Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 08:10 pm GMT

PDB ID	:	4BP7
EMDB ID	:	EMD-2365
Title	:	Asymmetric structure of a virus-receptor complex
Authors	:	Dent, K.C.; Thompson, R.; Barker, A.M.; Barr, J.N.; Hiscox, J.A.; Stockley, P.G.; Ranson, N.A.
Deposited on	:	2013-05-23
Resolution	:	39.00 Å(reported)
Based on initial model	:	2MS2

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:

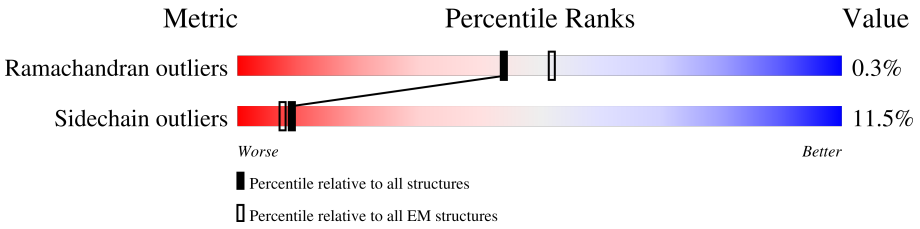
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 39.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	A0	129	5% 83% 14% ·
1	A1	129	5% 83% 14% ·
1	A2	129	83% 14% ·
1	A3	129	83% 14% ·
1	A4	129	83% 14% ·
1	A5	129	· 83% 14% ·
1	A6	129	83% 14% ·
1	A7	129	83% 14% ·
1	A8	129	83% 14% ·

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Mol	Chain	Length	Quality of chain
1	A9	129	83% 14%
1	AA	129	83% 14%
1	AB	129	83% 14%
1	AC	129	5% 83% 14%
1	AD	129	5% 83% 14%
1	AE	129	83% 14%
1	AF	129	83% 14%
1	AG	129	83% 14%
1	AH	129	83% 14%
1	AI	129	5% 83% 14%
1	AJ	129	83% 14%
1	AK	129	83% 14%
1	AL	129	7% 83% 14%
1	AM	129	83% 14%
1	AN	129	83% 14%
1	AO	129	5% 83% 14%
1	AP	129	83% 14%
1	AQ	129	83% 14%
1	AR	129	83% 14%
1	AS	129	83% 14%
1	AT	129	83% 14%
1	AU	129	83% 14%
1	AV	129	83% 14%
1	AW	129	83% 14%
1	AX	129	83% 14%

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Mol	Chain	Length	Quality of chain
1	AY	129	83% 14%
1	AZ	129	83% 14%
1	Aa	129	83% 14%
1	Ab	129	83% 14%
1	Ac	129	83% 14%
1	Ad	129	83% 14%
1	Ae	129	83% 14%
1	Af	129	83% 14%
1	Ag	129	83% 14%
1	Ah	129	5% 83% 14%
1	Ai	129	83% 14%
1	Aj	129	83% 14%
1	Ak	129	83% 14%
1	Al	129	83% 14%
1	Am	129	83% 14%
1	An	129	83% 14%
1	Ao	129	83% 14%
1	Ap	129	83% 14%
1	Aq	129	83% 14%
1	Ar	129	14% 83% 14%
1	As	129	5% 83% 14%
1	At	129	83% 14%
1	Au	129	5% 83% 14%
1	Av	129	83% 14%
1	Aw	129	5% 83% 14%

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Mol	Chain	Length	Quality of chain
1	Ax	129	83% 14%
1	B0	129	88% 9%
1	B1	129	88% 9%
1	B2	129	6% 88% 9%
1	B3	129	5% 88% 9%
1	B4	129	87% 9%
1	B5	129	87% 9%
1	B6	129	88% 9%
1	B7	129	88% 9%
1	B8	129	87% 9%
1	B9	129	87% 9%
1	BA	129	5% 88% 9%
1	BB	129	5% 87% 9%
1	BC	129	88% 9%
1	BD	129	88% 9%
1	BE	129	87% 9%
1	BF	129	88% 9%
1	BG	129	87% 9%
1	BH	129	88% 9%
1	BI	129	88% 9%
1	BJ	129	87% 9%
1	BK	129	5% 88% 9%
1	BL	129	5% 87% 9%
1	BM	129	5% 88% 9%
1	BN	129	88% 9%

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Mol	Chain	Length	Quality of chain
1	BO	129	87% 9%
1	BP	129	88% 9%
1	BQ	129	88% 9%
1	BR	129	88% 9%
1	BS	129	87% 9%
1	BT	129	88% 9%
1	BU	129	87% 9%
1	BV	129	88% 9%
1	BW	129	88% 9%
1	BX	129	87% 9%
1	BY	129	88% 9%
1	BZ	129	88% 9%
1	Ba	129	88% 9%
1	Bb	129	87% 9%
1	Bc	129	88% 9%
1	Bd	129	87% 9%
1	Be	129	5% 87% 9%
1	Bf	129	88% 9%
1	Bg	129	87% 9%
1	Bh	129	87% 9%
1	Bi	129	87% 9%
1	Bj	129	87% 9%
1	Bk	129	88% 9%
1	Bl	129	88% 9%
1	Bm	129	87% 9%

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Mol	Chain	Length	Quality of chain
1	Bn	129	88% 9%
1	Bo	129	88% 9%
1	Bp	129	88% 9%
1	Bq	129	87% 9%
1	Br	129	87% 9%
1	Bs	129	87% 9%
1	Bt	129	88% 9%
1	Bu	129	88% 9%
1	Bv	129	88% 9%
1	Bw	129	5% 88% 9%
1	Bx	129	87% 9%
1	C0	129	84% 12%
1	C1	129	5% 84% 13%
1	C2	129	5% 84% 12%
1	C3	129	84% 12%
1	C4	129	84% 12%
1	C5	129	84% 12%
1	C6	129	84% 13%
1	C7	129	84% 12%
1	C8	129	84% 13%
1	C9	129	84% 13%
1	CA	129	84% 13%
1	CB	129	84% 13%
1	CC	129	5% 84% 13%
1	CD	129	84% 13%

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Mol	Chain	Length	Quality of chain
1	CE	129	84% 13%
1	CF	129	84% 12%
1	CG	129	84% 12%
1	CH	129	84% 13%
1	CI	129	84% 13%
1	CJ	129	5% 84% 12%
1	CK	129	84% 12%
1	CL	129	5% 84% 13%
1	CM	129	84% 12%
1	CN	129	84% 13%
1	CO	129	84% 12%
1	CP	129	84% 13%
1	CQ	129	84% 13%
1	CR	129	84% 12%
1	CS	129	84% 13%
1	CT	129	84% 13%
1	CU	129	84% 12%
1	CV	129	84% 13%
1	CW	129	84% 13%
1	CX	129	84% 12%
1	CY	129	84% 13%
1	CZ	129	84% 13%
1	Ca	129	84% 13%
1	Cb	129	84% 12%
1	Cc	129	84% 12%

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Mol	Chain	Length	Quality of chain
1	Cd	129	84% 13%
1	Ce	129	6% 84% 12%
1	Cf	129	5% 84% 13%
1	Cg	129	84% 12%
1	Ch	129	84% 12%
1	Ci	129	84% 12%
1	Cj	129	84% 12%
1	Ck	129	84% 13%
1	Cl	129	84% 12%
1	Cm	129	84% 12%
1	Cn	129	84% 12%
1	Co	129	84% 12%
1	Cp	129	5% 84% 13%
1	Cq	129	84% 13%
1	Cr	129	84% 12%
1	Cs	129	84% 12%
1	Ct	129	84% 13%
1	Cu	129	84% 13%
1	Cv	129	84% 13%
1	Cw	129	84% 12%
1	Cx	129	84% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 173700 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called COAT PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A1	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A2	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A3	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A4	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A5	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A6	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A7	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A8	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A9	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AA	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AB	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AC	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AD	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AE	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AF	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AG	129	Total	C	N	O	S	0	0
			965	606	165	190	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AH	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AI	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AJ	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AK	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AL	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AM	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AN	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AO	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AP	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AQ	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AR	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AS	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AT	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AU	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AV	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AW	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AX	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AY	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AZ	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Aa	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ab	129	Total	C	N	O	S	0	0
			965	606	165	190	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ac	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ad	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ae	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Af	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ag	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ah	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ai	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Aj	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ak	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Al	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Am	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	An	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ao	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ap	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Aq	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ar	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	As	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	At	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Au	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Av	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Aw	129	Total	C	N	O	S	0	0
			965	606	165	190	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ax	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	B0	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	B1	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	B2	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	B3	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	B4	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	B5	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	B6	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	B7	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	B8	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	B9	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BA	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BB	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BC	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BD	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BE	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BF	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BG	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BH	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BI	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BJ	129	Total	C	N	O	S	0	0
			965	606	165	190	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BK	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BL	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BM	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BN	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BO	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BP	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BQ	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BR	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BS	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BT	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BU	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BV	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BW	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BX	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BY	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	BZ	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ba	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bb	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bc	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bd	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Be	129	Total	C	N	O	S	0	0
			965	606	165	190	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bf	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bg	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bh	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bi	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bj	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bk	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bl	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bm	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bn	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bo	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bp	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bq	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Br	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bs	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bt	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bu	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bv	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bw	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Bx	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	C0	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	C1	129	Total	C	N	O	S	0	0
			965	606	165	190	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	C2	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	C3	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	C4	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	C5	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	C6	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	C7	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	C8	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	C9	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CA	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CB	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CC	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CD	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CE	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CF	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CG	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CH	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CI	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CJ	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CK	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CL	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CM	129	Total	C	N	O	S	0	0
			965	606	165	190	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CN	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CO	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CP	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CQ	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CR	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CS	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CT	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CU	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CV	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CW	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CX	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CY	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	CZ	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ca	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cb	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cc	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cd	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ce	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cf	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cg	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ch	129	Total	C	N	O	S	0	0
			965	606	165	190	4		

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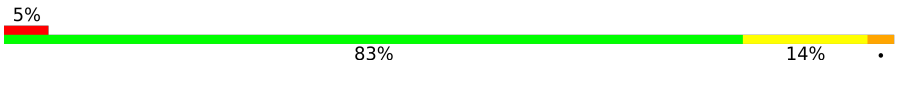
Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ci	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cj	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ck	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cl	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cm	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cn	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Co	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cp	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cq	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cr	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cs	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Ct	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cu	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cv	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cw	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	Cx	129	Total	C	N	O	S	0	0
			965	606	165	190	4		

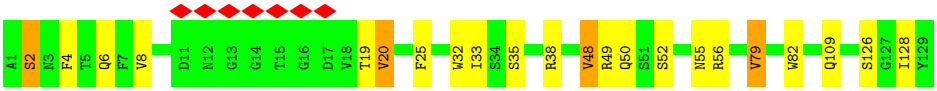
3 Residue-property plots (i)

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: COAT PROTEIN

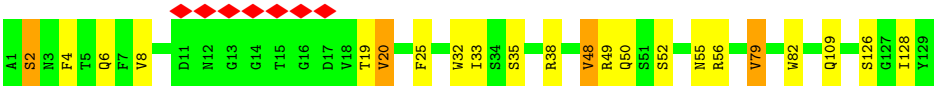
Chain A0:





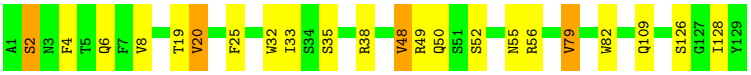
• Molecule 1: COAT PROTEIN

Chain A1:



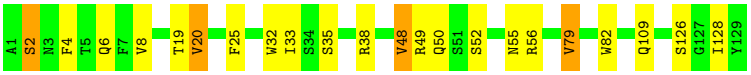
• Molecule 1: COAT PROTEIN

Chain A2:



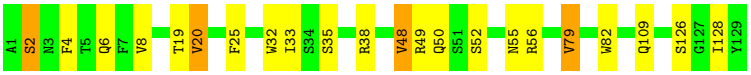
• Molecule 1: COAT PROTEIN

Chain A3:



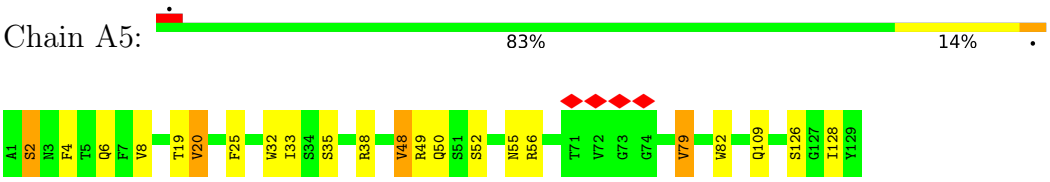
• Molecule 1: COAT PROTEIN

Chain A4:



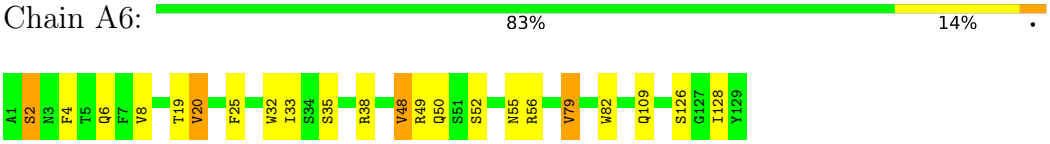
• Molecule 1: COAT PROTEIN

Chain A5:



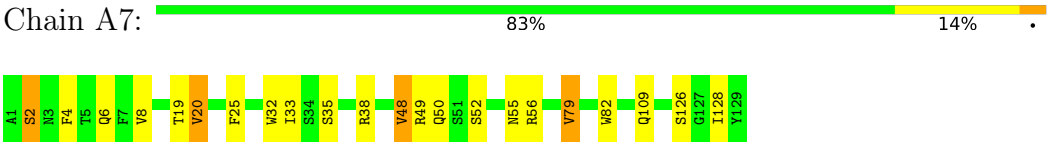
• Molecule 1: COAT PROTEIN

Chain A6:



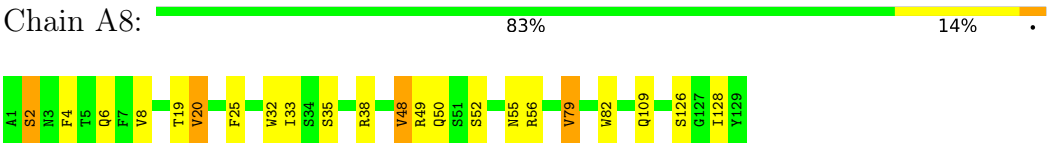
• Molecule 1: COAT PROTEIN

Chain A7:



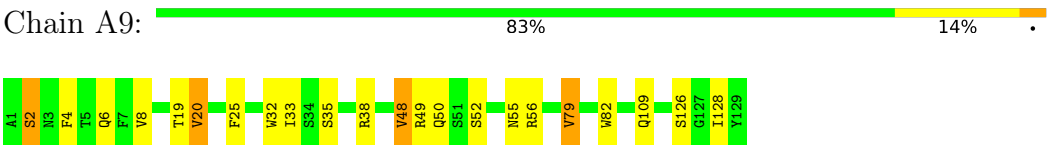
• Molecule 1: COAT PROTEIN

Chain A8:



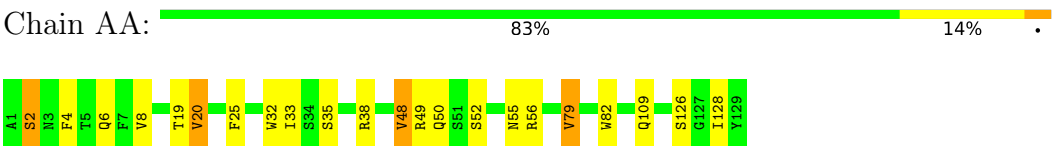
• Molecule 1: COAT PROTEIN

Chain A9:



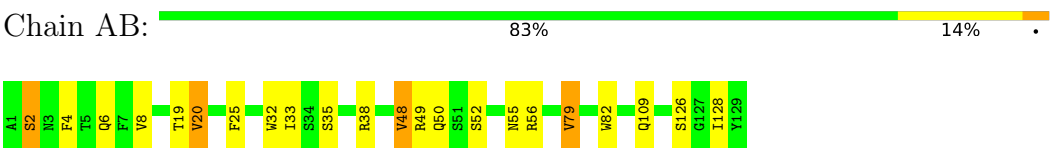
• Molecule 1: COAT PROTEIN

Chain AA:



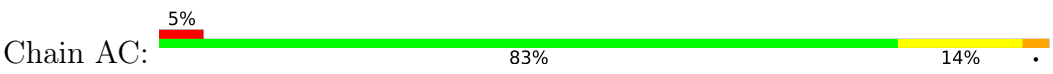
• Molecule 1: COAT PROTEIN

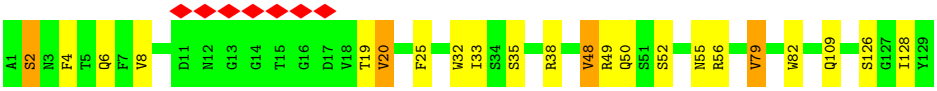
Chain AB:



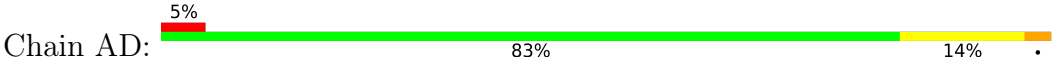
• Molecule 1: COAT PROTEIN

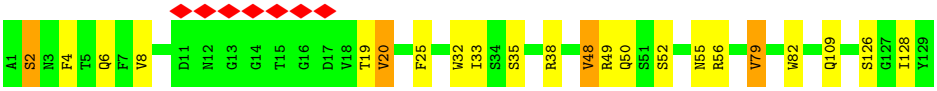
Chain AC:



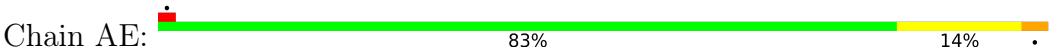


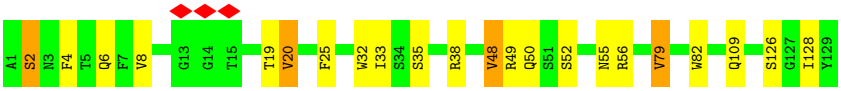
• Molecule 1: COAT PROTEIN



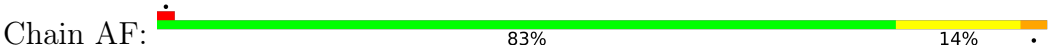


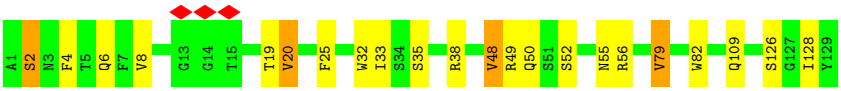
• Molecule 1: COAT PROTEIN



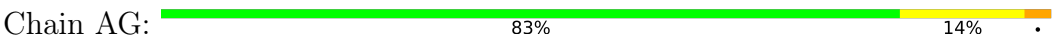


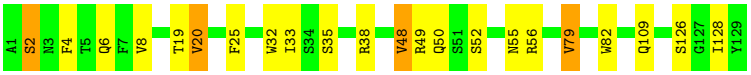
• Molecule 1: COAT PROTEIN



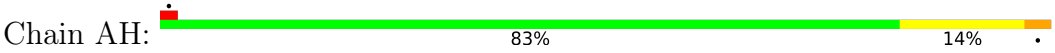


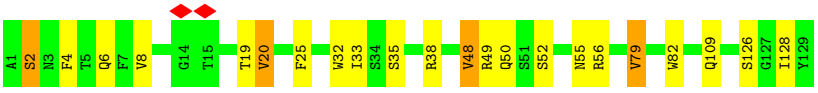
• Molecule 1: COAT PROTEIN



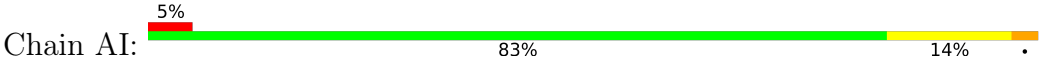


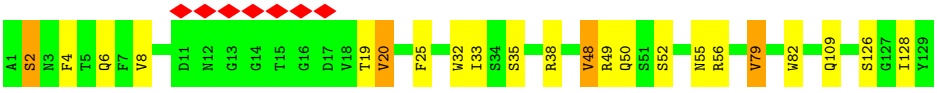
• Molecule 1: COAT PROTEIN



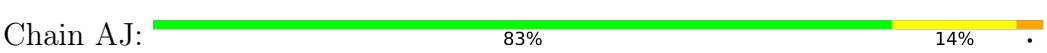


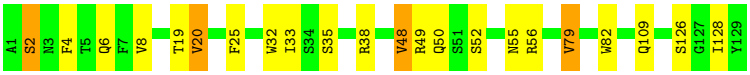
• Molecule 1: COAT PROTEIN





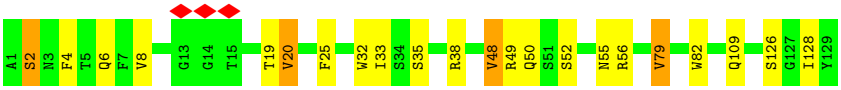
• Molecule 1: COAT PROTEIN





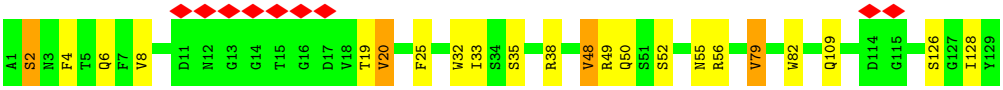
• Molecule 1: COAT PROTEIN

Chain AK:



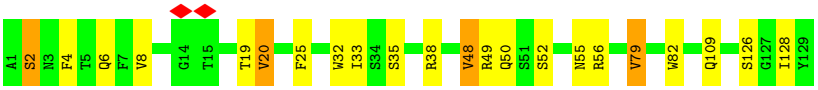
• Molecule 1: COAT PROTEIN

Chain AL:



• Molecule 1: COAT PROTEIN

Chain AM:

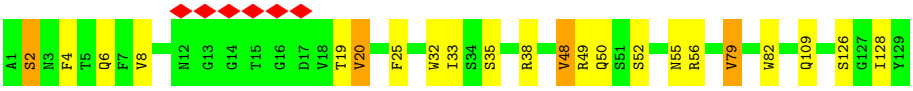


• Molecule 1: COAT PROTEIN

Chain AN:

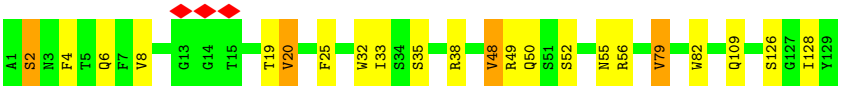
• Molecule 1: COAT PROTEIN

Chain AO:



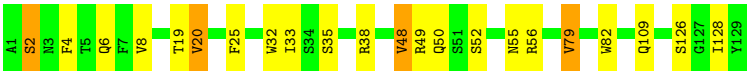
• Molecule 1: COAT PROTEIN

Chain AP:



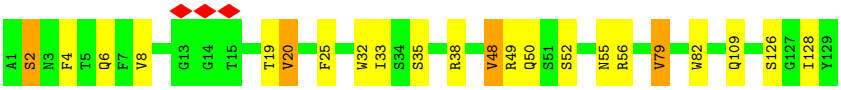
• Molecule 1: COAT PROTEIN

Chain AQ:



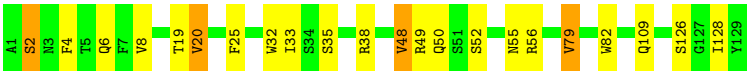
• Molecule 1: COAT PROTEIN

Chain AR:



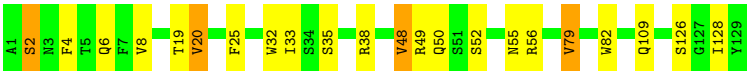
• Molecule 1: COAT PROTEIN

Chain AS:



• Molecule 1: COAT PROTEIN

Chain AT:

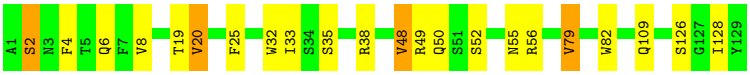


• Molecule 1: COAT PROTEIN

Chain AU:

• Molecule 1: COAT PROTEIN

Chain AV:

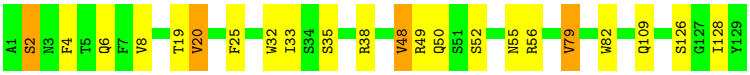


• Molecule 1: COAT PROTEIN

Chain AW:

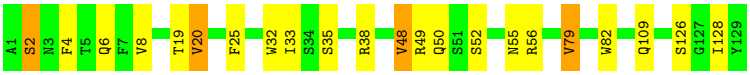
• Molecule 1: COAT PROTEIN

Chain AX:



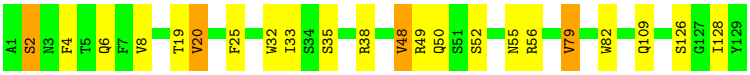
• Molecule 1: COAT PROTEIN

Chain AY:



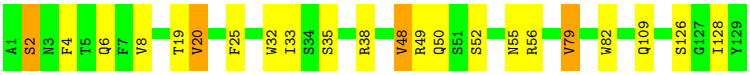
• Molecule 1: COAT PROTEIN

Chain AZ:



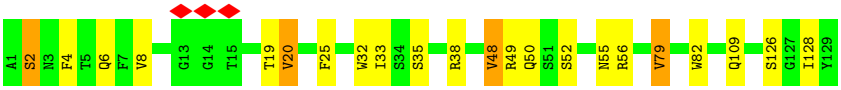
• Molecule 1: COAT PROTEIN

Chain Aa:



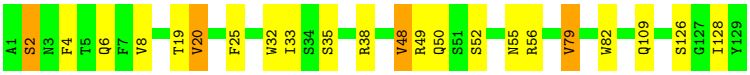
• Molecule 1: COAT PROTEIN

Chain Ab:



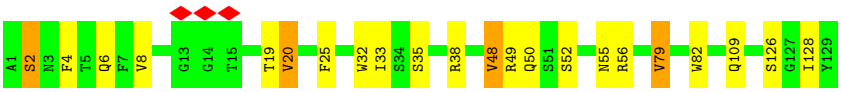
• Molecule 1: COAT PROTEIN

Chain Ac:



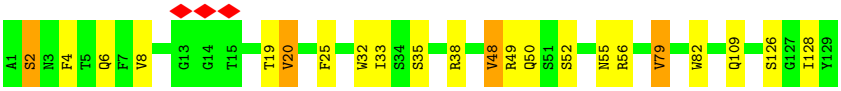
• Molecule 1: COAT PROTEIN

Chain Ad:



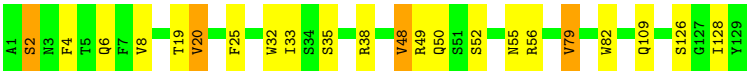
• Molecule 1: COAT PROTEIN

Chain Ae:



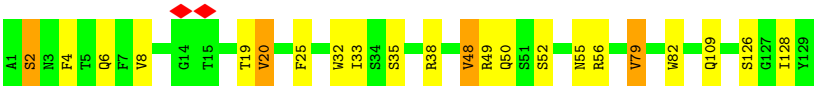
• Molecule 1: COAT PROTEIN

Chain Af:



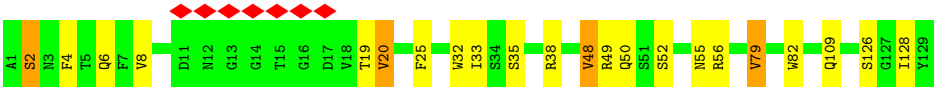
• Molecule 1: COAT PROTEIN

Chain Ag:



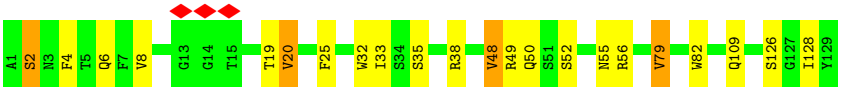
• Molecule 1: COAT PROTEIN

Chain Ah:



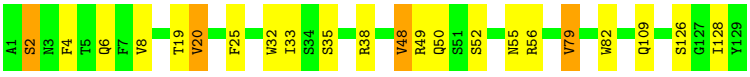
• Molecule 1: COAT PROTEIN

Chain Ai:



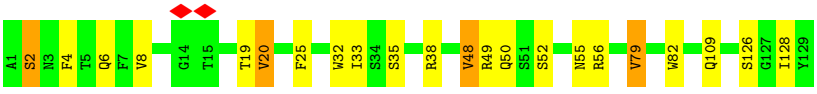
• Molecule 1: COAT PROTEIN

Chain Aj:



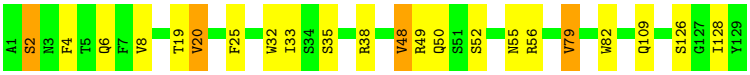
• Molecule 1: COAT PROTEIN

Chain Ak:



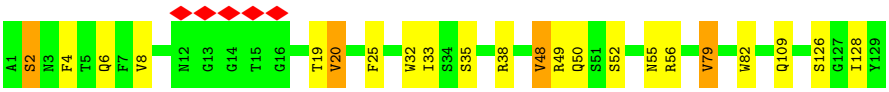
• Molecule 1: COAT PROTEIN

Chain Al:



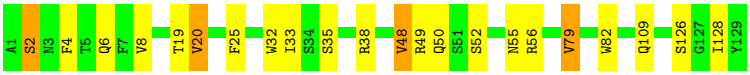
• Molecule 1: COAT PROTEIN

Chain Am:



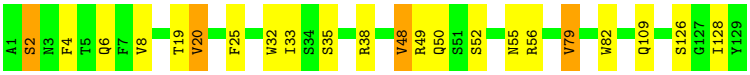
• Molecule 1: COAT PROTEIN

Chain An:



• Molecule 1: COAT PROTEIN

Chain Ao:

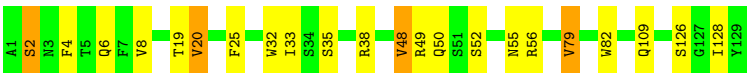


• Molecule 1: COAT PROTEIN

Chain Ap:

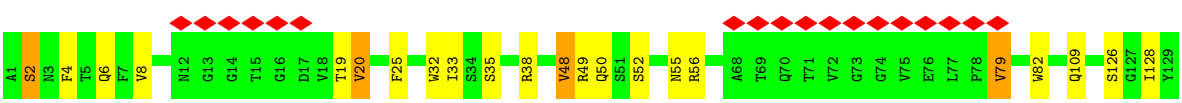
• Molecule 1: COAT PROTEIN

Chain Aq:



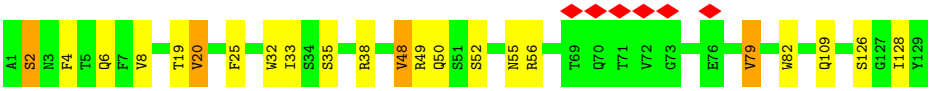
• Molecule 1: COAT PROTEIN

Chain Ar:



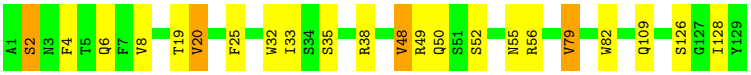
• Molecule 1: COAT PROTEIN

Chain As:



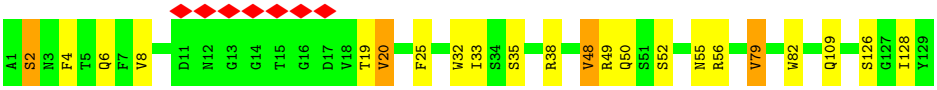
• Molecule 1: COAT PROTEIN

Chain At:



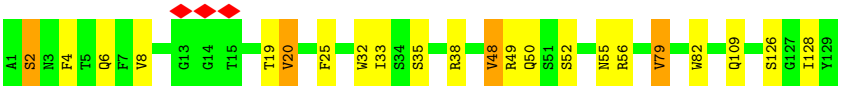
• Molecule 1: COAT PROTEIN

Chain Au:



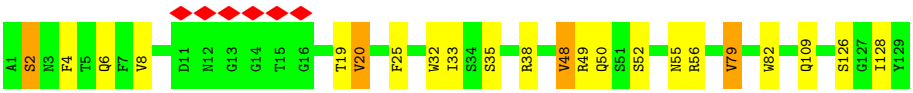
• Molecule 1: COAT PROTEIN

Chain Av:



• Molecule 1: COAT PROTEIN

Chain Aw:

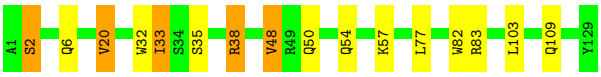


• Molecule 1: COAT PROTEIN

Chain Ax:

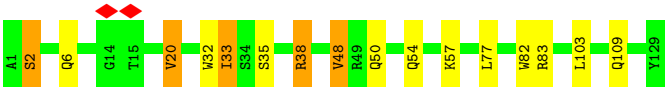
• Molecule 1: COAT PROTEIN

Chain B0:



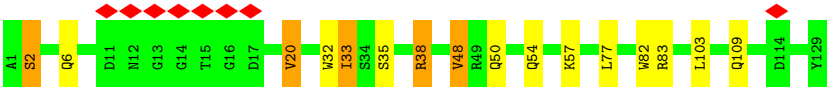
• Molecule 1: COAT PROTEIN

Chain B1:



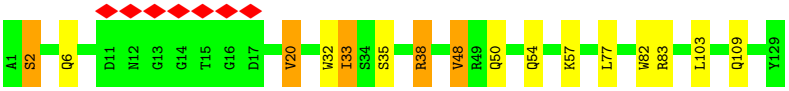
• Molecule 1: COAT PROTEIN

Chain B2:



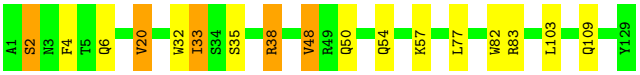
• Molecule 1: COAT PROTEIN

Chain B3:



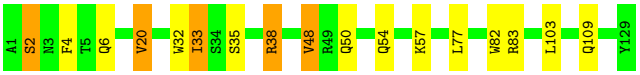
• Molecule 1: COAT PROTEIN

Chain B4:



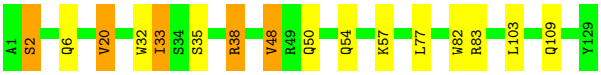
• Molecule 1: COAT PROTEIN

Chain B5:



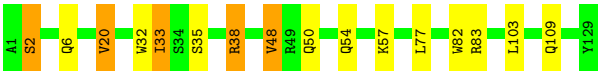
• Molecule 1: COAT PROTEIN

Chain B6:



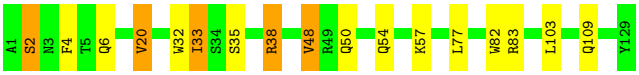
• Molecule 1: COAT PROTEIN

Chain B7:



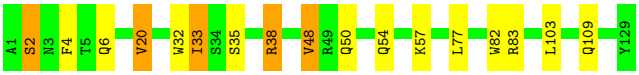
• Molecule 1: COAT PROTEIN

Chain B8:



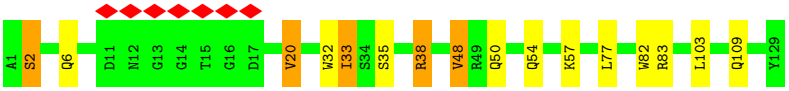
• Molecule 1: COAT PROTEIN

Chain B9:



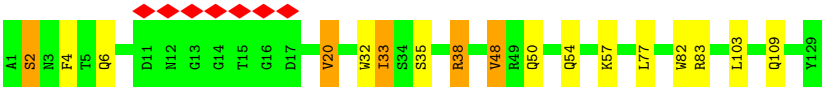
• Molecule 1: COAT PROTEIN

Chain BA:



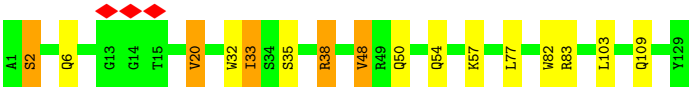
• Molecule 1: COAT PROTEIN

Chain BB:



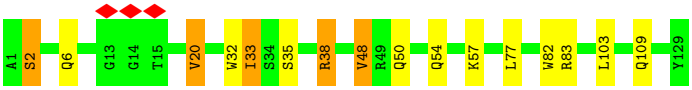
• Molecule 1: COAT PROTEIN

Chain BC:



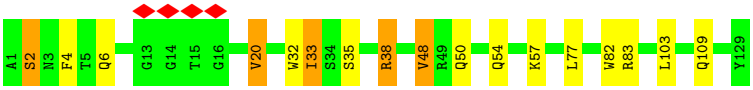
• Molecule 1: COAT PROTEIN

Chain BD:



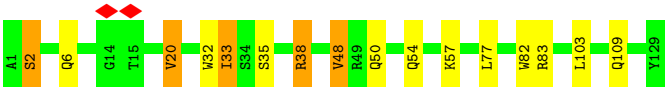
• Molecule 1: COAT PROTEIN

Chain BE:



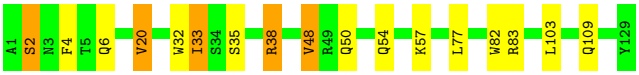
• Molecule 1: COAT PROTEIN

Chain BF:



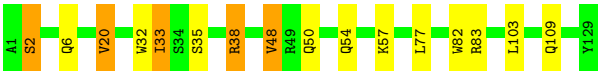
• Molecule 1: COAT PROTEIN

Chain BG:



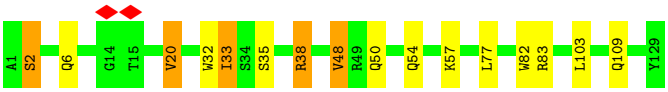
• Molecule 1: COAT PROTEIN

Chain BH:



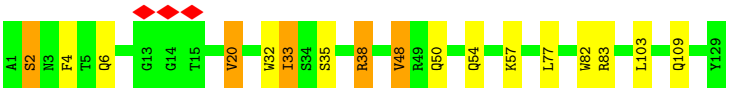
• Molecule 1: COAT PROTEIN

Chain BI:



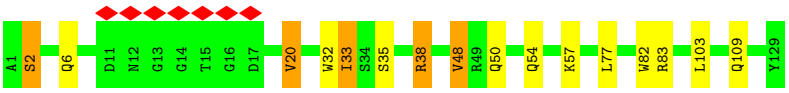
• Molecule 1: COAT PROTEIN

Chain BJ:



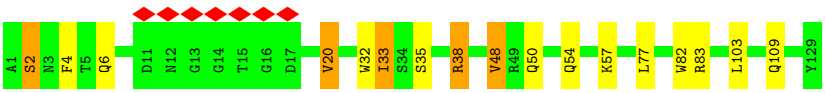
• Molecule 1: COAT PROTEIN

Chain BK:



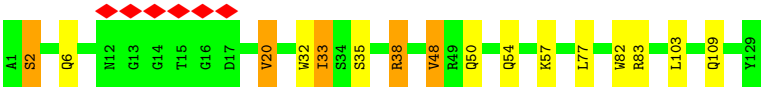
• Molecule 1: COAT PROTEIN

Chain BL:



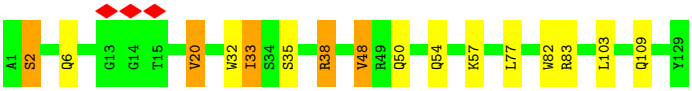
• Molecule 1: COAT PROTEIN

Chain BM:



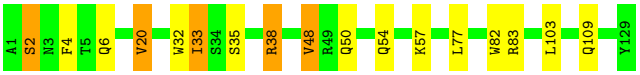
• Molecule 1: COAT PROTEIN

Chain BN:



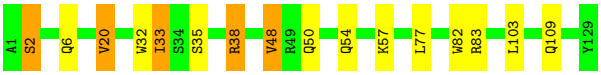
• Molecule 1: COAT PROTEIN

Chain BO:



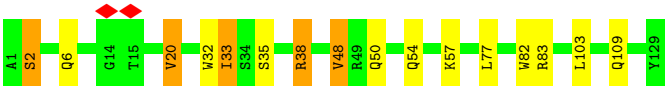
• Molecule 1: COAT PROTEIN

Chain BP:



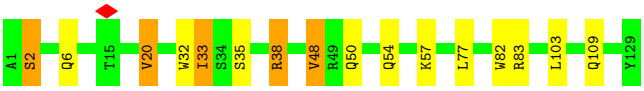
• Molecule 1: COAT PROTEIN

Chain BQ:



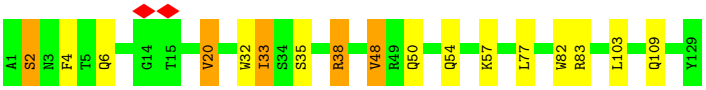
• Molecule 1: COAT PROTEIN

Chain BR:



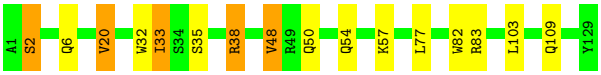
• Molecule 1: COAT PROTEIN

Chain BS:



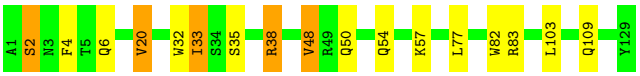
• Molecule 1: COAT PROTEIN

Chain BT:



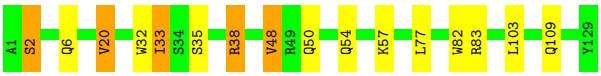
• Molecule 1: COAT PROTEIN

Chain BU:



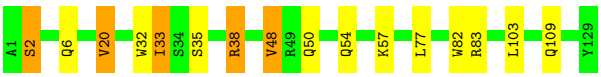
• Molecule 1: COAT PROTEIN

Chain BV:



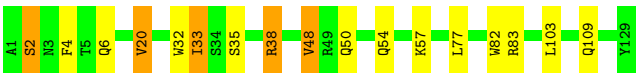
• Molecule 1: COAT PROTEIN

Chain BW:



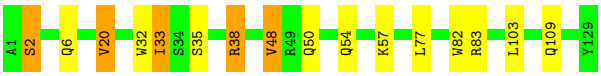
• Molecule 1: COAT PROTEIN

Chain BX:



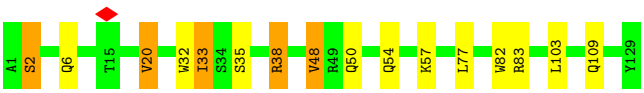
• Molecule 1: COAT PROTEIN

Chain BY:



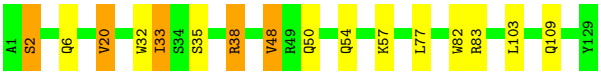
• Molecule 1: COAT PROTEIN

Chain BZ:



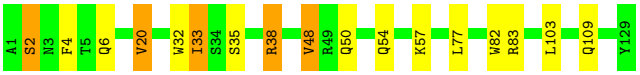
• Molecule 1: COAT PROTEIN

Chain Ba:



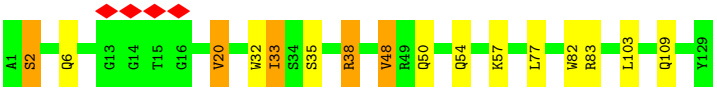
• Molecule 1: COAT PROTEIN

Chain Bb:



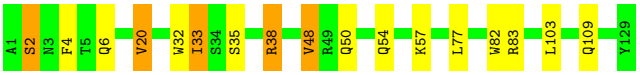
• Molecule 1: COAT PROTEIN

Chain Bc:



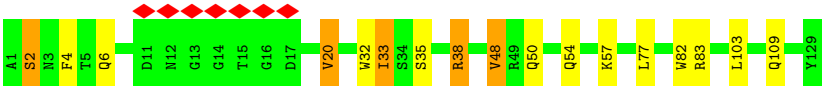
• Molecule 1: COAT PROTEIN

Chain Bd:



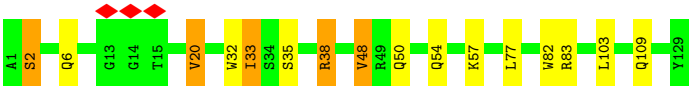
• Molecule 1: COAT PROTEIN

Chain Be:



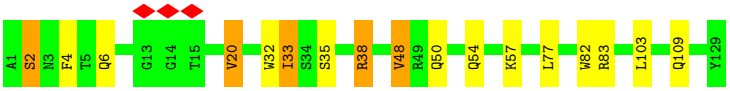
• Molecule 1: COAT PROTEIN

Chain Bf:



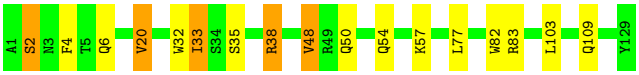
• Molecule 1: COAT PROTEIN

Chain Bg:



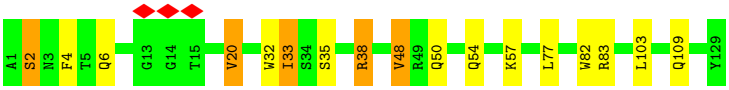
• Molecule 1: COAT PROTEIN

Chain Bh:



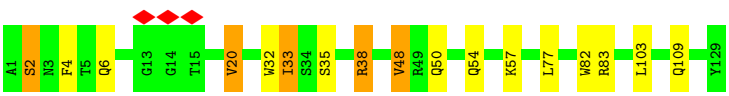
• Molecule 1: COAT PROTEIN

Chain Bi:



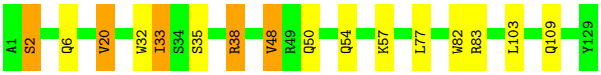
• Molecule 1: COAT PROTEIN

Chain Bj:



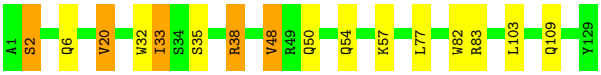
• Molecule 1: COAT PROTEIN

Chain Bk:



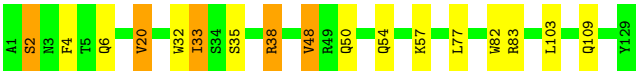
• Molecule 1: COAT PROTEIN

Chain Bl:



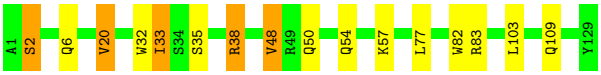
• Molecule 1: COAT PROTEIN

Chain Bm:



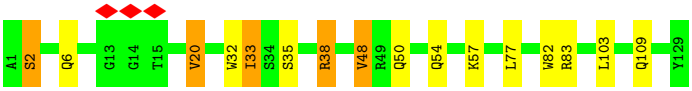
• Molecule 1: COAT PROTEIN

Chain Bn:



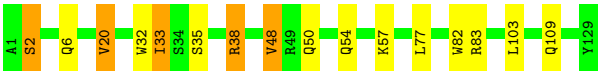
• Molecule 1: COAT PROTEIN

Chain Bo:



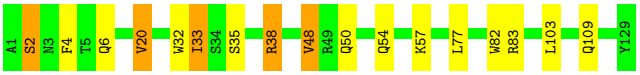
• Molecule 1: COAT PROTEIN

Chain Bp:



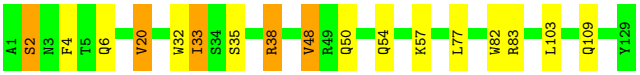
• Molecule 1: COAT PROTEIN

Chain Bq:



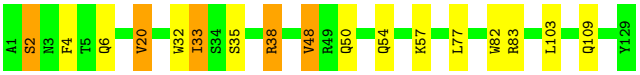
• Molecule 1: COAT PROTEIN

Chain Br:



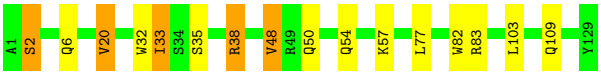
• Molecule 1: COAT PROTEIN

Chain Bs:



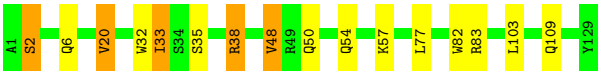
• Molecule 1: COAT PROTEIN

Chain Bt:



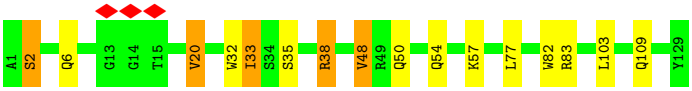
• Molecule 1: COAT PROTEIN

Chain Bu:



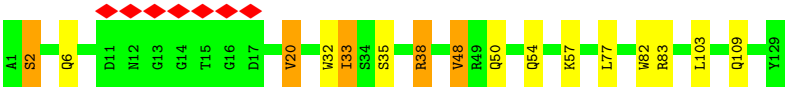
• Molecule 1: COAT PROTEIN

Chain Bv:



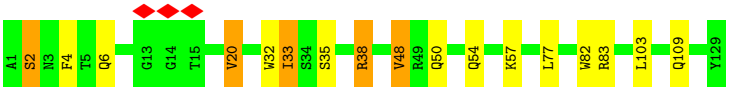
• Molecule 1: COAT PROTEIN

Chain Bw:



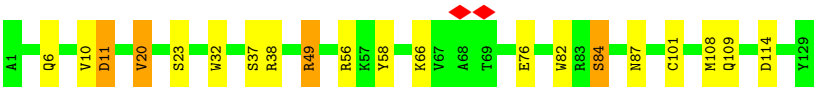
• Molecule 1: COAT PROTEIN

Chain Bx:



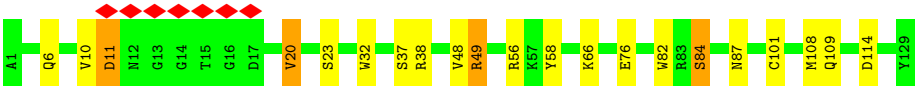
• Molecule 1: COAT PROTEIN

Chain C0:



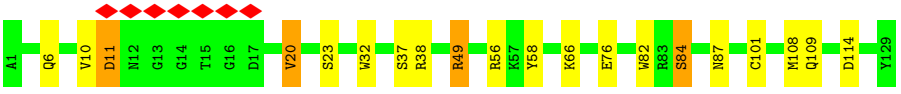
• Molecule 1: COAT PROTEIN

Chain C1:



• Molecule 1: COAT PROTEIN

Chain C2:

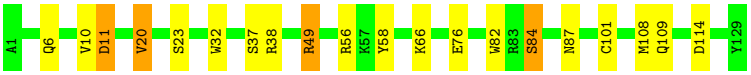


• Molecule 1: COAT PROTEIN

Chain C3:

• Molecule 1: COAT PROTEIN

Chain C4:



• Molecule 1: COAT PROTEIN

Chain C5:

• Molecule 1: COAT PROTEIN

Chain C6:

• Molecule 1: COAT PROTEIN

Chain C7:

• Molecule 1: COAT PROTEIN

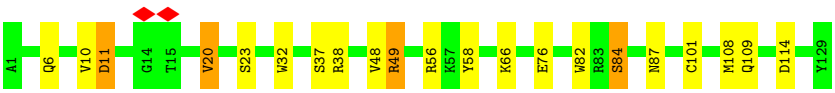
Chain C8:

• Molecule 1: COAT PROTEIN

Chain C9:

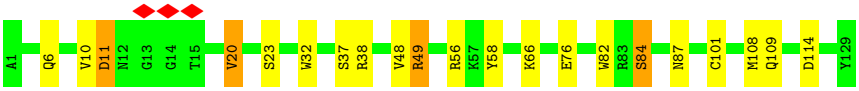
• Molecule 1: COAT PROTEIN

Chain CA:



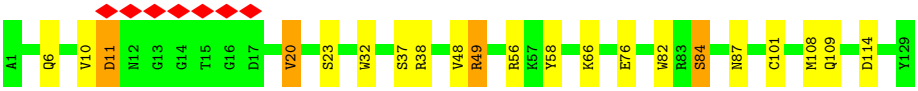
• Molecule 1: COAT PROTEIN

Chain CB:



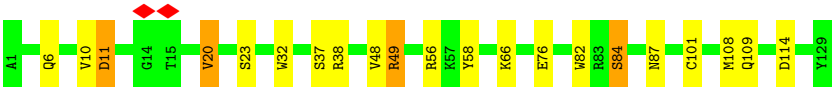
• Molecule 1: COAT PROTEIN

Chain CC:



• Molecule 1: COAT PROTEIN

Chain CD:

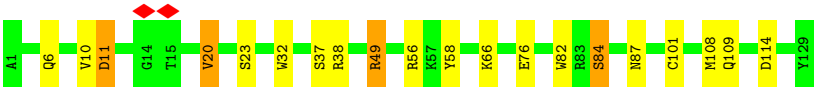


• Molecule 1: COAT PROTEIN

Chain CE:

• Molecule 1: COAT PROTEIN

Chain CF:



• Molecule 1: COAT PROTEIN

Chain CG:

• Molecule 1: COAT PROTEIN

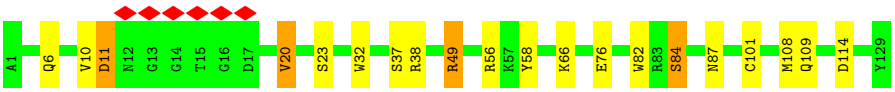
Chain CH:

• Molecule 1: COAT PROTEIN

Chain CI:

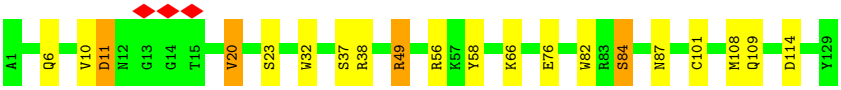
• Molecule 1: COAT PROTEIN

Chain CJ:



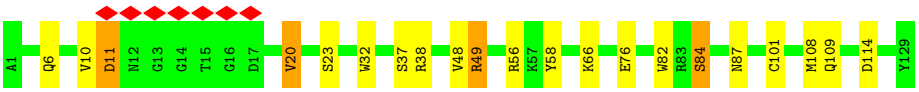
• Molecule 1: COAT PROTEIN

Chain CK:



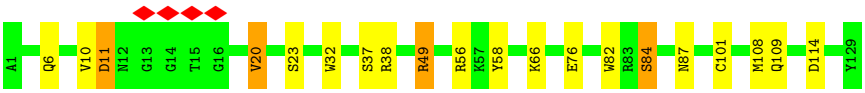
• Molecule 1: COAT PROTEIN

Chain CL:



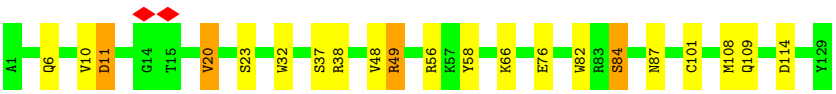
• Molecule 1: COAT PROTEIN

Chain CM:



• Molecule 1: COAT PROTEIN

Chain CN:



• Molecule 1: COAT PROTEIN

Chain CO:

• Molecule 1: COAT PROTEIN

Chain CP:

• Molecule 1: COAT PROTEIN

Chain CQ:

• Molecule 1: COAT PROTEIN

Chain CR:

• Molecule 1: COAT PROTEIN

Chain CS:

• Molecule 1: COAT PROTEIN

Chain CT:

• Molecule 1: COAT PROTEIN

Chain CU:

• Molecule 1: COAT PROTEIN

Chain CV:

• Molecule 1: COAT PROTEIN

Chain CW:

• Molecule 1: COAT PROTEIN

Chain CX:

• Molecule 1: COAT PROTEIN

Chain CY:

• Molecule 1: COAT PROTEIN

Chain CZ:

• Molecule 1: COAT PROTEIN

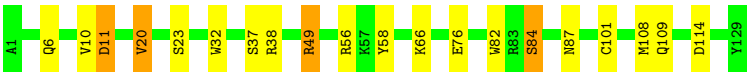
Chain Ca:

• Molecule 1: COAT PROTEIN

Chain Cb:

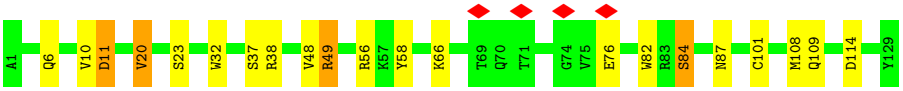
• Molecule 1: COAT PROTEIN

Chain Cc:



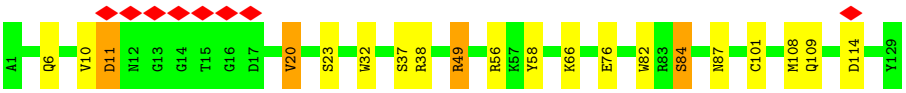
• Molecule 1: COAT PROTEIN

Chain Cd:



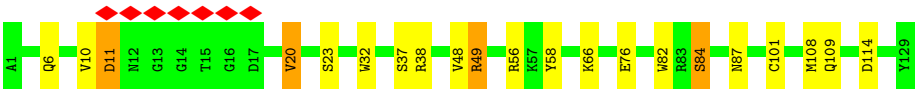
• Molecule 1: COAT PROTEIN

Chain Ce:



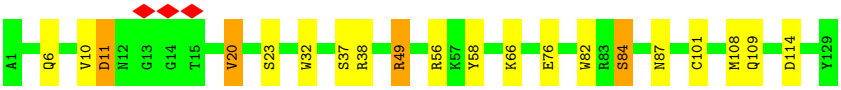
• Molecule 1: COAT PROTEIN

Chain Cf:



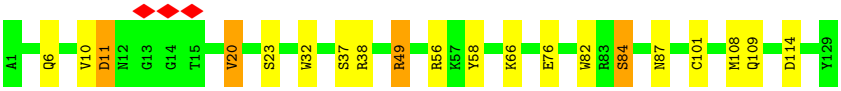
• Molecule 1: COAT PROTEIN

Chain Cg:



• Molecule 1: COAT PROTEIN

Chain Ch:

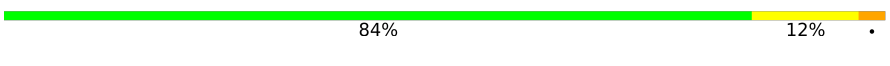


• Molecule 1: COAT PROTEIN

Chain Ci:

• Molecule 1: COAT PROTEIN

Chain Cj:



• Molecule 1: COAT PROTEIN

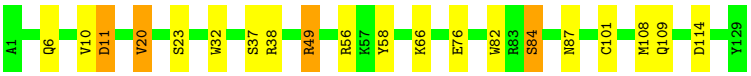
Chain Ck:

• Molecule 1: COAT PROTEIN

Chain Cl:

• Molecule 1: COAT PROTEIN

Chain Cm:



• Molecule 1: COAT PROTEIN

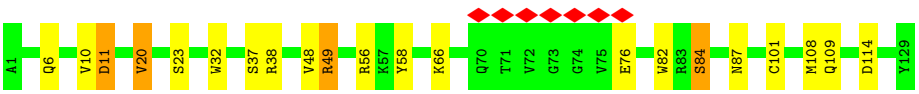
Chain Cn:

• Molecule 1: COAT PROTEIN

Chain Co:

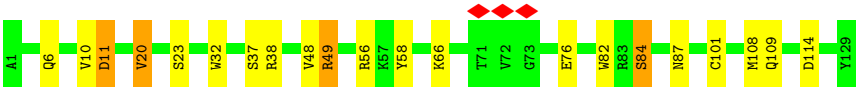
• Molecule 1: COAT PROTEIN

Chain Cp:



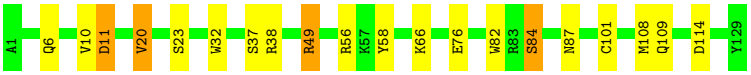
• Molecule 1: COAT PROTEIN

Chain Cq:



• Molecule 1: COAT PROTEIN

Chain Cr:

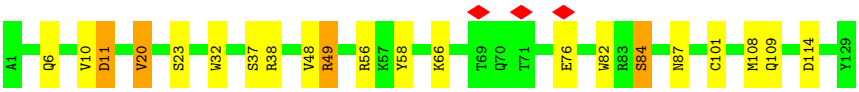


• Molecule 1: COAT PROTEIN

Chain Cs:

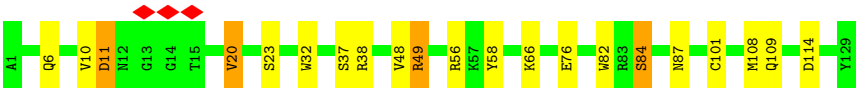
• Molecule 1: COAT PROTEIN

Chain Ct:



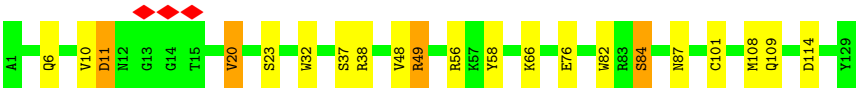
• Molecule 1: COAT PROTEIN

Chain Cu:



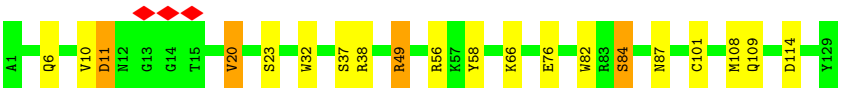
• Molecule 1: COAT PROTEIN

Chain Cv:



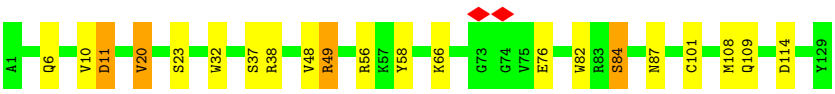
• Molecule 1: COAT PROTEIN

Chain Cw:



• Molecule 1: COAT PROTEIN

Chain Cx:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1500	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	23000	Depositor
Image detector	GATAN ULTRASCAN 10000 (10k x 10k)	Depositor
Maximum map value	7.490	Depositor
Minimum map value	-3.950	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.45	Depositor
Map size (Å)	583.68, 583.68, 583.68	wwPDB
Map dimensions	64, 64, 64	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	9.12, 9.12, 9.12	Depositor

5 Model quality

5.1 Standard geometry

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	A0	1.01	0/982	1.65	19/1337 (1.4%)
1	A1	1.01	0/982	1.65	19/1337 (1.4%)
1	A2	1.01	0/982	1.65	19/1337 (1.4%)
1	A3	1.01	0/982	1.65	19/1337 (1.4%)
1	A4	1.01	0/982	1.65	19/1337 (1.4%)
1	A5	1.01	0/982	1.65	19/1337 (1.4%)
1	A6	1.01	0/982	1.65	19/1337 (1.4%)
1	A7	1.01	0/982	1.65	19/1337 (1.4%)
1	A8	1.01	0/982	1.65	19/1337 (1.4%)
1	A9	1.01	0/982	1.65	19/1337 (1.4%)
1	AA	1.01	0/982	1.65	19/1337 (1.4%)
1	AB	1.01	0/982	1.65	19/1337 (1.4%)
1	AC	1.01	0/982	1.65	19/1337 (1.4%)
1	AD	1.01	0/982	1.65	19/1337 (1.4%)
1	AE	1.01	0/982	1.65	19/1337 (1.4%)
1	AF	1.01	0/982	1.65	19/1337 (1.4%)
1	AG	1.01	0/982	1.65	19/1337 (1.4%)
1	AH	1.01	0/982	1.65	19/1337 (1.4%)
1	AI	1.01	0/982	1.65	19/1337 (1.4%)
1	AJ	1.01	0/982	1.65	19/1337 (1.4%)
1	AK	1.01	0/982	1.65	19/1337 (1.4%)
1	AL	1.01	0/982	1.65	19/1337 (1.4%)
1	AM	1.01	0/982	1.65	19/1337 (1.4%)
1	AN	1.01	0/982	1.65	19/1337 (1.4%)
1	AO	1.01	0/982	1.65	19/1337 (1.4%)
1	AP	1.01	0/982	1.65	19/1337 (1.4%)
1	AQ	1.01	0/982	1.65	19/1337 (1.4%)
1	AR	1.01	0/982	1.65	19/1337 (1.4%)
1	AS	1.01	0/982	1.65	19/1337 (1.4%)
1	AT	1.01	0/982	1.65	19/1337 (1.4%)
1	AU	1.01	0/982	1.65	19/1337 (1.4%)
1	AV	1.01	0/982	1.65	19/1337 (1.4%)
1	AW	1.01	0/982	1.65	19/1337 (1.4%)
1	AX	1.01	0/982	1.65	19/1337 (1.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	AY	1.01	0/982	1.65	19/1337 (1.4%)
1	AZ	1.01	0/982	1.65	19/1337 (1.4%)
1	Aa	1.01	0/982	1.65	19/1337 (1.4%)
1	Ab	1.01	0/982	1.65	19/1337 (1.4%)
1	Ac	1.01	0/982	1.65	19/1337 (1.4%)
1	Ad	1.01	0/982	1.65	19/1337 (1.4%)
1	Ae	1.01	0/982	1.65	19/1337 (1.4%)
1	Af	1.01	0/982	1.65	19/1337 (1.4%)
1	Ag	1.01	0/982	1.65	19/1337 (1.4%)
1	Ah	1.01	0/982	1.65	19/1337 (1.4%)
1	Ai	1.01	0/982	1.65	19/1337 (1.4%)
1	Aj	1.01	0/982	1.65	19/1337 (1.4%)
1	Ak	1.01	0/982	1.65	19/1337 (1.4%)
1	Al	1.01	0/982	1.65	19/1337 (1.4%)
1	Am	1.01	0/982	1.65	19/1337 (1.4%)
1	An	1.01	0/982	1.65	19/1337 (1.4%)
1	Ao	1.01	0/982	1.65	19/1337 (1.4%)
1	Ap	1.01	0/982	1.65	19/1337 (1.4%)
1	Aq	1.01	0/982	1.65	19/1337 (1.4%)
1	Ar	1.01	0/982	1.65	19/1337 (1.4%)
1	As	1.01	0/982	1.65	19/1337 (1.4%)
1	At	1.01	0/982	1.65	19/1337 (1.4%)
1	Au	1.01	0/982	1.65	19/1337 (1.4%)
1	Av	1.01	0/982	1.65	19/1337 (1.4%)
1	Aw	1.01	0/982	1.65	19/1337 (1.4%)
1	Ax	1.01	0/982	1.65	19/1337 (1.4%)
1	B0	1.02	0/982	1.52	18/1337 (1.3%)
1	B1	1.02	0/982	1.52	19/1337 (1.4%)
1	B2	1.02	0/982	1.52	19/1337 (1.4%)
1	B3	1.02	0/982	1.52	18/1337 (1.3%)
1	B4	1.02	0/982	1.52	19/1337 (1.4%)
1	B5	1.02	0/982	1.52	18/1337 (1.3%)
1	B6	1.02	0/982	1.52	19/1337 (1.4%)
1	B7	1.02	0/982	1.52	18/1337 (1.3%)
1	B8	1.02	0/982	1.52	18/1337 (1.3%)
1	B9	1.02	0/982	1.52	18/1337 (1.3%)
1	BA	1.02	0/982	1.52	18/1337 (1.3%)
1	BB	1.02	0/982	1.52	18/1337 (1.3%)
1	BC	1.02	0/982	1.52	18/1337 (1.3%)
1	BD	1.02	0/982	1.52	18/1337 (1.3%)
1	BE	1.02	0/982	1.52	18/1337 (1.3%)
1	BF	1.02	0/982	1.52	18/1337 (1.3%)
1	BG	1.02	0/982	1.52	18/1337 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	BH	1.02	0/982	1.52	18/1337 (1.3%)
1	BI	1.02	0/982	1.52	18/1337 (1.3%)
1	BJ	1.02	0/982	1.52	18/1337 (1.3%)
1	BK	1.02	0/982	1.52	18/1337 (1.3%)
1	BL	1.02	0/982	1.52	19/1337 (1.4%)
1	BM	1.02	0/982	1.52	19/1337 (1.4%)
1	BN	1.02	0/982	1.52	18/1337 (1.3%)
1	BO	1.02	0/982	1.52	18/1337 (1.3%)
1	BP	1.02	0/982	1.52	18/1337 (1.3%)
1	BQ	1.02	0/982	1.52	18/1337 (1.3%)
1	BR	1.02	0/982	1.52	18/1337 (1.3%)
1	BS	1.02	0/982	1.52	19/1337 (1.4%)
1	BT	1.02	0/982	1.52	18/1337 (1.3%)
1	BU	1.02	0/982	1.52	18/1337 (1.3%)
1	BV	1.02	0/982	1.52	18/1337 (1.3%)
1	BW	1.02	0/982	1.52	18/1337 (1.3%)
1	BX	1.02	0/982	1.52	18/1337 (1.3%)
1	BY	1.02	0/982	1.52	18/1337 (1.3%)
1	BZ	1.02	0/982	1.52	18/1337 (1.3%)
1	Ba	1.02	0/982	1.52	18/1337 (1.3%)
1	Bb	1.02	0/982	1.52	19/1337 (1.4%)
1	Bc	1.02	0/982	1.52	18/1337 (1.3%)
1	Bd	1.02	0/982	1.52	18/1337 (1.3%)
1	Be	1.02	0/982	1.52	18/1337 (1.3%)
1	Bf	1.02	0/982	1.52	18/1337 (1.3%)
1	Bg	1.02	0/982	1.52	19/1337 (1.4%)
1	Bh	1.02	0/982	1.52	18/1337 (1.3%)
1	Bi	1.02	0/982	1.52	18/1337 (1.3%)
1	Bj	1.02	0/982	1.52	18/1337 (1.3%)
1	Bk	1.02	0/982	1.52	18/1337 (1.3%)
1	Bl	1.02	0/982	1.52	18/1337 (1.3%)
1	Bm	1.02	0/982	1.52	18/1337 (1.3%)
1	Bn	1.02	0/982	1.52	18/1337 (1.3%)
1	Bo	1.02	0/982	1.52	18/1337 (1.3%)
1	Bp	1.02	0/982	1.52	18/1337 (1.3%)
1	Bq	1.02	0/982	1.52	19/1337 (1.4%)
1	Br	1.02	0/982	1.52	19/1337 (1.4%)
1	Bs	1.02	0/982	1.52	18/1337 (1.3%)
1	Bt	1.02	0/982	1.52	18/1337 (1.3%)
1	Bu	1.02	0/982	1.52	18/1337 (1.3%)
1	Bv	1.02	0/982	1.52	18/1337 (1.3%)
1	Bw	1.02	0/982	1.52	18/1337 (1.3%)
1	Bx	1.02	0/982	1.52	18/1337 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	C0	0.94	0/982	1.67	22/1337 (1.6%)
1	C1	0.94	0/982	1.67	22/1337 (1.6%)
1	C2	0.94	0/982	1.67	22/1337 (1.6%)
1	C3	0.94	0/982	1.66	21/1337 (1.6%)
1	C4	0.94	0/982	1.66	21/1337 (1.6%)
1	C5	0.94	0/982	1.67	21/1337 (1.6%)
1	C6	0.94	0/982	1.67	22/1337 (1.6%)
1	C7	0.94	0/982	1.67	21/1337 (1.6%)
1	C8	0.94	0/982	1.67	22/1337 (1.6%)
1	C9	0.94	0/982	1.67	22/1337 (1.6%)
1	CA	0.94	0/982	1.67	22/1337 (1.6%)
1	CB	0.94	0/982	1.66	22/1337 (1.6%)
1	CC	0.94	0/982	1.67	22/1337 (1.6%)
1	CD	0.94	0/982	1.67	22/1337 (1.6%)
1	CE	0.94	0/982	1.67	22/1337 (1.6%)
1	CF	0.94	0/982	1.67	22/1337 (1.6%)
1	CG	0.94	0/982	1.67	21/1337 (1.6%)
1	CH	0.94	0/982	1.67	22/1337 (1.6%)
1	CI	0.94	0/982	1.66	22/1337 (1.6%)
1	CJ	0.94	0/982	1.67	21/1337 (1.6%)
1	CK	0.94	0/982	1.66	21/1337 (1.6%)
1	CL	0.94	0/982	1.67	22/1337 (1.6%)
1	CM	0.94	0/982	1.67	21/1337 (1.6%)
1	CN	0.94	0/982	1.67	22/1337 (1.6%)
1	CO	0.94	0/982	1.67	21/1337 (1.6%)
1	CP	0.94	0/982	1.67	23/1337 (1.7%)
1	CQ	0.94	0/982	1.67	22/1337 (1.6%)
1	CR	0.94	0/982	1.67	21/1337 (1.6%)
1	CS	0.94	0/982	1.66	22/1337 (1.6%)
1	CT	0.94	0/982	1.67	22/1337 (1.6%)
1	CU	0.94	0/982	1.66	21/1337 (1.6%)
1	CV	0.94	0/982	1.67	22/1337 (1.6%)
1	CW	0.94	0/982	1.67	22/1337 (1.6%)
1	CX	0.94	0/982	1.67	21/1337 (1.6%)
1	CY	0.94	0/982	1.67	22/1337 (1.6%)
1	CZ	0.94	0/982	1.67	22/1337 (1.6%)
1	Ca	0.94	0/982	1.67	22/1337 (1.6%)
1	Cb	0.94	0/982	1.67	21/1337 (1.6%)
1	Cc	0.94	0/982	1.67	21/1337 (1.6%)
1	Cd	0.94	0/982	1.67	22/1337 (1.6%)
1	Ce	0.94	0/982	1.67	21/1337 (1.6%)
1	Cf	0.94	0/982	1.67	22/1337 (1.6%)
1	Cg	0.94	0/982	1.67	21/1337 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	Ch	0.94	0/982	1.67	21/1337 (1.6%)
1	Ci	0.94	0/982	1.66	21/1337 (1.6%)
1	Cj	0.94	0/982	1.67	21/1337 (1.6%)
1	Ck	0.94	0/982	1.67	22/1337 (1.6%)
1	Cl	0.94	0/982	1.66	21/1337 (1.6%)
1	Cm	0.94	0/982	1.67	21/1337 (1.6%)
1	Cn	0.94	0/982	1.67	21/1337 (1.6%)
1	Co	0.94	0/982	1.67	21/1337 (1.6%)
1	Cp	0.94	0/982	1.67	22/1337 (1.6%)
1	Cq	0.94	0/982	1.67	22/1337 (1.6%)
1	Cr	0.94	0/982	1.67	21/1337 (1.6%)
1	Cs	0.94	0/982	1.66	21/1337 (1.6%)
1	Ct	0.94	0/982	1.67	22/1337 (1.6%)
1	Cu	0.94	0/982	1.67	22/1337 (1.6%)
1	Cv	0.94	0/982	1.67	22/1337 (1.6%)
1	Cw	0.94	0/982	1.67	21/1337 (1.6%)
1	Cx	0.94	0/982	1.67	22/1337 (1.6%)
All	All	0.99	0/176760	1.61	3526/240660 (1.5%)

There are no bond length outliers.

All (3526) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ac	56	ARG	NE-CZ-NH2	-20.60	110.00	120.30
1	A1	56	ARG	NE-CZ-NH2	-20.59	110.00	120.30
1	A3	56	ARG	NE-CZ-NH2	-20.56	110.02	120.30
1	AW	56	ARG	NE-CZ-NH2	-20.54	110.03	120.30
1	A9	56	ARG	NE-CZ-NH2	-20.54	110.03	120.30
1	AN	56	ARG	NE-CZ-NH2	-20.53	110.03	120.30
1	Av	56	ARG	NE-CZ-NH2	-20.52	110.04	120.30
1	Ax	56	ARG	NE-CZ-NH2	-20.51	110.05	120.30
1	Ar	56	ARG	NE-CZ-NH2	-20.50	110.05	120.30
1	AV	56	ARG	NE-CZ-NH2	-20.50	110.05	120.30
1	Ad	56	ARG	NE-CZ-NH2	-20.50	110.05	120.30
1	AA	56	ARG	NE-CZ-NH2	-20.49	110.05	120.30
1	AZ	56	ARG	NE-CZ-NH2	-20.49	110.05	120.30
1	As	56	ARG	NE-CZ-NH2	-20.49	110.06	120.30
1	A5	56	ARG	NE-CZ-NH2	-20.48	110.06	120.30
1	AD	56	ARG	NE-CZ-NH2	-20.48	110.06	120.30
1	Al	56	ARG	NE-CZ-NH2	-20.48	110.06	120.30
1	An	56	ARG	NE-CZ-NH2	-20.48	110.06	120.30
1	Ak	56	ARG	NE-CZ-NH2	-20.47	110.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A4	56	ARG	NE-CZ-NH2	-20.47	110.07	120.30
1	AT	56	ARG	NE-CZ-NH2	-20.47	110.07	120.30
1	Aw	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	Aj	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	Am	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	Ab	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	Au	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	AF	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	AU	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	Af	56	ARG	NE-CZ-NH2	-20.45	110.07	120.30
1	AB	56	ARG	NE-CZ-NH2	-20.45	110.07	120.30
1	A7	56	ARG	NE-CZ-NH2	-20.45	110.08	120.30
1	AH	56	ARG	NE-CZ-NH2	-20.45	110.08	120.30
1	AE	56	ARG	NE-CZ-NH2	-20.44	110.08	120.30
1	A6	56	ARG	NE-CZ-NH2	-20.44	110.08	120.30
1	Ae	56	ARG	NE-CZ-NH2	-20.44	110.08	120.30
1	A8	56	ARG	NE-CZ-NH2	-20.44	110.08	120.30
1	AM	56	ARG	NE-CZ-NH2	-20.44	110.08	120.30
1	AR	56	ARG	NE-CZ-NH2	-20.43	110.08	120.30
1	AX	56	ARG	NE-CZ-NH2	-20.43	110.08	120.30
1	A0	56	ARG	NE-CZ-NH2	-20.43	110.08	120.30
1	AI	56	ARG	NE-CZ-NH2	-20.43	110.08	120.30
1	A2	56	ARG	NE-CZ-NH2	-20.43	110.09	120.30
1	Ag	56	ARG	NE-CZ-NH2	-20.42	110.09	120.30
1	AK	56	ARG	NE-CZ-NH2	-20.42	110.09	120.30
1	Aa	56	ARG	NE-CZ-NH2	-20.40	110.10	120.30
1	AC	56	ARG	NE-CZ-NH2	-20.40	110.10	120.30
1	AL	56	ARG	NE-CZ-NH2	-20.40	110.10	120.30
1	Ap	56	ARG	NE-CZ-NH2	-20.40	110.10	120.30
1	AG	56	ARG	NE-CZ-NH2	-20.40	110.10	120.30
1	AO	56	ARG	NE-CZ-NH2	-20.39	110.10	120.30
1	Ah	56	ARG	NE-CZ-NH2	-20.39	110.11	120.30
1	AJ	56	ARG	NE-CZ-NH2	-20.39	110.11	120.30
1	AQ	56	ARG	NE-CZ-NH2	-20.38	110.11	120.30
1	Ao	56	ARG	NE-CZ-NH2	-20.37	110.11	120.30
1	AY	56	ARG	NE-CZ-NH2	-20.37	110.11	120.30
1	At	56	ARG	NE-CZ-NH2	-20.36	110.12	120.30
1	AP	56	ARG	NE-CZ-NH2	-20.36	110.12	120.30
1	Aq	56	ARG	NE-CZ-NH2	-20.33	110.14	120.30
1	AS	56	ARG	NE-CZ-NH2	-20.33	110.14	120.30
1	Ai	56	ARG	NE-CZ-NH2	-20.26	110.17	120.30
1	CR	11	ASP	CB-CA-C	-10.60	89.20	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CJ	11	ASP	CB-CA-C	-10.60	89.20	110.40
1	CV	11	ASP	CB-CA-C	-10.59	89.22	110.40
1	Cr	11	ASP	CB-CA-C	-10.59	89.22	110.40
1	Cg	11	ASP	CB-CA-C	-10.59	89.22	110.40
1	CL	11	ASP	CB-CA-C	-10.59	89.22	110.40
1	Cf	11	ASP	CB-CA-C	-10.59	89.23	110.40
1	Cp	11	ASP	CB-CA-C	-10.59	89.23	110.40
1	C5	11	ASP	CB-CA-C	-10.58	89.23	110.40
1	Cs	11	ASP	CB-CA-C	-10.58	89.23	110.40
1	CD	11	ASP	CB-CA-C	-10.58	89.24	110.40
1	C1	11	ASP	CB-CA-C	-10.58	89.24	110.40
1	CB	11	ASP	CB-CA-C	-10.58	89.24	110.40
1	CC	11	ASP	CB-CA-C	-10.58	89.24	110.40
1	CI	11	ASP	CB-CA-C	-10.58	89.25	110.40
1	Cd	11	ASP	CB-CA-C	-10.58	89.25	110.40
1	Ci	11	ASP	CB-CA-C	-10.58	89.25	110.40
1	Ck	11	ASP	CB-CA-C	-10.58	89.25	110.40
1	Co	11	ASP	CB-CA-C	-10.58	89.25	110.40
1	Cl	11	ASP	CB-CA-C	-10.57	89.25	110.40
1	CU	11	ASP	CB-CA-C	-10.57	89.25	110.40
1	CS	11	ASP	CB-CA-C	-10.57	89.26	110.40
1	CT	11	ASP	CB-CA-C	-10.57	89.26	110.40
1	Cc	11	ASP	CB-CA-C	-10.57	89.26	110.40
1	Ch	11	ASP	CB-CA-C	-10.57	89.26	110.40
1	Cj	11	ASP	CB-CA-C	-10.57	89.26	110.40
1	Cq	11	ASP	CB-CA-C	-10.57	89.26	110.40
1	CF	11	ASP	CB-CA-C	-10.57	89.27	110.40
1	Cn	11	ASP	CB-CA-C	-10.57	89.27	110.40
1	C0	11	ASP	CB-CA-C	-10.56	89.27	110.40
1	CQ	11	ASP	CB-CA-C	-10.56	89.27	110.40
1	CA	11	ASP	CB-CA-C	-10.56	89.27	110.40
1	C3	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	Ct	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	C6	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	CH	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	CK	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	CO	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	Ca	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	Cw	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	C9	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	CM	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	CZ	11	ASP	CB-CA-C	-10.56	89.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C2	11	ASP	CB-CA-C	-10.56	89.29	110.40
1	C4	11	ASP	CB-CA-C	-10.56	89.29	110.40
1	C8	11	ASP	CB-CA-C	-10.55	89.29	110.40
1	CE	11	ASP	CB-CA-C	-10.55	89.29	110.40
1	CY	11	ASP	CB-CA-C	-10.55	89.29	110.40
1	Cv	11	ASP	CB-CA-C	-10.55	89.29	110.40
1	Cx	11	ASP	CB-CA-C	-10.55	89.29	110.40
1	C7	11	ASP	CB-CA-C	-10.55	89.30	110.40
1	CN	11	ASP	CB-CA-C	-10.55	89.30	110.40
1	CP	11	ASP	CB-CA-C	-10.54	89.31	110.40
1	Cm	11	ASP	CB-CA-C	-10.54	89.31	110.40
1	Cu	11	ASP	CB-CA-C	-10.54	89.32	110.40
1	CG	11	ASP	CB-CA-C	-10.54	89.32	110.40
1	CW	11	ASP	CB-CA-C	-10.54	89.32	110.40
1	CX	11	ASP	CB-CA-C	-10.54	89.32	110.40
1	Cb	11	ASP	CB-CA-C	-10.54	89.33	110.40
1	Ce	11	ASP	CB-CA-C	-10.52	89.35	110.40
1	CF	11	ASP	N-CA-CB	10.22	129.00	110.60
1	CG	11	ASP	N-CA-CB	10.22	129.00	110.60
1	Cn	11	ASP	N-CA-CB	10.22	128.99	110.60
1	CM	11	ASP	N-CA-CB	10.22	128.99	110.60
1	Cb	11	ASP	N-CA-CB	10.21	128.99	110.60
1	Cf	11	ASP	N-CA-CB	10.21	128.98	110.60
1	Ce	11	ASP	N-CA-CB	10.21	128.97	110.60
1	Ct	11	ASP	N-CA-CB	10.21	128.97	110.60
1	CI	11	ASP	N-CA-CB	10.20	128.96	110.60
1	CX	11	ASP	N-CA-CB	10.20	128.97	110.60
1	C7	11	ASP	N-CA-CB	10.20	128.96	110.60
1	C2	11	ASP	N-CA-CB	10.20	128.95	110.60
1	CH	11	ASP	N-CA-CB	10.20	128.95	110.60
1	C0	11	ASP	N-CA-CB	10.19	128.95	110.60
1	CE	11	ASP	N-CA-CB	10.19	128.95	110.60
1	CA	11	ASP	N-CA-CB	10.19	128.94	110.60
1	Cj	11	ASP	N-CA-CB	10.19	128.94	110.60
1	Ck	11	ASP	N-CA-CB	10.19	128.94	110.60
1	CC	11	ASP	N-CA-CB	10.19	128.93	110.60
1	CD	11	ASP	N-CA-CB	10.19	128.93	110.60
1	CT	11	ASP	N-CA-CB	10.19	128.94	110.60
1	CN	11	ASP	N-CA-CB	10.19	128.93	110.60
1	Ch	11	ASP	N-CA-CB	10.19	128.93	110.60
1	C1	11	ASP	N-CA-CB	10.18	128.93	110.60
1	C3	11	ASP	N-CA-CB	10.18	128.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C9	11	ASP	N-CA-CB	10.18	128.93	110.60
1	CZ	11	ASP	N-CA-CB	10.18	128.93	110.60
1	Cm	11	ASP	N-CA-CB	10.18	128.93	110.60
1	Cc	11	ASP	N-CA-CB	10.18	128.93	110.60
1	Cx	11	ASP	N-CA-CB	10.18	128.93	110.60
1	C4	11	ASP	N-CA-CB	10.18	128.92	110.60
1	CO	11	ASP	N-CA-CB	10.18	128.92	110.60
1	C6	11	ASP	N-CA-CB	10.18	128.92	110.60
1	CP	11	ASP	N-CA-CB	10.18	128.92	110.60
1	C5	11	ASP	N-CA-CB	10.17	128.91	110.60
1	CK	11	ASP	N-CA-CB	10.17	128.91	110.60
1	CU	11	ASP	N-CA-CB	10.17	128.91	110.60
1	Cu	11	ASP	N-CA-CB	10.17	128.91	110.60
1	CW	11	ASP	N-CA-CB	10.17	128.91	110.60
1	Cw	11	ASP	N-CA-CB	10.17	128.91	110.60
1	C8	11	ASP	N-CA-CB	10.17	128.90	110.60
1	CB	11	ASP	N-CA-CB	10.17	128.90	110.60
1	CQ	11	ASP	N-CA-CB	10.17	128.90	110.60
1	CV	11	ASP	N-CA-CB	10.17	128.90	110.60
1	Cp	11	ASP	N-CA-CB	10.17	128.90	110.60
1	Cg	11	ASP	N-CA-CB	10.16	128.89	110.60
1	Cl	11	ASP	N-CA-CB	10.16	128.90	110.60
1	Cs	11	ASP	N-CA-CB	10.16	128.90	110.60
1	CR	11	ASP	N-CA-CB	10.16	128.89	110.60
1	Cq	11	ASP	N-CA-CB	10.16	128.89	110.60
1	Ci	11	ASP	N-CA-CB	10.16	128.89	110.60
1	Co	11	ASP	N-CA-CB	10.16	128.89	110.60
1	Cd	11	ASP	N-CA-CB	10.15	128.88	110.60
1	Cv	11	ASP	N-CA-CB	10.15	128.87	110.60
1	CY	11	ASP	N-CA-CB	10.15	128.87	110.60
1	Ca	11	ASP	N-CA-CB	10.15	128.87	110.60
1	Cr	11	ASP	N-CA-CB	10.15	128.86	110.60
1	CL	11	ASP	N-CA-CB	10.14	128.86	110.60
1	CJ	11	ASP	N-CA-CB	10.13	128.84	110.60
1	CS	11	ASP	N-CA-CB	10.12	128.82	110.60
1	AV	56	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	Aj	56	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	Ax	56	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	AB	56	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	Af	56	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	Ac	56	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	A1	56	ARG	NE-CZ-NH1	9.16	124.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AR	56	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	Ao	56	ARG	NE-CZ-NH1	9.15	124.87	120.30
1	As	56	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	Ah	56	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	Av	56	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	AT	56	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	Ag	56	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	AJ	56	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	Ab	56	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	AU	56	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	An	56	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	A0	56	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	AK	56	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	Au	56	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	AW	56	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	Aw	56	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	AN	56	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	Ad	56	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A5	56	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	AC	56	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A9	56	ARG	NE-CZ-NH1	9.09	124.85	120.30
1	Al	56	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	Ar	56	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	AQ	56	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	AM	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	AF	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	AO	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	Am	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A4	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A7	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	Ak	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	Aq	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A2	56	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	AZ	56	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A3	56	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	At	56	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	AI	56	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	Ap	56	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	AL	56	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	AP	56	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	A8	56	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	AX	56	ARG	NE-CZ-NH1	9.04	124.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AE	56	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	AG	56	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	AA	56	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	AD	56	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	A6	56	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	AH	56	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	AS	56	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	AY	56	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	Ae	56	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	Aa	56	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	Ai	56	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	Ck	56	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	Co	32	TRP	CE2-CD2-CG	-8.76	100.29	107.30
1	C0	32	TRP	CE2-CD2-CG	-8.76	100.30	107.30
1	Cm	32	TRP	CE2-CD2-CG	-8.76	100.30	107.30
1	CQ	56	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	Cx	32	TRP	CE2-CD2-CG	-8.74	100.31	107.30
1	CN	32	TRP	CE2-CD2-CG	-8.73	100.31	107.30
1	Ct	56	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	CH	32	TRP	CE2-CD2-CG	-8.73	100.32	107.30
1	Cd	32	TRP	CE2-CD2-CG	-8.73	100.32	107.30
1	CX	32	TRP	CE2-CD2-CG	-8.73	100.32	107.30
1	Cf	56	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	Cn	56	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	Ca	32	TRP	CE2-CD2-CG	-8.72	100.32	107.30
1	Ce	32	TRP	CE2-CD2-CG	-8.72	100.32	107.30
1	CL	32	TRP	CE2-CD2-CG	-8.72	100.32	107.30
1	C6	56	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	CE	32	TRP	CE2-CD2-CG	-8.72	100.33	107.30
1	CO	32	TRP	CE2-CD2-CG	-8.72	100.33	107.30
1	CV	32	TRP	CE2-CD2-CG	-8.72	100.33	107.30
1	C7	32	TRP	CE2-CD2-CG	-8.71	100.33	107.30
1	C5	32	TRP	CE2-CD2-CG	-8.71	100.33	107.30
1	CZ	32	TRP	CE2-CD2-CG	-8.71	100.33	107.30
1	CJ	32	TRP	CE2-CD2-CG	-8.71	100.33	107.30
1	CK	56	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	CT	32	TRP	CE2-CD2-CG	-8.71	100.33	107.30
1	C5	56	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	CD	32	TRP	CE2-CD2-CG	-8.70	100.34	107.30
1	CP	32	TRP	CE2-CD2-CG	-8.70	100.34	107.30
1	CM	32	TRP	CE2-CD2-CG	-8.70	100.34	107.30
1	CY	32	TRP	CE2-CD2-CG	-8.70	100.34	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Cv	32	TRP	CE2-CD2-CG	-8.70	100.34	107.30
1	Cp	32	TRP	CE2-CD2-CG	-8.69	100.34	107.30
1	C1	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	C9	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	CA	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	CC	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	Ch	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	Cr	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	CI	56	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	Cj	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	CH	56	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	CQ	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	Ca	56	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	Cc	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	CK	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	CB	32	TRP	CE2-CD2-CG	-8.68	100.35	107.30
1	C8	32	TRP	CE2-CD2-CG	-8.68	100.36	107.30
1	Cn	32	TRP	CE2-CD2-CG	-8.68	100.36	107.30
1	Cq	56	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	Cu	32	TRP	CE2-CD2-CG	-8.68	100.36	107.30
1	C2	32	TRP	CE2-CD2-CG	-8.68	100.36	107.30
1	CW	32	TRP	CE2-CD2-CG	-8.68	100.36	107.30
1	Cb	32	TRP	CE2-CD2-CG	-8.68	100.36	107.30
1	CS	32	TRP	CE2-CD2-CG	-8.67	100.36	107.30
1	Cj	56	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	Cw	56	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	Ci	32	TRP	CE2-CD2-CG	-8.67	100.36	107.30
1	C3	32	TRP	CE2-CD2-CG	-8.67	100.37	107.30
1	CR	32	TRP	CE2-CD2-CG	-8.67	100.37	107.30
1	Cw	32	TRP	CE2-CD2-CG	-8.67	100.36	107.30
1	C4	32	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	CG	32	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	CA	56	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	C6	32	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	Cf	32	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	CF	32	TRP	CE2-CD2-CG	-8.65	100.38	107.30
1	CV	56	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	Cq	32	TRP	CE2-CD2-CG	-8.65	100.38	107.30
1	C9	56	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	Ck	32	TRP	CE2-CD2-CG	-8.65	100.38	107.30
1	CC	56	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	Cg	32	TRP	CE2-CD2-CG	-8.65	100.38	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CW	56	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	CY	56	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	Cs	32	TRP	CE2-CD2-CG	-8.65	100.38	107.30
1	CT	56	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	Cl	32	TRP	CE2-CD2-CG	-8.64	100.39	107.30
1	CR	56	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	CX	56	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	C0	56	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	CU	32	TRP	CE2-CD2-CG	-8.63	100.39	107.30
1	C4	56	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	CP	56	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	Co	56	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	Ct	32	TRP	CE2-CD2-CG	-8.63	100.40	107.30
1	Ce	56	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	CJ	56	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	C7	56	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	CG	56	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	Ci	56	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	Cb	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	CL	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	Cr	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	CD	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	CF	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	Cc	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	CN	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	C8	56	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	CI	32	TRP	CE2-CD2-CG	-8.59	100.43	107.30
1	Ch	56	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	Cm	56	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	Cx	56	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	Cs	56	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	C3	56	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	CE	56	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	Cu	56	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	Cg	56	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	CU	56	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	Cv	56	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	CO	56	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	CS	56	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	C1	56	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	Cd	56	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	Cl	56	ARG	NE-CZ-NH2	-8.52	116.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C2	56	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	CB	56	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	CZ	56	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	Cp	56	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	CM	56	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B9	32	TRP	CD1-CG-CD2	8.35	112.98	106.30
1	Bw	32	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	B0	32	TRP	CD1-CG-CD2	8.29	112.94	106.30
1	Bv	32	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	BN	32	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	BH	32	TRP	CD1-CG-CD2	8.28	112.92	106.30
1	BP	32	TRP	CD1-CG-CD2	8.28	112.92	106.30
1	BW	32	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	Ba	32	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	Bu	32	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	Bc	32	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	Bf	32	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	B4	32	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	BD	32	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	B5	32	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	BA	32	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	B6	32	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	BY	32	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	BF	32	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	B7	32	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	Bs	32	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	BG	32	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	Bn	32	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	Bo	32	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	Bb	32	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	B2	32	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	BS	32	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	Bx	32	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	B3	32	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	Bd	32	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	BT	32	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	BQ	32	TRP	CD1-CG-CD2	8.22	112.87	106.30
1	Bp	32	TRP	CD1-CG-CD2	8.22	112.87	106.30
1	B1	32	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	BI	32	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	Bl	32	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	Cm	49	ARG	NE-CZ-NH2	-8.21	116.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BV	32	TRP	CD1-CG-CD2	8.20	112.86	106.30
1	Bm	32	TRP	CD1-CG-CD2	8.20	112.86	106.30
1	BX	32	TRP	CD1-CG-CD2	8.19	112.86	106.30
1	Bk	32	TRP	CD1-CG-CD2	8.19	112.86	106.30
1	Be	32	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	Bh	32	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	B8	32	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	BK	32	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	CA	49	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	Bt	32	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	BB	32	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	Bj	32	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	Bg	32	TRP	CD1-CG-CD2	8.17	112.84	106.30
1	BC	32	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	BZ	32	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	Br	32	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	BJ	32	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	BO	32	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	Bi	32	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	CZ	49	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	BL	32	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	Cj	49	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	AO	32	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	A7	32	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	BU	32	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	Co	49	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	BE	32	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	BR	32	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	BM	32	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	Ca	49	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	Bq	32	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	C1	49	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	AP	32	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	Au	32	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	CO	49	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	CW	49	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	Cl	49	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	C2	49	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	C3	49	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A3	32	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	C7	49	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	C8	49	ARG	NE-CZ-NH2	-8.10	116.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	32	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	AX	32	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	CG	49	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	CX	49	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	At	32	TRP	CD1-CG-CD2	8.09	112.78	106.30
1	AB	32	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	A9	32	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	AR	32	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	Cb	49	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	Ax	32	TRP	CD1-CG-CD2	8.08	112.77	106.30
1	CM	49	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	Aj	32	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	Ak	32	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	AF	32	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	BX	83	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	CE	49	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	CY	49	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	AA	32	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	AD	32	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	Cd	49	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	Ar	32	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	AN	32	TRP	CD1-CG-CD2	8.07	112.75	106.30
1	AW	32	TRP	CD1-CG-CD2	8.07	112.75	106.30
1	Ab	32	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	CF	49	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	AS	32	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	C9	49	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	AJ	32	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	Ac	32	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	Ap	32	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	CP	49	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A0	32	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	A6	32	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	AV	32	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	C5	49	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	Al	32	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	C0	49	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	Cf	49	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	AZ	32	TRP	CD1-CG-CD2	8.04	112.74	106.30
1	Af	32	TRP	CD1-CG-CD2	8.04	112.74	106.30
1	Av	32	TRP	CD1-CG-CD2	8.04	112.74	106.30
1	Aw	32	TRP	CD1-CG-CD2	8.04	112.73	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A2	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	AY	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	CD	49	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	CT	49	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	Cp	49	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A4	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	AQ	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	A8	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	AL	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	AM	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	Ao	32	TRP	CD1-CG-CD2	8.03	112.73	106.30
1	As	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	C4	49	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	Cw	49	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	Cx	49	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	AE	32	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	AT	32	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	Aa	32	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	AC	32	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	Am	32	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	CC	49	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	Cn	49	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	Cu	49	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	CN	49	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	Cc	49	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	Aq	32	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	Ce	49	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	Ad	32	TRP	CD1-CG-CD2	8.02	112.71	106.30
1	Ae	32	TRP	CD1-CG-CD2	8.02	112.71	106.30
1	AK	32	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	AI	32	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	A5	32	TRP	CD1-CG-CD2	8.01	112.70	106.30
1	Ah	32	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	AH	32	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	Cv	49	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B4	83	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	CR	49	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	AG	32	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	AU	32	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	CB	49	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	Cq	49	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	Bi	83	ARG	NE-CZ-NH2	-7.98	116.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Bo	83	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	CQ	49	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	BB	83	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	Ag	32	TRP	CD1-CG-CD2	7.98	112.68	106.30
1	An	32	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	B6	83	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	BL	83	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	CH	49	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	Ai	32	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	Bt	83	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	CJ	49	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	CL	49	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	Cs	49	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	Cg	49	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	Bx	83	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	Ci	49	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	BU	83	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	C6	49	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B7	83	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	Ct	49	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	CK	49	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	BR	83	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	CV	49	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	Ck	49	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	BM	83	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	Ch	49	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	CS	49	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	Bg	83	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	CP	32	TRP	CG-CD2-CE3	7.94	141.05	133.90
1	BQ	83	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	Cr	49	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	Be	83	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	Bp	83	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	CJ	32	TRP	CG-CD2-CE3	7.93	141.04	133.90
1	BG	83	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	C9	32	TRP	CG-CD2-CE3	7.93	141.03	133.90
1	CU	49	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	Br	83	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	Co	32	TRP	CG-CD2-CE3	7.92	141.03	133.90
1	B1	83	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	Bh	83	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	Bb	83	ARG	NE-CZ-NH2	-7.92	116.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CL	32	TRP	CG-CD2-CE3	7.92	141.03	133.90
1	CN	32	TRP	CG-CD2-CE3	7.92	141.03	133.90
1	Ca	32	TRP	CG-CD2-CE3	7.92	141.03	133.90
1	CB	32	TRP	CG-CD2-CE3	7.92	141.02	133.90
1	Bf	83	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	BV	83	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	Cq	32	TRP	CG-CD2-CE3	7.91	141.02	133.90
1	C1	32	TRP	CG-CD2-CE3	7.91	141.02	133.90
1	CY	32	TRP	CG-CD2-CE3	7.91	141.02	133.90
1	BF	83	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	BI	83	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	CI	49	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	Cm	32	TRP	CG-CD2-CE3	7.90	141.01	133.90
1	B2	83	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	BS	83	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	Bc	83	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	CA	32	TRP	CG-CD2-CE3	7.90	141.01	133.90
1	Ch	32	TRP	CG-CD2-CE3	7.90	141.01	133.90
1	BZ	83	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	BO	83	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	Cd	32	TRP	CG-CD2-CE3	7.90	141.01	133.90
1	CS	32	TRP	CG-CD2-CE3	7.89	141.00	133.90
1	Bq	83	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	Cv	32	TRP	CG-CD2-CE3	7.89	141.00	133.90
1	CD	32	TRP	CG-CD2-CE3	7.89	141.00	133.90
1	BJ	83	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	B5	83	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	BP	83	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	BT	83	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	Bj	83	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	BZ	82	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	Bs	82	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	C0	32	TRP	CG-CD2-CE3	7.88	140.99	133.90
1	CO	32	TRP	CG-CD2-CE3	7.88	140.99	133.90
1	Cc	32	TRP	CG-CD2-CE3	7.88	140.99	133.90
1	BH	82	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	Cg	32	TRP	CG-CD2-CE3	7.88	140.99	133.90
1	Bs	83	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	CU	32	TRP	CG-CD2-CE3	7.87	140.98	133.90
1	Ct	32	TRP	CG-CD2-CE3	7.87	140.98	133.90
1	Cw	32	TRP	CG-CD2-CE3	7.87	140.99	133.90
1	CE	32	TRP	CG-CD2-CE3	7.87	140.98	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CH	32	TRP	CG-CD2-CE3	7.87	140.98	133.90
1	CR	32	TRP	CG-CD2-CE3	7.87	140.98	133.90
1	Bu	83	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	CZ	32	TRP	CG-CD2-CE3	7.87	140.98	133.90
1	BA	83	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	CT	32	TRP	CG-CD2-CE3	7.86	140.98	133.90
1	AN	82	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	BY	83	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	Bm	83	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C2	32	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	C4	32	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	Ci	32	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	BA	82	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	BC	82	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	Cp	32	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	BE	82	TRP	CD1-CG-CD2	7.86	112.58	106.30
1	BE	83	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C6	32	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	Cu	32	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	Bj	82	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	B8	83	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	BH	83	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	AJ	82	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	Bp	82	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	AR	82	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	C3	32	TRP	CG-CD2-CE3	7.85	140.96	133.90
1	Bl	83	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	CX	32	TRP	CG-CD2-CE3	7.84	140.96	133.90
1	Cr	32	TRP	CG-CD2-CE3	7.84	140.96	133.90
1	BF	82	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	Bd	83	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	C8	32	TRP	CG-CD2-CE3	7.84	140.96	133.90
1	CQ	32	TRP	CG-CD2-CE3	7.84	140.96	133.90
1	Cj	32	TRP	CG-CD2-CE3	7.84	140.95	133.90
1	Ao	82	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	C7	32	TRP	CG-CD2-CE3	7.84	140.95	133.90
1	B4	82	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	Bm	82	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	Bn	83	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	C5	32	TRP	CG-CD2-CE3	7.83	140.95	133.90
1	CM	32	TRP	CG-CD2-CE3	7.83	140.95	133.90
1	Cb	32	TRP	CG-CD2-CE3	7.83	140.95	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BB	82	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	BD	82	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	Au	82	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	B3	83	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	BK	83	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	CV	32	TRP	CG-CD2-CE3	7.83	140.95	133.90
1	At	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	Ba	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	Bk	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	Bk	83	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	Ah	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	B2	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	AB	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	AD	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	Bf	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	CG	32	TRP	CG-CD2-CE3	7.82	140.94	133.90
1	B9	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	Ce	32	TRP	CG-CD2-CE3	7.82	140.94	133.90
1	Cx	32	TRP	CG-CD2-CE3	7.82	140.94	133.90
1	Ax	82	TRP	CD1-CG-CD2	7.82	112.55	106.30
1	Bd	82	TRP	CD1-CG-CD2	7.82	112.55	106.30
1	CF	32	TRP	CG-CD2-CE3	7.82	140.94	133.90
1	CW	32	TRP	CG-CD2-CE3	7.82	140.94	133.90
1	Cs	32	TRP	CG-CD2-CE3	7.82	140.93	133.90
1	AQ	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	B0	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	BI	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	BX	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	Br	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	Bo	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	CK	32	TRP	CG-CD2-CE3	7.81	140.93	133.90
1	BO	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	Bn	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	CI	32	TRP	CG-CD2-CE3	7.81	140.93	133.90
1	AA	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	Ar	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	BJ	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	BN	83	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	CA	32	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	Cd	32	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	Ap	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	BG	82	TRP	CD1-CG-CD2	7.80	112.54	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BM	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	BV	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Bg	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	CC	32	TRP	CG-CD2-CE3	7.80	140.92	133.90
1	CE	32	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Ck	32	TRP	CG-CD2-CE3	7.80	140.92	133.90
1	B6	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	BN	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	BW	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Cl	32	TRP	CG-CD2-CE3	7.80	140.92	133.90
1	AU	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Av	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	B3	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Be	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Af	82	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	B5	82	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	Bv	82	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	CL	32	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	B7	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	B8	82	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	B9	83	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	Bh	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Bt	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	C0	32	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	CH	32	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Co	32	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	A4	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	B1	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	AE	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Ag	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Bc	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Cf	32	TRP	CG-CD2-CE3	7.79	140.91	133.90
1	Cm	32	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	AF	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Ac	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	B0	83	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	Bq	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	CO	32	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Cn	32	TRP	CG-CD2-CE3	7.79	140.91	133.90
1	BP	82	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	CJ	32	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	A7	82	TRP	CD1-CG-CD2	7.78	112.53	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BT	82	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	Ca	32	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	A2	82	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	AW	82	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	AZ	82	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	BS	82	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	Bl	82	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	Bu	82	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A8	82	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	BL	82	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	Bx	82	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A1	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	Bb	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	AH	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	Ba	83	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	Aw	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	A3	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	AS	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	BY	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	BD	83	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	AP	82	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	BQ	82	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	BU	82	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	C6	32	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	CV	32	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	CZ	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Ch	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	A6	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	C7	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	CG	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Ce	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Cj	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	C1	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	CY	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	AV	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	BR	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	AT	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Bi	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	CB	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Cv	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	AG	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	AI	82	TRP	CD1-CG-CD2	7.76	112.50	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BK	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Bw	83	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	C5	32	TRP	CD1-CG-CD2	7.76	112.50	106.30
1	Cx	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Cc	32	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	C9	32	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	Aq	82	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	CM	32	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	Aa	82	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	Ad	82	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	BC	83	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	Cq	32	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	A9	82	TRP	CD1-CG-CD2	7.74	112.50	106.30
1	Ai	82	TRP	CD1-CG-CD2	7.74	112.50	106.30
1	Ak	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	Al	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	CN	32	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	AY	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	An	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	Bv	83	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	Cg	32	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	AK	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	Cb	32	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	AL	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	Bw	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	CT	32	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	Cw	32	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	AO	82	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	C2	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	CX	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	Ct	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	Ae	82	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	C4	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	CC	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	CD	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	CU	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	Am	82	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	As	82	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	Ci	32	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	CP	32	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	Cx	82	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	BW	83	ARG	NE-CZ-NH2	-7.72	116.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CS	32	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	CW	32	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	Cf	32	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	Ck	32	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	C2	82	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	CK	32	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	Au	32	TRP	CE2-CD2-CG	-7.71	101.13	107.30
1	C3	32	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	C6	82	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	CF	32	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	Ce	82	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	AX	82	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	CR	32	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	C8	32	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	Cr	32	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	Cs	32	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A5	82	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	CQ	32	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	CR	82	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	C9	82	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A0	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	C8	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	Cp	32	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	As	32	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	CD	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	Cn	32	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	Cu	32	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	AM	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	CI	32	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	CP	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	CX	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	Ca	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	Ch	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	Cr	82	TRP	CD1-CG-CD2	7.68	112.45	106.30
1	A9	32	TRP	CE2-CD2-CG	-7.68	101.15	107.30
1	CJ	82	TRP	CD1-CG-CD2	7.68	112.45	106.30
1	CW	82	TRP	CD1-CG-CD2	7.68	112.45	106.30
1	Cw	82	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	CM	82	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	Ct	82	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	Cl	32	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	AC	32	TRP	CE2-CD2-CG	-7.67	101.16	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AN	32	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	At	32	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	Cl	82	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	AD	32	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	CG	82	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	A5	32	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	AP	32	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	CS	82	TRP	CD1-CG-CD2	7.67	112.43	106.30
1	CF	82	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	CN	82	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	Cb	82	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	Cm	82	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	Cv	82	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	AW	32	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	A3	32	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	Cp	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	Ab	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	Aj	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	C0	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	Cq	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	Ap	32	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	CA	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	C1	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	C4	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	Ci	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	AC	82	TRP	CD1-CG-CD2	7.64	112.42	106.30
1	AT	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	Ae	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	Aj	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	CL	82	TRP	CD1-CG-CD2	7.64	112.42	106.30
1	Cg	82	TRP	CD1-CG-CD2	7.64	112.42	106.30
1	Cn	82	TRP	CD1-CG-CD2	7.64	112.42	106.30
1	AB	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	Ar	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	Ax	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	C5	82	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	CY	82	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	Cf	82	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	Am	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	A8	32	TRP	CE2-CD2-CG	-7.63	101.19	107.30
1	Cj	82	TRP	CD1-CG-CD2	7.63	112.41	106.30
1	CO	82	TRP	CD1-CG-CD2	7.63	112.41	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Av	32	TRP	CE2-CD2-CG	-7.63	101.19	107.30
1	AO	32	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	A7	32	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	Ac	32	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	CH	82	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	CU	82	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	Co	82	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	CZ	82	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	AJ	32	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	Cc	82	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	Cu	82	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	AI	32	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	C3	82	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	CT	82	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	CV	82	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	AS	32	TRP	CE2-CD2-CG	-7.62	101.21	107.30
1	Ao	32	TRP	CE2-CD2-CG	-7.62	101.21	107.30
1	CC	82	TRP	CD1-CG-CD2	7.62	112.39	106.30
1	AV	32	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	Cd	82	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	Af	32	TRP	CE2-CD2-CG	-7.61	101.22	107.30
1	A0	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	AQ	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	CE	82	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	A2	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A4	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	AA	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	AF	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	Ck	82	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	AM	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	AK	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	AR	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	Ab	32	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	Ak	32	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	Aw	32	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	AX	32	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	C7	82	TRP	CD1-CG-CD2	7.58	112.37	106.30
1	A1	32	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	CB	82	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	AL	32	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	AZ	32	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	AU	32	TRP	CE2-CD2-CG	-7.58	101.24	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Aq	32	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	CK	82	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	CQ	82	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	AH	32	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	Cs	82	TRP	CD1-CG-CD2	7.57	112.35	106.30
1	CI	82	TRP	CD1-CG-CD2	7.57	112.35	106.30
1	Ag	32	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	Ad	32	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	B9	32	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	Ah	32	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	An	32	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	A6	32	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	AE	32	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	BH	32	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	BY	32	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	AG	32	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	AY	32	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	Aa	32	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	Bf	32	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	BV	32	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	BN	32	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	Bw	32	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	Al	32	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	Bn	32	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	Ai	32	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	Bc	32	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	BC	32	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	Bv	32	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	Ba	32	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	B0	32	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	BD	32	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	BF	32	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	BW	32	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	B4	32	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	BK	32	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	BP	32	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	Bu	32	TRP	CE2-CD2-CG	-7.47	101.33	107.30
1	BQ	32	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	Br	32	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	BT	32	TRP	CE2-CD2-CG	-7.46	101.34	107.30
1	Bj	32	TRP	CE2-CD2-CG	-7.46	101.34	107.30
1	B7	32	TRP	CE2-CD2-CG	-7.45	101.34	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B8	32	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	Bg	32	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	BA	32	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	B6	32	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	B2	32	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	Bd	32	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	Bk	32	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	B5	32	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	BG	32	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	BL	32	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	Bb	32	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	Bh	32	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	BX	32	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	Bp	32	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	BB	32	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	BI	32	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	Bo	32	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	Be	32	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	Bt	32	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	BS	32	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	Bq	32	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	CE	32	TRP	CB-CG-CD1	-7.42	117.36	127.00
1	Cd	32	TRP	CB-CG-CD1	-7.42	117.36	127.00
1	BZ	32	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	Bs	32	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	Bx	32	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	CG	32	TRP	CB-CG-CD1	-7.41	117.36	127.00
1	CW	32	TRP	CB-CG-CD1	-7.41	117.37	127.00
1	Ca	32	TRP	CB-CG-CD1	-7.41	117.37	127.00
1	Ct	32	TRP	CB-CG-CD1	-7.41	117.37	127.00
1	B3	32	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	BM	32	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	Bm	32	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	Cj	32	TRP	CB-CG-CD1	-7.41	117.37	127.00
1	CH	32	TRP	CB-CG-CD1	-7.41	117.37	127.00
1	Co	32	TRP	CB-CG-CD1	-7.41	117.37	127.00
1	B1	32	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	Cx	32	TRP	CB-CG-CD1	-7.40	117.38	127.00
1	BR	32	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	CA	32	TRP	CB-CG-CD1	-7.40	117.38	127.00
1	Bl	32	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	C5	32	TRP	CB-CG-CD1	-7.40	117.38	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C6	32	TRP	CB-CG-CD1	-7.40	117.38	127.00
1	CI	32	TRP	CB-CG-CD1	-7.40	117.38	127.00
1	Cs	32	TRP	CB-CG-CD1	-7.40	117.38	127.00
1	BE	32	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	CZ	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	Cl	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	Bi	32	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	CY	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	Ck	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	CT	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	CU	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	CV	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	C7	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	Ch	32	TRP	CB-CG-CD1	-7.39	117.40	127.00
1	Cq	32	TRP	CB-CG-CD1	-7.39	117.40	127.00
1	C4	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	CC	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	C3	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	Ce	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	CM	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	Cc	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	Cm	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	Cv	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	C1	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	CQ	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	BJ	32	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	C0	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	C9	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	CX	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	Cb	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	Cf	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	C2	32	TRP	CB-CG-CD1	-7.37	117.41	127.00
1	Ci	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	C8	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	CK	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	CS	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	Cg	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	BU	32	TRP	CE2-CD2-CG	-7.37	101.41	107.30
1	CF	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	CO	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	Cn	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	CD	32	TRP	CB-CG-CD1	-7.37	117.43	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CR	32	TRP	CB-CG-CD1	-7.37	117.43	127.00
1	Cp	32	TRP	CB-CG-CD1	-7.36	117.43	127.00
1	Cr	32	TRP	CB-CG-CD1	-7.36	117.43	127.00
1	CJ	32	TRP	CB-CG-CD1	-7.36	117.43	127.00
1	Cw	32	TRP	CB-CG-CD1	-7.36	117.43	127.00
1	Cu	32	TRP	CB-CG-CD1	-7.36	117.43	127.00
1	Cr	108	MET	CG-SD-CE	-7.36	88.43	100.20
1	CL	32	TRP	CB-CG-CD1	-7.35	117.44	127.00
1	CB	32	TRP	CB-CG-CD1	-7.35	117.44	127.00
1	BO	32	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	CP	32	TRP	CB-CG-CD1	-7.34	117.45	127.00
1	Ck	108	MET	CG-SD-CE	-7.34	88.45	100.20
1	CN	32	TRP	CB-CG-CD1	-7.34	117.46	127.00
1	CS	108	MET	CG-SD-CE	-7.34	88.46	100.20
1	CI	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	CM	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	CR	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	CU	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	Ci	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	Cn	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	C4	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	C6	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	Ch	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	CV	108	MET	CG-SD-CE	-7.33	88.48	100.20
1	Cd	108	MET	CG-SD-CE	-7.33	88.48	100.20
1	Cg	108	MET	CG-SD-CE	-7.33	88.48	100.20
1	Ct	108	MET	CG-SD-CE	-7.33	88.48	100.20
1	C3	108	MET	CG-SD-CE	-7.32	88.48	100.20
1	CL	108	MET	CG-SD-CE	-7.32	88.48	100.20
1	Cc	108	MET	CG-SD-CE	-7.32	88.48	100.20
1	Cp	108	MET	CG-SD-CE	-7.32	88.49	100.20
1	CZ	108	MET	CG-SD-CE	-7.32	88.49	100.20
1	Ce	108	MET	CG-SD-CE	-7.32	88.49	100.20
1	C0	108	MET	CG-SD-CE	-7.32	88.49	100.20
1	C5	108	MET	CG-SD-CE	-7.32	88.49	100.20
1	CY	108	MET	CG-SD-CE	-7.32	88.49	100.20
1	C1	108	MET	CG-SD-CE	-7.32	88.50	100.20
1	Cs	108	MET	CG-SD-CE	-7.32	88.50	100.20
1	C8	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	C7	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	CG	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	CH	108	MET	CG-SD-CE	-7.31	88.50	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CQ	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	Cu	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	CA	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	CF	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	CP	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	Ca	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	Cv	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	C2	108	MET	CG-SD-CE	-7.31	88.51	100.20
1	Cb	108	MET	CG-SD-CE	-7.31	88.51	100.20
1	Cf	108	MET	CG-SD-CE	-7.31	88.51	100.20
1	Cw	108	MET	CG-SD-CE	-7.31	88.51	100.20
1	CC	108	MET	CG-SD-CE	-7.31	88.51	100.20
1	CK	108	MET	CG-SD-CE	-7.30	88.51	100.20
1	Cl	108	MET	CG-SD-CE	-7.30	88.51	100.20
1	Cm	108	MET	CG-SD-CE	-7.30	88.51	100.20
1	CJ	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	CB	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	CE	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	CO	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	CT	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	Cx	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	CW	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	CX	108	MET	CG-SD-CE	-7.30	88.53	100.20
1	Cj	108	MET	CG-SD-CE	-7.30	88.53	100.20
1	Cq	108	MET	CG-SD-CE	-7.29	88.53	100.20
1	Co	108	MET	CG-SD-CE	-7.29	88.53	100.20
1	C9	108	MET	CG-SD-CE	-7.29	88.53	100.20
1	CD	108	MET	CG-SD-CE	-7.29	88.53	100.20
1	CN	108	MET	CG-SD-CE	-7.29	88.53	100.20
1	AW	2	SER	N-CA-C	-7.27	91.37	111.00
1	A3	2	SER	N-CA-C	-7.27	91.38	111.00
1	Ag	2	SER	N-CA-C	-7.27	91.38	111.00
1	AD	2	SER	N-CA-C	-7.26	91.39	111.00
1	Ax	2	SER	N-CA-C	-7.26	91.39	111.00
1	AU	2	SER	N-CA-C	-7.26	91.39	111.00
1	AN	2	SER	N-CA-C	-7.26	91.39	111.00
1	AH	2	SER	N-CA-C	-7.26	91.40	111.00
1	A5	2	SER	N-CA-C	-7.26	91.41	111.00
1	Av	2	SER	N-CA-C	-7.26	91.41	111.00
1	A7	2	SER	N-CA-C	-7.25	91.42	111.00
1	An	2	SER	N-CA-C	-7.25	91.42	111.00
1	Ao	2	SER	N-CA-C	-7.25	91.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AL	2	SER	N-CA-C	-7.25	91.42	111.00
1	A0	2	SER	N-CA-C	-7.25	91.42	111.00
1	A2	2	SER	N-CA-C	-7.25	91.42	111.00
1	A8	2	SER	N-CA-C	-7.25	91.43	111.00
1	A9	2	SER	N-CA-C	-7.25	91.43	111.00
1	AE	2	SER	N-CA-C	-7.25	91.43	111.00
1	AP	2	SER	N-CA-C	-7.25	91.42	111.00
1	A1	2	SER	N-CA-C	-7.25	91.43	111.00
1	Aa	2	SER	N-CA-C	-7.25	91.43	111.00
1	Ah	2	SER	N-CA-C	-7.25	91.43	111.00
1	As	2	SER	N-CA-C	-7.25	91.43	111.00
1	At	2	SER	N-CA-C	-7.25	91.43	111.00
1	Au	2	SER	N-CA-C	-7.25	91.43	111.00
1	AB	2	SER	N-CA-C	-7.25	91.43	111.00
1	Ad	2	SER	N-CA-C	-7.25	91.43	111.00
1	Ap	2	SER	N-CA-C	-7.25	91.43	111.00
1	Ac	2	SER	N-CA-C	-7.25	91.44	111.00
1	Ak	2	SER	N-CA-C	-7.25	91.44	111.00
1	AJ	2	SER	N-CA-C	-7.24	91.44	111.00
1	AK	2	SER	N-CA-C	-7.24	91.44	111.00
1	Aw	2	SER	N-CA-C	-7.24	91.44	111.00
1	AF	2	SER	N-CA-C	-7.24	91.45	111.00
1	AS	2	SER	N-CA-C	-7.24	91.45	111.00
1	AZ	2	SER	N-CA-C	-7.24	91.45	111.00
1	Ae	2	SER	N-CA-C	-7.24	91.45	111.00
1	Af	2	SER	N-CA-C	-7.24	91.45	111.00
1	Aj	2	SER	N-CA-C	-7.24	91.45	111.00
1	Ar	2	SER	N-CA-C	-7.24	91.45	111.00
1	AY	2	SER	N-CA-C	-7.24	91.45	111.00
1	Aq	2	SER	N-CA-C	-7.24	91.45	111.00
1	AG	2	SER	N-CA-C	-7.24	91.45	111.00
1	AI	2	SER	N-CA-C	-7.24	91.46	111.00
1	AR	2	SER	N-CA-C	-7.24	91.46	111.00
1	AV	2	SER	N-CA-C	-7.24	91.46	111.00
1	Ai	2	SER	N-CA-C	-7.24	91.46	111.00
1	AQ	2	SER	N-CA-C	-7.24	91.47	111.00
1	AX	2	SER	N-CA-C	-7.24	91.46	111.00
1	Ab	2	SER	N-CA-C	-7.23	91.47	111.00
1	Al	2	SER	N-CA-C	-7.23	91.47	111.00
1	Am	2	SER	N-CA-C	-7.23	91.47	111.00
1	A6	2	SER	N-CA-C	-7.23	91.47	111.00
1	AA	2	SER	N-CA-C	-7.23	91.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AM	2	SER	N-CA-C	-7.23	91.47	111.00
1	AO	2	SER	N-CA-C	-7.23	91.47	111.00
1	A4	2	SER	N-CA-C	-7.23	91.48	111.00
1	AT	2	SER	N-CA-C	-7.23	91.48	111.00
1	CM	82	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	AC	2	SER	N-CA-C	-7.22	91.50	111.00
1	Cx	82	TRP	CE2-CD2-CG	-7.22	101.52	107.30
1	AD	82	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	At	82	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	Cb	82	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	AN	82	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	Au	82	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	CG	82	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	Cm	82	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	CX	82	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	Ah	82	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	A4	82	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	AH	82	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	C7	82	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	AE	82	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	Cc	82	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	CC	82	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	CO	82	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A9	82	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	AW	82	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	CR	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	Ao	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	C2	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	Ax	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A7	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	AQ	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	AS	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	CZ	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	Cn	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	Ap	82	TRP	CE2-CD2-CG	-7.14	101.58	107.30
1	Av	82	TRP	CE2-CD2-CG	-7.14	101.58	107.30
1	CT	82	TRP	CE2-CD2-CG	-7.14	101.58	107.30
1	An	82	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	C6	82	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	AA	82	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	CJ	82	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	Cr	82	TRP	CE2-CD2-CG	-7.14	101.59	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CV	82	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	Ch	82	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	Cp	82	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	CQ	82	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	BZ	48	VAL	CB-CA-C	-7.13	97.85	111.40
1	Cj	82	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	AB	82	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	Ag	82	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	BS	48	VAL	CB-CA-C	-7.13	97.86	111.40
1	C8	82	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	Ce	82	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	Cg	82	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	C3	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	Ck	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	A2	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	AL	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	AP	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	Be	48	VAL	CB-CA-C	-7.12	97.87	111.40
1	Ct	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	CS	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	Cq	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	AJ	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	Ar	82	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	BU	48	VAL	CB-CA-C	-7.12	97.88	111.40
1	A1	82	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	A3	82	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	Bq	48	VAL	CB-CA-C	-7.12	97.88	111.40
1	Bx	48	VAL	CB-CA-C	-7.12	97.88	111.40
1	CD	82	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	AF	82	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	BE	48	VAL	CB-CA-C	-7.12	97.88	111.40
1	Bj	48	VAL	CB-CA-C	-7.12	97.88	111.40
1	BX	48	VAL	CB-CA-C	-7.11	97.88	111.40
1	C1	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	Ci	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	C5	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	A8	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	BO	48	VAL	CB-CA-C	-7.11	97.89	111.40
1	CI	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	Ca	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	Cf	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	B2	48	VAL	CB-CA-C	-7.11	97.90	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BR	48	VAL	CB-CA-C	-7.11	97.90	111.40
1	CE	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	CK	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	AU	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	Af	82	TRP	CE2-CD2-CG	-7.11	101.62	107.30
1	Br	48	VAL	CB-CA-C	-7.11	97.90	111.40
1	Co	82	TRP	CE2-CD2-CG	-7.11	101.62	107.30
1	AO	82	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	Bb	48	VAL	CB-CA-C	-7.10	97.90	111.40
1	B7	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	Ba	48	VAL	CB-CA-C	-7.10	97.90	111.40
1	Bh	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	Bp	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	CW	82	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	Bi	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	Bm	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	Bv	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	CL	82	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	AT	82	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	B4	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	BA	48	VAL	CB-CA-C	-7.10	97.92	111.40
1	BJ	48	VAL	CB-CA-C	-7.10	97.92	111.40
1	Bc	48	VAL	CB-CA-C	-7.10	97.92	111.40
1	CF	82	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	BN	48	VAL	CB-CA-C	-7.09	97.92	111.40
1	Bg	48	VAL	CB-CA-C	-7.09	97.92	111.40
1	C9	82	TRP	CE2-CD2-CG	-7.09	101.62	107.30
1	CB	82	TRP	CE2-CD2-CG	-7.09	101.62	107.30
1	CU	82	TRP	CE2-CD2-CG	-7.09	101.62	107.30
1	BL	48	VAL	CB-CA-C	-7.09	97.92	111.40
1	Bf	48	VAL	CB-CA-C	-7.09	97.92	111.40
1	Ad	82	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	Bl	48	VAL	CB-CA-C	-7.09	97.92	111.40
1	AR	82	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	B0	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	B8	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	BG	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	BM	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	Bt	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	Cw	82	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	AZ	82	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	Aw	82	TRP	CE2-CD2-CG	-7.09	101.63	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BF	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	BP	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	Bo	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	B1	48	VAL	CB-CA-C	-7.09	97.94	111.40
1	BC	48	VAL	CB-CA-C	-7.09	97.94	111.40
1	Bk	48	VAL	CB-CA-C	-7.09	97.94	111.40
1	Bu	48	VAL	CB-CA-C	-7.09	97.94	111.40
1	B5	48	VAL	CB-CA-C	-7.08	97.94	111.40
1	B6	48	VAL	CB-CA-C	-7.08	97.94	111.40
1	Cv	82	TRP	CE2-CD2-CG	-7.08	101.63	107.30
1	BK	48	VAL	CB-CA-C	-7.08	97.94	111.40
1	BW	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	BY	48	VAL	CB-CA-C	-7.08	97.94	111.40
1	AV	82	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	Ak	82	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	CA	82	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	B9	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	BB	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	BD	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	Bd	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	Bs	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	As	82	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	B3	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	BH	48	VAL	CB-CA-C	-7.08	97.96	111.40
1	BQ	48	VAL	CB-CA-C	-7.07	97.96	111.40
1	BV	48	VAL	CB-CA-C	-7.07	97.96	111.40
1	Bw	48	VAL	CB-CA-C	-7.07	97.96	111.40
1	Bn	48	VAL	CB-CA-C	-7.07	97.96	111.40
1	BI	48	VAL	CB-CA-C	-7.07	97.97	111.40
1	C4	82	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	AI	82	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	BT	48	VAL	CB-CA-C	-7.07	97.98	111.40
1	Ac	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	Al	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	CN	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	Cd	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	Cl	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	Ai	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	Am	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	AG	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	Aq	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	CP	82	TRP	CE2-CD2-CG	-7.06	101.66	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ab	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	A6	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	Aa	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	Cu	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	CH	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	AK	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	AY	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	Ae	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	CY	82	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	AM	82	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	C0	82	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A0	82	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	AX	82	TRP	CE2-CD2-CG	-7.03	101.67	107.30
1	Aj	82	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	AC	82	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	Cs	82	TRP	CE2-CD2-CG	-7.02	101.68	107.30
1	A5	82	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	CW	58	TYR	CB-CG-CD2	-7.00	116.80	121.00
1	CN	58	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	Cg	58	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	Ca	58	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	CH	58	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	Cu	58	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	Cd	58	TYR	CB-CG-CD2	-6.96	116.83	121.00
1	CL	58	TYR	CB-CG-CD2	-6.94	116.84	121.00
1	Cr	58	TYR	CB-CG-CD2	-6.94	116.84	121.00
1	Ci	58	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	Cp	58	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	CR	58	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	CP	58	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	Co	58	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	CA	58	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	CB	58	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	CF	58	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	CJ	58	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	C0	58	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	C9	58	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	C8	58	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	Cw	58	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	Ch	58	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	C7	58	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	Cs	58	TYR	CB-CG-CD2	-6.87	116.88	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CY	58	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	Cv	58	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	CS	58	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	CC	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	CO	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	Ce	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	C1	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	CK	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	CT	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	Cb	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	C3	58	TYR	CB-CG-CD2	-6.86	116.89	121.00
1	CU	58	TYR	CB-CG-CD2	-6.86	116.89	121.00
1	Cn	58	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	C6	58	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	CD	58	TYR	CB-CG-CD2	-6.84	116.89	121.00
1	CI	58	TYR	CB-CG-CD2	-6.84	116.89	121.00
1	Cl	58	TYR	CB-CG-CD2	-6.84	116.89	121.00
1	Cx	58	TYR	CB-CG-CD2	-6.84	116.89	121.00
1	CG	58	TYR	CB-CG-CD2	-6.84	116.90	121.00
1	Cm	58	TYR	CB-CG-CD2	-6.84	116.90	121.00
1	CZ	58	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	C5	58	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	C2	58	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	CQ	58	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	C4	58	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	CX	58	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	Cq	58	TYR	CB-CG-CD2	-6.81	116.91	121.00
1	CE	58	TYR	CB-CG-CD2	-6.81	116.92	121.00
1	Cc	58	TYR	CB-CG-CD2	-6.81	116.91	121.00
1	Cj	58	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	CV	58	TYR	CB-CG-CD2	-6.78	116.94	121.00
1	Cf	58	TYR	CB-CG-CD2	-6.77	116.94	121.00
1	Ck	58	TYR	CB-CG-CD2	-6.77	116.94	121.00
1	CM	58	TYR	CB-CG-CD2	-6.76	116.94	121.00
1	Ct	58	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	BZ	82	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	BE	82	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	Bj	82	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	BX	82	TRP	CE2-CD2-CG	-6.69	101.95	107.30
1	BO	82	TRP	CE2-CD2-CG	-6.69	101.95	107.30
1	BJ	82	TRP	CE2-CD2-CG	-6.68	101.95	107.30
1	BC	82	TRP	CE2-CD2-CG	-6.68	101.95	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BG	82	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	Bs	82	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	Bq	82	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	B4	82	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	B8	82	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	BI	82	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	Be	82	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	B6	82	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	CT	20	VAL	N-CA-CB	-6.67	96.83	111.50
1	CB	20	VAL	N-CA-CB	-6.67	96.83	111.50
1	Bk	82	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	Bp	82	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	BH	82	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	Bh	82	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	CK	20	VAL	N-CA-CB	-6.66	96.85	111.50
1	BV	82	TRP	CE2-CD2-CG	-6.66	101.98	107.30
1	Cr	20	VAL	N-CA-CB	-6.66	96.86	111.50
1	BS	82	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	BU	82	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	Bc	82	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	C6	20	VAL	N-CA-CB	-6.65	96.87	111.50
1	Cq	20	VAL	N-CA-CB	-6.65	96.87	111.50
1	Ch	20	VAL	N-CA-CB	-6.65	96.87	111.50
1	Cp	20	VAL	N-CA-CB	-6.65	96.87	111.50
1	BR	82	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	Br	82	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	CG	20	VAL	N-CA-CB	-6.65	96.88	111.50
1	CM	20	VAL	N-CA-CB	-6.65	96.88	111.50
1	CV	20	VAL	N-CA-CB	-6.65	96.88	111.50
1	CW	20	VAL	N-CA-CB	-6.65	96.88	111.50
1	Cd	20	VAL	N-CA-CB	-6.65	96.87	111.50
1	Bm	82	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	CD	20	VAL	N-CA-CB	-6.65	96.88	111.50
1	BB	82	TRP	CE2-CD2-CG	-6.64	101.98	107.30
1	CI	20	VAL	N-CA-CB	-6.64	96.88	111.50
1	CP	20	VAL	N-CA-CB	-6.64	96.88	111.50
1	Ca	20	VAL	N-CA-CB	-6.64	96.88	111.50
1	Cf	20	VAL	N-CA-CB	-6.64	96.88	111.50
1	Cm	20	VAL	N-CA-CB	-6.64	96.88	111.50
1	Cx	20	VAL	N-CA-CB	-6.64	96.88	111.50
1	BF	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	C1	20	VAL	N-CA-CB	-6.64	96.89	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CC	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Co	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Bl	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	CR	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Bn	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	CX	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	CY	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Ci	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Ck	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Ct	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Cu	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Cw	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	B9	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	Cl	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	B3	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	BQ	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	Bd	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	C2	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	CH	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	CL	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	CU	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	Cb	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	Cc	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	Cj	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	CE	20	VAL	N-CA-CB	-6.63	96.90	111.50
1	CJ	20	VAL	N-CA-CB	-6.63	96.91	111.50
1	CQ	20	VAL	N-CA-CB	-6.63	96.90	111.50
1	CS	20	VAL	N-CA-CB	-6.63	96.90	111.50
1	Cg	20	VAL	N-CA-CB	-6.63	96.91	111.50
1	Cn	20	VAL	N-CA-CB	-6.63	96.90	111.50
1	Bf	82	TRP	CE2-CD2-CG	-6.63	101.99	107.30
1	C9	20	VAL	N-CA-CB	-6.63	96.91	111.50
1	CO	20	VAL	N-CA-CB	-6.63	96.91	111.50
1	Cv	20	VAL	N-CA-CB	-6.63	96.91	111.50
1	BL	82	TRP	CE2-CD2-CG	-6.63	102.00	107.30
1	C7	20	VAL	N-CA-CB	-6.63	96.92	111.50
1	B2	82	TRP	CE2-CD2-CG	-6.63	102.00	107.30
1	Bg	82	TRP	CE2-CD2-CG	-6.63	102.00	107.30
1	Bx	82	TRP	CE2-CD2-CG	-6.63	102.00	107.30
1	Ce	20	VAL	N-CA-CB	-6.63	96.92	111.50
1	CN	20	VAL	N-CA-CB	-6.63	96.92	111.50
1	BM	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BW	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	C5	20	VAL	N-CA-CB	-6.62	96.92	111.50
1	BA	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	Ba	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	BK	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	BT	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	Bt	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	C8	20	VAL	N-CA-CB	-6.62	96.93	111.50
1	CZ	20	VAL	N-CA-CB	-6.62	96.93	111.50
1	B0	82	TRP	CE2-CD2-CG	-6.62	102.01	107.30
1	BN	82	TRP	CE2-CD2-CG	-6.62	102.01	107.30
1	C3	20	VAL	N-CA-CB	-6.62	96.94	111.50
1	CF	20	VAL	N-CA-CB	-6.62	96.95	111.50
1	B5	82	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	C4	20	VAL	N-CA-CB	-6.61	96.95	111.50
1	Cs	20	VAL	N-CA-CB	-6.61	96.95	111.50
1	C0	20	VAL	N-CA-CB	-6.61	96.96	111.50
1	CA	20	VAL	N-CA-CB	-6.61	96.96	111.50
1	BP	82	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	Bb	82	TRP	CE2-CD2-CG	-6.61	102.02	107.30
1	Bu	82	TRP	CE2-CD2-CG	-6.61	102.02	107.30
1	BD	82	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	B7	82	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	B1	82	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	Bi	82	TRP	CE2-CD2-CG	-6.59	102.02	107.30
1	Bo	82	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	BY	82	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	Bv	82	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	Bw	82	TRP	CE2-CD2-CG	-6.57	102.04	107.30
1	A6	49	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	AE	49	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	BB	20	VAL	N-CA-CB	-6.49	97.22	111.50
1	BK	20	VAL	N-CA-CB	-6.49	97.22	111.50
1	Bu	20	VAL	N-CA-CB	-6.49	97.23	111.50
1	BS	20	VAL	N-CA-CB	-6.49	97.23	111.50
1	BT	20	VAL	N-CA-CB	-6.49	97.23	111.50
1	Bq	20	VAL	N-CA-CB	-6.49	97.23	111.50
1	B4	20	VAL	N-CA-CB	-6.48	97.24	111.50
1	BR	20	VAL	N-CA-CB	-6.48	97.24	111.50
1	B1	20	VAL	N-CA-CB	-6.48	97.24	111.50
1	BL	20	VAL	N-CA-CB	-6.48	97.24	111.50
1	Bo	20	VAL	N-CA-CB	-6.48	97.24	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B6	20	VAL	N-CA-CB	-6.48	97.25	111.50
1	Bn	20	VAL	N-CA-CB	-6.48	97.25	111.50
1	Bw	20	VAL	N-CA-CB	-6.48	97.25	111.50
1	BC	20	VAL	N-CA-CB	-6.47	97.26	111.50
1	BY	20	VAL	N-CA-CB	-6.47	97.25	111.50
1	B2	20	VAL	N-CA-CB	-6.47	97.26	111.50
1	B9	20	VAL	N-CA-CB	-6.47	97.26	111.50
1	BQ	20	VAL	N-CA-CB	-6.47	97.26	111.50
1	Bb	20	VAL	N-CA-CB	-6.47	97.26	111.50
1	B5	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	Bh	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	Br	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	B3	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	BI	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	BJ	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	Bp	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	AM	49	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	Bg	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	Bk	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	Bs	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	B7	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	BV	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	AG	49	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	BD	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	BO	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	BZ	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	Ba	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	Bi	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	BA	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	B0	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	BP	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	BU	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	Bc	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	Bj	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	Bt	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	BG	20	VAL	N-CA-CB	-6.46	97.30	111.50
1	Bl	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	Bx	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	BF	20	VAL	N-CA-CB	-6.45	97.30	111.50
1	BX	20	VAL	N-CA-CB	-6.45	97.30	111.50
1	BN	20	VAL	N-CA-CB	-6.45	97.31	111.50
1	Bf	20	VAL	N-CA-CB	-6.45	97.31	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Bd	20	VAL	N-CA-CB	-6.45	97.31	111.50
1	BE	20	VAL	N-CA-CB	-6.45	97.31	111.50
1	Bv	20	VAL	N-CA-CB	-6.45	97.31	111.50
1	B8	20	VAL	N-CA-CB	-6.45	97.32	111.50
1	BW	20	VAL	N-CA-CB	-6.45	97.32	111.50
1	BM	20	VAL	N-CA-CB	-6.44	97.32	111.50
1	Bm	20	VAL	N-CA-CB	-6.44	97.33	111.50
1	Aw	49	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	BH	20	VAL	N-CA-CB	-6.44	97.33	111.50
1	Be	20	VAL	N-CA-CB	-6.44	97.34	111.50
1	AO	49	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	Au	49	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	Ad	49	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	Ao	49	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	AH	49	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	AR	49	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	Ai	49	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	AX	49	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	Ag	49	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	Aa	49	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	Ah	49	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	Al	49	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	AY	49	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	AU	49	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	Ak	49	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	Bf	2	SER	N-CA-C	-6.36	93.84	111.00
1	Am	49	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A4	49	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	BH	2	SER	N-CA-C	-6.35	93.85	111.00
1	BV	2	SER	N-CA-C	-6.35	93.85	111.00
1	Bg	2	SER	N-CA-C	-6.35	93.85	111.00
1	BB	2	SER	N-CA-C	-6.35	93.85	111.00
1	Bw	2	SER	N-CA-C	-6.35	93.86	111.00
1	AS	49	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	BJ	2	SER	N-CA-C	-6.35	93.86	111.00
1	BS	2	SER	N-CA-C	-6.35	93.86	111.00
1	BY	2	SER	N-CA-C	-6.35	93.86	111.00
1	BK	2	SER	N-CA-C	-6.35	93.86	111.00
1	BR	2	SER	N-CA-C	-6.35	93.86	111.00
1	Bc	2	SER	N-CA-C	-6.35	93.86	111.00
1	BD	2	SER	N-CA-C	-6.34	93.87	111.00
1	BZ	2	SER	N-CA-C	-6.34	93.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ba	2	SER	N-CA-C	-6.34	93.87	111.00
1	Bk	2	SER	N-CA-C	-6.34	93.87	111.00
1	Bm	2	SER	N-CA-C	-6.34	93.87	111.00
1	Br	2	SER	N-CA-C	-6.34	93.87	111.00
1	Bv	2	SER	N-CA-C	-6.34	93.87	111.00
1	B0	2	SER	N-CA-C	-6.34	93.87	111.00
1	Bi	2	SER	N-CA-C	-6.34	93.88	111.00
1	B7	2	SER	N-CA-C	-6.34	93.88	111.00
1	BE	2	SER	N-CA-C	-6.34	93.88	111.00
1	BL	2	SER	N-CA-C	-6.34	93.88	111.00
1	BP	2	SER	N-CA-C	-6.34	93.88	111.00
1	Be	2	SER	N-CA-C	-6.34	93.88	111.00
1	Bh	2	SER	N-CA-C	-6.34	93.88	111.00
1	Bn	2	SER	N-CA-C	-6.34	93.88	111.00
1	Bp	2	SER	N-CA-C	-6.34	93.88	111.00
1	Ap	49	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	BN	2	SER	N-CA-C	-6.34	93.88	111.00
1	BW	2	SER	N-CA-C	-6.34	93.88	111.00
1	B8	2	SER	N-CA-C	-6.34	93.89	111.00
1	Bt	2	SER	N-CA-C	-6.34	93.89	111.00
1	B2	2	SER	N-CA-C	-6.34	93.89	111.00
1	BC	2	SER	N-CA-C	-6.34	93.89	111.00
1	BM	2	SER	N-CA-C	-6.34	93.89	111.00
1	BT	2	SER	N-CA-C	-6.34	93.89	111.00
1	Bl	2	SER	N-CA-C	-6.34	93.89	111.00
1	Bq	2	SER	N-CA-C	-6.34	93.89	111.00
1	B3	2	SER	N-CA-C	-6.33	93.89	111.00
1	BG	2	SER	N-CA-C	-6.33	93.90	111.00
1	BQ	2	SER	N-CA-C	-6.33	93.90	111.00
1	Bo	2	SER	N-CA-C	-6.33	93.90	111.00
1	Bb	2	SER	N-CA-C	-6.33	93.90	111.00
1	Aq	49	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B4	2	SER	N-CA-C	-6.33	93.91	111.00
1	BO	2	SER	N-CA-C	-6.33	93.90	111.00
1	BX	2	SER	N-CA-C	-6.33	93.91	111.00
1	B6	2	SER	N-CA-C	-6.33	93.91	111.00
1	BI	2	SER	N-CA-C	-6.33	93.91	111.00
1	B5	2	SER	N-CA-C	-6.33	93.91	111.00
1	Bx	2	SER	N-CA-C	-6.33	93.92	111.00
1	Ar	49	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	BA	2	SER	N-CA-C	-6.33	93.92	111.00
1	AN	49	ARG	NE-CZ-NH1	6.32	123.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BF	2	SER	N-CA-C	-6.32	93.93	111.00
1	BU	2	SER	N-CA-C	-6.32	93.92	111.00
1	Bd	2	SER	N-CA-C	-6.32	93.93	111.00
1	Bj	2	SER	N-CA-C	-6.32	93.92	111.00
1	Bu	2	SER	N-CA-C	-6.32	93.92	111.00
1	AJ	49	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	AV	49	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B1	2	SER	N-CA-C	-6.32	93.94	111.00
1	Bs	2	SER	N-CA-C	-6.32	93.94	111.00
1	B9	2	SER	N-CA-C	-6.32	93.94	111.00
1	A3	49	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	AL	49	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A7	49	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	AI	49	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A1	49	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	Ae	49	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	BZ	33	ILE	CA-CB-CG1	-6.29	99.05	111.00
1	Be	33	ILE	CA-CB-CG1	-6.29	99.05	111.00
1	Br	33	ILE	CA-CB-CG1	-6.29	99.05	111.00
1	AF	49	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	BJ	33	ILE	CA-CB-CG1	-6.29	99.05	111.00
1	Bq	33	ILE	CA-CB-CG1	-6.29	99.05	111.00
1	B4	33	ILE	CA-CB-CG1	-6.29	99.06	111.00
1	BD	33	ILE	CA-CB-CG1	-6.29	99.06	111.00
1	BH	33	ILE	CA-CB-CG1	-6.29	99.06	111.00
1	BP	33	ILE	CA-CB-CG1	-6.29	99.06	111.00
1	Bx	33	ILE	CA-CB-CG1	-6.29	99.06	111.00
1	B9	33	ILE	CA-CB-CG1	-6.28	99.06	111.00
1	BR	33	ILE	CA-CB-CG1	-6.28	99.06	111.00
1	A2	49	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	BX	33	ILE	CA-CB-CG1	-6.28	99.06	111.00
1	AD	49	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	BB	33	ILE	CA-CB-CG1	-6.28	99.07	111.00
1	Bb	33	ILE	CA-CB-CG1	-6.28	99.07	111.00
1	Bf	33	ILE	CA-CB-CG1	-6.28	99.06	111.00
1	Bi	33	ILE	CA-CB-CG1	-6.28	99.07	111.00
1	Bu	33	ILE	CA-CB-CG1	-6.28	99.07	111.00
1	Bv	33	ILE	CA-CB-CG1	-6.28	99.06	111.00
1	Av	49	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	Bs	33	ILE	CA-CB-CG1	-6.28	99.07	111.00
1	Ac	49	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	Bd	33	ILE	CA-CB-CG1	-6.28	99.07	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BA	33	ILE	CA-CB-CG1	-6.28	99.08	111.00
1	Bh	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	B6	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	BL	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	BU	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	BW	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	BY	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	Bo	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	B1	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	B8	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	BO	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	Bp	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	AZ	49	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B0	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	BM	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	BV	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	B2	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	BF	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	Aj	49	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	BK	33	ILE	CA-CB-CG1	-6.26	99.10	111.00
1	BG	33	ILE	CA-CB-CG1	-6.26	99.10	111.00
1	Bj	33	ILE	CA-CB-CG1	-6.26	99.10	111.00
1	B3	33	ILE	CA-CB-CG1	-6.26	99.10	111.00
1	Bm	33	ILE	CA-CB-CG1	-6.26	99.10	111.00
1	Bn	33	ILE	CA-CB-CG1	-6.26	99.10	111.00
1	AC	49	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	BN	33	ILE	CA-CB-CG1	-6.26	99.11	111.00
1	B5	33	ILE	CA-CB-CG1	-6.26	99.11	111.00
1	Bl	33	ILE	CA-CB-CG1	-6.26	99.11	111.00
1	Bt	33	ILE	CA-CB-CG1	-6.26	99.11	111.00
1	Bw	33	ILE	CA-CB-CG1	-6.26	99.11	111.00
1	AQ	49	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	BI	33	ILE	CA-CB-CG1	-6.25	99.11	111.00
1	AT	49	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	An	49	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B7	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	BT	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	Ba	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	Bc	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	BS	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	Bk	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	AB	49	ARG	NE-CZ-NH1	6.25	123.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BQ	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	At	49	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	AW	49	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	Bg	33	ILE	CA-CB-CG1	-6.24	99.14	111.00
1	BC	33	ILE	CA-CB-CG1	-6.24	99.14	111.00
1	BE	33	ILE	CA-CB-CG1	-6.24	99.14	111.00
1	AA	49	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A0	49	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	Ax	49	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	As	49	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A8	49	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	Af	49	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	AK	49	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	Ae	20	VAL	N-CA-CB	-6.21	97.85	111.50
1	Aw	20	VAL	N-CA-CB	-6.20	97.85	111.50
1	A5	49	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	Ab	20	VAL	N-CA-CB	-6.20	97.86	111.50
1	Ac	20	VAL	N-CA-CB	-6.19	97.87	111.50
1	AP	49	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A9	49	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	AI	20	VAL	N-CA-CB	-6.19	97.89	111.50
1	AK	20	VAL	N-CA-CB	-6.19	97.89	111.50
1	As	20	VAL	N-CA-CB	-6.19	97.89	111.50
1	A3	20	VAL	N-CA-CB	-6.18	97.89	111.50
1	A5	20	VAL	N-CA-CB	-6.18	97.89	111.50
1	Aq	20	VAL	N-CA-CB	-6.18	97.89	111.50
1	AB	20	VAL	N-CA-CB	-6.18	97.90	111.50
1	Ap	20	VAL	N-CA-CB	-6.18	97.90	111.50
1	AQ	20	VAL	N-CA-CB	-6.18	97.90	111.50
1	AT	20	VAL	N-CA-CB	-6.18	97.90	111.50
1	Ab	49	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A4	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	A7	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	AU	20	VAL	N-CA-CB	-6.18	97.90	111.50
1	AV	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	Ad	20	VAL	N-CA-CB	-6.18	97.90	111.50
1	Av	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	A1	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	AR	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	AZ	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	Af	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	Ai	20	VAL	N-CA-CB	-6.18	97.91	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AE	20	VAL	N-CA-CB	-6.17	97.92	111.50
1	AM	20	VAL	N-CA-CB	-6.17	97.92	111.50
1	Ah	20	VAL	N-CA-CB	-6.17	97.92	111.50
1	Aj	20	VAL	N-CA-CB	-6.17	97.92	111.50
1	Ak	20	VAL	N-CA-CB	-6.17	97.91	111.50
1	An	20	VAL	N-CA-CB	-6.17	97.92	111.50
1	Al	20	VAL	N-CA-CB	-6.17	97.92	111.50
1	AA	20	VAL	N-CA-CB	-6.17	97.93	111.50
1	AO	20	VAL	N-CA-CB	-6.17	97.93	111.50
1	AX	20	VAL	N-CA-CB	-6.17	97.93	111.50
1	Aa	20	VAL	N-CA-CB	-6.17	97.93	111.50
1	A6	20	VAL	N-CA-CB	-6.17	97.94	111.50
1	AC	20	VAL	N-CA-CB	-6.17	97.93	111.50
1	Am	20	VAL	N-CA-CB	-6.17	97.93	111.50
1	Ar	20	VAL	N-CA-CB	-6.17	97.94	111.50
1	AG	20	VAL	N-CA-CB	-6.17	97.94	111.50
1	A0	20	VAL	N-CA-CB	-6.16	97.94	111.50
1	AJ	20	VAL	N-CA-CB	-6.16	97.94	111.50
1	AL	20	VAL	N-CA-CB	-6.16	97.94	111.50
1	Ax	20	VAL	N-CA-CB	-6.16	97.94	111.50
1	A2	20	VAL	N-CA-CB	-6.16	97.94	111.50
1	AF	20	VAL	N-CA-CB	-6.16	97.95	111.50
1	Ag	20	VAL	N-CA-CB	-6.16	97.95	111.50
1	AP	20	VAL	N-CA-CB	-6.16	97.95	111.50
1	AS	20	VAL	N-CA-CB	-6.16	97.95	111.50
1	A9	20	VAL	N-CA-CB	-6.16	97.95	111.50
1	AH	20	VAL	N-CA-CB	-6.16	97.95	111.50
1	AW	20	VAL	N-CA-CB	-6.16	97.96	111.50
1	AN	20	VAL	N-CA-CB	-6.15	97.96	111.50
1	AY	20	VAL	N-CA-CB	-6.15	97.96	111.50
1	Ao	20	VAL	N-CA-CB	-6.15	97.96	111.50
1	At	20	VAL	N-CA-CB	-6.15	97.96	111.50
1	AD	20	VAL	N-CA-CB	-6.15	97.97	111.50
1	Au	20	VAL	N-CA-CB	-6.14	97.99	111.50
1	A8	20	VAL	N-CA-CB	-6.13	98.00	111.50
1	CK	10	VAL	CA-C-N	6.07	130.55	117.20
1	Cf	10	VAL	CA-C-N	6.06	130.53	117.20
1	CY	10	VAL	CA-C-N	6.06	130.53	117.20
1	CV	10	VAL	CA-C-N	6.06	130.53	117.20
1	Cn	10	VAL	CA-C-N	6.06	130.53	117.20
1	Ck	10	VAL	CA-C-N	6.05	130.52	117.20
1	CI	10	VAL	CA-C-N	6.05	130.52	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CH	10	VAL	CA-C-N	6.05	130.51	117.20
1	Cc	10	VAL	CA-C-N	6.05	130.50	117.20
1	Cu	10	VAL	CA-C-N	6.05	130.50	117.20
1	C6	10	VAL	CA-C-N	6.04	130.50	117.20
1	CF	10	VAL	CA-C-N	6.04	130.50	117.20
1	CT	10	VAL	CA-C-N	6.04	130.50	117.20
1	CW	10	VAL	CA-C-N	6.04	130.50	117.20
1	Cb	10	VAL	CA-C-N	6.04	130.50	117.20
1	Ct	10	VAL	CA-C-N	6.04	130.50	117.20
1	Cw	10	VAL	CA-C-N	6.04	130.49	117.20
1	CC	10	VAL	CA-C-N	6.04	130.49	117.20
1	Cs	10	VAL	CA-C-N	6.04	130.49	117.20
1	CN	10	VAL	CA-C-N	6.04	130.48	117.20
1	Ce	10	VAL	CA-C-N	6.04	130.48	117.20
1	C1	10	VAL	CA-C-N	6.03	130.47	117.20
1	C7	10	VAL	CA-C-N	6.03	130.47	117.20
1	CP	10	VAL	CA-C-N	6.03	130.47	117.20
1	CR	10	VAL	CA-C-N	6.03	130.47	117.20
1	C8	10	VAL	CA-C-N	6.03	130.47	117.20
1	C9	10	VAL	CA-C-N	6.03	130.47	117.20
1	CX	10	VAL	CA-C-N	6.03	130.47	117.20
1	Ca	10	VAL	CA-C-N	6.03	130.47	117.20
1	Ch	10	VAL	CA-C-N	6.03	130.46	117.20
1	C4	10	VAL	CA-C-N	6.03	130.46	117.20
1	CQ	10	VAL	CA-C-N	6.03	130.46	117.20
1	Cl	10	VAL	CA-C-N	6.03	130.46	117.20
1	Cx	10	VAL	CA-C-N	6.03	130.46	117.20
1	CG	10	VAL	CA-C-N	6.03	130.46	117.20
1	CM	10	VAL	CA-C-N	6.03	130.46	117.20
1	CA	10	VAL	CA-C-N	6.02	130.45	117.20
1	CO	10	VAL	CA-C-N	6.02	130.45	117.20
1	Cv	10	VAL	CA-C-N	6.02	130.45	117.20
1	Av	79	VAL	N-CA-CB	-6.02	98.25	111.50
1	C3	10	VAL	CA-C-N	6.02	130.45	117.20
1	CU	10	VAL	CA-C-N	6.02	130.45	117.20
1	CZ	10	VAL	CA-C-N	6.02	130.45	117.20
1	Cg	10	VAL	CA-C-N	6.02	130.45	117.20
1	C2	10	VAL	CA-C-N	6.02	130.45	117.20
1	Cm	10	VAL	CA-C-N	6.02	130.44	117.20
1	Cp	10	VAL	CA-C-N	6.02	130.45	117.20
1	Cj	10	VAL	CA-C-N	6.02	130.44	117.20
1	An	79	VAL	N-CA-CB	-6.02	98.26	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Co	10	VAL	CA-C-N	6.02	130.44	117.20
1	CE	10	VAL	CA-C-N	6.02	130.44	117.20
1	Au	79	VAL	N-CA-CB	-6.01	98.27	111.50
1	C0	10	VAL	CA-C-N	6.01	130.43	117.20
1	CD	10	VAL	CA-C-N	6.01	130.43	117.20
1	CJ	10	VAL	CA-C-N	6.01	130.43	117.20
1	Cr	10	VAL	CA-C-N	6.01	130.43	117.20
1	AE	79	VAL	N-CA-CB	-6.01	98.28	111.50
1	AN	79	VAL	N-CA-CB	-6.01	98.28	111.50
1	C5	10	VAL	CA-C-N	6.01	130.42	117.20
1	CB	10	VAL	CA-C-N	6.01	130.42	117.20
1	Ci	10	VAL	CA-C-N	6.01	130.42	117.20
1	Cq	10	VAL	CA-C-N	6.01	130.42	117.20
1	A9	79	VAL	N-CA-CB	-6.01	98.28	111.50
1	AP	79	VAL	N-CA-CB	-6.01	98.29	111.50
1	AU	79	VAL	N-CA-CB	-6.00	98.29	111.50
1	AW	79	VAL	N-CA-CB	-6.00	98.29	111.50
1	At	79	VAL	N-CA-CB	-6.00	98.29	111.50
1	CL	10	VAL	CA-C-N	6.00	130.41	117.20
1	Aw	79	VAL	N-CA-CB	-6.00	98.29	111.50
1	CS	10	VAL	CA-C-N	6.00	130.41	117.20
1	A7	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	AK	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	Aj	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	AT	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	Cd	10	VAL	CA-C-N	6.00	130.40	117.20
1	A1	32	TRP	CB-CG-CD1	-6.00	119.20	127.00
1	A2	79	VAL	N-CA-CB	-6.00	98.31	111.50
1	A4	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	A8	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	AH	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	AD	79	VAL	N-CA-CB	-6.00	98.31	111.50
1	AF	32	TRP	CB-CG-CD1	-6.00	119.20	127.00
1	AL	79	VAL	N-CA-CB	-6.00	98.31	111.50
1	AR	79	VAL	N-CA-CB	-6.00	98.31	111.50
1	Ax	79	VAL	N-CA-CB	-6.00	98.31	111.50
1	A1	79	VAL	N-CA-CB	-6.00	98.31	111.50
1	A3	79	VAL	N-CA-CB	-5.99	98.31	111.50
1	A6	79	VAL	N-CA-CB	-5.99	98.31	111.50
1	AQ	79	VAL	N-CA-CB	-5.99	98.31	111.50
1	Ab	79	VAL	N-CA-CB	-5.99	98.31	111.50
1	Ag	79	VAL	N-CA-CB	-5.99	98.31	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ak	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	AC	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	AX	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	AZ	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	AA	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	AG	79	VAL	N-CA-CB	-5.99	98.33	111.50
1	AI	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	Ac	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	AV	79	VAL	N-CA-CB	-5.99	98.33	111.50
1	Aa	79	VAL	N-CA-CB	-5.99	98.33	111.50
1	Ae	79	VAL	N-CA-CB	-5.99	98.33	111.50
1	Ak	32	TRP	CB-CG-CD1	-5.99	119.22	127.00
1	Al	79	VAL	N-CA-CB	-5.99	98.33	111.50
1	Ap	79	VAL	N-CA-CB	-5.99	98.33	111.50
1	At	32	TRP	CB-CG-CD1	-5.99	119.22	127.00
1	AM	79	VAL	N-CA-CB	-5.98	98.33	111.50
1	AS	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	AY	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	Ad	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	AJ	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	Ar	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	As	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	A0	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	A6	32	TRP	CB-CG-CD1	-5.98	119.23	127.00
1	AO	32	TRP	CB-CG-CD1	-5.98	119.23	127.00
1	Am	79	VAL	N-CA-CB	-5.98	98.35	111.50
1	Aq	79	VAL	N-CA-CB	-5.98	98.35	111.50
1	Ac	32	TRP	CB-CG-CD1	-5.98	119.23	127.00
1	Af	79	VAL	N-CA-CB	-5.98	98.35	111.50
1	A5	79	VAL	N-CA-CB	-5.97	98.36	111.50
1	AF	79	VAL	N-CA-CB	-5.97	98.35	111.50
1	AO	79	VAL	N-CA-CB	-5.97	98.36	111.50
1	Ah	79	VAL	N-CA-CB	-5.97	98.36	111.50
1	AB	79	VAL	N-CA-CB	-5.97	98.36	111.50
1	A3	32	TRP	CB-CG-CD1	-5.97	119.24	127.00
1	AA	32	TRP	CB-CG-CD1	-5.97	119.24	127.00
1	An	32	TRP	CB-CG-CD1	-5.97	119.24	127.00
1	Ao	79	VAL	N-CA-CB	-5.96	98.38	111.50
1	Ai	79	VAL	N-CA-CB	-5.96	98.39	111.50
1	A7	32	TRP	CB-CG-CD1	-5.96	119.25	127.00
1	Ax	32	TRP	CB-CG-CD1	-5.96	119.25	127.00
1	AR	32	TRP	CB-CG-CD1	-5.96	119.26	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AX	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	Ab	32	TRP	CB-CG-CD1	-5.95	119.26	127.00
1	A0	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	Ar	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	AP	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	Au	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	AB	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	AY	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	AE	32	TRP	CB-CG-CD1	-5.94	119.27	127.00
1	Af	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	Aa	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	Aw	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	AQ	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	Ad	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	Al	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	AW	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	A2	32	TRP	CB-CG-CD1	-5.93	119.28	127.00
1	AH	32	TRP	CB-CG-CD1	-5.93	119.28	127.00
1	AV	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	Aj	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	A8	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	AI	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	AL	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	AZ	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	Av	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	Bb	32	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	A9	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	Ao	32	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	AD	32	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	A4	32	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	AG	32	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	AU	32	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	Bm	32	TRP	CG-CD1-NE1	-5.92	104.18	110.10
1	AJ	32	TRP	CB-CG-CD1	-5.92	119.31	127.00
1	AS	32	TRP	CB-CG-CD1	-5.92	119.31	127.00
1	Ag	32	TRP	CB-CG-CD1	-5.92	119.31	127.00
1	B9	32	TRP	CG-CD1-NE1	-5.92	104.18	110.10
1	AK	32	TRP	CB-CG-CD1	-5.92	119.31	127.00
1	Ai	32	TRP	CB-CG-CD1	-5.92	119.31	127.00
1	B5	32	TRP	CG-CD1-NE1	-5.92	104.18	110.10
1	AM	32	TRP	CB-CG-CD1	-5.91	119.31	127.00
1	Ae	32	TRP	CB-CG-CD1	-5.91	119.32	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AN	32	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	Aq	32	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	Am	32	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	AT	32	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	As	32	TRP	CB-CG-CD1	-5.90	119.33	127.00
1	Ap	32	TRP	CB-CG-CD1	-5.90	119.34	127.00
1	Bp	32	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	Ah	32	TRP	CB-CG-CD1	-5.89	119.34	127.00
1	BX	32	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	AC	32	TRP	CB-CG-CD1	-5.89	119.34	127.00
1	BA	32	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	Bs	32	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	A5	32	TRP	CB-CG-CD1	-5.89	119.34	127.00
1	Bl	32	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	BH	32	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	B3	32	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	BS	32	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	B6	32	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	BJ	32	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	B8	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	BB	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	Bd	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	Bv	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	Bx	50	GLN	CA-CB-CG	-5.87	100.48	113.40
1	B9	50	GLN	CA-CB-CG	-5.87	100.49	113.40
1	B4	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	BG	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	BP	50	GLN	CA-CB-CG	-5.87	100.50	113.40
1	BZ	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	Bo	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	B1	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BL	50	GLN	CA-CB-CG	-5.86	100.50	113.40
1	BR	50	GLN	CA-CB-CG	-5.86	100.50	113.40
1	Bf	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BI	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BP	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BQ	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BZ	50	GLN	CA-CB-CG	-5.86	100.51	113.40
1	Ba	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	Bk	50	GLN	CA-CB-CG	-5.86	100.51	113.40
1	Bx	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BI	50	GLN	CA-CB-CG	-5.86	100.51	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Bc	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	B0	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BK	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	BO	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	Ba	50	GLN	CA-CB-CG	-5.86	100.51	113.40
1	Bc	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	Bg	50	GLN	CA-CB-CG	-5.86	100.51	113.40
1	BA	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	BJ	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	BS	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	Bm	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	Br	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	Bu	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	Bu	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	BM	50	GLN	CA-CB-CG	-5.85	100.52	113.40
1	BV	50	GLN	CA-CB-CG	-5.85	100.52	113.40
1	Bi	50	GLN	CA-CB-CG	-5.85	100.52	113.40
1	BG	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	BO	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	BW	50	GLN	CA-CB-CG	-5.85	100.52	113.40
1	BY	50	GLN	CA-CB-CG	-5.85	100.52	113.40
1	Bh	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	B2	32	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	BH	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	BF	32	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	Bs	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	Bw	32	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	B7	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	Be	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	Bj	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	Bn	50	GLN	CA-CB-CG	-5.85	100.54	113.40
1	Bt	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	B3	50	GLN	CA-CB-CG	-5.85	100.54	113.40
1	BX	50	GLN	CA-CB-CG	-5.85	100.54	113.40
1	Bq	50	GLN	CA-CB-CG	-5.85	100.54	113.40
1	B8	50	GLN	CA-CB-CG	-5.84	100.54	113.40
1	Bi	32	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	B0	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	BT	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	Bo	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	B4	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	BE	50	GLN	CA-CB-CG	-5.84	100.55	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BN	32	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	Bp	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	B2	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	B5	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	B7	32	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	BC	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	BQ	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	Bb	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	BU	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	Bw	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	B1	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	BD	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	BN	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	BU	32	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	Be	32	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	Bg	32	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	Bl	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	BM	32	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	Bf	50	GLN	CA-CB-CG	-5.83	100.57	113.40
1	Bj	32	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	BE	32	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	BB	50	GLN	CA-CB-CG	-5.83	100.58	113.40
1	BD	32	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	BF	50	GLN	CA-CB-CG	-5.83	100.58	113.40
1	BY	32	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	Bv	50	GLN	CA-CB-CG	-5.83	100.58	113.40
1	BR	32	TRP	CG-CD1-NE1	-5.83	104.28	110.10
1	Bd	50	GLN	CA-CB-CG	-5.83	100.58	113.40
1	Bh	32	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	BW	32	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	B6	50	GLN	CA-CB-CG	-5.82	100.60	113.40
1	BT	32	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	Br	32	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	BL	32	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	Bn	32	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	Bt	32	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	BV	32	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	Bq	32	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	Bk	32	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	BC	32	TRP	CG-CD1-NE1	-5.79	104.31	110.10
1	BK	32	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	Bf	82	TRP	CG-CD1-NE1	-5.71	104.39	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Bk	82	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	B2	82	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	Bd	82	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	BA	82	TRP	CG-CD1-NE1	-5.70	104.40	110.10
1	Bm	82	TRP	CG-CD1-NE1	-5.70	104.40	110.10
1	B4	82	TRP	CG-CD1-NE1	-5.70	104.40	110.10
1	BD	82	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	BF	82	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	Bn	82	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	BW	82	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	Bs	82	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	A9	32	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	BJ	38	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	Bf	38	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B5	82	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	BH	82	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	BX	82	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	BY	82	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	BC	82	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	BV	82	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	B0	82	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	At	32	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	BF	20	VAL	CB-CA-C	5.68	122.19	111.40
1	BJ	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	BZ	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	B9	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	BE	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	B7	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	AP	32	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	BO	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	A7	32	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	Au	32	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	B4	20	VAL	CB-CA-C	5.67	122.17	111.40
1	B7	38	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	BI	38	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	Bt	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	B3	20	VAL	CB-CA-C	5.66	122.16	111.40
1	B6	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	Bb	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	Bo	20	VAL	CB-CA-C	5.66	122.16	111.40
1	BB	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	BK	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Bn	38	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	CW	11	ASP	CA-CB-CG	5.66	125.85	113.40
1	BP	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	Bg	38	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	Bo	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	Bp	20	VAL	CB-CA-C	5.66	122.15	111.40
1	Bf	20	VAL	CB-CA-C	5.66	122.15	111.40
1	Cm	11	ASP	CA-CB-CG	5.66	125.85	113.40
1	Ax	32	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	B1	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	Bj	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	BQ	82	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Bt	20	VAL	CB-CA-C	5.65	122.14	111.40
1	CY	11	ASP	CA-CB-CG	5.65	125.84	113.40
1	A1	32	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	AO	32	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Ba	82	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Bp	82	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Bu	82	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	AB	32	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Ab	32	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	BE	20	VAL	CB-CA-C	5.65	122.14	111.40
1	BG	20	VAL	CB-CA-C	5.65	122.14	111.40
1	Bd	20	VAL	CB-CA-C	5.65	122.14	111.40
1	Bi	38	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	Cb	11	ASP	CA-CB-CG	5.65	125.83	113.40
1	Ak	32	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	BA	20	VAL	CB-CA-C	5.65	122.13	111.40
1	BD	20	VAL	CB-CA-C	5.65	122.13	111.40
1	AX	32	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Bi	20	VAL	CB-CA-C	5.65	122.13	111.40
1	Bl	82	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Cv	11	ASP	CA-CB-CG	5.65	125.83	113.40
1	B7	20	VAL	CB-CA-C	5.65	122.13	111.40
1	BF	38	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	Bg	20	VAL	CB-CA-C	5.65	122.13	111.40
1	Bq	20	VAL	CB-CA-C	5.65	122.13	111.40
1	Cu	11	ASP	CA-CB-CG	5.65	125.82	113.40
1	AA	32	TRP	CG-CD1-NE1	-5.64	104.45	110.10
1	BI	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	BO	20	VAL	CB-CA-C	5.64	122.12	111.40
1	Bn	20	VAL	CB-CA-C	5.64	122.12	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C6	56	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	Cn	56	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B2	20	VAL	CB-CA-C	5.64	122.12	111.40
1	BB	20	VAL	CB-CA-C	5.64	122.12	111.40
1	BK	20	VAL	CB-CA-C	5.64	122.12	111.40
1	Be	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	Br	20	VAL	CB-CA-C	5.64	122.12	111.40
1	AF	32	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	Be	20	VAL	CB-CA-C	5.64	122.12	111.40
1	Bw	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	C8	11	ASP	CA-CB-CG	5.64	125.81	113.40
1	B8	20	VAL	CB-CA-C	5.64	122.11	111.40
1	BV	20	VAL	CB-CA-C	5.64	122.12	111.40
1	Bh	20	VAL	CB-CA-C	5.64	122.11	111.40
1	CG	11	ASP	CA-CB-CG	5.64	125.81	113.40
1	BM	20	VAL	CB-CA-C	5.64	122.11	111.40
1	Bc	20	VAL	CB-CA-C	5.64	122.11	111.40
1	Bc	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	Bx	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	C4	11	ASP	CA-CB-CG	5.64	125.80	113.40
1	A6	32	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	Ad	55	ASN	CB-CA-C	-5.64	99.13	110.40
1	BL	20	VAL	CB-CA-C	5.64	122.11	111.40
1	BM	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	BS	20	VAL	CB-CA-C	5.64	122.11	111.40
1	BS	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	Bw	20	VAL	CB-CA-C	5.64	122.11	111.40
1	C1	11	ASP	CA-CB-CG	5.64	125.80	113.40
1	CK	11	ASP	CA-CB-CG	5.64	125.80	113.40
1	Av	32	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	B1	20	VAL	CB-CA-C	5.63	122.11	111.40
1	BC	20	VAL	CB-CA-C	5.63	122.11	111.40
1	BJ	20	VAL	CB-CA-C	5.63	122.11	111.40
1	BN	82	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	BP	20	VAL	CB-CA-C	5.63	122.11	111.40
1	BU	20	VAL	CB-CA-C	5.63	122.11	111.40
1	BX	20	VAL	CB-CA-C	5.63	122.11	111.40
1	Bg	82	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	Bl	20	VAL	CB-CA-C	5.63	122.11	111.40
1	CX	11	ASP	CA-CB-CG	5.63	125.79	113.40
1	Cq	11	ASP	CA-CB-CG	5.63	125.80	113.40
1	AD	32	TRP	CG-CD1-NE1	-5.63	104.47	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AY	32	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	B3	82	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	BQ	20	VAL	CB-CA-C	5.63	122.10	111.40
1	BT	20	VAL	CB-CA-C	5.63	122.10	111.40
1	Bx	20	VAL	CB-CA-C	5.63	122.10	111.40
1	BH	32	TRP	CG-CD2-CE3	5.63	138.97	133.90
1	BR	20	VAL	CB-CA-C	5.63	122.10	111.40
1	Bs	20	VAL	CB-CA-C	5.63	122.10	111.40
1	CO	11	ASP	CA-CB-CG	5.63	125.79	113.40
1	CP	11	ASP	CA-CB-CG	5.63	125.79	113.40
1	Ca	11	ASP	CA-CB-CG	5.63	125.79	113.40
1	Cw	11	ASP	CA-CB-CG	5.63	125.79	113.40
1	B7	32	TRP	CG-CD2-CE3	5.63	138.97	133.90
1	BN	20	VAL	CB-CA-C	5.63	122.10	111.40
1	CS	11	ASP	CA-CB-CG	5.63	125.78	113.40
1	A3	32	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	A8	32	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	AD	55	ASN	CB-CA-C	-5.63	99.14	110.40
1	AG	55	ASN	CB-CA-C	-5.63	99.14	110.40
1	AO	55	ASN	CB-CA-C	-5.63	99.14	110.40
1	AT	32	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	Ar	55	ASN	CB-CA-C	-5.63	99.14	110.40
1	B8	82	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	B9	20	VAL	CB-CA-C	5.63	122.09	111.40
1	Bc	38	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	Bi	82	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	Bu	20	VAL	CB-CA-C	5.63	122.09	111.40
1	Bv	20	VAL	CB-CA-C	5.63	122.09	111.40
1	C0	11	ASP	CA-CB-CG	5.63	125.78	113.40
1	C2	11	ASP	CA-CB-CG	5.63	125.78	113.40
1	CX	56	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	Ce	11	ASP	CA-CB-CG	5.63	125.78	113.40
1	AW	55	ASN	CB-CA-C	-5.63	99.14	110.40
1	AY	55	ASN	CB-CA-C	-5.63	99.15	110.40
1	Au	55	ASN	CB-CA-C	-5.63	99.15	110.40
1	B6	20	VAL	CB-CA-C	5.63	122.09	111.40
1	BH	20	VAL	CB-CA-C	5.63	122.09	111.40
1	BZ	20	VAL	CB-CA-C	5.63	122.09	111.40
1	Bb	20	VAL	CB-CA-C	5.63	122.09	111.40
1	C3	11	ASP	CA-CB-CG	5.63	125.78	113.40
1	C6	11	ASP	CA-CB-CG	5.63	125.78	113.40
1	Cj	11	ASP	CA-CB-CG	5.63	125.78	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AW	32	TRP	CG-CD1-NE1	-5.62	104.47	110.10
1	Ai	55	ASN	CB-CA-C	-5.62	99.15	110.40
1	B5	20	VAL	CB-CA-C	5.62	122.09	111.40
1	BI	20	VAL	CB-CA-C	5.62	122.09	111.40
1	BY	20	VAL	CB-CA-C	5.62	122.09	111.40
1	Bc	32	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	Bj	20	VAL	CB-CA-C	5.62	122.09	111.40
1	Bk	32	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	Cr	11	ASP	CA-CB-CG	5.62	125.78	113.40
1	A0	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	Am	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	B9	32	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	BG	82	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	CJ	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	CM	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	CN	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	CV	56	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A2	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	A4	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	A6	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	A7	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	AE	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	AS	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	Ac	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	Ap	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	As	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	Bk	20	VAL	CB-CA-C	5.62	122.08	111.40
1	CF	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	Cd	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	Co	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	Cs	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	A8	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	AF	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	AR	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	C9	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	Cl	11	ASP	CA-CB-CG	5.62	125.76	113.40
1	AI	55	ASN	CB-CA-C	-5.62	99.17	110.40
1	AK	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	AN	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	Ac	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	Aj	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	Ak	55	ASN	CB-CA-C	-5.62	99.16	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B0	20	VAL	CB-CA-C	5.62	122.07	111.40
1	BL	38	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	BQ	38	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	BT	32	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	BT	82	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	C7	11	ASP	CA-CB-CG	5.62	125.76	113.40
1	CZ	11	ASP	CA-CB-CG	5.62	125.76	113.40
1	Cx	11	ASP	CA-CB-CG	5.62	125.76	113.40
1	Bh	82	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	Bm	20	VAL	CB-CA-C	5.62	122.07	111.40
1	Br	82	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	CE	11	ASP	CA-CB-CG	5.62	125.76	113.40
1	CQ	11	ASP	CA-CB-CG	5.62	125.76	113.40
1	AH	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	AH	55	ASN	CB-CA-C	-5.62	99.17	110.40
1	AL	55	ASN	CB-CA-C	-5.62	99.17	110.40
1	AV	55	ASN	CB-CA-C	-5.62	99.17	110.40
1	Af	55	ASN	CB-CA-C	-5.62	99.17	110.40
1	Al	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	At	55	ASN	CB-CA-C	-5.62	99.17	110.40
1	BY	38	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	Ba	20	VAL	CB-CA-C	5.62	122.07	111.40
1	Ch	11	ASP	CA-CB-CG	5.62	125.75	113.40
1	A5	55	ASN	CB-CA-C	-5.61	99.17	110.40
1	AA	55	ASN	CB-CA-C	-5.61	99.17	110.40
1	AQ	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	AZ	55	ASN	CB-CA-C	-5.61	99.17	110.40
1	Aa	55	ASN	CB-CA-C	-5.61	99.17	110.40
1	Ar	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	AG	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	AK	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	AX	55	ASN	CB-CA-C	-5.61	99.17	110.40
1	Ad	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	BS	38	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	BU	82	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	BW	20	VAL	CB-CA-C	5.61	122.06	111.40
1	A0	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	AV	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	Av	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	BK	32	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	BN	32	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	Bf	32	TRP	CG-CD2-CE3	5.61	138.95	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Bq	82	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	Bv	82	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	CA	11	ASP	CA-CB-CG	5.61	125.74	113.40
1	CL	11	ASP	CA-CB-CG	5.61	125.75	113.40
1	CT	11	ASP	CA-CB-CG	5.61	125.74	113.40
1	Cp	11	ASP	CA-CB-CG	5.61	125.74	113.40
1	AJ	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	Ab	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	Ax	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	CH	11	ASP	CA-CB-CG	5.61	125.74	113.40
1	AC	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	AE	55	ASN	CB-CA-C	-5.61	99.19	110.40
1	AI	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	AP	55	ASN	CB-CA-C	-5.61	99.19	110.40
1	Aq	55	ASN	CB-CA-C	-5.61	99.19	110.40
1	As	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	Bn	32	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	CU	11	ASP	CA-CB-CG	5.61	125.73	113.40
1	Cc	11	ASP	CA-CB-CG	5.61	125.74	113.40
1	Ci	11	ASP	CA-CB-CG	5.61	125.74	113.40
1	Aw	55	ASN	CB-CA-C	-5.61	99.19	110.40
1	Br	38	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	CD	11	ASP	CA-CB-CG	5.61	125.73	113.40
1	CR	11	ASP	CA-CB-CG	5.61	125.73	113.40
1	Ck	11	ASP	CA-CB-CG	5.61	125.73	113.40
1	A1	55	ASN	CB-CA-C	-5.60	99.19	110.40
1	A9	55	ASN	CB-CA-C	-5.60	99.19	110.40
1	AM	55	ASN	CB-CA-C	-5.60	99.19	110.40
1	Am	55	ASN	CB-CA-C	-5.60	99.19	110.40
1	Ck	56	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A2	55	ASN	CB-CA-C	-5.60	99.19	110.40
1	AM	32	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	Ao	55	ASN	CB-CA-C	-5.60	99.20	110.40
1	B0	32	TRP	CG-CD2-CE3	5.60	138.94	133.90
1	Bp	38	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	CI	11	ASP	CA-CB-CG	5.60	125.72	113.40
1	Cn	11	ASP	CA-CB-CG	5.60	125.73	113.40
1	Ct	11	ASP	CA-CB-CG	5.60	125.73	113.40
1	AN	32	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	An	55	ASN	CB-CA-C	-5.60	99.20	110.40
1	Aa	32	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	Aw	32	TRP	CG-CD1-NE1	-5.60	104.50	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Bt	38	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	CC	11	ASP	CA-CB-CG	5.60	125.72	113.40
1	CV	11	ASP	CA-CB-CG	5.60	125.72	113.40
1	Cg	11	ASP	CA-CB-CG	5.60	125.72	113.40
1	AB	55	ASN	CB-CA-C	-5.60	99.20	110.40
1	AR	55	ASN	CB-CA-C	-5.60	99.21	110.40
1	AU	55	ASN	CB-CA-C	-5.60	99.20	110.40
1	C5	11	ASP	CA-CB-CG	5.60	125.72	113.40
1	AT	55	ASN	CB-CA-C	-5.60	99.21	110.40
1	Ae	55	ASN	CB-CA-C	-5.60	99.21	110.40
1	Al	55	ASN	CB-CA-C	-5.60	99.21	110.40
1	Bo	38	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	CQ	56	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A3	55	ASN	CB-CA-C	-5.59	99.21	110.40
1	Ae	32	TRP	CG-CD1-NE1	-5.59	104.50	110.10
1	Aj	55	ASN	CB-CA-C	-5.59	99.21	110.40
1	Bh	38	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	CC	56	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	CI	56	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	Ag	55	ASN	CB-CA-C	-5.59	99.21	110.40
1	AZ	32	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	Bw	32	TRP	CG-CD2-CE3	5.59	138.93	133.90
1	CB	11	ASP	CA-CB-CG	5.59	125.70	113.40
1	CI	20	VAL	CB-CA-C	5.59	122.02	111.40
1	CW	20	VAL	CB-CA-C	5.59	122.02	111.40
1	AJ	32	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	An	32	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	BK	38	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	BT	38	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	CK	56	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	Cw	20	VAL	CB-CA-C	5.59	122.02	111.40
1	AL	32	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	A5	32	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	C8	20	VAL	CB-CA-C	5.59	122.02	111.40
1	A4	32	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	Ah	55	ASN	CB-CA-C	-5.58	99.23	110.40
1	BL	82	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	BW	32	TRP	CG-CD2-CE3	5.58	138.93	133.90
1	Cn	20	VAL	CB-CA-C	5.58	122.01	111.40
1	Ct	20	VAL	CB-CA-C	5.58	122.01	111.40
1	Aq	32	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	Ba	32	TRP	CG-CD2-CE3	5.58	138.92	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C4	20	VAL	CB-CA-C	5.58	122.00	111.40
1	CL	20	VAL	CB-CA-C	5.58	122.00	111.40
1	CS	20	VAL	CB-CA-C	5.58	122.01	111.40
1	CV	20	VAL	CB-CA-C	5.58	122.00	111.40
1	Ce	56	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	AU	32	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	BR	82	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	Bx	38	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	CP	20	VAL	CB-CA-C	5.58	122.00	111.40
1	Cu	20	VAL	CB-CA-C	5.58	122.00	111.40
1	Ah	32	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	BR	38	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	CM	20	VAL	CB-CA-C	5.58	122.00	111.40
1	Cc	20	VAL	CB-CA-C	5.58	122.00	111.40
1	Ap	32	TRP	CG-CD1-NE1	-5.58	104.53	110.10
1	BM	38	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	Bk	38	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C0	56	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	CJ	20	VAL	CB-CA-C	5.58	122.00	111.40
1	Ck	20	VAL	CB-CA-C	5.58	121.99	111.40
1	AQ	55	ASN	CB-CA-C	-5.57	99.25	110.40
1	Af	32	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	BY	32	TRP	CG-CD2-CE3	5.57	138.92	133.90
1	C0	20	VAL	CB-CA-C	5.57	121.99	111.40
1	C2	20	VAL	CB-CA-C	5.57	121.99	111.40
1	CO	20	VAL	CB-CA-C	5.57	121.99	111.40
1	CR	20	VAL	CB-CA-C	5.57	121.99	111.40
1	CT	56	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	CU	20	VAL	CB-CA-C	5.57	121.99	111.40
1	Cp	20	VAL	CB-CA-C	5.57	121.99	111.40
1	AC	32	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	Ai	32	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	Cg	20	VAL	CB-CA-C	5.57	121.99	111.40
1	Co	20	VAL	CB-CA-C	5.57	121.99	111.40
1	BI	32	TRP	CG-CD2-CE3	5.57	138.91	133.90
1	CB	20	VAL	CB-CA-C	5.57	121.98	111.40
1	CC	20	VAL	CB-CA-C	5.57	121.98	111.40
1	CQ	20	VAL	CB-CA-C	5.57	121.98	111.40
1	Cq	20	VAL	CB-CA-C	5.57	121.98	111.40
1	C1	20	VAL	CB-CA-C	5.57	121.98	111.40
1	BV	32	TRP	CG-CD2-CE3	5.57	138.91	133.90
1	CD	20	VAL	CB-CA-C	5.57	121.98	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CN	20	VAL	CB-CA-C	5.57	121.98	111.40
1	Cf	11	ASP	CA-CB-CG	5.57	125.65	113.40
1	Cf	20	VAL	CB-CA-C	5.57	121.98	111.40
1	C7	56	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C9	20	VAL	CB-CA-C	5.57	121.97	111.40
1	CF	20	VAL	CB-CA-C	5.57	121.97	111.40
1	CK	20	VAL	CB-CA-C	5.57	121.97	111.40
1	Cd	20	VAL	CB-CA-C	5.57	121.97	111.40
1	Cs	20	VAL	CB-CA-C	5.57	121.97	111.40
1	B2	32	TRP	CG-CD2-CE3	5.56	138.91	133.90
1	CA	20	VAL	CB-CA-C	5.56	121.97	111.40
1	Ci	20	VAL	CB-CA-C	5.56	121.97	111.40
1	Cl	20	VAL	CB-CA-C	5.56	121.97	111.40
1	Cv	20	VAL	CB-CA-C	5.56	121.97	111.40
1	Ao	32	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	BP	32	TRP	CG-CD2-CE3	5.56	138.91	133.90
1	BX	32	TRP	CG-CD2-CE3	5.56	138.91	133.90
1	C6	20	VAL	CB-CA-C	5.56	121.97	111.40
1	Ch	20	VAL	CB-CA-C	5.56	121.97	111.40
1	Cj	20	VAL	CB-CA-C	5.56	121.97	111.40
1	BC	32	TRP	CG-CD2-CE3	5.56	138.90	133.90
1	Bx	32	TRP	CG-CD2-CE3	5.56	138.90	133.90
1	BQ	32	TRP	CG-CD2-CE3	5.56	138.90	133.90
1	CH	20	VAL	CB-CA-C	5.56	121.96	111.40
1	AS	32	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	Ag	32	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	Bl	32	TRP	CG-CD2-CE3	5.56	138.90	133.90
1	CX	20	VAL	CB-CA-C	5.55	121.95	111.40
1	CZ	20	VAL	CB-CA-C	5.55	121.95	111.40
1	B4	38	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	BD	32	TRP	CG-CD2-CE3	5.55	138.90	133.90
1	Ca	20	VAL	CB-CA-C	5.55	121.95	111.40
1	Cm	20	VAL	CB-CA-C	5.55	121.95	111.40
1	Cx	20	VAL	CB-CA-C	5.55	121.95	111.40
1	B1	38	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B6	32	TRP	CG-CD2-CE3	5.55	138.90	133.90
1	CO	56	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	CT	20	VAL	CB-CA-C	5.55	121.95	111.40
1	BG	32	TRP	CG-CD2-CE3	5.55	138.90	133.90
1	BV	38	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	C5	56	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	CY	20	VAL	CB-CA-C	5.55	121.94	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ce	20	VAL	CB-CA-C	5.55	121.95	111.40
1	Cr	20	VAL	CB-CA-C	5.55	121.94	111.40
1	Bd	38	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	Bt	32	TRP	CG-CD2-CE3	5.55	138.89	133.90
1	C5	20	VAL	CB-CA-C	5.55	121.94	111.40
1	BF	32	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	Bo	32	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	Bp	32	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	Bs	38	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	Bu	32	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	C3	20	VAL	CB-CA-C	5.54	121.93	111.40
1	BB	38	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	Bs	32	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	CN	56	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	BS	32	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	Bg	32	TRP	CG-CD2-CE3	5.54	138.88	133.90
1	C2	56	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	Cj	56	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	CG	20	VAL	CB-CA-C	5.54	121.92	111.40
1	Be	32	TRP	CG-CD2-CE3	5.54	138.88	133.90
1	CE	20	VAL	CB-CA-C	5.54	121.92	111.40
1	B1	32	TRP	CG-CD2-CE3	5.53	138.88	133.90
1	BX	38	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	Bl	38	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	C4	56	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B4	32	TRP	CG-CD2-CE3	5.53	138.88	133.90
1	C7	20	VAL	CB-CA-C	5.53	121.91	111.40
1	Cb	20	VAL	CB-CA-C	5.53	121.91	111.40
1	Ct	56	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	CZ	56	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B8	32	TRP	CG-CD2-CE3	5.53	138.87	133.90
1	BZ	38	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	CA	56	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B2	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B6	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	BC	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	BU	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	Cl	56	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	Bd	32	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	Bj	32	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	Bq	32	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	CW	56	ARG	NE-CZ-NH1	5.52	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ca	56	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	BN	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	Bb	32	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	B3	32	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	BD	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B3	38	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	BB	32	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	Cb	56	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	Br	32	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	CF	56	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	Bm	38	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C3	56	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B5	32	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	Ba	38	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	Bh	32	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	BO	38	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	BA	32	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	BA	38	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	CL	56	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B5	38	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	BJ	32	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	BW	38	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	Bv	38	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	BZ	32	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	Bu	38	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	Bv	32	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	Cc	56	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	Co	56	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	BL	32	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	Bq	38	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	Bw	38	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	Bi	32	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	Bv	32	TRP	CB-CG-CD1	-5.49	119.86	127.00
1	Cf	56	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	BH	38	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	BO	32	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	BU	32	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	Cm	56	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	Cx	56	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B8	38	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B9	38	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	Bm	32	TRP	CG-CD2-CE3	5.48	138.83	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AB	32	TRP	CG-CD2-CE3	5.48	138.83	133.90
1	Bj	38	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	Cs	56	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	BR	32	TRP	CG-CD2-CE3	5.48	138.83	133.90
1	BM	32	TRP	CG-CD2-CE3	5.47	138.83	133.90
1	BE	32	TRP	CG-CD2-CE3	5.47	138.82	133.90
1	Cv	56	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	BS	32	TRP	CB-CG-CD1	-5.46	119.89	127.00
1	Ch	56	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B3	32	TRP	CB-CG-CD1	-5.46	119.90	127.00
1	BB	32	TRP	CB-CG-CD1	-5.46	119.90	127.00
1	B5	32	TRP	CB-CG-CD1	-5.46	119.90	127.00
1	B6	32	TRP	CB-CG-CD1	-5.46	119.90	127.00
1	A2	35	SER	N-CA-CB	-5.46	102.31	110.50
1	Bb	32	TRP	CB-CG-CD1	-5.46	119.90	127.00
1	Cr	56	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	AE	35	SER	N-CA-CB	-5.46	102.31	110.50
1	AG	35	SER	N-CA-CB	-5.46	102.32	110.50
1	B9	32	TRP	CB-CG-CD1	-5.46	119.91	127.00
1	CJ	56	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A7	35	SER	N-CA-CB	-5.45	102.32	110.50
1	Ai	35	SER	N-CA-CB	-5.45	102.32	110.50
1	CM	56	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	CY	56	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	AD	35	SER	N-CA-CB	-5.45	102.32	110.50
1	AJ	32	TRP	CG-CD2-CE3	5.45	138.81	133.90
1	Ab	35	SER	N-CA-CB	-5.45	102.33	110.50
1	An	35	SER	N-CA-CB	-5.45	102.32	110.50
1	Ar	35	SER	N-CA-CB	-5.45	102.32	110.50
1	BP	32	TRP	CB-CG-CD1	-5.45	119.91	127.00
1	Bx	32	TRP	CB-CG-CD1	-5.45	119.91	127.00
1	A6	38	ARG	CG-CD-NE	-5.45	100.36	111.80
1	AA	35	SER	N-CA-CB	-5.45	102.33	110.50
1	AE	38	ARG	CG-CD-NE	-5.45	100.36	111.80
1	Ak	35	SER	N-CA-CB	-5.45	102.33	110.50
1	Ap	32	TRP	CG-CD2-CE3	5.45	138.80	133.90
1	At	35	SER	N-CA-CB	-5.45	102.33	110.50
1	Cu	56	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	Bm	32	TRP	CB-CG-CD1	-5.45	119.92	127.00
1	Cd	56	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	Bp	32	TRP	CB-CG-CD1	-5.45	119.92	127.00
1	CE	56	ARG	NE-CZ-NH1	5.45	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A0	35	SER	N-CA-CB	-5.44	102.33	110.50
1	Ak	38	ARG	CG-CD-NE	-5.44	100.37	111.80
1	A1	38	ARG	CG-CD-NE	-5.44	100.37	111.80
1	AN	35	SER	N-CA-CB	-5.44	102.33	110.50
1	AO	35	SER	N-CA-CB	-5.44	102.33	110.50
1	AY	35	SER	N-CA-CB	-5.44	102.34	110.50
1	AY	38	ARG	CG-CD-NE	-5.44	100.37	111.80
1	Ac	35	SER	N-CA-CB	-5.44	102.33	110.50
1	BF	32	TRP	CB-CG-CD1	-5.44	119.92	127.00
1	Bi	32	TRP	CB-CG-CD1	-5.44	119.92	127.00
1	A9	38	ARG	CG-CD-NE	-5.44	100.37	111.80
1	AG	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	AZ	35	SER	N-CA-CB	-5.44	102.34	110.50
1	As	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	BA	32	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	BO	32	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	Bo	32	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	CS	101	CYS	CA-CB-SG	-5.44	104.21	114.00
1	AC	35	SER	N-CA-CB	-5.44	102.34	110.50
1	AO	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	Ad	35	SER	N-CA-CB	-5.44	102.34	110.50
1	B1	32	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	Bl	32	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	Cq	56	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	AM	35	SER	N-CA-CB	-5.44	102.34	110.50
1	AQ	35	SER	N-CA-CB	-5.44	102.34	110.50
1	AR	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	Aa	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	Ai	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	Av	35	SER	N-CA-CB	-5.44	102.34	110.50
1	CD	101	CYS	CA-CB-SG	-5.44	104.21	114.00
1	A2	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	A3	35	SER	N-CA-CB	-5.44	102.35	110.50
1	AL	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	Ah	38	ARG	CG-CD-NE	-5.44	100.39	111.80
1	BN	32	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	AM	38	ARG	CG-CD-NE	-5.43	100.39	111.80
1	Ag	38	ARG	CG-CD-NE	-5.43	100.39	111.80
1	B0	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	B4	32	TRP	CB-CG-CD1	-5.43	119.93	127.00
1	C8	56	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	CG	101	CYS	CA-CB-SG	-5.43	104.22	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CU	101	CYS	CA-CB-SG	-5.43	104.22	114.00
1	AZ	38	ARG	CG-CD-NE	-5.43	100.39	111.80
1	Ad	38	ARG	CG-CD-NE	-5.43	100.39	111.80
1	Au	35	SER	N-CA-CB	-5.43	102.35	110.50
1	BL	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	Bb	38	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	CJ	101	CYS	CA-CB-SG	-5.43	104.22	114.00
1	CR	56	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	Cw	56	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	Aw	35	SER	N-CA-CB	-5.43	102.35	110.50
1	BW	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	C3	101	CYS	CA-CB-SG	-5.43	104.22	114.00
1	C9	56	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	Ci	101	CYS	CA-CB-SG	-5.43	104.22	114.00
1	A5	35	SER	N-CA-CB	-5.43	102.36	110.50
1	AA	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	AC	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	AI	35	SER	N-CA-CB	-5.43	102.36	110.50
1	AX	35	SER	N-CA-CB	-5.43	102.36	110.50
1	Af	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	Ao	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	Ax	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	BX	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	Bd	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	CN	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cp	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cv	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cw	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	A1	35	SER	N-CA-CB	-5.43	102.36	110.50
1	Ag	35	SER	N-CA-CB	-5.43	102.36	110.50
1	Au	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	Bu	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	CB	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Ct	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	AF	35	SER	N-CA-CB	-5.43	102.36	110.50
1	AH	38	ARG	CG-CD-NE	-5.43	100.41	111.80
1	AS	32	TRP	CG-CD2-CE3	5.43	138.78	133.90
1	AS	38	ARG	CG-CD-NE	-5.43	100.41	111.80
1	Aa	35	SER	N-CA-CB	-5.43	102.36	110.50
1	An	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	BG	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	BJ	32	TRP	CB-CG-CD1	-5.43	119.94	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BQ	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	C4	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cc	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cm	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cq	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cx	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	AB	38	ARG	CG-CD-NE	-5.42	100.41	111.80
1	AH	35	SER	N-CA-CB	-5.42	102.36	110.50
1	AX	38	ARG	CG-CD-NE	-5.42	100.41	111.80
1	Al	35	SER	N-CA-CB	-5.42	102.36	110.50
1	Ap	35	SER	N-CA-CB	-5.42	102.36	110.50
1	Ap	38	ARG	CG-CD-NE	-5.42	100.41	111.80
1	B8	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	BR	57	LYS	CB-CA-C	-5.42	99.55	110.40
1	BU	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	BZ	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	Bf	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	CH	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	CR	101	CYS	CA-CB-SG	-5.42	104.23	114.00
1	CT	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	CU	56	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A3	38	ARG	CG-CD-NE	-5.42	100.41	111.80
1	AJ	38	ARG	CG-CD-NE	-5.42	100.41	111.80
1	AW	35	SER	N-CA-CB	-5.42	102.36	110.50
1	Aj	35	SER	N-CA-CB	-5.42	102.37	110.50
1	Ax	35	SER	N-CA-CB	-5.42	102.37	110.50
1	B1	57	LYS	CB-CA-C	-5.42	99.55	110.40
1	Ba	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	Bg	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	Bs	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	CE	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	Ch	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	Cj	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	AP	35	SER	N-CA-CB	-5.42	102.37	110.50
1	AU	38	ARG	CG-CD-NE	-5.42	100.41	111.80
1	Ac	38	ARG	CG-CD-NE	-5.42	100.42	111.80
1	Af	32	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	B8	57	LYS	CB-CA-C	-5.42	99.56	110.40
1	Bq	57	LYS	CB-CA-C	-5.42	99.56	110.40
1	Bw	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	C7	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	CF	101	CYS	CA-CB-SG	-5.42	104.24	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CP	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	Cn	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	Cp	56	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	Cs	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	Cu	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	Ah	32	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	BZ	57	LYS	CB-CA-C	-5.42	99.56	110.40
1	Be	38	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C5	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	CL	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	A0	38	ARG	CG-CD-NE	-5.42	100.42	111.80
1	A8	35	SER	N-CA-CB	-5.42	102.37	110.50
1	Aq	35	SER	N-CA-CB	-5.42	102.37	110.50
1	Aq	38	ARG	CG-CD-NE	-5.42	100.42	111.80
1	As	35	SER	N-CA-CB	-5.42	102.37	110.50
1	Av	38	ARG	CG-CD-NE	-5.42	100.42	111.80
1	BH	32	TRP	CB-CG-CD1	-5.42	119.96	127.00
1	Be	32	TRP	CB-CG-CD1	-5.42	119.96	127.00
1	C8	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	C9	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	CW	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	CX	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	CY	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	Cg	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	A4	35	SER	N-CA-CB	-5.42	102.38	110.50
1	AF	38	ARG	CG-CD-NE	-5.42	100.43	111.80
1	AL	32	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	AW	32	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	Af	35	SER	N-CA-CB	-5.42	102.38	110.50
1	Ar	38	ARG	CG-CD-NE	-5.42	100.42	111.80
1	Aw	38	ARG	CG-CD-NE	-5.42	100.42	111.80
1	Bt	32	TRP	CB-CG-CD1	-5.42	119.96	127.00
1	CA	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	CK	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	CM	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	BD	57	LYS	CB-CA-C	-5.42	99.57	110.40
1	BI	32	TRP	CB-CG-CD1	-5.42	119.96	127.00
1	Bm	57	LYS	CB-CA-C	-5.42	99.57	110.40
1	C1	56	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	CI	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	AA	32	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	AL	35	SER	N-CA-CB	-5.41	102.38	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BD	32	TRP	CB-CG-CD1	-5.41	119.96	127.00
1	C0	101	CYS	CA-CB-SG	-5.41	104.25	114.00
1	CZ	101	CYS	CA-CB-SG	-5.41	104.25	114.00
1	Ck	101	CYS	CA-CB-SG	-5.41	104.25	114.00
1	Cr	101	CYS	CA-CB-SG	-5.41	104.25	114.00
1	A8	38	ARG	CG-CD-NE	-5.41	100.43	111.80
1	A9	35	SER	N-CA-CB	-5.41	102.38	110.50
1	AR	35	SER	N-CA-CB	-5.41	102.38	110.50
1	BH	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	A4	38	ARG	CG-CD-NE	-5.41	100.44	111.80
1	Am	35	SER	N-CA-CB	-5.41	102.38	110.50
1	BE	38	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	BU	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	BY	32	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	Bj	32	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	Bj	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	Bl	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	Bo	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	C2	101	CYS	CA-CB-SG	-5.41	104.26	114.00
1	CB	56	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	CG	56	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	AC	32	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	AK	35	SER	N-CA-CB	-5.41	102.39	110.50
1	AP	38	ARG	CG-CD-NE	-5.41	100.44	111.80
1	Ao	32	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	BG	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	Be	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	CO	101	CYS	CA-CB-SG	-5.41	104.27	114.00
1	Ce	101	CYS	CA-CB-SG	-5.41	104.26	114.00
1	A3	32	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	A7	32	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	AI	38	ARG	CG-CD-NE	-5.41	100.45	111.80
1	AQ	38	ARG	CG-CD-NE	-5.41	100.44	111.80
1	BE	57	LYS	CB-CA-C	-5.41	99.59	110.40
1	BL	57	LYS	CB-CA-C	-5.41	99.59	110.40
1	A7	38	ARG	CG-CD-NE	-5.41	100.45	111.80
1	AS	35	SER	N-CA-CB	-5.41	102.39	110.50
1	Ab	38	ARG	CG-CD-NE	-5.41	100.45	111.80
1	At	38	ARG	CG-CD-NE	-5.41	100.45	111.80
1	BR	32	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	Bc	32	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	CQ	101	CYS	CA-CB-SG	-5.41	104.27	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Cb	101	CYS	CA-CB-SG	-5.41	104.27	114.00
1	Cd	101	CYS	CA-CB-SG	-5.41	104.27	114.00
1	Cf	101	CYS	CA-CB-SG	-5.41	104.27	114.00
1	Cl	101	CYS	CA-CB-SG	-5.41	104.27	114.00
1	AN	32	TRP	CG-CD2-CE3	5.40	138.76	133.90
1	AV	38	ARG	CG-CD-NE	-5.40	100.45	111.80
1	Al	38	ARG	CG-CD-NE	-5.40	100.45	111.80
1	BE	32	TRP	CB-CG-CD1	-5.40	119.97	127.00
1	BX	57	LYS	CB-CA-C	-5.40	99.59	110.40
1	A5	38	ARG	CG-CD-NE	-5.40	100.45	111.80
1	AJ	35	SER	N-CA-CB	-5.40	102.40	110.50
1	AT	38	ARG	CG-CD-NE	-5.40	100.46	111.80
1	AW	38	ARG	CG-CD-NE	-5.40	100.45	111.80
1	Ae	35	SER	N-CA-CB	-5.40	102.39	110.50
1	Ae	38	ARG	CG-CD-NE	-5.40	100.46	111.80
1	B0	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	BG	38	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	BM	32	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	Bh	32	TRP	CB-CG-CD1	-5.40	119.97	127.00
1	Bk	32	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	Bn	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	CH	56	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	Ca	101	CYS	CA-CB-SG	-5.40	104.28	114.00
1	AB	35	SER	N-CA-CB	-5.40	102.40	110.50
1	BB	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	BF	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	Br	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	Bu	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	A6	35	SER	N-CA-CB	-5.40	102.40	110.50
1	AD	38	ARG	CG-CD-NE	-5.40	100.46	111.80
1	B9	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	Bb	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	Br	32	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	Bx	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	CV	101	CYS	CA-CB-SG	-5.40	104.28	114.00
1	AN	38	ARG	CG-CD-NE	-5.40	100.47	111.80
1	BT	32	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	C6	101	CYS	CA-CB-SG	-5.40	104.28	114.00
1	Am	38	ARG	CG-CD-NE	-5.40	100.47	111.80
1	BC	32	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	Bn	32	TRP	CB-CG-CD1	-5.40	119.99	127.00
1	Aj	38	ARG	CG-CD-NE	-5.39	100.47	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ak	32	TRP	CG-CD2-CE3	5.39	138.76	133.90
1	Am	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	BJ	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	Ba	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	Bd	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	Bh	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	Bq	32	TRP	CB-CG-CD1	-5.39	119.99	127.00
1	CC	101	CYS	CA-CB-SG	-5.39	104.29	114.00
1	AR	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	Aq	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	B2	32	TRP	CB-CG-CD1	-5.39	119.99	127.00
1	B2	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	B3	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	B4	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	BO	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	BS	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	AP	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	BY	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	Bg	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	Bw	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	A0	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	A4	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	AD	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	AT	35	SER	N-CA-CB	-5.39	102.42	110.50
1	AX	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	B7	32	TRP	CB-CG-CD1	-5.39	120.00	127.00
1	BP	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	Bi	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	Bv	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	C1	101	CYS	CA-CB-SG	-5.39	104.30	114.00
1	AK	38	ARG	CG-CD-NE	-5.39	100.49	111.80
1	AV	35	SER	N-CA-CB	-5.39	102.42	110.50
1	Bs	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	AF	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	Ah	35	SER	N-CA-CB	-5.39	102.42	110.50
1	Aw	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	BM	57	LYS	CB-CA-C	-5.39	99.63	110.40
1	A9	32	TRP	CG-CD2-CE3	5.38	138.75	133.90
1	Au	32	TRP	CG-CD2-CE3	5.38	138.75	133.90
1	BT	57	LYS	CB-CA-C	-5.38	99.63	110.40
1	BV	32	TRP	CB-CG-CD1	-5.38	120.00	127.00
1	Co	101	CYS	CA-CB-SG	-5.38	104.31	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ab	32	TRP	CG-CD2-CE3	5.38	138.75	133.90
1	Aj	32	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	B5	57	LYS	CB-CA-C	-5.38	99.63	110.40
1	B7	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	BC	57	LYS	CB-CA-C	-5.38	99.63	110.40
1	Ci	56	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B6	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	BI	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	BA	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	Bc	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	A5	32	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	BN	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	BV	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	Ao	35	SER	N-CA-CB	-5.38	102.44	110.50
1	AU	35	SER	N-CA-CB	-5.38	102.44	110.50
1	Bf	57	LYS	CB-CA-C	-5.38	99.65	110.40
1	AO	32	TRP	CG-CD2-CE3	5.37	138.74	133.90
1	Ar	32	TRP	CG-CD2-CE3	5.37	138.74	133.90
1	At	32	TRP	CG-CD2-CE3	5.37	138.74	133.90
1	BK	32	TRP	CB-CG-CD1	-5.37	120.02	127.00
1	Bk	57	LYS	CB-CA-C	-5.37	99.66	110.40
1	Bp	57	LYS	CB-CA-C	-5.37	99.66	110.40
1	AZ	32	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	Ag	32	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	BK	57	LYS	CB-CA-C	-5.37	99.66	110.40
1	BW	57	LYS	CB-CA-C	-5.37	99.66	110.40
1	Bt	57	LYS	CB-CA-C	-5.37	99.66	110.40
1	A8	32	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	AV	32	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	Ax	32	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	CS	56	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	BP	38	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	Ct	49	ARG	N-CA-CB	-5.36	100.94	110.60
1	AK	32	TRP	CG-CD2-CE3	5.36	138.73	133.90
1	A1	32	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	AT	32	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	Ac	32	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	BQ	57	LYS	CB-CA-C	-5.36	99.68	110.40
1	Cg	56	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A2	32	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	AI	32	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	AQ	32	TRP	CG-CD2-CE3	5.36	138.72	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CD	56	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	Al	32	TRP	CG-CD2-CE3	5.35	138.72	133.90
1	CR	49	ARG	N-CA-CB	-5.35	100.96	110.60
1	CV	49	ARG	N-CA-CB	-5.35	100.96	110.60
1	Cd	49	ARG	N-CA-CB	-5.35	100.96	110.60
1	AM	32	TRP	CG-CD2-CE3	5.35	138.72	133.90
1	Ad	32	TRP	CG-CD2-CE3	5.35	138.72	133.90
1	C6	49	ARG	N-CA-CB	-5.35	100.97	110.60
1	CP	56	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	Cu	49	ARG	N-CA-CB	-5.35	100.96	110.60
1	CC	49	ARG	N-CA-CB	-5.35	100.97	110.60
1	C0	49	ARG	N-CA-CB	-5.35	100.97	110.60
1	CH	49	ARG	N-CA-CB	-5.35	100.97	110.60
1	CP	49	ARG	N-CA-CB	-5.35	100.97	110.60
1	CI	49	ARG	N-CA-CB	-5.35	100.98	110.60
1	Cg	49	ARG	N-CA-CB	-5.35	100.98	110.60
1	As	32	TRP	CG-CD2-CE3	5.35	138.71	133.90
1	CW	49	ARG	N-CA-CB	-5.35	100.98	110.60
1	Cc	49	ARG	N-CA-CB	-5.35	100.98	110.60
1	Cl	49	ARG	N-CA-CB	-5.34	100.98	110.60
1	Cv	49	ARG	N-CA-CB	-5.34	100.98	110.60
1	Cw	49	ARG	N-CA-CB	-5.34	100.98	110.60
1	Av	32	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	Cf	49	ARG	N-CA-CB	-5.34	100.99	110.60
1	Cq	49	ARG	N-CA-CB	-5.34	100.98	110.60
1	CT	49	ARG	N-CA-CB	-5.34	100.99	110.60
1	Cr	49	ARG	N-CA-CB	-5.34	100.99	110.60
1	Ae	32	TRP	CG-CD2-CE3	5.34	138.70	133.90
1	Ch	49	ARG	N-CA-CB	-5.34	100.99	110.60
1	AE	32	TRP	CG-CD2-CE3	5.33	138.70	133.90
1	C5	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	C4	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	C9	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	CK	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	CL	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	CS	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	C3	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	CN	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	B0	38	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C2	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	C7	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	C8	49	ARG	N-CA-CB	-5.33	101.01	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CF	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	CJ	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	CY	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	Ci	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	Cn	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	Cp	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	Ca	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	AU	32	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	CX	49	ARG	N-CA-CB	-5.32	101.02	110.60
1	Ck	49	ARG	N-CA-CB	-5.32	101.02	110.60
1	AY	32	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	CU	49	ARG	N-CA-CB	-5.32	101.02	110.60
1	CO	49	ARG	N-CA-CB	-5.32	101.02	110.60
1	Cb	49	ARG	N-CA-CB	-5.32	101.02	110.60
1	Cs	49	ARG	N-CA-CB	-5.32	101.03	110.60
1	Cj	49	ARG	N-CA-CB	-5.32	101.03	110.60
1	Cm	49	ARG	N-CA-CB	-5.32	101.03	110.60
1	C1	49	ARG	N-CA-CB	-5.32	101.03	110.60
1	AH	32	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	CE	49	ARG	N-CA-CB	-5.31	101.03	110.60
1	An	32	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	CZ	49	ARG	N-CA-CB	-5.31	101.04	110.60
1	Aa	32	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	Ai	32	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	CA	49	ARG	N-CA-CB	-5.31	101.04	110.60
1	CB	49	ARG	N-CA-CB	-5.31	101.04	110.60
1	Co	49	ARG	N-CA-CB	-5.31	101.04	110.60
1	AG	32	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	CG	49	ARG	N-CA-CB	-5.31	101.05	110.60
1	CQ	49	ARG	N-CA-CB	-5.31	101.05	110.60
1	Cx	49	ARG	N-CA-CB	-5.31	101.05	110.60
1	A6	32	TRP	CG-CD2-CE3	5.30	138.67	133.90
1	CD	49	ARG	N-CA-CB	-5.30	101.06	110.60
1	Ce	49	ARG	N-CA-CB	-5.30	101.06	110.60
1	Ba	6	GLN	N-CA-CB	-5.30	101.06	110.60
1	CM	49	ARG	N-CA-CB	-5.30	101.07	110.60
1	Bv	6	GLN	N-CA-CB	-5.29	101.07	110.60
1	BN	6	GLN	N-CA-CB	-5.29	101.07	110.60
1	Bu	6	GLN	N-CA-CB	-5.29	101.07	110.60
1	BD	6	GLN	N-CA-CB	-5.29	101.08	110.60
1	Bn	6	GLN	N-CA-CB	-5.29	101.07	110.60
1	Bw	6	GLN	N-CA-CB	-5.29	101.08	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B7	6	GLN	N-CA-CB	-5.29	101.09	110.60
1	BH	6	GLN	N-CA-CB	-5.29	101.09	110.60
1	B0	6	GLN	N-CA-CB	-5.28	101.09	110.60
1	BI	6	GLN	N-CA-CB	-5.28	101.09	110.60
1	Bc	6	GLN	N-CA-CB	-5.28	101.09	110.60
1	BO	6	GLN	N-CA-CB	-5.28	101.09	110.60
1	Bk	6	GLN	N-CA-CB	-5.28	101.09	110.60
1	Bq	6	GLN	N-CA-CB	-5.28	101.10	110.60
1	B4	6	GLN	N-CA-CB	-5.28	101.10	110.60
1	Bf	6	GLN	N-CA-CB	-5.28	101.10	110.60
1	BG	6	GLN	N-CA-CB	-5.28	101.10	110.60
1	BC	6	GLN	N-CA-CB	-5.28	101.10	110.60
1	BY	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	C2	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	Ce	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	B9	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	BP	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	Bt	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	Bp	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	B5	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	BV	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	BK	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	BX	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	C3	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	CD	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	CM	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	B6	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	B8	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	C7	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	Bo	6	GLN	N-CA-CB	-5.26	101.12	110.60
1	Bs	6	GLN	N-CA-CB	-5.26	101.12	110.60
1	C0	6	GLN	N-CA-CB	-5.26	101.12	110.60
1	CG	6	GLN	N-CA-CB	-5.26	101.12	110.60
1	CX	6	GLN	N-CA-CB	-5.26	101.12	110.60
1	Cg	6	GLN	N-CA-CB	-5.26	101.12	110.60
1	BE	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	CC	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Ca	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Cc	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Bl	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Bx	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Co	6	GLN	N-CA-CB	-5.26	101.13	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ct	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Bj	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	CU	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Cs	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	B2	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	BT	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	BU	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	Bd	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	Bh	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	Bi	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	Bm	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	C4	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	C8	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	C9	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	CA	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	CE	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	CO	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	BA	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	BB	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	BW	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	BL	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	BS	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	C6	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	CI	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	CQ	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	CS	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	Cn	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	Cw	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	CK	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	Cb	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	Cj	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	BM	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	BQ	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	CW	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	CY	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	CJ	6	GLN	N-CA-CB	-5.25	101.16	110.60
1	Cf	6	GLN	N-CA-CB	-5.25	101.16	110.60
1	C5	6	GLN	N-CA-CB	-5.25	101.16	110.60
1	Cp	6	GLN	N-CA-CB	-5.25	101.16	110.60
1	Cx	6	GLN	N-CA-CB	-5.25	101.16	110.60
1	BZ	6	GLN	N-CA-CB	-5.24	101.16	110.60
1	Bb	6	GLN	N-CA-CB	-5.24	101.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Be	6	GLN	N-CA-CB	-5.24	101.16	110.60
1	CZ	6	GLN	N-CA-CB	-5.24	101.16	110.60
1	Cq	6	GLN	N-CA-CB	-5.24	101.16	110.60
1	Cv	6	GLN	N-CA-CB	-5.24	101.16	110.60
1	Ck	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	BJ	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	BR	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	CN	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	Cd	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	Cl	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	Br	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	CL	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	CP	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	CH	6	GLN	N-CA-CB	-5.24	101.18	110.60
1	Ch	6	GLN	N-CA-CB	-5.24	101.18	110.60
1	CT	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	Cm	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	B3	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	BF	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	Bg	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	CF	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	CV	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	Ci	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	Cr	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	Cu	6	GLN	N-CA-CB	-5.23	101.19	110.60
1	B1	6	GLN	N-CA-CB	-5.23	101.19	110.60
1	CB	6	GLN	N-CA-CB	-5.23	101.19	110.60
1	C1	6	GLN	N-CA-CB	-5.22	101.19	110.60
1	A3	56	ARG	NH1-CZ-NH2	5.22	125.14	119.40
1	CR	6	GLN	N-CA-CB	-5.22	101.21	110.60
1	AD	56	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	AJ	82	TRP	CB-CG-CD1	-5.21	120.22	127.00
1	Ae	56	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	AA	56	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	CM	84	SER	N-CA-CB	5.21	118.31	110.50
1	Aa	56	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	AH	56	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	A9	56	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	AW	56	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	AB	82	TRP	CB-CG-CD1	-5.20	120.25	127.00
1	AN	56	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	Ac	56	ARG	NH1-CZ-NH2	5.20	125.11	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Cp	84	SER	N-CA-CB	5.20	118.29	110.50
1	A1	56	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	A6	56	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	AZ	56	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	CA	84	SER	N-CA-CB	5.19	118.28	110.50
1	Ar	56	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	AR	82	TRP	CB-CG-CD1	-5.19	120.26	127.00
1	CR	84	SER	N-CA-CB	5.19	118.28	110.50
1	CX	84	SER	N-CA-CB	5.18	118.28	110.50
1	AE	56	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	AU	82	TRP	CB-CG-CD1	-5.18	120.26	127.00
1	Ad	56	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	AY	56	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	Ak	56	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	CE	84	SER	N-CA-CB	5.18	118.27	110.50
1	Ce	84	SER	N-CA-CB	5.18	118.27	110.50
1	A4	56	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	A8	56	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	Al	56	ARG	NH1-CZ-NH2	5.18	125.09	119.40
1	A5	56	ARG	NH1-CZ-NH2	5.18	125.09	119.40
1	AX	56	ARG	NH1-CZ-NH2	5.18	125.09	119.40
1	Cg	84	SER	N-CA-CB	5.18	118.27	110.50
1	Cm	84	SER	N-CA-CB	5.18	118.26	110.50
1	Am	56	ARG	NH1-CZ-NH2	5.17	125.09	119.40
1	Av	56	ARG	NH1-CZ-NH2	5.17	125.09	119.40
1	CS	84	SER	N-CA-CB	5.17	118.26	110.50
1	AF	56	ARG	NH1-CZ-NH2	5.17	125.09	119.40
1	C7	84	SER	N-CA-CB	5.17	118.26	110.50
1	Cx	84	SER	N-CA-CB	5.17	118.25	110.50
1	A7	56	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	Af	82	TRP	CB-CG-CD1	-5.17	120.28	127.00
1	C6	84	SER	N-CA-CB	5.17	118.25	110.50
1	CB	84	SER	N-CA-CB	5.17	118.25	110.50
1	CZ	84	SER	N-CA-CB	5.17	118.25	110.50
1	Cc	84	SER	N-CA-CB	5.17	118.25	110.50
1	An	56	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	B4	83	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	CG	84	SER	N-CA-CB	5.17	118.25	110.50
1	AI	56	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	Aw	56	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	Cb	84	SER	N-CA-CB	5.17	118.25	110.50
1	Ao	82	TRP	CB-CG-CD1	-5.16	120.29	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Cl	84	SER	N-CA-CB	5.16	118.25	110.50
1	Co	84	SER	N-CA-CB	5.16	118.25	110.50
1	AG	56	ARG	NH1-CZ-NH2	5.16	125.08	119.40
1	C1	84	SER	N-CA-CB	5.16	118.24	110.50
1	C8	84	SER	N-CA-CB	5.16	118.24	110.50
1	CC	84	SER	N-CA-CB	5.16	118.24	110.50
1	CO	84	SER	N-CA-CB	5.16	118.24	110.50
1	A2	56	ARG	NH1-CZ-NH2	5.16	125.08	119.40
1	AM	56	ARG	NH1-CZ-NH2	5.16	125.08	119.40
1	Ah	82	TRP	CB-CG-CD1	-5.16	120.29	127.00
1	Ai	56	ARG	NH1-CZ-NH2	5.16	125.08	119.40
1	Au	56	ARG	NH1-CZ-NH2	5.16	125.08	119.40
1	Ch	84	SER	N-CA-CB	5.16	118.24	110.50
1	A6	82	TRP	CB-CG-CD1	-5.16	120.29	127.00
1	Cw	84	SER	N-CA-CB	5.16	118.24	110.50
1	C3	84	SER	N-CA-CB	5.16	118.24	110.50
1	Ab	56	ARG	NH1-CZ-NH2	5.16	125.07	119.40
1	Ai	82	TRP	CB-CG-CD1	-5.16	120.30	127.00
1	As	56	ARG	NH1-CZ-NH2	5.16	125.07	119.40
1	Cf	84	SER	N-CA-CB	5.16	118.23	110.50
1	Ci	84	SER	N-CA-CB	5.16	118.23	110.50
1	AU	56	ARG	NH1-CZ-NH2	5.15	125.07	119.40
1	Cr	84	SER	N-CA-CB	5.15	118.23	110.50
1	AA	82	TRP	CB-CG-CD1	-5.15	120.30	127.00
1	AD	82	TRP	CB-CG-CD1	-5.15	120.30	127.00
1	CI	84	SER	N-CA-CB	5.15	118.23	110.50
1	AL	56	ARG	NH1-CZ-NH2	5.15	125.07	119.40
1	AT	56	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	Ap	56	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	CJ	84	SER	N-CA-CB	5.15	118.22	110.50
1	CW	84	SER	N-CA-CB	5.15	118.23	110.50
1	Cs	84	SER	N-CA-CB	5.15	118.23	110.50
1	Ct	84	SER	N-CA-CB	5.15	118.22	110.50
1	A5	82	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	AS	56	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	As	82	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	Aw	82	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	A0	56	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	Av	82	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	Ac	82	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	Cu	84	SER	N-CA-CB	5.15	118.22	110.50
1	A8	82	TRP	CB-CG-CD1	-5.14	120.31	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ap	82	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	CF	84	SER	N-CA-CB	5.14	118.22	110.50
1	AO	56	ARG	NH1-CZ-NH2	5.14	125.06	119.40
1	AP	56	ARG	NH1-CZ-NH2	5.14	125.06	119.40
1	AT	82	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	AY	82	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	Cj	84	SER	N-CA-CB	5.14	118.22	110.50
1	A3	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	AK	56	ARG	NH1-CZ-NH2	5.14	125.06	119.40
1	Cn	84	SER	N-CA-CB	5.14	118.21	110.50
1	AW	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	Al	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	Aq	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	C4	84	SER	N-CA-CB	5.14	118.21	110.50
1	Ck	84	SER	N-CA-CB	5.14	118.21	110.50
1	AC	56	ARG	NH1-CZ-NH2	5.14	125.05	119.40
1	AM	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	Aa	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	Ar	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	Ax	56	ARG	NH1-CZ-NH2	5.14	125.05	119.40
1	C5	84	SER	N-CA-CB	5.14	118.20	110.50
1	CD	84	SER	N-CA-CB	5.14	118.20	110.50
1	CH	84	SER	N-CA-CB	5.14	118.20	110.50
1	CN	84	SER	N-CA-CB	5.14	118.20	110.50
1	Cq	84	SER	N-CA-CB	5.14	118.21	110.50
1	A5	48	VAL	CB-CA-C	-5.13	101.64	111.40
1	Ae	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	Ax	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	CK	84	SER	N-CA-CB	5.13	118.20	110.50
1	CQ	84	SER	N-CA-CB	5.13	118.20	110.50
1	CT	84	SER	N-CA-CB	5.13	118.20	110.50
1	CY	84	SER	N-CA-CB	5.13	118.20	110.50
1	AL	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	AX	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	Ag	56	ARG	NH1-CZ-NH2	5.13	125.05	119.40
1	At	56	ARG	NH1-CZ-NH2	5.13	125.05	119.40
1	C9	84	SER	N-CA-CB	5.13	118.20	110.50
1	CU	84	SER	N-CA-CB	5.13	118.20	110.50
1	Ca	84	SER	N-CA-CB	5.13	118.20	110.50
1	AG	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	AK	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	AP	82	TRP	CB-CG-CD1	-5.13	120.33	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AZ	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	CP	84	SER	N-CA-CB	5.13	118.20	110.50
1	AQ	56	ARG	NH1-CZ-NH2	5.13	125.04	119.40
1	Ak	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	AR	56	ARG	NH1-CZ-NH2	5.13	125.04	119.40
1	Af	56	ARG	NH1-CZ-NH2	5.13	125.04	119.40
1	AN	82	TRP	CB-CG-CD1	-5.13	120.34	127.00
1	AS	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	Ag	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	C2	84	SER	N-CA-CB	5.13	118.19	110.50
1	CL	84	SER	N-CA-CB	5.13	118.19	110.50
1	Cd	84	SER	N-CA-CB	5.13	118.19	110.50
1	A2	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	AI	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	AE	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	AQ	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	AV	56	ARG	NH1-CZ-NH2	5.12	125.04	119.40
1	Cv	84	SER	N-CA-CB	5.12	118.19	110.50
1	AF	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	AV	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	Am	48	VAL	CB-CA-C	-5.12	101.67	111.40
1	At	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	C0	84	SER	N-CA-CB	5.12	118.18	110.50
1	A1	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	An	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	AB	56	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	AJ	56	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	AO	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	Aj	82	TRP	CB-CG-CD1	-5.12	120.35	127.00
1	AI	48	VAL	CB-CA-C	-5.12	101.68	111.40
1	Ad	82	TRP	CB-CG-CD1	-5.12	120.35	127.00
1	AK	48	VAL	CB-CA-C	-5.12	101.68	111.40
1	Aj	48	VAL	CB-CA-C	-5.12	101.68	111.40
1	Aq	56	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	CV	84	SER	N-CA-CB	5.12	118.17	110.50
1	A0	82	TRP	CB-CG-CD1	-5.11	120.35	127.00
1	AC	82	TRP	CB-CG-CD1	-5.11	120.35	127.00
1	A7	82	TRP	CB-CG-CD1	-5.11	120.35	127.00
1	AC	48	VAL	CB-CA-C	-5.11	101.69	111.40
1	Ah	56	ARG	NH1-CZ-NH2	5.11	125.02	119.40
1	AH	48	VAL	CB-CA-C	-5.11	101.69	111.40
1	Ae	48	VAL	CB-CA-C	-5.11	101.69	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Aj	56	ARG	NH1-CZ-NH2	5.11	125.02	119.40
1	Au	82	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	A4	82	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	Ak	48	VAL	CB-CA-C	-5.11	101.70	111.40
1	AH	82	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	AG	48	VAL	CB-CA-C	-5.10	101.70	111.40
1	AT	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	Ao	56	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	Ar	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	Ad	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	Am	82	TRP	CB-CG-CD1	-5.10	120.37	127.00
1	AN	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	Au	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	A8	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	AD	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	Ax	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	A2	48	VAL	CB-CA-C	-5.10	101.72	111.40
1	Ab	48	VAL	CB-CA-C	-5.10	101.72	111.40
1	AV	48	VAL	CB-CA-C	-5.09	101.72	111.40
1	Ab	82	TRP	CB-CG-CD1	-5.09	120.38	127.00
1	Ag	48	VAL	CB-CA-C	-5.09	101.72	111.40
1	Al	48	VAL	CB-CA-C	-5.09	101.72	111.40
1	Aw	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	A0	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	A1	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	AA	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	AE	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	AX	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	As	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	B6	83	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	AP	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	At	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	A9	82	TRP	CB-CG-CD1	-5.09	120.39	127.00
1	AQ	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	AY	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	AZ	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	Ac	48	VAL	CB-CA-C	-5.09	101.74	111.40
1	A6	48	VAL	CB-CA-C	-5.08	101.74	111.40
1	A4	48	VAL	CB-CA-C	-5.08	101.74	111.40
1	A9	48	VAL	CB-CA-C	-5.08	101.74	111.40
1	BS	83	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	AB	48	VAL	CB-CA-C	-5.08	101.75	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AS	48	VAL	CB-CA-C	-5.08	101.75	111.40
1	AU	48	VAL	CB-CA-C	-5.08	101.75	111.40
1	A3	48	VAL	CB-CA-C	-5.08	101.75	111.40
1	A7	48	VAL	CB-CA-C	-5.08	101.75	111.40
1	Ai	48	VAL	CB-CA-C	-5.08	101.75	111.40
1	AF	48	VAL	CB-CA-C	-5.08	101.76	111.40
1	Aa	48	VAL	CB-CA-C	-5.08	101.76	111.40
1	AW	48	VAL	CB-CA-C	-5.07	101.76	111.40
1	AO	48	VAL	CB-CA-C	-5.07	101.77	111.40
1	Bg	83	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	Ao	48	VAL	CB-CA-C	-5.07	101.77	111.40
1	AM	48	VAL	CB-CA-C	-5.07	101.77	111.40
1	AR	48	VAL	CB-CA-C	-5.07	101.78	111.40
1	An	48	VAL	CB-CA-C	-5.06	101.78	111.40
1	Av	48	VAL	CB-CA-C	-5.06	101.78	111.40
1	Ap	48	VAL	CB-CA-C	-5.06	101.78	111.40
1	AL	48	VAL	CB-CA-C	-5.06	101.79	111.40
1	Ah	48	VAL	CB-CA-C	-5.06	101.79	111.40
1	Aq	48	VAL	CB-CA-C	-5.06	101.79	111.40
1	AJ	48	VAL	CB-CA-C	-5.05	101.81	111.40
1	Af	48	VAL	CB-CA-C	-5.04	101.81	111.40
1	CS	48	VAL	CB-CA-C	-5.04	101.81	111.40
1	CN	48	VAL	CB-CA-C	-5.03	101.84	111.40
1	Cf	48	VAL	CB-CA-C	-5.03	101.84	111.40
1	CP	82	TRP	CB-CG-CD1	-5.03	120.46	127.00
1	Cp	48	VAL	CB-CA-C	-5.03	101.84	111.40
1	B2	83	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	CC	48	VAL	CB-CA-C	-5.03	101.84	111.40
1	BM	83	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	CY	48	VAL	CB-CA-C	-5.03	101.85	111.40
1	C9	48	VAL	CB-CA-C	-5.03	101.85	111.40
1	CV	48	VAL	CB-CA-C	-5.03	101.85	111.40
1	CQ	48	VAL	CB-CA-C	-5.02	101.86	111.40
1	C0	82	TRP	CB-CG-CD1	-5.02	120.47	127.00
1	CP	48	VAL	CB-CA-C	-5.02	101.86	111.40
1	CW	48	VAL	CB-CA-C	-5.02	101.86	111.40
1	Ca	48	VAL	CB-CA-C	-5.02	101.86	111.40
1	Ck	48	VAL	CB-CA-C	-5.02	101.86	111.40
1	Ct	48	VAL	CB-CA-C	-5.02	101.86	111.40
1	B1	83	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	Bq	83	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C6	48	VAL	CB-CA-C	-5.02	101.87	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BL	83	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	CH	48	VAL	CB-CA-C	-5.02	101.87	111.40
1	CI	48	VAL	CB-CA-C	-5.01	101.87	111.40
1	CL	48	VAL	CB-CA-C	-5.01	101.87	111.40
1	CT	48	VAL	CB-CA-C	-5.01	101.87	111.40
1	Cu	48	VAL	CB-CA-C	-5.01	101.87	111.40
1	C1	48	VAL	CB-CA-C	-5.01	101.88	111.40
1	CE	48	VAL	CB-CA-C	-5.01	101.88	111.40
1	CB	48	VAL	CB-CA-C	-5.01	101.89	111.40
1	CD	48	VAL	CB-CA-C	-5.01	101.89	111.40
1	CZ	48	VAL	CB-CA-C	-5.01	101.89	111.40
1	Bb	83	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	Br	83	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	Cq	48	VAL	CB-CA-C	-5.00	101.89	111.40
1	Cv	48	VAL	CB-CA-C	-5.00	101.89	111.40
1	Cx	48	VAL	CB-CA-C	-5.00	101.89	111.40
1	CF	82	TRP	CB-CG-CD1	-5.00	120.50	127.00
1	Cd	48	VAL	CB-CA-C	-5.00	101.89	111.40
1	C2	82	TRP	CB-CG-CD1	-5.00	120.50	127.00
1	C8	48	VAL	CB-CA-C	-5.00	101.90	111.40
1	CA	48	VAL	CB-CA-C	-5.00	101.90	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A1	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A2	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A3	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A4	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	A5	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A6	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A7	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A8	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A9	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AA	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AB	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AC	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AD	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AE	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AF	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AG	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AH	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AI	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AJ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AK	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AL	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AM	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AN	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AO	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AP	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AQ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AR	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AS	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AT	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AU	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AV	127/129 (98%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AX	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AY	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AZ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Aa	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ab	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ac	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	Ad	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ae	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Af	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ag	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ah	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ai	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Aj	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ak	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Al	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Am	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	An	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ao	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ap	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Aq	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ar	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	As	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	At	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Au	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Av	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Aw	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ax	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	B0	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	B1	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	B2	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B3	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	B4	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	B5	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	B6	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	B7	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	B8	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	B9	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BA	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BB	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BC	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BD	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BE	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BF	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BG	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BH	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BI	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BJ	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BK	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BL	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BM	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BN	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BO	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BP	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BQ	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BR	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BS	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BT	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BU	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BV	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BW	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BX	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BY	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	BZ	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Ba	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bb	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bc	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bd	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Be	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bf	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bg	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bh	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bi	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bj	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bk	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bl	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bm	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bn	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bo	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bp	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bq	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Br	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bs	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bt	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bu	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bv	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bw	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	Bx	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	60
1	C0	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C1	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C2	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C3	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C4	127/129 (98%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C5	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C6	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C7	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C8	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C9	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CA	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CB	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CC	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CD	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CE	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CF	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CG	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CH	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CI	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CJ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CK	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CL	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CM	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CN	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CO	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CP	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CQ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CR	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CS	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CT	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CU	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CV	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CX	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CY	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CZ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ca	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cb	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cc	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cd	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ce	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cf	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cg	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ch	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ci	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cj	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ck	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cl	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cm	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cn	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Co	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cp	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cq	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cr	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cs	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ct	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cu	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cv	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cw	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cx	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
All	All	22860/23220 (98%)	22138 (97%)	662 (3%)	60 (0%)	44	77

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B0	2	SER
1	B1	2	SER
1	B2	2	SER
1	B3	2	SER
1	B4	2	SER

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Mol	Chain	Res	Type
1	B5	2	SER
1	B6	2	SER
1	B7	2	SER
1	B8	2	SER
1	B9	2	SER
1	BA	2	SER
1	BB	2	SER
1	BC	2	SER
1	BD	2	SER
1	BE	2	SER
1	BF	2	SER
1	BG	2	SER
1	BH	2	SER
1	BI	2	SER
1	BJ	2	SER
1	BK	2	SER
1	BL	2	SER
1	BM	2	SER
1	BN	2	SER
1	BO	2	SER
1	BP	2	SER
1	BQ	2	SER
1	BR	2	SER
1	BS	2	SER
1	BT	2	SER
1	BU	2	SER
1	BV	2	SER
1	BW	2	SER
1	BX	2	SER
1	BY	2	SER
1	BZ	2	SER
1	Ba	2	SER
1	Bb	2	SER
1	Bc	2	SER
1	Bd	2	SER
1	Be	2	SER
1	Bf	2	SER
1	Bg	2	SER
1	Bh	2	SER
1	Bi	2	SER
1	Bj	2	SER
1	Bk	2	SER

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Mol	Chain	Res	Type
1	Bl	2	SER
1	Bm	2	SER
1	Bn	2	SER
1	Bo	2	SER
1	Bp	2	SER
1	Bq	2	SER
1	Br	2	SER
1	Bs	2	SER
1	Bt	2	SER
1	Bu	2	SER
1	Bv	2	SER
1	Bw	2	SER
1	Bx	2	SER

5.3.2 Protein sidechains (i)

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	A0	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	A1	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	A2	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	A3	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	A4	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	A5	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	A6	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	A7	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	A8	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	A9	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	AA	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	AB	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	AC	106/106 (100%)	91 (86%)	15 (14%)	3 16
1	AD	106/106 (100%)	91 (86%)	15 (14%)	3 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AE	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AF	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AG	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AH	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AI	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AJ	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AK	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AL	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AM	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AN	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AO	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AP	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AQ	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AR	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AS	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AT	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AU	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AV	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AW	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AX	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AY	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	AZ	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Aa	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Ab	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Ac	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Ad	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Ae	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Af	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Ag	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Ah	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Ai	106/106 (100%)	91 (86%)	15 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aj	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Ak	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Al	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Am	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	An	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Ao	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Ap	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Aq	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Ar	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	As	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	At	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Au	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Av	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Aw	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	Ax	106/106 (100%)	91 (86%)	15 (14%)	3	16
1	B0	106/106 (100%)	97 (92%)	9 (8%)	10	33
1	B1	106/106 (100%)	97 (92%)	9 (8%)	10	33
1	B2	106/106 (100%)	97 (92%)	9 (8%)	10	33
1	B3	106/106 (100%)	97 (92%)	9 (8%)	10	33
1	B4	106/106 (100%)	96 (91%)	10 (9%)	8	28
1	B5	106/106 (100%)	96 (91%)	10 (9%)	8	28
1	B6	106/106 (100%)	97 (92%)	9 (8%)	10	33
1	B7	106/106 (100%)	97 (92%)	9 (8%)	10	33
1	B8	106/106 (100%)	96 (91%)	10 (9%)	8	28
1	B9	106/106 (100%)	96 (91%)	10 (9%)	8	28
1	BA	106/106 (100%)	97 (92%)	9 (8%)	10	33
1	BB	106/106 (100%)	96 (91%)	10 (9%)	8	28
1	BC	106/106 (100%)	97 (92%)	9 (8%)	10	33
1	BD	106/106 (100%)	97 (92%)	9 (8%)	10	33
1	BE	106/106 (100%)	96 (91%)	10 (9%)	8	28
1	BF	106/106 (100%)	97 (92%)	9 (8%)	10	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	BG	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	BH	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	BI	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	BJ	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	BK	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	BL	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	BM	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	BN	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	BO	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	BP	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	BQ	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	BR	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	BS	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	BT	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	BU	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	BV	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	BW	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	BX	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	BY	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	BZ	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	Ba	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	Bb	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	Bc	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	Bd	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	Be	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	Bf	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	Bg	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	Bh	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	Bi	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	Bj	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	Bk	106/106 (100%)	97 (92%)	9 (8%)	10 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Bl	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	Bm	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	Bn	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	Bo	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	Bp	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	Bq	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	Br	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	Bs	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	Bt	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	Bu	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	Bv	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	Bw	106/106 (100%)	97 (92%)	9 (8%)	10 33
1	Bx	106/106 (100%)	96 (91%)	10 (9%)	8 28
1	C0	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	C1	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	C2	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	C3	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	C4	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	C5	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	C6	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	C7	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	C8	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	C9	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CA	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CB	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CC	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CD	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CE	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CF	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CG	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CH	106/106 (100%)	94 (89%)	12 (11%)	6 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	CI	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CJ	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CK	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CL	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CM	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CN	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CO	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CP	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CQ	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CR	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CS	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CT	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CU	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CV	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CW	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CX	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CY	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	CZ	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Ca	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Cb	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Cc	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Cd	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Ce	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Cf	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Cg	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Ch	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Ci	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Cj	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Ck	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Cl	106/106 (100%)	94 (89%)	12 (11%)	6 21
1	Cm	106/106 (100%)	94 (89%)	12 (11%)	6 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Cn	106/106 (100%)	94 (89%)	12 (11%)	6	21
1	Co	106/106 (100%)	94 (89%)	12 (11%)	6	21
1	Cp	106/106 (100%)	94 (89%)	12 (11%)	6	21
1	Cq	106/106 (100%)	94 (89%)	12 (11%)	6	21
1	Cr	106/106 (100%)	94 (89%)	12 (11%)	6	21
1	Cs	106/106 (100%)	94 (89%)	12 (11%)	6	21
1	Ct	106/106 (100%)	94 (89%)	12 (11%)	6	21
1	Cu	106/106 (100%)	94 (89%)	12 (11%)	6	21
1	Cv	106/106 (100%)	94 (89%)	12 (11%)	6	21
1	Cw	106/106 (100%)	94 (89%)	12 (11%)	6	21
1	Cx	106/106 (100%)	94 (89%)	12 (11%)	6	21
All	All	19080/19080 (100%)	16895 (88%)	2185 (12%)	9	21

All (2185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	2	SER
1	A0	4	PHE
1	A0	6	GLN
1	A0	8	VAL
1	A0	19	THR
1	A0	20	VAL
1	A0	25	PHE
1	A0	33	ILE
1	A0	48	VAL
1	A0	50	GLN
1	A0	52	SER
1	A0	79	VAL
1	A0	109	GLN
1	A0	126	SER
1	A0	128	ILE
1	A1	2	SER
1	A1	4	PHE
1	A1	6	GLN
1	A1	8	VAL
1	A1	19	THR
1	A1	20	VAL
1	A1	25	PHE

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Mol	Chain	Res	Type
1	A1	33	ILE
1	A1	48	VAL
1	A1	50	GLN
1	A1	52	SER
1	A1	79	VAL
1	A1	109	GLN
1	A1	126	SER
1	A1	128	ILE
1	A2	2	SER
1	A2	4	PHE
1	A2	6	GLN
1	A2	8	VAL
1	A2	19	THR
1	A2	20	VAL
1	A2	25	PHE
1	A2	33	ILE
1	A2	48	VAL
1	A2	50	GLN
1	A2	52	SER
1	A2	79	VAL
1	A2	109	GLN
1	A2	126	SER
1	A2	128	ILE
1	A3	2	SER
1	A3	4	PHE
1	A3	6	GLN
1	A3	8	VAL
1	A3	19	THR
1	A3	20	VAL
1	A3	25	PHE
1	A3	33	ILE
1	A3	48	VAL
1	A3	50	GLN
1	A3	52	SER
1	A3	79	VAL
1	A3	109	GLN
1	A3	126	SER
1	A3	128	ILE
1	A4	2	SER
1	A4	4	PHE
1	A4	6	GLN
1	A4	8	VAL

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Mol	Chain	Res	Type
1	A4	19	THR
1	A4	20	VAL
1	A4	25	PHE
1	A4	33	ILE
1	A4	48	VAL
1	A4	50	GLN
1	A4	52	SER
1	A4	79	VAL
1	A4	109	GLN
1	A4	126	SER
1	A4	128	ILE
1	A5	2	SER
1	A5	4	PHE
1	A5	6	GLN
1	A5	8	VAL
1	A5	19	THR
1	A5	20	VAL
1	A5	25	PHE
1	A5	33	ILE
1	A5	48	VAL
1	A5	50	GLN
1	A5	52	SER
1	A5	79	VAL
1	A5	109	GLN
1	A5	126	SER
1	A5	128	ILE
1	A6	2	SER
1	A6	4	PHE
1	A6	6	GLN
1	A6	8	VAL
1	A6	19	THR
1	A6	20	VAL
1	A6	25	PHE
1	A6	33	ILE
1	A6	48	VAL
1	A6	50	GLN
1	A6	52	SER
1	A6	79	VAL
1	A6	109	GLN
1	A6	126	SER
1	A6	128	ILE
1	A7	2	SER

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Mol	Chain	Res	Type
1	A7	4	PHE
1	A7	6	GLN
1	A7	8	VAL
1	A7	19	THR
1	A7	20	VAL
1	A7	25	PHE
1	A7	33	ILE
1	A7	48	VAL
1	A7	50	GLN
1	A7	52	SER
1	A7	79	VAL
1	A7	109	GLN
1	A7	126	SER
1	A7	128	ILE
1	A8	2	SER
1	A8	4	PHE
1	A8	6	GLN
1	A8	8	VAL
1	A8	19	THR
1	A8	20	VAL
1	A8	25	PHE
1	A8	33	ILE
1	A8	48	VAL
1	A8	50	GLN
1	A8	52	SER
1	A8	79	VAL
1	A8	109	GLN
1	A8	126	SER
1	A8	128	ILE
1	A9	2	SER
1	A9	4	PHE
1	A9	6	GLN
1	A9	8	VAL
1	A9	19	THR
1	A9	20	VAL
1	A9	25	PHE
1	A9	33	ILE
1	A9	48	VAL
1	A9	50	GLN
1	A9	52	SER
1	A9	79	VAL
1	A9	109	GLN

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Mol	Chain	Res	Type
1	A9	126	SER
1	A9	128	ILE
1	AA	2	SER
1	AA	4	PHE
1	AA	6	GLN
1	AA	8	VAL
1	AA	19	THR
1	AA	20	VAL
1	AA	25	PHE
1	AA	33	ILE
1	AA	48	VAL
1	AA	50	GLN
1	AA	52	SER
1	AA	79	VAL
1	AA	109	GLN
1	AA	126	SER
1	AA	128	ILE
1	AB	2	SER
1	AB	4	PHE
1	AB	6	GLN
1	AB	8	VAL
1	AB	19	THR
1	AB	20	VAL
1	AB	25	PHE
1	AB	33	ILE
1	AB	48	VAL
1	AB	50	GLN
1	AB	52	SER
1	AB	79	VAL
1	AB	109	GLN
1	AB	126	SER
1	AB	128	ILE
1	AC	2	SER
1	AC	4	PHE
1	AC	6	GLN
1	AC	8	VAL
1	AC	19	THR
1	AC	20	VAL
1	AC	25	PHE
1	AC	33	ILE
1	AC	48	VAL
1	AC	50	GLN

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Mol	Chain	Res	Type
1	AC	52	SER
1	AC	79	VAL
1	AC	109	GLN
1	AC	126	SER
1	AC	128	ILE
1	AD	2	SER
1	AD	4	PHE
1	AD	6	GLN
1	AD	8	VAL
1	AD	19	THR
1	AD	20	VAL
1	AD	25	PHE
1	AD	33	ILE
1	AD	48	VAL
1	AD	50	GLN
1	AD	52	SER
1	AD	79	VAL
1	AD	109	GLN
1	AD	126	SER
1	AD	128	ILE
1	AE	2	SER
1	AE	4	PHE
1	AE	6	GLN
1	AE	8	VAL
1	AE	19	THR
1	AE	20	VAL
1	AE	25	PHE
1	AE	33	ILE
1	AE	48	VAL
1	AE	50	GLN
1	AE	52	SER
1	AE	79	VAL
1	AE	109	GLN
1	AE	126	SER
1	AE	128	ILE
1	AF	2	SER
1	AF	4	PHE
1	AF	6	GLN
1	AF	8	VAL
1	AF	19	THR
1	AF	20	VAL
1	AF	25	PHE

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Mol	Chain	Res	Type
1	AF	33	ILE
1	AF	48	VAL
1	AF	50	GLN
1	AF	52	SER
1	AF	79	VAL
1	AF	109	GLN
1	AF	126	SER
1	AF	128	ILE
1	AG	2	SER
1	AG	4	PHE
1	AG	6	GLN
1	AG	8	VAL
1	AG	19	THR
1	AG	20	VAL
1	AG	25	PHE
1	AG	33	ILE
1	AG	48	VAL
1	AG	50	GLN
1	AG	52	SER
1	AG	79	VAL
1	AG	109	GLN
1	AG	126	SER
1	AG	128	ILE
1	AH	2	SER
1	AH	4	PHE
1	AH	6	GLN
1	AH	8	VAL
1	AH	19	THR
1	AH	20	VAL
1	AH	25	PHE
1	AH	33	ILE
1	AH	48	VAL
1	AH	50	GLN
1	AH	52	SER
1	AH	79	VAL
1	AH	109	GLN
1	AH	126	SER
1	AH	128	ILE
1	AI	2	SER
1	AI	4	PHE
1	AI	6	GLN
1	AI	8	VAL

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Mol	Chain	Res	Type
1	AI	19	THR
1	AI	20	VAL
1	AI	25	PHE
1	AI	33	ILE
1	AI	48	VAL
1	AI	50	GLN
1	AI	52	SER
1	AI	79	VAL
1	AI	109	GLN
1	AI	126	SER
1	AI	128	ILE
1	AJ	2	SER
1	AJ	4	PHE
1	AJ	6	GLN
1	AJ	8	VAL
1	AJ	19	THR
1	AJ	20	VAL
1	AJ	25	PHE
1	AJ	33	ILE
1	AJ	48	VAL
1	AJ	50	GLN
1	AJ	52	SER
1	AJ	79	VAL
1	AJ	109	GLN
1	AJ	126	SER
1	AJ	128	ILE
1	AK	2	SER
1	AK	4	PHE
1	AK	6	GLN
1	AK	8	VAL
1	AK	19	THR
1	AK	20	VAL
1	AK	25	PHE
1	AK	33	ILE
1	AK	48	VAL
1	AK	50	GLN
1	AK	52	SER
1	AK	79	VAL
1	AK	109	GLN
1	AK	126	SER
1	AK	128	ILE
1	AL	2	SER

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Mol	Chain	Res	Type
1	AL	4	PHE
1	AL	6	GLN
1	AL	8	VAL
1	AL	19	THR
1	AL	20	VAL
1	AL	25	PHE
1	AL	33	ILE
1	AL	48	VAL
1	AL	50	GLN
1	AL	52	SER
1	AL	79	VAL
1	AL	109	GLN
1	AL	126	SER
1	AL	128	ILE
1	AM	2	SER
1	AM	4	PHE
1	AM	6	GLN
1	AM	8	VAL
1	AM	19	THR
1	AM	20	VAL
1	AM	25	PHE
1	AM	33	ILE
1	AM	48	VAL
1	AM	50	GLN
1	AM	52	SER
1	AM	79	VAL
1	AM	109	GLN
1	AM	126	SER
1	AM	128	ILE
1	AN	2	SER
1	AN	4	PHE
1	AN	6	GLN
1	AN	8	VAL
1	AN	19	THR
1	AN	20	VAL
1	AN	25	PHE
1	AN	33	ILE
1	AN	48	VAL
1	AN	50	GLN
1	AN	52	SER
1	AN	79	VAL
1	AN	109	GLN

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Mol	Chain	Res	Type
1	AN	126	SER
1	AN	128	ILE
1	AO	2	SER
1	AO	4	PHE
1	AO	6	GLN
1	AO	8	VAL
1	AO	19	THR
1	AO	20	VAL
1	AO	25	PHE
1	AO	33	ILE
1	AO	48	VAL
1	AO	50	GLN
1	AO	52	SER
1	AO	79	VAL
1	AO	109	GLN
1	AO	126	SER
1	AO	128	ILE
1	AP	2	SER
1	AP	4	PHE
1	AP	6	GLN
1	AP	8	VAL
1	AP	19	THR
1	AP	20	VAL
1	AP	25	PHE
1	AP	33	ILE
1	AP	48	VAL
1	AP	50	GLN
1	AP	52	SER
1	AP	79	VAL
1	AP	109	GLN
1	AP	126	SER
1	AP	128	ILE
1	AQ	2	SER
1	AQ	4	PHE
1	AQ	6	GLN
1	AQ	8	VAL
1	AQ	19	THR
1	AQ	20	VAL
1	AQ	25	PHE
1	AQ	33	ILE
1	AQ	48	VAL
1	AQ	50	GLN

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Mol	Chain	Res	Type
1	AQ	52	SER
1	AQ	79	VAL
1	AQ	109	GLN
1	AQ	126	SER
1	AQ	128	ILE
1	AR	2	SER
1	AR	4	PHE
1	AR	6	GLN
1	AR	8	VAL
1	AR	19	THR
1	AR	20	VAL
1	AR	25	PHE
1	AR	33	ILE
1	AR	48	VAL
1	AR	50	GLN
1	AR	52	SER
1	AR	79	VAL
1	AR	109	GLN
1	AR	126	SER
1	AR	128	ILE
1	AS	2	SER
1	AS	4	PHE
1	AS	6	GLN
1	AS	8	VAL
1	AS	19	THR
1	AS	20	VAL
1	AS	25	PHE
1	AS	33	ILE
1	AS	48	VAL
1	AS	50	GLN
1	AS	52	SER
1	AS	79	VAL
1	AS	109	GLN
1	AS	126	SER
1	AS	128	ILE
1	AT	2	SER
1	AT	4	PHE
1	AT	6	GLN
1	AT	8	VAL
1	AT	19	THR
1	AT	20	VAL
1	AT	25	PHE

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Mol	Chain	Res	Type
1	AT	33	ILE
1	AT	48	VAL
1	AT	50	GLN
1	AT	52	SER
1	AT	79	VAL
1	AT	109	GLN
1	AT	126	SER
1	AT	128	ILE
1	AU	2	SER
1	AU	4	PHE
1	AU	6	GLN
1	AU	8	VAL
1	AU	19	THR
1	AU	20	VAL
1	AU	25	PHE
1	AU	33	ILE
1	AU	48	VAL
1	AU	50	GLN
1	AU	52	SER
1	AU	79	VAL
1	AU	109	GLN
1	AU	126	SER
1	AU	128	ILE
1	AV	2	SER
1	AV	4	PHE
1	AV	6	GLN
1	AV	8	VAL
1	AV	19	THR
1	AV	20	VAL
1	AV	25	PHE
1	AV	33	ILE
1	AV	48	VAL
1	AV	50	GLN
1	AV	52	SER
1	AV	79	VAL
1	AV	109	GLN
1	AV	126	SER
1	AV	128	ILE
1	AW	2	SER
1	AW	4	PHE
1	AW	6	GLN
1	AW	8	VAL

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Mol	Chain	Res	Type
1	AW	19	THR
1	AW	20	VAL
1	AW	25	PHE
1	AW	33	ILE
1	AW	48	VAL
1	AW	50	GLN
1	AW	52	SER
1	AW	79	VAL
1	AW	109	GLN
1	AW	126	SER
1	AW	128	ILE
1	AX	2	SER
1	AX	4	PHE
1	AX	6	GLN
1	AX	8	VAL
1	AX	19	THR
1	AX	20	VAL
1	AX	25	PHE
1	AX	33	ILE
1	AX	48	VAL
1	AX	50	GLN
1	AX	52	SER
1	AX	79	VAL
1	AX	109	GLN
1	AX	126	SER
1	AX	128	ILE
1	AY	2	SER
1	AY	4	PHE
1	AY	6	GLN
1	AY	8	VAL
1	AY	19	THR
1	AY	20	VAL
1	AY	25	PHE
1	AY	33	ILE
1	AY	48	VAL
1	AY	50	GLN
1	AY	52	SER
1	AY	79	VAL
1	AY	109	GLN
1	AY	126	SER
1	AY	128	ILE
1	AZ	2	SER

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Mol	Chain	Res	Type
1	AZ	4	PHE
1	AZ	6	GLN
1	AZ	8	VAL
1	AZ	19	THR
1	AZ	20	VAL
1	AZ	25	PHE
1	AZ	33	ILE
1	AZ	48	VAL
1	AZ	50	GLN
1	AZ	52	SER
1	AZ	79	VAL
1	AZ	109	GLN
1	AZ	126	SER
1	AZ	128	ILE
1	Aa	2	SER
1	Aa	4	PHE
1	Aa	6	GLN
1	Aa	8	VAL
1	Aa	19	THR
1	Aa	20	VAL
1	Aa	25	PHE
1	Aa	33	ILE
1	Aa	48	VAL
1	Aa	50	GLN
1	Aa	52	SER
1	Aa	79	VAL
1	Aa	109	GLN
1	Aa	126	SER
1	Aa	128	ILE
1	Ab	2	SER
1	Ab	4	PHE
1	Ab	6	GLN
1	Ab	8	VAL
1	Ab	19	THR
1	Ab	20	VAL
1	Ab	25	PHE
1	Ab	33	ILE
1	Ab	48	VAL
1	Ab	50	GLN
1	Ab	52	SER
1	Ab	79	VAL
1	Ab	109	GLN

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Mol	Chain	Res	Type
1	Ab	126	SER
1	Ab	128	ILE
1	Ac	2	SER
1	Ac	4	PHE
1	Ac	6	GLN
1	Ac	8	VAL
1	Ac	19	THR
1	Ac	20	VAL
1	Ac	25	PHE
1	Ac	33	ILE
1	Ac	48	VAL
1	Ac	50	GLN
1	Ac	52	SER
1	Ac	79	VAL
1	Ac	109	GLN
1	Ac	126	SER
1	Ac	128	ILE
1	Ad	2	SER
1	Ad	4	PHE
1	Ad	6	GLN
1	Ad	8	VAL
1	Ad	19	THR
1	Ad	20	VAL
1	Ad	25	PHE
1	Ad	33	ILE
1	Ad	48	VAL
1	Ad	50	GLN
1	Ad	52	SER
1	Ad	79	VAL
1	Ad	109	GLN
1	Ad	126	SER
1	Ad	128	ILE
1	Ae	2	SER
1	Ae	4	PHE
1	Ae	6	GLN
1	Ae	8	VAL
1	Ae	19	THR
1	Ae	20	VAL
1	Ae	25	PHE
1	Ae	33	ILE
1	Ae	48	VAL
1	Ae	50	GLN

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Mol	Chain	Res	Type
1	Ae	52	SER
1	Ae	79	VAL
1	Ae	109	GLN
1	Ae	126	SER
1	Ae	128	ILE
1	Af	2	SER
1	Af	4	PHE
1	Af	6	GLN
1	Af	8	VAL
1	Af	19	THR
1	Af	20	VAL
1	Af	25	PHE
1	Af	33	ILE
1	Af	48	VAL
1	Af	50	GLN
1	Af	52	SER
1	Af	79	VAL
1	Af	109	GLN
1	Af	126	SER
1	Af	128	ILE
1	Ag	2	SER
1	Ag	4	PHE
1	Ag	6	GLN
1	Ag	8	VAL
1	Ag	19	THR
1	Ag	20	VAL
1	Ag	25	PHE
1	Ag	33	ILE
1	Ag	48	VAL
1	Ag	50	GLN
1	Ag	52	SER
1	Ag	79	VAL
1	Ag	109	GLN
1	Ag	126	SER
1	Ag	128	ILE
1	Ah	2	SER
1	Ah	4	PHE
1	Ah	6	GLN
1	Ah	8	VAL
1	Ah	19	THR
1	Ah	20	VAL
1	Ah	25	PHE

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Mol	Chain	Res	Type
1	Ah	33	ILE
1	Ah	48	VAL
1	Ah	50	GLN
1	Ah	52	SER
1	Ah	79	VAL
1	Ah	109	GLN
1	Ah	126	SER
1	Ah	128	ILE
1	Ai	2	SER
1	Ai	4	PHE
1	Ai	6	GLN
1	Ai	8	VAL
1	Ai	19	THR
1	Ai	20	VAL
1	Ai	25	PHE
1	Ai	33	ILE
1	Ai	48	VAL
1	Ai	50	GLN
1	Ai	52	SER
1	Ai	79	VAL
1	Ai	109	GLN
1	Ai	126	SER
1	Ai	128	ILE
1	Aj	2	SER
1	Aj	4	PHE
1	Aj	6	GLN
1	Aj	8	VAL
1	Aj	19	THR
1	Aj	20	VAL
1	Aj	25	PHE
1	Aj	33	ILE
1	Aj	48	VAL
1	Aj	50	GLN
1	Aj	52	SER
1	Aj	79	VAL
1	Aj	109	GLN
1	Aj	126	SER
1	Aj	128	ILE
1	Ak	2	SER
1	Ak	4	PHE
1	Ak	6	GLN
1	Ak	8	VAL

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Mol	Chain	Res	Type
1	Ak	19	THR
1	Ak	20	VAL
1	Ak	25	PHE
1	Ak	33	ILE
1	Ak	48	VAL
1	Ak	50	GLN
1	Ak	52	SER
1	Ak	79	VAL
1	Ak	109	GLN
1	Ak	126	SER
1	Ak	128	ILE
1	Al	2	SER
1	Al	4	PHE
1	Al	6	GLN
1	Al	8	VAL
1	Al	19	THR
1	Al	20	VAL
1	Al	25	PHE
1	Al	33	ILE
1	Al	48	VAL
1	Al	50	GLN
1	Al	52	SER
1	Al	79	VAL
1	Al	109	GLN
1	Al	126	SER
1	Al	128	ILE
1	Am	2	SER
1	Am	4	PHE
1	Am	6	GLN
1	Am	8	VAL
1	Am	19	THR
1	Am	20	VAL
1	Am	25	PHE
1	Am	33	ILE
1	Am	48	VAL
1	Am	50	GLN
1	Am	52	SER
1	Am	79	VAL
1	Am	109	GLN
1	Am	126	SER
1	Am	128	ILE
1	An	2	SER

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Mol	Chain	Res	Type
1	An	4	PHE
1	An	6	GLN
1	An	8	VAL
1	An	19	THR
1	An	20	VAL
1	An	25	PHE
1	An	33	ILE
1	An	48	VAL
1	An	50	GLN
1	An	52	SER
1	An	79	VAL
1	An	109	GLN
1	An	126	SER
1	An	128	ILE
1	Ao	2	SER
1	Ao	4	PHE
1	Ao	6	GLN
1	Ao	8	VAL
1	Ao	19	THR
1	Ao	20	VAL
1	Ao	25	PHE
1	Ao	33	ILE
1	Ao	48	VAL
1	Ao	50	GLN
1	Ao	52	SER
1	Ao	79	VAL
1	Ao	109	GLN
1	Ao	126	SER
1	Ao	128	ILE
1	Ap	2	SER
1	Ap	4	PHE
1	Ap	6	GLN
1	Ap	8	VAL
1	Ap	19	THR
1	Ap	20	VAL
1	Ap	25	PHE
1	Ap	33	ILE
1	Ap	48	VAL
1	Ap	50	GLN
1	Ap	52	SER
1	Ap	79	VAL
1	Ap	109	GLN

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Mol	Chain	Res	Type
1	Ap	126	SER
1	Ap	128	ILE
1	Aq	2	SER
1	Aq	4	PHE
1	Aq	6	GLN
1	Aq	8	VAL
1	Aq	19	THR
1	Aq	20	VAL
1	Aq	25	PHE
1	Aq	33	ILE
1	Aq	48	VAL
1	Aq	50	GLN
1	Aq	52	SER
1	Aq	79	VAL
1	Aq	109	GLN
1	Aq	126	SER
1	Aq	128	ILE
1	Ar	2	SER
1	Ar	4	PHE
1	Ar	6	GLN
1	Ar	8	VAL
1	Ar	19	THR
1	Ar	20	VAL
1	Ar	25	PHE
1	Ar	33	ILE
1	Ar	48	VAL
1	Ar	50	GLN
1	Ar	52	SER
1	Ar	79	VAL
1	Ar	109	GLN
1	Ar	126	SER
1	Ar	128	ILE
1	As	2	SER
1	As	4	PHE
1	As	6	GLN
1	As	8	VAL
1	As	19	THR
1	As	20	VAL
1	As	25	PHE
1	As	33	ILE
1	As	48	VAL
1	As	50	GLN

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Mol	Chain	Res	Type
1	As	52	SER
1	As	79	VAL
1	As	109	GLN
1	As	126	SER
1	As	128	ILE
1	At	2	SER
1	At	4	PHE
1	At	6	GLN
1	At	8	VAL
1	At	19	THR
1	At	20	VAL
1	At	25	PHE
1	At	33	ILE
1	At	48	VAL
1	At	50	GLN
1	At	52	SER
1	At	79	VAL
1	At	109	GLN
1	At	126	SER
1	At	128	ILE
1	Au	2	SER
1	Au	4	PHE
1	Au	6	GLN
1	Au	8	VAL
1	Au	19	THR
1	Au	20	VAL
1	Au	25	PHE
1	Au	33	ILE
1	Au	48	VAL
1	Au	50	GLN
1	Au	52	SER
1	Au	79	VAL
1	Au	109	GLN
1	Au	126	SER
1	Au	128	ILE
1	Av	2	SER
1	Av	4	PHE
1	Av	6	GLN
1	Av	8	VAL
1	Av	19	THR
1	Av	20	VAL
1	Av	25	PHE

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Mol	Chain	Res	Type
1	Av	33	ILE
1	Av	48	VAL
1	Av	50	GLN
1	Av	52	SER
1	Av	79	VAL
1	Av	109	GLN
1	Av	126	SER
1	Av	128	ILE
1	Aw	2	SER
1	Aw	4	PHE
1	Aw	6	GLN
1	Aw	8	VAL
1	Aw	19	THR
1	Aw	20	VAL
1	Aw	25	PHE
1	Aw	33	ILE
1	Aw	48	VAL
1	Aw	50	GLN
1	Aw	52	SER
1	Aw	79	VAL
1	Aw	109	GLN
1	Aw	126	SER
1	Aw	128	ILE
1	Ax	2	SER
1	Ax	4	PHE
1	Ax	6	GLN
1	Ax	8	VAL
1	Ax	19	THR
1	Ax	20	VAL
1	Ax	25	PHE
1	Ax	33	ILE
1	Ax	48	VAL
1	Ax	50	GLN
1	Ax	52	SER
1	Ax	79	VAL
1	Ax	109	GLN
1	Ax	126	SER
1	Ax	128	ILE
1	B0	20	VAL
1	B0	33	ILE
1	B0	35	SER
1	B0	38	ARG

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Mol	Chain	Res	Type
1	B0	48	VAL
1	B0	54	GLN
1	B0	77	LEU
1	B0	103	LEU
1	B0	109	GLN
1	B1	20	VAL
1	B1	33	ILE
1	B1	35	SER
1	B1	38	ARG
1	B1	48	VAL
1	B1	54	GLN
1	B1	77	LEU
1	B1	103	LEU
1	B1	109	GLN
1	B2	20	VAL
1	B2	33	ILE
1	B2	35	SER
1	B2	38	ARG
1	B2	48	VAL
1	B2	54	GLN
1	B2	77	LEU
1	B2	103	LEU
1	B2	109	GLN
1	B3	20	VAL
1	B3	33	ILE
1	B3	35	SER
1	B3	38	ARG
1	B3	48	VAL
1	B3	54	GLN
1	B3	77	LEU
1	B3	103	LEU
1	B3	109	GLN
1	B4	4	PHE
1	B4	20	VAL
1	B4	33	ILE
1	B4	35	SER
1	B4	38	ARG
1	B4	48	VAL
1	B4	54	GLN
1	B4	77	LEU
1	B4	103	LEU
1	B4	109	GLN

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Mol	Chain	Res	Type
1	B5	4	PHE
1	B5	20	VAL
1	B5	33	ILE
1	B5	35	SER
1	B5	38	ARG
1	B5	48	VAL
1	B5	54	GLN
1	B5	77	LEU
1	B5	103	LEU
1	B5	109	GLN
1	B6	20	VAL
1	B6	33	ILE
1	B6	35	SER
1	B6	38	ARG
1	B6	48	VAL
1	B6	54	GLN
1	B6	77	LEU
1	B6	103	LEU
1	B6	109	GLN
1	B7	20	VAL
1	B7	33	ILE
1	B7	35	SER
1	B7	38	ARG
1	B7	48	VAL
1	B7	54	GLN
1	B7	77	LEU
1	B7	103	LEU
1	B7	109	GLN
1	B8	4	PHE
1	B8	20	VAL
1	B8	33	ILE
1	B8	35	SER
1	B8	38	ARG
1	B8	48	VAL
1	B8	54	GLN
1	B8	77	LEU
1	B8	103	LEU
1	B8	109	GLN
1	B9	4	PHE
1	B9	20	VAL
1	B9	33	ILE
1	B9	35	SER

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Mol	Chain	Res	Type
1	B9	38	ARG
1	B9	48	VAL
1	B9	54	GLN
1	B9	77	LEU
1	B9	103	LEU
1	B9	109	GLN
1	BA	20	VAL
1	BA	33	ILE
1	BA	35	SER
1	BA	38	ARG
1	BA	48	VAL
1	BA	54	GLN
1	BA	77	LEU
1	BA	103	LEU
1	BA	109	GLN
1	BB	4	PHE
1	BB	20	VAL
1	BB	33	ILE
1	BB	35	SER
1	BB	38	ARG
1	BB	48	VAL
1	BB	54	GLN
1	BB	77	LEU
1	BB	103	LEU
1	BB	109	GLN
1	BC	20	VAL
1	BC	33	ILE
1	BC	35	SER
1	BC	38	ARG
1	BC	48	VAL
1	BC	54	GLN
1	BC	77	LEU
1	BC	103	LEU
1	BC	109	GLN
1	BD	20	VAL
1	BD	33	ILE
1	BD	35	SER
1	BD	38	ARG
1	BD	48	VAL
1	BD	54	GLN
1	BD	77	LEU
1	BD	103	LEU

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Mol	Chain	Res	Type
1	BD	109	GLN
1	BE	4	PHE
1	BE	20	VAL
1	BE	33	ILE
1	BE	35	SER
1	BE	38	ARG
1	BE	48	VAL
1	BE	54	GLN
1	BE	77	LEU
1	BE	103	LEU
1	BE	109	GLN
1	BF	20	VAL
1	BF	33	ILE
1	BF	35	SER
1	BF	38	ARG
1	BF	48	VAL
1	BF	54	GLN
1	BF	77	LEU
1	BF	103	LEU
1	BF	109	GLN
1	BG	4	PHE
1	BG	20	VAL
1	BG	33	ILE
1	BG	35	SER
1	BG	38	ARG
1	BG	48	VAL
1	BG	54	GLN
1	BG	77	LEU
1	BG	103	LEU
1	BG	109	GLN
1	BH	20	VAL
1	BH	33	ILE
1	BH	35	SER
1	BH	38	ARG
1	BH	48	VAL
1	BH	54	GLN
1	BH	77	LEU
1	BH	103	LEU
1	BH	109	GLN
1	BI	20	VAL
1	BI	33	ILE
1	BI	35	SER

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Mol	Chain	Res	Type
1	BI	38	ARG
1	BI	48	VAL
1	BI	54	GLN
1	BI	77	LEU
1	BI	103	LEU
1	BI	109	GLN
1	BJ	4	PHE
1	BJ	20	VAL
1	BJ	33	ILE
1	BJ	35	SER
1	BJ	38	ARG
1	BJ	48	VAL
1	BJ	54	GLN
1	BJ	77	LEU
1	BJ	103	LEU
1	BJ	109	GLN
1	BK	20	VAL
1	BK	33	ILE
1	BK	35	SER
1	BK	38	ARG
1	BK	48	VAL
1	BK	54	GLN
1	BK	77	LEU
1	BK	103	LEU
1	BK	109	GLN
1	BL	4	PHE
1	BL	20	VAL
1	BL	33	ILE
1	BL	35	SER
1	BL	38	ARG
1	BL	48	VAL
1	BL	54	GLN
1	BL	77	LEU
1	BL	103	LEU
1	BL	109	GLN
1	BM	20	VAL
1	BM	33	ILE
1	BM	35	SER
1	BM	38	ARG
1	BM	48	VAL
1	BM	54	GLN
1	BM	77	LEU

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Mol	Chain	Res	Type
1	BM	103	LEU
1	BM	109	GLN
1	BN	20	VAL
1	BN	33	ILE
1	BN	35	SER
1	BN	38	ARG
1	BN	48	VAL
1	BN	54	GLN
1	BN	77	LEU
1	BN	103	LEU
1	BN	109	GLN
1	BO	4	PHE
1	BO	20	VAL
1	BO	33	ILE
1	BO	35	SER
1	BO	38	ARG
1	BO	48	VAL
1	BO	54	GLN
1	BO	77	LEU
1	BO	103	LEU
1	BO	109	GLN
1	BP	20	VAL
1	BP	33	ILE
1	BP	35	SER
1	BP	38	ARG
1	BP	48	VAL
1	BP	54	GLN
1	BP	77	LEU
1	BP	103	LEU
1	BP	109	GLN
1	BQ	20	VAL
1	BQ	33	ILE
1	BQ	35	SER
1	BQ	38	ARG
1	BQ	48	VAL
1	BQ	54	GLN
1	BQ	77	LEU
1	BQ	103	LEU
1	BQ	109	GLN
1	BR	20	VAL
1	BR	33	ILE
1	BR	35	SER

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Mol	Chain	Res	Type
1	BR	38	ARG
1	BR	48	VAL
1	BR	54	GLN
1	BR	77	LEU
1	BR	103	LEU
1	BR	109	GLN
1	BS	4	PHE
1	BS	20	VAL
1	BS	33	ILE
1	BS	35	SER
1	BS	38	ARG
1	BS	48	VAL
1	BS	54	GLN
1	BS	77	LEU
1	BS	103	LEU
1	BS	109	GLN
1	BT	20	VAL
1	BT	33	ILE
1	BT	35	SER
1	BT	38	ARG
1	BT	48	VAL
1	BT	54	GLN
1	BT	77	LEU
1	BT	103	LEU
1	BT	109	GLN
1	BU	4	PHE
1	BU	20	VAL
1	BU	33	ILE
1	BU	35	SER
1	BU	38	ARG
1	BU	48	VAL
1	BU	54	GLN
1	BU	77	LEU
1	BU	103	LEU
1	BU	109	GLN
1	BV	20	VAL
1	BV	33	ILE
1	BV	35	SER
1	BV	38	ARG
1	BV	48	VAL
1	BV	54	GLN
1	BV	77	LEU

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Mol	Chain	Res	Type
1	BV	103	LEU
1	BV	109	GLN
1	BW	20	VAL
1	BW	33	ILE
1	BW	35	SER
1	BW	38	ARG
1	BW	48	VAL
1	BW	54	GLN
1	BW	77	LEU
1	BW	103	LEU
1	BW	109	GLN
1	BX	4	PHE
1	BX	20	VAL
1	BX	33	ILE
1	BX	35	SER
1	BX	38	ARG
1	BX	48	VAL
1	BX	54	GLN
1	BX	77	LEU
1	BX	103	LEU
1	BX	109	GLN
1	BY	20	VAL
1	BY	33	ILE
1	BY	35	SER
1	BY	38	ARG
1	BY	48	VAL
1	BY	54	GLN
1	BY	77	LEU
1	BY	103	LEU
1	BY	109	GLN
1	BZ	20	VAL
1	BZ	33	ILE
1	BZ	35	SER
1	BZ	38	ARG
1	BZ	48	VAL
1	BZ	54	GLN
1	BZ	77	LEU
1	BZ	103	LEU
1	BZ	109	GLN
1	Ba	20	VAL
1	Ba	33	ILE
1	Ba	35	SER

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Mol	Chain	Res	Type
1	Ba	38	ARG
1	Ba	48	VAL
1	Ba	54	GLN
1	Ba	77	LEU
1	Ba	103	LEU
1	Ba	109	GLN
1	Bb	4	PHE
1	Bb	20	VAL
1	Bb	33	ILE
1	Bb	35	SER
1	Bb	38	ARG
1	Bb	48	VAL
1	Bb	54	GLN
1	Bb	77	LEU
1	Bb	103	LEU
1	Bb	109	GLN
1	Bc	20	VAL
1	Bc	33	ILE
1	Bc	35	SER
1	Bc	38	ARG
1	Bc	48	VAL
1	Bc	54	GLN
1	Bc	77	LEU
1	Bc	103	LEU
1	Bc	109	GLN
1	Bd	4	PHE
1	Bd	20	VAL
1	Bd	33	ILE
1	Bd	35	SER
1	Bd	38	ARG
1	Bd	48	VAL
1	Bd	54	GLN
1	Bd	77	LEU
1	Bd	103	LEU
1	Bd	109	GLN
1	Be	4	PHE
1	Be	20	VAL
1	Be	33	ILE
1	Be	35	SER
1	Be	38	ARG
1	Be	48	VAL
1	Be	54	GLN

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Mol	Chain	Res	Type
1	Be	77	LEU
1	Be	103	LEU
1	Be	109	GLN
1	Bf	20	VAL
1	Bf	33	ILE
1	Bf	35	SER
1	Bf	38	ARG
1	Bf	48	VAL
1	Bf	54	GLN
1	Bf	77	LEU
1	Bf	103	LEU
1	Bf	109	GLN
1	Bg	4	PHE
1	Bg	20	VAL
1	Bg	33	ILE
1	Bg	35	SER
1	Bg	38	ARG
1	Bg	48	VAL
1	Bg	54	GLN
1	Bg	77	LEU
1	Bg	103	LEU
1	Bg	109	GLN
1	Bh	4	PHE
1	Bh	20	VAL
1	Bh	33	ILE
1	Bh	35	SER
1	Bh	38	ARG
1	Bh	48	VAL
1	Bh	54	GLN
1	Bh	77	LEU
1	Bh	103	LEU
1	Bh	109	GLN
1	Bi	4	PHE
1	Bi	20	VAL
1	Bi	33	ILE
1	Bi	35	SER
1	Bi	38	ARG
1	Bi	48	VAL
1	Bi	54	GLN
1	Bi	77	LEU
1	Bi	103	LEU
1	Bi	109	GLN

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Mol	Chain	Res	Type
1	Bj	4	PHE
1	Bj	20	VAL
1	Bj	33	ILE
1	Bj	35	SER
1	Bj	38	ARG
1	Bj	48	VAL
1	Bj	54	GLN
1	Bj	77	LEU
1	Bj	103	LEU
1	Bj	109	GLN
1	Bk	20	VAL
1	Bk	33	ILE
1	Bk	35	SER
1	Bk	38	ARG
1	Bk	48	VAL
1	Bk	54	GLN
1	Bk	77	LEU
1	Bk	103	LEU
1	Bk	109	GLN
1	Bl	20	VAL
1	Bl	33	ILE
1	Bl	35	SER
1	Bl	38	ARG
1	Bl	48	VAL
1	Bl	54	GLN
1	Bl	77	LEU
1	Bl	103	LEU
1	Bl	109	GLN
1	Bm	4	PHE
1	Bm	20	VAL
1	Bm	33	ILE
1	Bm	35	SER
1	Bm	38	ARG
1	Bm	48	VAL
1	Bm	54	GLN
1	Bm	77	LEU
1	Bm	103	LEU
1	Bm	109	GLN
1	Bn	20	VAL
1	Bn	33	ILE
1	Bn	35	SER
1	Bn	38	ARG

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Mol	Chain	Res	Type
1	Bn	48	VAL
1	Bn	54	GLN
1	Bn	77	LEU
1	Bn	103	LEU
1	Bn	109	GLN
1	Bo	20	VAL
1	Bo	33	ILE
1	Bo	35	SER
1	Bo	38	ARG
1	Bo	48	VAL
1	Bo	54	GLN
1	Bo	77	LEU
1	Bo	103	LEU
1	Bo	109	GLN
1	Bp	20	VAL
1	Bp	33	ILE
1	Bp	35	SER
1	Bp	38	ARG
1	Bp	48	VAL
1	Bp	54	GLN
1	Bp	77	LEU
1	Bp	103	LEU
1	Bp	109	GLN
1	Bq	4	PHE
1	Bq	20	VAL
1	Bq	33	ILE
1	Bq	35	SER
1	Bq	38	ARG
1	Bq	48	VAL
1	Bq	54	GLN
1	Bq	77	LEU
1	Bq	103	LEU
1	Bq	109	GLN
1	Br	4	PHE
1	Br	20	VAL
1	Br	33	ILE
1	Br	35	SER
1	Br	38	ARG
1	Br	48	VAL
1	Br	54	GLN
1	Br	77	LEU
1	Br	103	LEU

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Mol	Chain	Res	Type
1	Br	109	GLN
1	Bs	4	PHE
1	Bs	20	VAL
1	Bs	33	ILE
1	Bs	35	SER
1	Bs	38	ARG
1	Bs	48	VAL
1	Bs	54	GLN
1	Bs	77	LEU
1	Bs	103	LEU
1	Bs	109	GLN
1	Bt	20	VAL
1	Bt	33	ILE
1	Bt	35	SER
1	Bt	38	ARG
1	Bt	48	VAL
1	Bt	54	GLN
1	Bt	77	LEU
1	Bt	103	LEU
1	Bt	109	GLN
1	Bu	20	VAL
1	Bu	33	ILE
1	Bu	35	SER
1	Bu	38	ARG
1	Bu	48	VAL
1	Bu	54	GLN
1	Bu	77	LEU
1	Bu	103	LEU
1	Bu	109	GLN
1	Bv	20	VAL
1	Bv	33	ILE
1	Bv	35	SER
1	Bv	38	ARG
1	Bv	48	VAL
1	Bv	54	GLN
1	Bv	77	LEU
1	Bv	103	LEU
1	Bv	109	GLN
1	Bw	20	VAL
1	Bw	33	ILE
1	Bw	35	SER
1	Bw	38	ARG

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Mol	Chain	Res	Type
1	Bw	48	VAL
1	Bw	54	GLN
1	Bw	77	LEU
1	Bw	103	LEU
1	Bw	109	GLN
1	Bx	4	PHE
1	Bx	20	VAL
1	Bx	33	ILE
1	Bx	35	SER
1	Bx	38	ARG
1	Bx	48	VAL
1	Bx	54	GLN
1	Bx	77	LEU
1	Bx	103	LEU
1	Bx	109	GLN
1	C0	11	ASP
1	C0	20	VAL
1	C0	23	SER
1	C0	37	SER
1	C0	38	ARG
1	C0	49	ARG
1	C0	66	LYS
1	C0	76	GLU
1	C0	84	SER
1	C0	87	ASN
1	C0	109	GLN
1	C0	114	ASP
1	C1	11	ASP
1	C1	20	VAL
1	C1	23	SER
1	C1	37	SER
1	C1	38	ARG
1	C1	49	ARG
1	C1	66	LYS
1	C1	76	GLU
1	C1	84	SER
1	C1	87	ASN
1	C1	109	GLN
1	C1	114	ASP
1	C2	11	ASP
1	C2	20	VAL
1	C2	23	SER

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Mol	Chain	Res	Type
1	C2	37	SER
1	C2	38	ARG
1	C2	49	ARG
1	C2	66	LYS
1	C2	76	GLU
1	C2	84	SER
1	C2	87	ASN
1	C2	109	GLN
1	C2	114	ASP
1	C3	11	ASP
1	C3	20	VAL
1	C3	23	SER
1	C3	37	SER
1	C3	38	ARG
1	C3	49	ARG
1	C3	66	LYS
1	C3	76	GLU
1	C3	84	SER
1	C3	87	ASN
1	C3	109	GLN
1	C3	114	ASP
1	C4	11	ASP
1	C4	20	VAL
1	C4	23	SER
1	C4	37	SER
1	C4	38	ARG
1	C4	49	ARG
1	C4	66	LYS
1	C4	76	GLU
1	C4	84	SER
1	C4	87	ASN
1	C4	109	GLN
1	C4	114	ASP
1	C5	11	ASP
1	C5	20	VAL
1	C5	23	SER
1	C5	37	SER
1	C5	38	ARG
1	C5	49	ARG
1	C5	66	LYS
1	C5	76	GLU
1	C5	84	SER

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Mol	Chain	Res	Type
1	C5	87	ASN
1	C5	109	GLN
1	C5	114	ASP
1	C6	11	ASP
1	C6	20	VAL
1	C6	23	SER
1	C6	37	SER
1	C6	38	ARG
1	C6	49	ARG
1	C6	66	LYS
1	C6	76	GLU
1	C6	84	SER
1	C6	87	ASN
1	C6	109	GLN
1	C6	114	ASP
1	C7	11	ASP
1	C7	20	VAL
1	C7	23	SER
1	C7	37	SER
1	C7	38	ARG
1	C7	49	ARG
1	C7	66	LYS
1	C7	76	GLU
1	C7	84	SER
1	C7	87	ASN
1	C7	109	GLN
1	C7	114	ASP
1	C8	11	ASP
1	C8	20	VAL
1	C8	23	SER
1	C8	37	SER
1	C8	38	ARG
1	C8	49	ARG
1	C8	66	LYS
1	C8	76	GLU
1	C8	84	SER
1	C8	87	ASN
1	C8	109	GLN
1	C8	114	ASP
1	C9	11	ASP
1	C9	20	VAL
1	C9	23	SER

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Mol	Chain	Res	Type
1	C9	37	SER
1	C9	38	ARG
1	C9	49	ARG
1	C9	66	LYS
1	C9	76	GLU
1	C9	84	SER
1	C9	87	ASN
1	C9	109	GLN
1	C9	114	ASP
1	CA	11	ASP
1	CA	20	VAL
1	CA	23	SER
1	CA	37	SER
1	CA	38	ARG
1	CA	49	ARG
1	CA	66	LYS
1	CA	76	GLU
1	CA	84	SER
1	CA	87	ASN
1	CA	109	GLN
1	CA	114	ASP
1	CB	11	ASP
1	CB	20	VAL
1	CB	23	SER
1	CB	37	SER
1	CB	38	ARG
1	CB	49	ARG
1	CB	66	LYS
1	CB	76	GLU
1	CB	84	SER
1	CB	87	ASN
1	CB	109	GLN
1	CB	114	ASP
1	CC	11	ASP
1	CC	20	VAL
1	CC	23	SER
1	CC	37	SER
1	CC	38	ARG
1	CC	49	ARG
1	CC	66	LYS
1	CC	76	GLU
1	CC	84	SER

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Mol	Chain	Res	Type
1	CC	87	ASN
1	CC	109	GLN
1	CC	114	ASP
1	CD	11	ASP
1	CD	20	VAL
1	CD	23	SER
1	CD	37	SER
1	CD	38	ARG
1	CD	49	ARG
1	CD	66	LYS
1	CD	76	GLU
1	CD	84	SER
1	CD	87	ASN
1	CD	109	GLN
1	CD	114	ASP
1	CE	11	ASP
1	CE	20	VAL
1	CE	23	SER
1	CE	37	SER
1	CE	38	ARG
1	CE	49	ARG
1	CE	66	LYS
1	CE	76	GLU
1	CE	84	SER
1	CE	87	ASN
1	CE	109	GLN
1	CE	114	ASP
1	CF	11	ASP
1	CF	20	VAL
1	CF	23	SER
1	CF	37	SER
1	CF	38	ARG
1	CF	49	ARG
1	CF	66	LYS
1	CF	76	GLU
1	CF	84	SER
1	CF	87	ASN
1	CF	109	GLN
1	CF	114	ASP
1	CG	11	ASP
1	CG	20	VAL
1	CG	23	SER

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Mol	Chain	Res	Type
1	CG	37	SER
1	CG	38	ARG
1	CG	49	ARG
1	CG	66	LYS
1	CG	76	GLU
1	CG	84	SER
1	CG	87	ASN
1	CG	109	GLN
1	CG	114	ASP
1	CH	11	ASP
1	CH	20	VAL
1	CH	23	SER
1	CH	37	SER
1	CH	38	ARG
1	CH	49	ARG
1	CH	66	LYS
1	CH	76	GLU
1	CH	84	SER
1	CH	87	ASN
1	CH	109	GLN
1	CH	114	ASP
1	CI	11	ASP
1	CI	20	VAL
1	CI	23	SER
1	CI	37	SER
1	CI	38	ARG
1	CI	49	ARG
1	CI	66	LYS
1	CI	76	GLU
1	CI	84	SER
1	CI	87	ASN
1	CI	109	GLN
1	CI	114	ASP
1	CJ	11	ASP
1	CJ	20	VAL
1	CJ	23	SER
1	CJ	37	SER
1	CJ	38	ARG
1	CJ	49	ARG
1	CJ	66	LYS
1	CJ	76	GLU
1	CJ	84	SER

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Mol	Chain	Res	Type
1	CJ	87	ASN
1	CJ	109	GLN
1	CJ	114	ASP
1	CK	11	ASP
1	CK	20	VAL
1	CK	23	SER
1	CK	37	SER
1	CK	38	ARG
1	CK	49	ARG
1	CK	66	LYS
1	CK	76	GLU
1	CK	84	SER
1	CK	87	ASN
1	CK	109	GLN
1	CK	114	ASP
1	CL	11	ASP
1	CL	20	VAL
1	CL	23	SER
1	CL	37	SER
1	CL	38	ARG
1	CL	49	ARG
1	CL	66	LYS
1	CL	76	GLU
1	CL	84	SER
1	CL	87	ASN
1	CL	109	GLN
1	CL	114	ASP
1	CM	11	ASP
1	CM	20	VAL
1	CM	23	SER
1	CM	37	SER
1	CM	38	ARG
1	CM	49	ARG
1	CM	66	LYS
1	CM	76	GLU
1	CM	84	SER
1	CM	87	ASN
1	CM	109	GLN
1	CM	114	ASP
1	CN	11	ASP
1	CN	20	VAL
1	CN	23	SER

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Mol	Chain	Res	Type
1	CN	37	SER
1	CN	38	ARG
1	CN	49	ARG
1	CN	66	LYS
1	CN	76	GLU
1	CN	84	SER
1	CN	87	ASN
1	CN	109	GLN
1	CN	114	ASP
1	CO	11	ASP
1	CO	20	VAL
1	CO	23	SER
1	CO	37	SER
1	CO	38	ARG
1	CO	49	ARG
1	CO	66	LYS
1	CO	76	GLU
1	CO	84	SER
1	CO	87	ASN
1	CO	109	GLN
1	CO	114	ASP
1	CP	11	ASP
1	CP	20	VAL
1	CP	23	SER
1	CP	37	SER
1	CP	38	ARG
1	CP	49	ARG
1	CP	66	LYS
1	CP	76	GLU
1	CP	84	SER
1	CP	87	ASN
1	CP	109	GLN
1	CP	114	ASP
1	CQ	11	ASP
1	CQ	20	VAL
1	CQ	23	SER
1	CQ	37	SER
1	CQ	38	ARG
1	CQ	49	ARG
1	CQ	66	LYS
1	CQ	76	GLU
1	CQ	84	SER

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Mol	Chain	Res	Type
1	CQ	87	ASN
1	CQ	109	GLN
1	CQ	114	ASP
1	CR	11	ASP
1	CR	20	VAL
1	CR	23	SER
1	CR	37	SER
1	CR	38	ARG
1	CR	49	ARG
1	CR	66	LYS
1	CR	76	GLU
1	CR	84	SER
1	CR	87	ASN
1	CR	109	GLN
1	CR	114	ASP
1	CS	11	ASP
1	CS	20	VAL
1	CS	23	SER
1	CS	37	SER
1	CS	38	ARG
1	CS	49	ARG
1	CS	66	LYS
1	CS	76	GLU
1	CS	84	SER
1	CS	87	ASN
1	CS	109	GLN
1	CS	114	ASP
1	CT	11	ASP
1	CT	20	VAL
1	CT	23	SER
1	CT	37	SER
1	CT	38	ARG
1	CT	49	ARG
1	CT	66	LYS
1	CT	76	GLU
1	CT	84	SER
1	CT	87	ASN
1	CT	109	GLN
1	CT	114	ASP
1	CU	11	ASP
1	CU	20	VAL
1	CU	23	SER

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Mol	Chain	Res	Type
1	CU	37	SER
1	CU	38	ARG
1	CU	49	ARG
1	CU	66	LYS
1	CU	76	GLU
1	CU	84	SER
1	CU	87	ASN
1	CU	109	GLN
1	CU	114	ASP
1	CV	11	ASP
1	CV	20	VAL
1	CV	23	SER
1	CV	37	SER
1	CV	38	ARG
1	CV	49	ARG
1	CV	66	LYS
1	CV	76	GLU
1	CV	84	SER
1	CV	87	ASN
1	CV	109	GLN
1	CV	114	ASP
1	CW	11	ASP
1	CW	20	VAL
1	CW	23	SER
1	CW	37	SER
1	CW	38	ARG
1	CW	49	ARG
1	CW	66	LYS
1	CW	76	GLU
1	CW	84	SER
1	CW	87	ASN
1	CW	109	GLN
1	CW	114	ASP
1	CX	11	ASP
1	CX	20	VAL
1	CX	23	SER
1	CX	37	SER
1	CX	38	ARG
1	CX	49	ARG
1	CX	66	LYS
1	CX	76	GLU
1	CX	84	SER

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Mol	Chain	Res	Type
1	CX	87	ASN
1	CX	109	GLN
1	CX	114	ASP
1	CY	11	ASP
1	CY	20	VAL
1	CY	23	SER
1	CY	37	SER
1	CY	38	ARG
1	CY	49	ARG
1	CY	66	LYS
1	CY	76	GLU
1	CY	84	SER
1	CY	87	ASN
1	CY	109	GLN
1	CY	114	ASP
1	CZ	11	ASP
1	CZ	20	VAL
1	CZ	23	SER
1	CZ	37	SER
1	CZ	38	ARG
1	CZ	49	ARG
1	CZ	66	LYS
1	CZ	76	GLU
1	CZ	84	SER
1	CZ	87	ASN
1	CZ	109	GLN
1	CZ	114	ASP
1	Ca	11	ASP
1	Ca	20	VAL
1	Ca	23	SER
1	Ca	37	SER
1	Ca	38	ARG
1	Ca	49	ARG
1	Ca	66	LYS
1	Ca	76	GLU
1	Ca	84	SER
1	Ca	87	ASN
1	Ca	109	GLN
1	Ca	114	ASP
1	Cb	11	ASP
1	Cb	20	VAL
1	Cb	23	SER

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Mol	Chain	Res	Type
1	Cb	37	SER
1	Cb	38	ARG
1	Cb	49	ARG
1	Cb	66	LYS
1	Cb	76	GLU
1	Cb	84	SER
1	Cb	87	ASN
1	Cb	109	GLN
1	Cb	114	ASP
1	Cc	11	ASP
1	Cc	20	VAL
1	Cc	23	SER
1	Cc	37	SER
1	Cc	38	ARG
1	Cc	49	ARG
1	Cc	66	LYS
1	Cc	76	GLU
1	Cc	84	SER
1	Cc	87	ASN
1	Cc	109	GLN
1	Cc	114	ASP
1	Cd	11	ASP
1	Cd	20	VAL
1	Cd	23	SER
1	Cd	37	SER
1	Cd	38	ARG
1	Cd	49	ARG
1	Cd	66	LYS
1	Cd	76	GLU
1	Cd	84	SER
1	Cd	87	ASN
1	Cd	109	GLN
1	Cd	114	ASP
1	Ce	11	ASP
1	Ce	20	VAL
1	Ce	23	SER
1	Ce	37	SER
1	Ce	38	ARG
1	Ce	49	ARG
1	Ce	66	LYS
1	Ce	76	GLU
1	Ce	84	SER

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Mol	Chain	Res	Type
1	Ce	87	ASN
1	Ce	109	GLN
1	Ce	114	ASP
1	Cf	11	ASP
1	Cf	20	VAL
1	Cf	23	SER
1	Cf	37	SER
1	Cf	38	ARG
1	Cf	49	ARG
1	Cf	66	LYS
1	Cf	76	GLU
1	Cf	84	SER
1	Cf	87	ASN
1	Cf	109	GLN
1	Cf	114	ASP
1	Cg	11	ASP
1	Cg	20	VAL
1	Cg	23	SER
1	Cg	37	SER
1	Cg	38	ARG
1	Cg	49	ARG
1	Cg	66	LYS
1	Cg	76	GLU
1	Cg	84	SER
1	Cg	87	ASN
1	Cg	109	GLN
1	Cg	114	ASP
1	Ch	11	ASP
1	Ch	20	VAL
1	Ch	23	SER
1	Ch	37	SER
1	Ch	38	ARG
1	Ch	49	ARG
1	Ch	66	LYS
1	Ch	76	GLU
1	Ch	84	SER
1	Ch	87	ASN
1	Ch	109	GLN
1	Ch	114	ASP
1	Ci	11	ASP
1	Ci	20	VAL
1	Ci	23	SER

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Mol	Chain	Res	Type
1	Ci	37	SER
1	Ci	38	ARG
1	Ci	49	ARG
1	Ci	66	LYS
1	Ci	76	GLU
1	Ci	84	SER
1	Ci	87	ASN
1	Ci	109	GLN
1	Ci	114	ASP
1	Cj	11	ASP
1	Cj	20	VAL
1	Cj	23	SER
1	Cj	37	SER
1	Cj	38	ARG
1	Cj	49	ARG
1	Cj	66	LYS
1	Cj	76	GLU
1	Cj	84	SER
1	Cj	87	ASN
1	Cj	109	GLN
1	Cj	114	ASP
1	Ck	11	ASP
1	Ck	20	VAL
1	Ck	23	SER
1	Ck	37	SER
1	Ck	38	ARG
1	Ck	49	ARG
1	Ck	66	LYS
1	Ck	76	GLU
1	Ck	84	SER
1	Ck	87	ASN
1	Ck	109	GLN
1	Ck	114	ASP
1	Cl	11	ASP
1	Cl	20	VAL
1	Cl	23	SER
1	Cl	37	SER
1	Cl	38	ARG
1	Cl	49	ARG
1	Cl	66	LYS
1	Cl	76	GLU
1	Cl	84	SER

Continued on next page...

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Mol	Chain	Res	Type
1	Cl	87	ASN
1	Cl	109	GLN
1	Cl	114	ASP
1	Cm	11	ASP
1	Cm	20	VAL
1	Cm	23	SER
1	Cm	37	SER
1	Cm	38	ARG
1	Cm	49	ARG
1	Cm	66	LYS
1	Cm	76	GLU
1	Cm	84	SER
1	Cm	87	ASN
1	Cm	109	GLN
1	Cm	114	ASP
1	Cn	11	ASP
1	Cn	20	VAL
1	Cn	23	SER
1	Cn	37	SER
1	Cn	38	ARG
1	Cn	49	ARG
1	Cn	66	LYS
1	Cn	76	GLU
1	Cn	84	SER
1	Cn	87	ASN
1	Cn	109	GLN
1	Cn	114	ASP
1	Co	11	ASP
1	Co	20	VAL
1	Co	23	SER
1	Co	37	SER
1	Co	38	ARG
1	Co	49	ARG
1	Co	66	LYS
1	Co	76	GLU
1	Co	84	SER
1	Co	87	ASN
1	Co	109	GLN
1	Co	114	ASP
1	Cp	11	ASP
1	Cp	20	VAL
1	Cp	23	SER

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Mol	Chain	Res	Type
1	Cp	37	SER
1	Cp	38	ARG
1	Cp	49	ARG
1	Cp	66	LYS
1	Cp	76	GLU
1	Cp	84	SER
1	Cp	87	ASN
1	Cp	109	GLN
1	Cp	114	ASP
1	Cq	11	ASP
1	Cq	20	VAL
1	Cq	23	SER
1	Cq	37	SER
1	Cq	38	ARG
1	Cq	49	ARG
1	Cq	66	LYS
1	Cq	76	GLU
1	Cq	84	SER
1	Cq	87	ASN
1	Cq	109	GLN
1	Cq	114	ASP
1	Cr	11	ASP
1	Cr	20	VAL
1	Cr	23	SER
1	Cr	37	SER
1	Cr	38	ARG
1	Cr	49	ARG
1	Cr	66	LYS
1	Cr	76	GLU
1	Cr	84	SER
1	Cr	87	ASN
1	Cr	109	GLN
1	Cr	114	ASP
1	Cs	11	ASP
1	Cs	20	VAL
1	Cs	23	SER
1	Cs	37	SER
1	Cs	38	ARG
1	Cs	49	ARG
1	Cs	66	LYS
1	Cs	76	GLU
1	Cs	84	SER

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Mol	Chain	Res	Type
1	Cs	87	ASN
1	Cs	109	GLN
1	Cs	114	ASP
1	Ct	11	ASP
1	Ct	20	VAL
1	Ct	23	SER
1	Ct	37	SER
1	Ct	38	ARG
1	Ct	49	ARG
1	Ct	66	LYS
1	Ct	76	GLU
1	Ct	84	SER
1	Ct	87	ASN
1	Ct	109	GLN
1	Ct	114	ASP
1	Cu	11	ASP
1	Cu	20	VAL
1	Cu	23	SER
1	Cu	37	SER
1	Cu	38	ARG
1	Cu	49	ARG
1	Cu	66	LYS
1	Cu	76	GLU
1	Cu	84	SER
1	Cu	87	ASN
1	Cu	109	GLN
1	Cu	114	ASP
1	Cv	11	ASP
1	Cv	20	VAL
1	Cv	23	SER
1	Cv	37	SER
1	Cv	38	ARG
1	Cv	49	ARG
1	Cv	66	LYS
1	Cv	76	GLU
1	Cv	84	SER
1	Cv	87	ASN
1	Cv	109	GLN
1	Cv	114	ASP
1	Cw	11	ASP
1	Cw	20	VAL
1	Cw	23	SER

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Mol	Chain	Res	Type
1	Cw	37	SER
1	Cw	38	ARG
1	Cw	49	ARG
1	Cw	66	LYS
1	Cw	76	GLU
1	Cw	84	SER
1	Cw	87	ASN
1	Cw	109	GLN
1	Cw	114	ASP
1	Cx	11	ASP
1	Cx	20	VAL
1	Cx	23	SER
1	Cx	37	SER
1	Cx	38	ARG
1	Cx	49	ARG
1	Cx	66	LYS
1	Cx	76	GLU
1	Cx	84	SER
1	Cx	87	ASN
1	Cx	109	GLN
1	Cx	114	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (229) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	40	GLN
1	A0	109	GLN
1	A1	40	GLN
1	A1	109	GLN
1	A2	40	GLN
1	A2	109	GLN
1	A3	40	GLN
1	A3	109	GLN
1	A4	40	GLN
1	A4	109	GLN
1	A5	40	GLN
1	A5	109	GLN
1	A6	40	GLN
1	A6	109	GLN
1	A7	40	GLN
1	A7	109	GLN
1	A8	40	GLN

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Mol	Chain	Res	Type
1	A8	109	GLN
1	A9	40	GLN
1	A9	109	GLN
1	AA	40	GLN
1	AA	109	GLN
1	AB	40	GLN
1	AB	109	GLN
1	AC	40	GLN
1	AC	109	GLN
1	AD	40	GLN
1	AD	109	GLN
1	AE	40	GLN
1	AE	109	GLN
1	AF	40	GLN
1	AG	40	GLN
1	AG	109	GLN
1	AH	40	GLN
1	AI	40	GLN
1	AI	109	GLN
1	AJ	40	GLN
1	AJ	109	GLN
1	AK	40	GLN
1	AL	40	GLN
1	AL	109	GLN
1	AM	40	GLN
1	AM	109	GLN
1	AN	40	GLN
1	AN	109	GLN
1	AO	40	GLN
1	AO	109	GLN
1	AP	40	GLN
1	AP	109	GLN
1	AQ	40	GLN
1	AR	40	GLN
1	AR	109	GLN
1	AS	40	GLN
1	AS	109	GLN
1	AT	40	GLN
1	AT	109	GLN
1	AU	109	GLN
1	AV	40	GLN
1	AV	109	GLN

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Mol	Chain	Res	Type
1	AW	40	GLN
1	AW	109	GLN
1	AX	40	GLN
1	AY	40	GLN
1	AY	109	GLN
1	AZ	40	GLN
1	Aa	40	GLN
1	Aa	109	GLN
1	Ab	40	GLN
1	Ac	40	GLN
1	Ac	109	GLN
1	Ad	40	GLN
1	Ad	109	GLN
1	Ae	40	GLN
1	Ae	109	GLN
1	Af	40	GLN
1	Af	109	GLN
1	Ag	40	GLN
1	Ag	109	GLN
1	Ah	40	GLN
1	Ah	109	GLN
1	Ai	40	GLN
1	Ai	109	GLN
1	Aj	40	GLN
1	Aj	109	GLN
1	Ak	40	GLN
1	Ak	109	GLN
1	Al	40	GLN
1	Al	109	GLN
1	Am	40	GLN
1	Am	109	GLN
1	An	40	GLN
1	An	109	GLN
1	Ao	40	GLN
1	Ap	40	GLN
1	Ap	109	GLN
1	Aq	40	GLN
1	Ar	40	GLN
1	Ar	109	GLN
1	As	40	GLN
1	As	109	GLN
1	At	40	GLN

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Mol	Chain	Res	Type
1	At	109	GLN
1	Au	40	GLN
1	Av	40	GLN
1	Av	109	GLN
1	Aw	40	GLN
1	Aw	109	GLN
1	Ax	40	GLN
1	Ax	109	GLN
1	B0	3	ASN
1	B0	36	ASN
1	B1	3	ASN
1	B1	36	ASN
1	B2	3	ASN
1	B2	36	ASN
1	B3	3	ASN
1	B3	36	ASN
1	B4	3	ASN
1	B4	36	ASN
1	B5	3	ASN
1	B5	36	ASN
1	B6	3	ASN
1	B6	36	ASN
1	B7	3	ASN
1	B7	36	ASN
1	B8	3	ASN
1	B8	36	ASN
1	B9	3	ASN
1	B9	36	ASN
1	BA	3	ASN
1	BA	36	ASN
1	BB	3	ASN
1	BB	36	ASN
1	BC	3	ASN
1	BC	36	ASN
1	BD	3	ASN
1	BD	36	ASN
1	BE	3	ASN
1	BE	36	ASN
1	BF	3	ASN
1	BF	36	ASN
1	BG	3	ASN
1	BG	36	ASN

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Mol	Chain	Res	Type
1	BH	3	ASN
1	BH	36	ASN
1	BI	3	ASN
1	BI	36	ASN
1	BJ	3	ASN
1	BJ	36	ASN
1	BK	3	ASN
1	BK	36	ASN
1	BL	3	ASN
1	BL	36	ASN
1	BM	3	ASN
1	BM	36	ASN
1	BN	3	ASN
1	BN	36	ASN
1	BO	3	ASN
1	BO	36	ASN
1	BP	3	ASN
1	BP	36	ASN
1	BQ	3	ASN
1	BQ	36	ASN
1	BR	3	ASN
1	BR	36	ASN
1	BS	3	ASN
1	BS	36	ASN
1	BT	3	ASN
1	BT	36	ASN
1	BU	3	ASN
1	BU	36	ASN
1	BV	3	ASN
1	BV	36	ASN
1	BW	3	ASN
1	BW	36	ASN
1	BX	3	ASN
1	BX	36	ASN
1	BY	3	ASN
1	BY	36	ASN
1	BZ	3	ASN
1	BZ	36	ASN
1	Ba	3	ASN
1	Ba	36	ASN
1	Bb	3	ASN
1	Bb	36	ASN

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Mol	Chain	Res	Type
1	Bc	3	ASN
1	Bc	36	ASN
1	Bd	3	ASN
1	Bd	36	ASN
1	Be	3	ASN
1	Be	36	ASN
1	Bf	3	ASN
1	Bf	36	ASN
1	Bg	3	ASN
1	Bg	36	ASN
1	Bh	3	ASN
1	Bh	36	ASN
1	Bi	3	ASN
1	Bi	36	ASN
1	Bj	3	ASN
1	Bj	36	ASN
1	Bk	3	ASN
1	Bk	36	ASN
1	Bl	3	ASN
1	Bl	36	ASN
1	Bm	3	ASN
1	Bm	36	ASN
1	Bn	3	ASN
1	Bn	36	ASN
1	Bo	3	ASN
1	Bo	36	ASN
1	Bp	3	ASN
1	Bp	36	ASN
1	Bq	3	ASN
1	Bq	36	ASN
1	Br	3	ASN
1	Br	36	ASN
1	Bs	3	ASN
1	Bs	36	ASN
1	Bt	3	ASN
1	Bt	36	ASN
1	Bu	3	ASN
1	Bu	36	ASN
1	Bv	3	ASN
1	Bv	36	ASN
1	Bw	3	ASN
1	Bw	36	ASN

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Mol	Chain	Res	Type
1	Bx	3	ASN
1	Bx	36	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

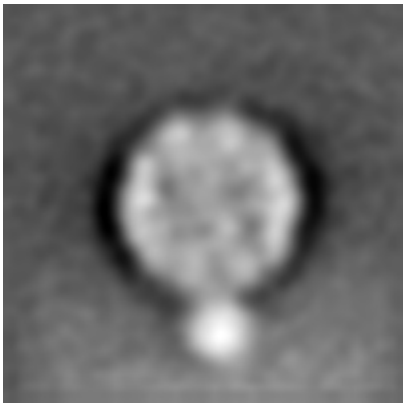
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2365. These allow visual inspection of the internal detail of the map and identification of artifacts.

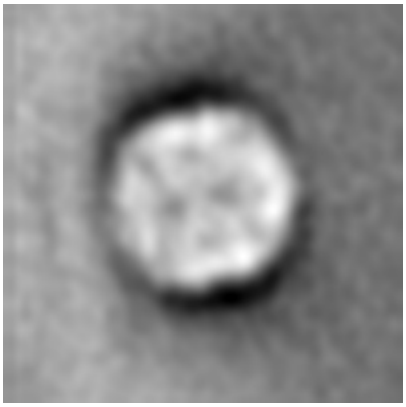
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

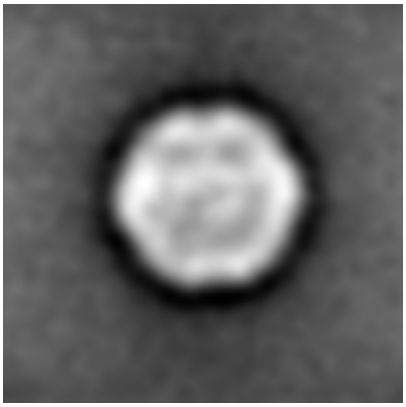
6.1.1 Primary map



X



Y

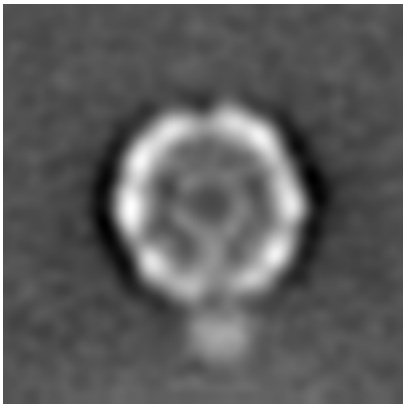


Z

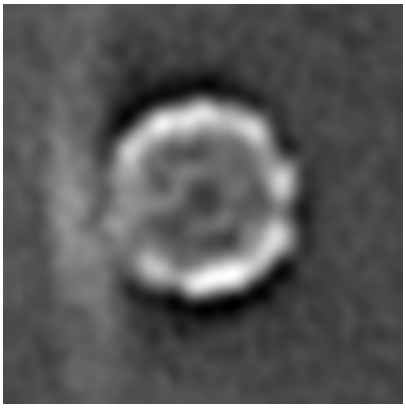
The images above show the map projected in three orthogonal directions.

6.2 Central slices

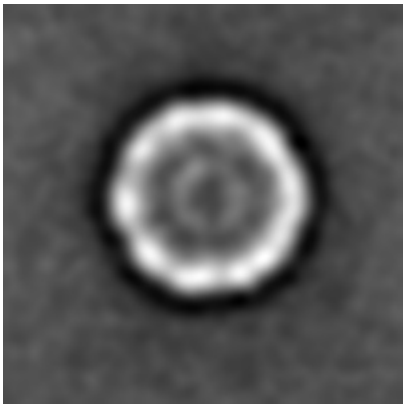
6.2.1 Primary map



X Index: 32



Y Index: 32

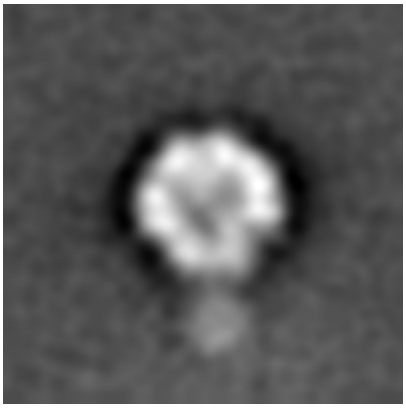


Z Index: 32

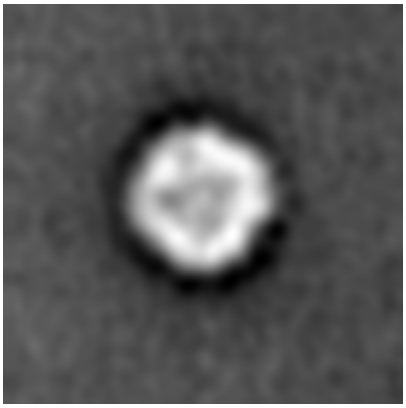
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

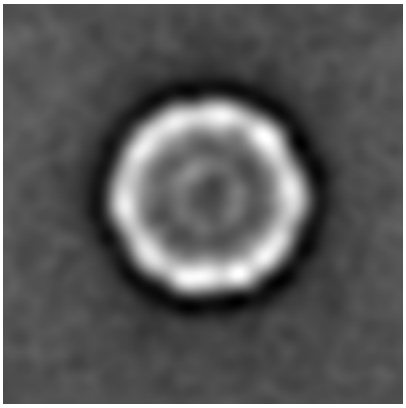
6.3.1 Primary map



X Index: 22



Y Index: 22



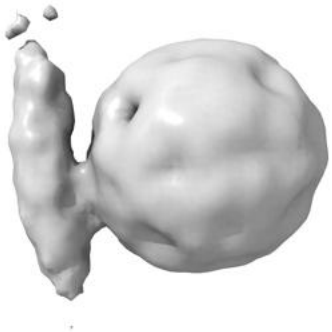
Z Index: 31

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

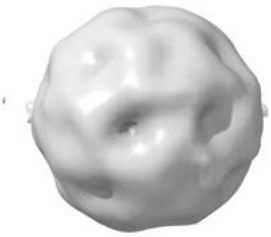
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

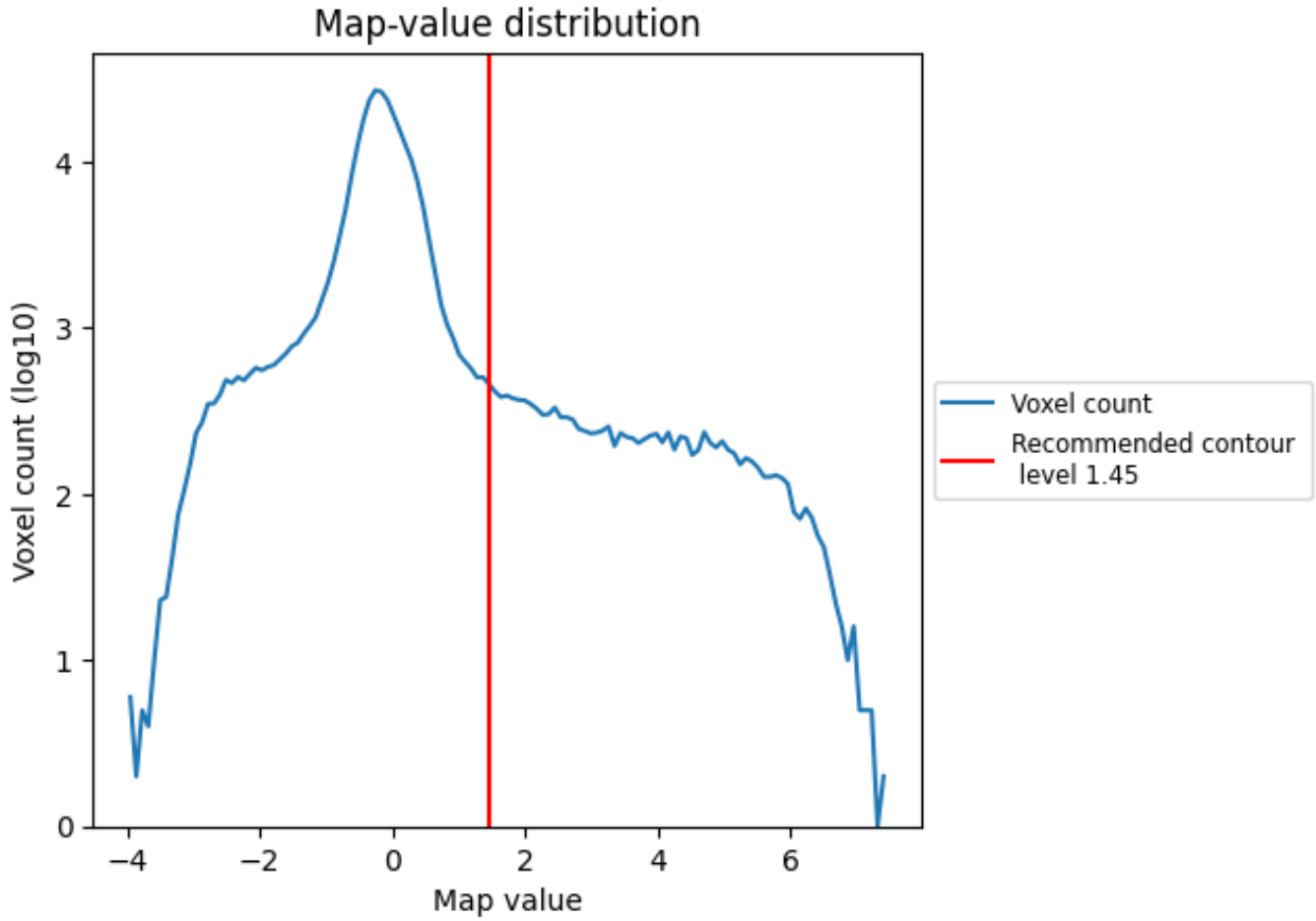
6.5 Mask visualisation (i)

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

7 Map analysis

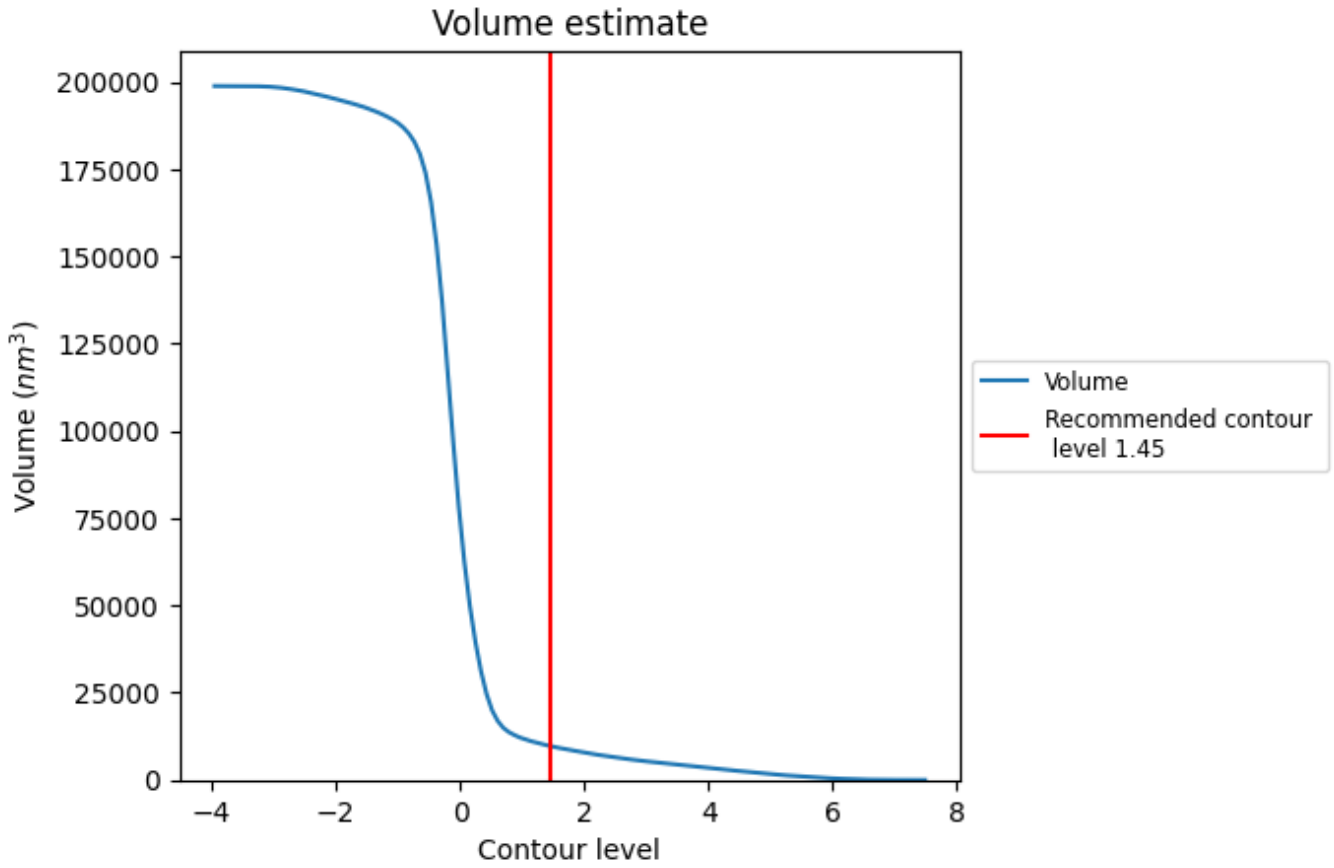
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

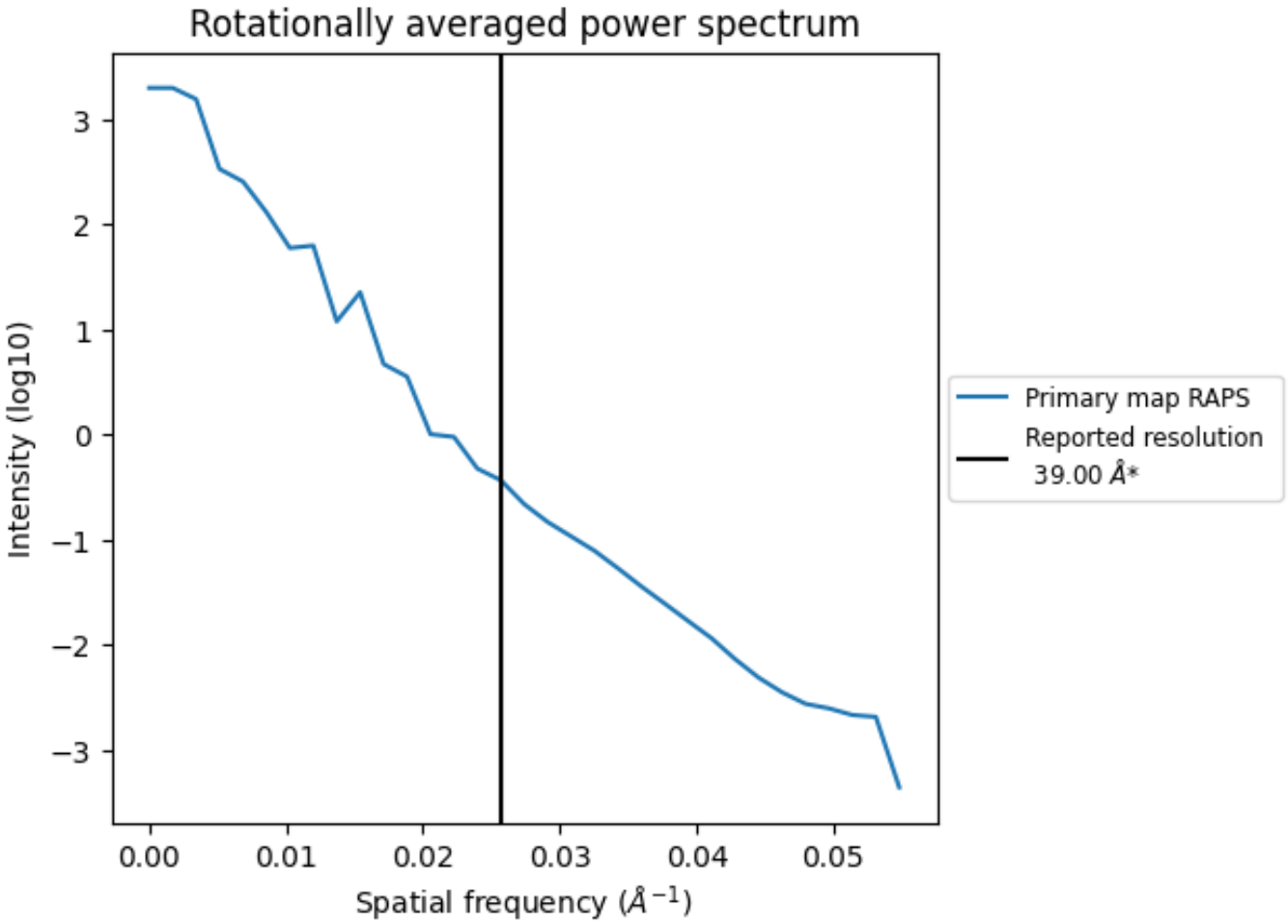
7.2 Volume estimate



The volume at the recommended contour level is 9733 nm^3; this corresponds to an approximate mass of 8792 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.026 Å^{-1}

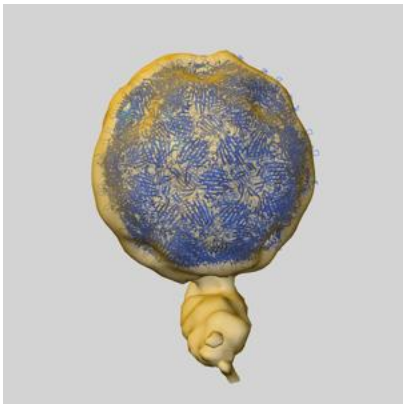
8 Fourier-Shell correlation

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

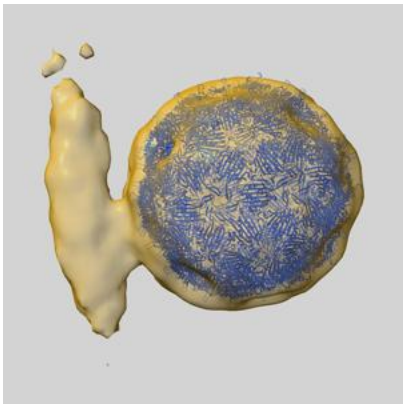
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2365 and PDB model 4BP7. Per-residue inclusion information can be found in section 3 on page 19.

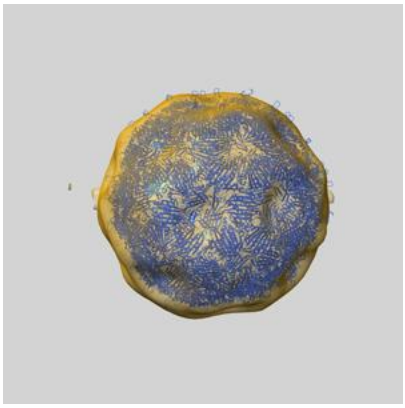
9.1 Map-model overlay



X



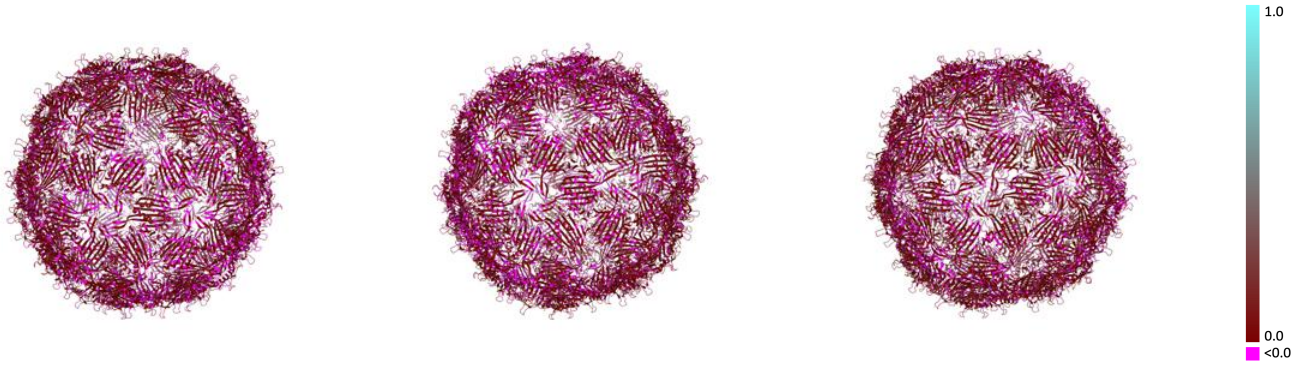
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.45 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.

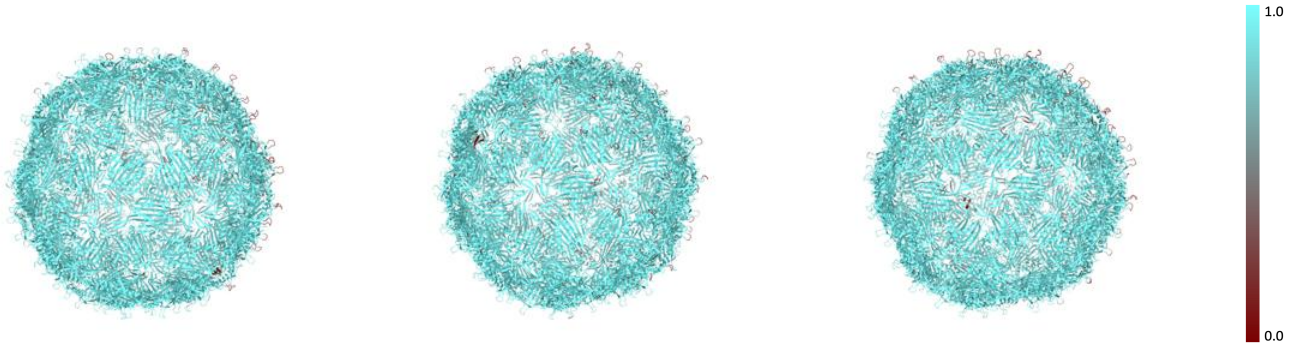
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

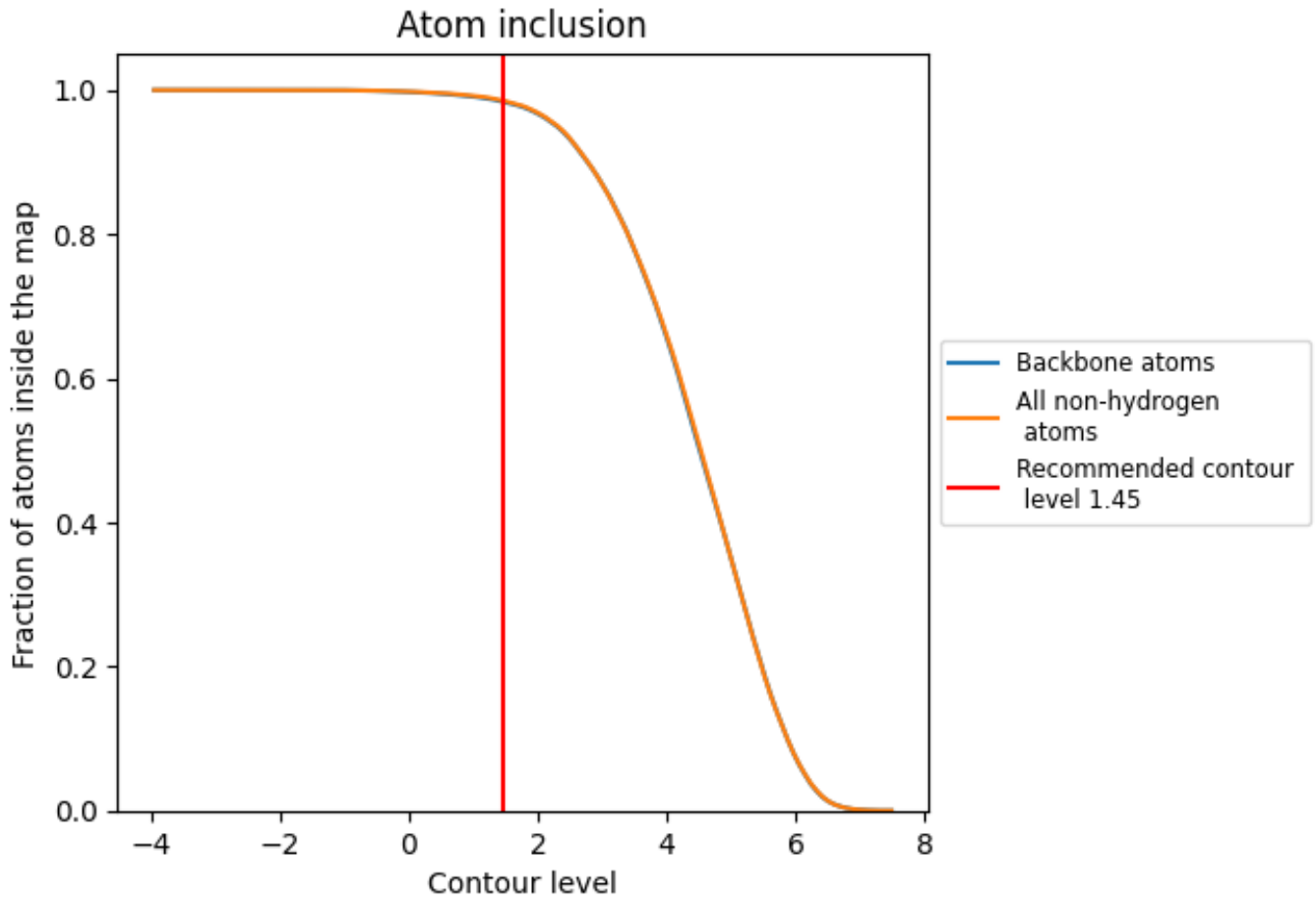
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (1.45).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 99% 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 (1.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9855	0.0430
A0	0.9506	0.0420
A1	0.9527	0.0270
A2	0.9905	0.0460
A3	1.0000	0.0530
A4	1.0000	0.0540
A5	0.9727	0.0270
A6	1.0000	0.0500
A7	0.9968	0.0520
A8	0.9968	0.0400
A9	1.0000	0.0350
AA	0.9958	0.0340
AB	0.9937	0.0460
AC	0.9590	0.0320
AD	0.9464	0.0340
AE	0.9842	0.0600
AF	0.9842	0.0320
AG	1.0000	0.0400
AH	0.9905	0.0480
AI	0.9600	0.0300
AJ	0.9947	0.0520
AK	0.9790	0.0320
AL	0.9264	0.0290
AM	0.9842	0.0480
AN	0.9989	0.0630
AO	0.9569	0.0310
AP	0.9832	0.0510
AQ	0.9989	0.0620
AR	0.9821	0.0440
AS	1.0000	0.0450
AT	0.9958	0.0320
AU	1.0000	0.0460
AV	1.0000	0.0510
AW	1.0000	0.0500
AX	0.9989	0.0260

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Chain	Atom inclusion	Q-score
AY	1.0000	0.0540
AZ	1.0000	0.0400
Aa	1.0000	0.0380
Ab	0.9853	0.0530
Ac	1.0000	0.0580
Ad	0.9832	0.0470
Ae	0.9758	0.0570
Af	1.0000	0.0590
Ag	0.9874	0.0480
Ah	0.9506	0.0340
Ai	0.9811	0.0450
Aj	0.9968	0.0280
Ak	0.9853	0.0420
Al	1.0000	0.0470
Am	0.9674	0.0400
An	1.0000	0.0410
Ao	1.0000	0.0510
Ap	0.9958	0.0310
Aq	0.9979	0.0350
Ar	0.8822	0.0190
As	0.9558	0.0210
At	0.9989	0.0400
Au	0.9569	0.0340
Av	0.9769	0.0320
Aw	0.9621	0.0440
Ax	1.0000	0.0330
B0	0.9968	0.0420
B1	0.9905	0.0290
B2	0.9232	0.0220
B3	0.9569	0.0430
B4	1.0000	0.0470
B5	1.0000	0.0550
B6	1.0000	0.0500
B7	1.0000	0.0330
B8	1.0000	0.0450
B9	1.0000	0.0600
BA	0.9548	0.0170
BB	0.9590	0.0290
BC	0.9800	0.0460
BD	0.9832	0.0560
BE	0.9737	0.0340
BF	0.9895	0.0520

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Chain	Atom inclusion	Q-score
BG	0.9968	0.0490
BH	0.9958	0.0400
BI	0.9874	0.0430
BJ	0.9790	0.0370
BK	0.9443	0.0230
BL	0.9506	0.0300
BM	0.9600	0.0270
BN	0.9800	0.0470
BO	0.9968	0.0660
BP	0.9958	0.0490
BQ	0.9905	0.0480
BR	0.9926	0.0490
BS	0.9884	0.0490
BT	1.0000	0.0570
BU	1.0000	0.0530
BV	1.0000	0.0440
BW	0.9968	0.0450
BX	1.0000	0.0530
BY	1.0000	0.0530
BZ	0.9947	0.0270
Ba	1.0000	0.0430
Bb	0.9968	0.0540
Bc	0.9716	0.0330
Bd	0.9968	0.0530
Be	0.9359	0.0330
Bf	0.9685	0.0520
Bg	0.9758	0.0580
Bh	0.9989	0.0620
Bi	0.9800	0.0540
Bj	0.9779	0.0500
Bk	0.9979	0.0360
Bl	1.0000	0.0470
Bm	1.0000	0.0370
Bn	0.9968	0.0640
Bo	0.9821	0.0380
Bp	1.0000	0.0170
Bq	1.0000	0.0350
Br	0.9968	0.0440
Bs	1.0000	0.0610
Bt	1.0000	0.0570
Bu	0.9926	0.0460
Bv	0.9800	0.0450

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Chain	Atom inclusion	Q-score
Bw	0.9590	0.0350
Bx	0.9874	0.0330
C0	0.9821	0.0380
C1	0.9558	0.0310
C2	0.9548	0.0330
C3	1.0000	0.0610
C4	1.0000	0.0290
C5	1.0000	0.0430
C6	1.0000	0.0330
C7	1.0000	0.0440
C8	1.0000	0.0460
C9	1.0000	0.0670
CA	0.9884	0.0560
CB	0.9811	0.0410
CC	0.9453	0.0270
CD	0.9863	0.0460
CE	0.9989	0.0680
CF	0.9884	0.0410
CG	0.9958	0.0330
CH	1.0000	0.0440
CI	0.9989	0.0500
CJ	0.9621	0.0310
CK	0.9874	0.0350
CL	0.9453	0.0310
CM	0.9653	0.0390
CN	0.9853	0.0420
CO	0.9937	0.0510
CP	0.9926	0.0600
CQ	0.9968	0.0380
CR	1.0000	0.0640
CS	1.0000	0.0610
CT	1.0000	0.0590
CU	1.0000	0.0380
CV	1.0000	0.0470
CW	1.0000	0.0570
CX	1.0000	0.0470
CY	1.0000	0.0620
CZ	1.0000	0.0360
Ca	1.0000	0.0470
Cb	1.0000	0.0400
Cc	1.0000	0.0580
Cd	0.9695	0.0360

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Chain	Atom inclusion	Q-score
Ce	0.9369	0.0320
Cf	0.9537	0.0460
Cg	0.9842	0.0500
Ch	0.9811	0.0550
Ci	0.9853	0.0510
Cj	1.0000	0.0410
Ck	1.0000	0.0540
Cl	1.0000	0.0320
Cm	1.0000	0.0400
Cn	1.0000	0.0590
Co	1.0000	0.0490
Cp	0.9495	0.0180
Cq	0.9811	0.0400
Cr	1.0000	0.0040
Cs	0.9926	0.0550
Ct	0.9716	0.0060
Cu	0.9832	0.0340
Cv	0.9558	0.0260
Cw	0.9842	0.0380
Cx	0.9916	0.0400