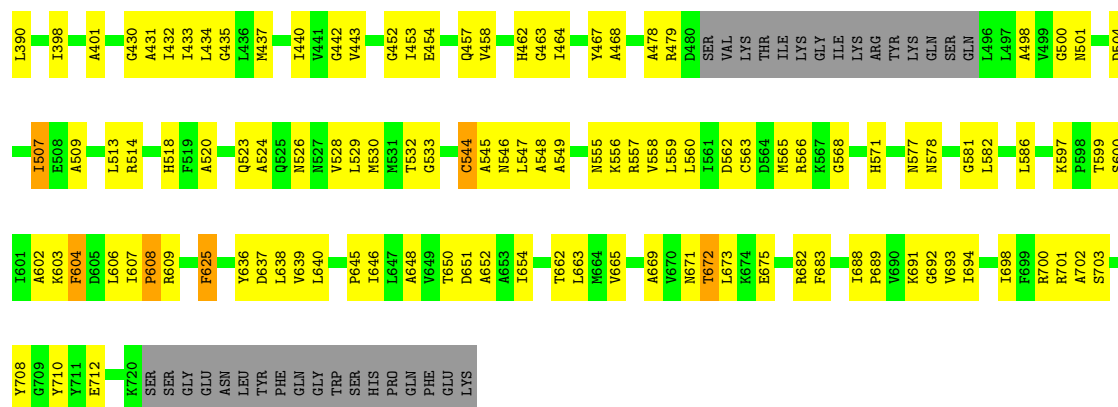


- Molecule 2: Tyrosine-protein kinase wzc



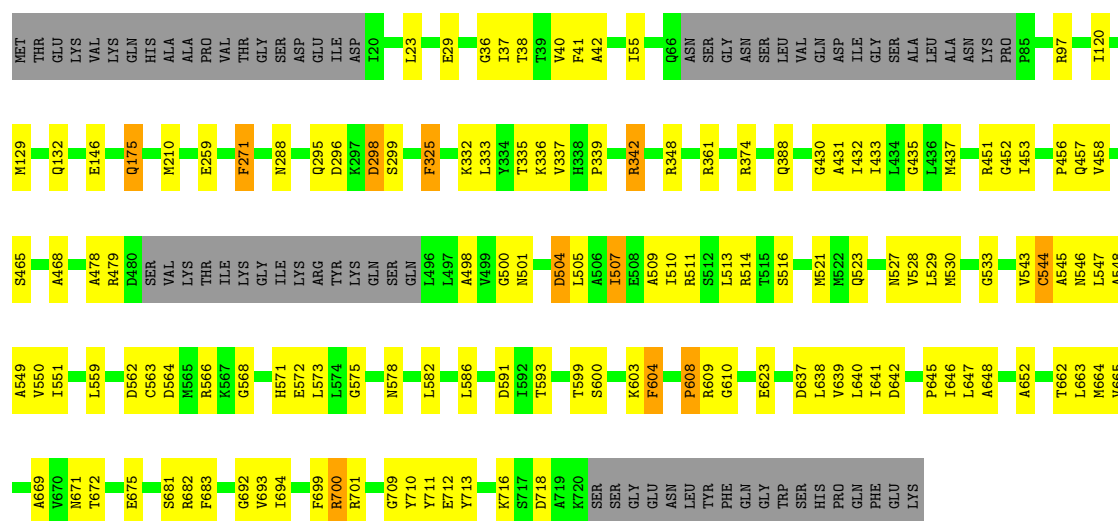
- Molecule 2: Tyrosine-protein kinase wzc





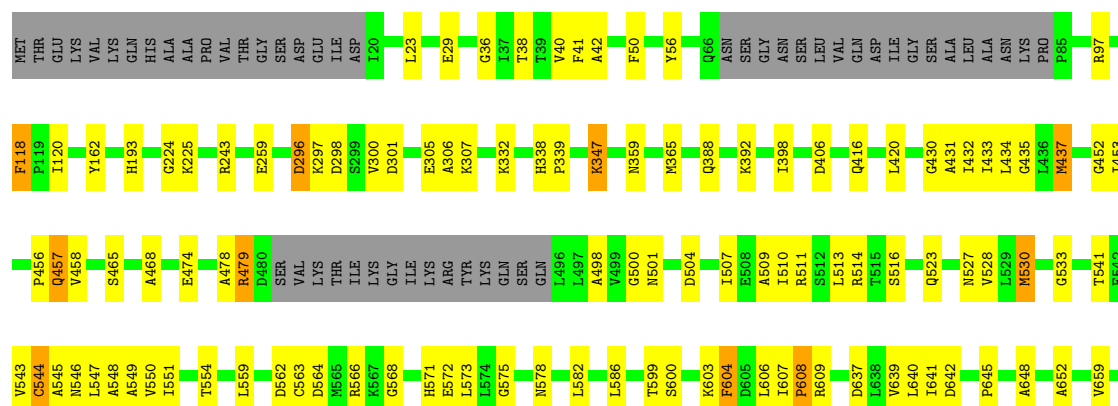
• Molecule 2: Tyrosine-protein kinase wzc

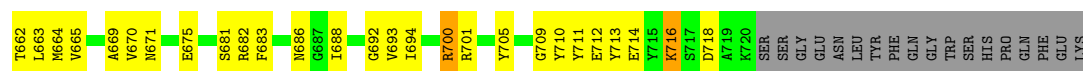
Chain M: 72% 17% 9%



• Molecule 2: Tyrosine-protein kinase wzc

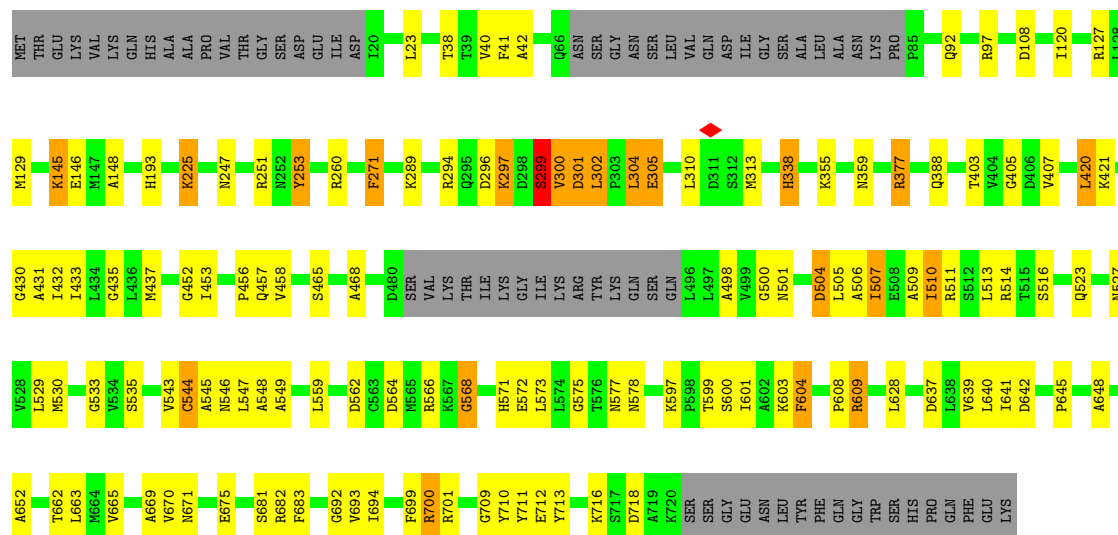
Chain N: 72% 17% 9%





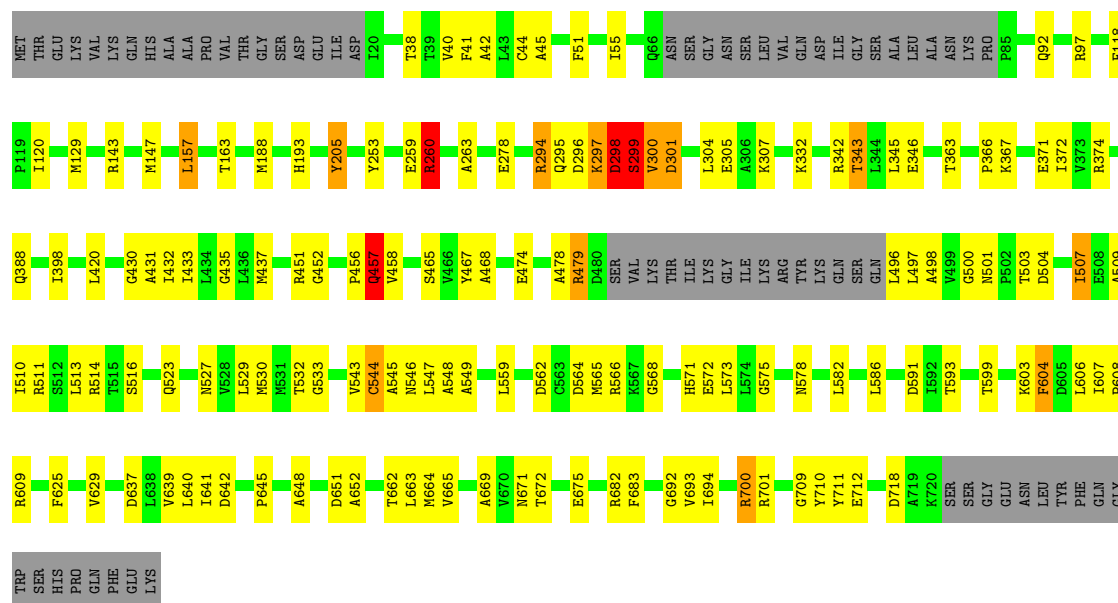
• Molecule 2: Tyrosine-protein kinase wzc

Chain O: 72% 15% 9%



• Molecule 2: Tyrosine-protein kinase wzc

Chain P: 71% 18% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	59128	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.222	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	546.0, 546.0, 546.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.91, 0.91, 0.91	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.12	12/2836 (0.4%)	1.36	27/3862 (0.7%)
1	B	0.98	9/2836 (0.3%)	1.14	23/3862 (0.6%)
1	C	1.09	10/2836 (0.4%)	1.26	40/3862 (1.0%)
1	D	0.85	5/2836 (0.2%)	1.07	18/3862 (0.5%)
1	E	0.88	6/2836 (0.2%)	1.10	26/3862 (0.7%)
1	F	1.06	13/2836 (0.5%)	1.22	35/3862 (0.9%)
1	G	0.93	11/2836 (0.4%)	1.09	22/3862 (0.6%)
1	H	1.26	25/2836 (0.9%)	1.40	48/3862 (1.2%)
1	a	1.21	12/2836 (0.4%)	1.36	46/3862 (1.2%)
1	b	1.04	16/2836 (0.6%)	1.26	25/3862 (0.6%)
1	c	0.91	7/2836 (0.2%)	1.13	36/3862 (0.9%)
1	d	0.87	5/2836 (0.2%)	1.08	26/3862 (0.7%)
1	e	1.23	24/2836 (0.8%)	1.34	52/3862 (1.3%)
1	f	1.19	21/2836 (0.7%)	1.34	45/3862 (1.2%)
1	g	1.14	21/2836 (0.7%)	1.34	40/3862 (1.0%)
1	h	0.88	6/2836 (0.2%)	1.12	30/3862 (0.8%)
2	I	1.42	47/5260 (0.9%)	1.65	146/7126 (2.0%)
2	J	1.59	52/5260 (1.0%)	1.83	194/7126 (2.7%)
2	K	0.71	0/5260	1.28	16/7126 (0.2%)
2	L	1.57	54/5260 (1.0%)	1.77	167/7126 (2.3%)
2	M	1.40	46/5260 (0.9%)	1.62	139/7126 (2.0%)
2	N	1.41	44/5260 (0.8%)	1.62	143/7126 (2.0%)
2	O	1.39	43/5260 (0.8%)	1.62	131/7126 (1.8%)
2	P	1.42	46/5260 (0.9%)	1.63	135/7126 (1.9%)
All	All	1.22	535/87456 (0.6%)	1.44	1610/118800 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	a	0	1
1	b	0	1
1	c	0	1
1	f	0	2
1	g	0	2
1	h	0	3
2	I	0	6
2	J	0	4
2	K	0	10
2	L	0	6
2	M	0	4
2	N	0	5
2	O	0	2
2	P	0	7
All	All	0	64

All (535) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	571	HIS	CE1-NE2	-8.87	1.23	1.32
1	f	217	HIS	ND1-CE1	-8.86	1.23	1.32
2	M	571	HIS	CE1-NE2	-8.83	1.23	1.32
1	g	217	HIS	ND1-CE1	-8.81	1.23	1.32
2	P	571	HIS	CE1-NE2	-8.79	1.23	1.32
2	L	571	HIS	CE1-NE2	-8.74	1.23	1.32
2	J	571	HIS	CE1-NE2	-8.74	1.23	1.32
2	N	571	HIS	CE1-NE2	-8.72	1.23	1.32
2	J	658	HIS	CE1-NE2	-8.71	1.23	1.32
2	I	571	HIS	CE1-NE2	-8.71	1.23	1.32
2	L	462	HIS	ND1-CE1	-8.69	1.23	1.32
1	e	217	HIS	ND1-CE1	-8.68	1.23	1.32
1	H	217	HIS	ND1-CE1	-8.68	1.23	1.32
1	a	239	ARG	CZ-NH2	-8.54	1.22	1.33
1	b	251	ARG	CZ-NH2	-8.51	1.22	1.33
1	b	211	ARG	CZ-NH2	-8.50	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	251	ARG	CZ-NH2	-8.50	1.22	1.33
1	g	251	ARG	CZ-NH2	-8.49	1.22	1.33
1	g	66	ARG	CZ-NH2	-8.49	1.22	1.33
1	g	211	ARG	CZ-NH2	-8.49	1.22	1.33
1	g	223	ARG	CZ-NH2	-8.47	1.22	1.33
1	b	71	ARG	CZ-NH2	-8.46	1.22	1.33
1	e	239	ARG	CZ-NH2	-8.45	1.22	1.33
1	f	251	ARG	CZ-NH2	-8.45	1.22	1.33
1	B	86	ARG	CZ-NH2	-8.44	1.22	1.33
1	E	86	ARG	CZ-NH2	-8.42	1.22	1.33
2	M	609	ARG	CZ-NH2	-8.40	1.22	1.33
1	F	86	ARG	CZ-NH2	-8.40	1.22	1.33
1	e	220	ARG	CZ-NH2	-8.39	1.22	1.33
1	e	223	ARG	CZ-NH2	-8.38	1.22	1.33
1	g	220	ARG	CZ-NH2	-8.38	1.22	1.33
2	I	566	ARG	CZ-NH2	-8.36	1.22	1.33
1	f	223	ARG	CZ-NH2	-8.36	1.22	1.33
1	G	86	ARG	CZ-NH2	-8.34	1.22	1.33
1	A	211	ARG	CZ-NH2	-8.34	1.22	1.33
1	H	66	ARG	CZ-NH2	-8.32	1.22	1.33
1	H	251	ARG	CZ-NH2	-8.32	1.22	1.33
2	O	514	ARG	CZ-NH2	-8.30	1.22	1.33
2	O	609	ARG	CZ-NH2	-8.30	1.22	1.33
1	H	211	ARG	CZ-NH2	-8.29	1.22	1.33
2	P	566	ARG	CZ-NH2	-8.30	1.22	1.33
1	F	251	ARG	CZ-NH2	-8.29	1.22	1.33
1	f	71	ARG	CZ-NH2	-8.29	1.22	1.33
2	M	701	ARG	CZ-NH2	-8.28	1.22	1.33
1	f	220	ARG	CZ-NH2	-8.28	1.22	1.33
1	A	71	ARG	CZ-NH2	-8.27	1.22	1.33
2	P	514	ARG	CZ-NH2	-8.27	1.22	1.33
1	H	220	ARG	CZ-NH2	-8.26	1.22	1.33
2	N	479	ARG	CZ-NH2	-8.26	1.22	1.33
2	P	682	ARG	CZ-NH2	-8.25	1.22	1.33
2	I	511	ARG	CZ-NH2	-8.24	1.22	1.33
1	H	335	ARG	CZ-NH2	-8.24	1.22	1.33
2	L	566	ARG	CZ-NH2	-8.24	1.22	1.33
1	H	223	ARG	CZ-NH2	-8.24	1.22	1.33
2	I	700	ARG	CZ-NH2	-8.24	1.22	1.33
2	O	701	ARG	CZ-NH2	-8.24	1.22	1.33
2	N	566	ARG	CZ-NH2	-8.23	1.22	1.33
2	O	682	ARG	CZ-NH2	-8.22	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	701	ARG	CZ-NH2	-8.22	1.22	1.33
2	N	609	ARG	CZ-NH2	-8.22	1.22	1.33
2	P	479	ARG	CZ-NH2	-8.22	1.22	1.33
2	I	514	ARG	CZ-NH2	-8.22	1.22	1.33
2	M	514	ARG	CZ-NH2	-8.22	1.22	1.33
2	L	479	ARG	CZ-NH2	-8.21	1.22	1.33
2	M	566	ARG	CZ-NH2	-8.21	1.22	1.33
2	P	700	ARG	CZ-NH2	-8.21	1.22	1.33
2	M	682	ARG	CZ-NH2	-8.21	1.22	1.33
2	N	682	ARG	CZ-NH2	-8.21	1.22	1.33
2	N	514	ARG	CZ-NH2	-8.21	1.22	1.33
2	J	511	ARG	CZ-NH2	-8.20	1.22	1.33
2	P	701	ARG	CZ-NH2	-8.20	1.22	1.33
2	N	511	ARG	CZ-NH2	-8.19	1.22	1.33
2	N	700	ARG	CZ-NH2	-8.18	1.22	1.33
2	I	682	ARG	CZ-NH2	-8.18	1.22	1.33
2	M	700	ARG	CZ-NH2	-8.18	1.22	1.33
2	J	514	ARG	CZ-NH2	-8.17	1.22	1.33
2	M	511	ARG	CZ-NH2	-8.17	1.22	1.33
2	P	511	ARG	CZ-NH2	-8.17	1.22	1.33
2	N	701	ARG	CZ-NH2	-8.16	1.22	1.33
2	M	479	ARG	CZ-NH2	-8.16	1.22	1.33
2	O	566	ARG	CZ-NH2	-8.15	1.22	1.33
2	J	700	ARG	CZ-NH2	-8.15	1.22	1.33
2	I	609	ARG	CZ-NH2	-8.14	1.22	1.33
2	L	682	ARG	CZ-NH2	-8.14	1.22	1.33
2	P	609	ARG	CZ-NH2	-8.14	1.22	1.33
2	N	571	HIS	CD2-NE2	-8.14	1.28	1.37
2	O	571	HIS	CD2-NE2	-8.14	1.28	1.37
2	O	700	ARG	CZ-NH2	-8.13	1.22	1.33
2	I	479	ARG	CZ-NH2	-8.13	1.22	1.33
2	L	701	ARG	CZ-NH2	-8.13	1.22	1.33
2	J	624	ARG	CZ-NH2	-8.12	1.22	1.33
2	J	701	ARG	CZ-NH2	-8.12	1.22	1.33
2	L	571	HIS	CD2-NE2	-8.11	1.28	1.37
2	L	557	ARG	CZ-NH2	-8.11	1.23	1.33
2	L	609	ARG	CZ-NH2	-8.11	1.23	1.33
2	O	511	ARG	CZ-NH2	-8.10	1.23	1.33
2	J	571	HIS	CD2-NE2	-8.09	1.28	1.37
2	I	571	HIS	CD2-NE2	-8.07	1.28	1.37
2	L	31	ARG	CZ-NH2	-8.06	1.23	1.33
2	J	479	ARG	CZ-NH2	-8.04	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	658	HIS	CD2-NE2	-8.04	1.29	1.37
2	L	700	ARG	CZ-NH2	-8.02	1.23	1.33
2	J	22	ARG	CZ-NH2	-8.01	1.23	1.33
2	L	22	ARG	CZ-NH2	-8.00	1.23	1.33
2	P	571	HIS	CD2-NE2	-7.99	1.29	1.37
2	J	446	ARG	CZ-NH2	-7.97	1.23	1.33
2	M	571	HIS	CD2-NE2	-7.96	1.29	1.37
1	a	183	GLY	N-CA	-7.77	1.38	1.45
1	a	228	ALA	CA-CB	-7.50	1.41	1.53
2	P	452	GLY	N-CA	-7.50	1.37	1.45
2	N	568	GLY	N-CA	-7.50	1.37	1.45
2	P	568	GLY	N-CA	-7.46	1.37	1.45
2	O	568	GLY	N-CA	-7.39	1.38	1.45
1	b	228	ALA	CA-CB	-7.39	1.41	1.53
2	L	452	GLY	N-CA	-7.37	1.38	1.45
2	L	568	GLY	N-CA	-7.37	1.38	1.45
2	M	568	GLY	N-CA	-7.35	1.38	1.45
1	H	228	ALA	CA-CB	-7.33	1.42	1.53
1	h	197	ALA	CA-CB	-7.30	1.42	1.53
2	I	452	GLY	N-CA	-7.29	1.38	1.45
1	g	208	ALA	CA-CB	-7.29	1.41	1.53
2	I	568	GLY	N-CA	-7.25	1.38	1.45
1	C	197	ALA	CA-CB	-7.24	1.42	1.53
1	f	228	ALA	CA-CB	-7.23	1.42	1.53
1	e	197	ALA	CA-CB	-7.23	1.42	1.53
1	c	197	ALA	CA-CB	-7.20	1.42	1.53
1	G	142	ALA	CA-CB	-7.17	1.42	1.53
1	g	228	ALA	CA-CB	-7.17	1.42	1.53
1	B	81	ALA	CA-CB	-7.15	1.42	1.53
1	A	228	ALA	CA-CB	-7.15	1.42	1.53
2	M	548	ALA	CA-CB	-7.11	1.42	1.53
2	P	509	ALA	CA-CB	-7.11	1.42	1.53
2	O	509	ALA	CA-CB	-7.10	1.42	1.53
2	N	545	ALA	CA-CB	-7.09	1.42	1.53
1	C	81	ALA	CA-CB	-7.08	1.42	1.53
2	N	509	ALA	CA-CB	-7.07	1.42	1.53
2	J	549	ALA	CA-CB	-7.06	1.42	1.53
2	M	545	ALA	CA-CB	-7.06	1.42	1.53
2	O	548	ALA	CA-CB	-7.06	1.42	1.53
2	P	545	ALA	CA-CB	-7.05	1.42	1.53
2	M	549	ALA	CA-CB	-7.04	1.42	1.53
2	I	533	GLY	N-CA	-7.03	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	548	ALA	CA-CB	-7.03	1.42	1.53
1	f	208	ALA	CA-CB	-7.03	1.41	1.53
2	N	669	ALA	CA-CB	-7.02	1.43	1.53
2	M	533	GLY	N-CA	-7.02	1.38	1.45
1	H	208	ALA	CA-CB	-7.02	1.42	1.53
1	h	81	ALA	CA-CB	-7.01	1.42	1.53
1	A	208	ALA	CA-CB	-7.01	1.42	1.53
1	E	81	ALA	CA-CB	-7.01	1.42	1.53
2	N	533	GLY	N-CA	-7.00	1.38	1.45
2	I	545	ALA	CA-CB	-7.00	1.42	1.53
2	O	549	ALA	CA-CB	-7.00	1.42	1.53
2	J	548	ALA	CA-CB	-7.00	1.42	1.53
2	M	509	ALA	CA-CB	-7.00	1.42	1.53
2	P	548	ALA	CA-CB	-6.99	1.42	1.53
2	N	548	ALA	CA-CB	-6.99	1.42	1.53
2	I	509	ALA	CA-CB	-6.99	1.42	1.53
1	b	208	ALA	CA-CB	-6.98	1.41	1.53
2	L	533	GLY	N-CA	-6.98	1.38	1.45
2	O	545	ALA	CA-CB	-6.97	1.42	1.53
2	N	549	ALA	CA-CB	-6.96	1.42	1.53
2	P	549	ALA	CA-CB	-6.96	1.42	1.53
1	e	239	ARG	CZ-NH1	-6.95	1.23	1.32
2	I	549	ALA	CA-CB	-6.95	1.42	1.53
2	O	669	ALA	CA-CB	-6.95	1.43	1.53
1	b	70	ALA	CA-CB	-6.94	1.41	1.53
1	b	211	ARG	CZ-NH1	-6.93	1.23	1.32
2	L	30	ALA	CA-CB	-6.93	1.43	1.53
2	P	652	ALA	CA-CB	-6.93	1.42	1.53
1	f	251	ARG	CZ-NH1	-6.92	1.23	1.32
2	I	669	ALA	CA-CB	-6.91	1.43	1.53
2	L	652	ALA	CA-CB	-6.90	1.42	1.53
2	M	669	ALA	CA-CB	-6.90	1.43	1.53
2	P	669	ALA	CA-CB	-6.89	1.43	1.53
1	g	211	ARG	CZ-NH1	-6.89	1.23	1.32
1	g	251	ARG	CZ-NH1	-6.88	1.23	1.32
1	e	223	ARG	CZ-NH1	-6.88	1.23	1.32
1	g	223	ARG	CZ-NH1	-6.88	1.23	1.32
1	a	239	ARG	CZ-NH1	-6.87	1.23	1.32
2	J	545	ALA	CA-CB	-6.86	1.42	1.53
1	c	81	ALA	CA-CB	-6.86	1.42	1.53
2	L	509	ALA	CA-CB	-6.85	1.42	1.53
1	e	251	ARG	CZ-NH1	-6.84	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	86	ARG	CZ-NH1	-6.84	1.23	1.32
1	b	251	ARG	CZ-NH1	-6.84	1.23	1.32
1	b	71	ARG	CZ-NH1	-6.84	1.23	1.32
1	e	201	ALA	CA-CB	-6.83	1.42	1.53
2	L	520	ALA	CA-CB	-6.83	1.42	1.53
1	D	81	ALA	CA-CB	-6.83	1.42	1.53
2	J	669	ALA	CA-CB	-6.82	1.43	1.53
2	J	626	ALA	CA-CB	-6.82	1.42	1.53
1	d	81	ALA	CA-CB	-6.82	1.42	1.53
2	L	548	ALA	CA-CB	-6.82	1.42	1.53
2	L	545	ALA	CA-CB	-6.81	1.42	1.53
1	A	211	ARG	CZ-NH1	-6.81	1.23	1.32
1	a	70	ALA	CA-CB	-6.80	1.41	1.53
1	e	220	ARG	CZ-NH1	-6.80	1.23	1.32
1	g	220	ARG	CZ-NH1	-6.80	1.23	1.32
2	L	549	ALA	CA-CB	-6.79	1.42	1.53
1	g	66	ARG	CZ-NH1	-6.79	1.23	1.32
1	F	251	ARG	CZ-NH1	-6.79	1.23	1.32
1	E	86	ARG	CZ-NH1	-6.78	1.23	1.32
1	B	186	ALA	CA-CB	-6.78	1.42	1.53
1	d	186	ALA	CA-CB	-6.78	1.42	1.53
2	J	509	ALA	CA-CB	-6.78	1.42	1.53
2	L	609	ARG	CZ-NH1	-6.78	1.23	1.32
2	L	669	ALA	CA-CB	-6.77	1.43	1.53
1	F	186	ALA	CA-CB	-6.77	1.42	1.53
1	C	200	ALA	CA-CB	-6.77	1.42	1.53
1	F	86	ARG	CZ-NH1	-6.76	1.23	1.32
2	J	300	VAL	N-CA	6.76	1.54	1.46
1	f	220	ARG	CZ-NH1	-6.76	1.23	1.32
2	I	609	ARG	CZ-NH1	-6.76	1.23	1.32
1	f	70	ALA	CA-CB	-6.75	1.42	1.53
1	H	251	ARG	CZ-NH1	-6.75	1.23	1.32
1	f	223	ARG	CZ-NH1	-6.75	1.23	1.32
1	B	86	ARG	CZ-NH1	-6.74	1.23	1.32
1	H	211	ARG	CZ-NH1	-6.73	1.23	1.32
1	H	220	ARG	CZ-NH1	-6.73	1.23	1.32
1	H	335	ARG	CZ-NH1	-6.73	1.23	1.32
2	N	511	ARG	CZ-NH1	-6.73	1.23	1.32
1	e	200	ALA	CA-CB	-6.73	1.42	1.53
2	M	514	ARG	CZ-NH1	-6.72	1.23	1.32
2	N	648	ALA	CA-CB	-6.72	1.42	1.53
1	D	186	ALA	CA-CB	-6.72	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	514	ARG	CZ-NH1	-6.71	1.23	1.32
2	O	682	ARG	CZ-NH1	-6.71	1.23	1.32
2	O	701	ARG	CZ-NH1	-6.71	1.23	1.32
2	J	514	ARG	CZ-NH1	-6.71	1.23	1.32
2	N	514	ARG	CZ-NH1	-6.70	1.23	1.32
1	c	200	ALA	CA-CB	-6.70	1.42	1.53
1	H	223	ARG	CZ-NH1	-6.70	1.23	1.32
2	L	566	ARG	CZ-NH1	-6.70	1.23	1.32
2	O	566	ARG	CZ-NH1	-6.69	1.23	1.32
2	I	479	ARG	CZ-NH1	-6.69	1.23	1.32
2	O	514	ARG	CZ-NH1	-6.68	1.23	1.32
2	N	479	ARG	CZ-NH1	-6.68	1.23	1.32
2	N	682	ARG	CZ-NH1	-6.68	1.23	1.32
2	M	609	ARG	CZ-NH1	-6.67	1.23	1.32
1	H	66	ARG	CZ-NH1	-6.67	1.23	1.32
2	P	479	ARG	CZ-NH1	-6.67	1.23	1.32
2	P	609	ARG	CZ-NH1	-6.67	1.23	1.32
1	f	71	ARG	CZ-NH1	-6.67	1.23	1.32
2	M	652	ALA	CA-CB	-6.66	1.42	1.53
2	I	652	ALA	CA-CB	-6.66	1.42	1.53
2	N	701	ARG	CZ-NH1	-6.66	1.23	1.32
1	h	200	ALA	CA-CB	-6.66	1.42	1.53
2	L	648	ALA	CA-CB	-6.66	1.42	1.53
2	O	700	ARG	CZ-NH1	-6.65	1.23	1.32
2	N	566	ARG	CZ-NH1	-6.65	1.23	1.32
2	N	700	ARG	CZ-NH1	-6.65	1.23	1.32
2	M	566	ARG	CZ-NH1	-6.65	1.23	1.32
2	P	701	ARG	CZ-NH1	-6.65	1.23	1.32
1	A	71	ARG	CZ-NH1	-6.64	1.23	1.32
2	L	479	ARG	CZ-NH1	-6.64	1.23	1.32
2	P	566	ARG	CZ-NH1	-6.64	1.23	1.32
2	P	700	ARG	CZ-NH1	-6.64	1.23	1.32
2	M	511	ARG	CZ-NH1	-6.63	1.23	1.32
2	P	511	ARG	CZ-NH1	-6.63	1.23	1.32
2	J	511	ARG	CZ-NH1	-6.63	1.23	1.32
2	I	700	ARG	CZ-NH1	-6.63	1.23	1.32
2	M	682	ARG	CZ-NH1	-6.63	1.23	1.32
2	I	701	ARG	CZ-NH1	-6.62	1.23	1.32
2	I	566	ARG	CZ-NH1	-6.62	1.23	1.32
2	N	609	ARG	CZ-NH1	-6.62	1.23	1.32
1	a	201	ALA	CA-CB	-6.62	1.42	1.53
2	I	682	ARG	CZ-NH1	-6.61	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	498	ALA	CA-CB	-6.61	1.42	1.53
1	c	186	ALA	CA-CB	-6.61	1.42	1.53
1	A	70	ALA	CA-CB	-6.61	1.42	1.53
1	E	186	ALA	CA-CB	-6.61	1.42	1.53
2	L	682	ARG	CZ-NH1	-6.61	1.23	1.32
2	M	479	ARG	CZ-NH1	-6.61	1.23	1.32
2	O	533	GLY	N-CA	-6.61	1.38	1.45
2	O	498	ALA	CA-CB	-6.61	1.42	1.53
2	O	511	ARG	CZ-NH1	-6.61	1.23	1.32
1	C	201	ALA	CA-CB	-6.59	1.42	1.53
2	O	652	ALA	CA-CB	-6.59	1.42	1.53
2	P	682	ARG	CZ-NH1	-6.59	1.23	1.32
2	I	511	ARG	CZ-NH1	-6.59	1.23	1.32
2	P	648	ALA	CA-CB	-6.59	1.42	1.53
2	M	701	ARG	CZ-NH1	-6.59	1.23	1.32
2	O	648	ALA	CA-CB	-6.58	1.42	1.53
2	O	609	ARG	CZ-NH1	-6.58	1.23	1.32
2	M	700	ARG	CZ-NH1	-6.58	1.23	1.32
2	J	700	ARG	CZ-NH1	-6.57	1.23	1.32
2	P	468	ALA	CA-CB	-6.57	1.42	1.53
2	P	514	ARG	CZ-NH1	-6.57	1.23	1.32
2	N	652	ALA	CA-CB	-6.56	1.42	1.53
1	G	186	ALA	CA-CB	-6.55	1.42	1.53
1	C	186	ALA	CA-CB	-6.54	1.42	1.53
2	I	648	ALA	CA-CB	-6.53	1.42	1.53
2	J	446	ARG	CZ-NH1	-6.53	1.23	1.32
2	J	479	ARG	CZ-NH1	-6.53	1.23	1.32
2	N	498	ALA	CA-CB	-6.53	1.42	1.53
2	I	498	ALA	CA-CB	-6.52	1.42	1.53
2	J	22	ARG	CZ-NH1	-6.52	1.23	1.32
2	L	524	ALA	CA-CB	-6.52	1.42	1.53
2	M	648	ALA	CA-CB	-6.51	1.42	1.53
2	L	557	ARG	CZ-NH1	-6.50	1.23	1.32
2	J	533	GLY	N-CA	-6.50	1.38	1.45
2	L	700	ARG	CZ-NH1	-6.50	1.23	1.32
2	O	452	GLY	N-CA	-6.50	1.37	1.45
2	L	22	ARG	CZ-NH1	-6.50	1.23	1.32
1	C	70	ALA	CA-CB	-6.50	1.42	1.53
2	L	31	ARG	CZ-NH1	-6.50	1.23	1.32
2	J	498	ALA	CA-CB	-6.49	1.42	1.53
2	J	701	ARG	CZ-NH1	-6.49	1.23	1.32
2	I	478	ALA	CA-CB	-6.47	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	701	ARG	CZ-NH1	-6.47	1.23	1.32
2	L	478	ALA	CA-CB	-6.44	1.42	1.53
2	J	624	ARG	CZ-NH1	-6.43	1.23	1.32
2	N	452	GLY	N-CA	-6.43	1.37	1.45
2	P	533	GLY	N-CA	-6.40	1.38	1.45
2	P	498	ALA	CA-CB	-6.40	1.42	1.53
2	L	602	ALA	CA-CB	-6.39	1.42	1.53
2	J	652	ALA	CA-CB	-6.37	1.42	1.53
2	L	468	ALA	CA-CB	-6.37	1.43	1.53
2	O	468	ALA	CA-CB	-6.35	1.42	1.53
2	N	468	ALA	CA-CB	-6.33	1.42	1.53
2	J	500	GLY	N-CA	-6.33	1.38	1.45
2	L	498	ALA	CA-CB	-6.33	1.43	1.53
2	M	500	GLY	N-CA	-6.30	1.38	1.45
2	O	500	GLY	N-CA	-6.29	1.38	1.45
2	M	468	ALA	CA-CB	-6.28	1.43	1.53
2	M	478	ALA	CA-CB	-6.24	1.42	1.53
2	N	500	GLY	N-CA	-6.24	1.38	1.45
2	I	500	GLY	N-CA	-6.23	1.38	1.45
2	L	435	GLY	N-CA	-6.22	1.38	1.45
2	N	478	ALA	CA-CB	-6.22	1.42	1.53
2	J	478	ALA	CA-CB	-6.21	1.43	1.53
2	J	435	GLY	N-CA	-6.21	1.38	1.45
2	I	435	GLY	N-CA	-6.19	1.38	1.45
1	D	189	ASN	C-N	-6.17	1.28	1.33
2	P	500	GLY	N-CA	-6.17	1.38	1.45
2	O	435	GLY	N-CA	-6.16	1.38	1.45
2	P	435	GLY	N-CA	-6.16	1.38	1.45
2	L	500	GLY	N-CA	-6.15	1.38	1.45
1	G	189	ASN	C-N	-6.14	1.28	1.33
2	N	435	GLY	N-CA	-6.14	1.38	1.45
2	M	435	GLY	N-CA	-6.13	1.38	1.45
2	P	478	ALA	CA-CB	-6.12	1.42	1.53
2	J	468	ALA	CA-CB	-6.08	1.43	1.53
2	J	581	GLY	N-CA	-6.05	1.37	1.45
2	J	442	GLY	N-CA	-6.02	1.38	1.45
2	L	25	GLY	N-CA	-5.96	1.38	1.45
2	P	430	GLY	N-CA	-5.95	1.38	1.45
2	L	702	ALA	CA-CB	-5.92	1.43	1.53
2	J	430	GLY	N-CA	-5.91	1.38	1.45
1	H	67	PRO	CA-CB	-5.91	1.46	1.53
2	O	430	GLY	N-CA	-5.89	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	430	GLY	N-CA	-5.83	1.38	1.45
2	M	42	ALA	CA-CB	-5.72	1.44	1.53
1	f	233	GLY	N-CA	-5.72	1.37	1.45
2	I	42	ALA	CA-CB	-5.71	1.44	1.53
2	N	42	ALA	CA-CB	-5.71	1.44	1.53
2	J	431	ALA	CA-CB	-5.71	1.44	1.53
2	L	431	ALA	CA-CB	-5.70	1.44	1.53
2	I	431	ALA	CA-CB	-5.70	1.44	1.53
2	J	452	GLY	N-CA	-5.70	1.37	1.45
2	J	42	ALA	CA-CB	-5.70	1.44	1.53
2	J	689	PRO	CA-CB	-5.68	1.46	1.53
2	M	430	GLY	N-CA	-5.68	1.38	1.45
2	M	431	ALA	CA-CB	-5.67	1.44	1.53
2	O	431	ALA	CA-CB	-5.67	1.44	1.53
2	P	45	ALA	CA-CB	-5.67	1.44	1.53
1	E	86	ARG	CD-NE	-5.67	1.38	1.46
1	G	86	ARG	CD-NE	-5.67	1.38	1.46
2	N	431	ALA	CA-CB	-5.67	1.44	1.53
2	J	45	ALA	CA-CB	-5.66	1.44	1.53
2	O	535	SER	CA-CB	-5.66	1.47	1.53
2	L	692	GLY	N-CA	-5.66	1.38	1.45
2	P	431	ALA	CA-CB	-5.66	1.44	1.53
2	L	42	ALA	CA-CB	-5.66	1.44	1.53
2	P	42	ALA	CA-CB	-5.66	1.44	1.53
1	b	233	GLY	N-CA	-5.65	1.37	1.45
1	F	86	ARG	CD-NE	-5.65	1.38	1.46
2	O	42	ALA	CA-CB	-5.65	1.44	1.53
2	I	45	ALA	CA-CB	-5.63	1.44	1.53
1	B	86	ARG	CD-NE	-5.63	1.38	1.46
1	a	239	ARG	CD-NE	-5.60	1.38	1.46
1	g	223	ARG	CD-NE	-5.58	1.38	1.46
1	e	223	ARG	CD-NE	-5.58	1.38	1.46
1	C	233	GLY	N-CA	-5.55	1.37	1.45
2	O	682	ARG	CD-NE	-5.53	1.38	1.46
1	e	239	ARG	CD-NE	-5.52	1.38	1.46
2	P	682	ARG	CD-NE	-5.52	1.38	1.46
1	A	233	GLY	N-CA	-5.49	1.37	1.45
1	a	233	GLY	N-CA	-5.49	1.37	1.45
2	M	682	ARG	CD-NE	-5.49	1.38	1.46
2	J	568	GLY	N-CA	-5.48	1.38	1.45
1	H	335	ARG	CD-NE	-5.48	1.38	1.46
2	I	682	ARG	CD-NE	-5.48	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	624	ARG	CD-NE	-5.47	1.38	1.46
1	g	66	ARG	CD-NE	-5.47	1.38	1.46
2	L	22	ARG	CD-NE	-5.46	1.38	1.46
2	I	468	ALA	CA-CB	-5.46	1.42	1.53
2	L	31	ARG	CD-NE	-5.46	1.38	1.46
2	L	479	ARG	CD-NE	-5.45	1.38	1.46
1	f	177	GLY	N-CA	-5.43	1.37	1.45
2	I	300	VAL	CA-C	-5.43	1.45	1.52
2	J	22	ARG	CD-NE	-5.42	1.38	1.46
1	F	177	GLY	N-CA	-5.42	1.37	1.45
1	f	223	ARG	CD-NE	-5.42	1.38	1.46
2	P	511	ARG	CD-NE	-5.42	1.38	1.46
1	H	211	ARG	CD-NE	-5.41	1.38	1.46
1	b	211	ARG	CD-NE	-5.41	1.38	1.46
1	g	211	ARG	CD-NE	-5.40	1.38	1.46
2	L	682	ARG	CD-NE	-5.40	1.38	1.46
2	I	479	ARG	CD-NE	-5.40	1.38	1.46
2	M	452	GLY	N-CA	-5.39	1.37	1.45
1	H	177	GLY	N-CA	-5.39	1.37	1.45
1	b	71	ARG	CD-NE	-5.39	1.38	1.46
2	J	479	ARG	CD-NE	-5.38	1.38	1.46
1	e	251	ARG	CD-NE	-5.38	1.38	1.46
1	f	220	ARG	CD-NE	-5.37	1.38	1.46
1	H	66	ARG	CD-NE	-5.37	1.38	1.46
1	g	251	ARG	CD-NE	-5.37	1.38	1.46
2	O	701	ARG	CD-NE	-5.36	1.38	1.46
2	N	682	ARG	CD-NE	-5.36	1.38	1.46
1	g	220	ARG	CD-NE	-5.36	1.38	1.46
2	J	446	ARG	CD-NE	-5.35	1.38	1.46
2	J	700	ARG	CD-NE	-5.35	1.38	1.46
1	H	220	ARG	CD-NE	-5.34	1.38	1.46
1	C	174	TYR	CA-CB	-5.34	1.45	1.53
2	N	479	ARG	CD-NE	-5.34	1.38	1.46
2	I	700	ARG	CD-NE	-5.33	1.38	1.46
1	G	124	GLY	N-CA	-5.33	1.37	1.45
1	e	177	GLY	N-CA	-5.33	1.37	1.45
1	B	243	PRO	CA-CB	-5.32	1.46	1.53
2	M	514	ARG	CD-NE	-5.32	1.38	1.46
2	N	514	ARG	CD-NE	-5.32	1.38	1.46
1	B	89	PRO	CA-CB	-5.31	1.46	1.53
2	I	566	ARG	CD-NE	-5.31	1.38	1.46
2	L	21	GLY	N-CA	-5.31	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	88	GLY	N-CA	-5.30	1.37	1.44
1	e	220	ARG	CD-NE	-5.30	1.38	1.46
1	A	211	ARG	CD-NE	-5.30	1.38	1.46
2	L	701	ARG	CD-NE	-5.30	1.38	1.46
2	J	511	ARG	CD-NE	-5.29	1.38	1.46
1	c	174	TYR	CA-CB	-5.29	1.45	1.53
2	L	566	ARG	CD-NE	-5.29	1.38	1.46
1	H	219	GLY	N-CA	-5.28	1.37	1.45
2	M	610	GLY	N-CA	-5.28	1.37	1.45
2	I	701	ARG	CD-NE	-5.28	1.38	1.46
1	b	338	PRO	CA-CB	-5.28	1.46	1.53
1	h	243	PRO	CA-CB	-5.28	1.46	1.53
1	H	251	ARG	CD-NE	-5.28	1.38	1.46
2	L	557	ARG	CD-NE	-5.28	1.38	1.46
2	P	566	ARG	CD-NE	-5.27	1.38	1.46
2	M	479	ARG	CD-NE	-5.27	1.38	1.46
2	M	566	ARG	CD-NE	-5.27	1.38	1.46
2	I	511	ARG	CD-NE	-5.26	1.38	1.46
1	f	219	GLY	N-CA	-5.26	1.37	1.45
1	b	251	ARG	CD-NE	-5.26	1.38	1.46
1	F	243	PRO	CA-CB	-5.26	1.46	1.53
2	M	700	ARG	CD-NE	-5.25	1.38	1.46
2	N	511	ARG	CD-NE	-5.25	1.38	1.46
2	O	514	ARG	CD-NE	-5.25	1.38	1.46
1	A	71	ARG	CD-NE	-5.25	1.38	1.46
1	H	223	ARG	CD-NE	-5.25	1.38	1.46
2	P	701	ARG	CD-NE	-5.25	1.39	1.46
2	M	701	ARG	CD-NE	-5.24	1.39	1.46
2	P	700	ARG	CD-NE	-5.24	1.39	1.46
2	I	514	ARG	CD-NE	-5.24	1.39	1.46
1	F	251	ARG	CD-NE	-5.24	1.39	1.46
2	J	514	ARG	CD-NE	-5.24	1.39	1.46
2	O	566	ARG	CD-NE	-5.24	1.39	1.46
1	d	243	PRO	CA-CB	-5.24	1.46	1.53
1	e	219	GLY	N-CA	-5.24	1.37	1.45
1	B	88	GLY	N-CA	-5.23	1.37	1.44
2	P	514	ARG	CD-NE	-5.23	1.39	1.46
2	O	511	ARG	CD-NE	-5.23	1.39	1.46
1	f	251	ARG	CD-NE	-5.22	1.39	1.46
2	N	700	ARG	CD-NE	-5.22	1.39	1.46
1	g	219	GLY	N-CA	-5.22	1.37	1.45
2	L	700	ARG	CD-NE	-5.22	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	PRO	CA-CB	-5.21	1.46	1.53
2	N	701	ARG	CD-NE	-5.21	1.39	1.46
2	P	479	ARG	CD-NE	-5.21	1.39	1.46
2	I	645	PRO	CA-CB	-5.21	1.46	1.53
2	J	701	ARG	CD-NE	-5.21	1.39	1.46
2	N	566	ARG	CD-NE	-5.21	1.39	1.46
1	G	191	PRO	CA-CB	-5.20	1.47	1.53
2	N	609	ARG	CD-NE	-5.20	1.39	1.46
1	F	219	GLY	N-CA	-5.18	1.37	1.45
2	O	700	ARG	CD-NE	-5.18	1.39	1.46
2	M	609	ARG	CD-NE	-5.18	1.39	1.46
1	E	191	PRO	CA-CB	-5.17	1.47	1.53
1	G	88	GLY	N-CA	-5.17	1.37	1.44
2	M	511	ARG	CD-NE	-5.17	1.39	1.46
2	O	609	ARG	CD-NE	-5.17	1.39	1.46
1	h	191	PRO	CA-CB	-5.16	1.46	1.53
2	P	609	ARG	CD-NE	-5.15	1.39	1.46
2	I	575	GLY	N-CA	-5.14	1.38	1.45
1	H	275	GLY	N-CA	-5.11	1.38	1.45
1	f	178	GLN	CD-NE2	-5.11	1.22	1.33
1	B	191	PRO	CA-CB	-5.10	1.46	1.53
1	G	90	GLY	N-CA	-5.09	1.37	1.45
1	e	199	ASN	CG-ND2	-5.09	1.22	1.33
1	e	178	GLN	CD-NE2	-5.08	1.22	1.33
1	a	178	GLN	CD-NE2	-5.07	1.22	1.33
1	G	171	GLN	CD-NE2	-5.07	1.22	1.33
2	P	575	GLY	N-CA	-5.06	1.38	1.45
1	f	231	GLN	CD-NE2	-5.05	1.22	1.33
1	a	180	ASN	CG-ND2	-5.05	1.22	1.33
2	O	575	GLY	N-CA	-5.04	1.38	1.45
1	g	67	PRO	CA-CB	-5.04	1.46	1.53
1	C	238	ASN	CG-ND2	-5.04	1.22	1.33
1	g	227	GLN	CD-NE2	-5.04	1.22	1.33
1	a	231	GLN	CD-NE2	-5.04	1.22	1.33
1	e	238	ASN	CG-ND2	-5.04	1.22	1.33
2	O	300	VAL	N-CA	5.04	1.52	1.46
1	c	191	PRO	CA-CB	-5.04	1.47	1.53
2	N	575	GLY	N-CA	-5.03	1.38	1.45
1	h	184	GLN	CD-NE2	-5.03	1.22	1.33
1	A	199	ASN	CG-ND2	-5.03	1.22	1.33
1	e	237	GLN	CD-NE2	-5.03	1.22	1.33
1	C	191	PRO	CA-CB	-5.02	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	71	ARG	CD-NE	-5.02	1.39	1.46
1	D	171	GLN	CD-NE2	-5.02	1.22	1.33
1	b	227	GLN	CD-NE2	-5.02	1.22	1.33
1	F	178	GLN	CD-NE2	-5.02	1.22	1.33
2	M	575	GLY	N-CA	-5.02	1.38	1.45
1	e	180	ASN	CG-ND2	-5.02	1.22	1.33
1	F	191	PRO	CA-CB	-5.01	1.47	1.53
2	J	575	GLY	N-CA	-5.01	1.38	1.45
1	a	237	GLN	CD-NE2	-5.01	1.22	1.33
1	F	185	GLN	CD-NE2	-5.00	1.22	1.33
1	c	199	ASN	CG-ND2	-5.00	1.22	1.33
1	d	191	PRO	CA-CB	-5.00	1.47	1.53
1	b	231	GLN	CD-NE2	-5.00	1.22	1.33
1	d	173	ALA	CA-CB	-5.00	1.42	1.53
1	e	178	GLN	CA-CB	-5.00	1.46	1.52

All (1610) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	317	ASP	CA-CB-CG	10.40	123.00	112.60
1	G	189	ASN	CA-C-N	9.48	131.58	123.33
1	G	189	ASN	C-N-CA	9.48	131.58	123.33
2	L	608	PRO	CA-N-CD	-9.45	98.77	112.00
1	D	189	ASN	CA-C-N	9.44	131.54	123.33
1	D	189	ASN	C-N-CA	9.44	131.54	123.33
2	I	608	PRO	CA-N-CD	-9.27	99.02	112.00
2	O	301	ASP	CA-C-N	9.22	136.09	121.62
2	O	301	ASP	C-N-CA	9.22	136.09	121.62
2	I	532	THR	CA-C-N	9.15	128.66	121.61
2	I	532	THR	C-N-CA	9.15	128.66	121.61
2	K	339	PRO	CA-N-CD	-8.65	99.89	112.00
2	L	500	GLY	CA-C-N	8.50	129.76	122.28
2	L	500	GLY	C-N-CA	8.50	129.76	122.28
2	N	500	GLY	CA-C-N	8.20	129.50	122.28
2	N	500	GLY	C-N-CA	8.20	129.50	122.28
2	L	325	PHE	CA-CB-CG	8.18	121.98	113.80
2	M	500	GLY	CA-C-N	8.14	129.44	122.28
2	M	500	GLY	C-N-CA	8.14	129.44	122.28
2	O	500	GLY	CA-C-N	8.13	129.43	122.28
2	O	500	GLY	C-N-CA	8.13	129.43	122.28
2	I	500	GLY	CA-C-N	8.13	129.43	122.28
2	I	500	GLY	C-N-CA	8.13	129.43	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	218	ASN	CA-CB-CG	7.88	120.48	112.60
2	J	325	PHE	CA-C-O	7.80	129.46	120.96
1	g	218	ASN	CA-CB-CG	7.80	120.40	112.60
1	h	183	GLY	N-CA-C	7.79	120.35	110.38
1	f	218	ASN	CA-CB-CG	7.76	120.36	112.60
2	L	532	THR	CA-C-N	7.75	128.82	121.46
2	L	532	THR	C-N-CA	7.75	128.82	121.46
2	J	326	LYS	CA-C-N	7.74	136.32	121.54
2	J	326	LYS	C-N-CA	7.74	136.32	121.54
2	P	301	ASP	CB-CA-C	7.70	123.25	109.38
2	O	296	ASP	CA-C-O	7.69	129.08	121.00
1	F	218	ASN	CA-CB-CG	7.69	120.29	112.60
1	H	218	ASN	CA-CB-CG	7.63	120.23	112.60
1	F	183	GLY	N-CA-C	7.62	120.14	110.38
2	K	658	HIS	CB-CG-CD2	-7.58	121.35	131.20
1	a	238	ASN	CA-CB-CG	7.54	120.14	112.60
1	b	273	PHE	CA-CB-CG	7.52	121.32	113.80
1	f	273	PHE	CA-CB-CG	7.52	121.32	113.80
1	e	238	ASN	CA-CB-CG	7.50	120.10	112.60
1	C	238	ASN	CA-CB-CG	7.50	120.09	112.60
1	D	196	ASP	CA-CB-CG	7.45	120.05	112.60
2	J	604	PHE	CA-CB-CG	7.44	121.24	113.80
2	J	580	ASN	CA-CB-CG	7.40	120.00	112.60
1	d	196	ASP	CA-CB-CG	7.40	120.00	112.60
1	g	273	PHE	CA-CB-CG	7.39	121.19	113.80
1	e	196	ASP	CA-CB-CG	7.38	119.98	112.60
1	B	196	ASP	CA-CB-CG	7.36	119.96	112.60
2	L	683	PHE	CA-CB-CG	7.35	121.15	113.80
2	N	604	PHE	CA-CB-CG	7.35	121.15	113.80
1	E	196	ASP	CA-CB-CG	7.35	119.95	112.60
2	M	604	PHE	CA-CB-CG	7.35	121.15	113.80
1	A	273	PHE	CA-CB-CG	7.32	121.12	113.80
2	O	604	PHE	CA-CB-CG	7.32	121.11	113.80
1	a	245	ASP	CA-CB-CG	7.31	119.91	112.60
2	O	683	PHE	CA-CB-CG	7.31	121.11	113.80
1	g	236	ASN	CA-CB-CG	7.29	119.89	112.60
2	N	683	PHE	CA-CB-CG	7.29	121.09	113.80
1	a	180	ASN	CA-CB-CG	7.28	119.88	112.60
2	J	532	THR	CA-C-N	7.28	128.85	121.35
2	J	532	THR	C-N-CA	7.28	128.85	121.35
2	I	604	PHE	CA-CB-CG	7.28	121.08	113.80
2	P	683	PHE	CA-CB-CG	7.28	121.08	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	296	ASP	CA-C-O	7.27	128.39	120.90
2	P	604	PHE	CA-CB-CG	7.27	121.07	113.80
2	I	324	THR	CA-CB-CG2	7.26	122.85	110.50
1	F	180	ASN	CA-CB-CG	7.26	119.86	112.60
1	g	206	ASP	CA-CB-CG	7.25	119.86	112.60
1	c	196	ASP	CA-CB-CG	7.25	119.85	112.60
2	P	532	THR	CA-C-N	7.25	128.82	121.35
2	P	532	THR	C-N-CA	7.25	128.82	121.35
2	J	683	PHE	CA-CB-CG	7.24	121.04	113.80
1	e	180	ASN	CA-CB-CG	7.24	119.84	112.60
2	L	430	GLY	CA-C-N	7.23	129.84	120.44
2	L	430	GLY	C-N-CA	7.23	129.84	120.44
1	h	196	ASP	CA-CB-CG	7.23	119.83	112.60
2	N	504	ASP	CA-CB-CG	7.22	119.82	112.60
2	N	338	HIS	CA-C-N	7.22	128.86	119.84
2	N	338	HIS	C-N-CA	7.22	128.86	119.84
2	M	683	PHE	CA-CB-CG	7.21	121.01	113.80
1	A	206	ASP	CA-CB-CG	7.20	119.80	112.60
2	L	604	PHE	CA-CB-CG	7.19	120.99	113.80
1	C	196	ASP	CA-CB-CG	7.19	119.79	112.60
1	b	206	ASP	CA-CB-CG	7.18	119.78	112.60
1	d	245	ASP	CA-CB-CG	7.15	119.75	112.60
1	F	196	ASP	CA-CB-CG	7.13	119.73	112.60
2	I	504	ASP	CA-CB-CG	7.13	119.73	112.60
1	H	206	ASP	CA-CB-CG	7.13	119.73	112.60
1	f	206	ASP	CA-CB-CG	7.12	119.72	112.60
1	G	91	ASP	CA-CB-CG	7.11	119.71	112.60
2	K	302	LEU	N-CA-C	7.10	125.51	109.81
1	C	180	ASN	CA-CB-CG	7.10	119.70	112.60
1	c	245	ASP	CA-CB-CG	7.08	119.68	112.60
1	E	245	ASP	CA-CB-CG	7.08	119.68	112.60
1	b	68	ASN	CA-CB-CG	7.08	119.68	112.60
1	e	199	ASN	CA-CB-CG	7.08	119.68	112.60
1	h	245	ASP	CA-CB-CG	7.08	119.68	112.60
1	C	245	ASP	CA-CB-CG	7.07	119.67	112.60
1	G	196	ASP	CA-CB-CG	7.07	119.67	112.60
1	F	245	ASP	CA-CB-CG	7.06	119.66	112.60
1	H	245	ASP	CA-CB-CG	7.06	119.66	112.60
2	P	504	ASP	CA-CB-CG	7.06	119.66	112.60
2	N	546	ASN	CA-CB-CG	7.05	119.65	112.60
1	e	73	ASN	CA-CB-CG	7.05	119.65	112.60
1	c	199	ASN	CA-CB-CG	7.05	119.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	253	ASP	CA-CB-CG	7.04	119.64	112.60
2	J	504	ASP	CA-CB-CG	7.03	119.63	112.60
2	J	630	ASN	CA-CB-CG	7.03	119.62	112.60
2	P	718	ASP	CA-CB-CG	7.00	119.60	112.60
2	J	301	ASP	CA-C-N	6.99	138.86	121.80
2	J	301	ASP	C-N-CA	6.99	138.86	121.80
2	M	504	ASP	CA-CB-CG	6.99	119.59	112.60
2	I	718	ASP	CA-CB-CG	6.99	119.59	112.60
1	C	199	ASN	CA-CB-CG	6.98	119.58	112.60
1	E	189	ASN	CA-C-N	6.97	129.40	123.33
1	E	189	ASN	C-N-CA	6.97	129.40	123.33
2	P	546	ASN	CA-CB-CG	6.97	119.57	112.60
2	O	299	SER	CA-C-N	6.97	132.05	120.62
2	O	299	SER	C-N-CA	6.97	132.05	120.62
2	O	504	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	199	ASN	CA-CB-CG	6.96	119.56	112.60
2	L	625	PHE	CA-CB-CG	6.96	120.76	113.80
1	A	253	ASP	CA-CB-CG	6.95	119.55	112.60
2	M	546	ASN	CA-CB-CG	6.95	119.55	112.60
2	J	625	PHE	CA-CB-CG	6.94	120.74	113.80
2	J	546	ASN	CA-CB-CG	6.94	119.54	112.60
1	f	223	ARG	CA-C-N	6.93	132.04	123.10
1	f	223	ARG	C-N-CA	6.93	132.04	123.10
2	M	41	PHE	CA-CB-CG	6.93	120.73	113.80
2	O	718	ASP	CA-CB-CG	6.92	119.52	112.60
2	I	546	ASN	CA-CB-CG	6.92	119.52	112.60
2	L	546	ASN	CA-CB-CG	6.91	119.51	112.60
1	b	253	ASP	CA-CB-CG	6.91	119.51	112.60
1	H	236	ASN	CA-CB-CG	6.91	119.51	112.60
2	L	578	ASN	CA-CB-CG	6.90	119.50	112.60
2	O	546	ASN	CA-CB-CG	6.90	119.50	112.60
1	a	223	ARG	CA-C-N	6.89	131.99	123.10
1	a	223	ARG	C-N-CA	6.89	131.99	123.10
1	a	232	ASN	CA-CB-CG	6.89	119.49	112.60
2	L	41	PHE	CA-CB-CG	6.89	120.69	113.80
2	P	41	PHE	CA-CB-CG	6.89	120.69	113.80
2	M	718	ASP	CA-CB-CG	6.89	119.49	112.60
2	J	645	PRO	CA-C-N	6.88	129.37	120.56
2	J	645	PRO	C-N-CA	6.88	129.37	120.56
2	L	504	ASP	CA-CB-CG	6.88	119.48	112.60
1	f	236	ASN	CA-CB-CG	6.86	119.46	112.60
2	N	718	ASP	CA-CB-CG	6.85	119.45	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	564	ASP	CA-CB-CG	6.85	119.45	112.60
2	O	564	ASP	CA-CB-CG	6.84	119.44	112.60
1	b	232	ASN	CA-CB-CG	6.84	119.44	112.60
2	J	718	ASP	CA-CB-CG	6.84	119.44	112.60
2	I	564	ASP	CA-CB-CG	6.84	119.44	112.60
1	c	82	ASN	CA-CB-CG	6.84	119.44	112.60
1	C	232	ASN	CA-CB-CG	6.83	119.43	112.60
1	C	82	ASN	CA-CB-CG	6.83	119.42	112.60
1	A	232	ASN	CA-CB-CG	6.82	119.42	112.60
2	P	562	ASP	CA-CB-CG	6.82	119.42	112.60
2	O	41	PHE	CA-CB-CG	6.80	120.61	113.80
2	N	564	ASP	CA-CB-CG	6.80	119.40	112.60
1	a	234	ASP	CA-CB-CG	6.80	119.40	112.60
1	a	183	GLY	N-CA-C	6.80	120.35	110.63
2	O	578	ASN	CA-CB-CG	6.80	119.40	112.60
2	P	642	ASP	CA-CB-CG	6.80	119.40	112.60
1	e	223	ARG	CA-C-N	6.80	131.87	123.10
1	e	223	ARG	C-N-CA	6.80	131.87	123.10
2	J	41	PHE	CA-CB-CG	6.79	120.59	113.80
1	f	232	ASN	CA-CB-CG	6.79	119.39	112.60
2	I	578	ASN	CA-CB-CG	6.79	119.39	112.60
2	I	642	ASP	CA-CB-CG	6.78	119.38	112.60
2	J	450	ASN	CA-CB-CG	6.77	119.37	112.60
1	A	234	ASP	CA-CB-CG	6.77	119.37	112.60
2	N	578	ASN	CA-CB-CG	6.77	119.37	112.60
2	I	41	PHE	CA-CB-CG	6.75	120.56	113.80
2	M	564	ASP	CA-CB-CG	6.75	119.36	112.60
2	J	562	ASP	CA-CB-CG	6.75	119.35	112.60
2	N	41	PHE	CA-CB-CG	6.75	120.55	113.80
2	K	271	PHE	CA-CB-CG	-6.75	107.05	113.80
2	N	562	ASP	CA-CB-CG	6.75	119.35	112.60
2	P	578	ASN	CA-CB-CG	6.75	119.34	112.60
1	H	234	ASP	CA-CB-CG	6.74	119.34	112.60
2	P	501	ASN	CA-CB-CG	6.74	119.34	112.60
2	O	501	ASN	CA-CB-CG	6.74	119.34	112.60
2	L	609	ARG	CD-NE-CZ	6.74	133.83	124.40
1	f	234	ASP	CA-CB-CG	6.74	119.34	112.60
2	I	501	ASN	CA-CB-CG	6.72	119.33	112.60
2	N	430	GLY	CA-C-N	6.72	129.62	120.54
2	N	430	GLY	C-N-CA	6.72	129.62	120.54
2	N	501	ASN	CA-CB-CG	6.72	119.33	112.60
2	M	578	ASN	CA-CB-CG	6.72	119.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	562	ASP	CA-CB-CG	6.72	119.32	112.60
2	M	562	ASP	CA-CB-CG	6.71	119.31	112.60
1	g	234	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	68	ASN	CA-CB-CG	6.71	119.31	112.60
2	O	562	ASP	CA-CB-CG	6.70	119.30	112.60
2	M	642	ASP	CA-CB-CG	6.70	119.30	112.60
1	c	186	ALA	CA-C-N	6.70	130.74	122.37
1	c	186	ALA	C-N-CA	6.70	130.74	122.37
2	M	501	ASN	CA-CB-CG	6.69	119.29	112.60
2	N	642	ASP	CA-CB-CG	6.69	119.29	112.60
2	J	500	GLY	CA-C-N	6.68	129.83	122.74
2	J	500	GLY	C-N-CA	6.68	129.83	122.74
2	L	562	ASP	CA-CB-CG	6.68	119.28	112.60
2	O	642	ASP	CA-CB-CG	6.68	119.28	112.60
2	L	501	ASN	CA-CB-CG	6.68	119.28	112.60
2	N	498	ALA	CA-C-N	6.67	130.22	122.35
2	N	498	ALA	C-N-CA	6.67	130.22	122.35
2	P	298	ASP	CA-C-N	6.67	134.28	121.54
2	P	298	ASP	C-N-CA	6.67	134.28	121.54
1	B	82	ASN	CA-CB-CG	6.66	119.26	112.60
2	O	377	ARG	NE-CZ-NH2	6.66	125.20	119.20
2	I	296	ASP	CA-C-O	6.66	127.81	120.82
2	I	297	LYS	CB-CA-C	6.66	123.67	110.42
2	J	642	ASP	CA-CB-CG	6.65	119.25	112.60
1	C	186	ALA	CA-C-N	6.65	130.81	122.43
1	C	186	ALA	C-N-CA	6.65	130.81	122.43
2	K	514	ARG	NE-CZ-NH2	6.65	125.19	119.20
1	d	82	ASN	CA-CB-CG	6.64	119.24	112.60
2	J	501	ASN	CA-CB-CG	6.63	119.23	112.60
1	E	186	ALA	CA-C-N	6.63	130.78	122.43
1	E	186	ALA	C-N-CA	6.63	130.78	122.43
1	H	68	ASN	CA-CB-CG	6.62	119.22	112.60
2	O	294	ARG	NE-CZ-NH2	6.62	125.16	119.20
1	G	168	PHE	CA-CB-CG	6.61	120.41	113.80
2	P	651	ASP	CA-CB-CG	6.59	119.19	112.60
2	L	462	HIS	CA-CB-CG	6.58	120.38	113.80
1	E	82	ASN	CA-CB-CG	6.57	119.17	112.60
2	O	600	SER	CA-C-N	6.57	131.21	122.93
2	O	600	SER	C-N-CA	6.57	131.21	122.93
1	F	82	ASN	CA-CB-CG	6.57	119.17	112.60
1	h	82	ASN	CA-CB-CG	6.57	119.17	112.60
2	N	671	ASN	CA-CB-CG	6.56	119.16	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	671	ASN	CA-CB-CG	6.54	119.14	112.60
2	M	325	PHE	CA-CB-CG	6.54	120.34	113.80
1	D	82	ASN	CA-CB-CG	6.54	119.14	112.60
1	g	212	ASN	CA-CB-CG	6.53	119.13	112.60
2	I	609	ARG	CD-NE-CZ	6.47	133.46	124.40
1	g	209	ASP	CA-CB-CG	6.47	119.08	112.60
2	N	118	PHE	CA-CB-CG	6.47	120.27	113.80
2	L	637	ASP	CA-CB-CG	6.46	119.06	112.60
1	H	212	ASN	CA-CB-CG	6.45	119.05	112.60
1	D	87	VAL	CA-C-N	6.44	131.97	121.87
1	D	87	VAL	C-N-CA	6.44	131.97	121.87
2	P	300	VAL	CA-CB-CG2	6.43	121.34	110.40
2	I	651	ASP	CA-CB-CG	6.43	119.03	112.60
2	O	671	ASN	CA-CB-CG	6.43	119.03	112.60
1	b	209	ASP	CA-CB-CG	6.43	119.03	112.60
1	g	203	GLY	CA-C-N	6.43	133.23	122.87
1	g	203	GLY	C-N-CA	6.43	133.23	122.87
1	H	209	ASP	CA-CB-CG	6.43	119.03	112.60
2	L	671	ASN	CA-CB-CG	6.43	119.03	112.60
2	L	651	ASP	CA-CB-CG	6.42	119.02	112.60
1	H	217	HIS	CA-CB-CG	6.41	120.21	113.80
1	H	135	HIS	CA-CB-CG	-6.41	107.39	113.80
1	e	217	HIS	CA-CB-CG	6.40	120.20	113.80
1	f	209	ASP	CA-CB-CG	6.39	118.99	112.60
2	I	301	ASP	CA-C-O	6.38	127.50	120.80
2	O	300	VAL	CB-CA-C	-6.37	102.75	112.05
1	A	209	ASP	CA-CB-CG	6.37	118.97	112.60
2	I	671	ASN	CA-CB-CG	6.37	118.97	112.60
2	J	453	ILE	N-CA-CB	6.36	117.81	110.49
2	J	651	ASP	CA-CB-CG	6.36	118.96	112.60
1	g	217	HIS	CA-CB-CG	6.34	120.14	113.80
2	P	671	ASN	CA-CB-CG	6.34	118.94	112.60
2	J	296	ASP	CA-C-O	6.33	127.47	120.82
2	P	500	GLY	CA-C-N	6.30	129.42	122.74
2	P	500	GLY	C-N-CA	6.30	129.42	122.74
1	f	215	LEU	CA-C-N	6.30	131.03	122.84
1	f	215	LEU	C-N-CA	6.30	131.03	122.84
1	f	217	HIS	CA-CB-CG	6.27	120.07	113.80
2	N	609	ARG	CD-NE-CZ	6.27	133.18	124.40
2	O	609	ARG	CD-NE-CZ	6.26	133.17	124.40
2	M	609	ARG	CD-NE-CZ	6.25	133.15	124.40
2	J	514	ARG	CD-NE-CZ	6.25	133.15	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	658	HIS	CA-CB-CG	6.22	120.02	113.80
1	c	147	ASP	CA-CB-CG	6.22	118.82	112.60
2	I	514	ARG	CD-NE-CZ	6.21	133.10	124.40
1	a	174	TYR	CA-C-N	6.20	130.64	122.95
1	a	174	TYR	C-N-CA	6.20	130.64	122.95
2	N	693	VAL	CA-C-N	6.20	130.83	122.90
2	N	693	VAL	C-N-CA	6.20	130.83	122.90
1	g	68	ASN	CA-CB-CG	6.20	118.80	112.60
1	d	186	ALA	CA-C-N	6.19	130.23	122.43
1	d	186	ALA	C-N-CA	6.19	130.23	122.43
1	D	186	ALA	CA-C-N	6.19	130.22	122.43
1	D	186	ALA	C-N-CA	6.19	130.22	122.43
2	L	693	VAL	CA-C-N	6.18	130.81	122.90
2	L	693	VAL	C-N-CA	6.18	130.81	122.90
1	h	174	TYR	CA-C-N	6.17	130.60	122.95
1	h	174	TYR	C-N-CA	6.17	130.60	122.95
2	P	693	VAL	CA-C-N	6.17	130.80	122.90
2	P	693	VAL	C-N-CA	6.17	130.80	122.90
2	J	560	LEU	CA-C-N	6.17	130.80	122.90
2	J	560	LEU	C-N-CA	6.17	130.80	122.90
2	N	514	ARG	CD-NE-CZ	6.17	133.04	124.40
2	P	609	ARG	CD-NE-CZ	6.17	133.03	124.40
1	A	203	GLY	CA-C-N	6.17	131.87	122.93
1	A	203	GLY	C-N-CA	6.17	131.87	122.93
1	G	186	ALA	CA-C-N	6.17	130.20	122.43
1	G	186	ALA	C-N-CA	6.17	130.20	122.43
2	J	606	LEU	CA-C-N	6.16	131.97	123.28
2	J	606	LEU	C-N-CA	6.16	131.97	123.28
2	L	689	PRO	CA-C-N	6.15	131.12	123.12
2	L	689	PRO	C-N-CA	6.15	131.12	123.12
1	F	215	LEU	CA-C-N	6.14	130.94	122.77
1	F	215	LEU	C-N-CA	6.14	130.94	122.77
2	M	514	ARG	CD-NE-CZ	6.14	133.00	124.40
2	P	694	ILE	CA-C-N	6.14	130.59	122.30
2	P	694	ILE	C-N-CA	6.14	130.59	122.30
1	F	174	TYR	CA-C-N	6.13	130.55	122.95
1	F	174	TYR	C-N-CA	6.13	130.55	122.95
2	O	514	ARG	CD-NE-CZ	6.13	132.98	124.40
2	J	689	PRO	CA-C-N	6.12	131.08	123.12
2	J	689	PRO	C-N-CA	6.12	131.08	123.12
2	J	693	VAL	CA-C-N	6.12	130.74	122.90
2	J	693	VAL	C-N-CA	6.12	130.74	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	694	ILE	CA-C-N	6.12	130.57	122.30
2	M	694	ILE	C-N-CA	6.12	130.57	122.30
2	J	694	ILE	CA-C-N	6.12	130.56	122.30
2	J	694	ILE	C-N-CA	6.12	130.56	122.30
2	O	693	VAL	CA-C-N	6.12	131.07	123.12
2	O	693	VAL	C-N-CA	6.12	131.07	123.12
1	g	220	ARG	CA-C-N	6.10	131.12	122.09
1	g	220	ARG	C-N-CA	6.10	131.12	122.09
2	M	701	ARG	CD-NE-CZ	6.10	132.94	124.40
2	P	514	ARG	CD-NE-CZ	6.10	132.94	124.40
2	O	694	ILE	CA-C-N	6.09	130.53	122.30
2	O	694	ILE	C-N-CA	6.09	130.53	122.30
1	B	186	ALA	CA-C-N	6.08	130.90	122.93
1	B	186	ALA	C-N-CA	6.08	130.90	122.93
2	J	701	ARG	CD-NE-CZ	6.08	132.91	124.40
2	J	527	ASN	CA-C-N	6.07	131.02	123.12
2	J	527	ASN	C-N-CA	6.07	131.02	123.12
2	L	638	LEU	CA-C-N	6.07	131.09	123.14
2	L	638	LEU	C-N-CA	6.07	131.09	123.14
1	G	100	HIS	CB-CG-CD2	-6.06	123.32	131.20
2	J	449	PHE	CA-CB-CG	6.06	119.86	113.80
2	N	700	ARG	CD-NE-CZ	6.05	132.88	124.40
2	N	701	ARG	CD-NE-CZ	6.05	132.88	124.40
2	P	701	ARG	CD-NE-CZ	6.05	132.88	124.40
1	b	251	ARG	CD-NE-CZ	6.05	132.88	124.40
2	J	654	ILE	CA-C-N	6.05	128.75	120.46
2	J	654	ILE	C-N-CA	6.05	128.75	120.46
2	J	700	ARG	CD-NE-CZ	6.05	132.87	124.40
1	a	115	ASP	CA-CB-CG	6.05	118.65	112.60
2	N	193	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	F	251	ARG	CD-NE-CZ	6.04	132.85	124.40
1	f	251	ARG	CD-NE-CZ	6.04	132.85	124.40
1	E	109	GLN	CA-C-N	6.03	128.97	120.28
1	E	109	GLN	C-N-CA	6.03	128.97	120.28
2	I	701	ARG	CD-NE-CZ	6.03	132.84	124.40
2	I	694	ILE	CA-C-N	6.02	130.43	122.30
2	I	694	ILE	C-N-CA	6.02	130.43	122.30
2	N	416	GLN	OE1-CD-NE2	-6.02	116.58	122.60
2	O	700	ARG	CD-NE-CZ	6.02	132.83	124.40
2	N	465	SER	CA-C-N	6.02	130.94	123.12
2	N	465	SER	C-N-CA	6.02	130.94	123.12
2	L	645	PRO	CA-C-N	6.01	128.13	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	645	PRO	C-N-CA	6.01	128.13	120.56
2	L	701	ARG	CD-NE-CZ	6.01	132.82	124.40
2	N	511	ARG	CD-NE-CZ	6.01	132.82	124.40
1	e	215	LEU	CA-C-N	6.01	130.76	122.77
1	e	215	LEU	C-N-CA	6.01	130.76	122.77
1	g	216	THR	CA-C-N	6.01	131.28	122.39
1	g	216	THR	C-N-CA	6.01	131.28	122.39
2	M	641	ILE	CA-C-N	6.01	131.01	122.72
2	M	641	ILE	C-N-CA	6.01	131.01	122.72
2	O	465	SER	CA-C-N	6.01	130.93	123.12
2	O	465	SER	C-N-CA	6.01	130.93	123.12
2	P	700	ARG	CD-NE-CZ	6.01	132.81	124.40
2	I	713	TYR	CA-C-N	6.00	131.45	122.99
2	I	713	TYR	C-N-CA	6.00	131.45	122.99
1	f	220	ARG	CA-C-N	6.00	131.00	122.72
1	f	220	ARG	C-N-CA	6.00	131.00	122.72
1	F	186	ALA	CA-C-N	6.00	130.79	122.93
1	F	186	ALA	C-N-CA	6.00	130.79	122.93
2	O	511	ARG	CD-NE-CZ	6.00	132.80	124.40
2	O	641	ILE	CA-C-N	6.00	131.00	122.72
2	O	641	ILE	C-N-CA	6.00	131.00	122.72
2	L	700	ARG	CD-NE-CZ	6.00	132.79	124.40
2	O	566	ARG	CD-NE-CZ	6.00	132.79	124.40
2	M	692	GLY	CA-C-N	5.99	131.27	122.94
2	M	692	GLY	C-N-CA	5.99	131.27	122.94
2	L	557	ARG	CD-NE-CZ	5.99	132.79	124.40
2	I	511	ARG	CD-NE-CZ	5.99	132.78	124.40
2	J	465	SER	CA-C-N	5.99	130.77	122.93
2	J	465	SER	C-N-CA	5.99	130.77	122.93
2	I	465	SER	CA-C-N	5.98	130.90	123.12
2	I	465	SER	C-N-CA	5.98	130.90	123.12
2	J	641	ILE	CA-C-N	5.98	130.97	122.72
2	J	641	ILE	C-N-CA	5.98	130.97	122.72
2	J	511	ARG	CD-NE-CZ	5.97	132.76	124.40
2	M	511	ARG	CD-NE-CZ	5.97	132.76	124.40
1	e	216	THR	CA-C-N	5.97	131.23	122.39
1	e	216	THR	C-N-CA	5.97	131.23	122.39
2	L	692	GLY	N-CA-C	5.97	119.21	110.80
2	J	709	GLY	CA-C-N	5.96	130.60	122.19
2	J	709	GLY	C-N-CA	5.96	130.60	122.19
2	M	465	SER	CA-C-N	5.96	130.87	123.12
2	M	465	SER	C-N-CA	5.96	130.87	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	259	GLU	CA-C-O	-5.96	114.56	120.82
2	O	701	ARG	CD-NE-CZ	5.96	132.75	124.40
1	g	251	ARG	CD-NE-CZ	5.96	132.74	124.40
2	I	640	LEU	CA-C-N	5.94	130.93	123.14
2	I	640	LEU	C-N-CA	5.94	130.93	123.14
2	L	560	LEU	CA-C-N	5.94	130.85	123.12
2	L	560	LEU	C-N-CA	5.94	130.85	123.12
2	L	692	GLY	CA-C-N	5.94	131.26	123.06
2	L	692	GLY	C-N-CA	5.94	131.26	123.06
1	F	191	PRO	CA-C-N	5.94	131.36	123.05
1	F	191	PRO	C-N-CA	5.94	131.36	123.05
2	L	640	LEU	CA-C-N	5.94	130.92	123.14
2	L	640	LEU	C-N-CA	5.94	130.92	123.14
2	P	709	GLY	CA-C-N	5.94	130.91	122.72
2	P	709	GLY	C-N-CA	5.94	130.91	122.72
2	M	709	GLY	CA-C-N	5.93	130.91	122.72
2	M	709	GLY	C-N-CA	5.93	130.91	122.72
2	I	298	ASP	CA-C-O	5.92	126.80	120.10
2	I	693	VAL	CA-C-N	5.92	130.82	123.12
2	I	693	VAL	C-N-CA	5.92	130.82	123.12
1	h	191	PRO	CA-C-N	5.92	131.34	123.05
1	h	191	PRO	C-N-CA	5.92	131.34	123.05
1	f	216	THR	CA-C-N	5.92	131.15	122.39
1	f	216	THR	C-N-CA	5.92	131.15	122.39
2	I	709	GLY	CA-C-N	5.92	130.53	122.19
2	I	709	GLY	C-N-CA	5.92	130.53	122.19
2	P	640	LEU	CA-C-N	5.92	130.89	123.14
2	P	640	LEU	C-N-CA	5.92	130.89	123.14
2	O	709	GLY	CA-C-N	5.91	130.88	122.72
2	O	709	GLY	C-N-CA	5.91	130.88	122.72
2	N	640	LEU	CA-C-N	5.90	130.87	123.14
2	N	640	LEU	C-N-CA	5.90	130.87	123.14
1	c	191	PRO	CA-C-N	5.90	131.15	123.00
1	c	191	PRO	C-N-CA	5.90	131.15	123.00
2	I	692	GLY	CA-C-N	5.90	131.14	122.94
2	I	692	GLY	C-N-CA	5.90	131.14	122.94
2	L	566	ARG	CD-NE-CZ	5.90	132.66	124.40
1	b	254	ASP	CA-CB-CG	5.89	118.49	112.60
2	K	193	HIS	CB-CG-CD2	-5.89	123.55	131.20
1	C	191	PRO	CA-C-N	5.88	131.12	123.00
1	C	191	PRO	C-N-CA	5.88	131.12	123.00
1	a	240	LEU	CA-C-N	5.88	129.90	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	240	LEU	C-N-CA	5.88	129.90	121.50
2	K	591	ASP	CA-CB-CG	-5.87	106.73	112.60
2	M	566	ARG	CD-NE-CZ	5.87	132.62	124.40
2	O	640	LEU	CA-C-N	5.87	130.83	123.14
2	O	640	LEU	C-N-CA	5.87	130.83	123.14
1	C	135	HIS	CA-CB-CG	-5.87	107.93	113.80
2	J	640	LEU	CA-C-N	5.86	130.82	123.14
2	J	640	LEU	C-N-CA	5.86	130.82	123.14
1	H	216	THR	CA-C-N	5.86	131.06	122.39
1	H	216	THR	C-N-CA	5.86	131.06	122.39
2	K	298	ASP	N-CA-CB	5.86	118.57	110.07
2	N	694	ILE	CA-C-N	5.86	130.56	122.77
2	N	694	ILE	C-N-CA	5.86	130.56	122.77
2	J	639	VAL	CA-C-N	5.85	131.08	123.00
2	J	639	VAL	C-N-CA	5.85	131.08	123.00
2	N	692	GLY	CA-C-N	5.85	131.08	122.94
2	N	692	GLY	C-N-CA	5.85	131.08	122.94
2	P	692	GLY	CA-C-N	5.85	131.07	122.94
2	P	692	GLY	C-N-CA	5.85	131.07	122.94
2	M	693	VAL	CA-C-N	5.85	130.72	123.12
2	M	693	VAL	C-N-CA	5.85	130.72	123.12
2	O	692	GLY	CA-C-N	5.85	131.13	123.06
2	O	692	GLY	C-N-CA	5.85	131.13	123.06
2	P	566	ARG	CD-NE-CZ	5.85	132.59	124.40
1	B	191	PRO	CA-C-N	5.84	131.23	123.05
1	B	191	PRO	C-N-CA	5.84	131.23	123.05
2	N	456	PRO	CA-C-N	5.84	128.38	120.38
2	N	456	PRO	C-N-CA	5.84	128.38	120.38
2	I	639	VAL	CA-C-N	5.84	131.06	123.00
2	I	639	VAL	C-N-CA	5.84	131.06	123.00
2	M	640	LEU	CA-C-N	5.84	130.79	123.14
2	M	640	LEU	C-N-CA	5.84	130.79	123.14
1	f	71	ARG	CD-NE-CZ	5.84	132.57	124.40
2	L	694	ILE	CA-C-N	5.83	130.53	122.77
2	L	694	ILE	C-N-CA	5.83	130.53	122.77
2	O	639	VAL	CA-C-N	5.83	131.04	123.00
2	O	639	VAL	C-N-CA	5.83	131.04	123.00
2	P	301	ASP	N-CA-C	-5.83	100.21	109.59
1	a	237	GLN	CA-C-N	5.83	129.75	121.42
1	a	237	GLN	C-N-CA	5.83	129.75	121.42
1	b	123	ASP	CA-CB-CG	5.83	118.43	112.60
2	I	540	MET	CA-C-N	5.83	128.34	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	540	MET	C-N-CA	5.83	128.34	120.65
2	I	566	ARG	CD-NE-CZ	5.83	132.56	124.40
2	J	692	GLY	CA-C-N	5.82	131.09	123.06
2	J	692	GLY	C-N-CA	5.82	131.09	123.06
2	J	468	ALA	CA-C-N	5.82	131.33	122.95
2	J	468	ALA	C-N-CA	5.82	131.33	122.95
2	N	641	ILE	CA-C-N	5.82	131.03	123.00
2	N	641	ILE	C-N-CA	5.82	131.03	123.00
2	P	645	PRO	CA-C-N	5.82	127.90	120.56
2	P	645	PRO	C-N-CA	5.82	127.90	120.56
2	N	566	ARG	CD-NE-CZ	5.82	132.55	124.40
2	P	641	ILE	CA-C-N	5.82	131.03	123.00
2	P	641	ILE	C-N-CA	5.82	131.03	123.00
2	M	713	TYR	CA-C-N	5.81	131.19	122.99
2	M	713	TYR	C-N-CA	5.81	131.19	122.99
2	I	645	PRO	CA-C-N	5.81	128.00	120.56
2	I	645	PRO	C-N-CA	5.81	128.00	120.56
2	J	299	SER	CA-C-N	5.81	132.43	121.97
2	J	299	SER	C-N-CA	5.81	132.43	121.97
2	J	713	TYR	CA-C-N	5.81	131.19	122.99
2	J	713	TYR	C-N-CA	5.81	131.19	122.99
2	I	348	ARG	NE-CZ-NH2	5.81	124.43	119.20
2	M	600	SER	CA-C-N	5.79	131.19	122.91
2	M	600	SER	C-N-CA	5.79	131.19	122.91
1	A	254	ASP	CA-CB-CG	5.79	118.39	112.60
2	P	51	PHE	CA-CB-CG	-5.79	108.01	113.80
1	f	223	ARG	CB-CG-CD	5.79	124.62	111.30
2	O	271	PHE	CA-CB-CG	-5.79	108.01	113.80
1	E	191	PRO	CA-C-N	5.79	131.15	123.05
1	E	191	PRO	C-N-CA	5.79	131.15	123.05
2	N	603	LYS	CA-C-N	5.79	130.83	122.44
2	N	603	LYS	C-N-CA	5.79	130.83	122.44
1	A	123	ASP	CA-CB-CG	5.78	118.38	112.60
1	F	178	GLN	CA-C-N	5.78	130.37	122.34
1	F	178	GLN	C-N-CA	5.78	130.37	122.34
2	P	468	ALA	CA-C-N	5.77	131.26	122.95
2	P	468	ALA	C-N-CA	5.77	131.26	122.95
2	M	342	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	F	181	LYS	CA-CB-CG	5.77	125.63	114.10
2	P	663	LEU	CA-C-N	5.75	130.94	123.00
2	P	663	LEU	C-N-CA	5.75	130.94	123.00
2	J	559	LEU	CA-C-N	5.75	130.42	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	559	LEU	C-N-CA	5.75	130.42	122.77
1	a	73	ASN	CA-C-N	5.75	127.99	120.28
1	a	73	ASN	C-N-CA	5.75	127.99	120.28
2	L	663	LEU	CA-C-N	5.75	130.94	123.00
2	L	663	LEU	C-N-CA	5.75	130.94	123.00
2	O	516	SER	CA-C-N	5.75	127.99	120.28
2	O	516	SER	C-N-CA	5.75	127.99	120.28
2	L	557	ARG	CA-C-N	5.75	130.99	123.06
2	L	557	ARG	C-N-CA	5.75	130.99	123.06
2	P	603	LYS	CA-C-N	5.75	131.02	122.86
2	P	603	LYS	C-N-CA	5.75	131.02	122.86
2	N	645	PRO	CA-C-N	5.75	127.80	120.56
2	N	645	PRO	C-N-CA	5.75	127.80	120.56
2	N	639	VAL	CA-C-N	5.74	131.09	122.99
2	N	639	VAL	C-N-CA	5.74	131.09	122.99
2	M	645	PRO	CA-C-N	5.74	127.79	120.56
2	M	645	PRO	C-N-CA	5.74	127.79	120.56
2	J	533	GLY	N-CA-C	5.74	119.51	110.96
2	J	516	SER	CA-C-N	5.74	127.97	120.28
2	J	516	SER	C-N-CA	5.74	127.97	120.28
2	O	543	VAL	N-CA-CB	5.74	117.26	110.55
1	h	240	LEU	CA-C-N	5.73	130.04	122.30
1	h	240	LEU	C-N-CA	5.73	130.04	122.30
2	J	600	SER	CA-C-N	5.73	131.11	122.91
2	J	600	SER	C-N-CA	5.73	131.11	122.91
2	P	465	SER	CA-C-N	5.73	130.90	123.11
2	P	465	SER	C-N-CA	5.73	130.90	123.11
1	d	240	LEU	CA-C-N	5.73	130.04	122.30
1	d	240	LEU	C-N-CA	5.73	130.04	122.30
2	N	663	LEU	CA-C-N	5.73	130.91	123.00
2	N	663	LEU	C-N-CA	5.73	130.91	123.00
1	c	240	LEU	CA-C-N	5.73	130.03	122.30
1	c	240	LEU	C-N-CA	5.73	130.03	122.30
2	L	558	VAL	CA-C-N	5.73	131.06	122.99
2	L	558	VAL	C-N-CA	5.73	131.06	122.99
2	P	533	GLY	CA-C-N	5.73	127.89	120.56
2	P	533	GLY	C-N-CA	5.73	127.89	120.56
1	b	176	SER	N-CA-C	5.72	116.10	108.38
2	J	581	GLY	CA-C-N	5.72	127.87	120.44
2	J	581	GLY	C-N-CA	5.72	127.87	120.44
2	L	600	SER	CA-C-N	5.71	131.08	122.91
2	L	600	SER	C-N-CA	5.71	131.08	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	254	ASP	CA-C-N	5.71	130.64	122.08
1	b	254	ASP	C-N-CA	5.71	130.64	122.08
2	L	361	ARG	NE-CZ-NH2	5.70	124.33	119.20
2	P	530	MET	CA-C-N	5.70	131.03	122.99
2	P	530	MET	C-N-CA	5.70	131.03	122.99
2	J	456	PRO	CA-C-N	5.70	128.19	120.38
2	J	456	PRO	C-N-CA	5.70	128.19	120.38
2	I	516	SER	CA-C-N	5.70	127.92	120.28
2	I	516	SER	C-N-CA	5.70	127.92	120.28
1	C	240	LEU	CA-C-N	5.70	129.99	122.30
1	C	240	LEU	C-N-CA	5.70	129.99	122.30
1	a	178	GLN	CA-C-N	5.70	130.26	122.34
1	a	178	GLN	C-N-CA	5.70	130.26	122.34
2	L	639	VAL	CA-C-N	5.69	131.01	122.99
2	L	639	VAL	C-N-CA	5.69	131.01	122.99
1	h	245	ASP	CA-C-N	5.69	130.52	123.12
1	h	245	ASP	C-N-CA	5.69	130.52	123.12
2	P	533	GLY	N-CA-C	5.69	119.44	110.96
2	M	603	LYS	CA-C-N	5.68	130.93	122.86
2	M	603	LYS	C-N-CA	5.68	130.93	122.86
2	P	639	VAL	CA-C-N	5.68	131.00	122.99
2	P	639	VAL	C-N-CA	5.68	131.00	122.99
2	P	516	SER	CA-C-N	5.68	127.89	120.28
2	P	516	SER	C-N-CA	5.68	127.89	120.28
2	L	581	GLY	CA-C-N	5.68	127.82	120.44
2	L	581	GLY	C-N-CA	5.68	127.82	120.44
2	I	663	LEU	CA-C-N	5.67	130.83	123.00
2	I	663	LEU	C-N-CA	5.67	130.83	123.00
1	F	240	LEU	CA-C-N	5.67	129.95	122.30
1	F	240	LEU	C-N-CA	5.67	129.95	122.30
2	I	456	PRO	CA-C-N	5.67	128.15	120.38
2	I	456	PRO	C-N-CA	5.67	128.15	120.38
2	K	609	ARG	NE-CZ-NH2	5.67	124.30	119.20
2	O	456	PRO	CA-C-N	5.67	128.15	120.38
2	O	456	PRO	C-N-CA	5.67	128.15	120.38
1	F	245	ASP	CA-C-N	5.66	130.48	123.12
1	F	245	ASP	C-N-CA	5.66	130.48	123.12
2	P	498	ALA	CA-C-N	5.66	130.03	121.65
2	P	498	ALA	C-N-CA	5.66	130.03	121.65
1	g	66	ARG	CB-CG-CD	5.66	124.32	111.30
2	M	700	ARG	CD-NE-CZ	5.66	132.32	124.40
2	N	600	SER	CA-C-N	5.66	131.00	122.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	600	SER	C-N-CA	5.66	131.00	122.91
2	I	377	ARG	NE-CZ-NH2	5.66	124.29	119.20
2	J	498	ALA	CA-C-N	5.66	130.02	121.65
2	J	498	ALA	C-N-CA	5.66	130.02	121.65
2	O	645	PRO	CA-C-N	5.66	127.80	120.56
2	O	645	PRO	C-N-CA	5.66	127.80	120.56
2	J	603	LYS	CA-C-N	5.65	131.09	122.95
2	J	603	LYS	C-N-CA	5.65	131.09	122.95
2	I	641	ILE	CA-C-N	5.65	130.96	123.05
2	I	641	ILE	C-N-CA	5.65	130.96	123.05
1	a	145	ARG	NE-CZ-NH2	5.65	124.28	119.20
2	N	709	GLY	CA-C-N	5.65	130.51	122.72
2	N	709	GLY	C-N-CA	5.65	130.51	122.72
1	A	254	ASP	CA-C-N	5.64	130.54	122.08
1	A	254	ASP	C-N-CA	5.64	130.54	122.08
1	B	240	LEU	CA-C-N	5.64	129.92	122.30
1	B	240	LEU	C-N-CA	5.64	129.92	122.30
2	I	700	ARG	CD-NE-CZ	5.64	132.30	124.40
2	O	713	TYR	CA-C-N	5.64	131.42	122.74
2	O	713	TYR	C-N-CA	5.64	131.42	122.74
2	O	603	LYS	CA-C-N	5.64	130.87	122.86
2	O	603	LYS	C-N-CA	5.64	130.87	122.86
2	O	663	LEU	CA-C-N	5.64	130.78	123.00
2	O	663	LEU	C-N-CA	5.64	130.78	123.00
2	M	516	SER	CA-C-N	5.63	127.83	120.28
2	M	516	SER	C-N-CA	5.63	127.83	120.28
2	L	533	GLY	N-CA-C	5.63	119.51	110.90
2	O	498	ALA	CA-C-N	5.63	129.98	121.65
2	O	498	ALA	C-N-CA	5.63	129.98	121.65
1	g	158	ASP	CA-CB-CG	5.63	118.23	112.60
2	J	325	PHE	N-CA-CB	5.62	118.20	109.48
2	O	544	CYS	CA-C-N	5.62	127.75	120.44
2	O	544	CYS	C-N-CA	5.62	127.75	120.44
1	e	220	ARG	CA-C-N	5.62	131.03	122.65
1	e	220	ARG	C-N-CA	5.62	131.03	122.65
2	N	530	MET	CA-C-N	5.62	130.92	122.99
2	N	530	MET	C-N-CA	5.62	130.92	122.99
2	I	193	HIS	CB-CG-CD2	-5.62	123.89	131.20
2	M	374	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	f	145	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	H	245	ASP	CA-C-N	5.61	130.42	123.12
1	H	245	ASP	C-N-CA	5.61	130.42	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	468	ALA	CA-C-N	5.61	131.26	123.07
2	O	468	ALA	C-N-CA	5.61	131.26	123.07
2	M	529	LEU	CA-C-N	5.61	131.06	122.93
2	M	529	LEU	C-N-CA	5.61	131.06	122.93
2	J	627	GLU	CA-C-N	5.61	127.73	120.44
2	J	627	GLU	C-N-CA	5.61	127.73	120.44
1	G	87	VAL	CA-C-N	5.60	130.67	121.87
1	G	87	VAL	C-N-CA	5.60	130.67	121.87
2	L	691	LYS	CA-C-N	5.60	128.51	120.56
2	L	691	LYS	C-N-CA	5.60	128.51	120.56
2	N	675	GLU	CA-C-N	5.60	127.61	120.56
2	N	675	GLU	C-N-CA	5.60	127.61	120.56
2	M	663	LEU	CA-C-N	5.60	130.72	123.00
2	M	663	LEU	C-N-CA	5.60	130.72	123.00
1	d	191	PRO	CA-C-N	5.60	131.24	123.07
1	d	191	PRO	C-N-CA	5.60	131.24	123.07
2	M	639	VAL	CA-C-N	5.59	130.88	122.99
2	M	639	VAL	C-N-CA	5.59	130.88	122.99
2	L	603	LYS	CA-C-N	5.59	130.80	122.86
2	L	603	LYS	C-N-CA	5.59	130.80	122.86
1	h	196	ASP	CA-C-N	5.59	127.71	120.44
1	h	196	ASP	C-N-CA	5.59	127.71	120.44
1	e	73	ASN	CA-C-N	5.59	127.77	120.28
1	e	73	ASN	C-N-CA	5.59	127.77	120.28
2	O	711	TYR	CA-C-N	5.59	131.32	122.60
2	O	711	TYR	C-N-CA	5.59	131.32	122.60
2	I	343	THR	CA-CB-CG2	5.59	120.00	110.50
1	e	237	GLN	CA-C-N	5.59	129.41	121.42
1	e	237	GLN	C-N-CA	5.59	129.41	121.42
1	a	172	LYS	CA-C-N	5.58	131.57	122.81
1	a	172	LYS	C-N-CA	5.58	131.57	122.81
1	e	196	ASP	CA-C-N	5.58	128.03	120.44
1	e	196	ASP	C-N-CA	5.58	128.03	120.44
2	L	533	GLY	CA-C-N	5.57	127.69	120.56
2	L	533	GLY	C-N-CA	5.57	127.69	120.56
2	P	193	HIS	CB-CG-CD2	-5.57	123.95	131.20
2	J	663	LEU	CA-C-N	5.57	130.69	123.00
2	J	663	LEU	C-N-CA	5.57	130.69	123.00
2	O	530	MET	CA-C-N	5.57	130.85	123.00
2	O	530	MET	C-N-CA	5.57	130.85	123.00
2	L	453	ILE	N-CA-CB	5.57	116.89	110.49
2	J	500	GLY	N-CA-C	5.57	118.95	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	675	GLU	CA-C-N	5.57	127.57	120.56
2	M	675	GLU	C-N-CA	5.57	127.57	120.56
2	L	21	GLY	CA-C-N	5.56	127.67	120.44
2	L	21	GLY	C-N-CA	5.56	127.67	120.44
1	A	196	ASP	CA-CB-CG	5.56	118.16	112.60
2	J	193	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	H	219	GLY	CA-C-N	5.56	130.67	123.00
1	H	219	GLY	C-N-CA	5.56	130.67	123.00
1	H	254	ASP	CA-C-N	5.56	130.42	122.08
1	H	254	ASP	C-N-CA	5.56	130.42	122.08
1	f	247	LEU	CA-C-N	5.56	130.83	123.05
1	f	247	LEU	C-N-CA	5.56	130.83	123.05
1	B	86	ARG	CB-CG-CD	5.55	124.07	111.30
2	L	27	VAL	CA-C-N	5.55	127.56	120.56
2	L	27	VAL	C-N-CA	5.55	127.56	120.56
2	L	332	LYS	N-CA-C	5.55	117.46	108.08
2	M	549	ALA	CA-C-N	5.55	128.07	120.46
2	M	549	ALA	C-N-CA	5.55	128.07	120.46
2	I	608	PRO	CA-C-N	5.55	127.72	120.28
2	I	608	PRO	C-N-CA	5.55	127.72	120.28
2	I	299	SER	CA-C-N	5.55	131.95	121.97
2	I	299	SER	C-N-CA	5.55	131.95	121.97
2	N	416	GLN	CB-CA-C	5.55	117.43	109.11
1	a	182	SER	CA-C-N	5.55	128.66	121.23
1	a	182	SER	C-N-CA	5.55	128.66	121.23
2	L	530	MET	CA-C-N	5.54	130.81	122.99
2	L	530	MET	C-N-CA	5.54	130.81	122.99
2	O	513	LEU	CA-C-N	5.54	127.65	120.44
2	O	513	LEU	C-N-CA	5.54	127.65	120.44
2	I	453	ILE	N-CA-CB	5.54	116.86	110.49
2	P	544	CYS	CA-C-N	5.54	127.64	120.44
2	P	544	CYS	C-N-CA	5.54	127.64	120.44
1	e	247	LEU	CA-C-N	5.54	130.81	123.05
1	e	247	LEU	C-N-CA	5.54	130.81	123.05
2	I	712	GLU	CA-CB-CG	5.54	125.18	114.10
1	H	223	ARG	CB-CG-CD	5.53	124.03	111.30
2	M	453	ILE	N-CA-CB	5.53	116.85	110.49
2	P	711	TYR	CA-C-N	5.53	131.23	122.60
2	P	711	TYR	C-N-CA	5.53	131.23	122.60
2	O	529	LEU	CA-C-N	5.53	130.95	122.93
2	O	529	LEU	C-N-CA	5.53	130.95	122.93
2	O	712	GLU	CA-CB-CG	5.53	125.16	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	194	ILE	CA-C-N	5.53	127.69	120.28
1	e	194	ILE	C-N-CA	5.53	127.69	120.28
1	G	86	ARG	CB-CG-CD	5.53	124.02	111.30
2	J	591	ASP	CA-C-N	5.53	127.52	120.56
2	J	591	ASP	C-N-CA	5.53	127.52	120.56
2	P	343	THR	CA-CB-OG1	5.53	117.89	109.60
2	O	675	GLU	CA-C-N	5.52	127.52	120.56
2	O	675	GLU	C-N-CA	5.52	127.52	120.56
2	N	453	ILE	N-CA-CB	5.52	116.84	110.49
2	N	712	GLU	CA-CB-CG	5.52	125.14	114.10
1	d	172	LYS	CA-C-N	5.52	131.48	122.81
1	d	172	LYS	C-N-CA	5.52	131.48	122.81
2	J	672	THR	CA-C-N	5.52	127.99	120.54
2	J	672	THR	C-N-CA	5.52	127.99	120.54
2	N	551	ILE	N-CA-CB	5.51	117.00	110.55
1	H	123	ASP	CA-CB-CG	5.51	118.11	112.60
2	I	603	LYS	CA-C-N	5.51	130.68	122.86
2	I	603	LYS	C-N-CA	5.51	130.68	122.86
2	J	588	GLY	CA-C-N	5.50	127.93	120.44
2	J	588	GLY	C-N-CA	5.50	127.93	120.44
1	C	237	GLN	CA-C-N	5.50	129.29	121.42
1	C	237	GLN	C-N-CA	5.50	129.29	121.42
1	e	178	GLN	CA-C-N	5.50	130.38	122.45
1	e	178	GLN	C-N-CA	5.50	130.38	122.45
2	I	533	GLY	CA-C-N	5.50	127.60	120.56
2	I	533	GLY	C-N-CA	5.50	127.60	120.56
2	M	544	CYS	CA-C-N	5.50	127.59	120.44
2	M	544	CYS	C-N-CA	5.50	127.59	120.44
2	P	529	LEU	CA-C-N	5.50	130.90	122.93
2	P	529	LEU	C-N-CA	5.50	130.90	122.93
1	a	181	LYS	CA-CB-CG	5.50	125.10	114.10
2	M	711	TYR	CA-C-N	5.50	131.17	122.60
2	M	711	TYR	C-N-CA	5.50	131.17	122.60
2	J	544	CYS	CA-C-N	5.50	127.58	120.44
2	J	544	CYS	C-N-CA	5.50	127.58	120.44
2	M	608	PRO	CA-C-N	5.50	127.64	120.28
2	M	608	PRO	C-N-CA	5.50	127.64	120.28
1	b	203	GLY	CA-C-N	5.50	130.90	122.93
1	b	203	GLY	C-N-CA	5.50	130.90	122.93
2	J	530	MET	CA-C-N	5.49	130.74	122.99
2	J	530	MET	C-N-CA	5.49	130.74	122.99
2	L	675	GLU	CA-C-N	5.49	127.48	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	675	GLU	C-N-CA	5.49	127.48	120.56
2	N	516	SER	CA-C-N	5.49	127.64	120.28
2	N	516	SER	C-N-CA	5.49	127.64	120.28
2	I	300	VAL	CA-CB-CG2	5.49	119.74	110.40
2	I	296	ASP	CA-C-N	5.49	132.02	121.54
2	I	296	ASP	C-N-CA	5.49	132.02	121.54
2	J	21	GLY	CA-C-N	5.49	127.63	120.28
2	J	21	GLY	C-N-CA	5.49	127.63	120.28
2	J	499	VAL	CA-C-N	5.49	126.03	119.94
2	J	499	VAL	C-N-CA	5.49	126.03	119.94
2	L	636	TYR	CA-C-N	5.49	128.08	120.29
2	L	636	TYR	C-N-CA	5.49	128.08	120.29
1	c	172	LYS	CA-C-N	5.49	131.42	122.81
1	c	172	LYS	C-N-CA	5.49	131.42	122.81
1	c	194	ILE	CA-C-N	5.49	127.57	120.44
1	c	194	ILE	C-N-CA	5.49	127.57	120.44
2	L	544	CYS	CA-C-N	5.48	127.57	120.44
2	L	544	CYS	C-N-CA	5.48	127.57	120.44
2	P	299	SER	CA-C-O	-5.48	112.67	120.51
2	O	716	LYS	CB-CG-CD	5.48	123.91	111.30
1	C	172	LYS	CA-C-N	5.48	131.42	122.81
1	C	172	LYS	C-N-CA	5.48	131.42	122.81
2	J	25	GLY	CA-C-N	5.48	127.56	120.44
2	J	25	GLY	C-N-CA	5.48	127.56	120.44
2	P	712	GLU	CA-CB-CG	5.48	125.05	114.10
1	E	240	LEU	CA-C-N	5.47	129.91	122.19
1	E	240	LEU	C-N-CA	5.47	129.91	122.19
2	I	530	MET	CA-C-N	5.47	131.17	122.74
2	I	530	MET	C-N-CA	5.47	131.17	122.74
1	f	203	GLY	CA-C-N	5.47	130.19	122.09
1	f	203	GLY	C-N-CA	5.47	130.19	122.09
2	N	711	TYR	CA-C-N	5.47	131.14	122.60
2	N	711	TYR	C-N-CA	5.47	131.14	122.60
2	M	468	ALA	CA-C-N	5.47	131.39	123.13
2	M	468	ALA	C-N-CA	5.47	131.39	123.13
2	P	433	ILE	CA-C-N	5.47	127.55	120.44
2	P	433	ILE	C-N-CA	5.47	127.55	120.44
2	M	513	LEU	CA-C-N	5.47	127.55	120.44
2	M	513	LEU	C-N-CA	5.47	127.55	120.44
2	I	675	GLU	CA-C-N	5.47	127.45	120.56
2	I	675	GLU	C-N-CA	5.47	127.45	120.56
2	N	713	TYR	CA-C-N	5.46	131.16	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	713	TYR	C-N-CA	5.46	131.16	122.74
1	e	251	ARG	CA-CB-CG	5.46	125.03	114.10
1	g	217	HIS	CE1-NE2-CD2	-5.46	103.54	109.00
2	L	498	ALA	CA-C-N	5.46	130.19	121.34
2	L	498	ALA	C-N-CA	5.46	130.19	121.34
2	P	513	LEU	CA-C-N	5.46	127.53	120.44
2	P	513	LEU	C-N-CA	5.46	127.53	120.44
1	F	247	LEU	CA-C-N	5.46	130.69	123.05
1	F	247	LEU	C-N-CA	5.46	130.69	123.05
2	I	301	ASP	CA-CB-CG	5.46	118.06	112.60
2	O	453	ILE	N-CA-CB	5.46	116.76	110.49
1	E	86	ARG	CB-CG-CD	5.45	123.84	111.30
2	J	716	LYS	CB-CG-CD	5.45	123.84	111.30
2	P	510	ILE	CA-C-N	5.45	127.53	120.44
2	P	510	ILE	C-N-CA	5.45	127.53	120.44
2	P	675	GLU	CA-C-N	5.45	127.43	120.56
2	P	675	GLU	C-N-CA	5.45	127.43	120.56
2	M	712	GLU	CA-CB-CG	5.45	125.00	114.10
1	f	217	HIS	CE1-NE2-CD2	-5.45	103.55	109.00
1	F	86	ARG	CB-CG-CD	5.45	123.83	111.30
2	L	712	GLU	CA-CB-CG	5.45	125.00	114.10
2	J	551	ILE	N-CA-CB	5.45	116.92	110.55
2	O	193	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	f	71	ARG	CA-CB-CG	5.44	124.98	114.10
1	A	269	LEU	CA-C-N	5.44	130.51	123.00
1	A	269	LEU	C-N-CA	5.44	130.51	123.00
2	I	458	VAL	CA-C-N	5.44	127.51	120.44
2	I	458	VAL	C-N-CA	5.44	127.51	120.44
2	L	559	LEU	CA-C-N	5.44	130.67	123.05
2	L	559	LEU	C-N-CA	5.44	130.67	123.05
2	K	260	ARG	NE-CZ-NH2	5.44	124.09	119.20
2	J	529	LEU	CA-C-N	5.44	130.81	122.93
2	J	529	LEU	C-N-CA	5.44	130.81	122.93
1	B	79	GLU	CA-C-N	5.43	127.41	120.56
1	B	79	GLU	C-N-CA	5.43	127.41	120.56
2	I	300	VAL	CA-C-O	-5.43	113.99	120.78
2	J	295	GLN	CB-CA-C	5.43	119.49	110.90
2	M	361	ARG	NE-CZ-NH2	5.43	124.09	119.20
2	M	716	LYS	CB-CG-CD	5.43	123.80	111.30
1	d	77	GLU	CA-C-N	5.43	127.50	120.44
1	d	77	GLU	C-N-CA	5.43	127.50	120.44
2	I	716	LYS	CB-CG-CD	5.43	123.79	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	462	HIS	CE1-NE2-CD2	-5.43	103.57	109.00
1	g	219	GLY	CA-C-N	5.43	130.65	122.99
1	g	219	GLY	C-N-CA	5.43	130.65	122.99
2	I	498	ALA	CA-C-N	5.42	130.13	121.34
2	I	498	ALA	C-N-CA	5.42	130.13	121.34
2	P	608	PRO	CA-C-N	5.42	127.49	120.44
2	P	608	PRO	C-N-CA	5.42	127.49	120.44
2	J	549	ALA	CA-C-N	5.42	127.39	120.56
2	J	549	ALA	C-N-CA	5.42	127.39	120.56
1	C	194	ILE	CA-C-N	5.42	127.48	120.44
1	C	194	ILE	C-N-CA	5.42	127.48	120.44
2	M	37	ILE	N-CA-CB	5.42	116.89	110.55
2	N	716	LYS	CB-CG-CD	5.42	123.76	111.30
1	E	172	LYS	CA-C-N	5.41	131.31	122.81
1	E	172	LYS	C-N-CA	5.41	131.31	122.81
2	K	120	ILE	CA-C-N	5.41	127.53	120.28
2	K	120	ILE	C-N-CA	5.41	127.53	120.28
1	G	86	ARG	CA-C-N	5.41	127.87	120.35
1	G	86	ARG	C-N-CA	5.41	127.87	120.35
1	c	196	ASP	CA-C-N	5.41	127.80	120.44
1	c	196	ASP	C-N-CA	5.41	127.80	120.44
1	e	217	HIS	CE1-NE2-CD2	-5.41	103.59	109.00
1	e	219	GLY	CA-C-N	5.41	130.62	122.99
1	e	219	GLY	C-N-CA	5.41	130.62	122.99
1	H	269	LEU	CA-C-N	5.41	130.46	123.00
1	H	269	LEU	C-N-CA	5.41	130.46	123.00
2	L	304	LEU	CA-C-N	5.40	127.52	120.28
2	L	304	LEU	C-N-CA	5.40	127.52	120.28
2	I	711	TYR	CA-C-N	5.40	131.03	122.60
2	I	711	TYR	C-N-CA	5.40	131.03	122.60
2	M	551	ILE	N-CA-CB	5.40	116.86	110.55
1	e	213	VAL	CA-C-N	5.39	130.13	123.12
1	e	213	VAL	C-N-CA	5.39	130.13	123.12
1	f	221	GLU	CA-C-N	5.39	131.03	122.62
1	f	221	GLU	C-N-CA	5.39	131.03	122.62
2	N	468	ALA	CA-C-N	5.39	131.27	123.13
2	N	468	ALA	C-N-CA	5.39	131.27	123.13
1	f	214	VAL	CA-C-N	5.39	130.76	123.11
1	f	214	VAL	C-N-CA	5.39	130.76	123.11
2	L	514	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	P	260	ARG	NE-CZ-NH2	5.38	124.05	119.20
2	P	496	LEU	CA-C-N	5.38	127.44	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	496	LEU	C-N-CA	5.38	127.44	120.44
2	J	662	THR	CA-C-N	5.38	131.03	122.74
2	J	662	THR	C-N-CA	5.38	131.03	122.74
2	L	463	GLY	CA-C-N	5.38	129.65	122.01
2	L	463	GLY	C-N-CA	5.38	129.65	122.01
2	N	433	ILE	CA-C-N	5.38	127.43	120.44
2	N	433	ILE	C-N-CA	5.38	127.43	120.44
1	d	135	HIS	CA-CB-CG	-5.38	108.42	113.80
1	e	214	VAL	CA-C-N	5.38	130.74	123.11
1	e	214	VAL	C-N-CA	5.38	130.74	123.11
1	C	196	ASP	CA-C-N	5.37	127.74	120.44
1	C	196	ASP	C-N-CA	5.37	127.74	120.44
2	I	474	GLU	CA-C-N	5.37	127.42	120.44
2	I	474	GLU	C-N-CA	5.37	127.42	120.44
1	H	335	ARG	CB-CG-CD	5.37	123.65	111.30
2	I	662	THR	CA-C-N	5.37	131.01	122.74
2	I	662	THR	C-N-CA	5.37	131.01	122.74
1	g	115	ASP	CA-CB-CG	5.37	117.97	112.60
2	J	433	ILE	CA-C-N	5.37	127.42	120.44
2	J	433	ILE	C-N-CA	5.37	127.42	120.44
2	L	546	ASN	CA-C-N	5.37	127.41	120.44
2	L	546	ASN	C-N-CA	5.37	127.41	120.44
2	L	565	MET	CA-CB-CG	5.36	124.83	114.10
1	f	69	VAL	CA-C-N	5.36	128.84	120.75
1	f	69	VAL	C-N-CA	5.36	128.84	120.75
2	O	548	ALA	CA-C-N	5.36	127.40	120.44
2	O	548	ALA	C-N-CA	5.36	127.40	120.44
2	L	458	VAL	CA-C-N	5.35	127.40	120.44
2	L	458	VAL	C-N-CA	5.35	127.40	120.44
2	M	530	MET	CA-C-N	5.35	130.55	123.00
2	M	530	MET	C-N-CA	5.35	130.55	123.00
1	c	151	ARG	NE-CZ-NH2	5.35	124.02	119.20
2	I	432	ILE	N-CA-CB	5.35	116.81	110.55
2	I	433	ILE	CA-C-N	5.35	127.40	120.44
2	I	433	ILE	C-N-CA	5.35	127.40	120.44
2	N	544	CYS	CA-C-N	5.35	127.39	120.44
2	N	544	CYS	C-N-CA	5.35	127.39	120.44
2	N	513	LEU	CA-C-N	5.35	127.39	120.44
2	N	513	LEU	C-N-CA	5.35	127.39	120.44
2	N	549	ALA	CA-C-N	5.35	127.30	120.56
2	N	549	ALA	C-N-CA	5.35	127.30	120.56
2	I	546	ASN	CA-C-N	5.34	127.39	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	546	ASN	C-N-CA	5.34	127.39	120.44
1	a	203	GLY	CA-C-N	5.34	130.00	122.09
1	a	203	GLY	C-N-CA	5.34	130.00	122.09
1	f	219	GLY	CA-C-N	5.34	130.52	122.99
1	f	219	GLY	C-N-CA	5.34	130.52	122.99
1	H	217	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
2	J	712	GLU	CA-CB-CG	5.34	124.78	114.10
1	f	213	VAL	CA-C-N	5.34	130.06	123.12
1	f	213	VAL	C-N-CA	5.34	130.06	123.12
1	H	280	GLU	N-CA-CB	5.34	117.75	110.01
2	P	457	GLN	CA-CB-CG	5.34	124.77	114.10
2	J	584	GLU	CA-C-N	5.33	127.28	120.56
2	J	584	GLU	C-N-CA	5.33	127.28	120.56
2	L	529	LEU	CA-C-N	5.33	130.94	122.94
2	L	529	LEU	C-N-CA	5.33	130.94	122.94
2	N	514	ARG	N-CA-CB	5.33	117.74	110.01
2	O	432	ILE	N-CA-CB	5.33	116.79	110.55
1	c	77	GLU	CA-C-N	5.33	127.37	120.44
1	c	77	GLU	C-N-CA	5.33	127.37	120.44
2	L	571	HIS	CA-C-N	5.33	127.36	120.44
2	L	571	HIS	C-N-CA	5.33	127.36	120.44
2	N	700	ARG	N-CA-CB	5.33	117.84	109.69
2	J	513	LEU	CA-C-N	5.32	127.36	120.44
2	J	513	LEU	C-N-CA	5.32	127.36	120.44
1	H	178	GLN	CA-C-N	5.32	129.74	122.34
1	H	178	GLN	C-N-CA	5.32	129.74	122.34
2	M	546	ASN	CA-C-N	5.32	127.36	120.44
2	M	546	ASN	C-N-CA	5.32	127.36	120.44
2	J	443	VAL	N-CA-CB	5.32	116.77	110.55
2	L	462	HIS	CG-CD2-NE2	5.32	112.52	107.20
2	I	551	ILE	N-CA-CB	5.32	116.77	110.55
2	M	432	ILE	N-CA-CB	5.32	116.77	110.55
2	O	559	LEU	CA-C-N	5.32	130.50	123.05
2	O	559	LEU	C-N-CA	5.32	130.50	123.05
2	O	701	ARG	CG-CD-NE	5.32	123.70	112.00
1	E	195	LEU	CA-C-N	5.32	127.35	120.44
1	E	195	LEU	C-N-CA	5.32	127.35	120.44
2	I	514	ARG	N-CA-CB	5.32	117.72	110.01
2	L	646	ILE	CA-C-N	5.32	127.94	120.28
2	L	646	ILE	C-N-CA	5.32	127.94	120.28
2	P	543	VAL	N-CA-CB	5.31	116.77	110.55
2	P	662	THR	CA-C-N	5.31	130.92	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	662	THR	C-N-CA	5.31	130.92	122.74
2	I	302	LEU	CB-CA-C	5.31	120.63	110.17
2	I	513	LEU	CA-C-N	5.31	127.34	120.44
2	I	513	LEU	C-N-CA	5.31	127.34	120.44
2	J	711	TYR	CA-C-N	5.31	131.30	122.54
2	J	711	TYR	C-N-CA	5.31	131.30	122.54
2	L	253	TYR	CB-CG-CD1	-5.31	112.84	120.80
2	L	443	VAL	N-CA-CB	5.31	116.76	110.55
2	L	555	ASN	CA-C-N	5.31	129.95	122.09
2	L	555	ASN	C-N-CA	5.31	129.95	122.09
2	P	565	MET	CA-CB-CG	5.31	124.71	114.10
2	M	664	MET	CA-C-N	5.31	130.50	122.91
2	M	664	MET	C-N-CA	5.31	130.50	122.91
1	a	214	VAL	CA-C-N	5.31	130.64	123.11
1	a	214	VAL	C-N-CA	5.31	130.64	123.11
1	E	169	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	N	543	VAL	CA-C-N	5.30	127.65	120.65
2	N	543	VAL	C-N-CA	5.30	127.65	120.65
1	c	135	HIS	CA-CB-CG	-5.30	108.50	113.80
2	P	546	ASN	CA-C-N	5.30	127.33	120.44
2	P	546	ASN	C-N-CA	5.30	127.33	120.44
1	d	195	LEU	CA-C-N	5.30	127.33	120.44
1	d	195	LEU	C-N-CA	5.30	127.33	120.44
2	L	432	ILE	N-CA-CB	5.30	116.75	110.55
2	L	526	ASN	CA-C-N	5.30	131.00	122.83
2	L	526	ASN	C-N-CA	5.30	131.00	122.83
2	O	433	ILE	CA-C-N	5.30	127.33	120.44
2	O	433	ILE	C-N-CA	5.30	127.33	120.44
2	O	609	ARG	CB-CG-CD	5.30	123.50	111.30
2	I	700	ARG	N-CA-CB	5.30	117.75	109.85
2	O	546	ASN	CA-C-N	5.30	127.33	120.44
2	O	546	ASN	C-N-CA	5.30	127.33	120.44
1	a	77	GLU	CA-C-N	5.30	127.33	120.44
1	a	77	GLU	C-N-CA	5.30	127.33	120.44
2	L	528	VAL	CA-C-N	5.30	130.89	122.94
2	L	528	VAL	C-N-CA	5.30	130.89	122.94
2	M	662	THR	CA-C-N	5.29	130.89	122.74
2	M	662	THR	C-N-CA	5.29	130.89	122.74
1	e	195	LEU	CA-C-N	5.29	127.32	120.44
1	e	195	LEU	C-N-CA	5.29	127.32	120.44
2	J	446	ARG	N-CA-CB	5.29	117.83	109.94
2	L	433	ILE	CA-C-N	5.29	127.32	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	433	ILE	C-N-CA	5.29	127.32	120.44
2	M	458	VAL	CA-C-N	5.29	127.32	120.44
2	M	458	VAL	C-N-CA	5.29	127.32	120.44
2	P	456	PRO	CA-C-N	5.29	128.11	120.38
2	P	456	PRO	C-N-CA	5.29	128.11	120.38
2	J	546	ASN	CA-C-N	5.29	127.32	120.44
2	J	546	ASN	C-N-CA	5.29	127.32	120.44
2	N	432	ILE	N-CA-CB	5.29	116.74	110.55
2	P	294	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	N	559	LEU	CA-C-N	5.29	130.45	123.05
2	N	559	LEU	C-N-CA	5.29	130.45	123.05
2	O	700	ARG	N-CA-CB	5.29	117.78	109.69
2	M	700	ARG	N-CA-CB	5.29	117.78	109.69
1	D	195	LEU	CA-C-N	5.28	127.31	120.44
1	D	195	LEU	C-N-CA	5.28	127.31	120.44
2	P	559	LEU	CA-C-N	5.28	130.45	123.05
2	P	559	LEU	C-N-CA	5.28	130.45	123.05
1	f	217	HIS	ND1-CG-CD2	-5.28	100.82	106.10
1	h	77	GLU	CA-C-N	5.28	127.30	120.44
1	h	77	GLU	C-N-CA	5.28	127.30	120.44
2	M	559	LEU	CA-C-N	5.28	130.44	123.05
2	M	559	LEU	C-N-CA	5.28	130.44	123.05
2	N	546	ASN	CA-C-N	5.28	127.30	120.44
2	N	546	ASN	C-N-CA	5.28	127.30	120.44
2	L	440	ILE	N-CA-CB	5.28	116.72	110.55
2	L	662	THR	CA-C-N	5.28	130.87	122.74
2	L	662	THR	C-N-CA	5.28	130.87	122.74
1	C	239	ARG	CA-C-N	5.28	129.42	122.30
1	C	239	ARG	C-N-CA	5.28	129.42	122.30
1	G	195	LEU	CA-C-N	5.28	127.30	120.44
1	G	195	LEU	C-N-CA	5.28	127.30	120.44
2	O	571	HIS	CA-C-N	5.28	127.30	120.44
2	O	571	HIS	C-N-CA	5.28	127.30	120.44
2	O	662	THR	CA-C-N	5.28	130.87	122.74
2	O	662	THR	C-N-CA	5.28	130.87	122.74
1	E	88	GLY	CA-C-N	5.27	125.74	120.52
1	E	88	GLY	C-N-CA	5.27	125.74	120.52
1	H	99	ASP	CA-CB-CG	5.27	117.87	112.60
2	J	432	ILE	N-CA-CB	5.27	116.72	110.55
2	L	462	HIS	ND1-CG-CD2	-5.27	100.83	106.10
2	P	432	ILE	N-CA-CB	5.27	116.72	110.55
1	a	193	THR	CA-C-N	5.27	127.20	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	193	THR	C-N-CA	5.27	127.20	120.56
2	N	648	ALA	CA-C-N	5.27	130.17	122.69
2	N	648	ALA	C-N-CA	5.27	130.17	122.69
2	O	608	PRO	CA-C-N	5.27	127.77	120.29
2	O	608	PRO	C-N-CA	5.27	127.77	120.29
1	c	239	ARG	CA-C-N	5.27	129.41	122.30
1	c	239	ARG	C-N-CA	5.27	129.41	122.30
2	L	25	GLY	CA-C-N	5.27	127.29	120.44
2	L	25	GLY	C-N-CA	5.27	127.29	120.44
1	b	227	GLN	N-CA-CB	5.27	117.60	109.91
2	P	565	MET	CA-C-N	5.27	129.50	120.71
2	P	565	MET	C-N-CA	5.27	129.50	120.71
1	h	195	LEU	CA-C-N	5.26	127.28	120.44
1	h	195	LEU	C-N-CA	5.26	127.28	120.44
1	D	83	TYR	N-CA-CB	5.26	117.63	109.48
1	H	221	GLU	CA-CB-CG	5.26	124.62	114.10
1	H	227	GLN	N-CA-CB	5.26	117.59	109.91
2	M	504	ASP	N-CA-CB	5.26	117.78	110.04
2	P	458	VAL	CA-C-N	5.26	127.28	120.44
2	P	458	VAL	C-N-CA	5.26	127.28	120.44
2	P	700	ARG	N-CA-CB	5.26	117.82	109.51
2	J	700	ARG	N-CA-CB	5.25	117.73	109.69
1	e	217	HIS	CG-CD2-NE2	5.25	112.45	107.20
2	O	338	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	c	195	LEU	CA-C-N	5.25	127.27	120.44
1	c	195	LEU	C-N-CA	5.25	127.27	120.44
2	L	548	ALA	CA-C-N	5.25	127.27	120.44
2	L	548	ALA	C-N-CA	5.25	127.27	120.44
2	I	559	LEU	CA-C-N	5.25	130.40	123.05
2	I	559	LEU	C-N-CA	5.25	130.40	123.05
2	M	550	VAL	CA-C-N	5.25	127.17	120.56
2	M	550	VAL	C-N-CA	5.25	127.17	120.56
1	f	217	HIS	CG-CD2-NE2	5.25	112.45	107.20
2	I	339	PRO	N-CA-CB	5.25	107.91	103.19
2	I	664	MET	CA-C-N	5.25	130.41	122.91
2	I	664	MET	C-N-CA	5.25	130.41	122.91
2	L	608	PRO	CA-C-N	5.25	127.57	120.44
2	L	608	PRO	C-N-CA	5.25	127.57	120.44
2	M	433	ILE	CA-C-N	5.25	127.26	120.44
2	M	433	ILE	C-N-CA	5.25	127.26	120.44
2	N	510	ILE	CA-C-N	5.25	127.26	120.44
2	N	510	ILE	C-N-CA	5.25	127.26	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	438	LEU	CA-C-N	5.24	127.26	120.44
2	J	438	LEU	C-N-CA	5.24	127.26	120.44
2	L	377	ARG	NE-CZ-NH2	5.24	123.92	119.20
2	M	510	ILE	CA-C-N	5.24	127.26	120.44
2	M	510	ILE	C-N-CA	5.24	127.26	120.44
2	M	548	ALA	CA-C-N	5.24	127.25	120.44
2	M	548	ALA	C-N-CA	5.24	127.25	120.44
2	J	329	GLU	N-CA-C	5.24	118.46	111.75
2	I	571	HIS	CA-C-N	5.24	127.25	120.44
2	I	571	HIS	C-N-CA	5.24	127.25	120.44
2	L	700	ARG	N-CA-CB	5.24	117.71	109.69
1	g	222	GLU	CA-C-N	5.24	130.23	123.00
1	g	222	GLU	C-N-CA	5.24	130.23	123.00
2	J	572	GLU	CA-C-N	5.23	127.24	120.44
2	J	572	GLU	C-N-CA	5.23	127.24	120.44
2	M	528	VAL	CA-C-N	5.23	130.80	122.74
2	M	528	VAL	C-N-CA	5.23	130.80	122.74
2	N	572	GLU	CA-C-N	5.23	127.24	120.44
2	N	572	GLU	C-N-CA	5.23	127.24	120.44
1	g	217	HIS	CG-CD2-NE2	5.23	112.43	107.20
2	J	609	ARG	NE-CZ-NH2	5.23	123.91	119.20
2	O	504	ASP	N-CA-CB	5.23	117.72	110.04
1	f	229	LEU	N-CA-CB	5.23	117.59	110.01
2	J	528	VAL	CA-C-N	5.22	130.79	122.74
2	J	528	VAL	C-N-CA	5.22	130.79	122.74
2	L	28	ILE	CA-C-N	5.22	127.23	120.44
2	L	28	ILE	C-N-CA	5.22	127.23	120.44
2	P	701	ARG	CG-CD-NE	5.22	123.49	112.00
1	b	104	THR	CA-C-N	5.22	126.88	122.28
1	b	104	THR	C-N-CA	5.22	126.88	122.28
2	L	464	ILE	N-CA-CB	5.22	117.45	111.39
2	N	548	ALA	CA-C-N	5.22	127.23	120.44
2	N	548	ALA	C-N-CA	5.22	127.23	120.44
1	F	195	LEU	CA-C-N	5.22	127.23	120.44
1	F	195	LEU	C-N-CA	5.22	127.23	120.44
1	e	217	HIS	ND1-CG-CD2	-5.22	100.88	106.10
1	B	195	LEU	CA-C-N	5.22	127.22	120.44
1	B	195	LEU	C-N-CA	5.22	127.22	120.44
1	H	217	HIS	ND1-CG-CD2	-5.22	100.88	106.10
2	N	608	PRO	CA-C-N	5.22	127.22	120.44
2	N	608	PRO	C-N-CA	5.22	127.22	120.44
1	e	75	THR	CA-C-N	5.22	127.27	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	75	THR	C-N-CA	5.22	127.27	120.28
1	g	217	HIS	ND1-CG-CD2	-5.22	100.88	106.10
2	J	548	ALA	CA-C-N	5.21	127.22	120.44
2	J	548	ALA	C-N-CA	5.21	127.22	120.44
2	N	571	HIS	CA-C-N	5.21	127.22	120.44
2	N	571	HIS	C-N-CA	5.21	127.22	120.44
1	H	220	ARG	CA-C-N	5.21	129.81	122.09
1	H	220	ARG	C-N-CA	5.21	129.81	122.09
1	C	195	LEU	CA-C-N	5.21	127.21	120.44
1	C	195	LEU	C-N-CA	5.21	127.21	120.44
1	a	229	LEU	N-CA-CB	5.21	117.57	110.01
2	J	513	LEU	N-CA-CB	5.21	117.70	109.94
2	L	654	ILE	CA-C-N	5.21	127.60	120.46
2	L	654	ILE	C-N-CA	5.21	127.60	120.46
2	M	36	GLY	CA-C-N	5.21	127.12	120.56
2	M	36	GLY	C-N-CA	5.21	127.12	120.56
2	I	549	ALA	CA-C-N	5.21	127.59	120.46
2	I	549	ALA	C-N-CA	5.21	127.59	120.46
1	h	239	ARG	CA-C-N	5.21	129.33	122.30
1	h	239	ARG	C-N-CA	5.21	129.33	122.30
2	I	600	SER	CA-C-N	5.20	130.83	122.50
2	I	600	SER	C-N-CA	5.20	130.83	122.50
2	L	504	ASP	N-CA-CB	5.20	117.68	109.83
1	G	170	SER	CA-C-N	5.20	130.32	122.99
1	G	170	SER	C-N-CA	5.20	130.32	122.99
1	A	229	LEU	N-CA-CB	5.20	117.55	110.01
1	C	229	LEU	N-CA-CB	5.20	117.55	110.01
2	I	670	VAL	CA-C-N	5.20	128.85	121.42
2	I	670	VAL	C-N-CA	5.20	128.85	121.42
1	E	184	GLN	CA-C-N	5.20	130.08	122.39
1	E	184	GLN	C-N-CA	5.20	130.08	122.39
2	M	571	HIS	CA-C-N	5.20	127.19	120.44
2	M	571	HIS	C-N-CA	5.20	127.19	120.44
2	P	511	ARG	CD-NE-CZ	5.20	131.68	124.40
2	J	625	PHE	N-CA-CB	5.19	117.54	110.01
2	I	431	ALA	CA-C-N	5.19	127.10	120.56
2	I	431	ALA	C-N-CA	5.19	127.10	120.56
1	H	217	HIS	CG-CD2-NE2	5.19	112.39	107.20
2	M	609	ARG	CB-CG-CD	5.19	123.23	111.30
2	N	474	GLU	CA-C-N	5.19	127.18	120.44
2	N	474	GLU	C-N-CA	5.19	127.18	120.44
2	P	118	PHE	CA-CB-CG	5.19	118.99	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	c	184	GLN	CA-C-N	5.19	130.06	122.39
1	c	184	GLN	C-N-CA	5.19	130.06	122.39
2	L	682	ARG	CD-NE-CZ	5.18	131.65	124.40
2	I	510	ILE	CA-C-N	5.18	127.18	120.44
2	I	510	ILE	C-N-CA	5.18	127.18	120.44
2	M	514	ARG	N-CA-CB	5.18	117.52	110.01
2	N	664	MET	CA-C-N	5.18	130.32	122.91
2	N	664	MET	C-N-CA	5.18	130.32	122.91
1	d	75	THR	CA-C-N	5.18	127.22	120.28
1	d	75	THR	C-N-CA	5.18	127.22	120.28
2	O	458	VAL	CA-C-N	5.18	127.17	120.44
2	O	458	VAL	C-N-CA	5.18	127.17	120.44
2	J	431	ALA	CA-C-N	5.18	127.08	120.56
2	J	431	ALA	C-N-CA	5.18	127.08	120.56
2	J	514	ARG	N-CA-CB	5.18	117.52	110.01
2	J	580	ASN	CA-C-N	5.17	128.24	122.55
2	J	580	ASN	C-N-CA	5.17	128.24	122.55
2	O	513	LEU	N-CA-CB	5.17	117.65	109.94
2	O	38	THR	CA-C-N	5.17	127.17	120.44
2	O	38	THR	C-N-CA	5.17	127.17	120.44
2	P	300	VAL	CB-CA-C	-5.17	102.81	111.29
1	A	227	GLN	N-CA-CB	5.17	117.46	109.91
2	J	458	VAL	CA-C-N	5.17	127.16	120.44
2	J	458	VAL	C-N-CA	5.17	127.16	120.44
2	L	625	PHE	N-CA-CB	5.17	117.51	110.01
2	N	682	ARG	CD-NE-CZ	5.17	131.64	124.40
2	P	474	GLU	CA-C-N	5.17	127.16	120.44
2	P	474	GLU	C-N-CA	5.17	127.16	120.44
2	J	681	SER	N-CA-CB	5.17	117.51	110.01
2	I	665	VAL	CA-C-N	5.17	130.68	122.62
2	I	665	VAL	C-N-CA	5.17	130.68	122.62
2	N	670	VAL	CA-C-N	5.17	128.81	121.42
2	N	670	VAL	C-N-CA	5.17	128.81	121.42
2	J	582	LEU	CA-C-N	5.17	127.15	120.44
2	J	582	LEU	C-N-CA	5.17	127.15	120.44
2	J	699	PHE	CA-C-N	5.17	128.10	120.82
2	J	699	PHE	C-N-CA	5.17	128.10	120.82
2	J	510	ILE	CA-C-N	5.16	127.15	120.44
2	J	510	ILE	C-N-CA	5.16	127.15	120.44
2	N	513	LEU	N-CA-CB	5.16	117.64	109.94
2	L	38	THR	CA-C-N	5.16	127.15	120.44
2	L	38	THR	C-N-CA	5.16	127.15	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	572	GLU	CA-C-N	5.16	127.15	120.44
2	P	572	GLU	C-N-CA	5.16	127.15	120.44
1	E	83	TYR	N-CA-CB	5.16	117.48	109.48
2	K	557	ARG	NE-CZ-NH2	5.16	123.84	119.20
2	O	510	ILE	CA-C-N	5.16	127.15	120.44
2	O	510	ILE	C-N-CA	5.16	127.15	120.44
2	P	664	MET	CA-C-N	5.16	130.29	122.91
2	P	664	MET	C-N-CA	5.16	130.29	122.91
2	N	388	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	C	184	GLN	CA-C-N	5.16	130.02	122.39
1	C	184	GLN	C-N-CA	5.16	130.02	122.39
2	J	316	ILE	CA-CB-CG1	5.16	119.17	110.40
2	J	452	GLY	CA-C-N	5.16	128.30	120.77
2	J	452	GLY	C-N-CA	5.16	128.30	120.77
2	J	457	GLN	CA-C-N	5.16	127.25	120.60
2	J	457	GLN	C-N-CA	5.16	127.25	120.60
2	N	437	MET	CA-C-N	5.16	127.14	120.44
2	N	437	MET	C-N-CA	5.16	127.14	120.44
1	E	79	GLU	CA-C-N	5.16	127.52	120.46
1	E	79	GLU	C-N-CA	5.16	127.52	120.46
1	e	193	THR	CA-C-N	5.16	127.06	120.56
1	e	193	THR	C-N-CA	5.16	127.06	120.56
1	F	172	LYS	CA-C-N	5.15	130.90	122.81
1	F	172	LYS	C-N-CA	5.15	130.90	122.81
1	e	221	GLU	CA-CB-CG	5.15	124.41	114.10
1	f	151	ARG	NE-CZ-NH2	5.15	123.84	119.20
2	I	550	VAL	CA-C-N	5.15	127.05	120.56
2	I	550	VAL	C-N-CA	5.15	127.05	120.56
2	J	377	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	f	205	THR	CA-C-N	5.15	127.60	120.29
1	f	205	THR	C-N-CA	5.15	127.60	120.29
1	A	73	ASN	CA-C-N	5.15	127.18	120.28
1	A	73	ASN	C-N-CA	5.15	127.18	120.28
1	G	84	GLN	CA-C-N	5.15	129.71	122.09
1	G	84	GLN	C-N-CA	5.15	129.71	122.09
1	a	239	ARG	CA-C-N	5.15	129.25	122.30
1	a	239	ARG	C-N-CA	5.15	129.25	122.30
2	M	431	ALA	CA-C-N	5.14	127.04	120.56
2	M	431	ALA	C-N-CA	5.14	127.04	120.56
2	P	513	LEU	N-CA-CB	5.14	117.60	109.94
1	a	75	THR	CA-C-N	5.14	127.17	120.28
1	a	75	THR	C-N-CA	5.14	127.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	672	THR	CA-C-N	5.14	127.12	120.44
2	L	672	THR	C-N-CA	5.14	127.12	120.44
2	N	665	VAL	CA-C-N	5.14	130.64	122.62
2	N	665	VAL	C-N-CA	5.14	130.64	122.62
1	h	184	GLN	CA-C-N	5.14	130.00	122.39
1	h	184	GLN	C-N-CA	5.14	130.00	122.39
2	L	665	VAL	CA-C-N	5.14	130.64	122.62
2	L	665	VAL	C-N-CA	5.14	130.64	122.62
2	O	300	VAL	CA-C-O	5.14	126.24	120.64
1	g	121	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	C	76	LEU	N-CA-CB	5.14	117.67	110.12
2	N	301	ASP	CB-CA-C	5.14	121.04	110.31
2	I	572	GLU	CA-C-N	5.13	127.11	120.44
2	I	572	GLU	C-N-CA	5.13	127.11	120.44
2	M	348	ARG	NE-CZ-NH2	5.13	123.82	119.20
2	M	513	LEU	N-CA-CB	5.13	117.59	109.94
1	c	76	LEU	N-CA-CB	5.13	117.67	110.12
1	B	137	VAL	N-CA-CB	5.13	116.62	110.31
1	e	76	LEU	N-CA-CB	5.13	117.67	110.12
2	I	513	LEU	N-CA-CB	5.13	117.58	109.94
2	L	22	ARG	CA-C-N	5.13	127.11	120.44
2	L	22	ARG	C-N-CA	5.13	127.11	120.44
2	P	504	ASP	N-CA-CB	5.13	117.58	110.04
2	L	431	ALA	CA-C-N	5.13	127.02	120.56
2	L	431	ALA	C-N-CA	5.13	127.02	120.56
2	O	431	ALA	CA-C-N	5.13	127.02	120.56
2	O	431	ALA	C-N-CA	5.13	127.02	120.56
1	a	76	LEU	N-CA-CB	5.13	117.66	110.12
2	J	458	VAL	N-CA-CB	5.13	116.20	110.51
2	L	513	LEU	N-CA-CB	5.13	117.58	109.94
2	L	520	ALA	CA-C-N	5.13	129.40	120.68
2	L	520	ALA	C-N-CA	5.13	129.40	120.68
2	O	359	ASN	CA-CB-CG	5.13	117.73	112.60
2	M	681	SER	CA-C-N	5.12	127.10	120.44
2	M	681	SER	C-N-CA	5.12	127.10	120.44
1	C	193	THR	CA-C-N	5.12	127.02	120.56
1	C	193	THR	C-N-CA	5.12	127.02	120.56
2	J	478	ALA	CA-C-N	5.12	129.34	120.58
2	J	478	ALA	C-N-CA	5.12	129.34	120.58
2	L	30	ALA	CA-C-N	5.12	127.40	120.38
2	L	30	ALA	C-N-CA	5.12	127.40	120.38
1	h	76	LEU	N-CA-CB	5.12	117.65	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	701	ARG	CG-CD-NE	5.12	123.27	112.00
2	M	456	PRO	CA-C-N	5.12	127.86	120.38
2	M	456	PRO	C-N-CA	5.12	127.86	120.38
2	M	665	VAL	CA-C-N	5.12	130.61	122.62
2	M	665	VAL	C-N-CA	5.12	130.61	122.62
2	M	41	PHE	CA-C-N	5.12	127.10	120.44
2	M	41	PHE	C-N-CA	5.12	127.10	120.44
2	N	528	VAL	CA-C-N	5.12	131.03	122.73
2	N	528	VAL	C-N-CA	5.12	131.03	122.73
2	J	38	THR	CA-C-N	5.12	127.09	120.44
2	J	38	THR	C-N-CA	5.12	127.09	120.44
2	N	701	ARG	CG-CD-NE	5.12	123.26	112.00
2	O	572	GLU	CA-C-N	5.12	127.09	120.44
2	O	572	GLU	C-N-CA	5.12	127.09	120.44
1	B	76	LEU	N-CA-CB	5.12	117.64	110.12
1	b	71	ARG	CA-CB-CG	5.12	124.33	114.10
1	e	145	ARG	NE-CZ-NH2	5.12	123.80	119.20
2	K	280	ARG	NE-CZ-NH2	5.11	123.80	119.20
2	L	442	GLY	CA-C-N	5.11	127.00	120.56
2	L	442	GLY	C-N-CA	5.11	127.00	120.56
2	M	699	PHE	CA-C-N	5.11	128.03	120.82
2	M	699	PHE	C-N-CA	5.11	128.03	120.82
2	N	458	VAL	CA-C-N	5.11	127.09	120.44
2	N	458	VAL	C-N-CA	5.11	127.09	120.44
2	M	573	LEU	N-CA-CB	5.11	117.42	110.01
2	M	572	GLU	CA-C-N	5.11	127.08	120.44
2	M	572	GLU	C-N-CA	5.11	127.08	120.44
1	g	221	GLU	CA-CB-CG	5.11	124.32	114.10
2	P	42	ALA	CA-C-N	5.11	127.08	120.44
2	P	42	ALA	C-N-CA	5.11	127.08	120.44
1	h	75	THR	CA-C-N	5.11	127.13	120.28
1	h	75	THR	C-N-CA	5.11	127.13	120.28
2	J	665	VAL	CA-C-N	5.11	130.59	122.62
2	J	665	VAL	C-N-CA	5.11	130.59	122.62
1	d	76	LEU	N-CA-CB	5.11	117.63	110.12
2	M	647	LEU	CA-C-N	5.11	129.24	120.71
2	M	647	LEU	C-N-CA	5.11	129.24	120.71
2	N	36	GLY	CA-C-N	5.11	126.99	120.56
2	N	36	GLY	C-N-CA	5.11	126.99	120.56
2	P	431	ALA	CA-C-N	5.11	126.99	120.56
2	P	431	ALA	C-N-CA	5.11	126.99	120.56
2	I	565	MET	CA-CB-CG	5.10	124.31	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	650	THR	CA-C-N	5.10	127.08	120.44
2	I	650	THR	C-N-CA	5.10	127.08	120.44
1	B	184	GLN	CA-C-N	5.10	129.94	122.39
1	B	184	GLN	C-N-CA	5.10	129.94	122.39
2	P	573	LEU	N-CA-CB	5.10	117.41	110.01
1	h	185	GLN	CB-CG-CD	5.10	121.27	112.60
2	L	650	THR	CA-C-N	5.10	127.07	120.44
2	L	650	THR	C-N-CA	5.10	127.07	120.44
2	M	646	ILE	CA-C-N	5.10	127.62	120.28
2	M	646	ILE	C-N-CA	5.10	127.62	120.28
2	O	573	LEU	N-CA-CB	5.10	117.41	110.01
1	d	184	GLN	CA-C-N	5.10	129.94	122.39
1	d	184	GLN	C-N-CA	5.10	129.94	122.39
1	g	251	ARG	CA-CB-CG	5.10	124.30	114.10
2	I	548	ALA	CA-C-N	5.10	127.07	120.44
2	I	548	ALA	C-N-CA	5.10	127.07	120.44
2	P	38	THR	CA-C-N	5.10	127.07	120.44
2	P	38	THR	C-N-CA	5.10	127.07	120.44
2	J	550	VAL	N-CA-CB	5.10	116.51	110.55
1	d	185	GLN	CB-CG-CD	5.10	121.26	112.60
2	I	42	ALA	CA-C-N	5.09	127.06	120.44
2	I	42	ALA	C-N-CA	5.09	127.06	120.44
2	N	38	THR	CA-C-N	5.09	127.06	120.44
2	N	38	THR	C-N-CA	5.09	127.06	120.44
2	N	431	ALA	CA-C-N	5.09	126.98	120.56
2	N	431	ALA	C-N-CA	5.09	126.98	120.56
2	O	681	SER	CA-C-N	5.09	127.06	120.44
2	O	681	SER	C-N-CA	5.09	127.06	120.44
1	C	83	TYR	N-CA-CB	5.09	117.53	110.04
1	H	251	ARG	CA-CB-CG	5.09	124.28	114.10
2	N	41	PHE	CA-C-N	5.09	127.06	120.44
2	N	41	PHE	C-N-CA	5.09	127.06	120.44
1	D	184	GLN	CA-C-N	5.09	129.93	122.39
1	D	184	GLN	C-N-CA	5.09	129.93	122.39
2	M	298	ASP	CA-C-N	5.09	131.26	121.54
2	M	298	ASP	C-N-CA	5.09	131.26	121.54
2	O	665	VAL	CA-C-N	5.09	130.56	122.62
2	O	665	VAL	C-N-CA	5.09	130.56	122.62
2	P	497	LEU	N-CA-CB	5.09	117.39	110.01
1	g	220	ARG	CD-NE-CZ	5.09	131.53	124.40
2	K	462	HIS	CB-CG-CD2	-5.09	124.58	131.20
2	L	524	ALA	CA-C-N	5.09	127.52	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	524	ALA	C-N-CA	5.09	127.52	120.29
1	c	78	SER	N-CA-CB	5.09	117.39	110.01
2	N	50	PHE	CA-CB-CG	-5.09	108.71	113.80
1	F	185	GLN	CB-CG-CD	5.09	121.25	112.60
2	L	42	ALA	CA-C-N	5.09	127.05	120.44
2	L	42	ALA	C-N-CA	5.09	127.05	120.44
1	G	83	TYR	CA-C-N	5.08	130.89	121.94
1	G	83	TYR	C-N-CA	5.08	130.89	121.94
2	L	37	ILE	N-CA-CB	5.08	116.50	110.55
2	M	38	THR	CA-C-N	5.08	127.05	120.44
2	M	38	THR	C-N-CA	5.08	127.05	120.44
1	G	83	TYR	N-CA-CB	5.08	117.36	109.48
2	M	648	ALA	CA-C-N	5.08	129.91	122.69
2	M	648	ALA	C-N-CA	5.08	129.91	122.69
1	g	252	ASN	CA-C-N	5.08	127.60	120.28
1	g	252	ASN	C-N-CA	5.08	127.60	120.28
2	J	464	ILE	N-CA-CB	5.08	117.38	111.90
1	C	79	GLU	CA-C-N	5.08	127.42	120.46
1	C	79	GLU	C-N-CA	5.08	127.42	120.46
1	a	79	GLU	CA-C-N	5.08	127.42	120.46
1	a	79	GLU	C-N-CA	5.08	127.42	120.46
2	J	507	ILE	CA-C-N	5.08	127.04	120.44
2	J	507	ILE	C-N-CA	5.08	127.04	120.44
1	f	121	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	h	79	GLU	CA-C-N	5.08	127.41	120.46
1	h	79	GLU	C-N-CA	5.08	127.41	120.46
2	J	131	ARG	NE-CZ-NH2	5.07	123.77	119.20
2	P	504	ASP	CA-C-N	5.07	127.59	120.28
2	P	504	ASP	C-N-CA	5.07	127.59	120.28
1	F	83	TYR	CA-C-N	5.07	130.87	121.94
1	F	83	TYR	C-N-CA	5.07	130.87	121.94
1	e	222	GLU	CA-CB-CG	5.07	124.24	114.10
1	F	184	GLN	CA-C-N	5.07	129.89	122.39
1	F	184	GLN	C-N-CA	5.07	129.89	122.39
2	J	625	PHE	CA-C-N	5.07	127.03	120.44
2	J	625	PHE	C-N-CA	5.07	127.03	120.44
2	I	544	CYS	CA-C-N	5.07	127.03	120.44
2	I	544	CYS	C-N-CA	5.07	127.03	120.44
2	N	42	ALA	CA-C-N	5.07	127.03	120.44
2	N	42	ALA	C-N-CA	5.07	127.03	120.44
1	g	227	GLN	N-CA-CB	5.07	117.53	109.82
2	P	665	VAL	CA-C-N	5.07	130.53	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	665	VAL	C-N-CA	5.07	130.53	122.62
1	f	227	GLN	CA-C-N	5.07	127.03	120.44
1	f	227	GLN	C-N-CA	5.07	127.03	120.44
1	g	247	LEU	CA-C-N	5.07	130.15	123.00
1	g	247	LEU	C-N-CA	5.07	130.15	123.00
2	I	681	SER	CA-C-N	5.07	127.03	120.44
2	I	681	SER	C-N-CA	5.07	127.03	120.44
1	g	227	GLN	CA-C-N	5.06	127.07	120.28
1	g	227	GLN	C-N-CA	5.06	127.07	120.28
2	N	504	ASP	N-CA-CB	5.06	117.60	110.36
2	N	550	VAL	N-CA-CB	5.06	116.47	110.55
1	D	185	GLN	CB-CG-CD	5.06	121.20	112.60
2	J	573	LEU	N-CA-CB	5.06	117.35	110.01
2	N	507	ILE	CA-C-N	5.06	127.02	120.44
2	N	507	ILE	C-N-CA	5.06	127.02	120.44
2	O	40	VAL	N-CA-CB	5.06	116.47	110.55
1	a	227	GLN	CA-C-N	5.06	127.02	120.44
1	a	227	GLN	C-N-CA	5.06	127.02	120.44
2	I	41	PHE	CA-C-N	5.06	127.02	120.44
2	I	41	PHE	C-N-CA	5.06	127.02	120.44
2	J	627	GLU	N-CA-CB	5.06	117.34	110.01
2	P	41	PHE	CA-C-N	5.06	127.02	120.44
2	P	41	PHE	C-N-CA	5.06	127.02	120.44
1	D	79	GLU	CA-C-N	5.06	127.39	120.46
1	D	79	GLU	C-N-CA	5.06	127.39	120.46
1	H	68	ASN	CA-C-N	5.06	129.97	122.94
1	H	68	ASN	C-N-CA	5.06	129.97	122.94
1	H	222	GLU	CA-CB-CG	5.06	124.22	114.10
2	I	38	THR	CA-C-N	5.06	127.02	120.44
2	I	38	THR	C-N-CA	5.06	127.02	120.44
2	J	22	ARG	CA-C-N	5.06	127.01	120.44
2	J	22	ARG	C-N-CA	5.06	127.01	120.44
2	J	40	VAL	N-CA-CB	5.06	116.47	110.55
2	M	543	VAL	CA-C-N	5.06	127.33	120.65
2	M	543	VAL	C-N-CA	5.06	127.33	120.65
2	O	670	VAL	CA-C-N	5.06	128.65	121.42
2	O	670	VAL	C-N-CA	5.06	128.65	121.42
2	M	40	VAL	N-CA-CB	5.05	116.46	110.55
2	O	377	ARG	CD-NE-CZ	5.05	131.48	124.40
2	P	514	ARG	N-CA-CB	5.05	117.34	110.01
1	c	79	GLU	CA-C-N	5.05	127.39	120.46
1	c	79	GLU	C-N-CA	5.05	127.39	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	442	GLY	CA-C-N	5.05	126.93	120.56
2	J	442	GLY	C-N-CA	5.05	126.93	120.56
1	a	184	GLN	CA-C-N	5.05	129.87	122.39
1	a	184	GLN	C-N-CA	5.05	129.87	122.39
1	B	77	GLU	CA-C-N	5.05	127.01	120.44
1	B	77	GLU	C-N-CA	5.05	127.01	120.44
2	L	648	ALA	CA-C-N	5.05	129.86	122.69
2	L	648	ALA	C-N-CA	5.05	129.86	122.69
1	H	334	PHE	CA-C-N	5.05	130.51	122.94
1	H	334	PHE	C-N-CA	5.05	130.51	122.94
2	P	571	HIS	CA-C-N	5.05	127.00	120.44
2	P	571	HIS	C-N-CA	5.05	127.00	120.44
1	e	181	LYS	CA-CB-CG	5.05	124.20	114.10
1	g	222	GLU	CA-CB-CG	5.05	124.20	114.10
2	I	507	ILE	CA-C-N	5.05	127.00	120.44
2	I	507	ILE	C-N-CA	5.05	127.00	120.44
2	O	42	ALA	CA-C-N	5.05	127.00	120.44
2	O	42	ALA	C-N-CA	5.05	127.00	120.44
1	c	75	THR	CA-C-N	5.05	127.05	120.28
1	c	75	THR	C-N-CA	5.05	127.05	120.28
1	A	217	HIS	CB-CG-CD2	-5.05	124.64	131.20
1	c	185	GLN	CB-CG-CD	5.05	121.18	112.60
1	e	177	GLY	CA-C-N	5.05	129.65	122.08
1	e	177	GLY	C-N-CA	5.05	129.65	122.08
1	B	75	THR	CA-C-N	5.04	127.04	120.28
1	B	75	THR	C-N-CA	5.04	127.04	120.28
1	C	185	GLN	CB-CG-CD	5.04	121.17	112.60
1	b	227	GLN	CA-C-N	5.04	127.04	120.28
1	b	227	GLN	C-N-CA	5.04	127.04	120.28
2	N	573	LEU	N-CA-CB	5.04	117.32	110.01
1	g	211	ARG	CA-CB-CG	5.04	124.19	114.10
1	D	170	SER	CA-C-N	5.04	130.10	122.99
1	D	170	SER	C-N-CA	5.04	130.10	122.99
1	H	208	ALA	CA-C-N	5.04	131.59	123.33
1	H	208	ALA	C-N-CA	5.04	131.59	123.33
2	J	628	LEU	CA-C-N	5.04	126.91	120.56
2	J	628	LEU	C-N-CA	5.04	126.91	120.56
2	L	518	HIS	CB-CG-CD2	-5.04	124.65	131.20
2	O	533	GLY	N-CA-C	5.04	120.24	110.66
1	H	220	ARG	CD-NE-CZ	5.04	131.45	124.40
2	J	571	HIS	CA-C-N	5.04	126.99	120.44
2	J	571	HIS	C-N-CA	5.04	126.99	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	703	SER	N-CA-CB	5.04	117.54	109.28
2	N	296	ASP	O-C-N	-5.04	116.79	122.03
1	C	75	THR	CA-C-N	5.04	127.03	120.28
1	C	75	THR	C-N-CA	5.04	127.03	120.28
2	L	22	ARG	CA-CB-CG	5.04	124.17	114.10
2	L	556	LYS	CA-C-N	5.04	129.10	122.30
2	L	556	LYS	C-N-CA	5.04	129.10	122.30
2	N	681	SER	CA-C-N	5.04	126.99	120.44
2	N	681	SER	C-N-CA	5.04	126.99	120.44
2	P	40	VAL	N-CA-CB	5.04	116.44	110.55
2	P	548	ALA	CA-C-N	5.04	127.30	120.65
2	P	548	ALA	C-N-CA	5.04	127.30	120.65
1	F	160	GLN	OE1-CD-NE2	-5.03	117.57	122.60
2	J	583	SER	CA-C-N	5.03	127.02	120.28
2	J	583	SER	C-N-CA	5.03	127.02	120.28
2	O	699	PHE	CA-C-N	5.03	127.92	120.82
2	O	699	PHE	C-N-CA	5.03	127.92	120.82
1	A	208	ALA	CA-C-N	5.03	131.58	123.33
1	A	208	ALA	C-N-CA	5.03	131.58	123.33
2	J	550	VAL	CA-C-N	5.03	126.90	120.56
2	J	550	VAL	C-N-CA	5.03	126.90	120.56
2	K	451	ARG	NE-CZ-NH2	5.03	123.73	119.20
2	L	454	GLU	CA-CB-CG	5.03	124.16	114.10
2	L	673	LEU	N-CA-CB	5.03	117.30	110.01
2	O	41	PHE	CA-C-N	5.03	126.98	120.44
2	O	41	PHE	C-N-CA	5.03	126.98	120.44
1	e	222	GLU	CA-C-N	5.03	130.09	123.05
1	e	222	GLU	C-N-CA	5.03	130.09	123.05
1	H	227	GLN	CA-C-N	5.03	126.98	120.44
1	H	227	GLN	C-N-CA	5.03	126.98	120.44
1	A	211	ARG	CD-NE-CZ	5.03	131.44	124.40
1	B	185	GLN	CB-CG-CD	5.02	121.14	112.60
2	I	40	VAL	N-CA-CB	5.02	116.43	110.55
2	M	701	ARG	CG-CD-NE	5.02	123.05	112.00
1	c	80	ILE	CA-C-N	5.02	127.01	120.28
1	c	80	ILE	C-N-CA	5.02	127.01	120.28
1	A	252	ASN	CA-C-N	5.02	127.51	120.28
1	A	252	ASN	C-N-CA	5.02	127.51	120.28
2	N	40	VAL	N-CA-CB	5.02	116.42	110.55
1	H	169	ARG	NE-CZ-NH2	5.02	123.72	119.20
2	P	44	CYS	N-CA-CB	5.02	117.29	110.01
1	b	272	ASP	CA-C-N	5.02	127.50	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	272	ASP	C-N-CA	5.02	127.50	120.28
2	J	388	GLN	OE1-CD-NE2	-5.01	117.59	122.60
2	J	511	ARG	CB-CG-CD	5.01	122.83	111.30
1	d	239	ARG	CA-C-N	5.01	129.44	122.77
1	d	239	ARG	C-N-CA	5.01	129.44	122.77
1	C	80	ILE	CA-C-N	5.01	127.00	120.28
1	C	80	ILE	C-N-CA	5.01	127.00	120.28
1	H	213	VAL	CA-C-N	5.01	129.63	123.12
1	H	213	VAL	C-N-CA	5.01	129.63	123.12
2	O	514	ARG	N-CA-CB	5.01	117.28	110.01
2	M	175	GLN	OE1-CD-NE2	-5.01	117.59	122.60
2	N	457	GLN	CA-CB-CG	5.01	124.12	114.10
2	O	127	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	d	79	GLU	CA-C-N	5.01	127.32	120.46
1	d	79	GLU	C-N-CA	5.01	127.32	120.46
1	B	80	ILE	N-CA-CB	5.01	116.41	110.55
2	I	710	TYR	N-CA-CB	5.01	118.42	110.16
2	I	479	ARG	CD-NE-CZ	5.01	131.41	124.40
2	J	629	VAL	N-CA-CB	5.01	116.41	110.55
1	h	80	ILE	CA-C-N	5.01	126.99	120.28
1	h	80	ILE	C-N-CA	5.01	126.99	120.28
2	J	42	ALA	CA-C-N	5.00	126.95	120.44
2	J	42	ALA	C-N-CA	5.00	126.95	120.44
1	a	185	GLN	CB-CG-CD	5.00	121.11	112.60
1	b	208	ALA	CA-C-N	5.00	131.54	123.33
1	b	208	ALA	C-N-CA	5.00	131.54	123.33
2	L	651	ASP	CA-C-N	5.00	126.98	120.28
2	L	651	ASP	C-N-CA	5.00	126.98	120.28
2	M	42	ALA	CA-C-N	5.00	126.94	120.44
2	M	42	ALA	C-N-CA	5.00	126.94	120.44
2	N	662	THR	CA-C-N	5.00	130.84	122.73
2	N	662	THR	C-N-CA	5.00	130.84	122.73
1	b	211	ARG	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	TYR	Sidechain
1	A	169	ARG	Sidechain
1	A	86	ARG	Sidechain
1	B	169	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	C	155	TYR	Sidechain
1	D	86	ARG	Sidechain
1	E	110	TYR	Sidechain
1	F	128	TYR	Sidechain
1	G	100	HIS	Sidechain
1	H	155	TYR	Sidechain
2	I	253	TYR	Sidechain
2	I	298	ASP	Mainchain
2	I	299	SER	Peptide
2	I	300	VAL	Mainchain
2	I	341	TYR	Sidechain
2	I	97	ARG	Sidechain
2	J	162	TYR	Sidechain
2	J	253	TYR	Sidechain
2	J	48	TYR	Sidechain
2	J	97	ARG	Sidechain
2	K	253	TYR	Sidechain
2	K	341	TYR	Sidechain
2	K	423	LYS	Peptide
2	K	467	TYR	Sidechain
2	K	636	TYR	Sidechain
2	K	658	HIS	Sidechain
2	K	708	TYR	Sidechain
2	K	710	TYR	Sidechain
2	K	711	TYR	Sidechain
2	K	97	ARG	Sidechain
2	L	143	ARG	Sidechain
2	L	205	TYR	Sidechain
2	L	253	TYR	Sidechain
2	L	467	TYR	Sidechain
2	L	708	TYR	Sidechain
2	L	97	ARG	Sidechain
2	M	271	PHE	Sidechain
2	M	295	GLN	Mainchain
2	M	342	ARG	Sidechain
2	M	97	ARG	Sidechain
2	N	162	TYR	Sidechain
2	N	243	ARG	Sidechain
2	N	296	ASP	Mainchain
2	N	56	TYR	Sidechain
2	N	97	ARG	Sidechain
2	O	253	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	O	97	ARG	Sidechain
2	P	143	ARG	Sidechain
2	P	205	TYR	Sidechain
2	P	253	TYR	Sidechain
2	P	260	ARG	Sidechain
2	P	296	ASP	Mainchain
2	P	342	ARG	Sidechain
2	P	97	ARG	Sidechain
1	a	155	TYR	Sidechain
1	b	86	ARG	Sidechain
1	c	110	TYR	Sidechain
1	f	110	TYR	Sidechain
1	f	155	TYR	Sidechain
1	g	130	TYR	Sidechain
1	g	86	ARG	Sidechain
1	h	110	TYR	Sidechain
1	h	145	ARG	Sidechain
1	h	86	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2783	2765	2764	4	0
1	B	2783	2765	2764	3	0
1	C	2783	2765	2764	7	0
1	D	2783	2765	2764	5	0
1	E	2783	2765	2764	6	0
1	F	2783	2765	2764	3	0
1	G	2783	2765	2764	21	0
1	H	2783	2765	2764	2	0
1	a	2783	2765	2764	5	0
1	b	2783	2765	2764	4	0
1	c	2783	2765	2762	13	0
1	d	2783	2765	2764	12	0
1	e	2783	2765	2764	3	0
1	f	2783	2765	2764	4	0
1	g	2783	2765	2764	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	h	2783	2765	2764	7	0
2	I	5185	5302	5300	39	0
2	J	5185	5302	5300	40	0
2	K	5185	5302	5300	29	0
2	L	5185	5302	5300	23	0
2	M	5185	5302	5300	26	0
2	N	5185	5302	5300	26	0
2	O	5185	5302	5300	33	0
2	P	5185	5302	5300	33	0
3	I	27	12	12	0	0
3	J	27	12	12	0	0
3	K	27	12	12	0	0
3	L	27	12	12	0	0
3	M	27	12	12	0	0
3	N	27	12	12	0	0
3	O	27	12	12	0	0
3	P	27	12	12	0	0
All	All	86224	86752	86718	304	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 2.

All (304) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:310:ARG:HD3	1:d:58:ARG:NH1	1.46	1.30
1:G:310:ARG:CD	1:d:58:ARG:NH1	2.01	1.23
1:G:310:ARG:CD	1:d:58:ARG:HH12	1.60	1.13
1:G:310:ARG:NE	1:d:58:ARG:NH1	1.97	1.12
1:G:310:ARG:HB3	1:c:40:GLN:OE1	1.52	1.08
1:G:310:ARG:NE	1:d:58:ARG:HH11	1.52	1.06
1:G:310:ARG:HB3	1:c:40:GLN:CD	1.48	1.05
1:G:310:ARG:CB	1:c:40:GLN:OE1	2.02	1.05
1:G:310:ARG:CB	1:c:40:GLN:CD	2.18	1.02
2:K:313:MET:SD	2:K:358:LEU:HD22	2.03	0.97
1:G:310:ARG:HD3	1:d:58:ARG:HH12	1.06	0.89
1:G:310:ARG:CA	1:c:40:GLN:OE1	2.22	0.87
2:J:599:THR:OG1	2:J:604:PHE:O	1.96	0.81
2:M:599:THR:OG1	2:M:604:PHE:O	1.98	0.81
2:I:599:THR:OG1	2:I:604:PHE:O	1.98	0.81
2:L:599:THR:OG1	2:L:604:PHE:O	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:599:THR:OG1	2:N:604:PHE:O	1.99	0.80
2:I:705:TYR:O	2:P:451:ARG:NH1	2.15	0.79
2:P:599:THR:OG1	2:P:604:PHE:O	2.01	0.77
2:O:599:THR:OG1	2:O:604:PHE:O	2.03	0.76
2:J:344:LEU:HG	2:J:347:LYS:HE3	1.70	0.74
2:J:344:LEU:CD1	2:J:347:LYS:HE3	2.19	0.73
2:J:300:VAL:C	2:J:302:LEU:H	1.98	0.72
2:I:309:VAL:HG13	2:I:362:VAL:HG22	1.70	0.72
2:J:344:LEU:CG	2:J:347:LYS:HE3	2.20	0.71
2:M:451:ARG:NH1	2:N:705:TYR:O	2.24	0.70
2:K:312:SER:HB2	2:K:313:MET:HE2	1.74	0.69
2:N:554:THR:HG22	2:N:554:THR:O	1.91	0.69
2:K:313:MET:HG3	2:K:358:LEU:HD13	1.74	0.68
2:J:523:GLN:N	2:J:523:GLN:OE1	2.27	0.68
2:P:297:LYS:C	2:P:299:SER:H	2.02	0.68
2:J:554:THR:HG22	2:J:554:THR:O	1.92	0.67
2:P:523:GLN:N	2:P:523:GLN:OE1	2.27	0.67
2:N:523:GLN:N	2:N:523:GLN:OE1	2.28	0.67
2:K:358:LEU:HG	2:K:359:ASN:N	2.08	0.67
2:I:320:LEU:HD22	2:I:351:LEU:HA	1.76	0.67
2:L:582:LEU:HD12	2:L:586:LEU:HD23	1.77	0.67
2:J:347:LYS:HD2	2:J:348:ARG:N	2.11	0.66
2:O:507:ILE:HD12	2:O:507:ILE:H	1.61	0.66
2:J:323:LEU:HG	2:J:347:LYS:HD3	1.79	0.65
2:P:582:LEU:HD12	2:P:586:LEU:HD23	1.77	0.65
2:K:312:SER:CB	2:K:313:MET:HE2	2.27	0.64
2:P:301:ASP:H	2:P:304:LEU:HB2	1.63	0.63
2:M:623:GLU:OE1	2:M:623:GLU:N	2.31	0.62
2:M:523:GLN:OE1	2:M:523:GLN:N	2.32	0.62
2:L:523:GLN:N	2:L:523:GLN:OE1	2.33	0.62
2:O:300:VAL:C	2:O:302:LEU:H	2.07	0.62
2:O:523:GLN:OE1	2:O:523:GLN:N	2.33	0.62
2:K:313:MET:CG	2:K:358:LEU:HD13	2.29	0.61
2:N:582:LEU:HD12	2:N:586:LEU:HD23	1.81	0.61
2:J:344:LEU:HA	2:J:347:LYS:HG3	1.81	0.61
2:L:157:LEU:HD21	2:L:163:THR:HG23	1.82	0.61
2:I:324:THR:HG23	2:I:347:LYS:HD3	1.81	0.61
2:K:313:MET:SD	2:K:358:LEU:CD2	2.85	0.60
2:I:309:VAL:CG1	2:I:362:VAL:HG22	2.30	0.60
2:J:582:LEU:HD12	2:J:586:LEU:HD23	1.83	0.60
1:G:310:ARG:HA	1:c:40:GLN:OE1	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:323:LEU:HB3	2:J:347:LYS:HE2	1.84	0.60
2:I:523:GLN:N	2:I:523:GLN:OE1	2.34	0.60
2:J:554:THR:O	2:J:554:THR:CG2	2.51	0.59
2:J:344:LEU:HD12	2:J:347:LYS:HE3	1.84	0.59
2:J:33:TRP:O	2:J:37:ILE:HG13	2.03	0.58
2:P:606:LEU:HD12	2:P:607:ILE:N	2.18	0.58
2:N:306:ALA:HB2	2:N:365:MET:SD	2.43	0.58
2:N:554:THR:O	2:N:554:THR:CG2	2.51	0.58
2:M:325:PHE:HA	2:N:347:LYS:HE3	1.84	0.58
2:K:313:MET:HE3	2:K:358:LEU:HB2	1.85	0.58
2:J:323:LEU:CG	2:J:347:LYS:HE2	2.35	0.57
2:I:294:ARG:HA	2:I:297:LYS:HB2	1.87	0.57
2:I:299:SER:HA	2:I:304:LEU:HG	1.87	0.56
2:J:323:LEU:HD12	2:J:347:LYS:HE2	1.86	0.56
2:N:582:LEU:N	2:N:608:PRO:O	2.36	0.56
2:J:323:LEU:CB	2:J:347:LYS:HE2	2.35	0.55
2:M:582:LEU:HD12	2:M:586:LEU:HD23	1.88	0.55
2:K:319:GLN:HA	2:K:322:GLU:HG2	1.89	0.54
2:K:507:ILE:HD12	2:K:507:ILE:H	1.72	0.54
2:I:700:ARG:NH2	2:I:710:TYR:O	2.40	0.54
1:D:272:ASP:OD1	1:D:272:ASP:N	2.41	0.54
2:P:157:LEU:HD21	2:P:163:THR:HG23	1.90	0.54
1:d:272:ASP:OD1	1:d:272:ASP:N	2.41	0.54
2:I:297:LYS:O	2:I:300:VAL:HA	2.08	0.53
1:A:272:ASP:OD1	1:A:272:ASP:N	2.42	0.53
2:O:297:LYS:C	2:O:299:SER:N	2.67	0.53
2:J:700:ARG:NH2	2:J:710:TYR:O	2.41	0.53
2:K:313:MET:HG3	2:K:358:LEU:CD1	2.39	0.52
1:f:110:TYR:HA	1:g:110:TYR:CE2	2.45	0.52
1:a:272:ASP:OD1	1:a:272:ASP:N	2.42	0.52
1:G:310:ARG:CZ	1:d:58:ARG:NH1	2.68	0.52
2:N:307:LYS:CA	2:O:304:LEU:HD13	2.40	0.52
2:O:271:PHE:CD1	2:P:398:ILE:HG12	2.45	0.52
2:L:33:TRP:O	2:L:37:ILE:HG13	2.10	0.52
2:J:527:ASN:ND2	2:J:637:ASP:O	2.42	0.52
1:H:157:ALA:HB1	2:K:337:VAL:HA	1.92	0.51
2:L:608:PRO:O	2:L:608:PRO:HD2	2.09	0.51
2:N:700:ARG:NH2	2:N:710:TYR:O	2.43	0.51
1:G:242:TYR:N	1:G:245:ASP:OD2	2.39	0.51
2:O:310:LEU:CD1	2:P:307:LYS:HE3	2.41	0.51
2:I:451:ARG:NH1	2:J:705:TYR:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:507:ILE:HD12	2:M:507:ILE:H	1.76	0.51
2:O:253:TYR:C	2:O:253:TYR:CD2	2.88	0.51
2:K:313:MET:CG	2:K:358:LEU:HD22	2.40	0.51
2:O:271:PHE:CD1	2:P:398:ILE:CG1	2.94	0.51
2:I:334:TYR:CG	2:I:335:THR:N	2.79	0.51
2:P:527:ASN:ND2	2:P:637:ASP:O	2.42	0.51
2:I:608:PRO:HD2	2:I:608:PRO:O	2.10	0.50
2:M:337:VAL:C	2:M:339:PRO:HD3	2.36	0.50
2:N:457:GLN:OE1	2:N:457:GLN:O	2.29	0.50
2:M:700:ARG:NH2	2:M:710:TYR:O	2.44	0.50
2:M:591:ASP:OD1	2:M:593:THR:HG22	2.12	0.50
2:L:688:ILE:N	2:L:688:ILE:HD12	2.27	0.49
2:P:297:LYS:HB2	2:P:299:SER:HB3	1.94	0.49
2:P:363:THR:O	2:P:366:PRO:HD2	2.13	0.49
1:A:329:VAL:HG21	1:F:315:ALA:HB2	1.94	0.49
2:I:298:ASP:C	2:I:300:VAL:H	2.19	0.49
2:I:527:ASN:ND2	2:I:637:ASP:O	2.41	0.49
2:O:247:ASN:C	2:O:251:ARG:HE	2.20	0.49
1:h:272:ASP:OD1	1:h:272:ASP:N	2.43	0.49
1:C:128:TYR:CD1	1:C:131:ILE:HD11	2.48	0.49
1:F:272:ASP:OD1	1:F:272:ASP:N	2.44	0.49
2:I:271:PHE:CD1	2:J:401:ALA:HB1	2.48	0.49
1:G:310:ARG:HE	1:d:58:ARG:HH11	1.48	0.49
2:K:293:PHE:CE2	2:K:297:LYS:HG2	2.47	0.49
2:M:23:LEU:HD12	2:M:23:LEU:H	1.77	0.49
2:I:343:THR:HG22	2:I:347:LYS:HE3	1.95	0.49
1:E:96:THR:HA	1:E:104:THR:HG23	1.94	0.48
2:J:344:LEU:HG	2:J:347:LYS:CE	2.41	0.48
2:K:338:HIS:C	2:K:340:ALA:H	2.20	0.48
2:P:625:PHE:CE1	2:P:629:VAL:HG11	2.48	0.48
1:a:329:VAL:HG21	1:f:315:ALA:HB2	1.94	0.48
1:C:221:GLU:OE2	1:C:223:ARG:NH2	2.46	0.48
1:G:310:ARG:HD3	1:d:58:ARG:CZ	2.31	0.48
2:K:271:PHE:CD1	2:L:401:ALA:HB3	2.48	0.48
2:I:23:LEU:HD12	2:I:23:LEU:H	1.77	0.48
2:N:347:LYS:HE2	2:N:347:LYS:HA	1.96	0.48
1:g:174:TYR:C	1:g:175:ILE:HD12	2.39	0.48
1:c:221:GLU:OE2	1:c:223:ARG:NH2	2.46	0.48
2:K:521:MET:HA	2:K:524:ALA:HB3	1.95	0.48
2:J:437:MET:SD	2:J:437:MET:C	2.96	0.47
2:L:507:ILE:HD12	2:L:507:ILE:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:504:ASP:OD1	2:M:505:LEU:N	2.47	0.47
1:G:272:ASP:OD1	1:G:272:ASP:N	2.43	0.47
2:M:582:LEU:N	2:M:608:PRO:O	2.46	0.47
2:N:527:ASN:ND2	2:N:637:ASP:O	2.43	0.47
2:I:145:LYS:C	2:I:145:LYS:HE2	2.39	0.47
2:N:23:LEU:HD12	2:N:23:LEU:H	1.80	0.47
2:O:504:ASP:OD1	2:O:505:LEU:N	2.47	0.47
2:P:591:ASP:OD1	2:P:593:THR:HG22	2.15	0.47
1:f:272:ASP:OD1	1:f:272:ASP:N	2.44	0.47
1:A:174:TYR:C	1:A:175:ILE:HD12	2.39	0.47
2:L:606:LEU:HD12	2:L:607:ILE:N	2.30	0.47
2:O:23:LEU:HD12	2:O:23:LEU:H	1.79	0.47
2:O:403:THR:HG22	2:O:405:GLY:H	1.79	0.47
2:P:295:GLN:HA	2:P:300:VAL:HG22	1.95	0.47
2:P:299:SER:O	2:P:301:ASP:C	2.58	0.47
1:D:129:PRO:HG2	1:E:98:TRP:CD2	2.50	0.47
2:P:298:ASP:C	2:P:300:VAL:H	2.23	0.47
2:I:297:LYS:O	2:I:300:VAL:CA	2.63	0.47
2:J:306:ALA:HB1	2:K:299:SER:HB3	1.97	0.47
2:N:307:LYS:N	2:O:304:LEU:HD13	2.30	0.47
2:O:457:GLN:OE1	2:O:457:GLN:O	2.33	0.47
2:M:337:VAL:HG13	1:h:158:ASP:CG	2.41	0.46
1:G:221:GLU:OE2	1:G:223:ARG:NH2	2.48	0.46
2:J:457:GLN:OE1	2:J:457:GLN:O	2.34	0.46
2:I:457:GLN:O	2:I:457:GLN:OE1	2.33	0.46
2:I:582:LEU:O	2:I:586:LEU:HD23	2.15	0.46
2:P:294:ARG:HG3	2:P:372:ILE:HD12	1.98	0.46
1:D:175:ILE:HD12	1:D:175:ILE:N	2.31	0.45
2:P:259:GLU:C	2:P:263:ALA:HB2	2.41	0.45
1:h:175:ILE:HD12	1:h:175:ILE:N	2.31	0.45
2:I:616:PRO:O	2:I:619:LEU:N	2.49	0.45
2:K:313:MET:SD	2:K:358:LEU:CB	3.03	0.45
2:P:625:PHE:CD1	2:P:625:PHE:C	2.93	0.45
1:d:175:ILE:N	1:d:175:ILE:HD12	2.31	0.45
1:e:102:GLU:CD	1:e:102:GLU:H	2.23	0.45
1:G:310:ARG:CG	1:c:40:GLN:OE1	2.62	0.45
2:I:688:ILE:HD12	2:I:688:ILE:N	2.31	0.45
2:J:323:LEU:CD1	2:J:347:LYS:HE2	2.46	0.45
2:O:577:ASN:OD1	2:O:597:LYS:NZ	2.37	0.45
2:P:700:ARG:NH2	2:P:710:TYR:O	2.49	0.45
1:C:242:TYR:N	1:C:245:ASP:OD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:174:TYR:C	1:b:175:ILE:HD12	2.41	0.45
1:B:272:ASP:OD1	1:B:272:ASP:N	2.46	0.45
1:E:175:ILE:N	1:E:175:ILE:HD12	2.31	0.45
2:I:580:ASN:N	2:I:584:GLU:OE1	2.48	0.45
2:O:299:SER:HA	2:O:305:GLU:HG3	1.98	0.45
2:O:568:GLY:O	2:O:609:ARG:NH2	2.49	0.45
2:J:146:GLU:H	2:J:146:GLU:CD	2.25	0.44
2:K:271:PHE:CD2	2:L:398:ILE:CG1	3.01	0.44
1:h:102:GLU:CD	1:h:102:GLU:H	2.25	0.44
2:P:294:ARG:HB3	2:P:299:SER:O	2.16	0.44
2:P:371:GLU:CD	2:P:374:ARG:HE	2.25	0.44
2:I:299:SER:CB	2:I:304:LEU:HB2	2.48	0.44
2:J:385:VAL:HG21	2:K:394:GLN:CD	2.42	0.44
2:P:507:ILE:HD12	2:P:507:ILE:H	1.83	0.44
2:J:23:LEU:HD12	2:J:23:LEU:H	1.83	0.44
2:J:337:VAL:HG13	2:J:338:HIS:H	1.83	0.44
2:L:293:PHE:CZ	2:L:297:LYS:HE3	2.52	0.44
2:M:457:GLN:C	2:M:457:GLN:CD	2.85	0.44
1:G:175:ILE:N	1:G:175:ILE:HD12	2.33	0.44
2:I:316:ILE:HG13	2:I:358:LEU:CD2	2.47	0.44
2:K:297:LYS:HA	2:K:301:ASP:CB	2.48	0.44
2:I:225:LYS:HE3	2:I:225:LYS:C	2.43	0.44
2:M:29:GLU:OE1	2:M:29:GLU:C	2.61	0.44
2:N:686:ASN:HB2	2:N:688:ILE:HD12	2.00	0.44
1:B:175:ILE:N	1:B:175:ILE:HD12	2.32	0.44
1:F:175:ILE:HD12	1:F:175:ILE:N	2.32	0.44
2:K:253:TYR:C	2:K:253:TYR:CD2	2.95	0.44
2:J:714:GLU:OE2	2:J:716:LYS:NZ	2.46	0.44
2:I:577:ASN:OD1	2:I:597:LYS:NZ	2.35	0.43
2:M:271:PHE:CE1	2:N:398:ILE:HG12	2.53	0.43
2:N:29:GLU:C	2:N:29:GLU:OE1	2.61	0.43
2:O:146:GLU:CD	2:O:146:GLU:H	2.26	0.43
2:O:527:ASN:ND2	2:O:637:ASP:O	2.44	0.43
1:B:329:VAL:HG23	1:E:303:PRO:HG3	2.00	0.43
1:C:175:ILE:HD12	1:C:175:ILE:N	2.33	0.43
2:I:320:LEU:HD21	2:I:354:GLU:CB	2.49	0.43
1:A:128:TYR:CG	1:A:129:PRO:HD2	2.54	0.43
1:E:242:TYR:N	1:E:245:ASP:OD2	2.45	0.43
2:I:368:THR:O	2:I:372:ILE:HD12	2.19	0.43
2:N:563:CYS:O	2:N:563:CYS:SG	2.77	0.43
2:N:714:GLU:OE2	2:N:716:LYS:NZ	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:242:TYR:N	1:c:245:ASP:OD2	2.46	0.43
2:L:370:GLN:HE22	2:M:288:ASN:N	2.17	0.43
1:c:103:LEU:C	1:c:103:LEU:HD13	2.44	0.43
1:b:102:GLU:H	1:b:102:GLU:CD	2.27	0.43
1:b:329:VAL:HG23	1:e:303:PRO:HG3	2.01	0.43
2:I:377:ARG:HG3	2:J:387:MET:SD	2.58	0.42
2:L:23:LEU:H	2:L:23:LEU:HD12	1.83	0.42
2:O:271:PHE:CD1	2:P:398:ILE:HG13	2.55	0.42
2:P:586:LEU:HD11	2:P:625:PHE:HB2	2.01	0.42
2:M:325:PHE:CA	2:N:347:LYS:HE3	2.50	0.42
1:a:174:TYR:OH	1:h:196:ASP:OD1	2.35	0.42
1:c:175:ILE:HD12	1:c:175:ILE:N	2.34	0.42
2:J:29:GLU:C	2:J:29:GLU:OE1	2.61	0.42
2:K:313:MET:HG3	2:K:358:LEU:HD22	2.02	0.42
2:L:259:GLU:O	2:L:263:ALA:N	2.49	0.42
2:P:457:GLN:C	2:P:457:GLN:OE1	2.62	0.42
1:a:175:ILE:HD12	1:a:175:ILE:N	2.34	0.42
1:f:102:GLU:CD	1:f:102:GLU:H	2.26	0.42
1:C:128:TYR:CD1	1:C:129:PRO:HD2	2.55	0.42
2:N:437:MET:C	2:N:437:MET:SD	3.02	0.42
2:P:298:ASP:C	2:P:300:VAL:N	2.76	0.42
2:O:700:ARG:NH2	2:O:710:TYR:O	2.52	0.42
2:J:344:LEU:HA	2:J:347:LYS:CG	2.48	0.42
2:L:563:CYS:O	2:L:563:CYS:SG	2.77	0.42
2:M:437:MET:SD	2:M:437:MET:C	3.03	0.42
2:K:223:ASN:HD21	2:K:231:SER:N	2.17	0.42
2:L:29:GLU:C	2:L:29:GLU:OE1	2.62	0.42
2:M:325:PHE:HA	2:N:347:LYS:HD2	2.02	0.42
2:M:521:MET:HE1	2:M:638:LEU:HD11	2.01	0.42
2:M:336:LYS:HG3	1:a:155:TYR:CE1	2.55	0.42
2:O:628:LEU:C	2:O:628:LEU:HD23	2.45	0.42
2:K:355:LYS:HA	2:K:358:LEU:HD23	2.02	0.42
2:L:437:MET:SD	2:L:437:MET:C	3.03	0.42
2:P:295:GLN:HA	2:P:300:VAL:CA	2.49	0.42
1:h:376:ILE:O	1:h:376:ILE:HG22	2.20	0.42
2:O:420:LEU:HG	2:O:421:LYS:H	1.85	0.42
1:g:221:GLU:OE2	1:g:223:ARG:NH2	2.53	0.42
1:h:130:TYR:HB3	1:h:155:TYR:CZ	2.55	0.42
2:I:563:CYS:O	2:I:563:CYS:SG	2.78	0.41
1:g:307:GLU:OE2	1:g:310:ARG:NH2	2.53	0.41
2:O:225:LYS:C	2:O:225:LYS:HE3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:437:MET:SD	2:P:437:MET:C	3.03	0.41
1:c:102:GLU:H	1:c:102:GLU:CD	2.28	0.41
1:d:303:PRO:HG3	1:e:329:VAL:HG23	2.02	0.41
2:I:316:ILE:CG1	2:I:358:LEU:HG	2.50	0.41
2:J:546:ASN:O	2:J:550:VAL:HG23	2.20	0.41
2:K:146:GLU:H	2:K:146:GLU:CD	2.27	0.41
2:O:437:MET:SD	2:O:437:MET:C	3.04	0.41
1:G:307:GLU:OE2	1:G:310:ARG:NH2	2.53	0.41
2:J:323:LEU:HB3	2:J:347:LYS:CE	2.48	0.41
2:L:577:ASN:OD1	2:L:597:LYS:NZ	2.46	0.41
2:O:628:LEU:HD23	2:O:628:LEU:O	2.19	0.41
1:C:110:TYR:CE1	1:D:110:TYR:CZ	3.09	0.41
2:I:299:SER:HA	2:I:304:LEU:CG	2.49	0.41
2:J:253:TYR:CD2	2:J:253:TYR:C	2.98	0.41
2:N:530:MET:HE2	2:N:659:VAL:HG11	2.02	0.41
2:P:301:ASP:HB2	2:P:304:LEU:HD13	2.03	0.41
1:D:303:PRO:HG3	1:E:329:VAL:HG23	2.02	0.41
2:L:698:ILE:HG21	2:L:710:TYR:HB2	2.03	0.41
2:O:313:MET:SD	2:O:355:LYS:HG3	2.61	0.41
2:O:506:ALA:O	2:O:510:ILE:HD12	2.19	0.41
2:L:333:LEU:HG	2:L:334:TYR:N	2.35	0.41
2:M:146:GLU:H	2:M:146:GLU:CD	2.29	0.41
2:O:271:PHE:CD1	2:O:271:PHE:C	2.99	0.41
2:I:56:TYR:CD2	2:I:239:ARG:HG2	2.56	0.41
2:I:437:MET:SD	2:I:437:MET:C	3.03	0.41
2:K:602:ALA:C	2:K:604:PHE:H	2.29	0.41
2:M:527:ASN:ND2	2:M:637:ASP:O	2.49	0.41
1:b:106:PRO:CB	1:g:99:ASP:H	2.34	0.41
1:c:272:ASP:OD1	1:c:272:ASP:N	2.47	0.41
2:J:324:THR:O	2:J:325:PHE:C	2.63	0.40
2:J:563:CYS:O	2:J:563:CYS:SG	2.78	0.40
2:K:530:MET:SD	2:K:643:THR:HG21	2.61	0.40
2:O:145:LYS:HE2	2:O:145:LYS:C	2.46	0.40
1:C:117:GLY:C	1:C:119:TRP:H	2.28	0.40
1:H:376:ILE:O	1:H:376:ILE:HG22	2.20	0.40
2:I:320:LEU:CD2	2:I:351:LEU:HA	2.48	0.40
2:L:322:GLU:CG	2:L:344:LEU:HD22	2.51	0.40
1:g:359:LEU:O	1:g:362:THR:HG22	2.21	0.40
2:M:563:CYS:O	2:M:563:CYS:SG	2.79	0.40
2:L:586:LEU:HD11	2:L:625:PHE:HB2	2.04	0.40
2:N:606:LEU:HD23	2:N:607:ILE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:145:LYS:HA	2:O:148:ALA:HB3	2.04	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	356/394 (90%)	333 (94%)	20 (6%)	3 (1%)	16	54
1	B	356/394 (90%)	337 (95%)	18 (5%)	1 (0%)	36	72
1	C	356/394 (90%)	342 (96%)	11 (3%)	3 (1%)	16	54
1	D	356/394 (90%)	339 (95%)	17 (5%)	0	100	100
1	E	356/394 (90%)	338 (95%)	16 (4%)	2 (1%)	21	59
1	F	356/394 (90%)	345 (97%)	11 (3%)	0	100	100
1	G	356/394 (90%)	345 (97%)	10 (3%)	1 (0%)	36	72
1	H	356/394 (90%)	338 (95%)	13 (4%)	5 (1%)	9	40
1	a	356/394 (90%)	339 (95%)	17 (5%)	0	100	100
1	b	356/394 (90%)	338 (95%)	18 (5%)	0	100	100
1	c	356/394 (90%)	345 (97%)	10 (3%)	1 (0%)	36	72
1	d	356/394 (90%)	345 (97%)	10 (3%)	1 (0%)	36	72
1	e	356/394 (90%)	340 (96%)	16 (4%)	0	100	100
1	f	356/394 (90%)	337 (95%)	18 (5%)	1 (0%)	36	72
1	g	356/394 (90%)	337 (95%)	19 (5%)	0	100	100
1	h	356/394 (90%)	341 (96%)	14 (4%)	1 (0%)	36	72
2	I	662/738 (90%)	637 (96%)	20 (3%)	5 (1%)	16	54
2	J	662/738 (90%)	630 (95%)	24 (4%)	8 (1%)	10	44
2	K	662/738 (90%)	622 (94%)	34 (5%)	6 (1%)	14	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	662/738 (90%)	636 (96%)	24 (4%)	2 (0%)	36	72
2	M	662/738 (90%)	636 (96%)	21 (3%)	5 (1%)	16	54
2	N	662/738 (90%)	637 (96%)	20 (3%)	5 (1%)	16	54
2	O	662/738 (90%)	640 (97%)	16 (2%)	6 (1%)	14	51
2	P	662/738 (90%)	633 (96%)	25 (4%)	4 (1%)	21	59
All	All	10992/12208 (90%)	10510 (96%)	422 (4%)	60 (0%)	26	63

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	300	VAL
2	J	301	ASP
2	J	326	LYS
2	J	327	GLU
2	J	328	ALA
2	K	339	PRO
2	M	298	ASP
2	M	335	THR
2	N	298	ASP
2	N	420	LEU
2	O	420	LEU
2	P	298	ASP
1	H	157	ALA
2	I	120	ILE
2	J	297	LYS
2	K	120	ILE
2	M	299	SER
2	M	333	LEU
2	N	120	ILE
2	O	297	LYS
2	O	299	SER
2	O	301	ASP
2	O	407	VAL
2	P	120	ILE
2	P	297	LYS
1	A	122	PRO
1	C	118	ASN
1	H	234	ASP
2	I	299	SER
2	J	338	HIS

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Mol	Chain	Res	Type
2	P	299	SER
1	C	130	TYR
1	H	99	ASP
2	K	536	PRO
2	K	603	LYS
2	L	120	ILE
1	c	130	TYR
1	d	130	TYR
1	h	130	TYR
1	A	120	VAL
1	H	130	TYR
2	K	333	LEU
2	K	407	VAL
2	M	120	ILE
1	f	180	ASN
1	B	158	ASP
1	E	105	THR
2	I	302	LEU
2	J	339	PRO
2	J	407	VAL
2	N	224	GLY
2	N	297	LYS
1	C	105	THR
1	H	159	PRO
2	I	337	VAL
2	O	120	ILE
1	A	158	ASP
2	L	338	HIS
1	E	122	PRO
1	G	131	ILE

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	307/342 (90%)	303 (99%)	4 (1%)	61 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	307/342 (90%)	305 (99%)	2 (1%)	76	81
1	C	307/342 (90%)	303 (99%)	4 (1%)	61	74
1	D	307/342 (90%)	304 (99%)	3 (1%)	68	78
1	E	307/342 (90%)	306 (100%)	1 (0%)	86	86
1	F	307/342 (90%)	299 (97%)	8 (3%)	40	62
1	G	307/342 (90%)	303 (99%)	4 (1%)	61	74
1	H	307/342 (90%)	305 (99%)	2 (1%)	76	81
1	a	307/342 (90%)	298 (97%)	9 (3%)	37	58
1	b	307/342 (90%)	304 (99%)	3 (1%)	68	78
1	c	307/342 (90%)	303 (99%)	4 (1%)	61	74
1	d	307/342 (90%)	305 (99%)	2 (1%)	76	81
1	e	307/342 (90%)	305 (99%)	2 (1%)	76	81
1	f	307/342 (90%)	302 (98%)	5 (2%)	55	70
1	g	307/342 (90%)	303 (99%)	4 (1%)	61	74
1	h	307/342 (90%)	302 (98%)	5 (2%)	55	70
2	I	570/630 (90%)	549 (96%)	21 (4%)	30	51
2	J	570/630 (90%)	554 (97%)	16 (3%)	38	60
2	K	570/630 (90%)	540 (95%)	30 (5%)	20	41
2	L	570/630 (90%)	548 (96%)	22 (4%)	28	49
2	M	570/630 (90%)	558 (98%)	12 (2%)	47	65
2	N	570/630 (90%)	554 (97%)	16 (3%)	38	60
2	O	570/630 (90%)	553 (97%)	17 (3%)	36	57
2	P	570/630 (90%)	545 (96%)	25 (4%)	25	47
All	All	9472/10512 (90%)	9251 (98%)	221 (2%)	44	64

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	TYR
1	A	179	VAL
1	A	216	THR
1	A	254	ASP
1	B	84	GLN
1	B	165	ILE

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Mol	Chain	Res	Type
1	C	84	GLN
1	C	96	THR
1	C	102	GLU
1	C	296	SER
1	D	103	LEU
1	D	118	ASN
1	D	130	TYR
1	E	140	THR
1	F	98	TRP
1	F	102	GLU
1	F	128	TYR
1	F	130	TYR
1	F	134	VAL
1	F	140	THR
1	F	175	ILE
1	F	182	SER
1	G	102	GLU
1	G	128	TYR
1	G	161	VAL
1	G	164	ASN
1	H	71	ARG
1	H	98	TRP
2	I	126	ASP
2	I	129	MET
2	I	145	LYS
2	I	181	LYS
2	I	225	LYS
2	I	259	GLU
2	I	261	LYS
2	I	301	ASP
2	I	316	ILE
2	I	326	LYS
2	I	332	LYS
2	I	334	TYR
2	I	346	GLU
2	I	348	ARG
2	I	351	LEU
2	I	372	ILE
2	I	479	ARG
2	I	544	CYS
2	I	547	LEU
2	I	601	ILE

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Mol	Chain	Res	Type
2	I	672	THR
2	J	23	LEU
2	J	53	THR
2	J	55	ILE
2	J	92	GLN
2	J	173	ARG
2	J	323	LEU
2	J	335	THR
2	J	342	ARG
2	J	347	LYS
2	J	354	GLU
2	J	384	GLN
2	J	392	LYS
2	J	467	TYR
2	J	544	CYS
2	J	547	LEU
2	J	697	SER
2	K	23	LEU
2	K	108	ASP
2	K	121	PHE
2	K	129	MET
2	K	147	MET
2	K	287	GLU
2	K	289	LYS
2	K	297	LYS
2	K	301	ASP
2	K	302	LEU
2	K	304	LEU
2	K	313	MET
2	K	358	LEU
2	K	367	LYS
2	K	388	GLN
2	K	392	LYS
2	K	409	ILE
2	K	479	ARG
2	K	587	ILE
2	K	609	ARG
2	K	618	GLU
2	K	634	LYS
2	K	637	ASP
2	K	649	VAL
2	K	657	ARG

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Mol	Chain	Res	Type
2	K	659	VAL
2	K	664	MET
2	K	682	ARG
2	K	708	TYR
2	K	713	TYR
2	L	37	ILE
2	L	55	ILE
2	L	118	PHE
2	L	129	MET
2	L	157	LEU
2	L	164	LEU
2	L	205	TYR
2	L	287	GLU
2	L	289	LYS
2	L	332	LYS
2	L	334	TYR
2	L	337	VAL
2	L	341	TYR
2	L	345	LEU
2	L	367	LYS
2	L	390	LEU
2	L	434	LEU
2	L	457	GLN
2	L	507	ILE
2	L	544	CYS
2	L	547	LEU
2	L	672	THR
2	M	55	ILE
2	M	129	MET
2	M	132	GLN
2	M	175	GLN
2	M	210	MET
2	M	259	GLU
2	M	332	LYS
2	M	388	GLN
2	M	507	ILE
2	M	544	CYS
2	M	547	LEU
2	M	672	THR
2	N	118	PHE
2	N	225	LYS
2	N	259	GLU

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Mol	Chain	Res	Type
2	N	300	VAL
2	N	305	GLU
2	N	332	LYS
2	N	339	PRO
2	N	347	LYS
2	N	359	ASN
2	N	392	LYS
2	N	406	ASP
2	N	434	LEU
2	N	479	ARG
2	N	541	THR
2	N	544	CYS
2	N	547	LEU
2	O	92	GLN
2	O	108	ASP
2	O	129	MET
2	O	145	LYS
2	O	225	LYS
2	O	260	ARG
2	O	289	LYS
2	O	302	LEU
2	O	304	LEU
2	O	305	GLU
2	O	338	HIS
2	O	377	ARG
2	O	388	GLN
2	O	507	ILE
2	O	544	CYS
2	O	547	LEU
2	O	601	ILE
2	P	55	ILE
2	P	92	GLN
2	P	129	MET
2	P	147	MET
2	P	157	LEU
2	P	188	MET
2	P	205	TYR
2	P	260	ARG
2	P	278	GLU
2	P	305	GLU
2	P	332	LYS
2	P	343	THR

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Mol	Chain	Res	Type
2	P	345	LEU
2	P	346	GLU
2	P	367	LYS
2	P	388	GLN
2	P	420	LEU
2	P	457	GLN
2	P	467	TYR
2	P	479	ARG
2	P	503	THR
2	P	507	ILE
2	P	544	CYS
2	P	547	LEU
2	P	672	THR
1	a	78	SER
1	a	99	ASP
1	a	102	GLU
1	a	115	ASP
1	a	116	THR
1	a	130	TYR
1	a	172	LYS
1	a	175	ILE
1	a	182	SER
1	b	102	GLU
1	b	179	VAL
1	b	254	ASP
1	c	94	ASN
1	c	102	GLU
1	c	103	LEU
1	c	105	THR
1	d	84	GLN
1	d	140	THR
1	e	102	GLU
1	e	140	THR
1	f	102	GLU
1	f	140	THR
1	f	154	THR
1	f	175	ILE
1	f	179	VAL
1	g	102	GLU
1	g	105	THR
1	g	143	GLU
1	g	158	ASP

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Mol	Chain	Res	Type
1	h	98	TRP
1	h	102	GLU
1	h	105	THR
1	h	172	LYS
1	h	175	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	118	ASN
1	C	94	ASN
1	C	164	ASN
1	D	40	GLN
1	D	94	ASN
1	D	135	HIS
1	D	164	ASN
1	D	184	GLN
1	E	135	HIS
1	E	189	ASN
1	E	236	ASN
1	F	94	ASN
1	F	109	GLN
1	F	135	HIS
1	F	236	ASN
1	G	68	ASN
1	G	94	ASN
1	G	232	ASN
1	H	68	ASN
1	H	94	ASN
2	I	66	GLN
2	I	161	ASN
2	I	175	GLN
2	I	178	GLN
2	I	193	HIS
2	I	555	ASN
2	I	630	ASN
2	J	369	GLN
2	J	476	GLN
2	J	580	ASN
2	K	275	GLN
2	K	359	ASN

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Mol	Chain	Res	Type
2	K	394	GLN
2	K	476	GLN
2	K	611	GLN
2	K	685	GLN
2	L	175	GLN
2	L	291	ASN
2	L	383	GLN
2	L	457	GLN
2	L	518	HIS
2	L	555	ASN
2	L	580	ASN
2	M	132	GLN
2	M	274	GLN
2	M	457	GLN
2	M	555	ASN
2	M	630	ASN
2	N	241	GLN
2	N	257	ASN
2	N	319	GLN
2	N	338	HIS
2	N	388	GLN
2	N	476	GLN
2	N	580	ASN
2	O	159	ASN
2	O	384	GLN
2	O	416	GLN
2	O	476	GLN
2	O	555	ASN
2	O	630	ASN
2	P	175	GLN
2	P	319	GLN
2	P	391	ASN
2	P	580	ASN
1	a	84	GLN
1	b	109	GLN
1	b	189	ASN
1	b	353	ASN
1	c	109	GLN
1	c	121	GLN
1	c	189	ASN
1	d	40	GLN
1	d	94	ASN

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Mol	Chain	Res	Type
1	d	164	ASN
1	d	184	GLN
1	e	84	GLN
1	e	94	ASN
1	f	94	ASN
1	f	236	ASN
1	g	68	ASN
1	g	84	GLN
1	g	180	ASN
1	g	232	ASN
1	h	94	ASN
1	h	121	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	M	1000	-	27,29,29	0.98	1 (3%)	42,45,45	1.22	6 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	I	1000	-	27,29,29	0.95	0	42,45,45	1.27	7 (16%)
3	ADP	J	1000	-	27,29,29	1.04	0	42,45,45	1.31	6 (14%)
3	ADP	L	1000	-	27,29,29	0.97	1 (3%)	42,45,45	1.13	5 (11%)
3	ADP	N	1000	-	27,29,29	1.01	1 (3%)	42,45,45	1.29	5 (11%)
3	ADP	P	1000	-	27,29,29	0.95	0	42,45,45	1.28	8 (19%)
3	ADP	O	1000	-	27,29,29	0.95	1 (3%)	42,45,45	1.27	7 (16%)
3	ADP	K	1000	-	27,29,29	0.99	1 (3%)	42,45,45	1.29	7 (16%)

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	ADP	M	1000	-	-	8/16/32/32	0/3/3/3
3	ADP	I	1000	-	-	4/16/32/32	0/3/3/3
3	ADP	J	1000	-	-	4/16/32/32	0/3/3/3
3	ADP	L	1000	-	-	0/16/32/32	0/3/3/3
3	ADP	N	1000	-	-	4/16/32/32	0/3/3/3
3	ADP	P	1000	-	-	1/16/32/32	0/3/3/3
3	ADP	O	1000	-	-	1/16/32/32	0/3/3/3
3	ADP	K	1000	-	-	2/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1000	ADP	C8-N7	2.18	1.35	1.31
3	O	1000	ADP	C8-N7	2.17	1.35	1.31
3	K	1000	ADP	C8-N7	2.09	1.35	1.31
3	N	1000	ADP	C8-N7	2.08	1.35	1.31
3	L	1000	ADP	C8-N7	2.07	1.35	1.31

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1000	ADP	C5-C4-N3	-3.32	122.42	126.75
3	P	1000	ADP	C5-C4-N3	-3.16	122.63	126.75
3	I	1000	ADP	C5-C4-N3	-3.14	122.65	126.75
3	N	1000	ADP	C5-C4-N3	-3.03	122.80	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1000	ADP	O2B-PB-O3A	2.94	114.51	104.64
3	K	1000	ADP	C5-C4-N3	-2.92	122.94	126.75
3	M	1000	ADP	O3B-PB-O3A	2.88	114.30	104.64
3	M	1000	ADP	C5-C4-N3	-2.85	123.03	126.75
3	L	1000	ADP	PA-O3A-PB	-2.78	123.30	132.83
3	L	1000	ADP	C5-C4-N3	-2.77	123.14	126.75
3	O	1000	ADP	C5-C4-N3	-2.68	123.25	126.75
3	J	1000	ADP	C4-C5-N7	2.68	113.89	110.62
3	J	1000	ADP	C5-C6-N1	2.60	122.98	117.39
3	K	1000	ADP	C4-C5-N7	2.59	113.77	110.62
3	I	1000	ADP	C4-C5-N7	2.59	113.77	110.62
3	P	1000	ADP	C4-C5-N7	2.48	113.64	110.62
3	J	1000	ADP	N3-C4-N9	2.48	131.17	127.08
3	O	1000	ADP	C4-C5-N7	2.48	113.64	110.62
3	K	1000	ADP	PA-O3A-PB	-2.46	124.37	132.83
3	I	1000	ADP	PA-O3A-PB	-2.44	124.46	132.83
3	I	1000	ADP	N3-C4-N9	2.41	131.06	127.08
3	O	1000	ADP	O2B-PB-O3A	2.40	112.69	104.64
3	P	1000	ADP	C5-C6-N1	2.39	122.52	117.39
3	K	1000	ADP	C5-C6-N1	2.39	122.51	117.39
3	P	1000	ADP	PA-O3A-PB	-2.38	124.67	132.83
3	M	1000	ADP	N6-C6-N1	-2.37	113.17	118.35
3	I	1000	ADP	C5-C6-N1	2.34	122.42	117.39
3	O	1000	ADP	PA-O3A-PB	-2.33	124.82	132.83
3	M	1000	ADP	C5-C6-N1	2.31	122.36	117.39
3	K	1000	ADP	O3B-PB-O3A	2.31	112.37	104.64
3	O	1000	ADP	C5-C6-N1	2.30	122.33	117.39
3	M	1000	ADP	C4-C5-N7	2.27	113.38	110.62
3	N	1000	ADP	C5-C6-N1	2.26	122.24	117.39
3	L	1000	ADP	C5-C6-N1	2.25	122.23	117.39
3	K	1000	ADP	O4'-C1'-C2'	-2.24	101.76	106.64
3	P	1000	ADP	O4'-C1'-C2'	-2.23	101.77	106.64
3	O	1000	ADP	O3B-PB-O3A	2.23	112.11	104.64
3	K	1000	ADP	N6-C6-N1	-2.23	113.47	118.35
3	P	1000	ADP	N3-C4-N9	2.21	130.72	127.08
3	L	1000	ADP	C4-C5-N7	2.20	113.30	110.62
3	N	1000	ADP	C4-C5-N7	2.20	113.29	110.62
3	N	1000	ADP	N6-C6-N1	-2.18	113.58	118.35
3	J	1000	ADP	C2-N1-C6	-2.12	115.13	118.77
3	I	1000	ADP	O4'-C4'-C3'	-2.11	100.93	105.11
3	P	1000	ADP	O3B-PB-O3A	2.11	111.70	104.64
3	L	1000	ADP	N6-C6-N1	-2.09	113.77	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1000	ADP	N6-C6-N1	-2.09	113.78	118.35
3	J	1000	ADP	PA-O3A-PB	-2.07	125.74	132.83
3	M	1000	ADP	PA-O3A-PB	-2.05	125.79	132.83
3	P	1000	ADP	C2-N1-C6	-2.03	115.28	118.77
3	I	1000	ADP	C2-N1-C6	-2.00	115.33	118.77

There are no chirality outliers.

All (24) torsion outliers are listed below:

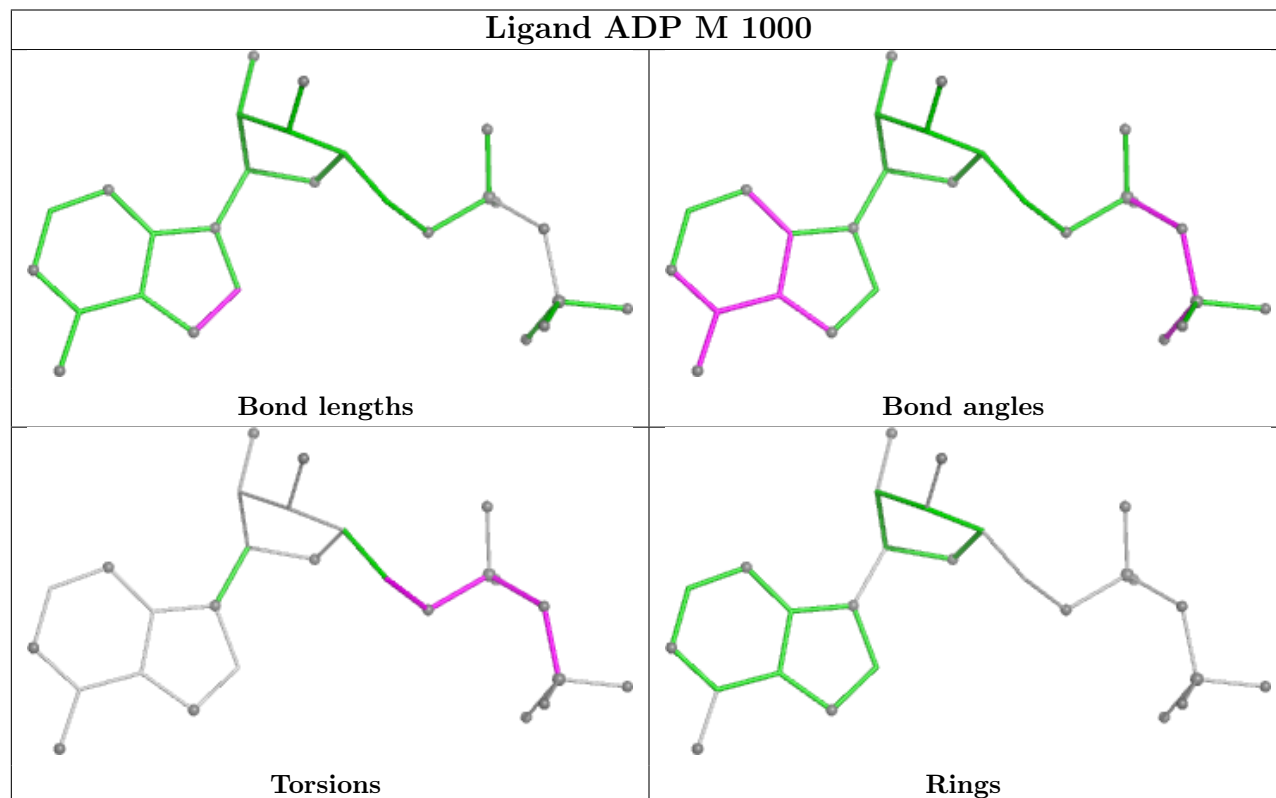
Mol	Chain	Res	Type	Atoms
3	J	1000	ADP	PA-O3A-PB-O3B
3	M	1000	ADP	PA-O3A-PB-O2B
3	M	1000	ADP	PA-O3A-PB-O3B
3	M	1000	ADP	C5'-O5'-PA-O1A
3	M	1000	ADP	C5'-O5'-PA-O2A
3	I	1000	ADP	C3'-C4'-C5'-O5'
3	N	1000	ADP	O4'-C4'-C5'-O5'
3	M	1000	ADP	C4'-C5'-O5'-PA
3	N	1000	ADP	C3'-C4'-C5'-O5'
3	J	1000	ADP	C3'-C4'-C5'-O5'
3	I	1000	ADP	O4'-C4'-C5'-O5'
3	N	1000	ADP	PA-O3A-PB-O1B
3	O	1000	ADP	PB-O3A-PA-O1A
3	J	1000	ADP	C4'-C5'-O5'-PA
3	M	1000	ADP	PB-O3A-PA-O5'
3	N	1000	ADP	PB-O3A-PA-O5'
3	J	1000	ADP	O4'-C4'-C5'-O5'
3	I	1000	ADP	PA-O3A-PB-O2B
3	M	1000	ADP	C5'-O5'-PA-O3A
3	K	1000	ADP	PB-O3A-PA-O1A
3	I	1000	ADP	C2'-C1'-N9-C8
3	M	1000	ADP	PA-O3A-PB-O1B
3	K	1000	ADP	PB-O3A-PA-O2A
3	P	1000	ADP	PB-O3A-PA-O2A

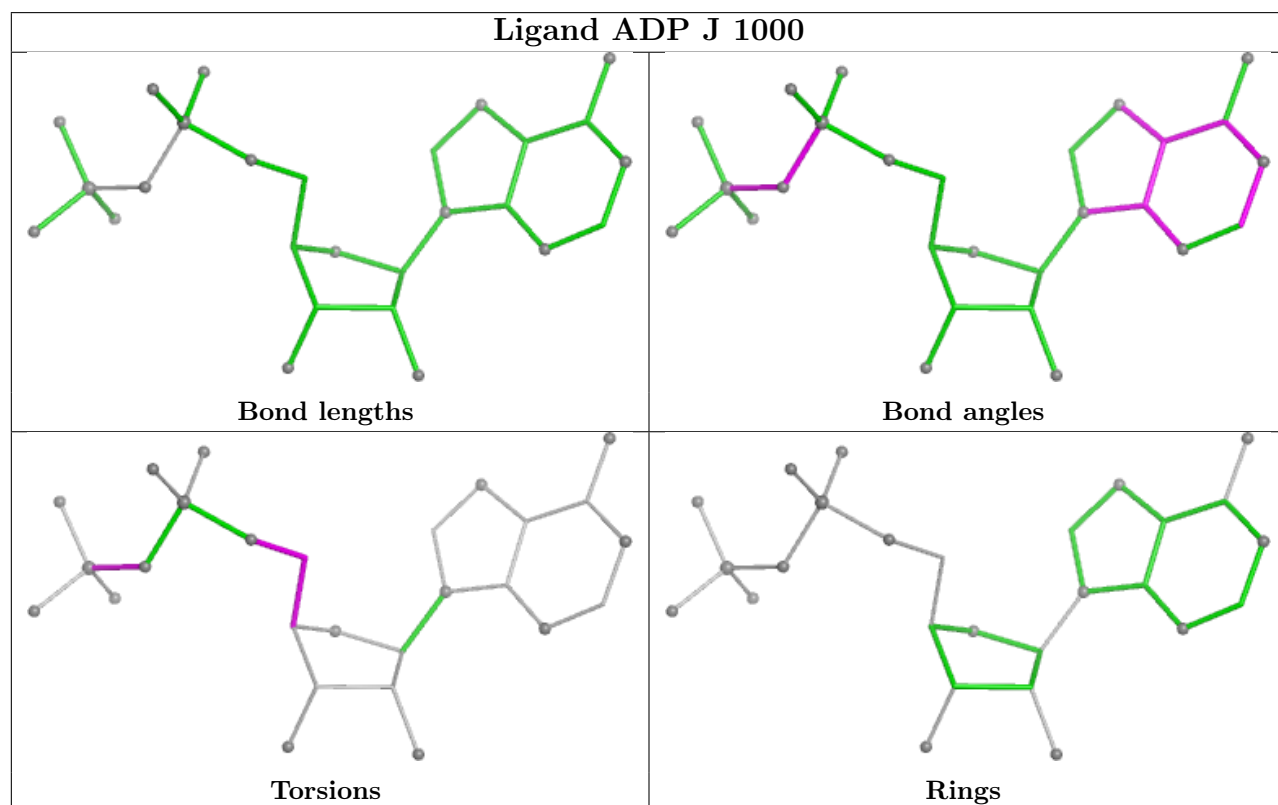
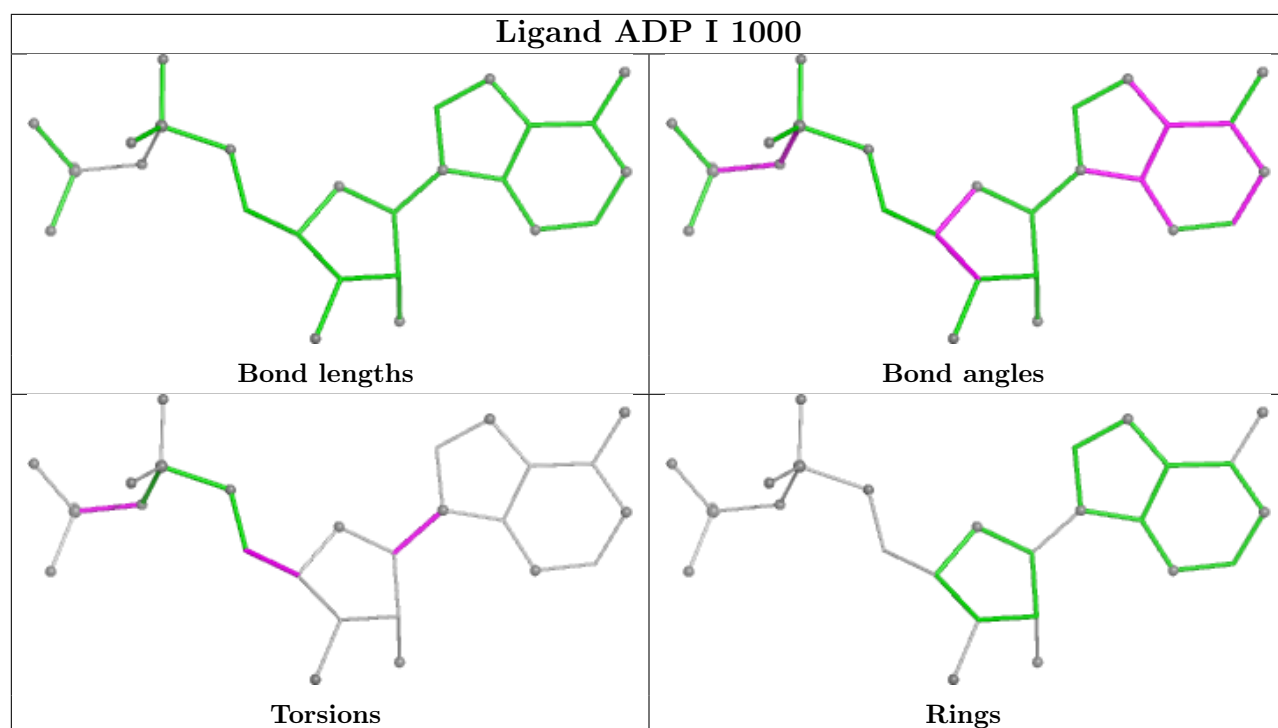
There are no ring outliers.

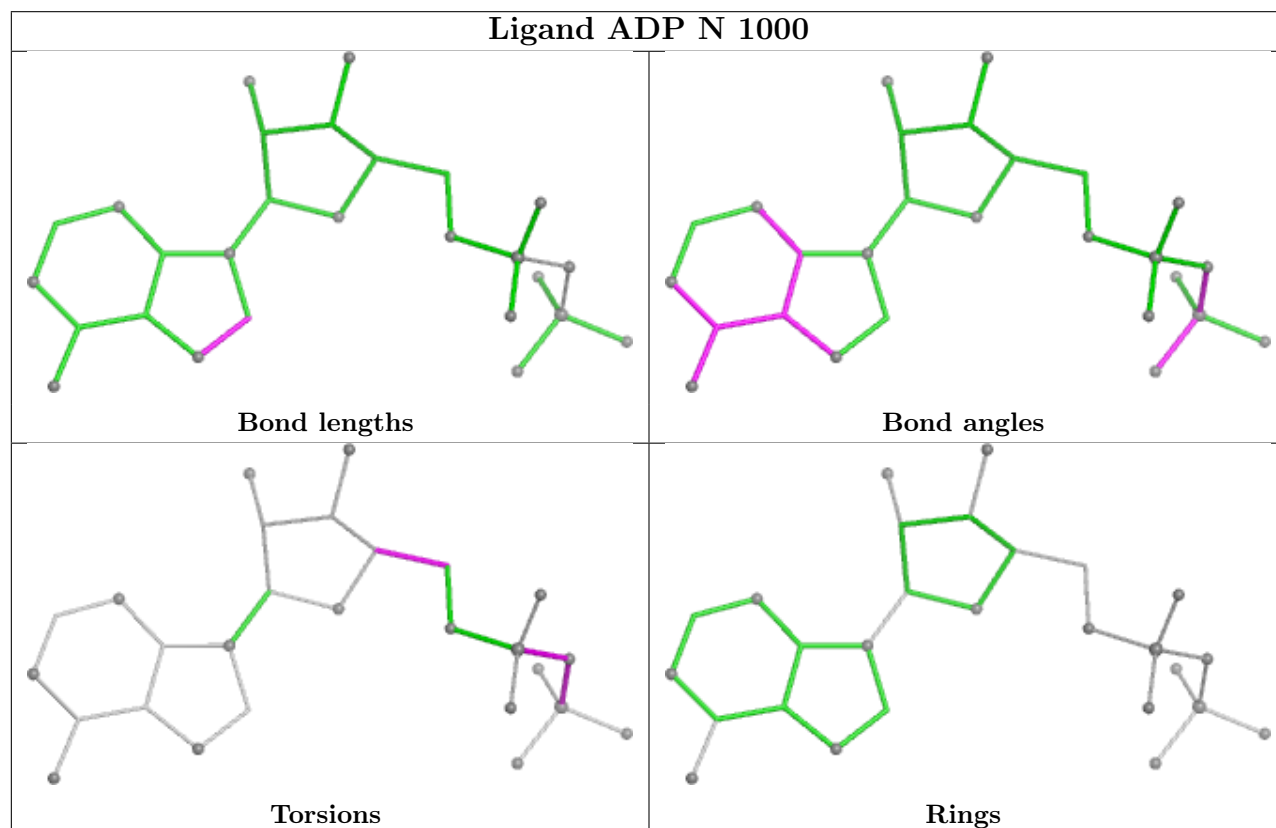
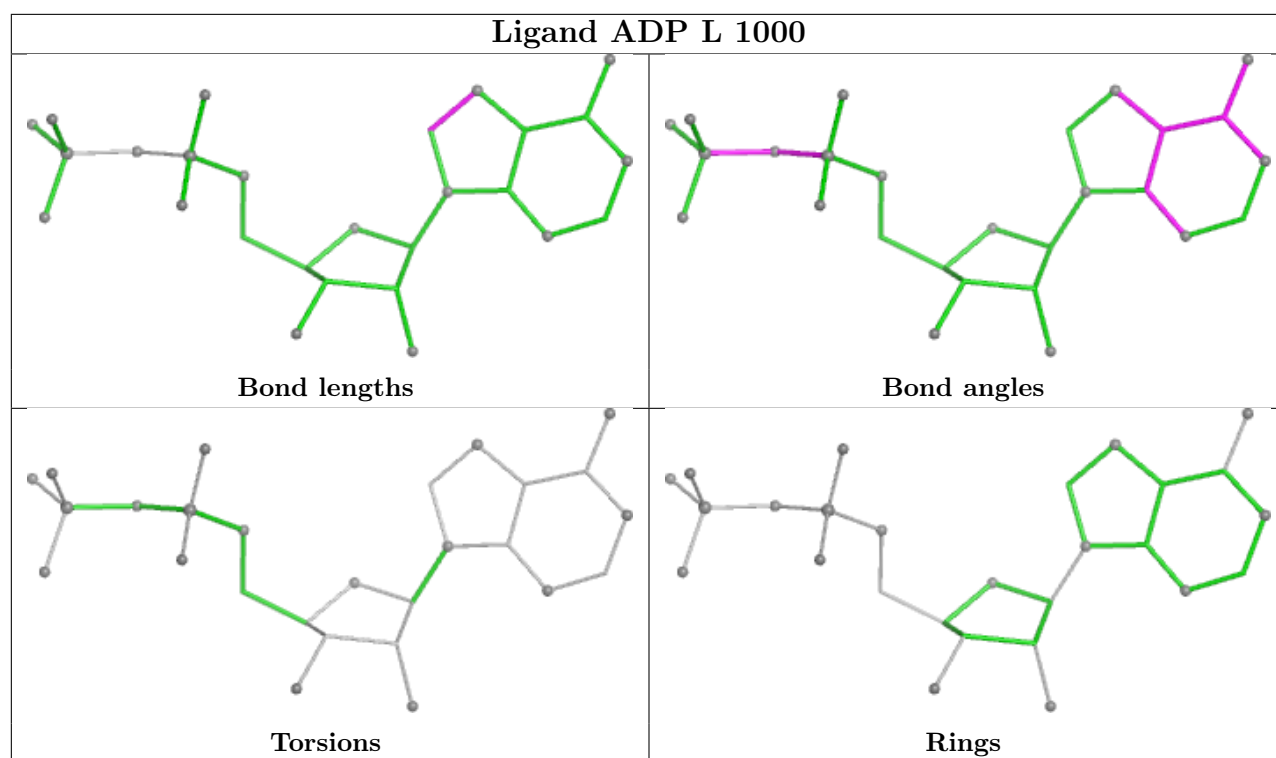
No monomer is involved in short contacts.

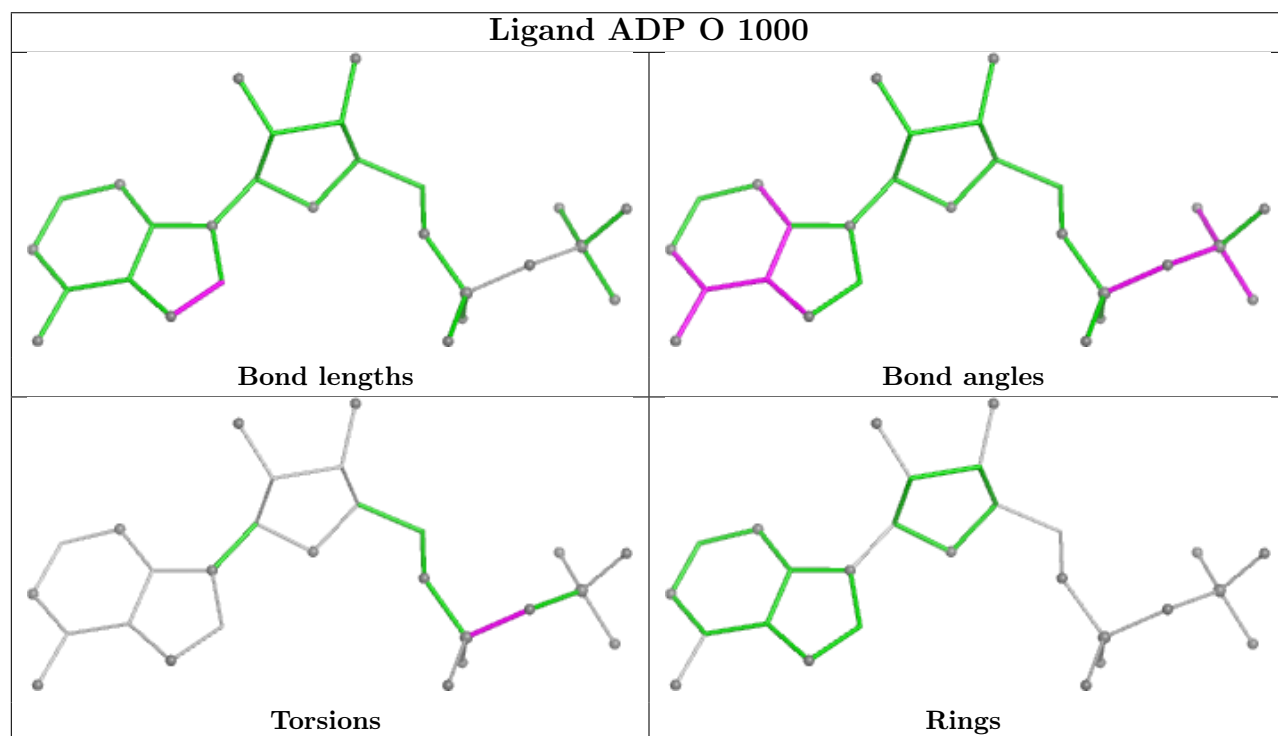
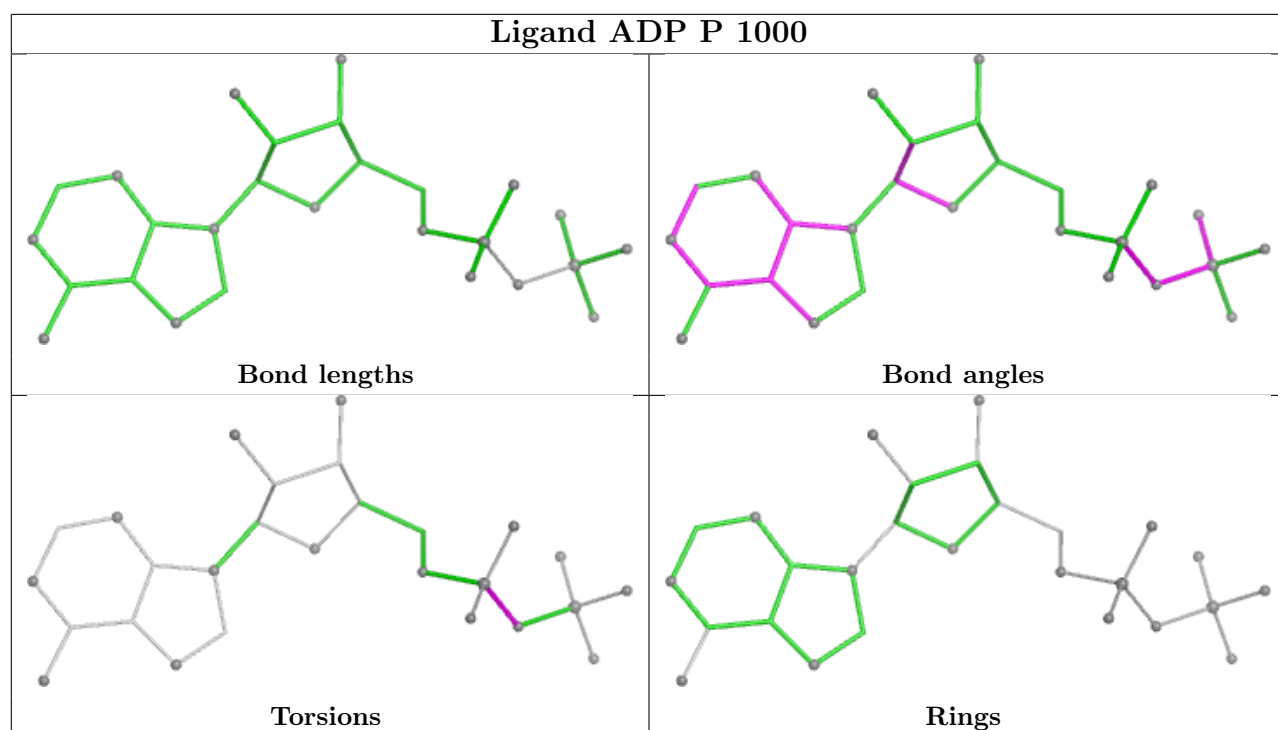
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

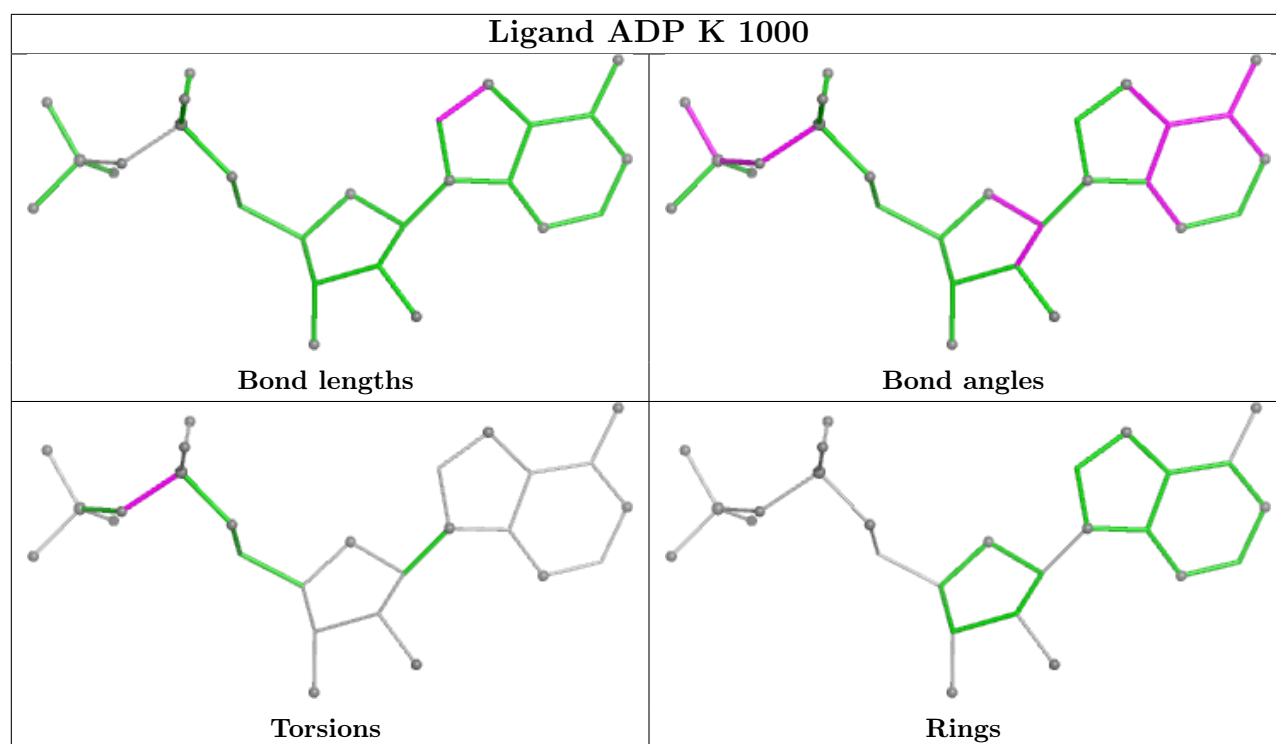
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53610. These allow visual inspection of the internal detail of the map and identification of artifacts.

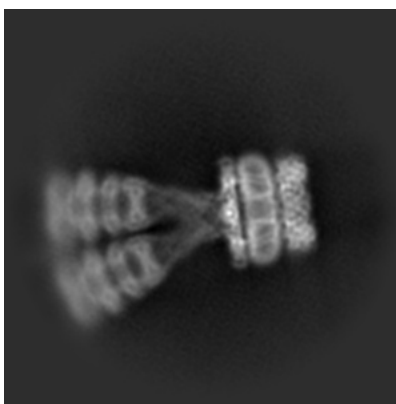
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

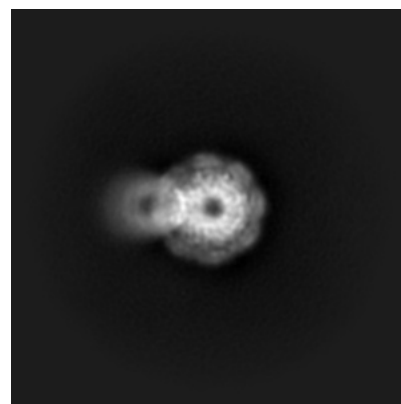
6.1.1 Primary map



X

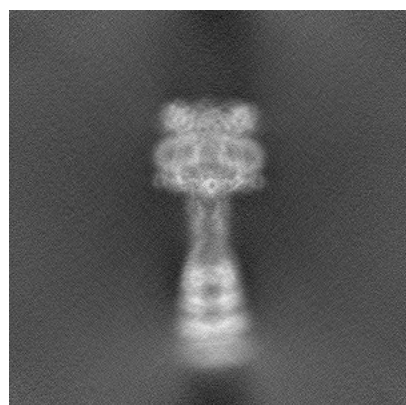


Y

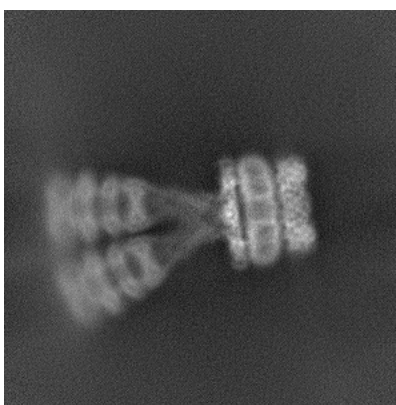


Z

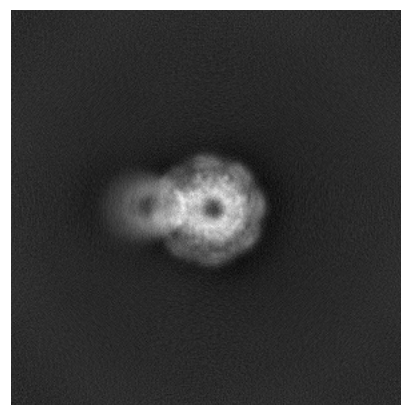
6.1.2 Raw map



X



Y

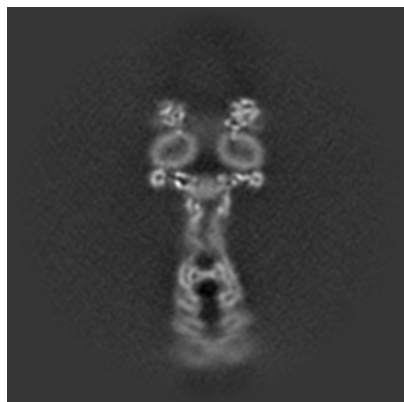


Z

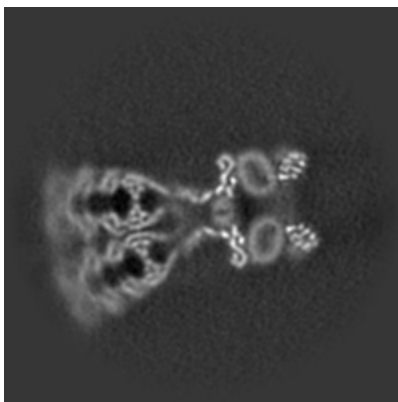
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

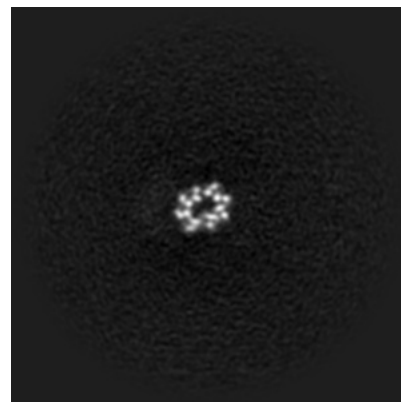
6.2.1 Primary map



X Index: 300

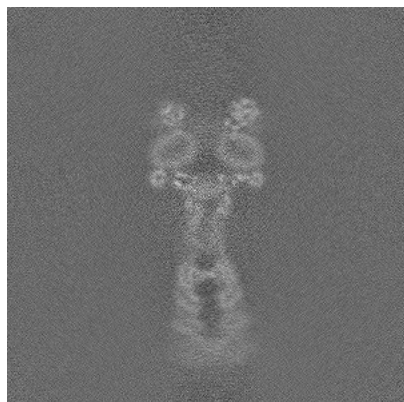


Y Index: 300

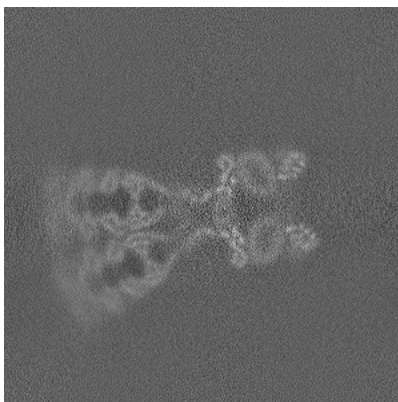


Z Index: 300

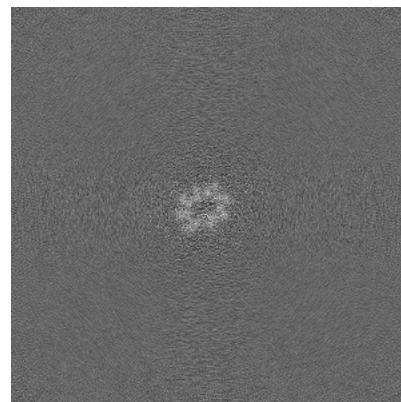
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

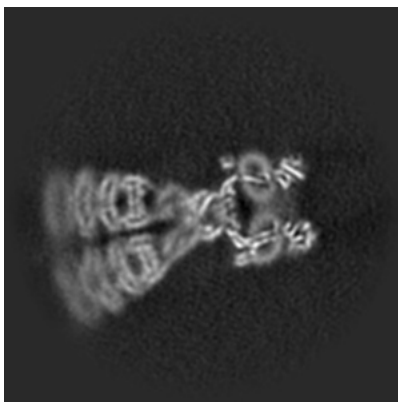
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

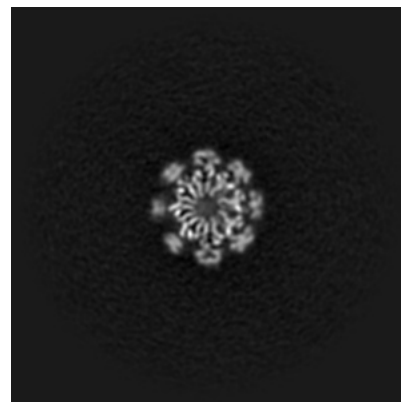
6.3.1 Primary map



X Index: 281



Y Index: 284

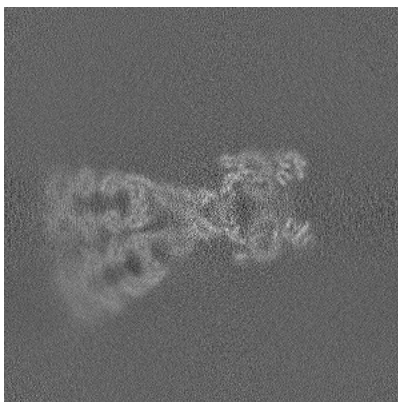


Z Index: 343

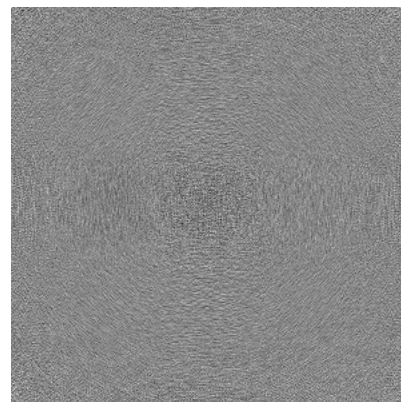
6.3.2 Raw map



X Index: 284



Y Index: 314



Z Index: 0

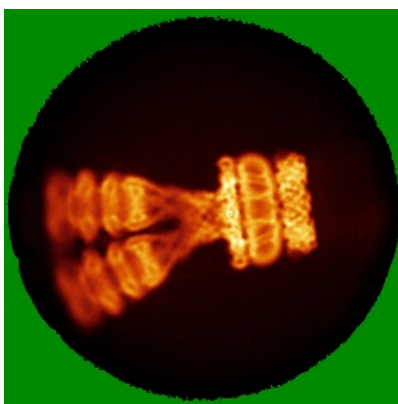
The images above show the largest variance slices of the map in three orthogonal directions.

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

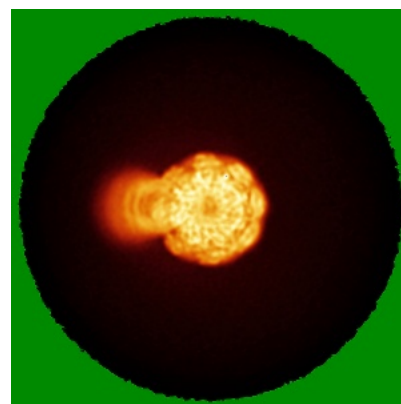
6.4.1 Primary map



X

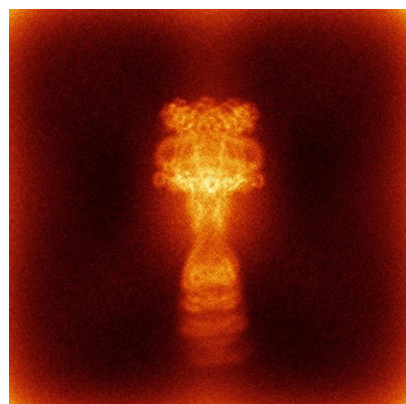


Y

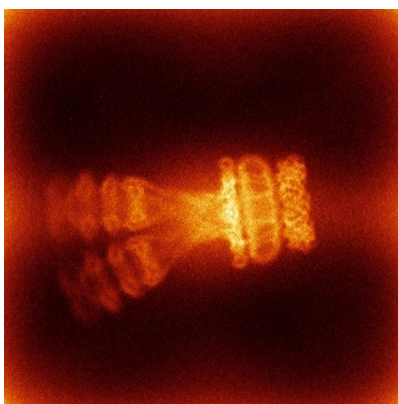


Z

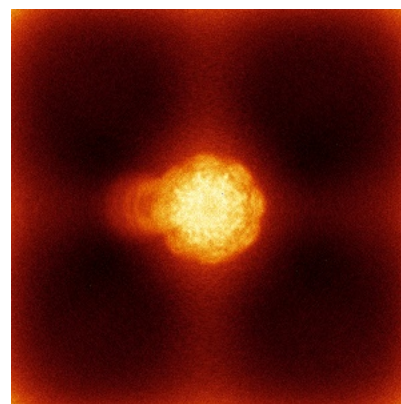
6.4.2 Raw map



X



Y

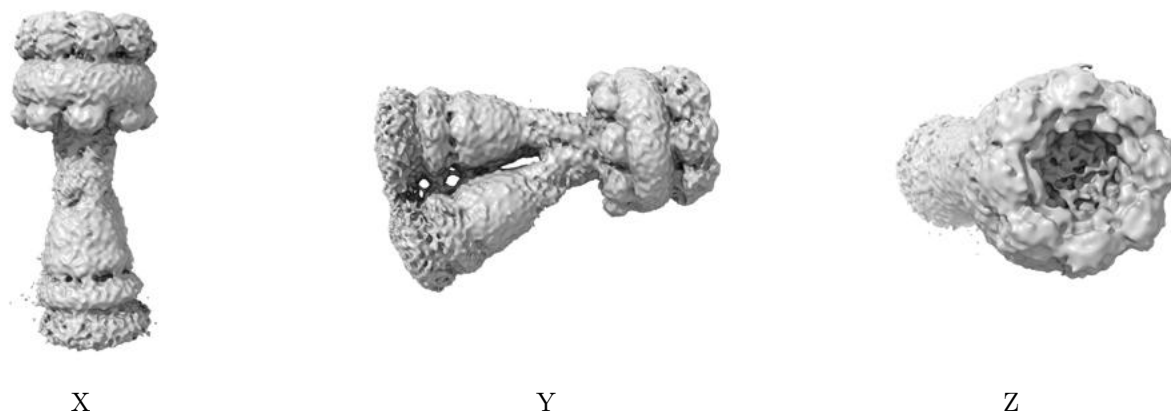


Z

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

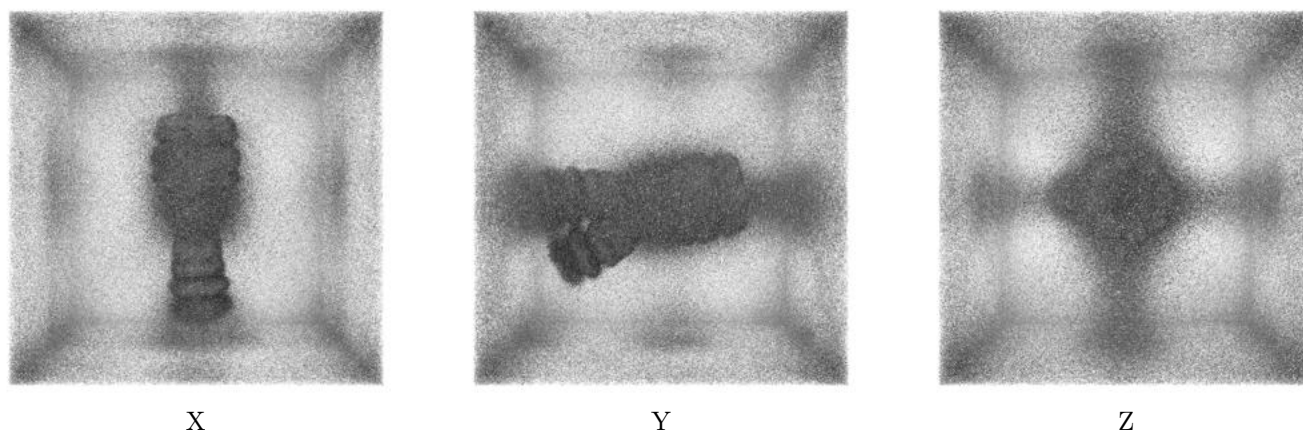
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

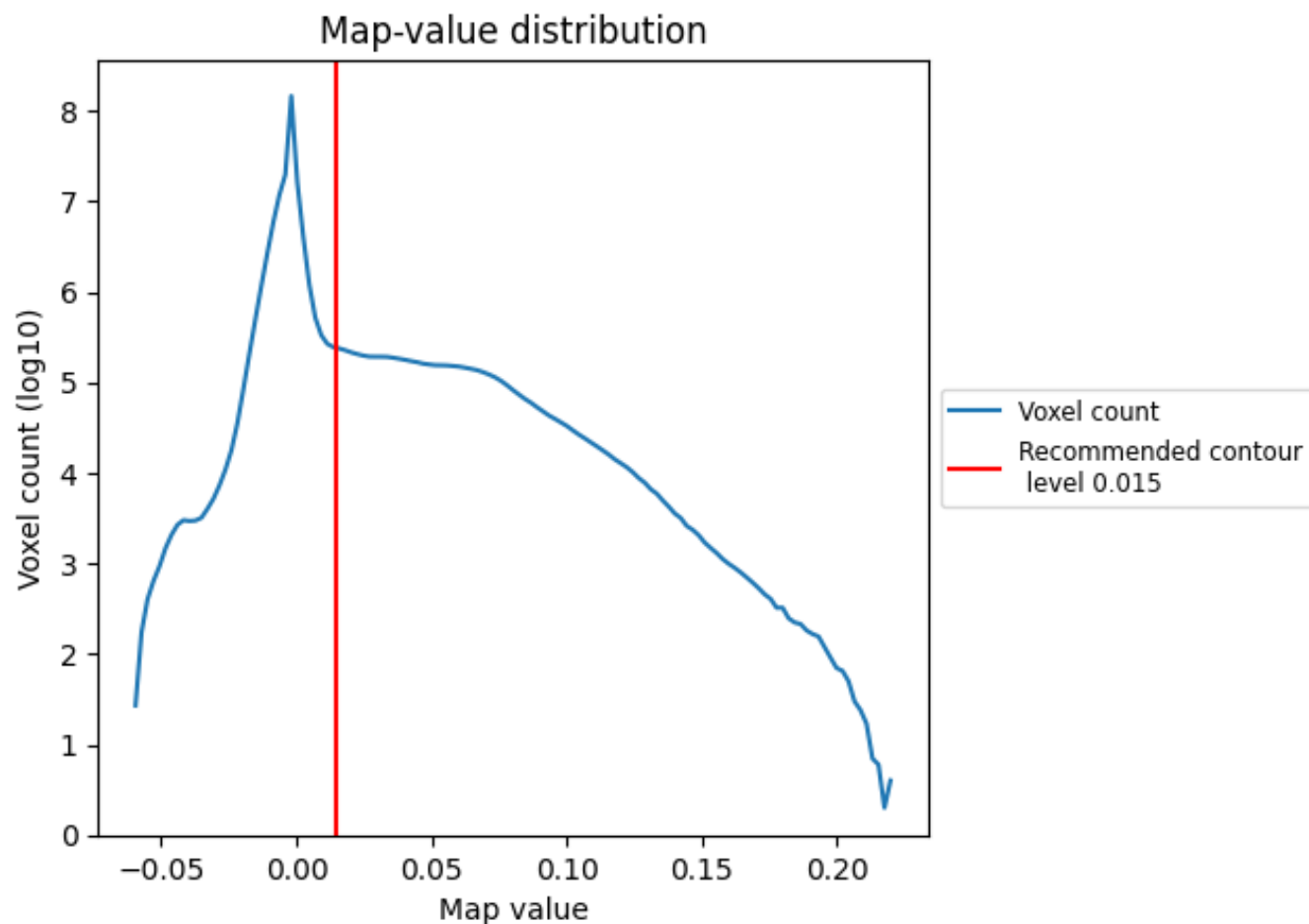
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

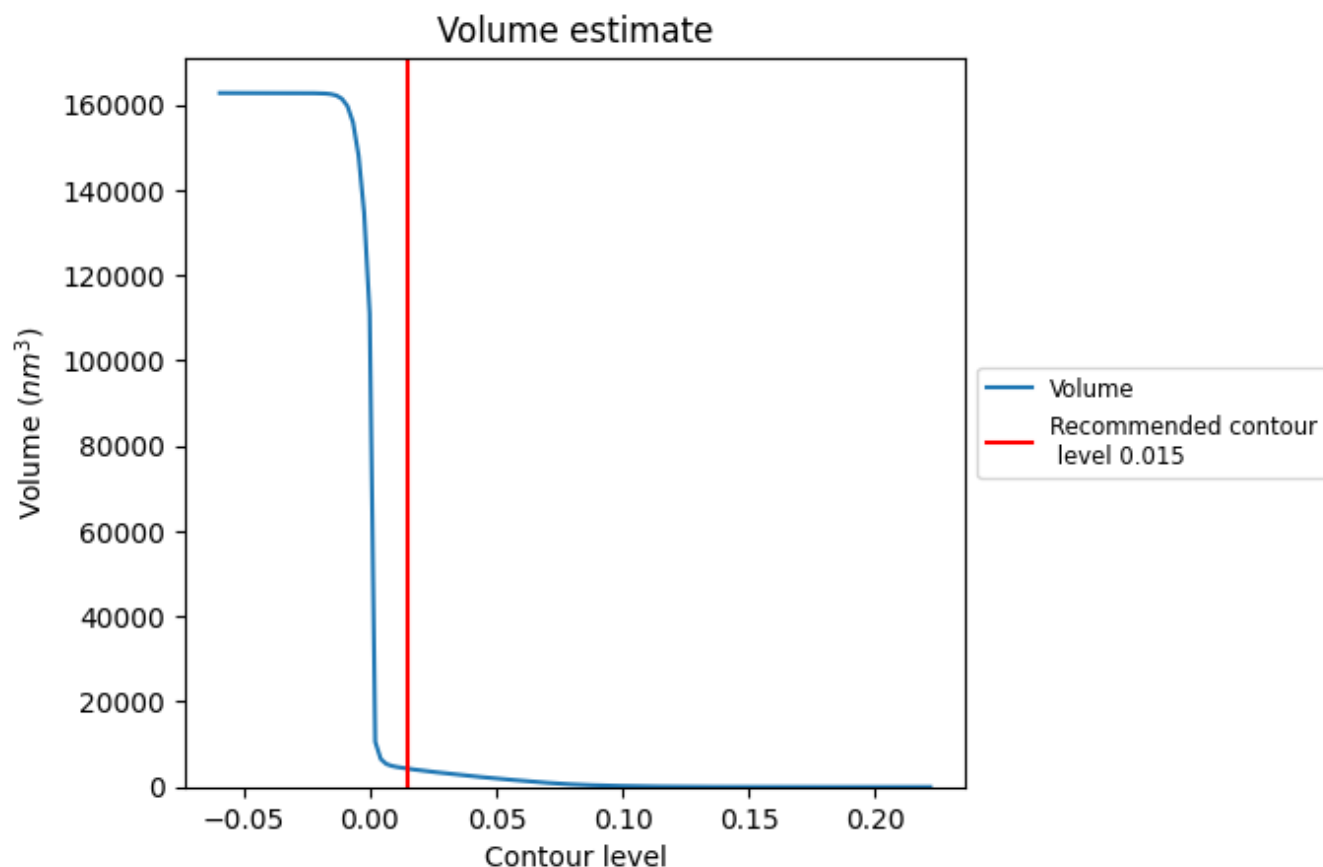
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

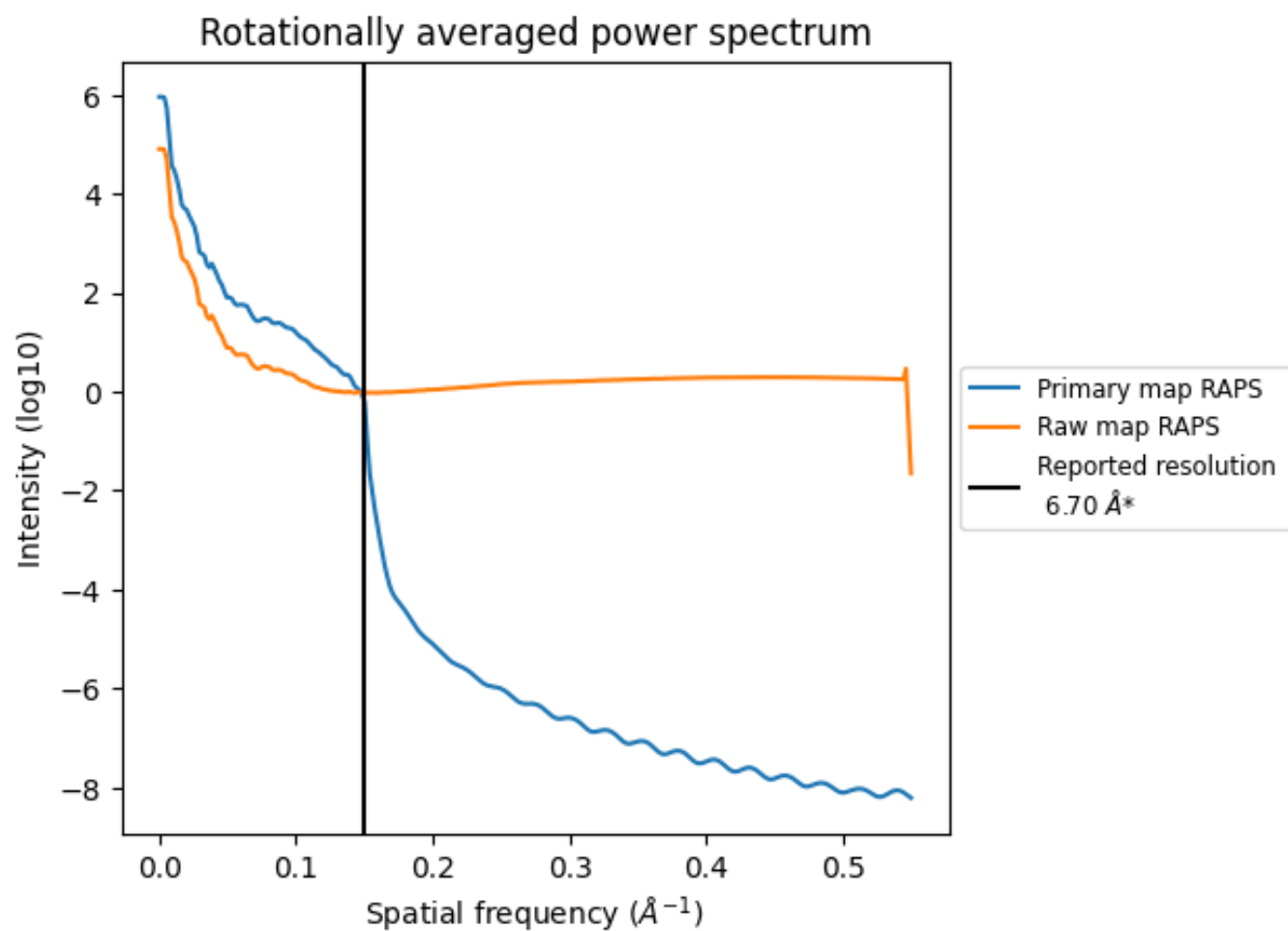
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4293 nm^3 ; this corresponds to an approximate mass of 3878 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

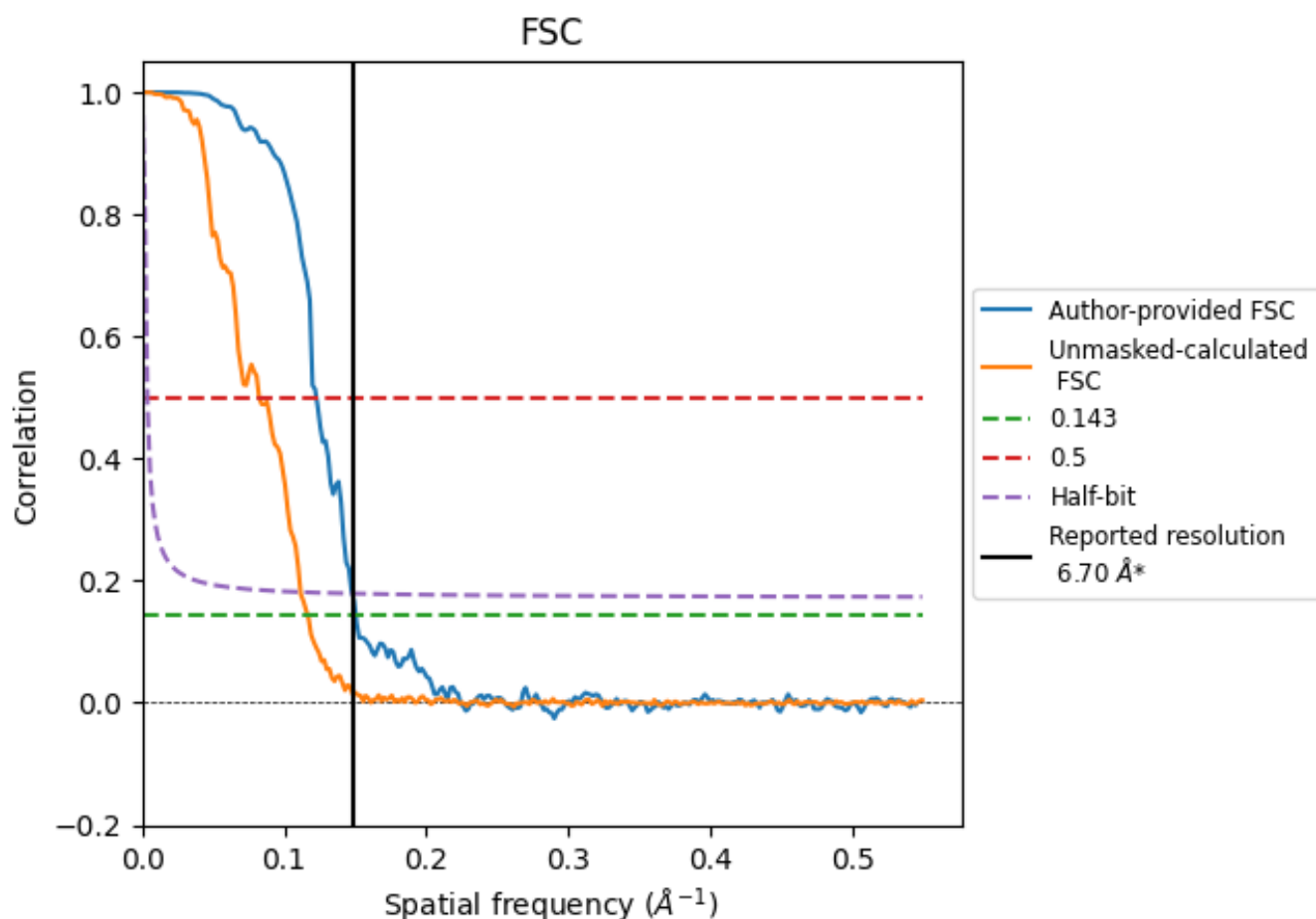


*Reported resolution corresponds to spatial frequency of 0.149 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.149 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

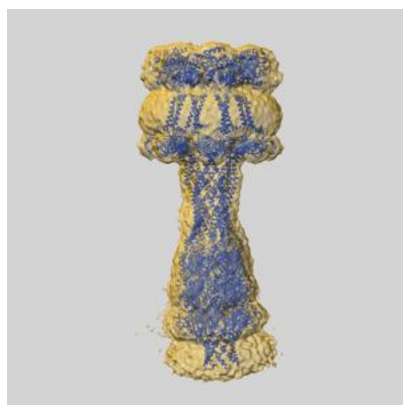
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.70	-	-
Author-provided FSC curve	6.65	8.15	6.76
Unmasked-calculated*	8.58	12.14	8.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.58 differs from the reported value 6.7 by more than 10 %

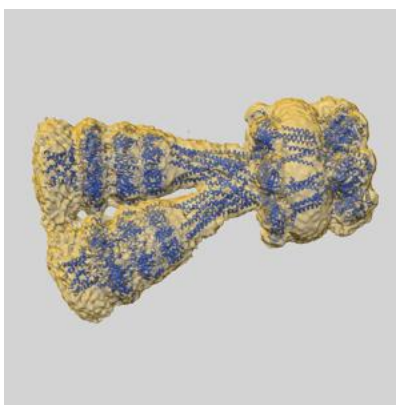
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53610 and PDB model 9R6C. Per-residue inclusion information can be found in section [3](#) on page [16](#).

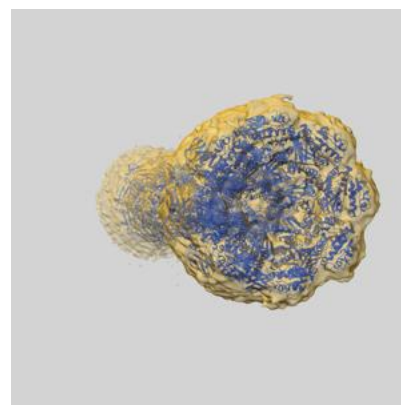
9.1 Map-model overlay [i](#)



X



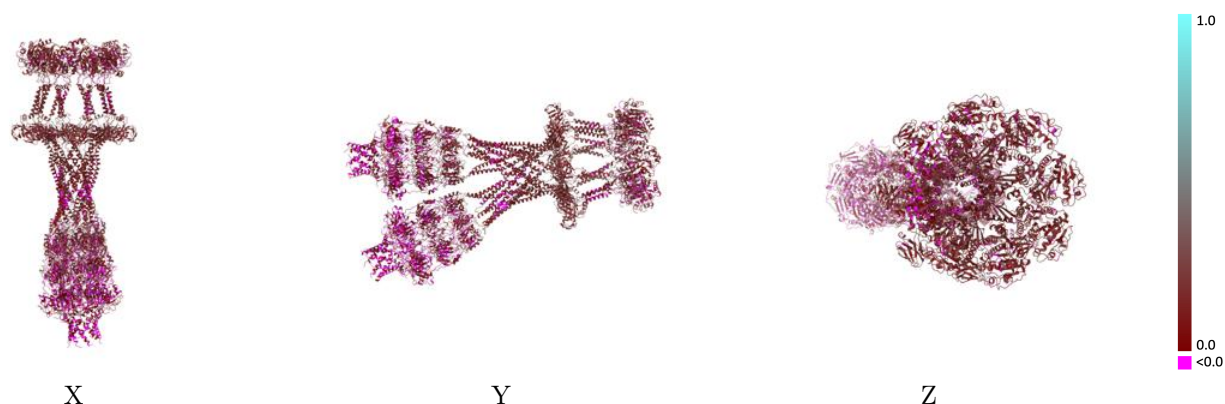
Y



Z

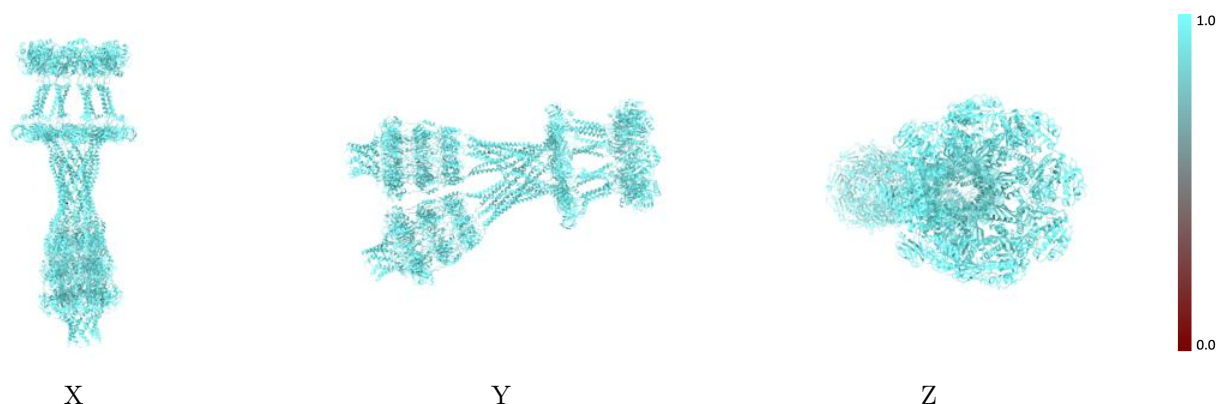
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



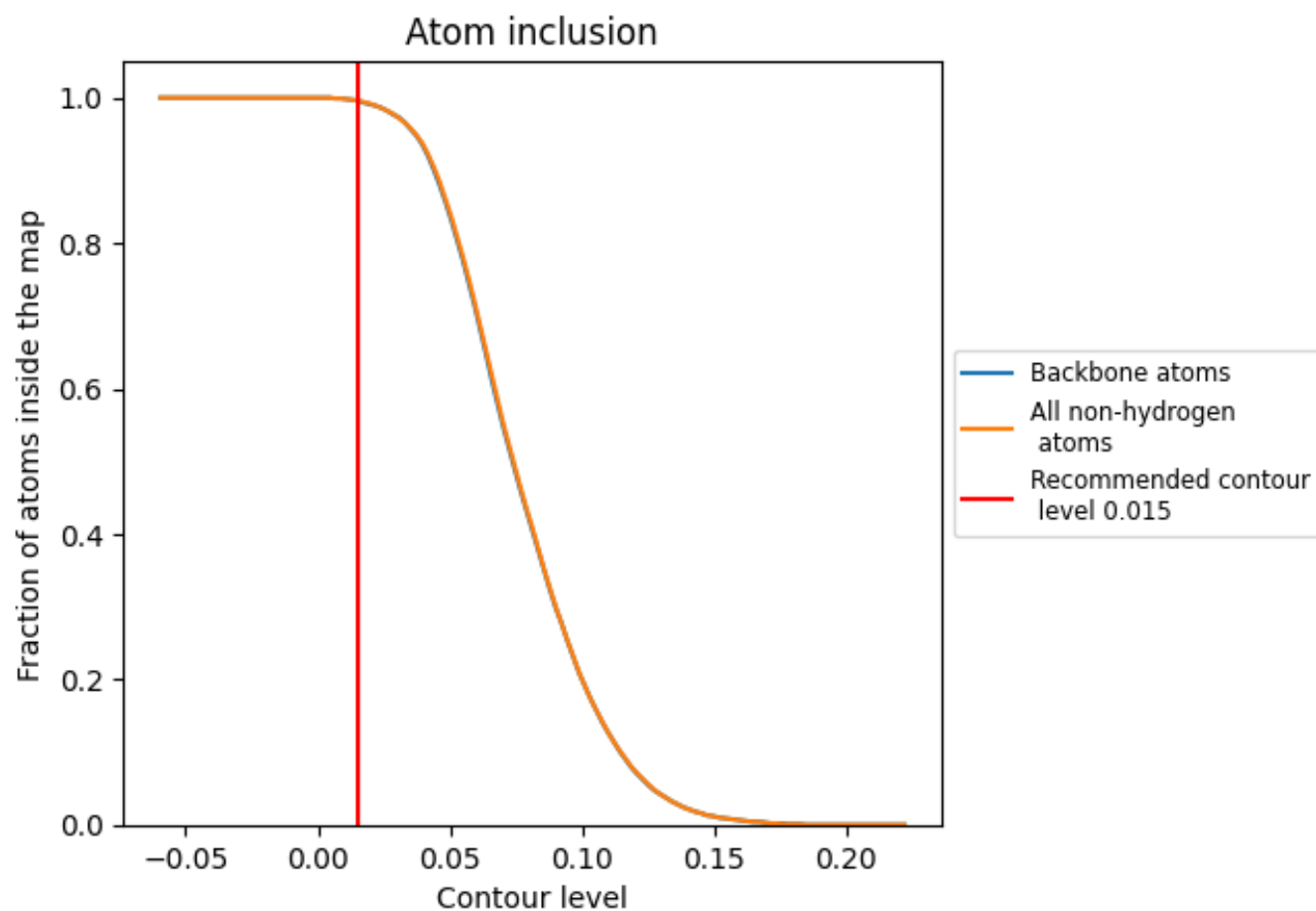
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9960	 0.1280
A	 0.9990	 0.0610
B	 0.9990	 0.0680
C	 0.9970	 0.0680
D	 0.9980	 0.0690
E	 0.9990	 0.0580
F	 0.9910	 0.0760
G	 0.9920	 0.0840
H	 0.9990	 0.0840
I	 0.9980	 0.1700
J	 0.9970	 0.1770
K	 0.9960	 0.1830
L	 0.9960	 0.1580
M	 0.9950	 0.1570
N	 0.9960	 0.1670
O	 0.9930	 0.1680
P	 0.9970	 0.1740
a	 0.9980	 0.1110
b	 1.0000	 0.1080
c	 0.9960	 0.1100
d	 0.9950	 0.1150
e	 0.9990	 0.1060
f	 0.9970	 0.1000
g	 0.9960	 0.1070
h	 0.9980	 0.1130

