Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 01:33 pm GMT

PDB ID	:	4CTG
EMDB ID	:	EMD-2390
Title	:	The limits of structural plasticity in a picornavirus capsid revealed by a massively expanded equine rhinitis A virus particle
Authors	:	Bakker, S.E.; Groppelli, E.; Pearson, A.R.; Stockley, P.G.; Rowlands, D.J.; Ranson, N.A.
Deposited on	:	2014-03-13
Resolution	:	17.00 Å(reported)
Based on initial model	:	2WFF

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:

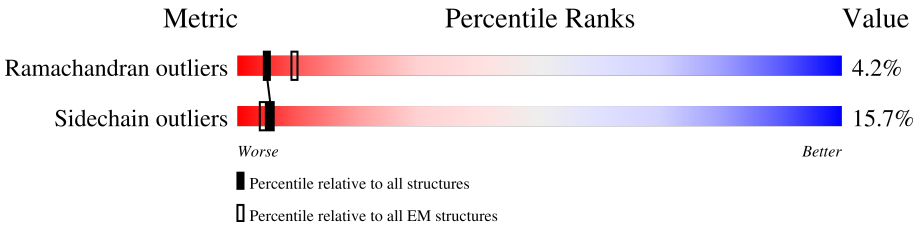
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 17.00 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	246	10% 82% 15% ·
1	A1	246	9% 82% 15% ·
1	A2	246	9% 82% 15% ·
1	A3	246	11% 82% 15% ·
1	A4	246	9% 82% 15% ·
1	A5	246	9% 82% 15% ·
1	A6	246	9% 82% 15% ·
1	A7	246	9% 82% 15% · ·
1	A8	246	11% 82% 15% ·

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Mol	Chain	Length	Quality of chain
1	A9	246	10% 82% 15%
1	AA	246	8% 82% 15%
1	AB	246	8% 82% 15%
1	AC	246	9% 82% 15%
1	AD	246	10% 82% 15%
1	AE	246	8% 82% 15%
1	AF	246	11% 82% 15%
1	AG	246	9% 82% 15%
1	AH	246	12% 82% 15%
1	AI	246	12% 82% 15%
1	AJ	246	9% 82% 15%
1	AK	246	8% 82% 15%
1	AL	246	10% 82% 15%
1	AM	246	10% 82% 15%
1	AN	246	6% 82% 15%
1	AO	246	9% 82% 15%
1	AP	246	7% 82% 15%
1	AQ	246	10% 82% 15%
1	AR	246	10% 82% 15%
1	AS	246	8% 82% 15%
1	AT	246	11% 82% 15%
1	AU	246	10% 82% 15%
1	AV	246	13% 82% 15%
1	AW	246	11% 81% 15%
1	AX	246	13% 82% 15%

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Mol	Chain	Length	Quality of chain
1	AY	246	8% 82% 15%
1	AZ	246	9% 82% 15%
1	Aa	246	13% 82% 15%
1	Ab	246	13% 82% 15%
1	Ac	246	12% 82% 15%
1	Ad	246	9% 82% 15%
1	Ae	246	7% 81% 15%
1	Af	246	11% 82% 15%
1	Ag	246	9% 82% 15%
1	Ah	246	8% 82% 15%
1	Ai	246	8% 82% 15%
1	Aj	246	7% 82% 15%
1	Ak	246	11% 82% 15%
1	Al	246	9% 82% 15%
1	Am	246	11% 82% 15%
1	An	246	12% 82% 15%
1	Ao	246	10% 82% 15%
1	DC	246	11% 82% 15%
1	DD	246	13% 82% 15%
1	DE	246	9% 82% 15%
1	DF	246	8% 82% 15%
1	DG	246	9% 81% 15%
1	DH	246	8% 82% 15%
1	DI	246	7% 82% 15%
1	DJ	246	9% 82% 15%

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Mol	Chain	Length	Quality of chain
1	DK	246	9% 82% 15%
2	B0	200	8% 81% 17%
2	B1	200	8% 81% 17%
2	B2	200	7% 81% 17%
2	B3	200	11% 81% 17%
2	B4	200	8% 81% 16%
2	B5	200	10% 81% 17%
2	B6	200	8% 81% 16%
2	B7	200	8% 81% 17%
2	B8	200	5% 81% 17%
2	B9	200	5% 81% 17%
2	BA	200	6% 81% 16%
2	BB	200	8% 81% 16%
2	BC	200	9% 81% 17%
2	BD	200	6% 81% 16%
2	BE	200	10% 81% 16%
2	BF	200	6% 81% 16%
2	BG	200	6% 81% 17%
2	BH	200	6% 81% 17%
2	BI	200	81% 16%
2	BJ	200	6% 81% 16%
2	BK	200	6% 81% 17%
2	BL	200	6% 81% 17%
2	BM	200	10% 81% 17%
2	BN	200	6% 81% 16%

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Mol	Chain	Length	Quality of chain
2	BO	200	6% 81% 17%
2	BP	200	8% 81% 17%
2	BQ	200	6% 81% 16%
2	BR	200	7% 81% 17%
2	BS	200	6% 81% 17%
2	BT	200	6% 81% 16%
2	BU	200	5% 81% 17%
2	BV	200	6% 81% 17%
2	BW	200	6% 81% 17%
2	BX	200	5% 81% 17%
2	BY	200	7% 81% 17%
2	BZ	200	6% 81% 17%
2	Ba	200	6% 81% 17%
2	Bb	200	6% 81% 16%
2	Bc	200	6% 81% 17%
2	Bd	200	6% 81% 17%
2	Be	200	6% 81% 16%
2	Bf	200	8% 81% 17%
2	Bg	200	6% 81% 17%
2	Bh	200	7% 81% 17%
2	Bi	200	6% 81% 17%
2	Bj	200	6% 81% 16%
2	Bk	200	81% 17%
2	Bl	200	6% 81% 16%
2	Bm	200	7% 81% 17%

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Mol	Chain	Length	Quality of chain
2	Bn	200	81% 17%
2	Bo	200	6% 81% 17%
2	Bp	200	7% 81% 17%
2	Bq	200	6% 81% 16%
2	Br	200	6% 81% 17%
2	Bs	200	9% 81% 16%
2	Bt	200	9% 81% 17%
2	Bu	200	6% 81% 17%
2	Bv	200	6% 81% 17%
2	Bw	200	6% 81% 17%
2	Bx	200	7% 81% 17%
3	C0	226	14% 80% 16%
3	C1	226	14% 80% 16%
3	C2	226	13% 80% 16%
3	C3	226	13% 80% 16%
3	C4	226	13% 80% 16%
3	C5	226	15% 80% 16%
3	C6	226	14% 80% 16%
3	C7	226	14% 80% 16%
3	C8	226	15% 80% 16%
3	C9	226	11% 80% 16%
3	CA	226	13% 80% 16%
3	CB	226	14% 80% 16%
3	CC	226	12% 80% 16%
3	CD	226	13% 80% 16%

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Mol	Chain	Length	Quality of chain
3	CE	226	13% 80% 16%
3	CF	226	9% 80% 16%
3	CG	226	12% 80% 16%
3	CH	226	12% 80% 16%
3	CI	226	10% 80% 16%
3	CJ	226	13% 80% 16%
3	CK	226	11% 80% 16%
3	CL	226	12% 80% 16%
3	CM	226	11% 80% 16%
3	CN	226	10% 80% 16%
3	CO	226	12% 80% 16%
3	CP	226	10% 80% 16%
3	CQ	226	12% 80% 16%
3	CR	226	10% 80% 16%
3	CS	226	9% 80% 16%
3	CT	226	14% 80% 16%
3	CU	226	10% 80% 16%
3	CV	226	13% 80% 16%
3	CW	226	11% 80% 16%
3	CX	226	10% 80% 16%
3	CY	226	13% 80% 16%
3	CZ	226	15% 80% 16%
3	Cc	226	12% 80% 16%
3	Cd	226	14% 80% 16%
3	Ce	226	12% 80% 16%

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Mol	Chain	Length	Quality of chain
3	Cf	226	12% 80% 16%
3	Cg	226	11% 80% 16%
3	Ch	226	10% 80% 16%
3	Ci	226	14% 80% 16%
3	Cj	226	11% 80% 16%
3	Ck	226	13% 80% 16%
3	Cl	226	10% 80% 16%
3	Cm	226	10% 80% 16%
3	Cn	226	12% 80% 16%
3	Co	226	9% 80% 16%
3	Cp	226	12% 80% 16%
3	Cq	226	12% 80% 16%
3	Cr	226	10% 80% 16%
3	Cs	226	13% 80% 16%
3	Ct	226	12% 80% 16%
3	Cu	226	12% 80% 16%
3	Cv	226	13% 80% 16%
3	Cw	226	13% 80% 16%
3	Cx	226	13% 80% 16%
3	DA	226	12% 80% 16%
3	DB	226	12% 80% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 311940 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 P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AB	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AC	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AD	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AE	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AF	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AG	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AH	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AI	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AJ	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AK	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AL	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AM	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AN	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AO	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AP	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AQ	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AR	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AS	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AT	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AU	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AV	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AW	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AX	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AY	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	AZ	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	A0	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	A1	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	A2	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	A3	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	A4	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	A5	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	A6	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	A7	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	A8	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	A9	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Aa	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Ab	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ac	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Ad	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Ae	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Af	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Ag	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Ah	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Ai	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Aj	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Ak	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Al	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Am	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	An	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	Ao	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	DC	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	DD	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	DE	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	DF	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	DG	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	DH	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	DI	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		
1	DJ	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DK	246	Total	C	N	O	S	0	0
			1928	1240	329	351	8		

- Molecule 2 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BB	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BC	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BD	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BE	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BF	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BG	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BH	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BI	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BJ	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BK	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BL	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BM	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BN	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BR	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BO	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BS	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BP	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	BQ	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BT	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BU	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BV	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BW	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BX	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BY	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	BZ	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B0	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B1	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B2	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B3	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B4	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B5	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B6	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B7	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B8	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	B9	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Ba	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bb	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bc	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bd	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Be	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bf	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bg	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bh	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bi	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bj	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bk	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bl	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bm	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bn	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bo	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bp	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bq	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Br	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bs	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bt	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bu	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bv	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bw	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		
2	Bx	200	Total	C	N	O	S	0	0
			1553	997	266	283	7		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	85	SER	GLY	conflict	UNP Q91B42
B1	85	SER	GLY	conflict	UNP Q91B42
B2	85	SER	GLY	conflict	UNP Q91B42
B3	85	SER	GLY	conflict	UNP Q91B42
B4	85	SER	GLY	conflict	UNP Q91B42
B5	85	SER	GLY	conflict	UNP Q91B42
B6	85	SER	GLY	conflict	UNP Q91B42
B7	85	SER	GLY	conflict	UNP Q91B42
B8	85	SER	GLY	conflict	UNP Q91B42
B9	85	SER	GLY	conflict	UNP Q91B42
BA	85	SER	GLY	conflict	UNP Q91B42
BB	85	SER	GLY	conflict	UNP Q91B42
BC	85	SER	GLY	conflict	UNP Q91B42
BD	85	SER	GLY	conflict	UNP Q91B42
BE	85	SER	GLY	conflict	UNP Q91B42
BF	85	SER	GLY	conflict	UNP Q91B42
BG	85	SER	GLY	conflict	UNP Q91B42
BH	85	SER	GLY	conflict	UNP Q91B42
BI	85	SER	GLY	conflict	UNP Q91B42
BJ	85	SER	GLY	conflict	UNP Q91B42
BK	85	SER	GLY	conflict	UNP Q91B42
BL	85	SER	GLY	conflict	UNP Q91B42
BM	85	SER	GLY	conflict	UNP Q91B42
BN	85	SER	GLY	conflict	UNP Q91B42
BO	85	SER	GLY	conflict	UNP Q91B42
BP	85	SER	GLY	conflict	UNP Q91B42
BQ	85	SER	GLY	conflict	UNP Q91B42
BR	85	SER	GLY	conflict	UNP Q91B42
BS	85	SER	GLY	conflict	UNP Q91B42
BT	85	SER	GLY	conflict	UNP Q91B42
BU	85	SER	GLY	conflict	UNP Q91B42
BV	85	SER	GLY	conflict	UNP Q91B42
BW	85	SER	GLY	conflict	UNP Q91B42
BX	85	SER	GLY	conflict	UNP Q91B42
BY	85	SER	GLY	conflict	UNP Q91B42
BZ	85	SER	GLY	conflict	UNP Q91B42
Ba	85	SER	GLY	conflict	UNP Q91B42
Bb	85	SER	GLY	conflict	UNP Q91B42
Bc	85	SER	GLY	conflict	UNP Q91B42
Bd	85	SER	GLY	conflict	UNP Q91B42
Be	85	SER	GLY	conflict	UNP Q91B42
Bf	85	SER	GLY	conflict	UNP Q91B42

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Chain	Residue	Modelled	Actual	Comment	Reference
Bg	85	SER	GLY	conflict	UNP Q91B42
Bh	85	SER	GLY	conflict	UNP Q91B42
Bi	85	SER	GLY	conflict	UNP Q91B42
Bj	85	SER	GLY	conflict	UNP Q91B42
Bk	85	SER	GLY	conflict	UNP Q91B42
Bl	85	SER	GLY	conflict	UNP Q91B42
Bm	85	SER	GLY	conflict	UNP Q91B42
Bn	85	SER	GLY	conflict	UNP Q91B42
Bo	85	SER	GLY	conflict	UNP Q91B42
Bp	85	SER	GLY	conflict	UNP Q91B42
Bq	85	SER	GLY	conflict	UNP Q91B42
Br	85	SER	GLY	conflict	UNP Q91B42
Bs	85	SER	GLY	conflict	UNP Q91B42
Bt	85	SER	GLY	conflict	UNP Q91B42
Bu	85	SER	GLY	conflict	UNP Q91B42
Bv	85	SER	GLY	conflict	UNP Q91B42
Bw	85	SER	GLY	conflict	UNP Q91B42
Bx	85	SER	GLY	conflict	UNP Q91B42

- Molecule 3 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CA	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CB	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CC	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CD	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CE	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CF	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CG	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CH	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CI	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CJ	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	CK	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CL	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CM	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CN	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CO	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CP	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CQ	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CR	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CS	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CT	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CU	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CV	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CW	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CX	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CY	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	CZ	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C0	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C1	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C2	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C3	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C4	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	C5	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C6	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C7	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C8	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	C9	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cc	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cd	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Ce	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cf	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cg	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Ch	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Ci	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cj	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Ck	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cl	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cm	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cn	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Co	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cp	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cq	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cr	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		

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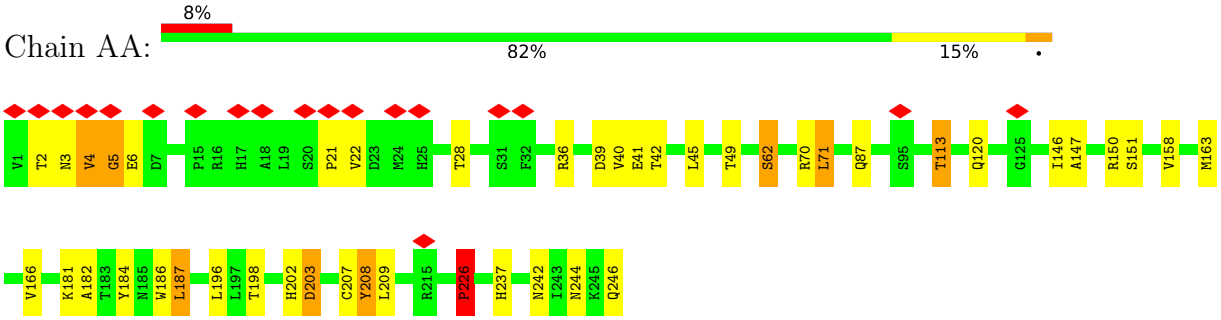
Mol	Chain	Residues	Atoms					AltConf	Trace
3	Cs	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Ct	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cu	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cv	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cw	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	Cx	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	DA	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		
3	DB	226	Total	C	N	O	S	0	0
			1718	1107	280	325	6		

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.

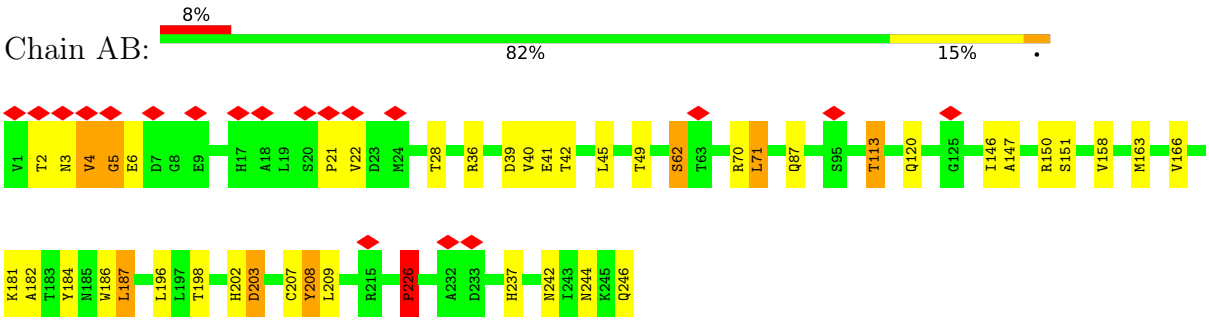
• Molecule 1: P1

Chain AA:



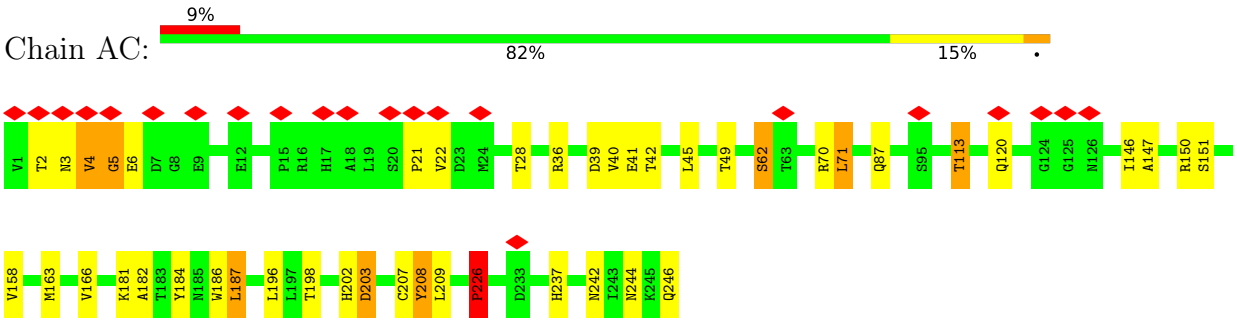
• Molecule 1: P1

Chain AB:



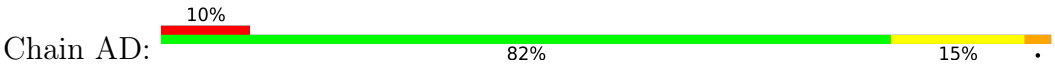
• Molecule 1: P1

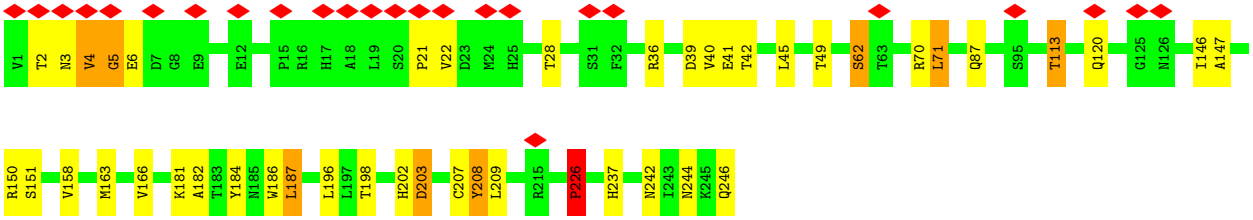
Chain AC:



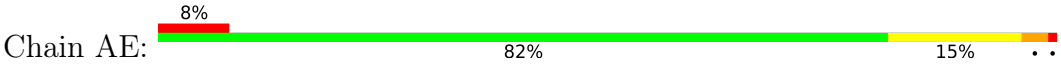
• Molecule 1: P1

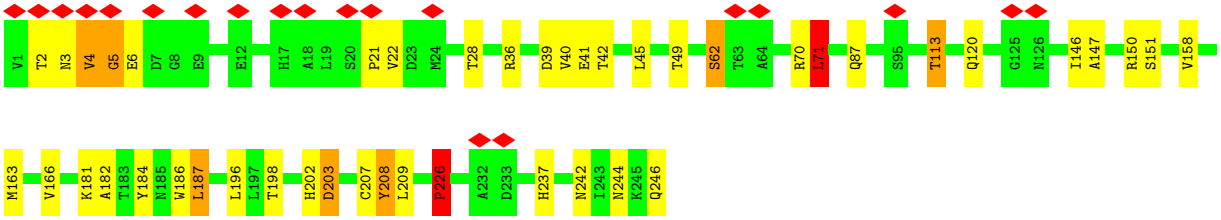
Chain AD:



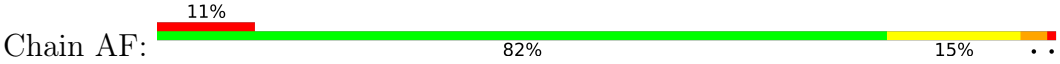


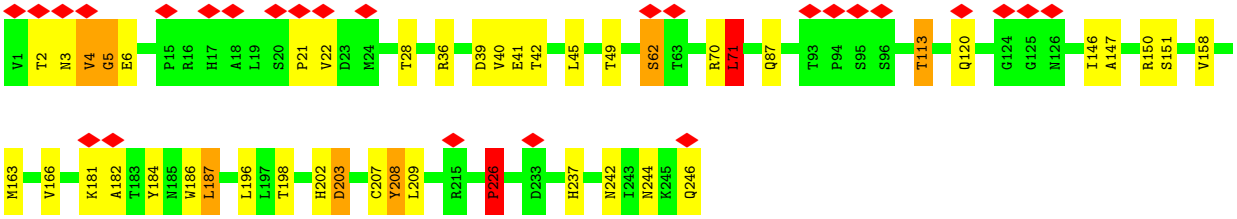
• Molecule 1: P1



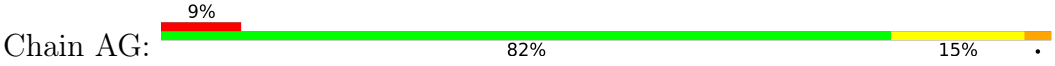


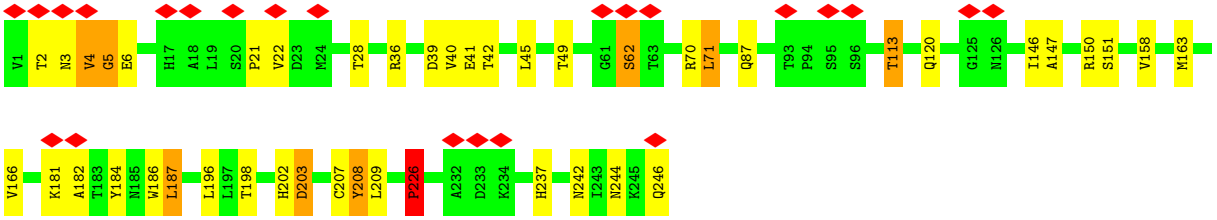
• Molecule 1: P1



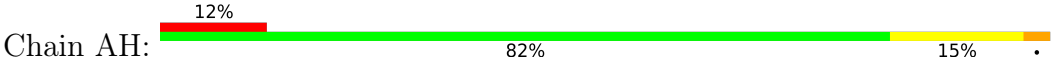


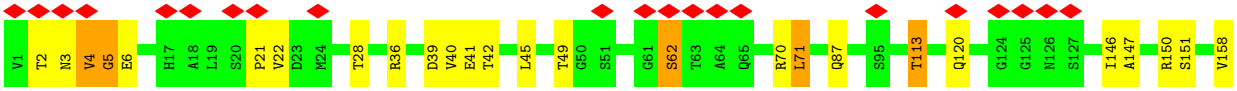
• Molecule 1: P1

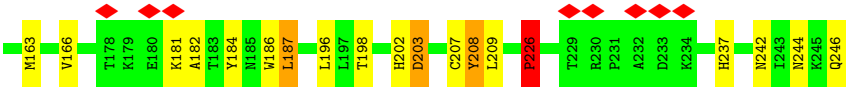




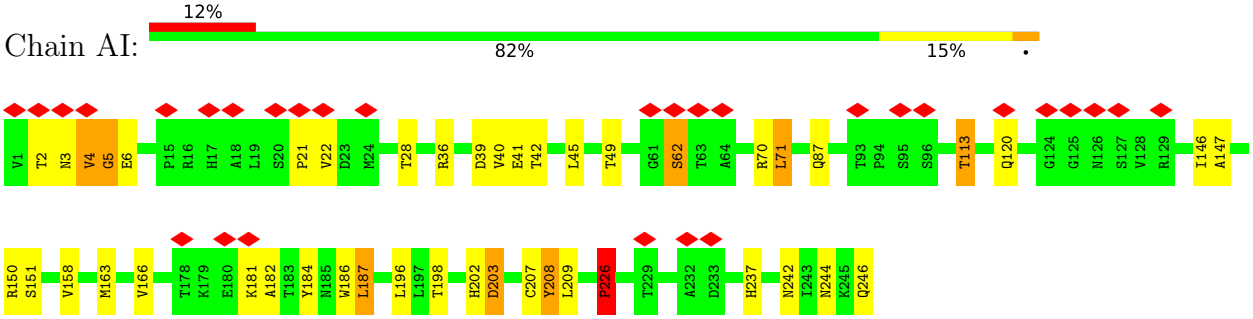
• Molecule 1: P1



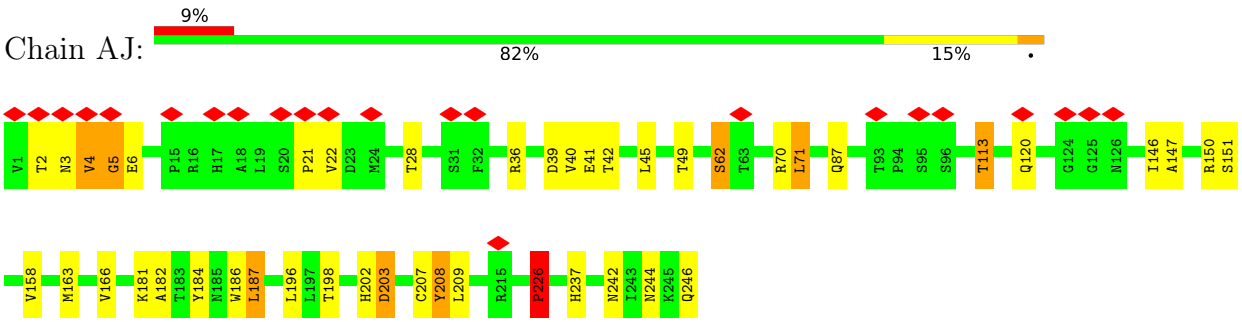




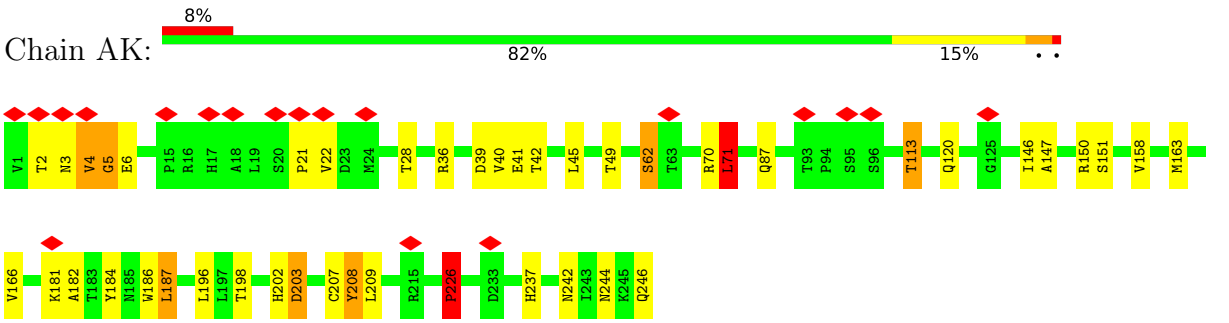
• Molecule 1: P1



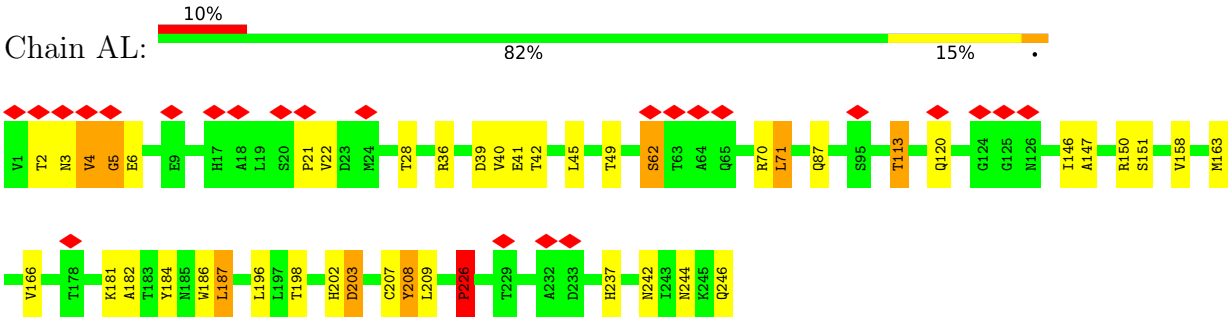
• Molecule 1: P1



• Molecule 1: P1

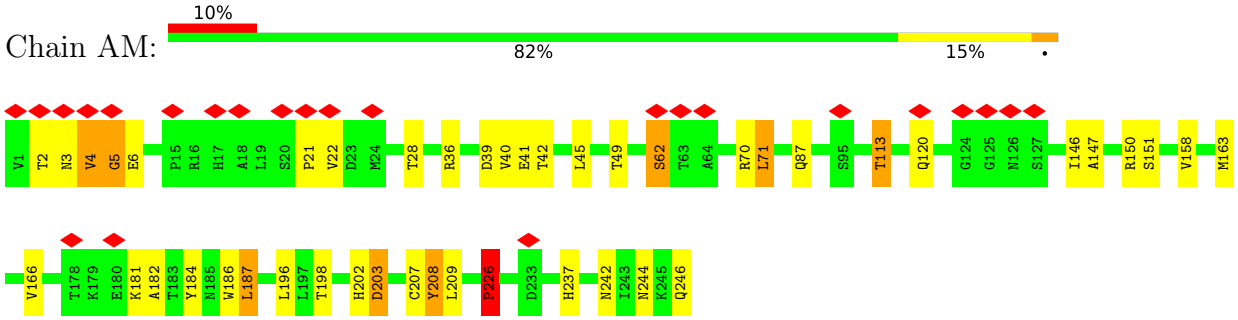


• Molecule 1: P1



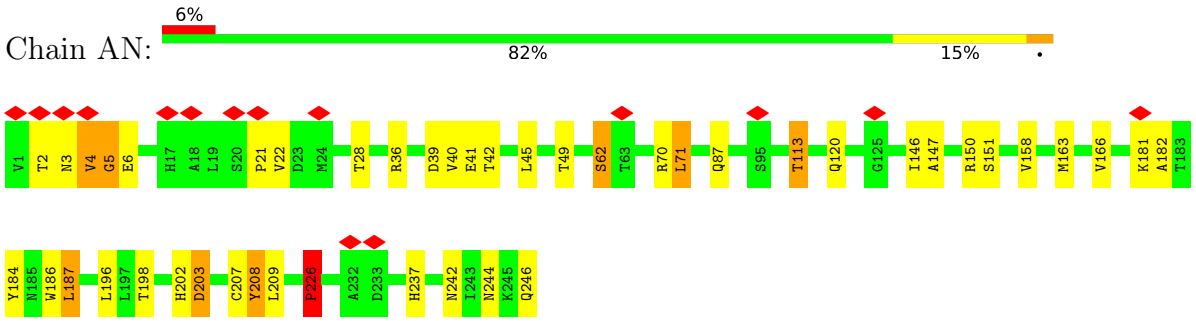
• Molecule 1: P1

Chain AM:



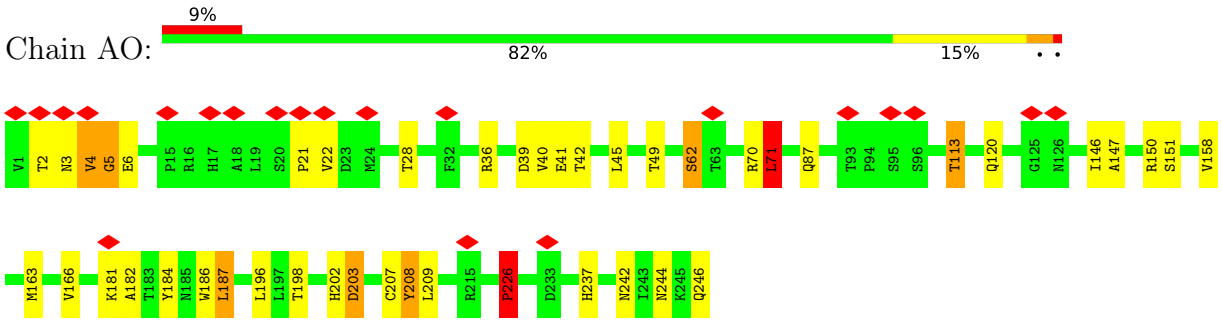
• Molecule 1: P1

Chain AN:



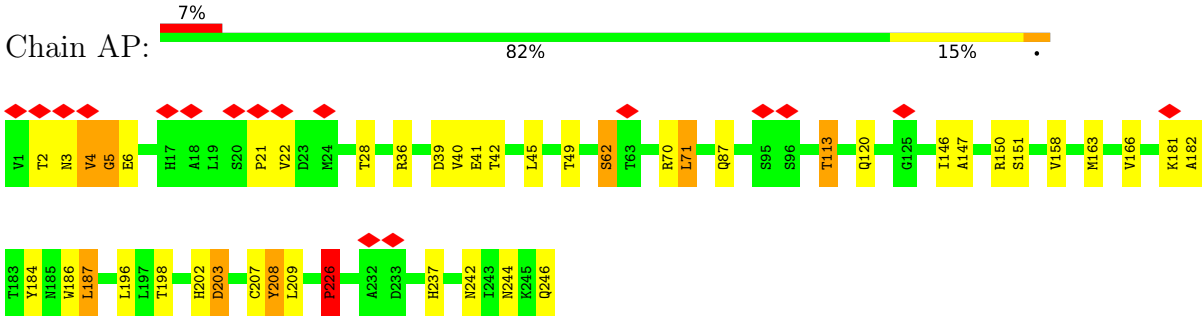
• Molecule 1: P1

Chain AO:



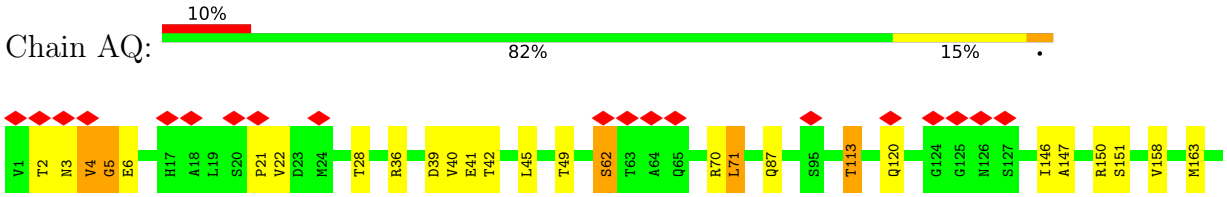
• Molecule 1: P1

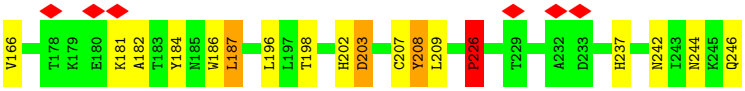
Chain AP:



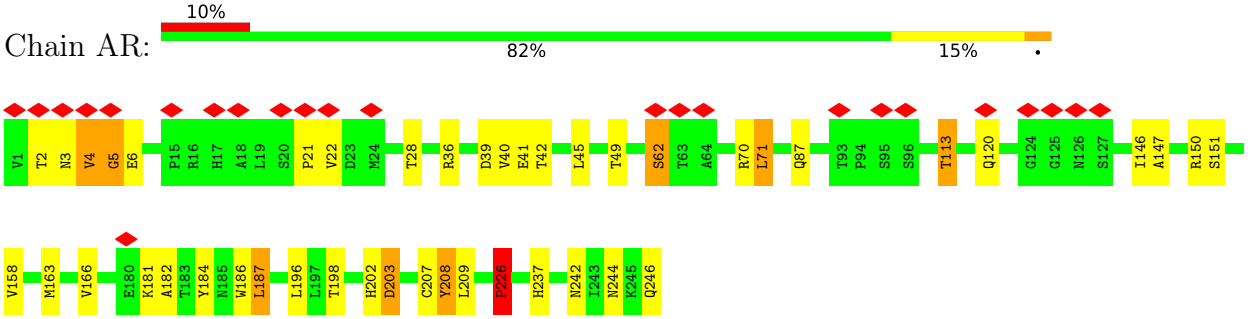
• Molecule 1: P1

Chain AQ:

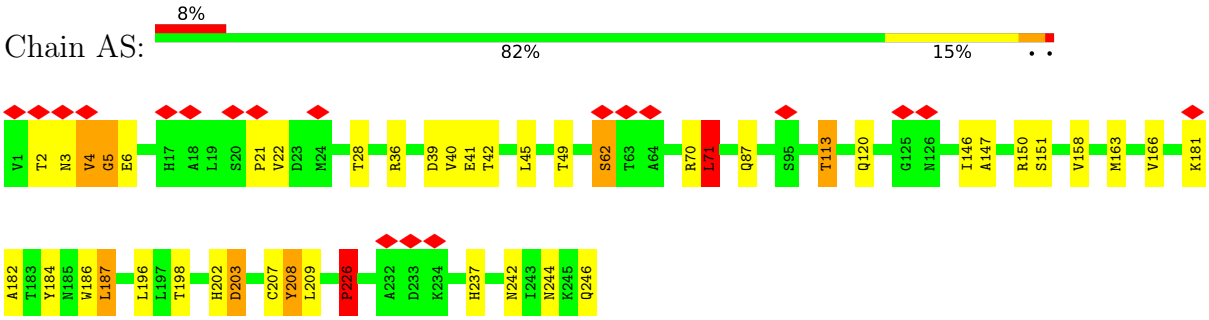




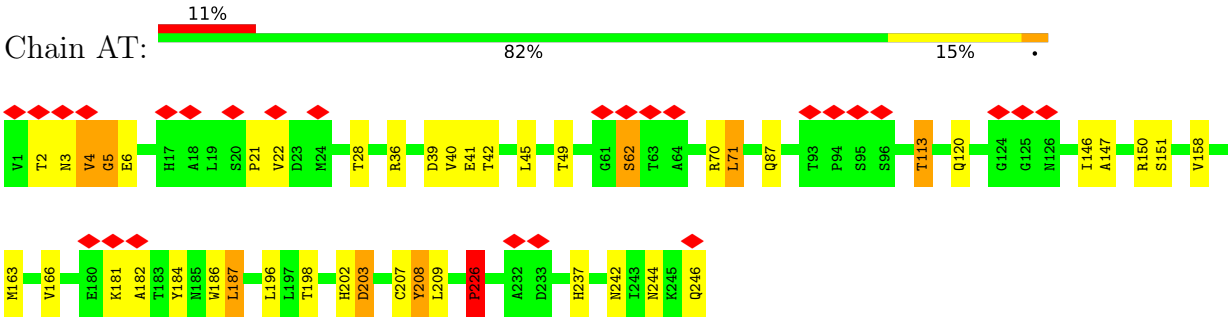
• Molecule 1: P1



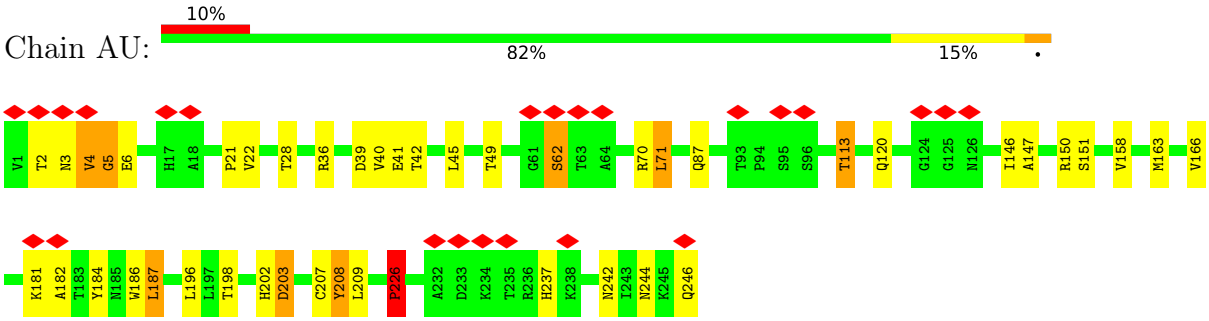
• Molecule 1: P1



• Molecule 1: P1

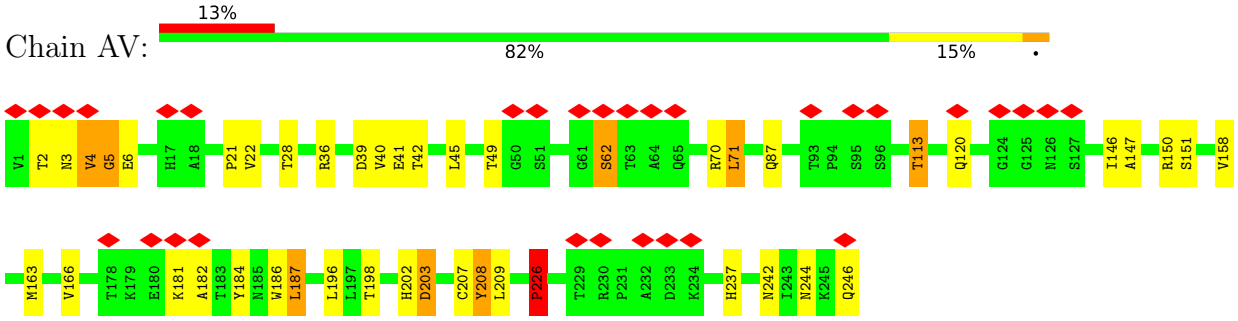


• Molecule 1: P1



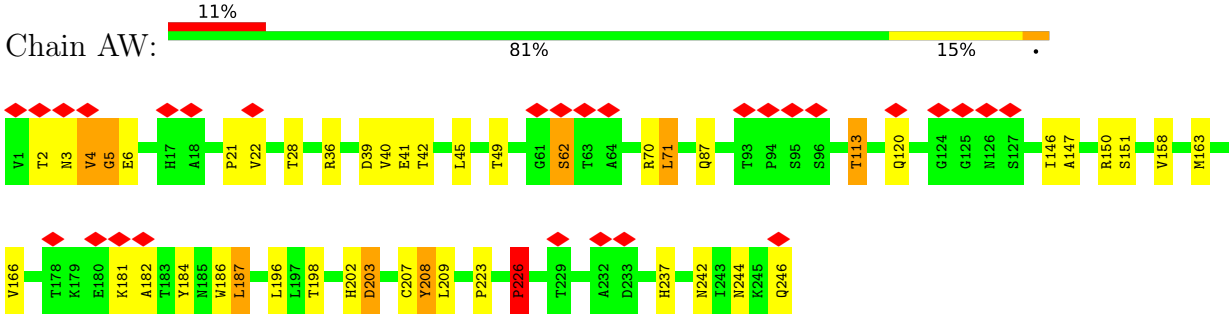
• Molecule 1: P1

Chain AV:



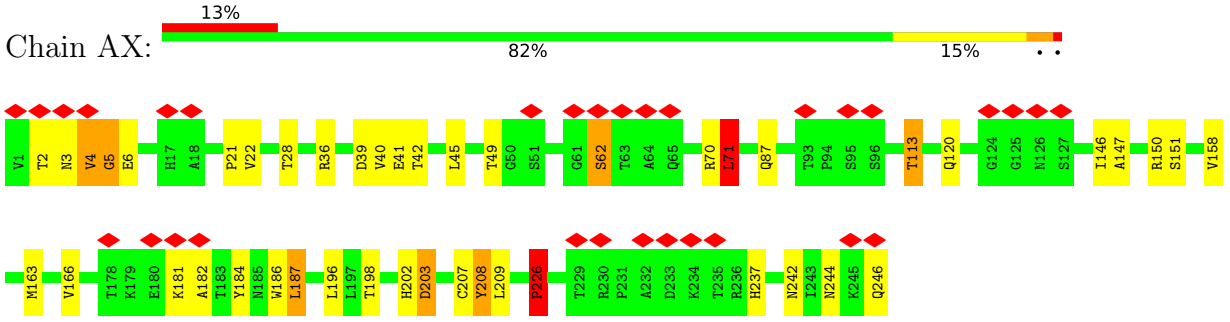
• Molecule 1: P1

Chain AW:



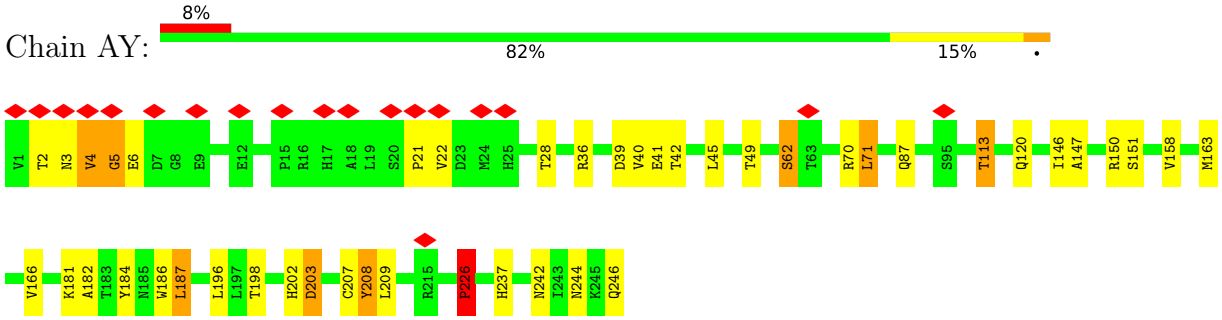
• Molecule 1: P1

Chain AX:



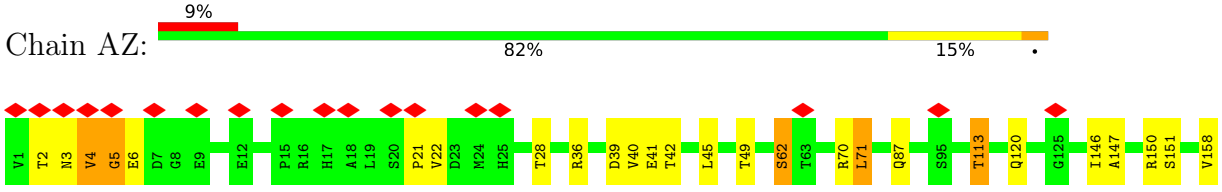
• Molecule 1: P1

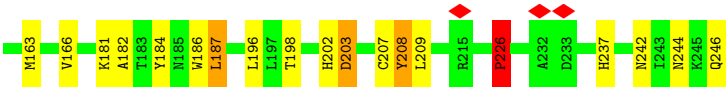
Chain AY:



• Molecule 1: P1

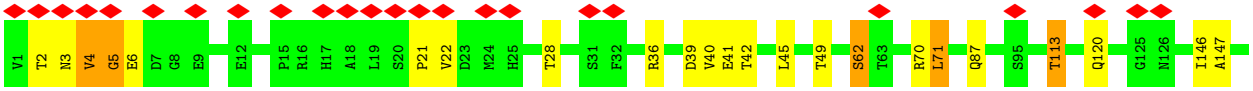
Chain AZ:

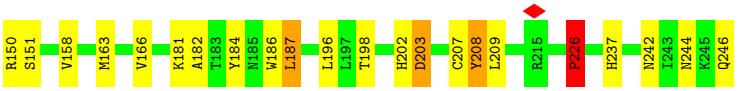




• Molecule 1: P1

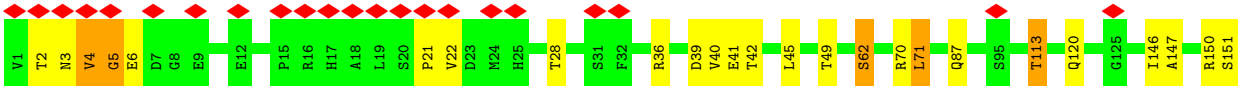
Chain A0:

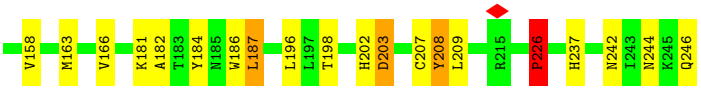




• Molecule 1: P1

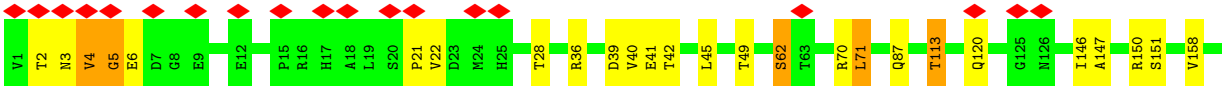
Chain A1:





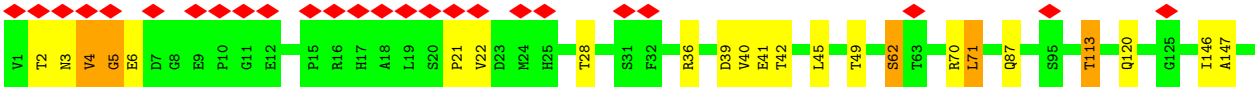
• Molecule 1: P1

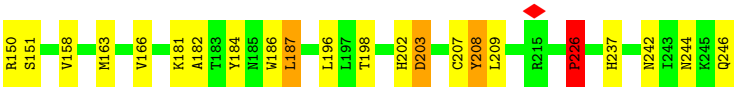
Chain A2:



• Molecule 1: P1

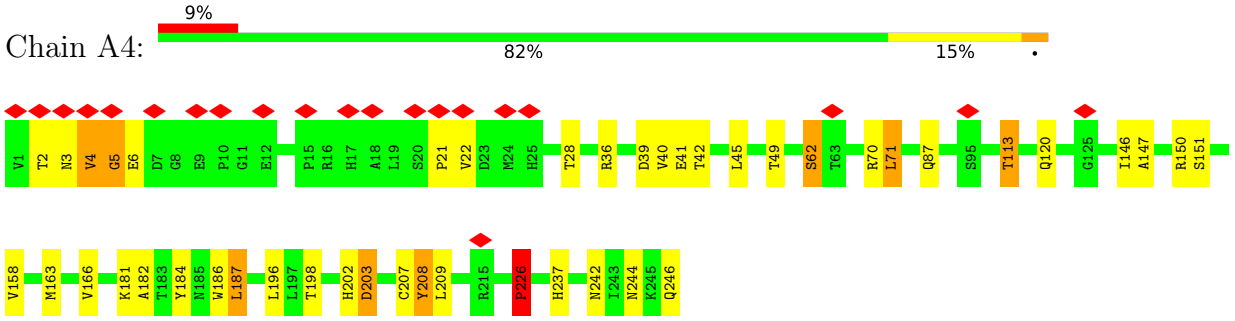
Chain A3:





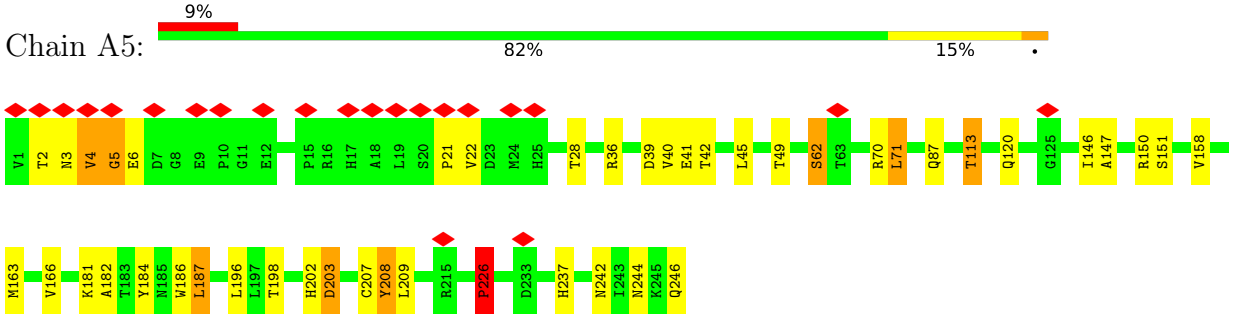
• Molecule 1: P1

Chain A4:



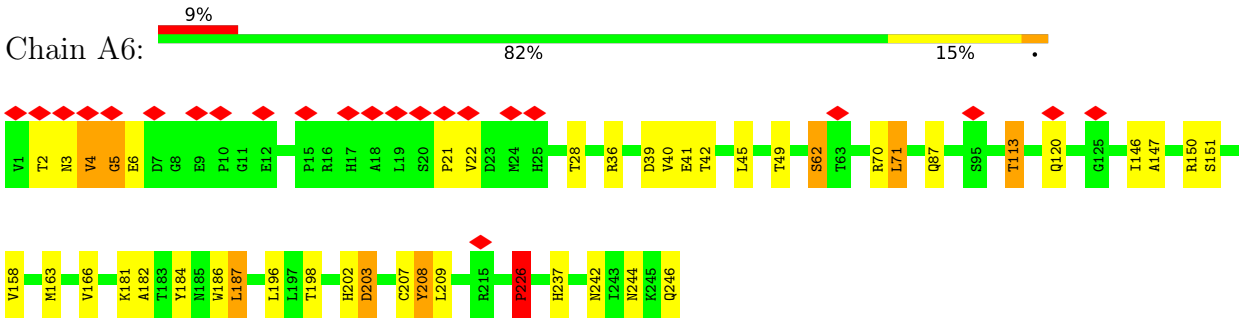
• Molecule 1: P1

Chain A5:



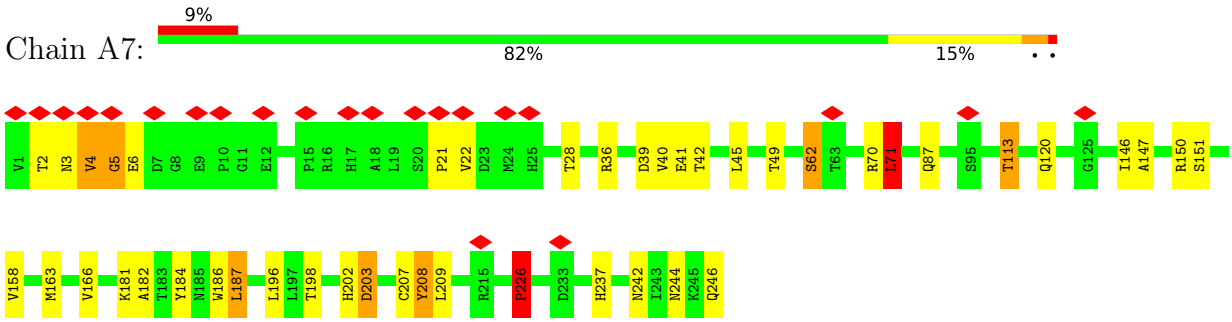
• Molecule 1: P1

Chain A6:



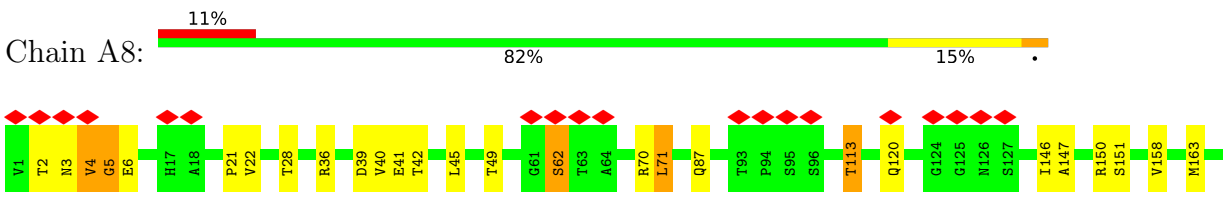
• Molecule 1: P1

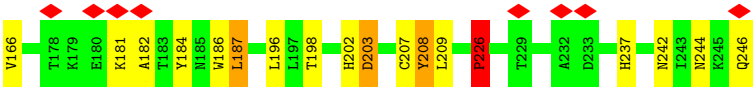
Chain A7:



• Molecule 1: P1

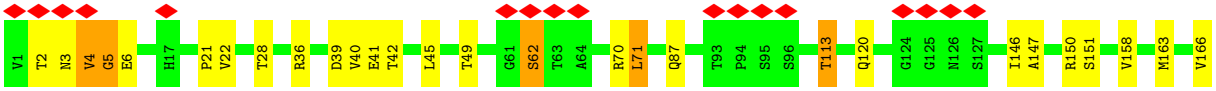
Chain A8:

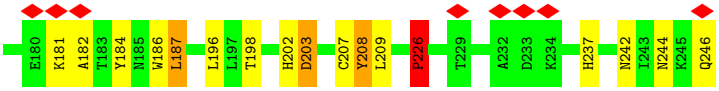




• Molecule 1: P1

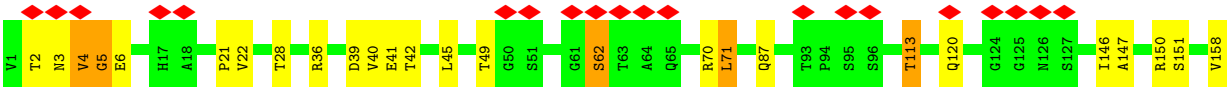
Chain A9:

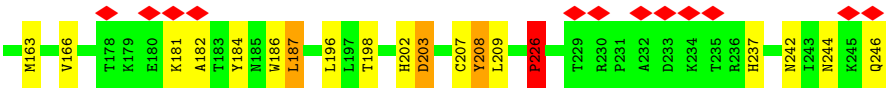




• Molecule 1: P1

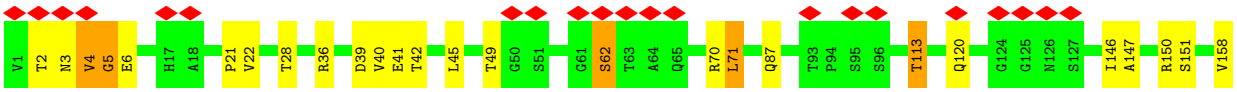
Chain Aa:

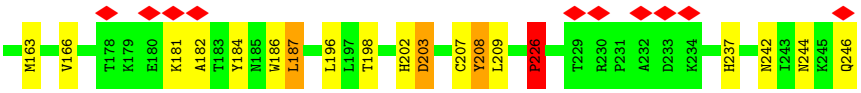




• Molecule 1: P1

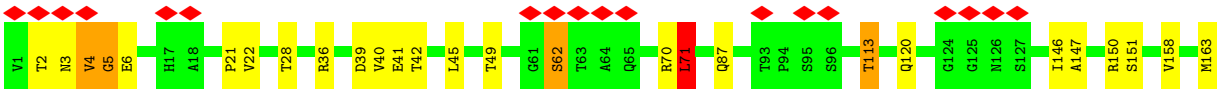
Chain Ab:

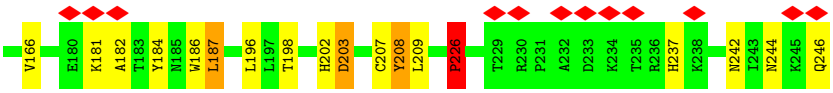




• Molecule 1: P1

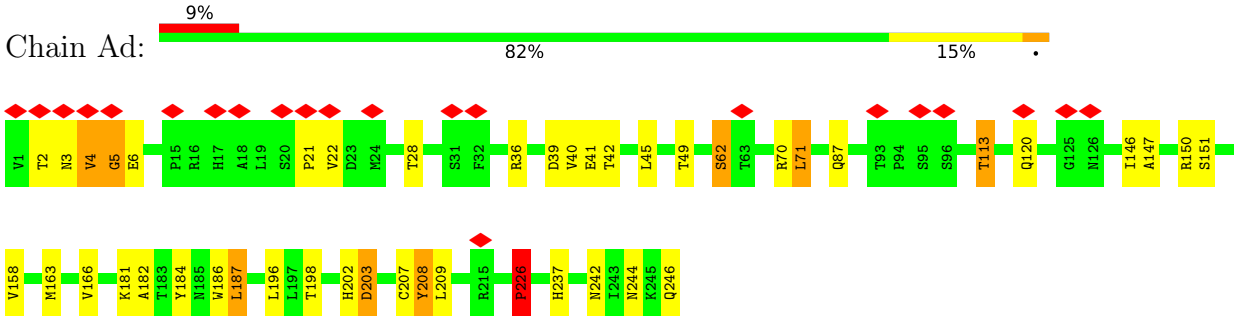
Chain Ac:





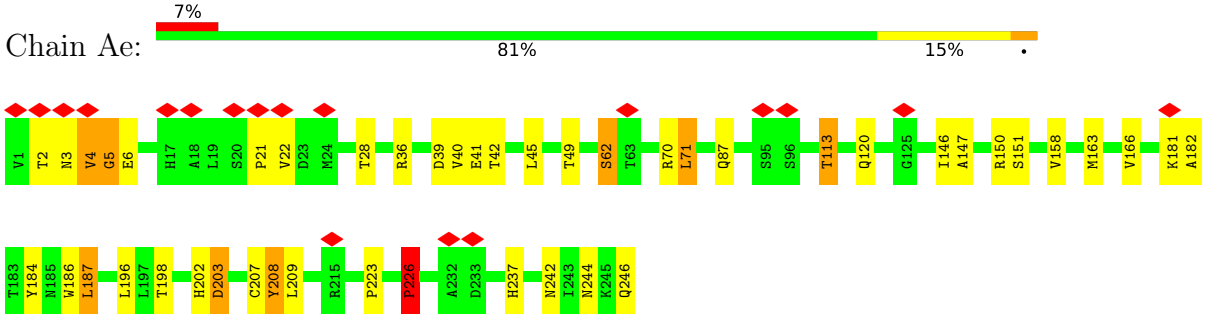
• Molecule 1: P1

Chain Ad:



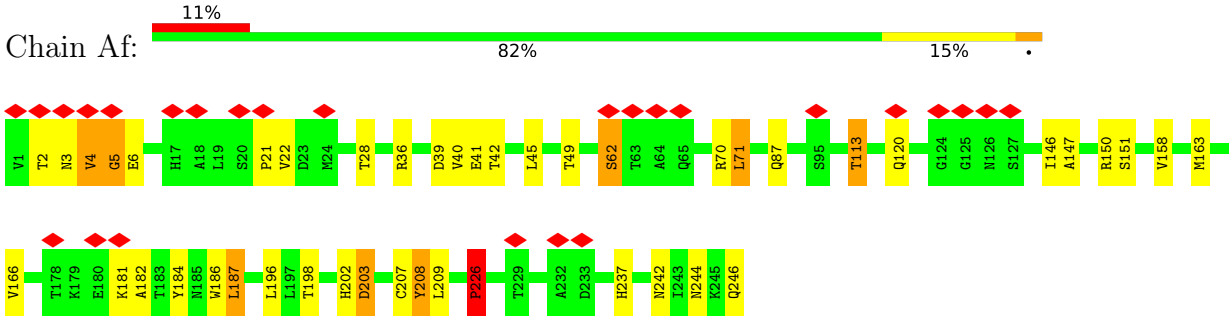
• Molecule 1: P1

Chain Ae:



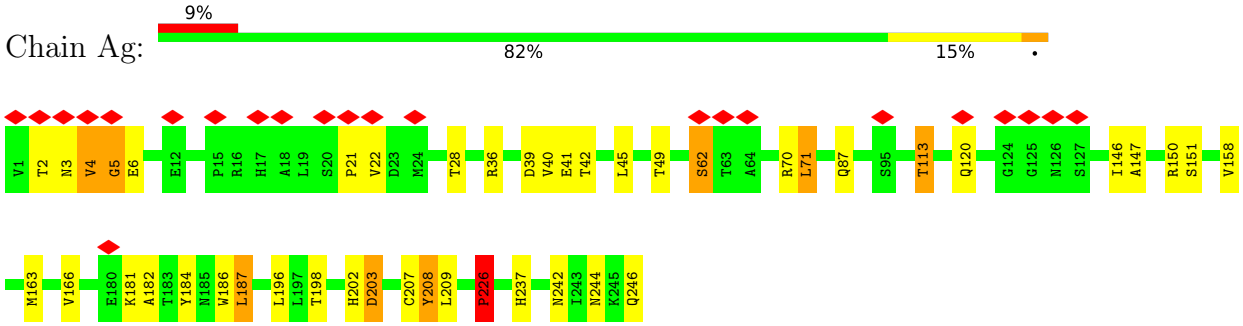
• Molecule 1: P1

Chain Af:



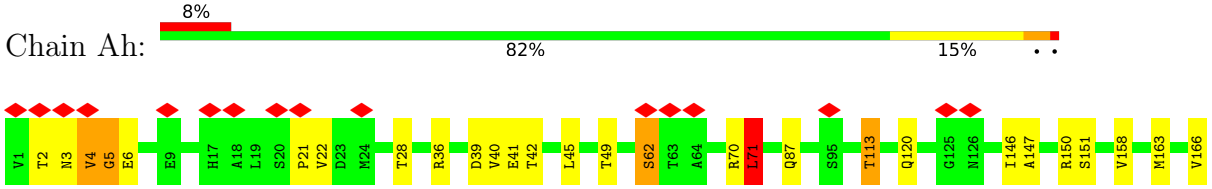
• Molecule 1: P1

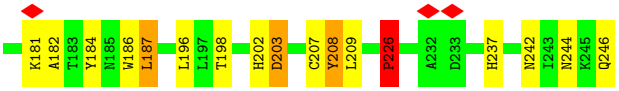
Chain Ag:



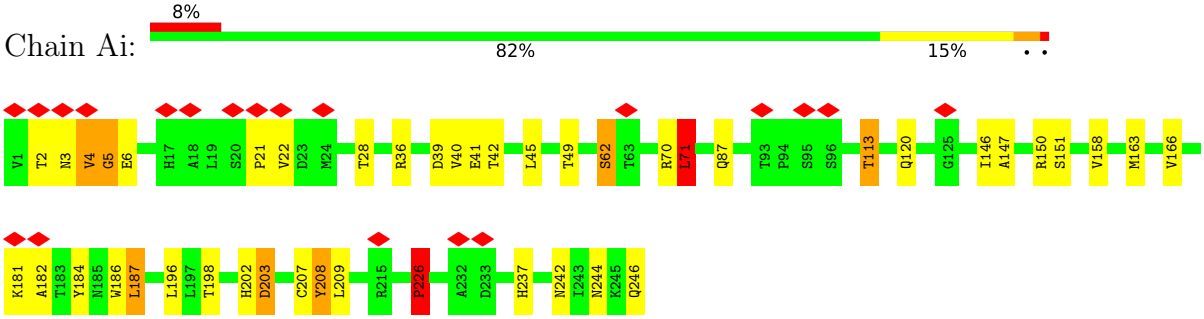
• Molecule 1: P1

Chain Ah:

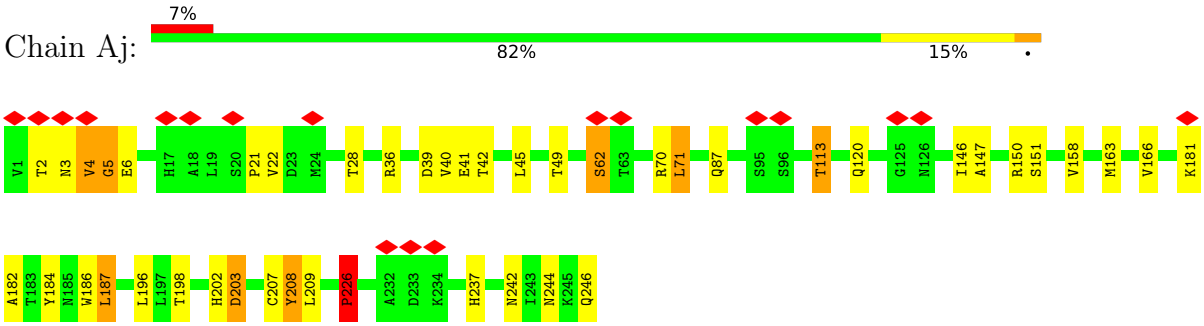




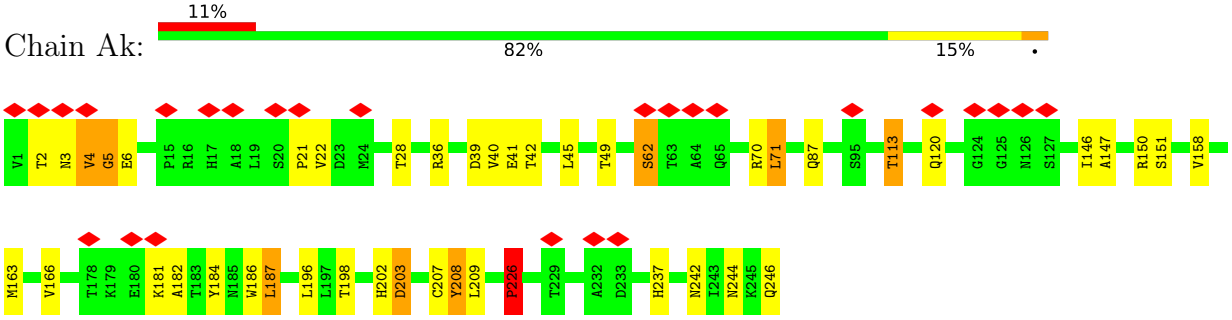
• Molecule 1: P1



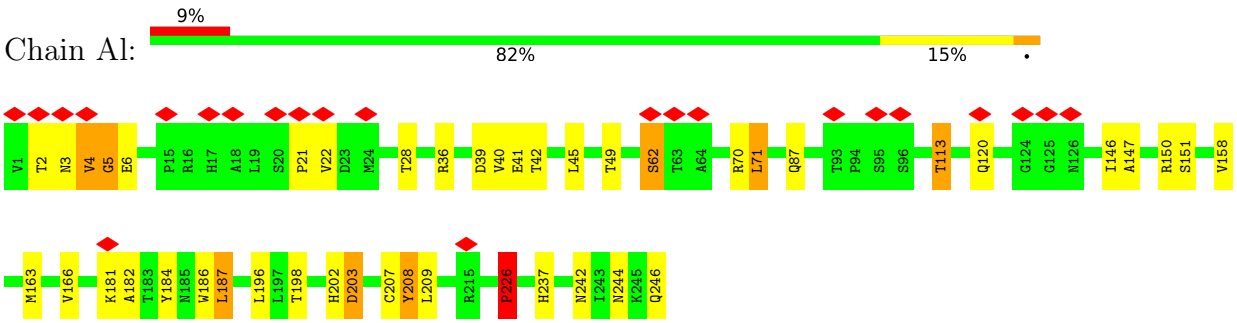
• Molecule 1: P1



• Molecule 1: P1

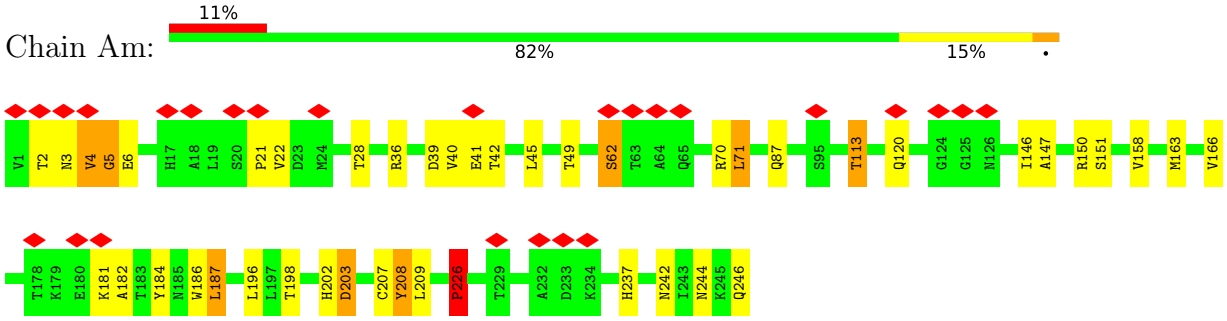


• Molecule 1: P1



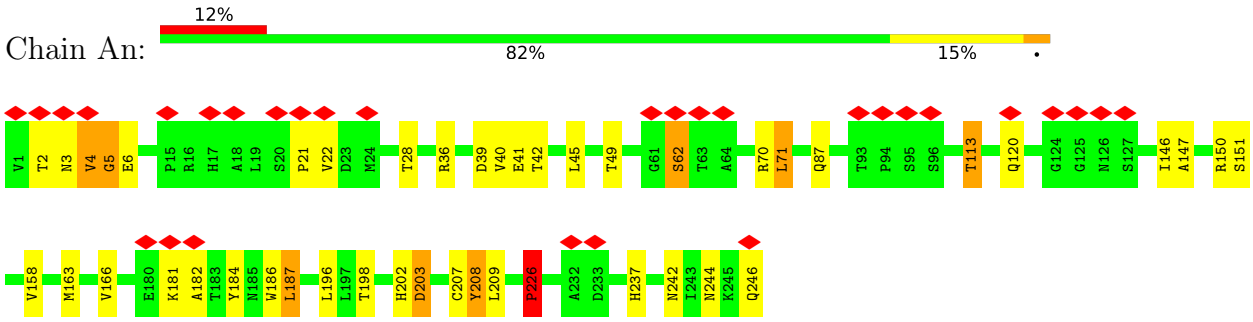
• Molecule 1: P1

Chain Am:



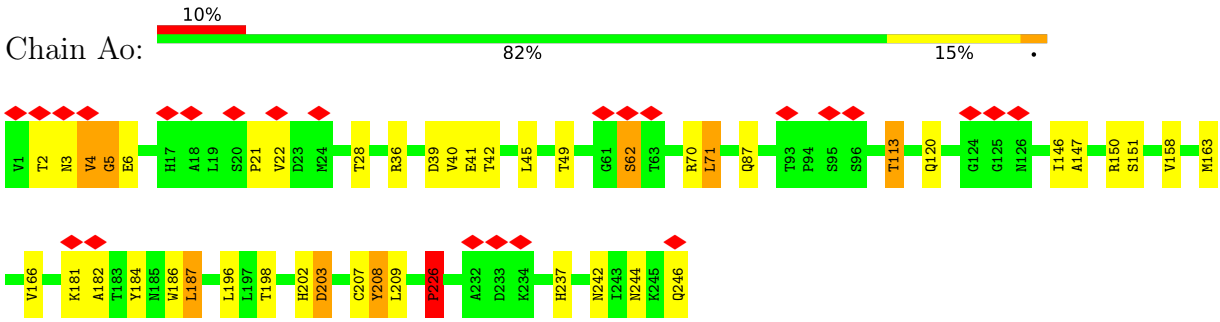
• Molecule 1: P1

Chain An:



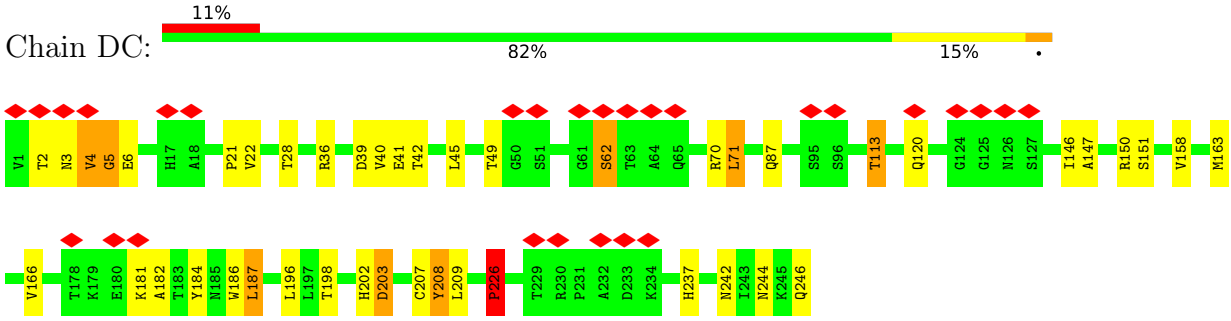
• Molecule 1: P1

Chain Ao:



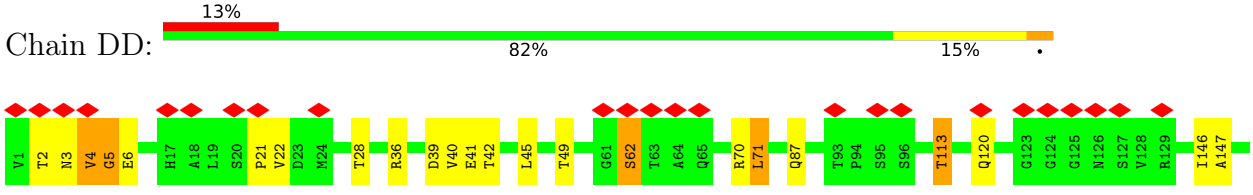
• Molecule 1: P1

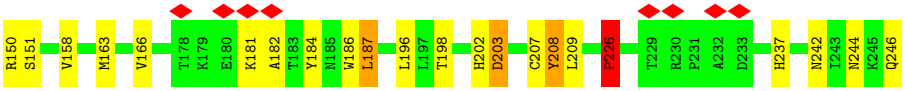
Chain DC:



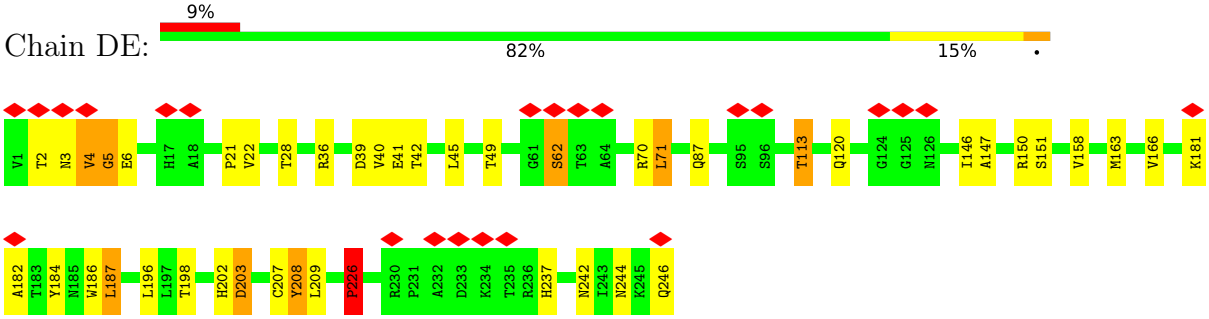
• Molecule 1: P1

Chain DD:

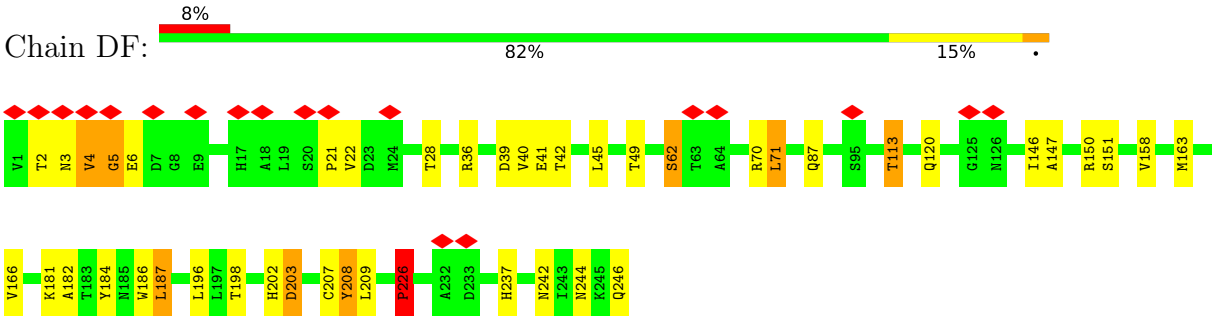




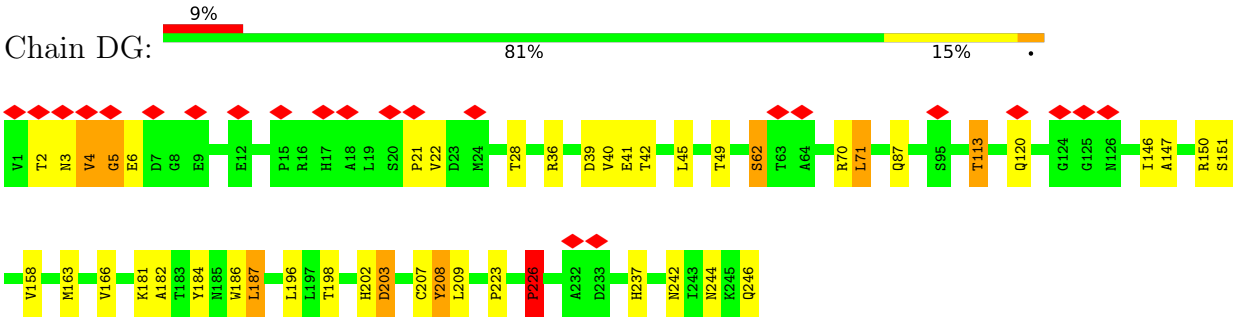
• Molecule 1: P1



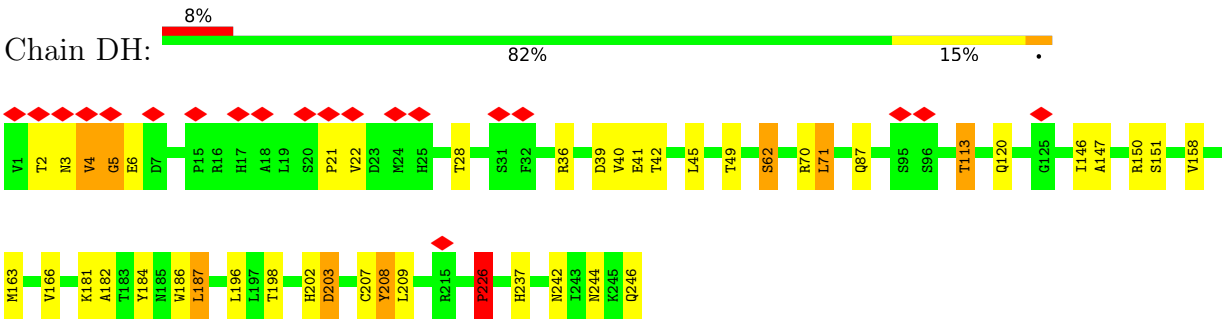
• Molecule 1: P1



• Molecule 1: P1

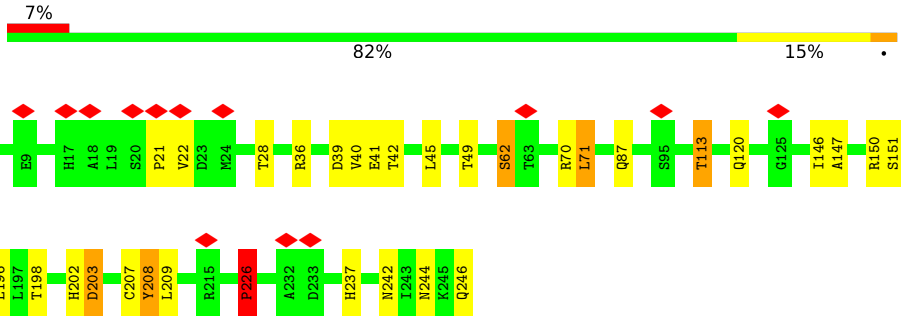


• Molecule 1: P1



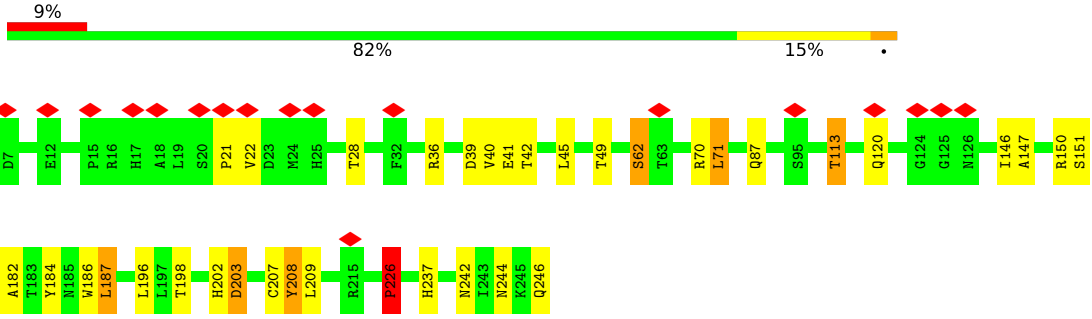
• Molecule 1: P1

Chain DI:



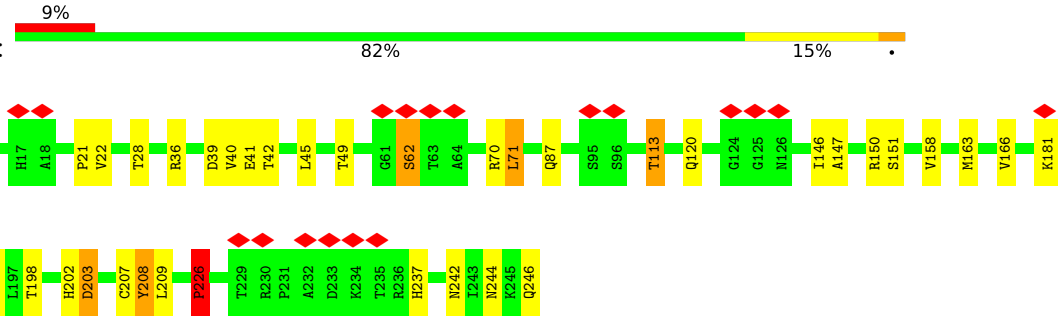
• Molecule 1: P1

Chain DJ:



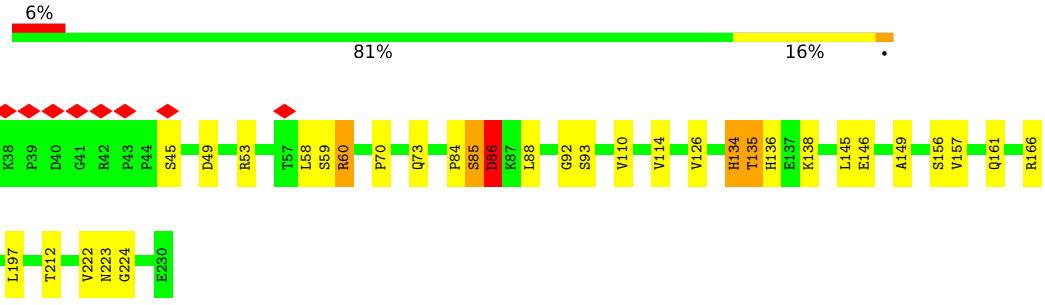
• Molecule 1: P1

Chain DK:



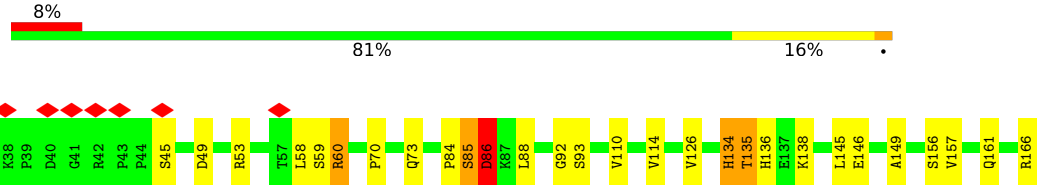
• Molecule 2: P1

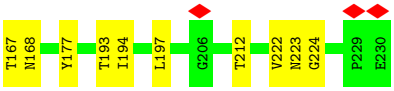
Chain BA:



• Molecule 2: P1

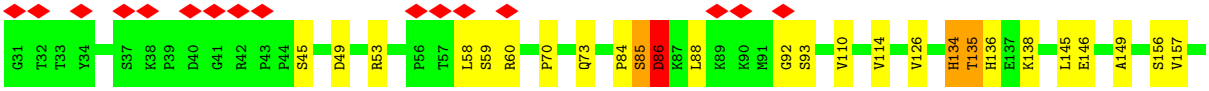
Chain BB:

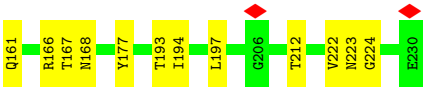




• Molecule 2: P1

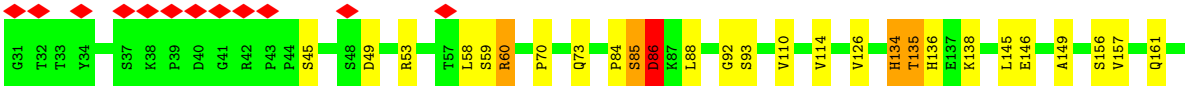
Chain BC:

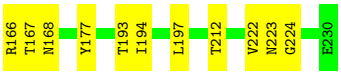




• Molecule 2: P1

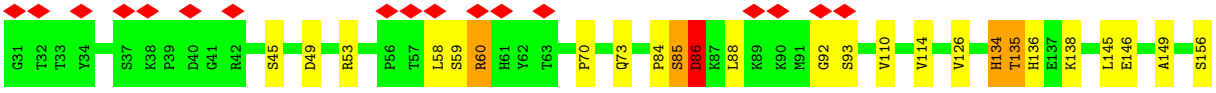
Chain BD:

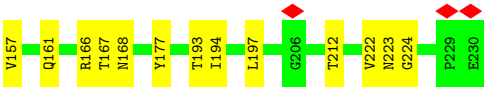




• Molecule 2: P1

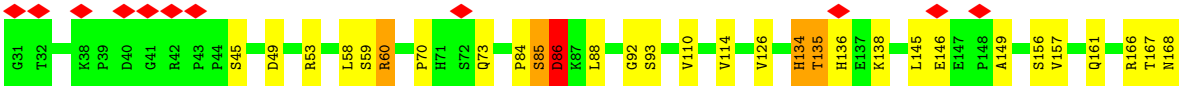
Chain BE:





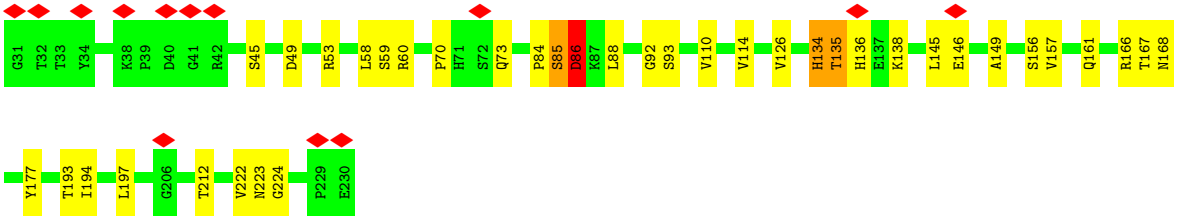
• Molecule 2: P1

Chain BF:

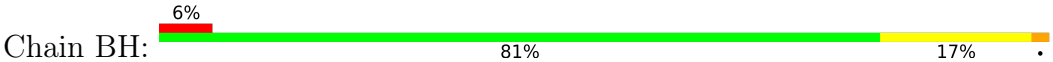


• Molecule 2: P1

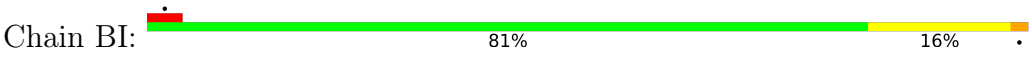
Chain BG:

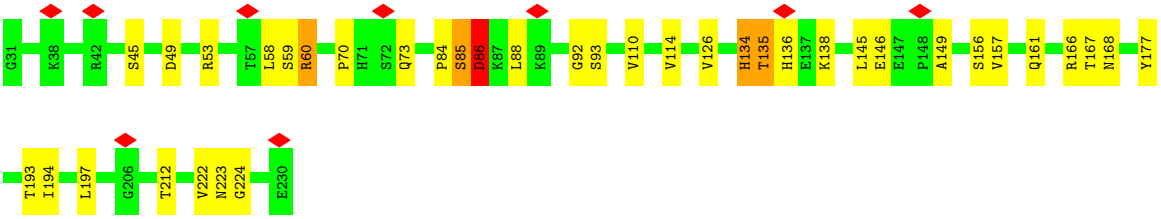


• Molecule 2: P1

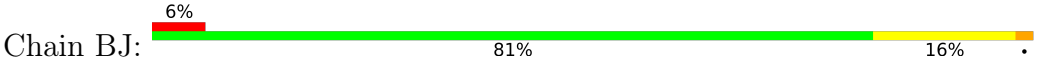


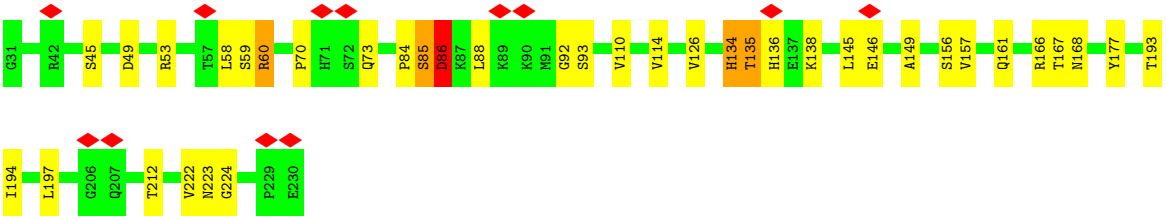
• Molecule 2: P1



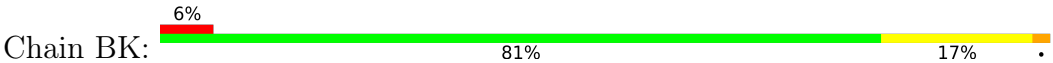


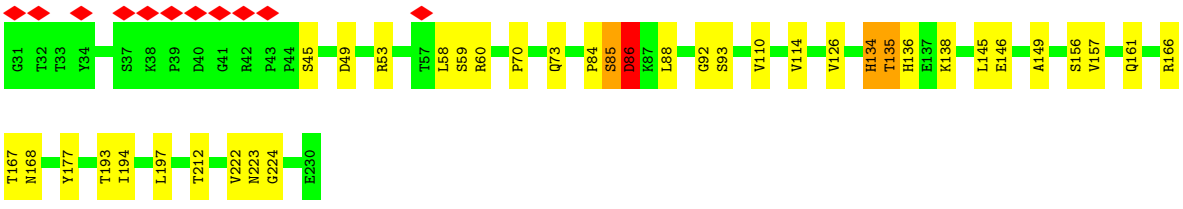
• Molecule 2: P1





• Molecule 2: P1





• Molecule 2: P1

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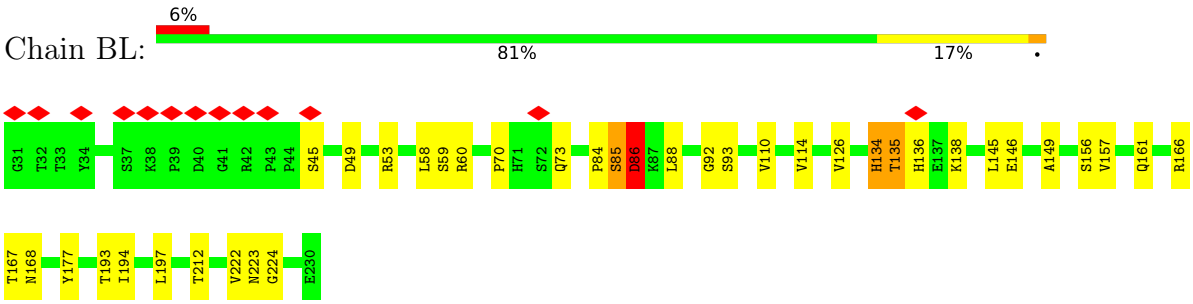

• Molecule 2: P1

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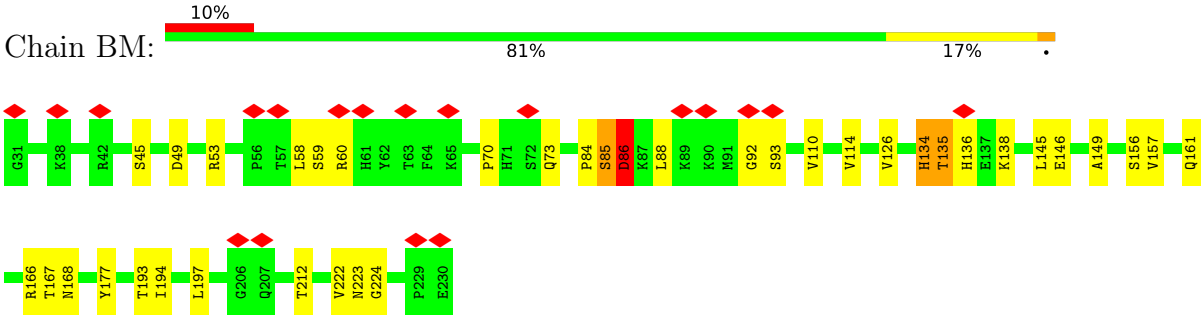
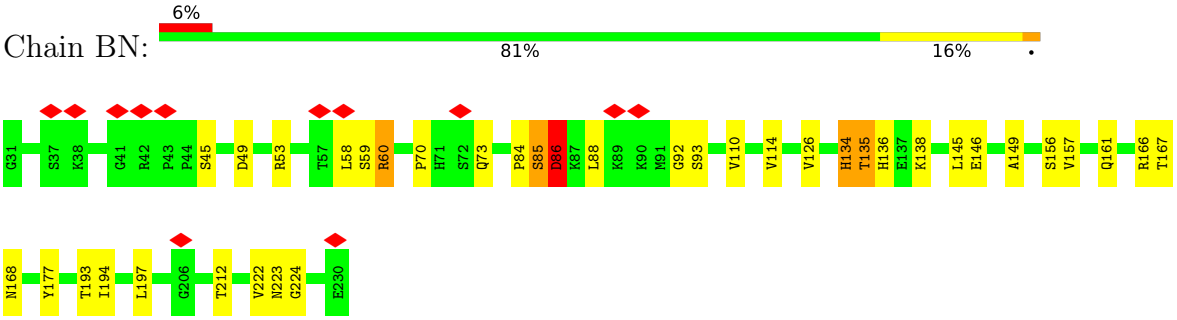


• Molecule 2: P1

Chain BN:



• Molecule 2: P1

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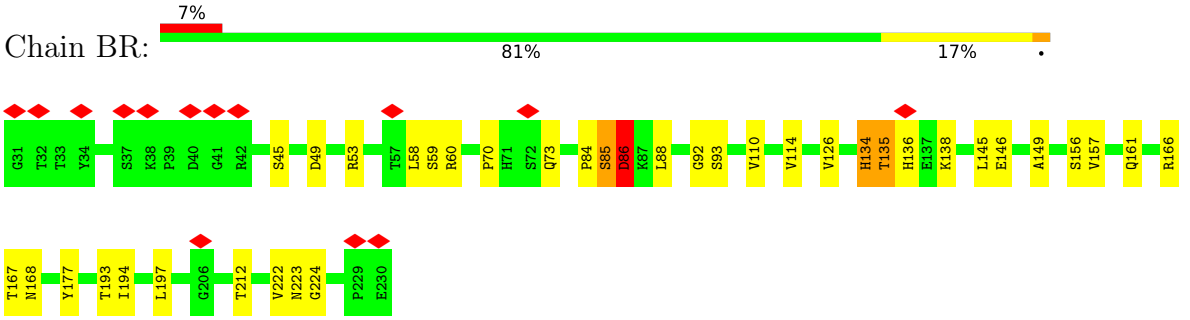

• Molecule 2: P1

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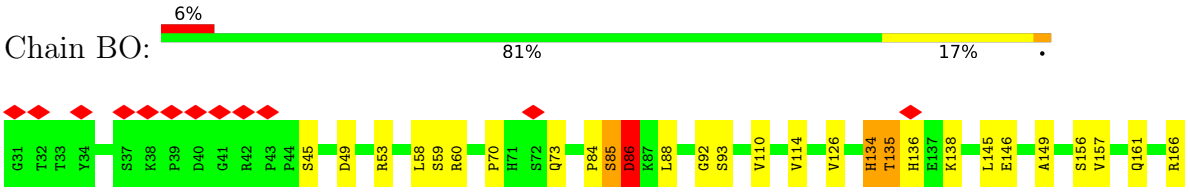
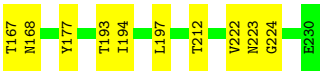
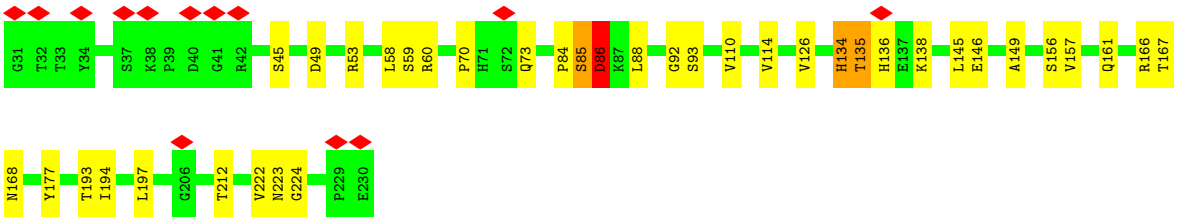




• Molecule 2: P1

Chain BS:



• Molecule 2: P1

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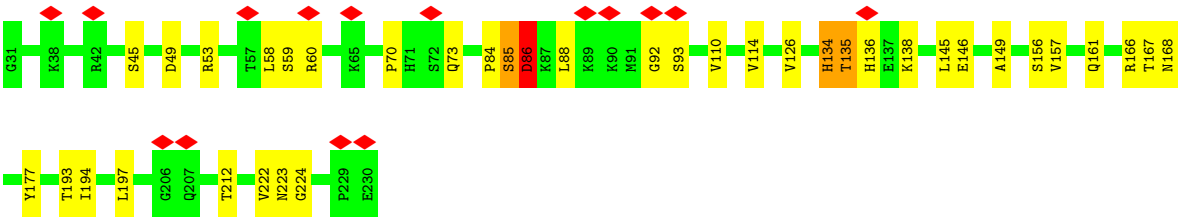
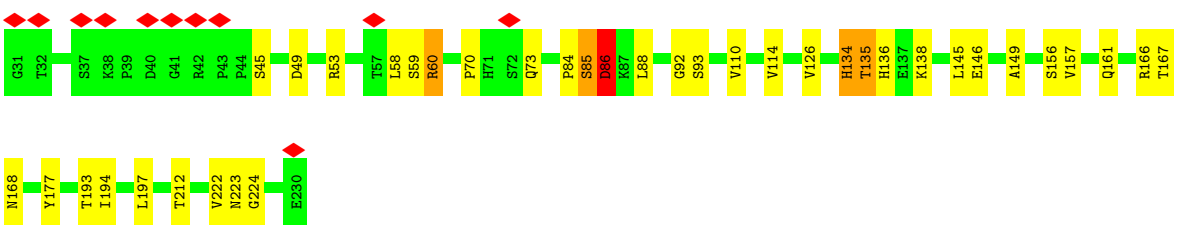


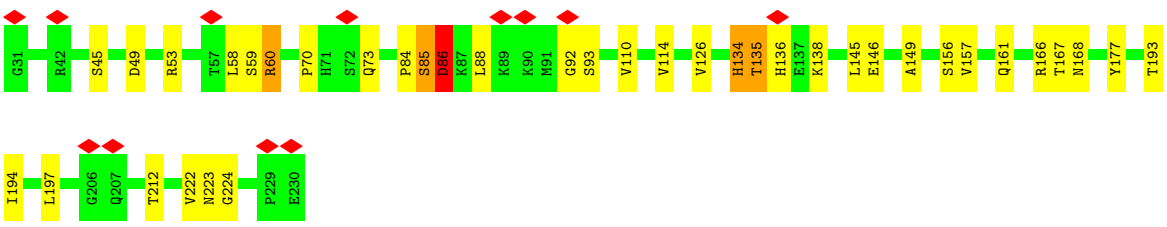
• Molecule 2: P1

Chain BQ:



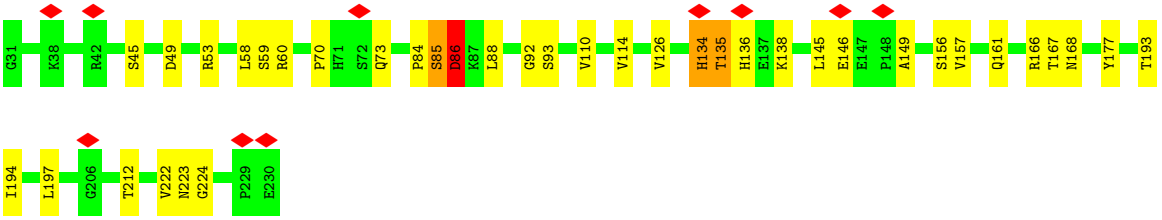
• Molecule 2: P1

Chain BT:



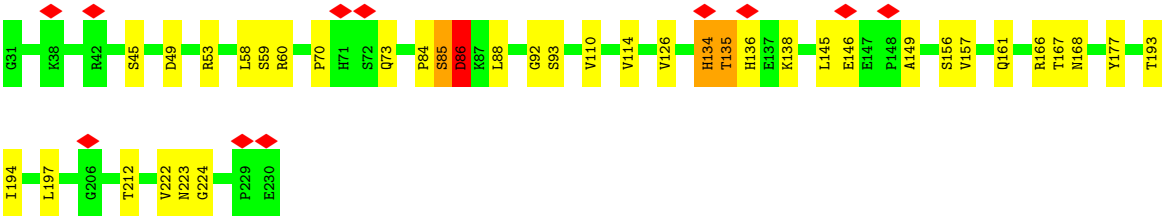
• Molecule 2: P1

Chain BU:



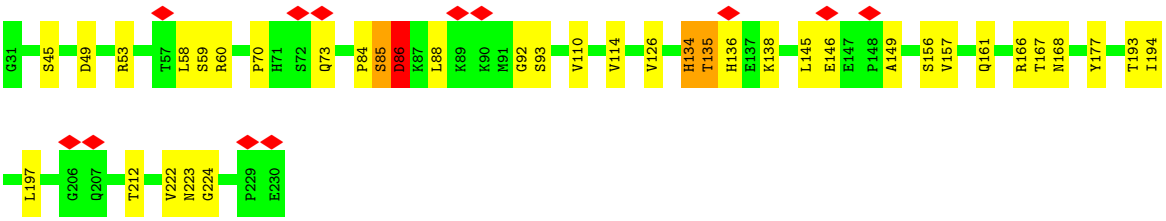
• Molecule 2: P1

Chain BV:



• Molecule 2: P1

Chain BW:



• Molecule 2: P1

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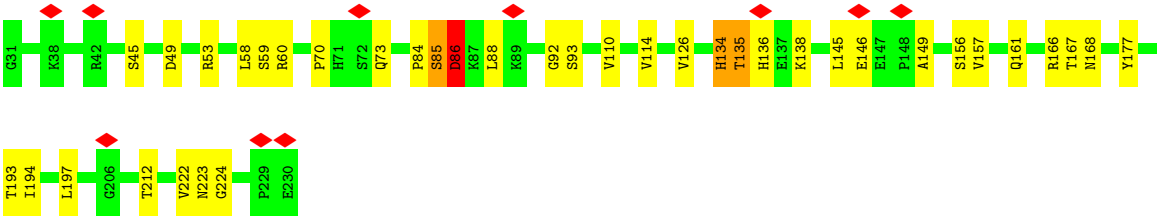
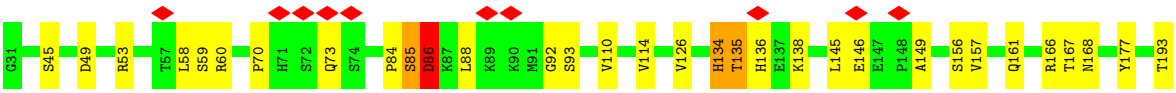
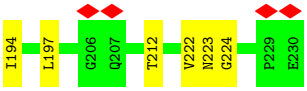


• Molecule 2: P1

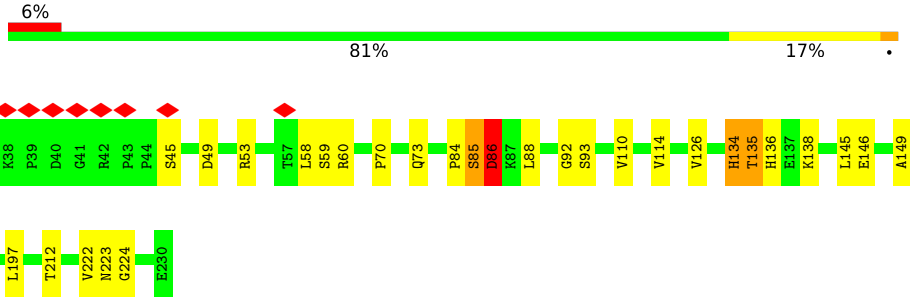
Chain BY:





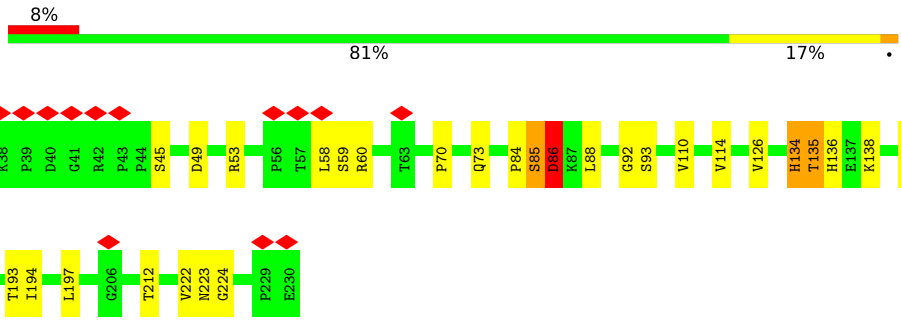
• Molecule 2: P1

Chain BZ:



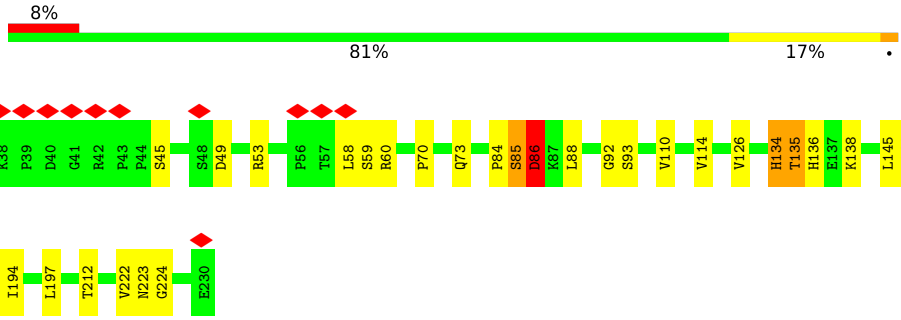
• Molecule 2: P1

Chain B0:



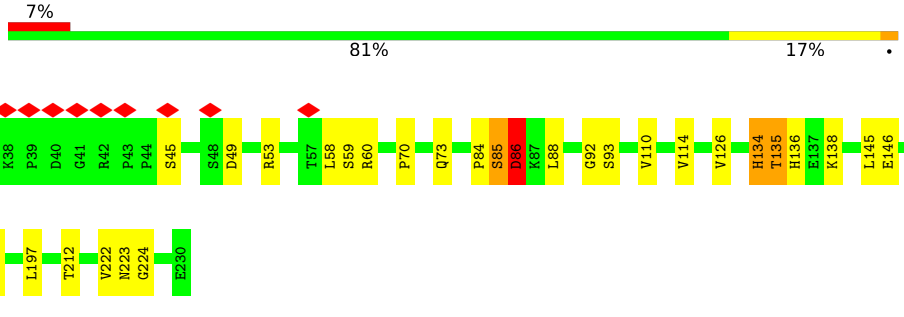
• Molecule 2: P1

Chain B1:



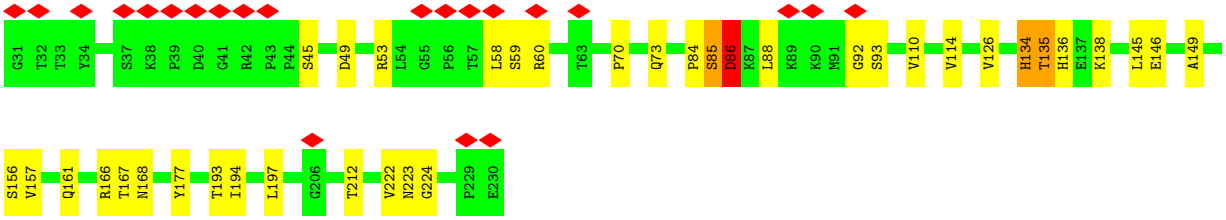
• Molecule 2: P1

Chain B2:



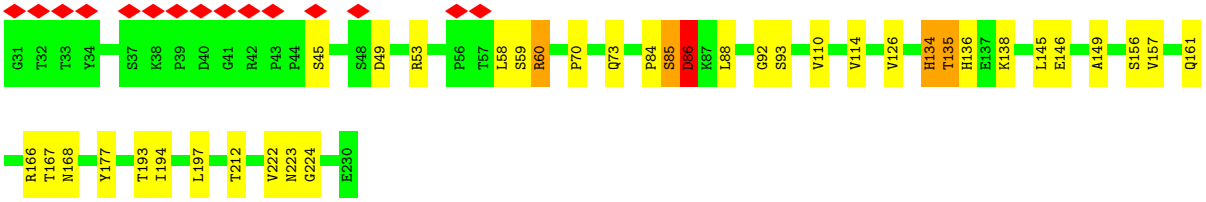
• Molecule 2: P1

Chain B3:



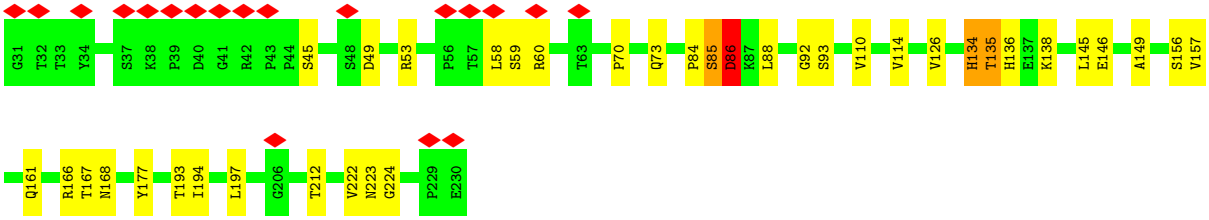
• Molecule 2: P1

Chain B4:



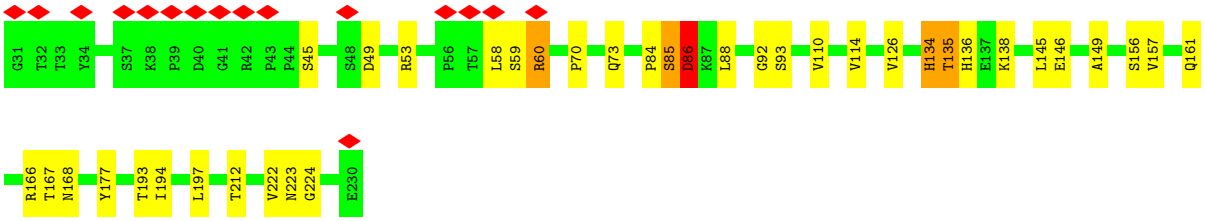
• Molecule 2: P1

Chain B5:



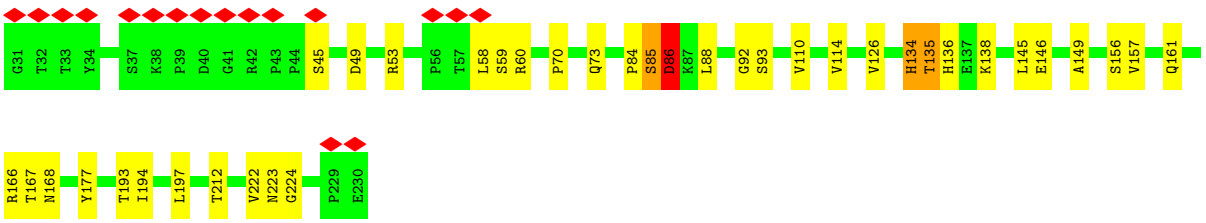
• Molecule 2: P1

Chain B6:



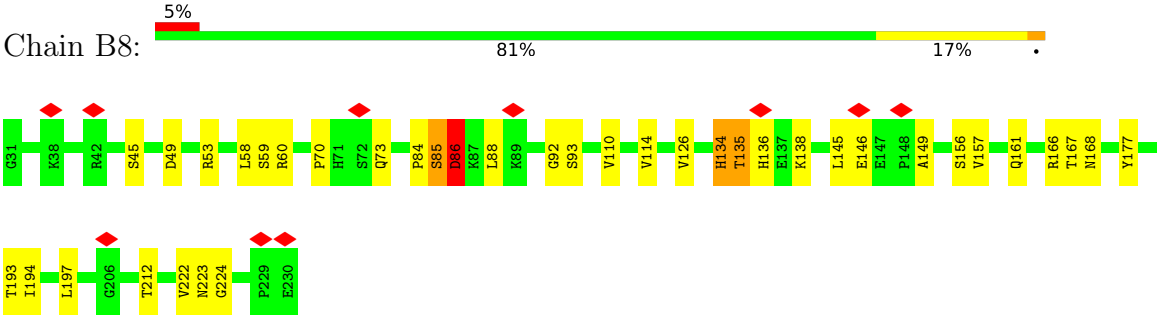
• Molecule 2: P1

Chain B7:



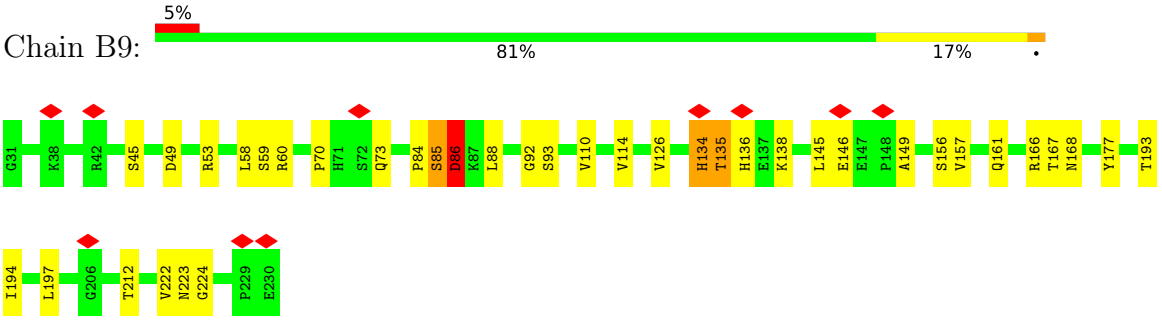
• Molecule 2: P1

Chain B8:



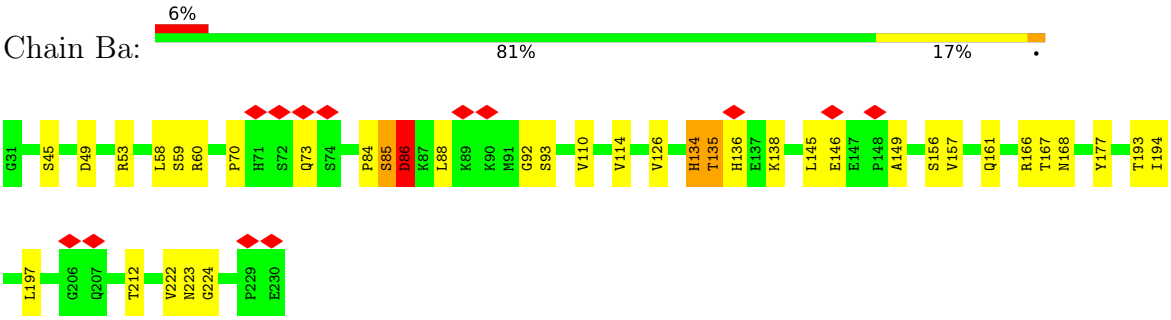
• Molecule 2: P1

Chain B9:



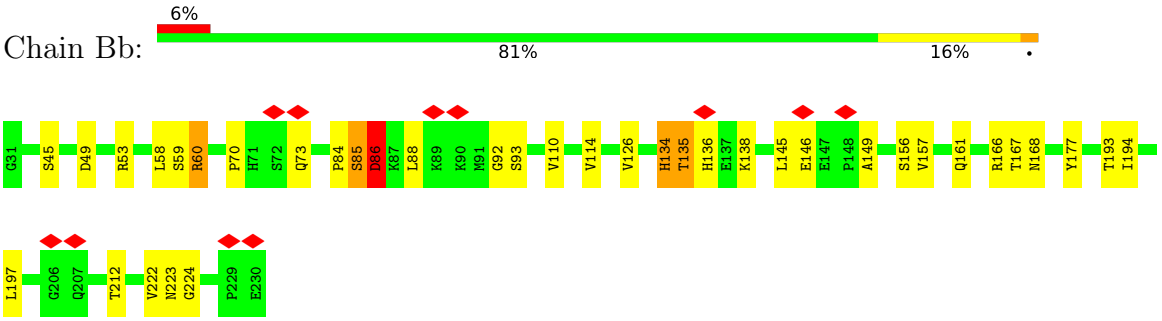
• Molecule 2: P1

Chain Ba:



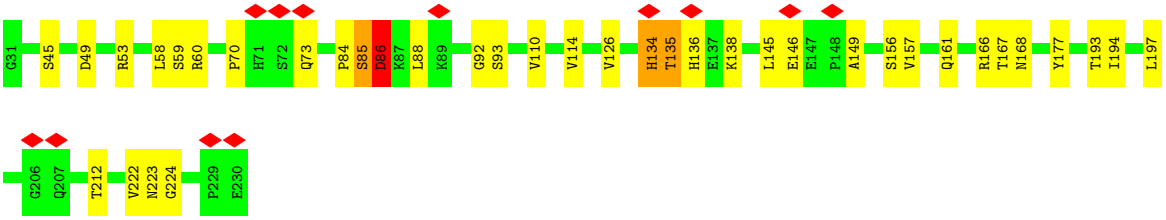
• Molecule 2: P1

Chain Bb:



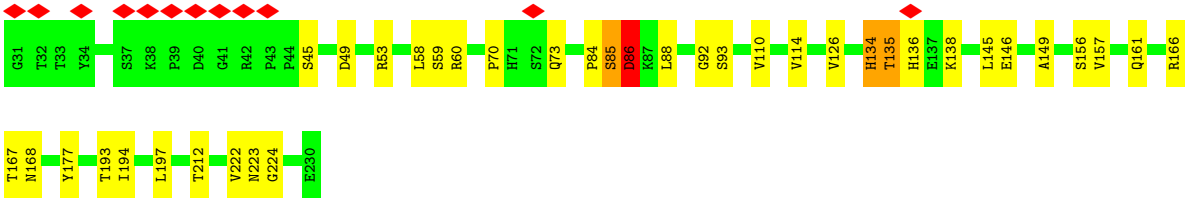
• Molecule 2: P1

Chain Bc:



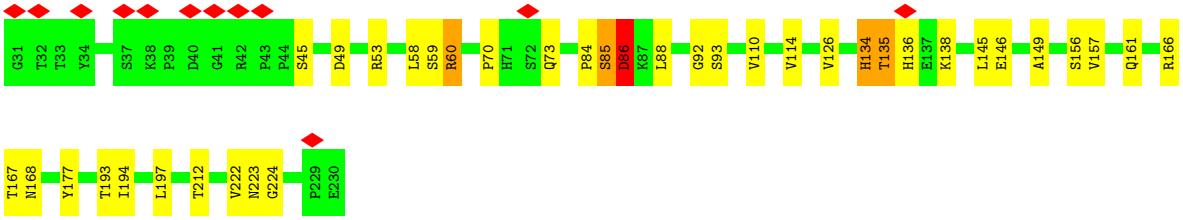
• Molecule 2: P1

Chain Bd:



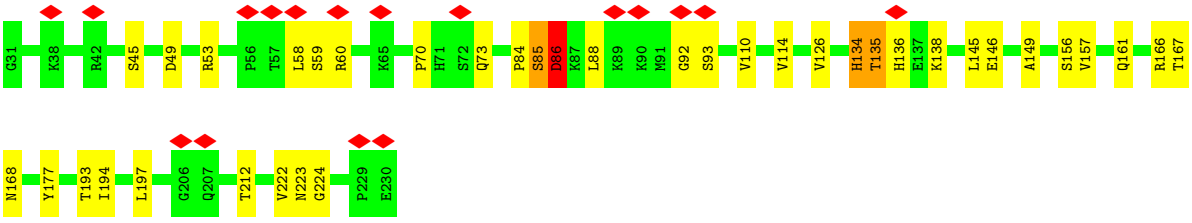
• Molecule 2: P1

Chain Be:



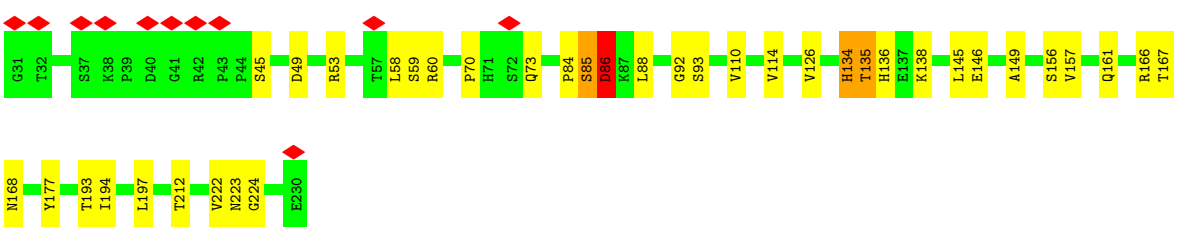
• Molecule 2: P1

Chain Bf:



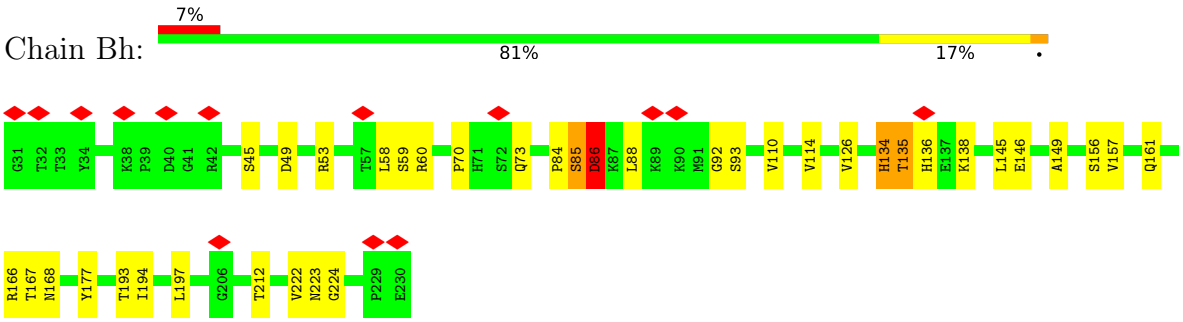
• Molecule 2: P1

Chain Bg:



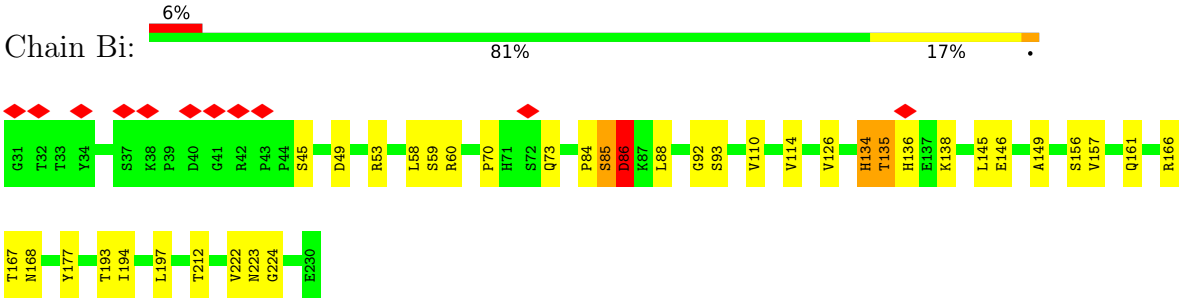
• Molecule 2: P1

Chain Bh:



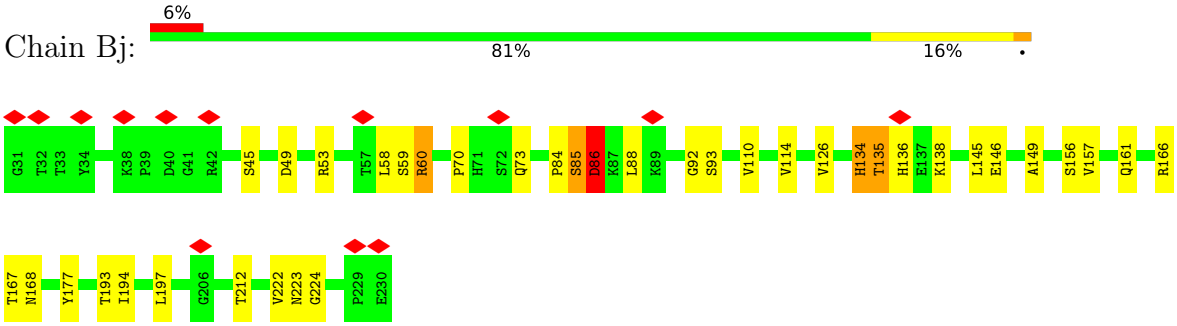
• Molecule 2: P1

Chain Bi:



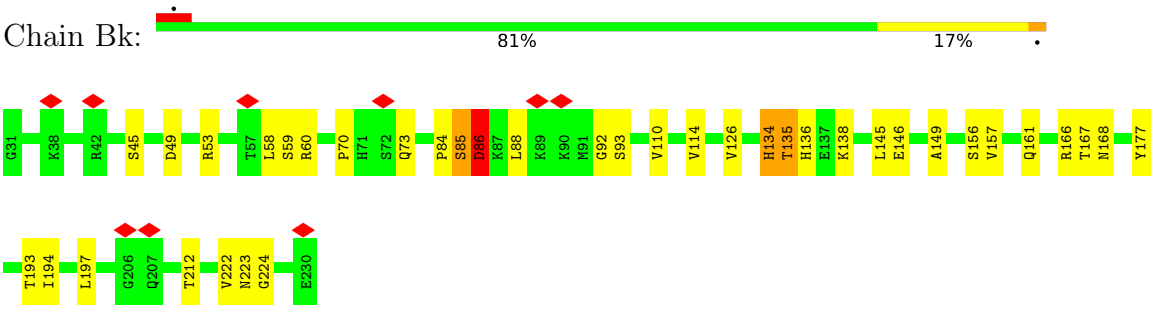
• Molecule 2: P1

Chain Bj:



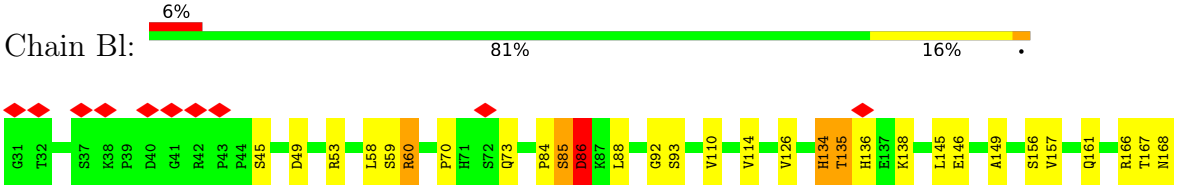
• Molecule 2: P1

Chain Bk:



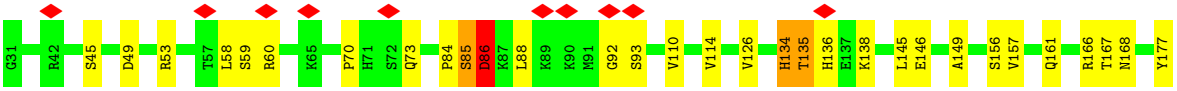
• Molecule 2: P1

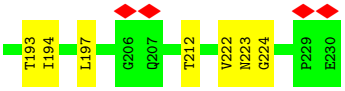
Chain Bl:



• Molecule 2: P1

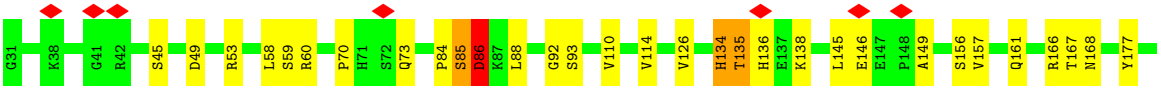
Chain Bm:

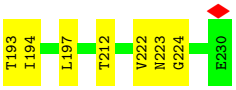




• Molecule 2: P1

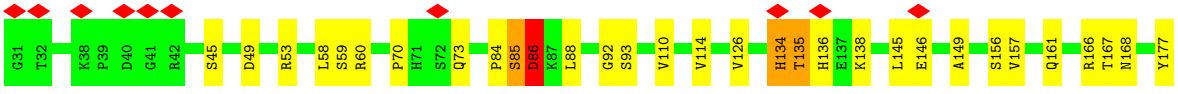
Chain Bn:

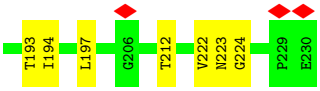




• Molecule 2: P1

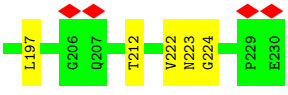
Chain Bo:





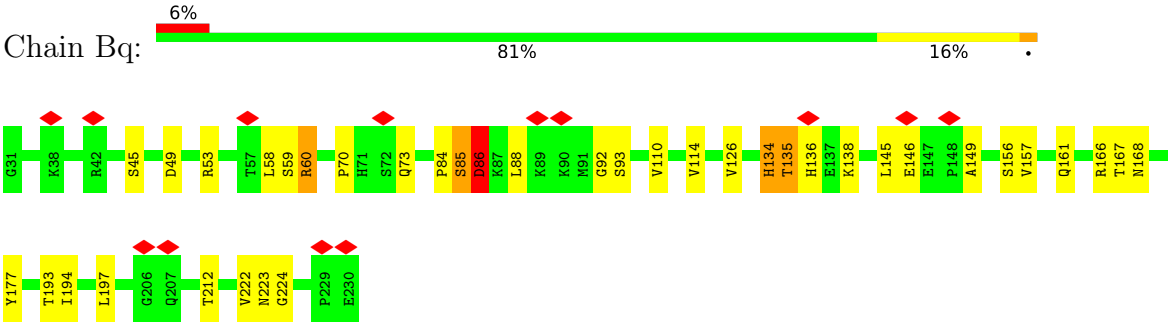
• Molecule 2: P1

Chain Bp:



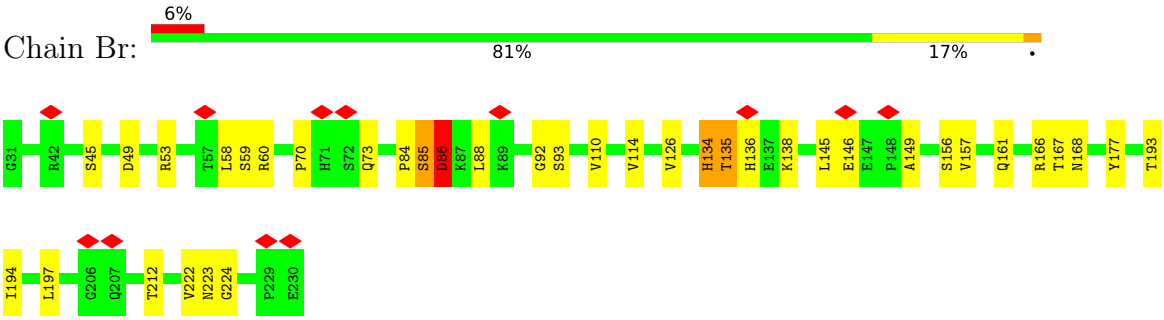
• Molecule 2: P1

Chain Bq:



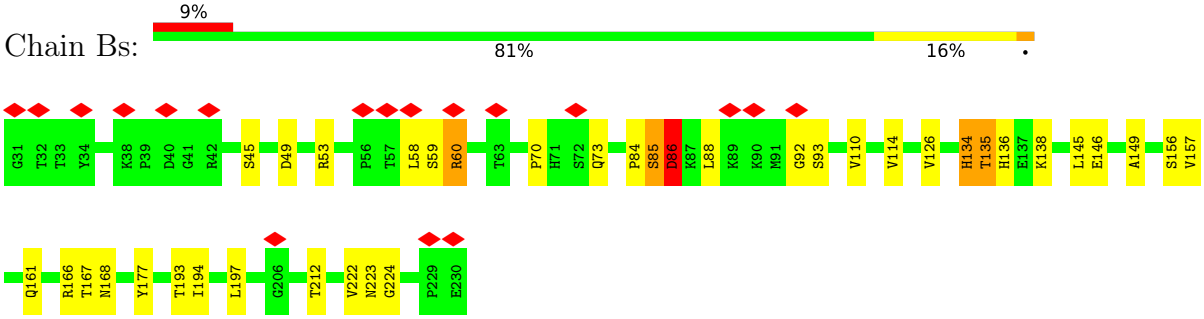
• Molecule 2: P1

Chain Br:



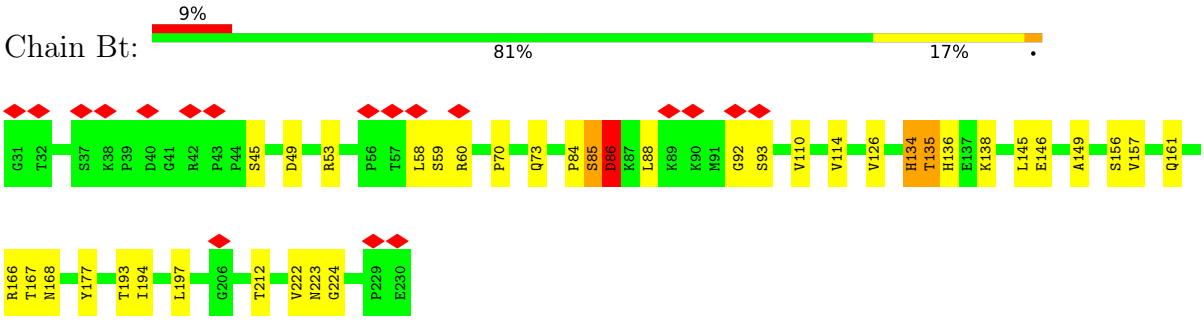
• Molecule 2: P1

Chain Bs:



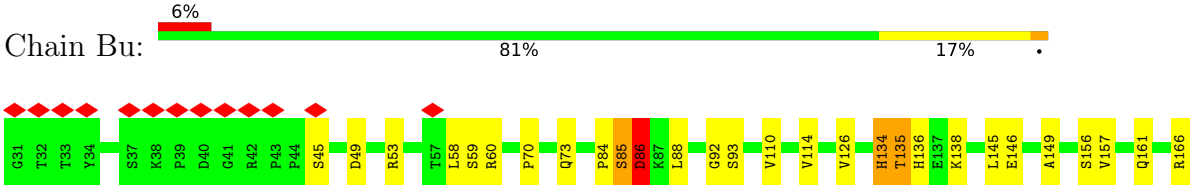
• Molecule 2: P1

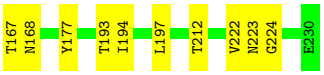
Chain Bt:



• Molecule 2: P1

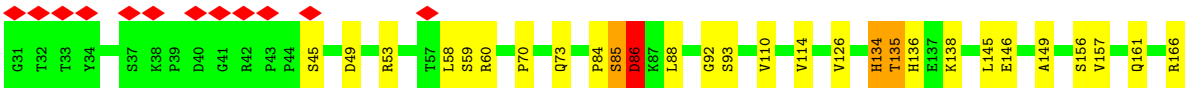
Chain Bu:





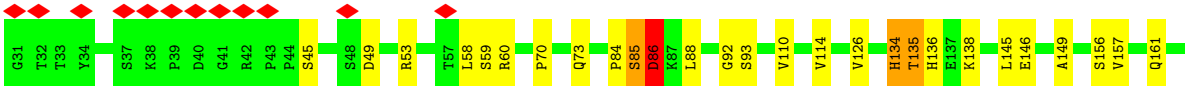
• Molecule 2: P1

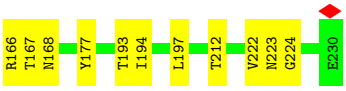
Chain Bv:



• Molecule 2: P1

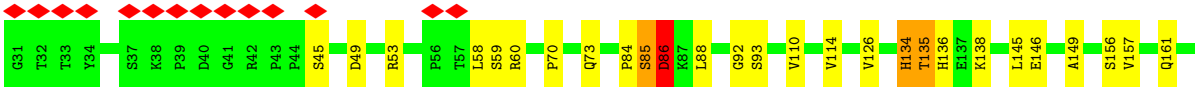
Chain Bw:

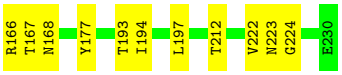




• Molecule 2: P1

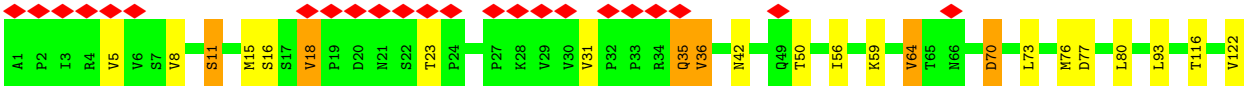
Chain Bx:

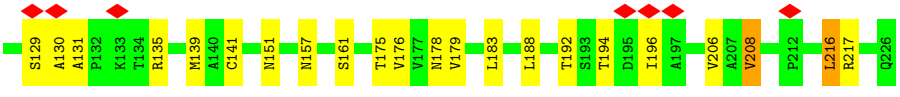




• Molecule 3: P1

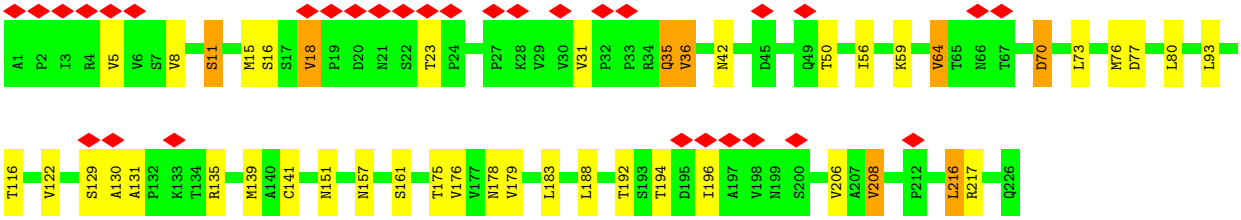
Chain CA:





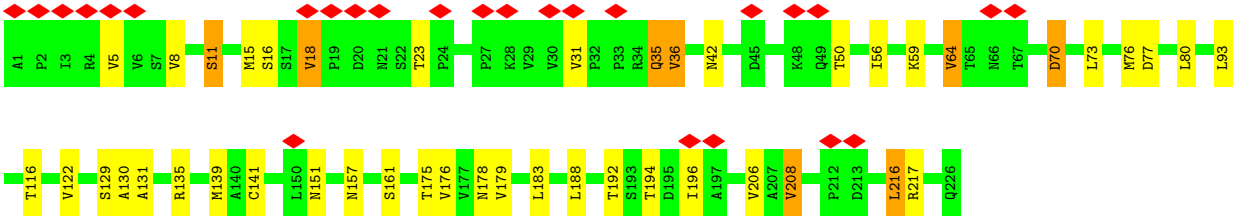
• Molecule 3: P1

Chain CB:



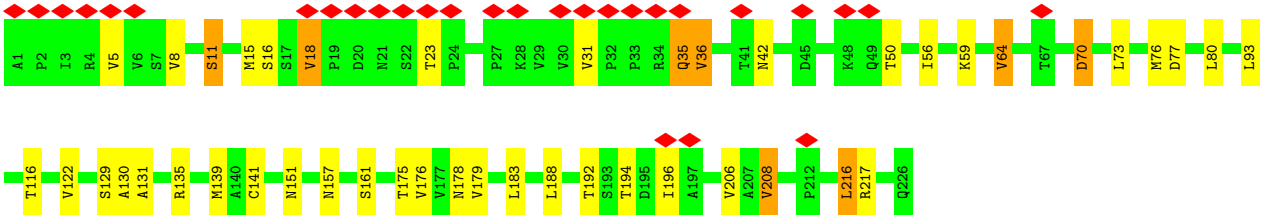
• Molecule 3: P1

Chain CC:



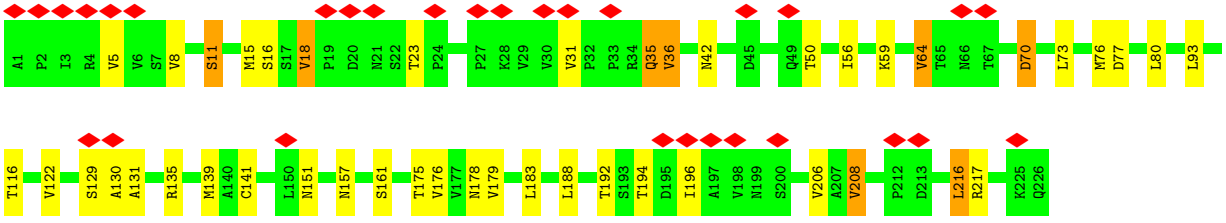
• Molecule 3: P1

Chain CD:



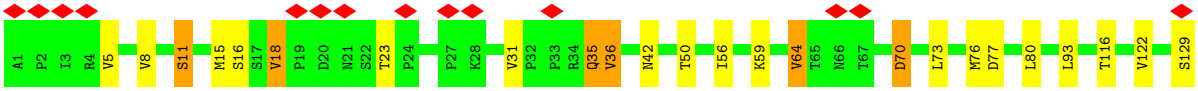
• Molecule 3: P1

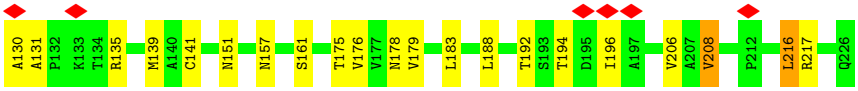
Chain CE:



• Molecule 3: P1

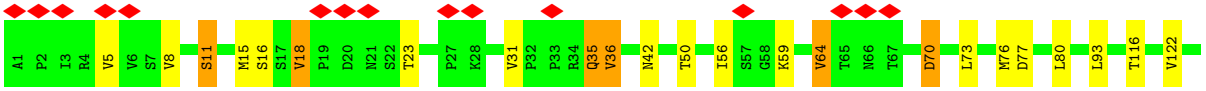
Chain CF:





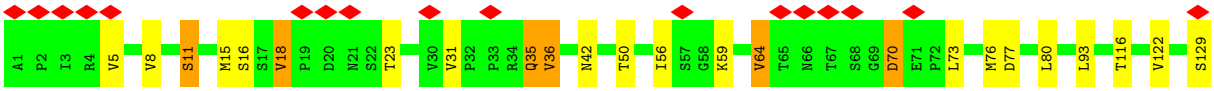
• Molecule 3: P1

Chain CG:



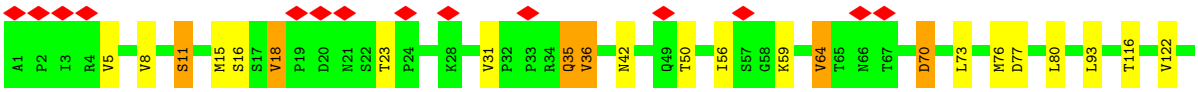
• Molecule 3: P1

Chain CH:



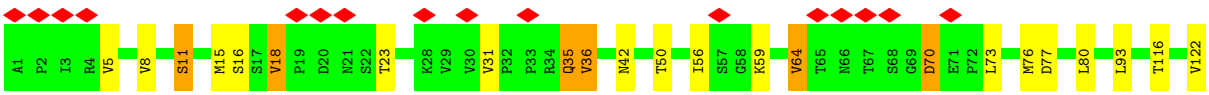
• Molecule 3: P1

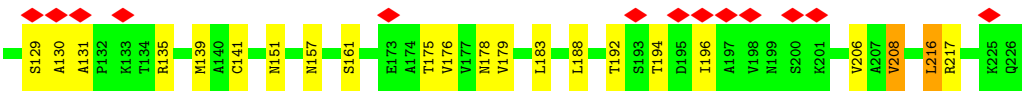
Chain CI:



• Molecule 3: P1

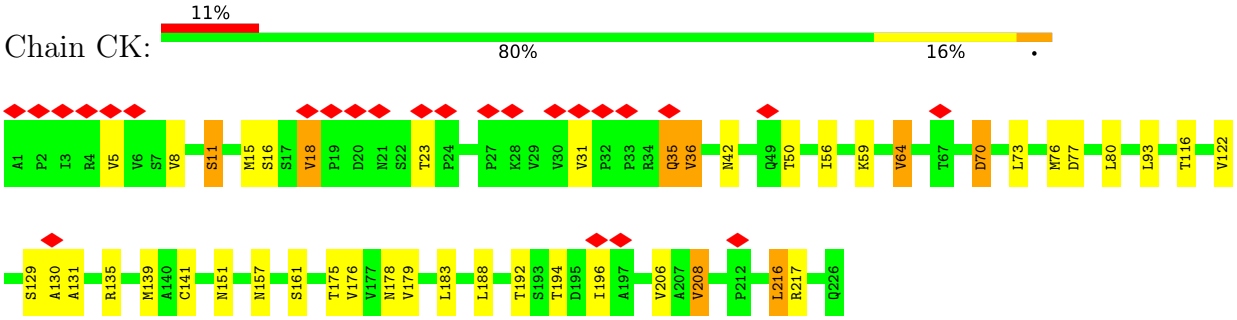
Chain CJ:





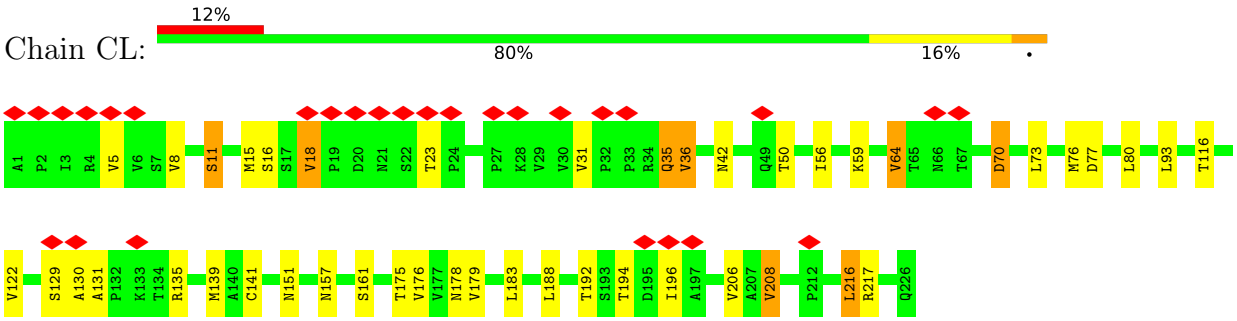
• Molecule 3: P1

Chain CK:



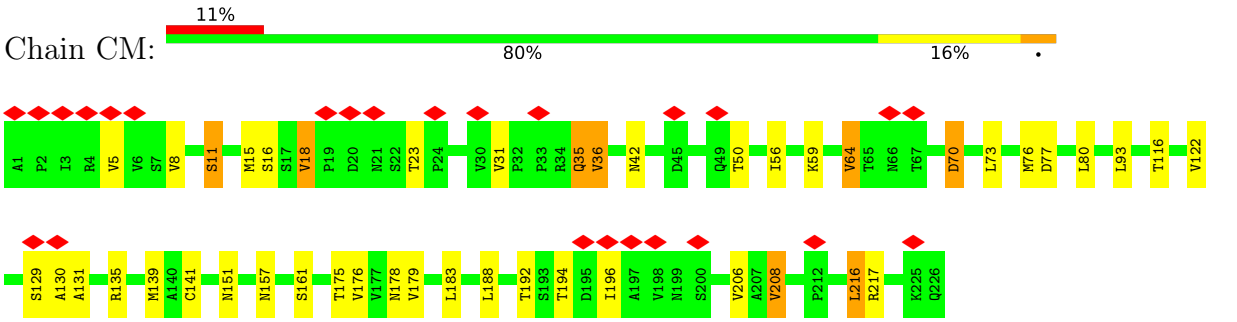
• Molecule 3: P1

Chain CL:



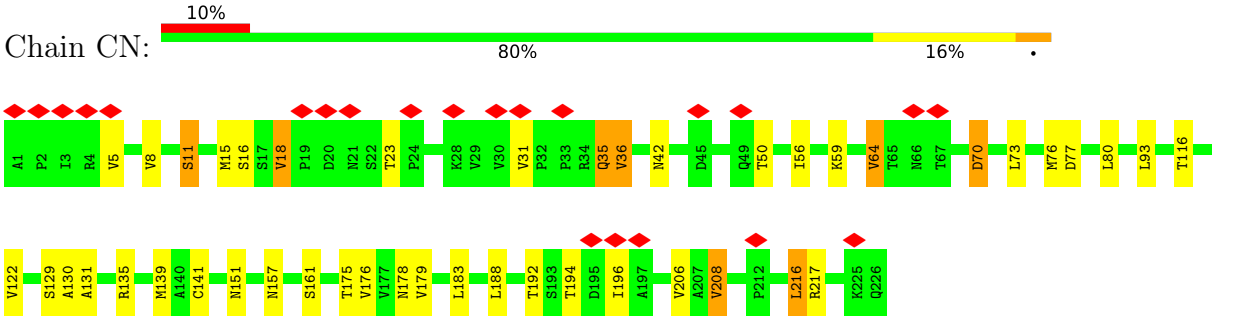
• Molecule 3: P1

Chain CM:



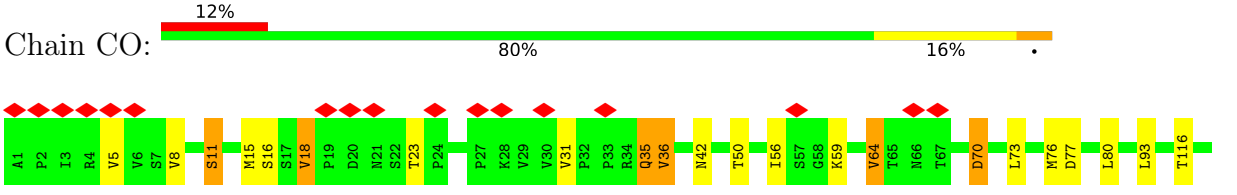
• Molecule 3: P1

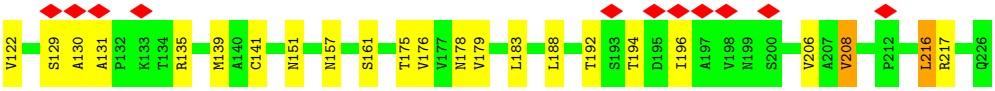
Chain CN:



• Molecule 3: P1

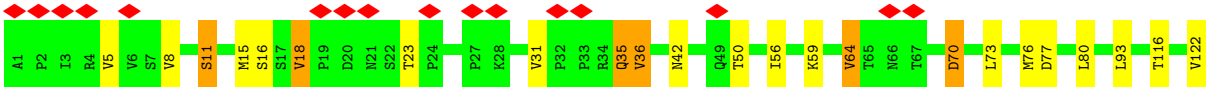
Chain CO:

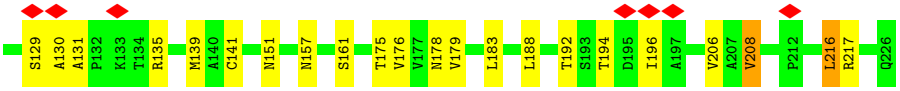




• Molecule 3: P1

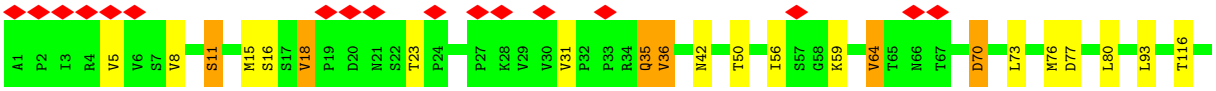
Chain CP:





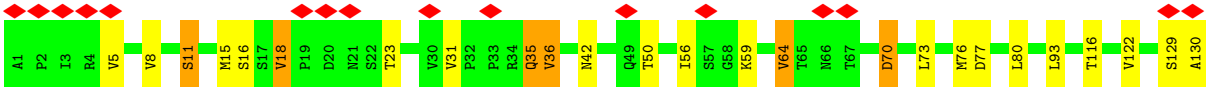
• Molecule 3: P1

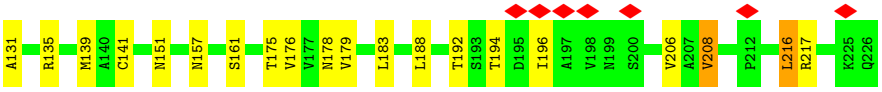
Chain CQ:



• Molecule 3: P1

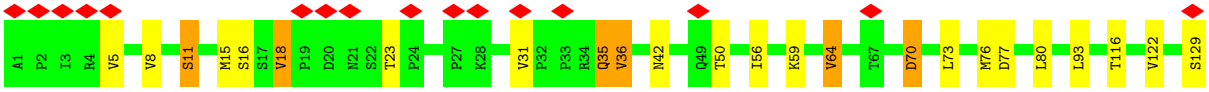
Chain CR:





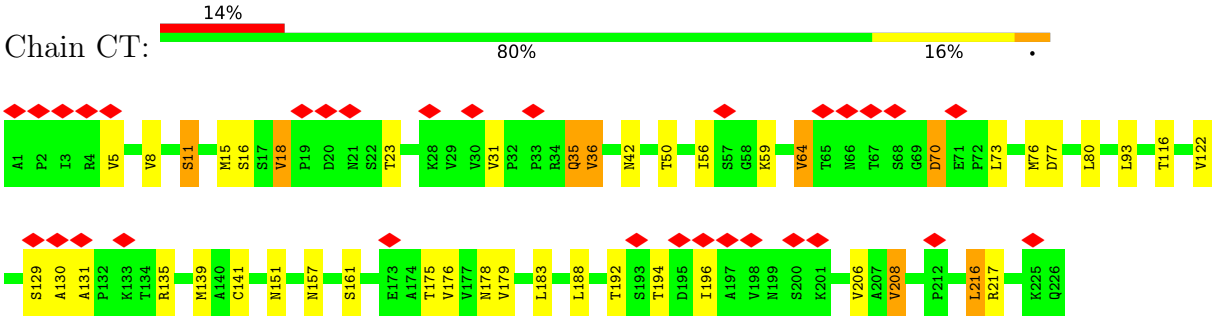
• Molecule 3: P1

Chain CS:



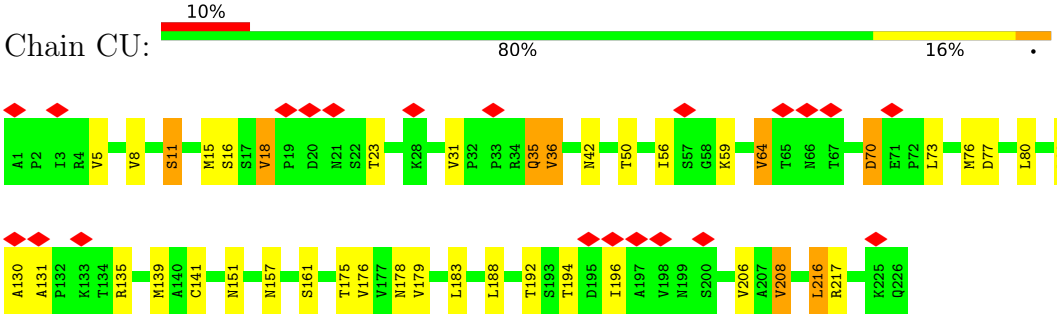
• Molecule 3: P1

Chain CT:



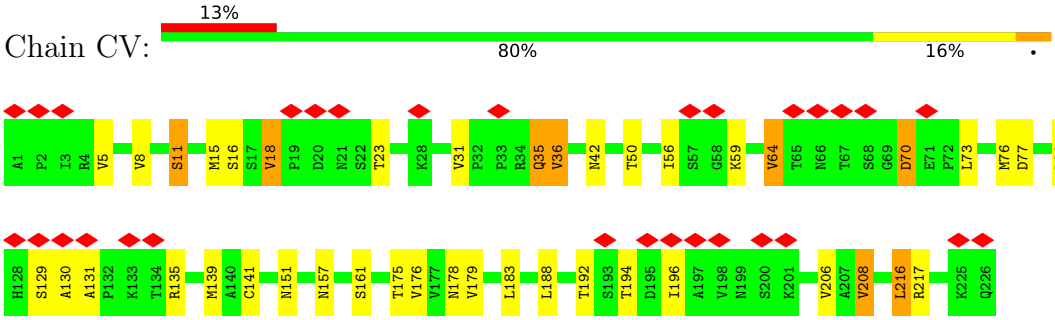
- Molecule 3: P1

Chain CU:



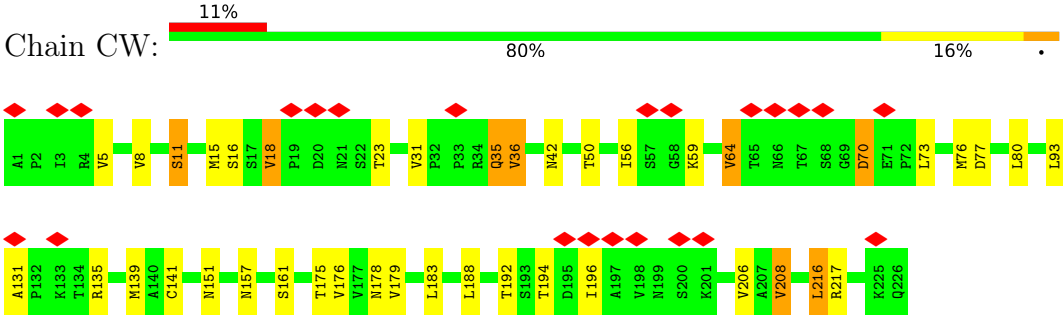
- Molecule 3: P1

Chain CV:



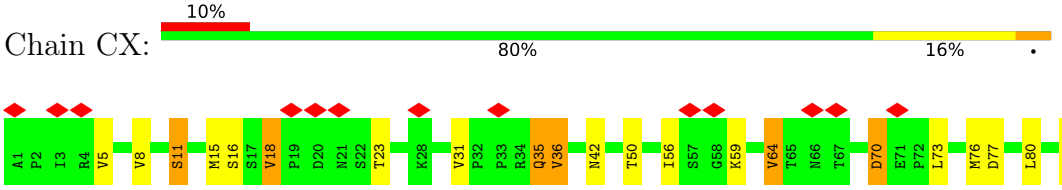
- Molecule 3: P1

Chain CW:



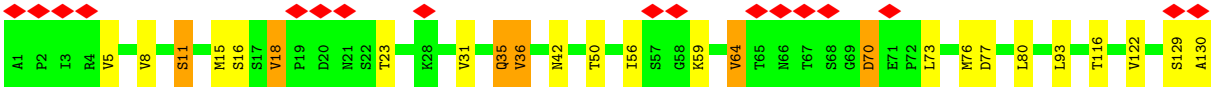
- Molecule 3: P1

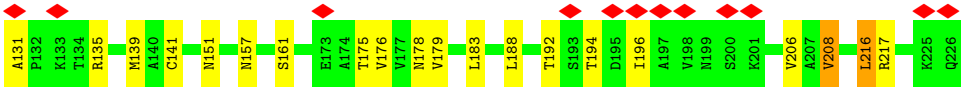
Chain CX:



• Molecule 3: P1

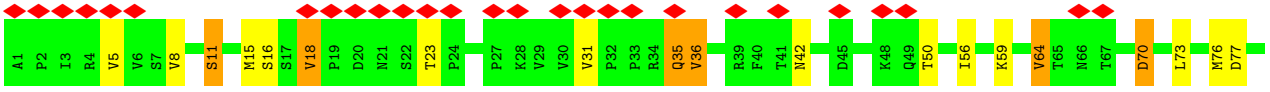
Chain CY:

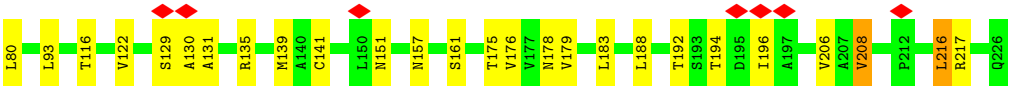




• Molecule 3: P1

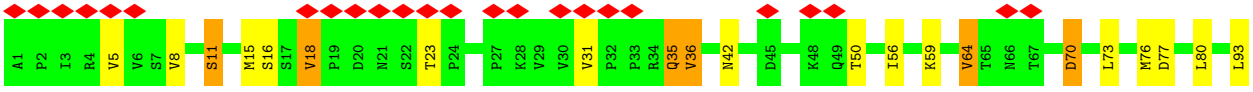
Chain CZ:





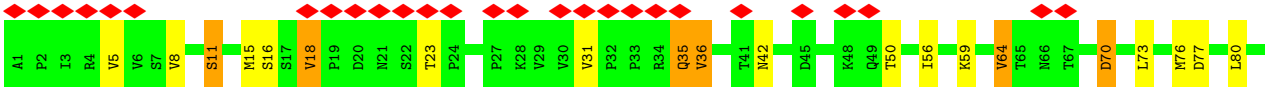
• Molecule 3: P1

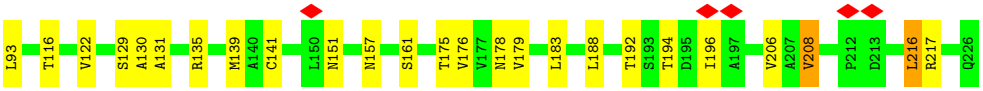
Chain C0:



• Molecule 3: P1

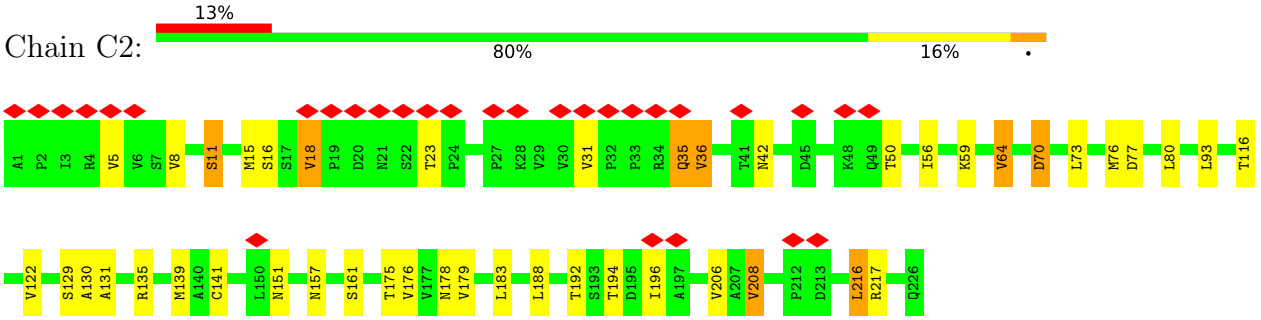
Chain C1:





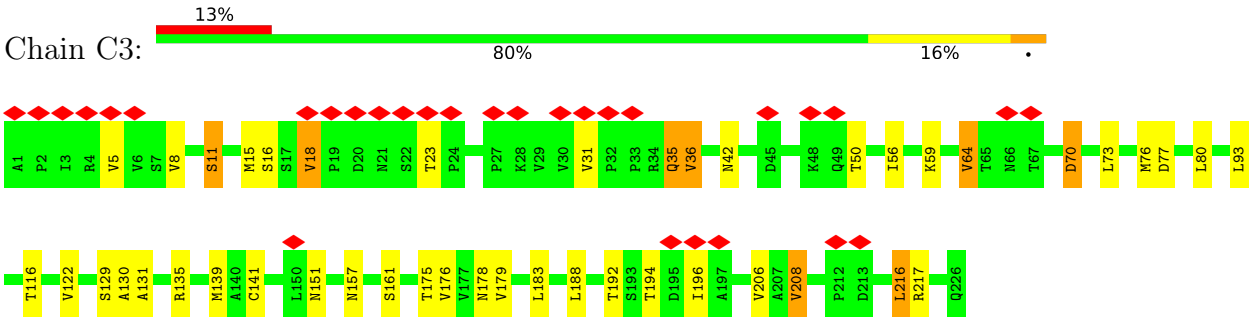
• Molecule 3: P1

Chain C2:



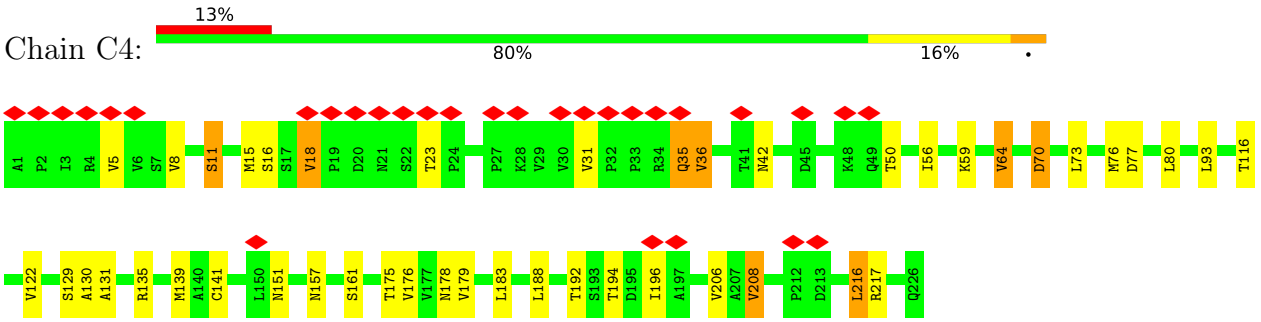
• Molecule 3: P1

Chain C3:



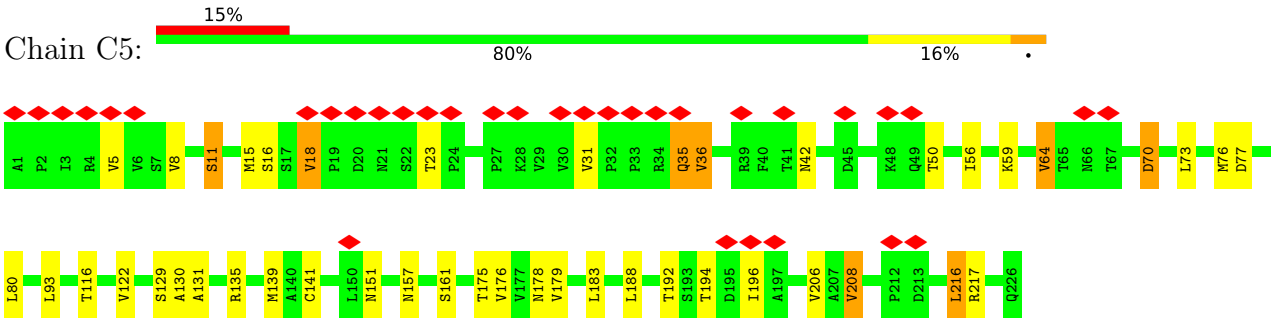
• Molecule 3: P1

Chain C4:



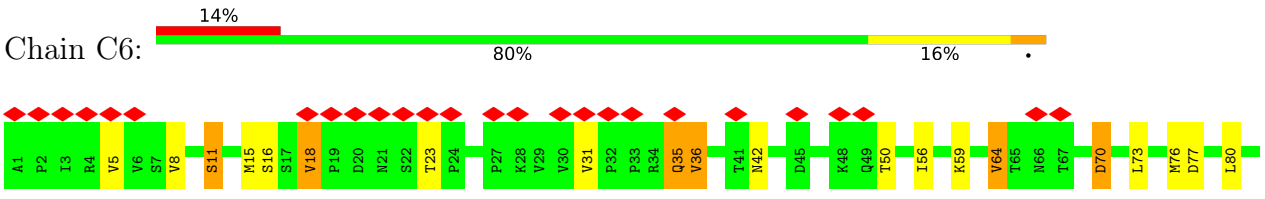
• Molecule 3: P1

Chain C5:



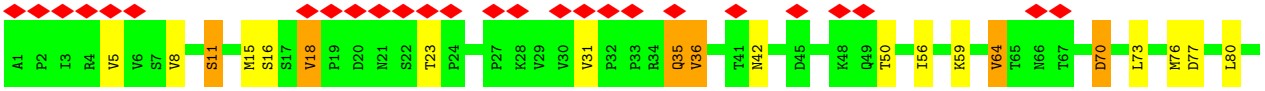
• Molecule 3: P1

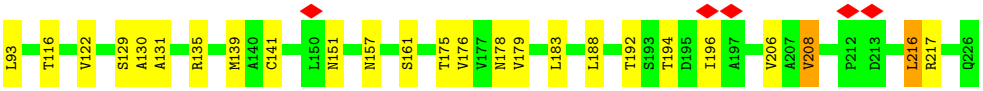
Chain C6:



• Molecule 3: P1

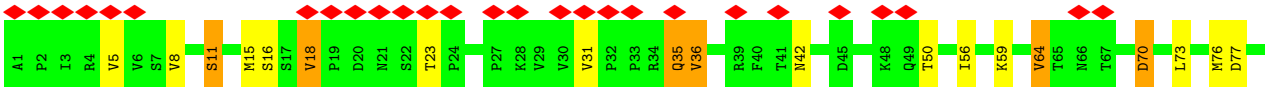
Chain C7:





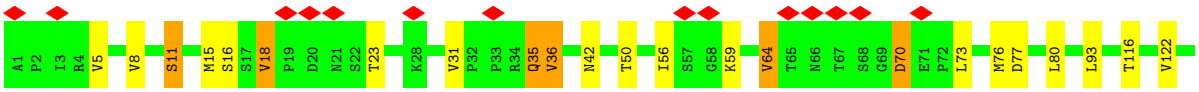
• Molecule 3: P1

Chain C8:



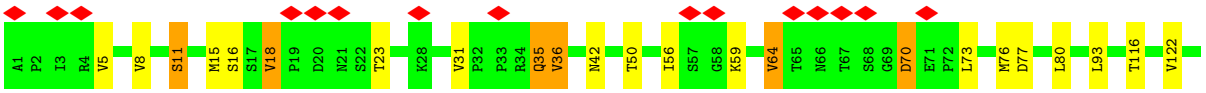
• Molecule 3: P1

Chain C9:



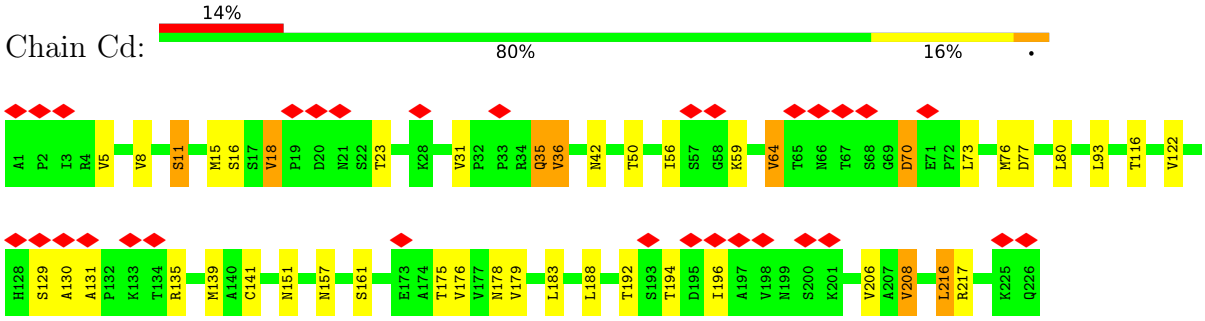
• Molecule 3: P1

Chain Cc:



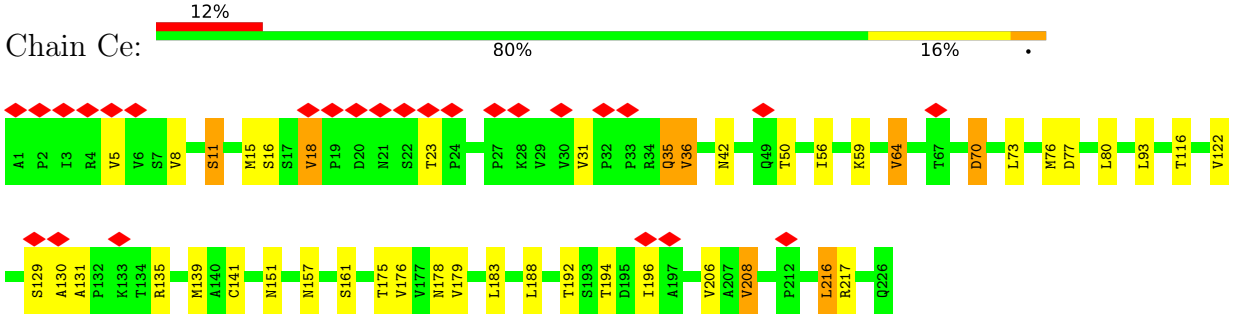
• Molecule 3: P1

Chain Cd:



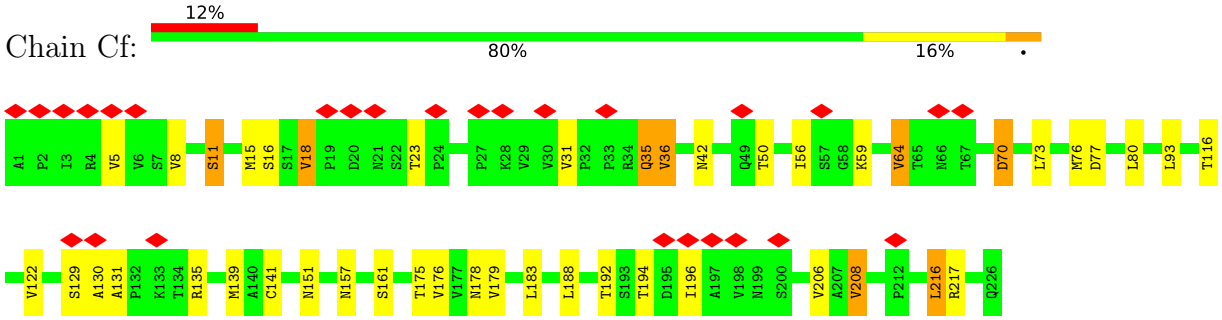
• Molecule 3: P1

Chain Ce:



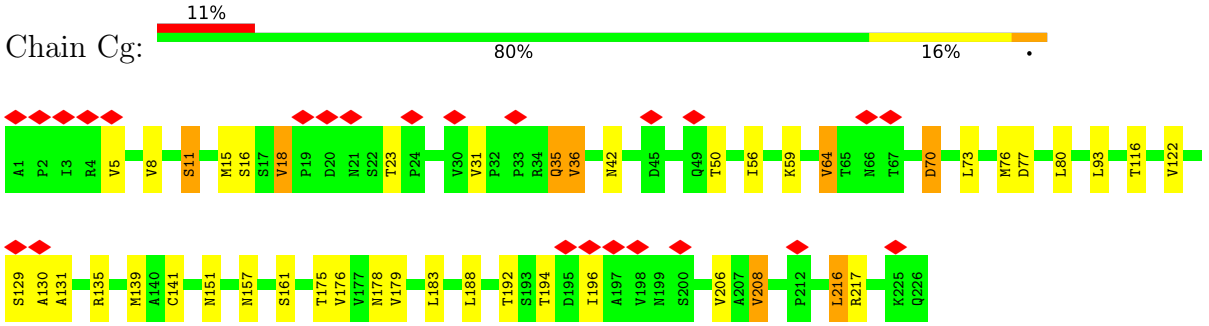
• Molecule 3: P1

Chain Cf:



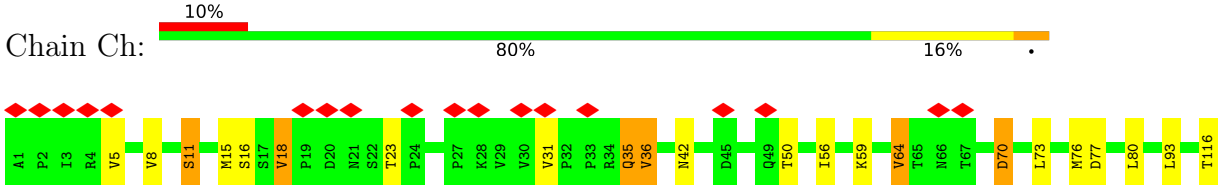
• Molecule 3: P1

Chain Cg:



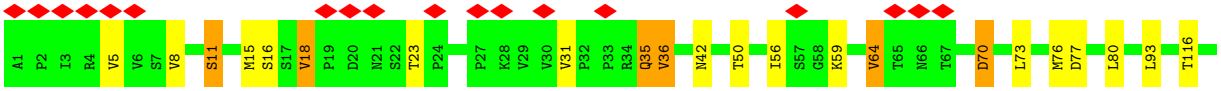
• Molecule 3: P1

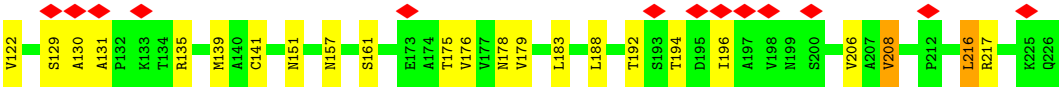
Chain Ch:



• Molecule 3: P1

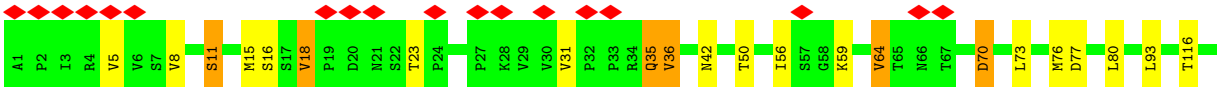
Chain Ci:

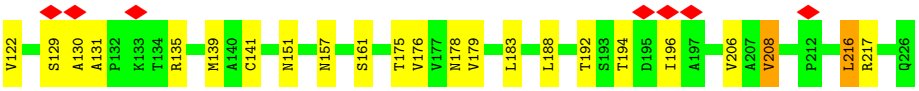




• Molecule 3: P1

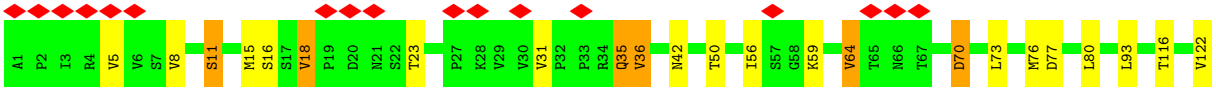
Chain Cj:





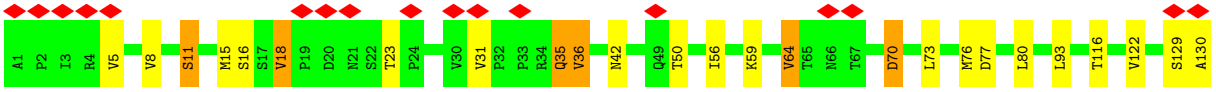
• Molecule 3: P1

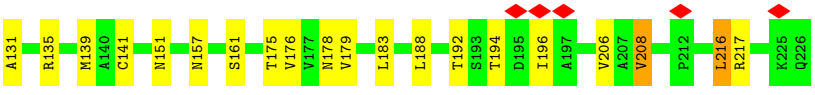
Chain Ck:



• Molecule 3: P1

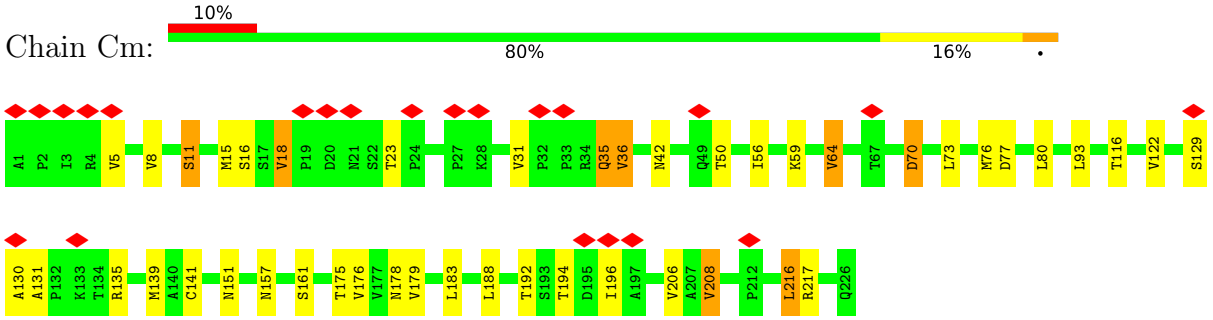
Chain Cl:





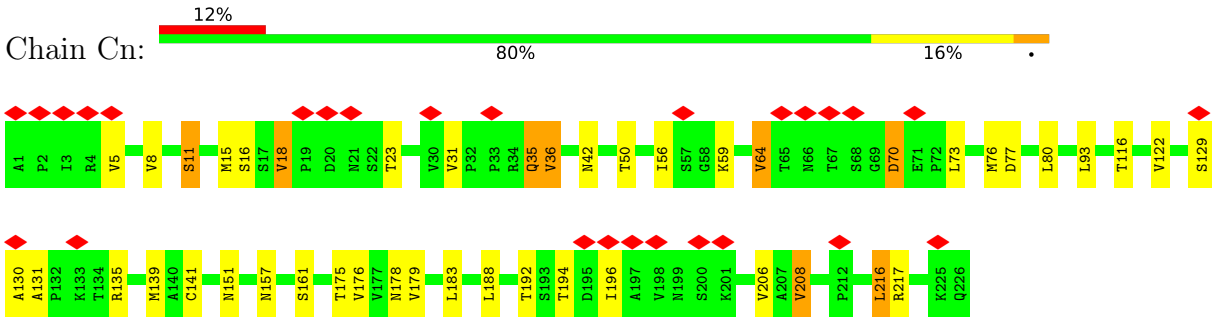
• Molecule 3: P1

Chain Cm:



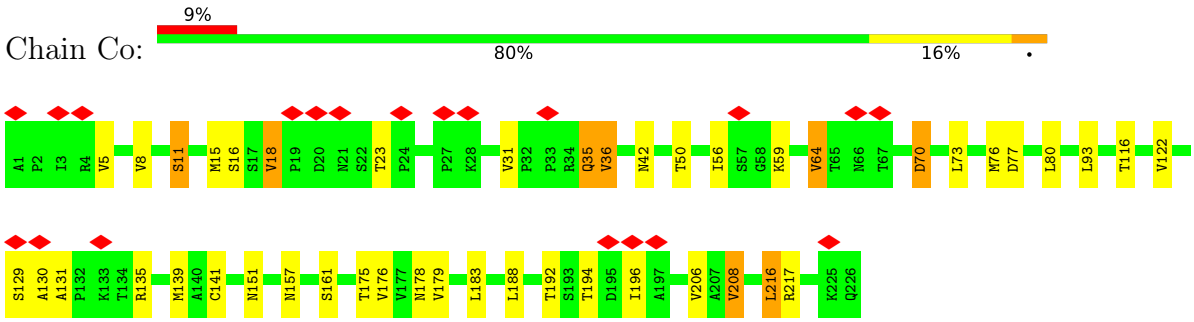
• Molecule 3: P1

Chain Cn:



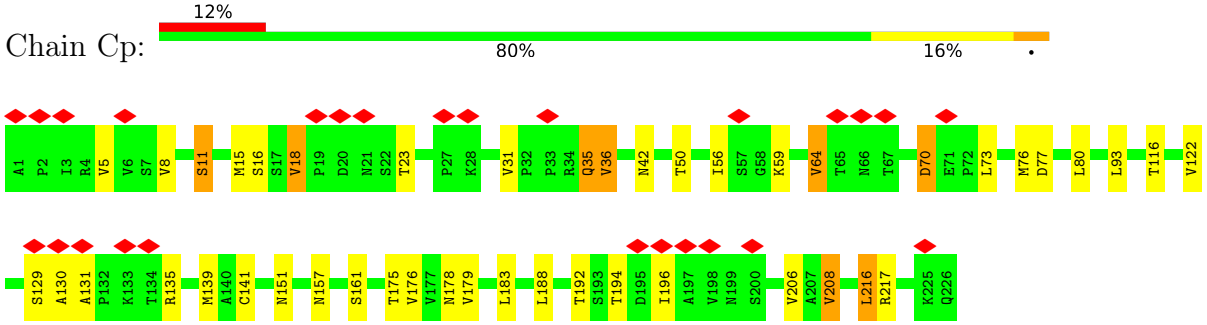
• Molecule 3: P1

Chain Co:



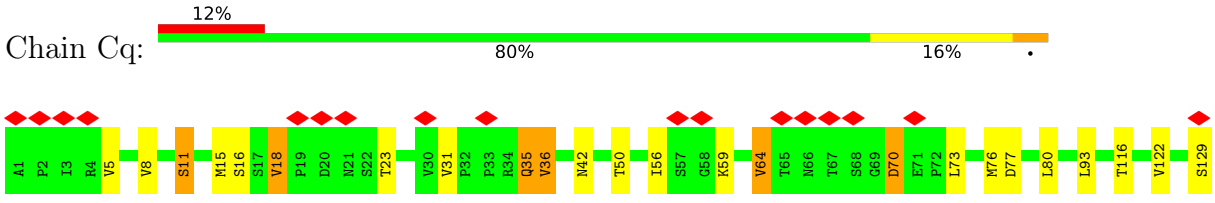
• Molecule 3: P1

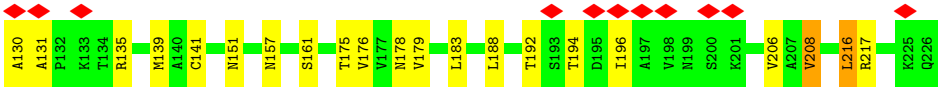
Chain Cp:



• Molecule 3: P1

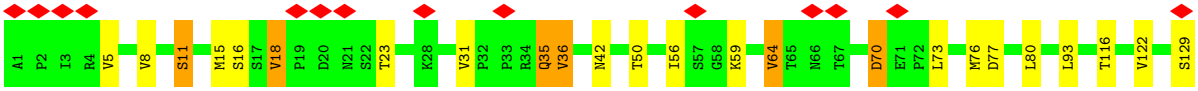
Chain Cq:





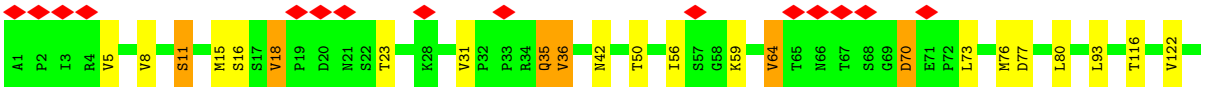
• Molecule 3: P1

Chain Cr:



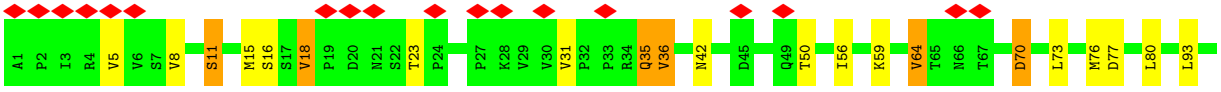
• Molecule 3: P1

Chain Cs:



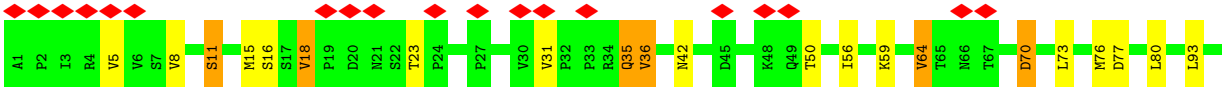
• Molecule 3: P1

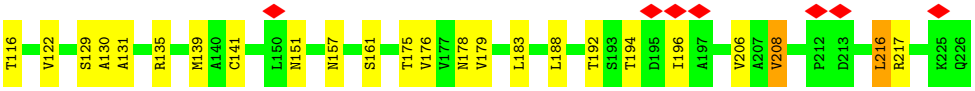
Chain Ct:



• Molecule 3: P1

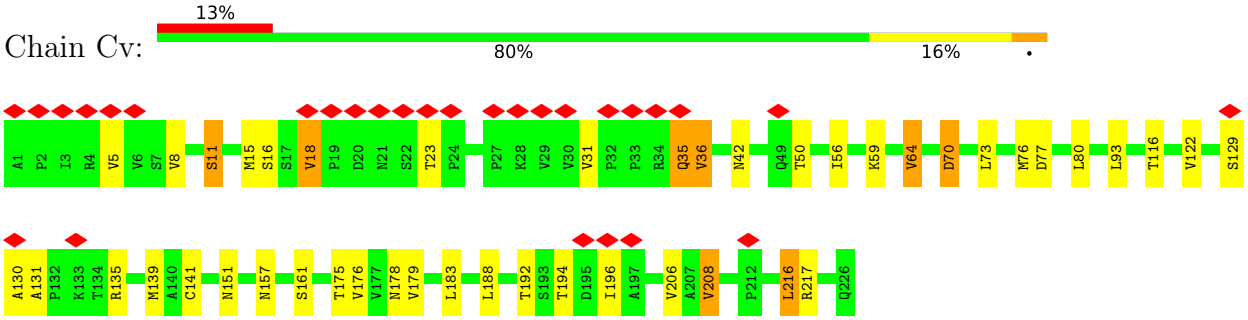
Chain Cu:





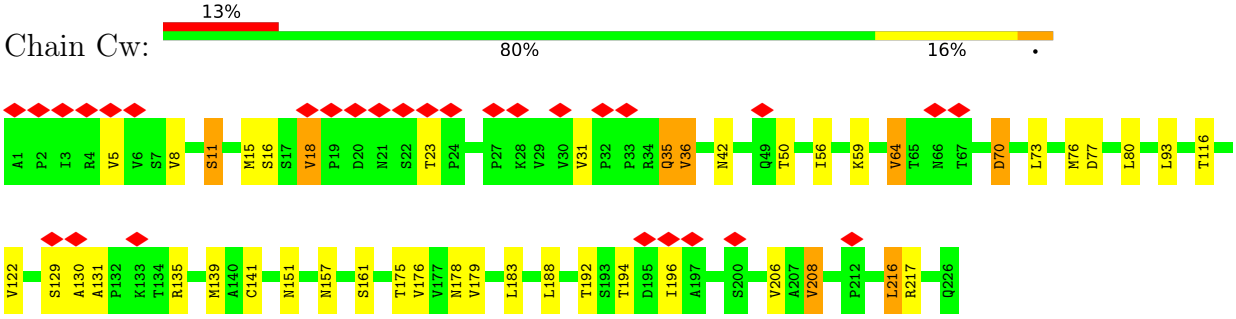
• Molecule 3: P1

Chain Cv:



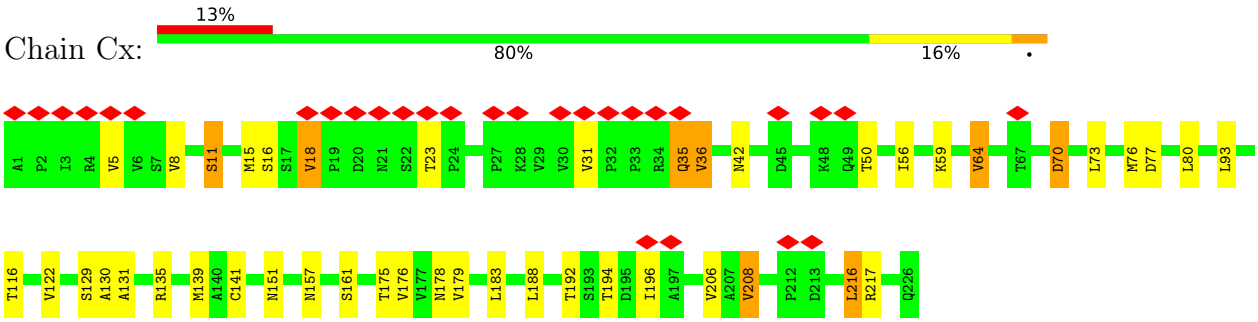
• Molecule 3: P1

Chain Cw:



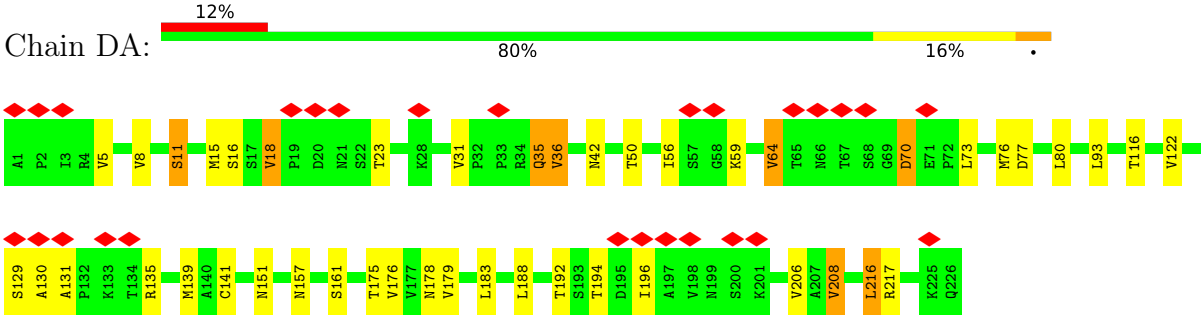
• Molecule 3: P1

Chain Cx:



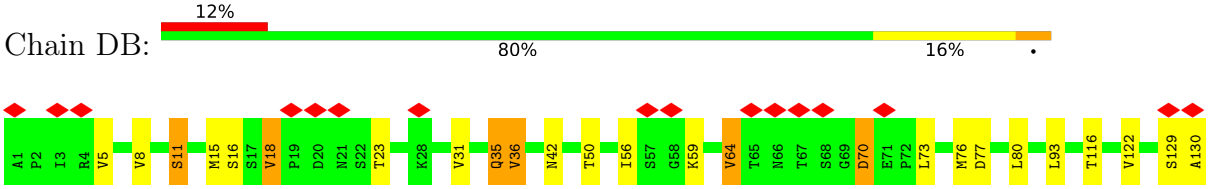
• Molecule 3: P1

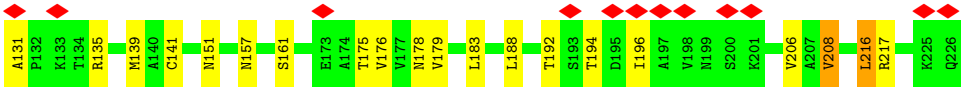
Chain DA:



• Molecule 3: P1

Chain DB:




A131
P132
K133
T134
R135
M139
A140
C141
N151
N157
S161
E173
A174
T175
V176
V177
N178
V179
L183
L188
T192
S193
T194
D195
I196
A197
V198
N199
S200
K201
V206
A207
V208
L216
R217
K225
Q226

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	227	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING, EACH PARTICLE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	87209	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	5.000	Depositor
Minimum map value	-3.303	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.982	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	412.80002, 412.80002, 412.80002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.72, 1.72, 1.72	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.77	0/1992	1.12	17/2721 (0.6%)
1	A1	0.76	0/1992	1.12	17/2721 (0.6%)
1	A2	0.76	0/1992	1.13	17/2721 (0.6%)
1	A3	0.76	0/1992	1.12	17/2721 (0.6%)
1	A4	0.76	0/1992	1.12	17/2721 (0.6%)
1	A5	0.76	0/1992	1.13	17/2721 (0.6%)
1	A6	0.77	0/1992	1.12	17/2721 (0.6%)
1	A7	0.76	0/1992	1.12	18/2721 (0.7%)
1	A8	0.76	0/1992	1.13	17/2721 (0.6%)
1	A9	0.76	0/1992	1.12	17/2721 (0.6%)
1	AA	0.76	0/1992	1.12	17/2721 (0.6%)
1	AB	0.76	0/1992	1.12	17/2721 (0.6%)
1	AC	0.76	0/1992	1.12	17/2721 (0.6%)
1	AD	0.76	0/1992	1.12	17/2721 (0.6%)
1	AE	0.76	0/1992	1.12	18/2721 (0.7%)
1	AF	0.76	0/1992	1.12	18/2721 (0.7%)
1	AG	0.76	0/1992	1.12	17/2721 (0.6%)
1	AH	0.76	0/1992	1.12	17/2721 (0.6%)
1	AI	0.76	0/1992	1.12	17/2721 (0.6%)
1	AJ	0.76	0/1992	1.12	17/2721 (0.6%)
1	AK	0.76	0/1992	1.12	18/2721 (0.7%)
1	AL	0.76	0/1992	1.12	17/2721 (0.6%)
1	AM	0.76	0/1992	1.12	17/2721 (0.6%)
1	AN	0.77	0/1992	1.12	17/2721 (0.6%)
1	AO	0.76	0/1992	1.12	18/2721 (0.7%)
1	AP	0.76	0/1992	1.12	17/2721 (0.6%)
1	AQ	0.77	0/1992	1.12	17/2721 (0.6%)
1	AR	0.76	0/1992	1.12	17/2721 (0.6%)
1	AS	0.76	0/1992	1.12	18/2721 (0.7%)
1	AT	0.76	0/1992	1.12	17/2721 (0.6%)
1	AU	0.76	0/1992	1.12	17/2721 (0.6%)
1	AV	0.76	0/1992	1.12	17/2721 (0.6%)
1	AW	0.76	0/1992	1.12	17/2721 (0.6%)
1	AX	0.76	0/1992	1.12	18/2721 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	AY	0.76	0/1992	1.12	17/2721 (0.6%)
1	AZ	0.77	0/1992	1.12	17/2721 (0.6%)
1	Aa	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ab	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ac	0.77	0/1992	1.12	18/2721 (0.7%)
1	Ad	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ae	0.76	0/1992	1.12	17/2721 (0.6%)
1	Af	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ag	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ah	0.76	0/1992	1.12	18/2721 (0.7%)
1	Ai	0.76	0/1992	1.12	18/2721 (0.7%)
1	Aj	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ak	0.76	0/1992	1.12	17/2721 (0.6%)
1	Al	0.76	0/1992	1.12	17/2721 (0.6%)
1	Am	0.76	0/1992	1.12	17/2721 (0.6%)
1	An	0.76	0/1992	1.12	17/2721 (0.6%)
1	Ao	0.76	0/1992	1.12	17/2721 (0.6%)
1	DC	0.76	0/1992	1.12	17/2721 (0.6%)
1	DD	0.76	0/1992	1.12	17/2721 (0.6%)
1	DE	0.76	0/1992	1.12	17/2721 (0.6%)
1	DF	0.76	0/1992	1.12	17/2721 (0.6%)
1	DG	0.76	0/1992	1.12	17/2721 (0.6%)
1	DH	0.76	0/1992	1.12	17/2721 (0.6%)
1	DI	0.76	0/1992	1.12	17/2721 (0.6%)
1	DJ	0.76	0/1992	1.12	17/2721 (0.6%)
1	DK	0.76	0/1992	1.12	17/2721 (0.6%)
2	B0	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B1	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B2	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B3	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B4	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	B5	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B6	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	B7	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B8	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	B9	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BA	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BB	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BC	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BD	0.78	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BE	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BF	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BG	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	BH	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BI	0.78	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BJ	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BK	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BL	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BM	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BN	0.78	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BO	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BP	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BQ	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BR	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BS	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BT	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	BU	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BV	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BW	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BX	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BY	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	BZ	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Ba	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bb	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	Bc	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bd	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Be	0.78	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	Bf	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bg	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bh	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bi	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bj	0.77	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	Bk	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bl	0.77	1/1607 (0.1%)	0.99	8/2208 (0.4%)
2	Bm	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bn	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bo	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bp	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bq	0.77	1/1607 (0.1%)	0.99	8/2208 (0.4%)
2	Br	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bs	0.78	1/1607 (0.1%)	0.99	7/2208 (0.3%)
2	Bt	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bu	0.78	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bv	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bw	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)
2	Bx	0.77	1/1607 (0.1%)	0.99	6/2208 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	C0	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C1	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C2	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C3	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C4	0.82	1/1768 (0.1%)	1.04	6/2420 (0.2%)
3	C5	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C6	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C7	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C8	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	C9	0.82	1/1768 (0.1%)	1.04	6/2420 (0.2%)
3	CA	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CB	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CC	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CD	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CE	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CF	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CG	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CH	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CI	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CJ	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CK	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CL	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CM	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CN	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CO	0.82	1/1768 (0.1%)	1.04	6/2420 (0.2%)
3	CP	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CQ	0.82	1/1768 (0.1%)	1.04	6/2420 (0.2%)
3	CR	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CS	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CT	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CU	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CV	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CW	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CX	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CY	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	CZ	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cc	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cd	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Ce	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cf	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cg	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Ch	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Ci	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	Cj	0.82	1/1768 (0.1%)	1.04	6/2420 (0.2%)
3	Ck	0.82	1/1768 (0.1%)	1.03	7/2420 (0.3%)
3	Cl	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cm	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cn	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Co	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cp	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cq	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cr	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cs	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Ct	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cu	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cv	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cw	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	Cx	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	DA	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
3	DB	0.82	1/1768 (0.1%)	1.03	6/2420 (0.2%)
All	All	0.79	120/322020 (0.0%)	1.06	1771/440940 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A0	0	1
1	A1	0	1
1	A2	0	1
1	A3	0	1
1	A4	0	1
1	A5	0	1
1	A6	0	1
1	A7	0	1
1	A8	0	1
1	A9	0	1
1	AA	0	1
1	AB	0	1
1	AC	0	1
1	AD	0	1
1	AE	0	1
1	AF	0	1
1	AG	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	AH	0	1
1	AI	0	1
1	AJ	0	1
1	AK	0	1
1	AL	0	1
1	AM	0	1
1	AN	0	1
1	AO	0	1
1	AP	0	1
1	AQ	0	1
1	AR	0	1
1	AS	0	1
1	AT	0	1
1	AU	0	1
1	AV	0	1
1	AW	0	1
1	AX	0	1
1	AY	0	1
1	AZ	0	1
1	Aa	0	1
1	Ab	0	1
1	Ac	0	1
1	Ad	0	1
1	Ae	0	1
1	Af	0	1
1	Ag	0	1
1	Ah	0	1
1	Ai	0	1
1	Aj	0	1
1	Ak	0	1
1	Al	0	1
1	Am	0	1
1	An	0	1
1	Ao	0	1
1	DC	0	1
1	DD	0	1
1	DE	0	1
1	DF	0	1
1	DG	0	1
1	DH	0	1
1	DI	0	1
1	DJ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	DK	0	1
2	B0	0	2
2	B1	0	2
2	B2	0	2
2	B3	0	2
2	B4	0	2
2	B5	0	2
2	B6	0	2
2	B7	0	2
2	B8	0	2
2	B9	0	2
2	BA	0	2
2	BB	0	2
2	BC	0	2
2	BD	0	2
2	BE	0	2
2	BF	0	2
2	BG	0	2
2	BH	0	2
2	BI	0	2
2	BJ	0	2
2	BK	0	2
2	BL	0	2
2	BM	0	2
2	BN	0	2
2	BO	0	2
2	BP	0	2
2	BQ	0	2
2	BR	0	2
2	BS	0	2
2	BT	0	2
2	BU	0	2
2	BV	0	2
2	BW	0	2
2	BX	0	2
2	BY	0	2
2	BZ	0	2
2	Ba	0	2
2	Bb	0	2
2	Bc	0	2
2	Bd	0	2
2	Be	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	Bf	0	2
2	Bg	0	2
2	Bh	0	2
2	Bi	0	2
2	Bj	0	2
2	Bk	0	2
2	Bl	0	2
2	Bm	0	2
2	Bn	0	2
2	Bo	0	2
2	Bp	0	2
2	Bq	0	2
2	Br	0	2
2	Bs	0	2
2	Bt	0	2
2	Bu	0	2
2	Bv	0	2
2	Bw	0	2
2	Bx	0	2
All	All	0	180

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B2	222	VAL	CB-CG1	-5.18	1.42	1.52
3	Cc	141	CYS	CB-SG	-5.17	1.73	1.81
3	Cg	141	CYS	CB-SG	-5.16	1.73	1.81
3	C1	141	CYS	CB-SG	-5.15	1.73	1.81
3	Cq	141	CYS	CB-SG	-5.15	1.73	1.81
3	CN	141	CYS	CB-SG	-5.15	1.73	1.81
2	BK	222	VAL	CB-CG1	-5.14	1.42	1.52
2	BO	222	VAL	CB-CG1	-5.14	1.42	1.52
2	BU	222	VAL	CB-CG1	-5.14	1.42	1.52
2	B4	222	VAL	CB-CG1	-5.14	1.42	1.52
2	B6	222	VAL	CB-CG1	-5.14	1.42	1.52
2	Bn	222	VAL	CB-CG1	-5.14	1.42	1.52
2	B3	222	VAL	CB-CG1	-5.14	1.42	1.52
2	BR	222	VAL	CB-CG1	-5.13	1.42	1.52
2	BX	222	VAL	CB-CG1	-5.13	1.42	1.52
3	C5	141	CYS	CB-SG	-5.13	1.73	1.81
3	Cf	141	CYS	CB-SG	-5.13	1.73	1.81
2	Bc	222	VAL	CB-CG1	-5.13	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Bg	222	VAL	CB-CG1	-5.13	1.42	1.52
2	Bm	222	VAL	CB-CG1	-5.13	1.42	1.52
3	CC	141	CYS	CB-SG	-5.13	1.73	1.81
3	Cx	141	CYS	CB-SG	-5.13	1.73	1.81
2	B8	222	VAL	CB-CG1	-5.12	1.42	1.52
2	BE	222	VAL	CB-CG1	-5.12	1.42	1.52
2	Bd	222	VAL	CB-CG1	-5.12	1.42	1.52
2	Bb	222	VAL	CB-CG1	-5.12	1.42	1.52
3	Ch	141	CYS	CB-SG	-5.12	1.73	1.81
2	BS	222	VAL	CB-CG1	-5.12	1.42	1.52
2	BT	222	VAL	CB-CG1	-5.12	1.42	1.52
3	CD	141	CYS	CB-SG	-5.12	1.73	1.81
3	Cv	141	CYS	CB-SG	-5.12	1.73	1.81
2	Bs	222	VAL	CB-CG1	-5.12	1.42	1.52
3	CW	141	CYS	CB-SG	-5.12	1.73	1.81
2	BD	222	VAL	CB-CG1	-5.12	1.42	1.52
2	Bo	222	VAL	CB-CG1	-5.12	1.42	1.52
2	BQ	222	VAL	CB-CG1	-5.12	1.42	1.52
2	Bh	222	VAL	CB-CG1	-5.12	1.42	1.52
3	C6	141	CYS	CB-SG	-5.12	1.73	1.81
3	Cr	141	CYS	CB-SG	-5.12	1.73	1.81
2	Bi	222	VAL	CB-CG1	-5.11	1.42	1.52
2	Bu	222	VAL	CB-CG1	-5.11	1.42	1.52
3	Cm	141	CYS	CB-SG	-5.11	1.73	1.81
2	Br	222	VAL	CB-CG1	-5.11	1.42	1.52
2	BA	222	VAL	CB-CG1	-5.11	1.42	1.52
2	BZ	222	VAL	CB-CG1	-5.11	1.42	1.52
2	Bw	222	VAL	CB-CG1	-5.11	1.42	1.52
3	CS	141	CYS	CB-SG	-5.11	1.73	1.81
3	C8	141	CYS	CB-SG	-5.11	1.73	1.81
2	BN	222	VAL	CB-CG1	-5.10	1.42	1.52
3	CA	141	CYS	CB-SG	-5.10	1.73	1.81
3	Ci	141	CYS	CB-SG	-5.10	1.73	1.81
2	Bj	222	VAL	CB-CG1	-5.10	1.42	1.52
2	Bv	222	VAL	CB-CG1	-5.10	1.42	1.52
2	BJ	222	VAL	CB-CG1	-5.10	1.42	1.52
2	B7	222	VAL	CB-CG1	-5.10	1.42	1.52
2	Bq	222	VAL	CB-CG1	-5.10	1.42	1.52
3	CL	141	CYS	CB-SG	-5.10	1.73	1.81
3	CR	141	CYS	CB-SG	-5.10	1.73	1.81
3	Cp	141	CYS	CB-SG	-5.10	1.73	1.81
2	BI	222	VAL	CB-CG1	-5.10	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CB	141	CYS	CB-SG	-5.10	1.73	1.81
3	Cw	141	CYS	CB-SG	-5.10	1.73	1.81
2	B0	222	VAL	CB-CG1	-5.10	1.42	1.52
3	C7	141	CYS	CB-SG	-5.09	1.73	1.81
2	B5	222	VAL	CB-CG1	-5.09	1.42	1.52
3	CV	141	CYS	CB-SG	-5.09	1.73	1.81
2	Bf	222	VAL	CB-CG1	-5.09	1.42	1.52
3	CM	141	CYS	CB-SG	-5.09	1.73	1.81
3	DA	141	CYS	CB-SG	-5.09	1.73	1.81
3	C2	141	CYS	CB-SG	-5.09	1.73	1.81
3	Cu	141	CYS	CB-SG	-5.09	1.73	1.81
2	Ba	222	VAL	CB-CG1	-5.09	1.42	1.52
3	CY	141	CYS	CB-SG	-5.09	1.73	1.81
3	C3	141	CYS	CB-SG	-5.09	1.73	1.81
3	CJ	141	CYS	CB-SG	-5.08	1.73	1.81
2	BB	222	VAL	CB-CG1	-5.08	1.42	1.52
2	BC	222	VAL	CB-CG1	-5.08	1.42	1.52
2	Bl	222	VAL	CB-CG1	-5.08	1.42	1.52
2	BM	222	VAL	CB-CG1	-5.08	1.42	1.52
3	DB	141	CYS	CB-SG	-5.08	1.73	1.81
2	BF	222	VAL	CB-CG1	-5.08	1.42	1.52
2	BP	222	VAL	CB-CG1	-5.08	1.42	1.52
2	Bp	222	VAL	CB-CG1	-5.08	1.42	1.52
3	CP	141	CYS	CB-SG	-5.08	1.73	1.81
2	BL	222	VAL	CB-CG1	-5.07	1.42	1.52
2	B9	222	VAL	CB-CG1	-5.07	1.42	1.52
3	CG	141	CYS	CB-SG	-5.07	1.73	1.81
3	CH	141	CYS	CB-SG	-5.07	1.73	1.81
3	CI	141	CYS	CB-SG	-5.07	1.73	1.81
3	CZ	141	CYS	CB-SG	-5.07	1.73	1.81
2	BW	222	VAL	CB-CG1	-5.07	1.42	1.52
2	B1	222	VAL	CB-CG1	-5.07	1.42	1.52
3	Cn	141	CYS	CB-SG	-5.07	1.73	1.81
2	Bk	222	VAL	CB-CG1	-5.07	1.42	1.52
3	Co	141	CYS	CB-SG	-5.07	1.73	1.81
3	Ce	141	CYS	CB-SG	-5.06	1.73	1.81
3	Ct	141	CYS	CB-SG	-5.06	1.73	1.81
2	BV	222	VAL	CB-CG1	-5.06	1.42	1.52
3	CF	141	CYS	CB-SG	-5.06	1.73	1.81
2	Bt	222	VAL	CB-CG1	-5.06	1.42	1.52
3	C9	141	CYS	CB-SG	-5.06	1.73	1.81
3	CU	141	CYS	CB-SG	-5.05	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CX	141	CYS	CB-SG	-5.05	1.73	1.81
3	C0	141	CYS	CB-SG	-5.05	1.73	1.81
3	Cs	141	CYS	CB-SG	-5.05	1.73	1.81
3	CQ	141	CYS	CB-SG	-5.05	1.73	1.81
3	Cd	141	CYS	CB-SG	-5.05	1.73	1.81
2	Be	222	VAL	CB-CG1	-5.05	1.42	1.52
3	Ck	141	CYS	CB-SG	-5.04	1.73	1.81
3	CE	141	CYS	CB-SG	-5.04	1.73	1.81
3	Cj	141	CYS	CB-SG	-5.04	1.73	1.81
2	BH	222	VAL	CB-CG1	-5.04	1.42	1.52
2	BY	222	VAL	CB-CG1	-5.04	1.42	1.52
2	Bx	222	VAL	CB-CG1	-5.04	1.42	1.52
3	CK	141	CYS	CB-SG	-5.04	1.73	1.81
3	C4	141	CYS	CB-SG	-5.03	1.73	1.81
3	CT	141	CYS	CB-SG	-5.02	1.73	1.81
3	Cl	141	CYS	CB-SG	-5.02	1.73	1.81
3	CO	141	CYS	CB-SG	-5.01	1.73	1.81
2	BG	222	VAL	CB-CG1	-5.00	1.42	1.52

All (1771) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DE	5	GLY	N-CA-C	10.76	140.00	113.10
1	Ah	5	GLY	N-CA-C	10.76	140.00	113.10
1	A1	5	GLY	N-CA-C	10.76	139.99	113.10
1	A2	5	GLY	N-CA-C	10.75	139.97	113.10
1	AM	5	GLY	N-CA-C	10.75	139.97	113.10
1	A5	5	GLY	N-CA-C	10.75	139.96	113.10
1	A7	5	GLY	N-CA-C	10.75	139.97	113.10
1	Am	5	GLY	N-CA-C	10.74	139.96	113.10
1	DI	5	GLY	N-CA-C	10.74	139.96	113.10
1	AV	5	GLY	N-CA-C	10.74	139.96	113.10
1	DK	5	GLY	N-CA-C	10.74	139.96	113.10
1	Ab	5	GLY	N-CA-C	10.74	139.95	113.10
1	AN	5	GLY	N-CA-C	10.74	139.94	113.10
1	A6	5	GLY	N-CA-C	10.74	139.94	113.10
1	Ai	5	GLY	N-CA-C	10.74	139.94	113.10
1	AS	5	GLY	N-CA-C	10.73	139.94	113.10
1	Ag	5	GLY	N-CA-C	10.73	139.93	113.10
1	AH	5	GLY	N-CA-C	10.73	139.93	113.10
1	DJ	5	GLY	N-CA-C	10.73	139.93	113.10
1	AC	5	GLY	N-CA-C	10.73	139.93	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AE	5	GLY	N-CA-C	10.73	139.93	113.10
1	AR	5	GLY	N-CA-C	10.73	139.93	113.10
1	AW	5	GLY	N-CA-C	10.73	139.93	113.10
1	Ad	5	GLY	N-CA-C	10.73	139.93	113.10
1	DD	5	GLY	N-CA-C	10.73	139.93	113.10
1	A9	5	GLY	N-CA-C	10.73	139.92	113.10
1	AP	5	GLY	N-CA-C	10.73	139.92	113.10
1	Aa	5	GLY	N-CA-C	10.73	139.92	113.10
1	Ac	5	GLY	N-CA-C	10.73	139.92	113.10
1	AX	5	GLY	N-CA-C	10.72	139.91	113.10
1	AI	5	GLY	N-CA-C	10.72	139.90	113.10
1	AY	5	GLY	N-CA-C	10.72	139.90	113.10
1	A4	5	GLY	N-CA-C	10.72	139.90	113.10
1	AB	5	GLY	N-CA-C	10.72	139.90	113.10
1	A0	5	GLY	N-CA-C	10.72	139.90	113.10
1	Ao	5	GLY	N-CA-C	10.72	139.90	113.10
1	AD	5	GLY	N-CA-C	10.72	139.89	113.10
1	AG	5	GLY	N-CA-C	10.72	139.89	113.10
1	AJ	5	GLY	N-CA-C	10.71	139.88	113.10
1	AQ	5	GLY	N-CA-C	10.71	139.89	113.10
1	AL	5	GLY	N-CA-C	10.71	139.88	113.10
1	AO	5	GLY	N-CA-C	10.71	139.88	113.10
1	AZ	5	GLY	N-CA-C	10.71	139.88	113.10
1	Ae	5	GLY	N-CA-C	10.71	139.88	113.10
1	Aj	5	GLY	N-CA-C	10.71	139.88	113.10
1	DC	5	GLY	N-CA-C	10.71	139.88	113.10
1	AU	5	GLY	N-CA-C	10.71	139.87	113.10
1	Af	5	GLY	N-CA-C	10.71	139.87	113.10
1	Al	5	GLY	N-CA-C	10.71	139.87	113.10
1	DH	5	GLY	N-CA-C	10.71	139.86	113.10
1	AA	5	GLY	N-CA-C	10.70	139.85	113.10
1	AK	5	GLY	N-CA-C	10.70	139.85	113.10
1	AF	5	GLY	N-CA-C	10.70	139.84	113.10
1	Ak	5	GLY	N-CA-C	10.70	139.85	113.10
1	DG	5	GLY	N-CA-C	10.70	139.85	113.10
1	A8	5	GLY	N-CA-C	10.70	139.84	113.10
1	AT	5	GLY	N-CA-C	10.69	139.82	113.10
1	DF	5	GLY	N-CA-C	10.69	139.82	113.10
1	A3	5	GLY	N-CA-C	10.68	139.81	113.10
1	An	5	GLY	N-CA-C	10.67	139.78	113.10
1	AS	207	CYS	N-CA-C	8.43	133.77	111.00
1	AG	207	CYS	N-CA-C	8.43	133.76	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AZ	207	CYS	N-CA-C	8.43	133.76	111.00
1	AR	207	CYS	N-CA-C	8.43	133.75	111.00
1	DH	207	CYS	N-CA-C	8.43	133.76	111.00
1	Ag	207	CYS	N-CA-C	8.43	133.75	111.00
1	Ao	207	CYS	N-CA-C	8.43	133.75	111.00
1	AL	207	CYS	N-CA-C	8.42	133.74	111.00
1	Aa	207	CYS	N-CA-C	8.42	133.74	111.00
1	AF	207	CYS	N-CA-C	8.42	133.74	111.00
1	A5	207	CYS	N-CA-C	8.42	133.74	111.00
1	AQ	207	CYS	N-CA-C	8.42	133.73	111.00
1	AW	207	CYS	N-CA-C	8.42	133.72	111.00
1	A9	207	CYS	N-CA-C	8.42	133.73	111.00
1	Ab	207	CYS	N-CA-C	8.42	133.73	111.00
1	AY	207	CYS	N-CA-C	8.42	133.72	111.00
1	A0	207	CYS	N-CA-C	8.42	133.72	111.00
1	Ac	207	CYS	N-CA-C	8.42	133.73	111.00
1	Af	207	CYS	N-CA-C	8.42	133.72	111.00
1	DG	207	CYS	N-CA-C	8.42	133.72	111.00
1	AK	207	CYS	N-CA-C	8.41	133.72	111.00
1	Al	207	CYS	N-CA-C	8.41	133.72	111.00
1	AC	207	CYS	N-CA-C	8.41	133.71	111.00
1	AP	207	CYS	N-CA-C	8.41	133.71	111.00
1	Aj	207	CYS	N-CA-C	8.41	133.71	111.00
1	DC	207	CYS	N-CA-C	8.41	133.70	111.00
1	AB	207	CYS	N-CA-C	8.41	133.70	111.00
1	AE	207	CYS	N-CA-C	8.41	133.70	111.00
1	AI	207	CYS	N-CA-C	8.41	133.70	111.00
1	AU	207	CYS	N-CA-C	8.41	133.70	111.00
1	Am	207	CYS	N-CA-C	8.40	133.69	111.00
1	An	207	CYS	N-CA-C	8.40	133.69	111.00
1	DJ	207	CYS	N-CA-C	8.40	133.69	111.00
1	AD	207	CYS	N-CA-C	8.40	133.68	111.00
1	AH	207	CYS	N-CA-C	8.40	133.69	111.00
1	AM	207	CYS	N-CA-C	8.40	133.68	111.00
1	A3	207	CYS	N-CA-C	8.40	133.68	111.00
1	Ad	207	CYS	N-CA-C	8.40	133.68	111.00
1	DD	207	CYS	N-CA-C	8.40	133.68	111.00
1	DE	207	CYS	N-CA-C	8.40	133.68	111.00
1	A7	207	CYS	N-CA-C	8.40	133.68	111.00
1	AA	207	CYS	N-CA-C	8.40	133.67	111.00
1	AJ	207	CYS	N-CA-C	8.40	133.67	111.00
1	AO	207	CYS	N-CA-C	8.40	133.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AT	207	CYS	N-CA-C	8.40	133.67	111.00
1	AV	207	CYS	N-CA-C	8.40	133.67	111.00
1	Ae	207	CYS	N-CA-C	8.40	133.67	111.00
1	A1	207	CYS	N-CA-C	8.39	133.67	111.00
1	A4	207	CYS	N-CA-C	8.39	133.66	111.00
1	A6	207	CYS	N-CA-C	8.39	133.67	111.00
1	A8	207	CYS	N-CA-C	8.39	133.66	111.00
1	DI	207	CYS	N-CA-C	8.39	133.66	111.00
1	A2	207	CYS	N-CA-C	8.39	133.65	111.00
1	Ak	207	CYS	N-CA-C	8.39	133.65	111.00
1	DK	207	CYS	N-CA-C	8.39	133.65	111.00
1	AX	207	CYS	N-CA-C	8.38	133.64	111.00
1	Ai	207	CYS	N-CA-C	8.38	133.64	111.00
1	DF	207	CYS	N-CA-C	8.38	133.61	111.00
1	Ah	207	CYS	N-CA-C	8.37	133.60	111.00
1	AN	207	CYS	N-CA-C	8.37	133.59	111.00
2	B8	138	LYS	N-CA-C	-7.74	90.11	111.00
2	B7	138	LYS	N-CA-C	-7.73	90.14	111.00
2	Bb	138	LYS	N-CA-C	-7.72	90.14	111.00
2	BQ	138	LYS	N-CA-C	-7.72	90.15	111.00
2	BX	138	LYS	N-CA-C	-7.72	90.15	111.00
2	Bu	138	LYS	N-CA-C	-7.72	90.15	111.00
2	Bd	138	LYS	N-CA-C	-7.72	90.16	111.00
2	Bh	138	LYS	N-CA-C	-7.72	90.16	111.00
2	Bj	138	LYS	N-CA-C	-7.72	90.16	111.00
2	Bn	138	LYS	N-CA-C	-7.72	90.16	111.00
2	BD	138	LYS	N-CA-C	-7.72	90.16	111.00
2	B6	138	LYS	N-CA-C	-7.72	90.16	111.00
2	BF	138	LYS	N-CA-C	-7.72	90.17	111.00
2	BI	138	LYS	N-CA-C	-7.72	90.17	111.00
2	BY	138	LYS	N-CA-C	-7.72	90.17	111.00
2	Bt	138	LYS	N-CA-C	-7.72	90.17	111.00
2	BK	138	LYS	N-CA-C	-7.71	90.17	111.00
2	Bl	138	LYS	N-CA-C	-7.71	90.17	111.00
2	Bp	138	LYS	N-CA-C	-7.71	90.17	111.00
2	Bv	138	LYS	N-CA-C	-7.71	90.17	111.00
2	BN	138	LYS	N-CA-C	-7.71	90.17	111.00
2	Ba	138	LYS	N-CA-C	-7.71	90.17	111.00
2	BP	138	LYS	N-CA-C	-7.71	90.18	111.00
2	Bg	138	LYS	N-CA-C	-7.71	90.18	111.00
2	Bm	138	LYS	N-CA-C	-7.71	90.18	111.00
2	Bs	138	LYS	N-CA-C	-7.71	90.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Bx	138	LYS	N-CA-C	-7.71	90.18	111.00
2	BO	138	LYS	N-CA-C	-7.71	90.18	111.00
2	BC	138	LYS	N-CA-C	-7.71	90.19	111.00
2	BJ	138	LYS	N-CA-C	-7.71	90.19	111.00
2	Be	138	LYS	N-CA-C	-7.71	90.19	111.00
2	Bw	138	LYS	N-CA-C	-7.71	90.19	111.00
2	BB	138	LYS	N-CA-C	-7.71	90.19	111.00
2	B1	138	LYS	N-CA-C	-7.71	90.19	111.00
2	B2	138	LYS	N-CA-C	-7.71	90.19	111.00
2	B3	138	LYS	N-CA-C	-7.71	90.19	111.00
2	B4	138	LYS	N-CA-C	-7.71	90.19	111.00
2	Bq	138	LYS	N-CA-C	-7.71	90.19	111.00
2	BE	138	LYS	N-CA-C	-7.70	90.20	111.00
2	BR	138	LYS	N-CA-C	-7.70	90.20	111.00
2	B5	138	LYS	N-CA-C	-7.70	90.20	111.00
2	Bi	138	LYS	N-CA-C	-7.70	90.20	111.00
2	BA	138	LYS	N-CA-C	-7.70	90.20	111.00
2	BW	138	LYS	N-CA-C	-7.70	90.20	111.00
2	Bo	138	LYS	N-CA-C	-7.70	90.20	111.00
2	BL	138	LYS	N-CA-C	-7.70	90.21	111.00
2	BZ	138	LYS	N-CA-C	-7.70	90.21	111.00
2	Bf	138	LYS	N-CA-C	-7.70	90.21	111.00
2	BM	138	LYS	N-CA-C	-7.70	90.22	111.00
2	BT	138	LYS	N-CA-C	-7.70	90.22	111.00
2	BG	138	LYS	N-CA-C	-7.70	90.22	111.00
2	BU	138	LYS	N-CA-C	-7.69	90.22	111.00
2	B9	138	LYS	N-CA-C	-7.69	90.23	111.00
2	BH	138	LYS	N-CA-C	-7.69	90.24	111.00
2	BS	138	LYS	N-CA-C	-7.69	90.24	111.00
2	B0	138	LYS	N-CA-C	-7.69	90.23	111.00
2	Br	138	LYS	N-CA-C	-7.69	90.23	111.00
2	Bk	138	LYS	N-CA-C	-7.69	90.24	111.00
2	Bc	138	LYS	N-CA-C	-7.69	90.24	111.00
2	BV	138	LYS	N-CA-C	-7.68	90.27	111.00
1	Aa	21	PRO	N-CA-C	7.63	131.93	112.10
1	Ah	21	PRO	N-CA-C	7.63	131.94	112.10
1	A2	21	PRO	N-CA-C	7.63	131.93	112.10
1	DJ	21	PRO	N-CA-C	7.63	131.93	112.10
1	Am	21	PRO	N-CA-C	7.62	131.92	112.10
1	An	21	PRO	N-CA-C	7.62	131.92	112.10
1	DG	21	PRO	N-CA-C	7.62	131.91	112.10
1	AE	21	PRO	N-CA-C	7.62	131.91	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DC	21	PRO	N-CA-C	7.62	131.90	112.10
1	AO	21	PRO	N-CA-C	7.62	131.90	112.10
1	AX	21	PRO	N-CA-C	7.62	131.90	112.10
1	DF	21	PRO	N-CA-C	7.62	131.90	112.10
1	AH	21	PRO	N-CA-C	7.61	131.89	112.10
1	DK	21	PRO	N-CA-C	7.61	131.90	112.10
1	A7	21	PRO	N-CA-C	7.61	131.89	112.10
1	AP	21	PRO	N-CA-C	7.61	131.89	112.10
1	Ad	21	PRO	N-CA-C	7.61	131.89	112.10
1	Ae	21	PRO	N-CA-C	7.61	131.89	112.10
1	AK	21	PRO	N-CA-C	7.61	131.88	112.10
1	AJ	21	PRO	N-CA-C	7.61	131.88	112.10
1	DE	21	PRO	N-CA-C	7.61	131.88	112.10
1	AT	21	PRO	N-CA-C	7.61	131.87	112.10
1	AG	21	PRO	N-CA-C	7.60	131.87	112.10
1	AQ	21	PRO	N-CA-C	7.60	131.87	112.10
1	Ao	21	PRO	N-CA-C	7.60	131.87	112.10
1	AA	21	PRO	N-CA-C	7.60	131.87	112.10
1	AV	21	PRO	N-CA-C	7.60	131.86	112.10
1	AY	21	PRO	N-CA-C	7.60	131.86	112.10
1	Af	21	PRO	N-CA-C	7.60	131.86	112.10
1	DI	21	PRO	N-CA-C	7.60	131.86	112.10
1	AS	21	PRO	N-CA-C	7.60	131.85	112.10
1	A4	21	PRO	N-CA-C	7.60	131.85	112.10
1	A8	21	PRO	N-CA-C	7.60	131.85	112.10
1	Ak	21	PRO	N-CA-C	7.60	131.85	112.10
1	AB	21	PRO	N-CA-C	7.59	131.85	112.10
1	AM	21	PRO	N-CA-C	7.59	131.84	112.10
1	Ac	21	PRO	N-CA-C	7.59	131.84	112.10
1	AC	21	PRO	N-CA-C	7.59	131.84	112.10
1	Ai	21	PRO	N-CA-C	7.59	131.83	112.10
1	AF	21	PRO	N-CA-C	7.59	131.83	112.10
1	AL	21	PRO	N-CA-C	7.59	131.83	112.10
1	AU	21	PRO	N-CA-C	7.59	131.82	112.10
1	Ab	21	PRO	N-CA-C	7.59	131.82	112.10
1	AZ	21	PRO	N-CA-C	7.58	131.82	112.10
1	A1	21	PRO	N-CA-C	7.58	131.82	112.10
1	A9	21	PRO	N-CA-C	7.58	131.82	112.10
1	AD	21	PRO	N-CA-C	7.58	131.81	112.10
1	A0	21	PRO	N-CA-C	7.58	131.81	112.10
1	A5	21	PRO	N-CA-C	7.58	131.81	112.10
1	DD	21	PRO	N-CA-C	7.58	131.81	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DH	21	PRO	N-CA-C	7.58	131.81	112.10
1	AR	21	PRO	N-CA-C	7.58	131.81	112.10
1	Aj	21	PRO	N-CA-C	7.58	131.80	112.10
1	A3	21	PRO	N-CA-C	7.58	131.80	112.10
1	Al	21	PRO	N-CA-C	7.57	131.79	112.10
1	AW	21	PRO	N-CA-C	7.57	131.79	112.10
1	AN	21	PRO	N-CA-C	7.57	131.78	112.10
1	AI	21	PRO	N-CA-C	7.56	131.76	112.10
1	Ag	21	PRO	N-CA-C	7.56	131.76	112.10
1	A6	21	PRO	N-CA-C	7.55	131.74	112.10
2	BU	86	ASP	CB-CA-C	7.03	124.46	110.40
2	B4	86	ASP	CB-CA-C	7.03	124.46	110.40
2	Bd	86	ASP	CB-CA-C	7.02	124.44	110.40
2	BA	86	ASP	CB-CA-C	7.02	124.44	110.40
2	Bn	86	ASP	CB-CA-C	7.02	124.43	110.40
2	BF	86	ASP	CB-CA-C	7.01	124.43	110.40
2	B6	86	ASP	CB-CA-C	7.01	124.43	110.40
2	BO	86	ASP	CB-CA-C	7.01	124.42	110.40
2	BQ	86	ASP	CB-CA-C	7.01	124.42	110.40
2	Bs	86	ASP	CB-CA-C	7.01	124.42	110.40
2	BI	86	ASP	CB-CA-C	7.01	124.42	110.40
2	Bi	86	ASP	CB-CA-C	7.01	124.42	110.40
2	Bv	86	ASP	CB-CA-C	7.01	124.41	110.40
2	BD	86	ASP	CB-CA-C	7.00	124.41	110.40
2	BX	86	ASP	CB-CA-C	7.00	124.40	110.40
2	BZ	86	ASP	CB-CA-C	7.00	124.40	110.40
2	B3	86	ASP	CB-CA-C	7.00	124.40	110.40
2	Bm	86	ASP	CB-CA-C	7.00	124.40	110.40
2	BP	86	ASP	CB-CA-C	7.00	124.39	110.40
2	BN	86	ASP	CB-CA-C	7.00	124.39	110.40
2	BS	86	ASP	CB-CA-C	7.00	124.39	110.40
2	B0	86	ASP	CB-CA-C	7.00	124.39	110.40
2	Bx	86	ASP	CB-CA-C	7.00	124.39	110.40
2	BK	86	ASP	CB-CA-C	6.99	124.39	110.40
2	Bb	86	ASP	CB-CA-C	6.99	124.39	110.40
2	Bc	86	ASP	CB-CA-C	6.99	124.39	110.40
2	Bl	86	ASP	CB-CA-C	6.99	124.39	110.40
2	Bt	86	ASP	CB-CA-C	6.99	124.39	110.40
2	BC	86	ASP	CB-CA-C	6.99	124.38	110.40
2	BV	86	ASP	CB-CA-C	6.99	124.38	110.40
2	BB	86	ASP	CB-CA-C	6.99	124.38	110.40
2	B8	86	ASP	CB-CA-C	6.99	124.38	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Bp	86	ASP	CB-CA-C	6.99	124.38	110.40
2	Bo	86	ASP	CB-CA-C	6.99	124.38	110.40
2	Bh	86	ASP	CB-CA-C	6.99	124.37	110.40
2	BE	86	ASP	CB-CA-C	6.99	124.37	110.40
2	B9	86	ASP	CB-CA-C	6.99	124.37	110.40
2	BG	86	ASP	CB-CA-C	6.98	124.37	110.40
2	BH	86	ASP	CB-CA-C	6.98	124.37	110.40
2	Bj	86	ASP	CB-CA-C	6.98	124.37	110.40
2	BT	86	ASP	CB-CA-C	6.98	124.36	110.40
2	Ba	86	ASP	CB-CA-C	6.98	124.36	110.40
2	Br	86	ASP	CB-CA-C	6.98	124.36	110.40
2	Bf	86	ASP	CB-CA-C	6.98	124.36	110.40
2	BJ	86	ASP	CB-CA-C	6.98	124.35	110.40
2	BY	86	ASP	CB-CA-C	6.98	124.35	110.40
2	BR	86	ASP	CB-CA-C	6.97	124.35	110.40
2	BL	86	ASP	CB-CA-C	6.97	124.34	110.40
2	B7	86	ASP	CB-CA-C	6.97	124.34	110.40
2	BM	86	ASP	CB-CA-C	6.97	124.34	110.40
2	Be	86	ASP	CB-CA-C	6.97	124.34	110.40
2	Bu	86	ASP	CB-CA-C	6.96	124.33	110.40
2	B5	86	ASP	CB-CA-C	6.96	124.32	110.40
2	Bk	86	ASP	CB-CA-C	6.96	124.32	110.40
2	Bg	86	ASP	CB-CA-C	6.96	124.32	110.40
2	Bq	86	ASP	CB-CA-C	6.96	124.31	110.40
2	B1	86	ASP	CB-CA-C	6.96	124.31	110.40
2	B2	86	ASP	CB-CA-C	6.96	124.31	110.40
2	Bw	86	ASP	CB-CA-C	6.95	124.31	110.40
2	BW	86	ASP	CB-CA-C	6.94	124.28	110.40
3	Cv	130	ALA	N-CA-C	6.90	129.62	111.00
3	Cx	130	ALA	N-CA-C	6.89	129.61	111.00
3	CE	130	ALA	N-CA-C	6.89	129.60	111.00
3	Cd	130	ALA	N-CA-C	6.89	129.60	111.00
3	Cm	130	ALA	N-CA-C	6.89	129.60	111.00
3	C6	130	ALA	N-CA-C	6.89	129.60	111.00
3	CF	130	ALA	N-CA-C	6.89	129.59	111.00
3	CM	130	ALA	N-CA-C	6.89	129.59	111.00
3	Ci	130	ALA	N-CA-C	6.89	129.60	111.00
3	Cn	130	ALA	N-CA-C	6.89	129.59	111.00
3	CT	130	ALA	N-CA-C	6.88	129.59	111.00
3	C3	130	ALA	N-CA-C	6.88	129.59	111.00
3	Co	130	ALA	N-CA-C	6.88	129.59	111.00
3	CN	130	ALA	N-CA-C	6.88	129.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C8	130	ALA	N-CA-C	6.88	129.58	111.00
3	CC	130	ALA	N-CA-C	6.88	129.58	111.00
3	CO	130	ALA	N-CA-C	6.88	129.58	111.00
3	CY	130	ALA	N-CA-C	6.88	129.58	111.00
3	C1	130	ALA	N-CA-C	6.88	129.58	111.00
3	CR	130	ALA	N-CA-C	6.88	129.58	111.00
3	Ct	130	ALA	N-CA-C	6.88	129.58	111.00
3	C5	130	ALA	N-CA-C	6.88	129.57	111.00
3	C7	130	ALA	N-CA-C	6.88	129.57	111.00
3	Cl	130	ALA	N-CA-C	6.88	129.57	111.00
3	CW	130	ALA	N-CA-C	6.88	129.57	111.00
3	CH	130	ALA	N-CA-C	6.88	129.56	111.00
3	CU	130	ALA	N-CA-C	6.88	129.56	111.00
3	Cs	130	ALA	N-CA-C	6.88	129.56	111.00
3	CA	130	ALA	N-CA-C	6.87	129.56	111.00
3	Ce	130	ALA	N-CA-C	6.87	129.56	111.00
3	Ch	130	ALA	N-CA-C	6.87	129.56	111.00
3	Cw	130	ALA	N-CA-C	6.87	129.56	111.00
3	CI	130	ALA	N-CA-C	6.87	129.56	111.00
3	C2	130	ALA	N-CA-C	6.87	129.55	111.00
3	Cg	130	ALA	N-CA-C	6.87	129.56	111.00
3	Cj	130	ALA	N-CA-C	6.87	129.55	111.00
3	Cp	130	ALA	N-CA-C	6.87	129.56	111.00
3	CQ	130	ALA	N-CA-C	6.87	129.55	111.00
3	Ck	130	ALA	N-CA-C	6.87	129.54	111.00
3	Cq	130	ALA	N-CA-C	6.87	129.54	111.00
3	CV	130	ALA	N-CA-C	6.87	129.54	111.00
3	CZ	130	ALA	N-CA-C	6.87	129.54	111.00
3	DB	130	ALA	N-CA-C	6.87	129.54	111.00
3	CD	130	ALA	N-CA-C	6.86	129.53	111.00
3	CK	130	ALA	N-CA-C	6.86	129.53	111.00
3	CP	130	ALA	N-CA-C	6.86	129.53	111.00
3	C4	130	ALA	N-CA-C	6.86	129.53	111.00
3	Cc	130	ALA	N-CA-C	6.86	129.53	111.00
3	DA	130	ALA	N-CA-C	6.86	129.53	111.00
3	Cu	130	ALA	N-CA-C	6.86	129.52	111.00
3	Cf	130	ALA	N-CA-C	6.86	129.51	111.00
3	CG	130	ALA	N-CA-C	6.86	129.51	111.00
3	CL	130	ALA	N-CA-C	6.86	129.51	111.00
3	C0	130	ALA	N-CA-C	6.86	129.51	111.00
3	Cr	130	ALA	N-CA-C	6.86	129.51	111.00
3	CJ	130	ALA	N-CA-C	6.85	129.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CB	130	ALA	N-CA-C	6.85	129.49	111.00
3	C9	130	ALA	N-CA-C	6.85	129.49	111.00
3	CX	130	ALA	N-CA-C	6.85	129.48	111.00
3	CS	130	ALA	N-CA-C	6.84	129.48	111.00
2	BV	223	ASN	CB-CA-C	-6.64	97.12	110.40
2	BG	223	ASN	CB-CA-C	-6.63	97.13	110.40
2	BI	223	ASN	CB-CA-C	-6.63	97.14	110.40
2	Bo	223	ASN	CB-CA-C	-6.62	97.15	110.40
2	Bx	223	ASN	CB-CA-C	-6.62	97.15	110.40
2	BU	223	ASN	CB-CA-C	-6.62	97.16	110.40
2	B0	223	ASN	CB-CA-C	-6.61	97.18	110.40
2	Be	223	ASN	CB-CA-C	-6.61	97.18	110.40
2	Bl	223	ASN	CB-CA-C	-6.61	97.18	110.40
2	B9	223	ASN	CB-CA-C	-6.61	97.18	110.40
2	BN	223	ASN	CB-CA-C	-6.60	97.20	110.40
2	B2	223	ASN	CB-CA-C	-6.60	97.20	110.40
2	B6	223	ASN	CB-CA-C	-6.60	97.19	110.40
2	BB	223	ASN	CB-CA-C	-6.60	97.20	110.40
2	Bt	223	ASN	CB-CA-C	-6.60	97.20	110.40
2	Bd	223	ASN	CB-CA-C	-6.60	97.21	110.40
2	BS	223	ASN	CB-CA-C	-6.59	97.21	110.40
2	BZ	223	ASN	CB-CA-C	-6.59	97.21	110.40
2	Bj	223	ASN	CB-CA-C	-6.59	97.21	110.40
2	BT	223	ASN	CB-CA-C	-6.59	97.22	110.40
2	BL	223	ASN	CB-CA-C	-6.59	97.22	110.40
1	Ag	87	GLN	N-CA-C	6.59	128.79	111.00
2	BQ	223	ASN	CB-CA-C	-6.59	97.23	110.40
2	BK	223	ASN	CB-CA-C	-6.58	97.23	110.40
2	B8	223	ASN	CB-CA-C	-6.58	97.23	110.40
1	Ah	87	GLN	N-CA-C	6.58	128.77	111.00
2	BY	223	ASN	CB-CA-C	-6.58	97.24	110.40
2	Bq	223	ASN	CB-CA-C	-6.58	97.23	110.40
2	Bv	223	ASN	CB-CA-C	-6.58	97.24	110.40
2	BD	223	ASN	CB-CA-C	-6.58	97.24	110.40
1	AR	87	GLN	N-CA-C	6.58	128.76	111.00
2	BH	223	ASN	CB-CA-C	-6.58	97.25	110.40
1	AO	87	GLN	N-CA-C	6.58	128.76	111.00
1	AW	87	GLN	N-CA-C	6.58	128.76	111.00
2	Bg	223	ASN	CB-CA-C	-6.58	97.25	110.40
2	Bs	223	ASN	CB-CA-C	-6.58	97.25	110.40
1	AQ	87	GLN	N-CA-C	6.58	128.75	111.00
1	An	87	GLN	N-CA-C	6.58	128.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B3	223	ASN	CB-CA-C	-6.58	97.25	110.40
1	Al	87	GLN	N-CA-C	6.57	128.75	111.00
2	BF	223	ASN	CB-CA-C	-6.57	97.25	110.40
2	BM	223	ASN	CB-CA-C	-6.57	97.25	110.40
2	Bu	223	ASN	CB-CA-C	-6.57	97.25	110.40
1	AM	87	GLN	N-CA-C	6.57	128.74	111.00
1	Aa	87	GLN	N-CA-C	6.57	128.74	111.00
2	BW	223	ASN	CB-CA-C	-6.57	97.26	110.40
2	B5	223	ASN	CB-CA-C	-6.57	97.26	110.40
2	Bh	223	ASN	CB-CA-C	-6.57	97.26	110.40
1	DJ	87	GLN	N-CA-C	6.57	128.74	111.00
1	A5	87	GLN	N-CA-C	6.57	128.74	111.00
2	BX	223	ASN	CB-CA-C	-6.57	97.26	110.40
2	B4	223	ASN	CB-CA-C	-6.57	97.26	110.40
1	AL	87	GLN	N-CA-C	6.57	128.73	111.00
2	BJ	223	ASN	CB-CA-C	-6.57	97.26	110.40
2	Bb	223	ASN	CB-CA-C	-6.57	97.26	110.40
2	Bn	223	ASN	CB-CA-C	-6.57	97.27	110.40
2	Bf	223	ASN	CB-CA-C	-6.57	97.27	110.40
2	Bi	223	ASN	CB-CA-C	-6.57	97.27	110.40
1	DH	87	GLN	N-CA-C	6.57	128.72	111.00
1	DI	87	GLN	N-CA-C	6.57	128.73	111.00
1	AH	87	GLN	N-CA-C	6.56	128.72	111.00
1	AX	87	GLN	N-CA-C	6.56	128.72	111.00
1	A0	87	GLN	N-CA-C	6.56	128.72	111.00
1	A2	87	GLN	N-CA-C	6.56	128.72	111.00
1	Af	87	GLN	N-CA-C	6.56	128.72	111.00
2	Br	223	ASN	CB-CA-C	-6.56	97.27	110.40
1	AN	87	GLN	N-CA-C	6.56	128.71	111.00
2	Bp	223	ASN	CB-CA-C	-6.56	97.28	110.40
1	DD	87	GLN	N-CA-C	6.56	128.72	111.00
2	BA	223	ASN	CB-CA-C	-6.56	97.28	110.40
2	Bm	223	ASN	CB-CA-C	-6.56	97.28	110.40
1	AC	87	GLN	N-CA-C	6.56	128.70	111.00
1	AS	87	GLN	N-CA-C	6.56	128.70	111.00
1	AU	87	GLN	N-CA-C	6.56	128.70	111.00
1	A1	87	GLN	N-CA-C	6.56	128.71	111.00
1	A6	87	GLN	N-CA-C	6.56	128.70	111.00
1	Ak	87	GLN	N-CA-C	6.56	128.71	111.00
1	Am	87	GLN	N-CA-C	6.56	128.70	111.00
2	Bc	223	ASN	CB-CA-C	-6.56	97.28	110.40
1	AA	87	GLN	N-CA-C	6.56	128.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A7	87	GLN	N-CA-C	6.56	128.70	111.00
1	Ae	87	GLN	N-CA-C	6.56	128.70	111.00
2	Bw	223	ASN	CB-CA-C	-6.56	97.29	110.40
1	AE	87	GLN	N-CA-C	6.55	128.70	111.00
2	BE	223	ASN	CB-CA-C	-6.55	97.29	110.40
2	BO	223	ASN	CB-CA-C	-6.55	97.29	110.40
2	B1	223	ASN	CB-CA-C	-6.55	97.29	110.40
2	Ba	223	ASN	CB-CA-C	-6.55	97.29	110.40
1	DE	87	GLN	N-CA-C	6.55	128.70	111.00
1	A9	87	GLN	N-CA-C	6.55	128.69	111.00
1	AF	87	GLN	N-CA-C	6.55	128.69	111.00
1	AT	87	GLN	N-CA-C	6.55	128.69	111.00
1	AY	87	GLN	N-CA-C	6.55	128.69	111.00
1	AZ	87	GLN	N-CA-C	6.55	128.69	111.00
1	Ab	87	GLN	N-CA-C	6.55	128.69	111.00
2	BP	223	ASN	CB-CA-C	-6.55	97.30	110.40
1	AI	87	GLN	N-CA-C	6.55	128.68	111.00
1	Aj	87	GLN	N-CA-C	6.55	128.68	111.00
1	A8	87	GLN	N-CA-C	6.55	128.68	111.00
1	DF	87	GLN	N-CA-C	6.55	128.68	111.00
2	B7	223	ASN	CB-CA-C	-6.55	97.31	110.40
2	Bk	223	ASN	CB-CA-C	-6.55	97.31	110.40
1	DK	87	GLN	N-CA-C	6.55	128.68	111.00
1	Ad	87	GLN	N-CA-C	6.54	128.67	111.00
1	Ai	87	GLN	N-CA-C	6.54	128.67	111.00
1	DC	87	GLN	N-CA-C	6.54	128.67	111.00
1	AK	87	GLN	N-CA-C	6.54	128.67	111.00
1	AD	87	GLN	N-CA-C	6.54	128.66	111.00
1	AP	87	GLN	N-CA-C	6.54	128.66	111.00
1	A3	87	GLN	N-CA-C	6.54	128.66	111.00
1	Ac	87	GLN	N-CA-C	6.54	128.66	111.00
1	Ao	87	GLN	N-CA-C	6.54	128.66	111.00
2	BC	223	ASN	CB-CA-C	-6.54	97.32	110.40
1	AJ	87	GLN	N-CA-C	6.54	128.65	111.00
1	AV	87	GLN	N-CA-C	6.54	128.66	111.00
2	BR	223	ASN	CB-CA-C	-6.54	97.33	110.40
1	AB	87	GLN	N-CA-C	6.54	128.65	111.00
1	A4	87	GLN	N-CA-C	6.53	128.64	111.00
1	Ag	203	ASP	N-CA-C	-6.53	93.37	111.00
1	AG	87	GLN	N-CA-C	6.53	128.63	111.00
1	DG	87	GLN	N-CA-C	6.53	128.63	111.00
1	AM	203	ASP	N-CA-C	-6.53	93.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ab	203	ASP	N-CA-C	-6.52	93.39	111.00
1	Al	203	ASP	N-CA-C	-6.52	93.39	111.00
1	AD	203	ASP	N-CA-C	-6.52	93.40	111.00
1	DI	203	ASP	N-CA-C	-6.52	93.40	111.00
1	AG	203	ASP	N-CA-C	-6.52	93.40	111.00
1	AZ	203	ASP	N-CA-C	-6.52	93.41	111.00
1	AI	203	ASP	N-CA-C	-6.51	93.41	111.00
1	AU	203	ASP	N-CA-C	-6.51	93.42	111.00
1	A3	203	ASP	N-CA-C	-6.51	93.42	111.00
1	A9	203	ASP	N-CA-C	-6.51	93.42	111.00
1	Ai	203	ASP	N-CA-C	-6.51	93.43	111.00
1	Ao	203	ASP	N-CA-C	-6.51	93.43	111.00
1	Ah	203	ASP	N-CA-C	-6.51	93.43	111.00
1	AN	203	ASP	N-CA-C	-6.51	93.43	111.00
1	AP	203	ASP	N-CA-C	-6.51	93.43	111.00
1	AW	203	ASP	N-CA-C	-6.51	93.43	111.00
1	AY	203	ASP	N-CA-C	-6.51	93.43	111.00
1	AR	203	ASP	N-CA-C	-6.50	93.44	111.00
1	A6	203	ASP	N-CA-C	-6.50	93.44	111.00
1	Ad	203	ASP	N-CA-C	-6.50	93.44	111.00
1	AJ	203	ASP	N-CA-C	-6.50	93.45	111.00
1	AK	203	ASP	N-CA-C	-6.50	93.44	111.00
1	AX	203	ASP	N-CA-C	-6.50	93.45	111.00
1	A1	203	ASP	N-CA-C	-6.50	93.44	111.00
1	Ac	203	ASP	N-CA-C	-6.50	93.44	111.00
1	DD	203	ASP	N-CA-C	-6.50	93.45	111.00
1	AE	203	ASP	N-CA-C	-6.50	93.45	111.00
1	A0	203	ASP	N-CA-C	-6.50	93.45	111.00
1	A4	203	ASP	N-CA-C	-6.50	93.45	111.00
1	AB	203	ASP	N-CA-C	-6.50	93.46	111.00
1	AO	203	ASP	N-CA-C	-6.50	93.46	111.00
1	AS	203	ASP	N-CA-C	-6.50	93.46	111.00
1	AT	203	ASP	N-CA-C	-6.50	93.46	111.00
1	Ae	203	ASP	N-CA-C	-6.50	93.46	111.00
1	Aj	203	ASP	N-CA-C	-6.50	93.46	111.00
1	DE	203	ASP	N-CA-C	-6.50	93.46	111.00
1	Am	203	ASP	N-CA-C	-6.50	93.46	111.00
1	AA	203	ASP	N-CA-C	-6.49	93.47	111.00
1	AC	203	ASP	N-CA-C	-6.49	93.47	111.00
1	A2	203	ASP	N-CA-C	-6.49	93.47	111.00
1	DF	203	ASP	N-CA-C	-6.49	93.47	111.00
1	AQ	203	ASP	N-CA-C	-6.49	93.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A5	203	ASP	N-CA-C	-6.49	93.47	111.00
1	DG	203	ASP	N-CA-C	-6.49	93.47	111.00
1	A8	203	ASP	N-CA-C	-6.49	93.48	111.00
1	An	203	ASP	N-CA-C	-6.49	93.47	111.00
1	DK	203	ASP	N-CA-C	-6.49	93.48	111.00
1	AF	203	ASP	N-CA-C	-6.49	93.48	111.00
1	A7	203	ASP	N-CA-C	-6.49	93.49	111.00
1	AL	203	ASP	N-CA-C	-6.49	93.49	111.00
1	AV	203	ASP	N-CA-C	-6.49	93.49	111.00
1	Aa	203	ASP	N-CA-C	-6.49	93.49	111.00
1	DH	203	ASP	N-CA-C	-6.49	93.49	111.00
1	DJ	203	ASP	N-CA-C	-6.49	93.49	111.00
1	Ak	203	ASP	N-CA-C	-6.48	93.50	111.00
1	Af	203	ASP	N-CA-C	-6.48	93.50	111.00
1	AH	203	ASP	N-CA-C	-6.48	93.51	111.00
1	DC	203	ASP	N-CA-C	-6.47	93.53	111.00
1	Ai	146	ILE	CB-CA-C	-6.39	98.82	111.60
1	AJ	146	ILE	CB-CA-C	-6.39	98.83	111.60
1	AY	146	ILE	CB-CA-C	-6.38	98.84	111.60
1	Ad	146	ILE	CB-CA-C	-6.38	98.84	111.60
1	AO	146	ILE	CB-CA-C	-6.38	98.85	111.60
1	AF	146	ILE	CB-CA-C	-6.37	98.86	111.60
1	AA	146	ILE	CB-CA-C	-6.37	98.86	111.60
1	Ae	146	ILE	CB-CA-C	-6.37	98.87	111.60
1	A8	146	ILE	CB-CA-C	-6.37	98.87	111.60
1	AQ	146	ILE	CB-CA-C	-6.36	98.87	111.60
1	A9	146	ILE	CB-CA-C	-6.36	98.87	111.60
1	Ao	146	ILE	CB-CA-C	-6.36	98.87	111.60
1	AB	146	ILE	CB-CA-C	-6.36	98.88	111.60
1	A6	146	ILE	CB-CA-C	-6.36	98.88	111.60
1	AT	146	ILE	CB-CA-C	-6.36	98.88	111.60
1	AE	146	ILE	CB-CA-C	-6.36	98.89	111.60
1	A3	146	ILE	CB-CA-C	-6.36	98.89	111.60
1	Al	146	ILE	CB-CA-C	-6.35	98.89	111.60
1	AG	146	ILE	CB-CA-C	-6.35	98.90	111.60
1	AL	146	ILE	CB-CA-C	-6.35	98.90	111.60
1	DG	146	ILE	CB-CA-C	-6.35	98.90	111.60
1	AP	146	ILE	CB-CA-C	-6.35	98.90	111.60
1	Am	146	ILE	CB-CA-C	-6.35	98.90	111.60
1	DF	146	ILE	CB-CA-C	-6.35	98.90	111.60
1	DH	146	ILE	CB-CA-C	-6.35	98.90	111.60
1	Ak	146	ILE	CB-CA-C	-6.35	98.91	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	An	146	ILE	CB-CA-C	-6.35	98.91	111.60
1	AC	146	ILE	CB-CA-C	-6.34	98.91	111.60
1	DK	146	ILE	CB-CA-C	-6.34	98.91	111.60
1	DC	146	ILE	CB-CA-C	-6.34	98.92	111.60
1	AX	146	ILE	CB-CA-C	-6.34	98.92	111.60
1	Ag	146	ILE	CB-CA-C	-6.34	98.92	111.60
1	A2	146	ILE	CB-CA-C	-6.34	98.93	111.60
1	Ah	146	ILE	CB-CA-C	-6.34	98.93	111.60
1	Aj	146	ILE	CB-CA-C	-6.34	98.93	111.60
1	AD	146	ILE	CB-CA-C	-6.33	98.93	111.60
1	AW	146	ILE	CB-CA-C	-6.33	98.93	111.60
1	A0	146	ILE	CB-CA-C	-6.33	98.94	111.60
1	AV	146	ILE	CB-CA-C	-6.33	98.94	111.60
1	A7	146	ILE	CB-CA-C	-6.33	98.94	111.60
1	DE	146	ILE	CB-CA-C	-6.33	98.94	111.60
1	AM	146	ILE	CB-CA-C	-6.33	98.95	111.60
1	A5	146	ILE	CB-CA-C	-6.33	98.95	111.60
1	AH	146	ILE	CB-CA-C	-6.33	98.95	111.60
1	AK	146	ILE	CB-CA-C	-6.33	98.95	111.60
1	Af	146	ILE	CB-CA-C	-6.33	98.95	111.60
1	AZ	146	ILE	CB-CA-C	-6.32	98.95	111.60
1	Aa	146	ILE	CB-CA-C	-6.32	98.95	111.60
1	Ac	146	ILE	CB-CA-C	-6.32	98.95	111.60
1	DD	146	ILE	CB-CA-C	-6.32	98.95	111.60
1	AN	146	ILE	CB-CA-C	-6.32	98.96	111.60
1	A1	146	ILE	CB-CA-C	-6.32	98.96	111.60
1	AR	146	ILE	CB-CA-C	-6.32	98.96	111.60
1	AS	146	ILE	CB-CA-C	-6.32	98.97	111.60
1	DI	146	ILE	CB-CA-C	-6.32	98.97	111.60
1	DJ	146	ILE	CB-CA-C	-6.30	98.99	111.60
1	Ab	146	ILE	CB-CA-C	-6.30	99.00	111.60
1	AI	146	ILE	CB-CA-C	-6.30	99.01	111.60
1	A4	146	ILE	CB-CA-C	-6.30	99.01	111.60
1	AU	146	ILE	CB-CA-C	-6.29	99.02	111.60
3	CX	70	ASP	N-CA-C	6.25	127.87	111.00
3	Cd	70	ASP	N-CA-C	6.24	127.84	111.00
3	Cs	70	ASP	N-CA-C	6.24	127.84	111.00
3	CT	70	ASP	N-CA-C	6.23	127.83	111.00
3	CM	70	ASP	N-CA-C	6.23	127.82	111.00
3	C0	70	ASP	N-CA-C	6.23	127.81	111.00
3	Cn	70	ASP	N-CA-C	6.23	127.81	111.00
3	CS	70	ASP	N-CA-C	6.22	127.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C3	70	ASP	N-CA-C	6.22	127.80	111.00
3	CI	70	ASP	N-CA-C	6.22	127.80	111.00
3	C1	70	ASP	N-CA-C	6.22	127.80	111.00
3	C9	70	ASP	N-CA-C	6.22	127.80	111.00
3	CF	70	ASP	N-CA-C	6.22	127.80	111.00
3	CE	70	ASP	N-CA-C	6.22	127.79	111.00
3	C4	70	ASP	N-CA-C	6.22	127.79	111.00
3	Cj	70	ASP	N-CA-C	6.22	127.79	111.00
3	Cx	70	ASP	N-CA-C	6.22	127.80	111.00
3	C8	70	ASP	N-CA-C	6.22	127.79	111.00
3	Cm	70	ASP	N-CA-C	6.22	127.79	111.00
3	Ch	70	ASP	N-CA-C	6.22	127.78	111.00
3	Ct	70	ASP	N-CA-C	6.22	127.78	111.00
3	CJ	70	ASP	N-CA-C	6.21	127.78	111.00
3	CY	70	ASP	N-CA-C	6.21	127.77	111.00
3	Cr	70	ASP	N-CA-C	6.21	127.77	111.00
3	DB	70	ASP	N-CA-C	6.21	127.77	111.00
3	CD	70	ASP	N-CA-C	6.21	127.76	111.00
3	Cl	70	ASP	N-CA-C	6.21	127.76	111.00
3	CN	70	ASP	N-CA-C	6.21	127.76	111.00
3	CW	70	ASP	N-CA-C	6.21	127.75	111.00
3	C2	70	ASP	N-CA-C	6.21	127.75	111.00
3	Ce	70	ASP	N-CA-C	6.21	127.75	111.00
3	DA	70	ASP	N-CA-C	6.21	127.75	111.00
2	BT	85	SER	N-CA-C	6.20	127.75	111.00
3	CQ	70	ASP	N-CA-C	6.20	127.75	111.00
3	C6	70	ASP	N-CA-C	6.20	127.75	111.00
3	Cf	70	ASP	N-CA-C	6.20	127.75	111.00
3	Cu	70	ASP	N-CA-C	6.20	127.75	111.00
3	CU	70	ASP	N-CA-C	6.20	127.75	111.00
2	B5	134	HIS	N-CA-C	-6.20	94.26	111.00
3	CB	70	ASP	N-CA-C	6.20	127.74	111.00
3	Ci	70	ASP	N-CA-C	6.20	127.74	111.00
3	CC	70	ASP	N-CA-C	6.20	127.74	111.00
3	C5	70	ASP	N-CA-C	6.20	127.74	111.00
3	Cw	70	ASP	N-CA-C	6.20	127.74	111.00
3	CV	70	ASP	N-CA-C	6.20	127.73	111.00
3	C7	70	ASP	N-CA-C	6.20	127.73	111.00
3	Cv	70	ASP	N-CA-C	6.20	127.73	111.00
3	CG	70	ASP	N-CA-C	6.20	127.73	111.00
3	Co	70	ASP	N-CA-C	6.20	127.73	111.00
3	CL	70	ASP	N-CA-C	6.19	127.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Bn	85	SER	N-CA-C	6.19	127.72	111.00
3	CA	70	ASP	N-CA-C	6.19	127.72	111.00
3	CH	70	ASP	N-CA-C	6.19	127.72	111.00
3	CZ	70	ASP	N-CA-C	6.19	127.72	111.00
2	B7	85	SER	N-CA-C	6.19	127.72	111.00
2	B8	85	SER	N-CA-C	6.19	127.72	111.00
3	CK	70	ASP	N-CA-C	6.19	127.72	111.00
3	CO	70	ASP	N-CA-C	6.19	127.72	111.00
3	CP	70	ASP	N-CA-C	6.19	127.71	111.00
3	Cc	70	ASP	N-CA-C	6.19	127.71	111.00
2	BC	134	HIS	N-CA-C	-6.19	94.29	111.00
3	Cq	70	ASP	N-CA-C	6.19	127.71	111.00
2	BY	85	SER	N-CA-C	6.19	127.71	111.00
2	Bt	134	HIS	N-CA-C	-6.19	94.30	111.00
2	BN	134	HIS	N-CA-C	-6.18	94.30	111.00
2	Bq	85	SER	N-CA-C	6.18	127.70	111.00
2	BH	134	HIS	N-CA-C	-6.18	94.31	111.00
2	Bh	85	SER	N-CA-C	6.18	127.69	111.00
3	CR	70	ASP	N-CA-C	6.18	127.69	111.00
3	Cg	70	ASP	N-CA-C	6.18	127.69	111.00
2	Bm	85	SER	N-CA-C	6.18	127.69	111.00
2	Ba	134	HIS	N-CA-C	-6.18	94.31	111.00
2	Bb	134	HIS	N-CA-C	-6.18	94.31	111.00
2	Bf	134	HIS	N-CA-C	-6.18	94.32	111.00
3	Ck	70	ASP	N-CA-C	6.18	127.68	111.00
2	BF	134	HIS	N-CA-C	-6.18	94.32	111.00
2	BP	134	HIS	N-CA-C	-6.18	94.32	111.00
2	BZ	134	HIS	N-CA-C	-6.18	94.33	111.00
2	Bn	134	HIS	N-CA-C	-6.18	94.32	111.00
2	Bp	134	HIS	N-CA-C	-6.18	94.32	111.00
2	BI	134	HIS	N-CA-C	-6.17	94.33	111.00
2	BX	134	HIS	N-CA-C	-6.17	94.33	111.00
2	Bs	85	SER	N-CA-C	6.17	127.67	111.00
2	BV	134	HIS	N-CA-C	-6.17	94.33	111.00
3	Cp	70	ASP	N-CA-C	6.17	127.67	111.00
2	BD	134	HIS	N-CA-C	-6.17	94.34	111.00
2	BR	134	HIS	N-CA-C	-6.17	94.34	111.00
2	BU	134	HIS	N-CA-C	-6.17	94.34	111.00
2	BZ	85	SER	N-CA-C	6.17	127.66	111.00
2	B1	134	HIS	N-CA-C	-6.17	94.34	111.00
2	Bu	134	HIS	N-CA-C	-6.17	94.34	111.00
2	Bi	85	SER	N-CA-C	6.17	127.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BE	85	SER	N-CA-C	6.17	127.66	111.00
2	BJ	85	SER	N-CA-C	6.17	127.66	111.00
2	B2	134	HIS	N-CA-C	-6.17	94.34	111.00
2	Bw	134	HIS	N-CA-C	-6.17	94.35	111.00
2	BA	134	HIS	N-CA-C	-6.17	94.35	111.00
2	BW	134	HIS	N-CA-C	-6.17	94.35	111.00
2	B3	85	SER	N-CA-C	6.17	127.65	111.00
2	Bq	134	HIS	N-CA-C	-6.17	94.35	111.00
2	BK	134	HIS	N-CA-C	-6.17	94.36	111.00
2	BQ	134	HIS	N-CA-C	-6.17	94.35	111.00
2	Bd	85	SER	N-CA-C	6.17	127.64	111.00
2	Bh	134	HIS	N-CA-C	-6.17	94.36	111.00
2	Bi	134	HIS	N-CA-C	-6.17	94.36	111.00
2	BA	85	SER	N-CA-C	6.16	127.64	111.00
2	BE	134	HIS	N-CA-C	-6.16	94.36	111.00
2	BH	85	SER	N-CA-C	6.16	127.64	111.00
2	BO	85	SER	N-CA-C	6.16	127.64	111.00
2	Bc	85	SER	N-CA-C	6.16	127.64	111.00
2	Bg	134	HIS	N-CA-C	-6.16	94.36	111.00
2	Bl	134	HIS	N-CA-C	-6.16	94.36	111.00
2	Bv	85	SER	N-CA-C	6.16	127.64	111.00
2	BK	85	SER	N-CA-C	6.16	127.64	111.00
2	BU	85	SER	N-CA-C	6.16	127.64	111.00
2	B1	85	SER	N-CA-C	6.16	127.64	111.00
2	B6	85	SER	N-CA-C	6.16	127.64	111.00
2	Bk	85	SER	N-CA-C	6.16	127.64	111.00
2	BM	134	HIS	N-CA-C	-6.16	94.37	111.00
2	BS	85	SER	N-CA-C	6.16	127.63	111.00
2	BF	85	SER	N-CA-C	6.16	127.63	111.00
2	BS	134	HIS	N-CA-C	-6.16	94.37	111.00
2	BX	85	SER	N-CA-C	6.16	127.63	111.00
2	B4	134	HIS	N-CA-C	-6.16	94.37	111.00
2	B6	134	HIS	N-CA-C	-6.16	94.37	111.00
2	Bs	134	HIS	N-CA-C	-6.16	94.37	111.00
2	Bx	85	SER	N-CA-C	6.16	127.63	111.00
2	BP	85	SER	N-CA-C	6.16	127.62	111.00
2	BT	134	HIS	N-CA-C	-6.16	94.38	111.00
2	B3	134	HIS	N-CA-C	-6.16	94.38	111.00
2	Be	134	HIS	N-CA-C	-6.16	94.38	111.00
2	Bw	85	SER	N-CA-C	6.16	127.62	111.00
2	BB	134	HIS	N-CA-C	-6.16	94.38	111.00
2	BG	85	SER	N-CA-C	6.16	127.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BI	85	SER	N-CA-C	6.16	127.62	111.00
2	B5	85	SER	N-CA-C	6.16	127.62	111.00
2	Ba	85	SER	N-CA-C	6.16	127.62	111.00
2	Bc	134	HIS	N-CA-C	-6.16	94.38	111.00
2	BR	85	SER	N-CA-C	6.15	127.61	111.00
2	BO	134	HIS	N-CA-C	-6.15	94.38	111.00
2	BW	85	SER	N-CA-C	6.15	127.61	111.00
2	B0	85	SER	N-CA-C	6.15	127.61	111.00
2	B0	134	HIS	N-CA-C	-6.15	94.39	111.00
2	Bk	134	HIS	N-CA-C	-6.15	94.39	111.00
2	Bv	134	HIS	N-CA-C	-6.15	94.39	111.00
2	BG	134	HIS	N-CA-C	-6.15	94.39	111.00
2	BQ	85	SER	N-CA-C	6.15	127.61	111.00
2	Bg	85	SER	N-CA-C	6.15	127.61	111.00
2	Bj	134	HIS	N-CA-C	-6.15	94.40	111.00
2	Bo	134	HIS	N-CA-C	-6.15	94.39	111.00
2	Bp	85	SER	N-CA-C	6.15	127.61	111.00
2	Br	134	HIS	N-CA-C	-6.15	94.39	111.00
2	B4	85	SER	N-CA-C	6.15	127.60	111.00
2	B9	134	HIS	N-CA-C	-6.15	94.40	111.00
2	BD	85	SER	N-CA-C	6.15	127.60	111.00
2	BJ	134	HIS	N-CA-C	-6.15	94.40	111.00
2	Bb	85	SER	N-CA-C	6.15	127.60	111.00
2	Bd	134	HIS	N-CA-C	-6.15	94.40	111.00
2	Bo	85	SER	N-CA-C	6.15	127.60	111.00
2	BL	134	HIS	N-CA-C	-6.15	94.41	111.00
2	B9	85	SER	N-CA-C	6.15	127.59	111.00
2	BY	134	HIS	N-CA-C	-6.14	94.41	111.00
2	B7	134	HIS	N-CA-C	-6.14	94.41	111.00
2	Bj	85	SER	N-CA-C	6.14	127.59	111.00
2	Bx	134	HIS	N-CA-C	-6.14	94.41	111.00
2	BC	85	SER	N-CA-C	6.14	127.58	111.00
2	BL	85	SER	N-CA-C	6.14	127.58	111.00
2	BM	85	SER	N-CA-C	6.14	127.58	111.00
2	B8	134	HIS	N-CA-C	-6.14	94.41	111.00
2	Br	85	SER	N-CA-C	6.14	127.59	111.00
2	Bt	85	SER	N-CA-C	6.14	127.58	111.00
2	BN	85	SER	N-CA-C	6.14	127.58	111.00
2	Bu	85	SER	N-CA-C	6.14	127.57	111.00
2	Bf	85	SER	N-CA-C	6.14	127.57	111.00
2	Bl	85	SER	N-CA-C	6.14	127.57	111.00
2	Bm	134	HIS	N-CA-C	-6.14	94.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BB	85	SER	N-CA-C	6.13	127.56	111.00
2	B2	85	SER	N-CA-C	6.13	127.56	111.00
2	Be	85	SER	N-CA-C	6.13	127.56	111.00
3	CR	216	LEU	CA-CB-CG	6.13	129.40	115.30
3	Cx	216	LEU	CA-CB-CG	6.13	129.39	115.30
2	BV	85	SER	N-CA-C	6.12	127.53	111.00
3	Ct	216	LEU	CA-CB-CG	6.12	129.37	115.30
3	DB	216	LEU	CA-CB-CG	6.11	129.36	115.30
3	CM	216	LEU	CA-CB-CG	6.11	129.35	115.30
3	CW	216	LEU	CA-CB-CG	6.11	129.36	115.30
3	C3	216	LEU	CA-CB-CG	6.11	129.34	115.30
3	C6	216	LEU	CA-CB-CG	6.11	129.34	115.30
3	Ci	216	LEU	CA-CB-CG	6.10	129.33	115.30
3	CJ	216	LEU	CA-CB-CG	6.10	129.33	115.30
3	CV	216	LEU	CA-CB-CG	6.10	129.33	115.30
3	CZ	216	LEU	CA-CB-CG	6.10	129.33	115.30
3	Cn	216	LEU	CA-CB-CG	6.10	129.33	115.30
3	C1	216	LEU	CA-CB-CG	6.10	129.33	115.30
3	Ck	216	LEU	CA-CB-CG	6.10	129.33	115.30
3	Cg	216	LEU	CA-CB-CG	6.10	129.32	115.30
3	Cd	216	LEU	CA-CB-CG	6.09	129.32	115.30
3	Cj	216	LEU	CA-CB-CG	6.09	129.32	115.30
3	CL	216	LEU	CA-CB-CG	6.09	129.31	115.30
3	CQ	216	LEU	CA-CB-CG	6.09	129.31	115.30
3	Cr	216	LEU	CA-CB-CG	6.09	129.31	115.30
3	CC	216	LEU	CA-CB-CG	6.09	129.31	115.30
3	Cq	216	LEU	CA-CB-CG	6.09	129.31	115.30
3	CA	216	LEU	CA-CB-CG	6.09	129.31	115.30
3	CI	216	LEU	CA-CB-CG	6.09	129.31	115.30
3	Cs	216	LEU	CA-CB-CG	6.09	129.31	115.30
3	Cv	216	LEU	CA-CB-CG	6.09	129.31	115.30
3	C7	216	LEU	CA-CB-CG	6.09	129.30	115.30
3	CE	216	LEU	CA-CB-CG	6.09	129.30	115.30
3	CT	216	LEU	CA-CB-CG	6.09	129.30	115.30
3	C4	216	LEU	CA-CB-CG	6.09	129.30	115.30
3	C9	216	LEU	CA-CB-CG	6.09	129.30	115.30
3	Cf	216	LEU	CA-CB-CG	6.09	129.30	115.30
3	Cp	216	LEU	CA-CB-CG	6.09	129.30	115.30
3	C0	216	LEU	CA-CB-CG	6.08	129.29	115.30
3	C5	216	LEU	CA-CB-CG	6.08	129.29	115.30
1	Al	4	VAL	N-CA-C	6.08	127.42	111.00
3	CG	216	LEU	CA-CB-CG	6.08	129.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CS	216	LEU	CA-CB-CG	6.08	129.29	115.30
3	C2	216	LEU	CA-CB-CG	6.08	129.28	115.30
1	An	4	VAL	N-CA-C	6.08	127.41	111.00
3	DA	216	LEU	CA-CB-CG	6.08	129.28	115.30
3	CF	216	LEU	CA-CB-CG	6.08	129.28	115.30
3	CH	216	LEU	CA-CB-CG	6.08	129.28	115.30
1	DF	4	VAL	N-CA-C	6.08	127.40	111.00
3	Cc	216	LEU	CA-CB-CG	6.07	129.27	115.30
1	DI	4	VAL	N-CA-C	6.07	127.40	111.00
1	Af	4	VAL	N-CA-C	6.07	127.39	111.00
3	CX	216	LEU	CA-CB-CG	6.07	129.26	115.30
1	AO	4	VAL	N-CA-C	6.07	127.39	111.00
1	AQ	4	VAL	N-CA-C	6.07	127.39	111.00
1	AY	4	VAL	N-CA-C	6.07	127.39	111.00
1	A0	4	VAL	N-CA-C	6.07	127.39	111.00
1	Aj	4	VAL	N-CA-C	6.07	127.39	111.00
3	Co	216	LEU	CA-CB-CG	6.07	129.26	115.30
3	Cw	216	LEU	CA-CB-CG	6.07	129.26	115.30
1	AG	4	VAL	N-CA-C	6.07	127.39	111.00
3	CB	216	LEU	CA-CB-CG	6.07	129.26	115.30
3	CD	216	LEU	CA-CB-CG	6.07	129.26	115.30
3	CP	216	LEU	CA-CB-CG	6.07	129.26	115.30
3	Ce	216	LEU	CA-CB-CG	6.07	129.26	115.30
1	AB	4	VAL	N-CA-C	6.07	127.38	111.00
1	A9	4	VAL	N-CA-C	6.07	127.38	111.00
3	CN	216	LEU	CA-CB-CG	6.07	129.25	115.30
3	CU	216	LEU	CA-CB-CG	6.07	129.25	115.30
3	CY	216	LEU	CA-CB-CG	6.07	129.25	115.30
3	C8	216	LEU	CA-CB-CG	6.07	129.25	115.30
3	Cm	216	LEU	CA-CB-CG	6.07	129.25	115.30
1	AE	4	VAL	N-CA-C	6.06	127.37	111.00
1	A2	4	VAL	N-CA-C	6.06	127.37	111.00
1	A3	4	VAL	N-CA-C	6.06	127.37	111.00
1	AC	4	VAL	N-CA-C	6.06	127.37	111.00
1	Ae	4	VAL	N-CA-C	6.06	127.37	111.00
1	Ag	4	VAL	N-CA-C	6.06	127.37	111.00
3	Ch	216	LEU	CA-CB-CG	6.06	129.24	115.30
3	Cl	216	LEU	CA-CB-CG	6.06	129.24	115.30
1	AR	4	VAL	N-CA-C	6.06	127.37	111.00
1	Am	4	VAL	N-CA-C	6.06	127.36	111.00
1	A4	4	VAL	N-CA-C	6.06	127.36	111.00
1	Ah	4	VAL	N-CA-C	6.06	127.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CO	216	LEU	CA-CB-CG	6.06	129.24	115.30
3	Cu	216	LEU	CA-CB-CG	6.06	129.24	115.30
1	DG	4	VAL	N-CA-C	6.06	127.36	111.00
1	AW	4	VAL	N-CA-C	6.06	127.36	111.00
1	A7	4	VAL	N-CA-C	6.06	127.35	111.00
3	CK	216	LEU	CA-CB-CG	6.06	129.23	115.30
1	AN	4	VAL	N-CA-C	6.05	127.35	111.00
1	AU	4	VAL	N-CA-C	6.05	127.35	111.00
1	AZ	4	VAL	N-CA-C	6.05	127.35	111.00
1	Ad	4	VAL	N-CA-C	6.05	127.35	111.00
1	DD	4	VAL	N-CA-C	6.05	127.34	111.00
1	Ao	4	VAL	N-CA-C	6.05	127.34	111.00
1	AD	4	VAL	N-CA-C	6.05	127.34	111.00
1	AI	4	VAL	N-CA-C	6.05	127.34	111.00
1	AJ	4	VAL	N-CA-C	6.05	127.34	111.00
1	A8	4	VAL	N-CA-C	6.05	127.34	111.00
1	AP	4	VAL	N-CA-C	6.05	127.33	111.00
1	AS	4	VAL	N-CA-C	6.05	127.34	111.00
1	AT	4	VAL	N-CA-C	6.05	127.33	111.00
1	A1	4	VAL	N-CA-C	6.05	127.33	111.00
1	A6	4	VAL	N-CA-C	6.05	127.33	111.00
1	DJ	4	VAL	N-CA-C	6.05	127.32	111.00
1	AK	4	VAL	N-CA-C	6.04	127.32	111.00
1	AA	4	VAL	N-CA-C	6.04	127.31	111.00
1	AF	4	VAL	N-CA-C	6.04	127.31	111.00
1	AM	4	VAL	N-CA-C	6.04	127.31	111.00
1	AV	4	VAL	N-CA-C	6.04	127.31	111.00
1	Ac	4	VAL	N-CA-C	6.04	127.31	111.00
1	Ai	4	VAL	N-CA-C	6.04	127.31	111.00
1	Ak	4	VAL	N-CA-C	6.04	127.30	111.00
1	DH	4	VAL	N-CA-C	6.04	127.30	111.00
1	DK	4	VAL	N-CA-C	6.04	127.30	111.00
1	Aa	4	VAL	N-CA-C	6.04	127.30	111.00
1	AX	4	VAL	N-CA-C	6.04	127.30	111.00
1	Ab	4	VAL	N-CA-C	6.04	127.30	111.00
1	A5	4	VAL	N-CA-C	6.03	127.29	111.00
1	AH	4	VAL	N-CA-C	6.03	127.29	111.00
1	AL	4	VAL	N-CA-C	6.03	127.28	111.00
1	DE	4	VAL	N-CA-C	6.03	127.28	111.00
1	DC	4	VAL	N-CA-C	6.03	127.27	111.00
1	Al	151	SER	N-CA-C	-5.76	95.45	111.00
1	AM	151	SER	N-CA-C	-5.76	95.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DD	151	SER	N-CA-C	-5.75	95.47	111.00
1	AR	151	SER	N-CA-C	-5.74	95.50	111.00
1	AW	151	SER	N-CA-C	-5.74	95.49	111.00
1	DI	151	SER	N-CA-C	-5.74	95.49	111.00
1	Aa	151	SER	N-CA-C	-5.74	95.50	111.00
1	AI	151	SER	N-CA-C	-5.74	95.50	111.00
1	AH	151	SER	N-CA-C	-5.74	95.51	111.00
1	AX	151	SER	N-CA-C	-5.74	95.51	111.00
1	Ab	151	SER	N-CA-C	-5.74	95.50	111.00
1	AD	151	SER	N-CA-C	-5.74	95.51	111.00
1	AL	151	SER	N-CA-C	-5.74	95.51	111.00
1	DF	151	SER	N-CA-C	-5.74	95.52	111.00
1	A6	151	SER	N-CA-C	-5.73	95.52	111.00
1	AC	151	SER	N-CA-C	-5.73	95.52	111.00
1	AV	151	SER	N-CA-C	-5.73	95.52	111.00
1	AE	151	SER	N-CA-C	-5.73	95.53	111.00
1	AJ	151	SER	N-CA-C	-5.73	95.53	111.00
1	Ac	151	SER	N-CA-C	-5.73	95.53	111.00
1	Ah	151	SER	N-CA-C	-5.73	95.53	111.00
1	DJ	151	SER	N-CA-C	-5.73	95.53	111.00
1	DK	151	SER	N-CA-C	-5.73	95.53	111.00
1	A2	151	SER	N-CA-C	-5.73	95.53	111.00
1	A7	151	SER	N-CA-C	-5.73	95.53	111.00
1	AS	151	SER	N-CA-C	-5.73	95.54	111.00
1	AT	151	SER	N-CA-C	-5.73	95.53	111.00
1	Af	151	SER	N-CA-C	-5.73	95.54	111.00
1	Ag	151	SER	N-CA-C	-5.73	95.53	111.00
1	Ak	151	SER	N-CA-C	-5.73	95.53	111.00
1	An	151	SER	N-CA-C	-5.73	95.53	111.00
1	Ao	151	SER	N-CA-C	-5.73	95.53	111.00
1	AY	151	SER	N-CA-C	-5.73	95.54	111.00
1	A1	151	SER	N-CA-C	-5.72	95.55	111.00
1	AQ	151	SER	N-CA-C	-5.72	95.55	111.00
1	Am	151	SER	N-CA-C	-5.72	95.55	111.00
1	AN	151	SER	N-CA-C	-5.72	95.56	111.00
1	AA	151	SER	N-CA-C	-5.72	95.56	111.00
1	AK	151	SER	N-CA-C	-5.72	95.56	111.00
1	DE	151	SER	N-CA-C	-5.72	95.56	111.00
1	AO	151	SER	N-CA-C	-5.72	95.56	111.00
1	A5	151	SER	N-CA-C	-5.72	95.56	111.00
1	A8	151	SER	N-CA-C	-5.72	95.56	111.00
1	Ai	151	SER	N-CA-C	-5.72	95.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DG	151	SER	N-CA-C	-5.72	95.56	111.00
1	A0	151	SER	N-CA-C	-5.71	95.57	111.00
1	Aj	151	SER	N-CA-C	-5.71	95.57	111.00
1	AG	151	SER	N-CA-C	-5.71	95.58	111.00
1	AF	151	SER	N-CA-C	-5.71	95.58	111.00
1	DC	151	SER	N-CA-C	-5.71	95.58	111.00
1	AP	151	SER	N-CA-C	-5.71	95.59	111.00
1	Ae	151	SER	N-CA-C	-5.71	95.59	111.00
1	AB	151	SER	N-CA-C	-5.71	95.59	111.00
1	Ad	151	SER	N-CA-C	-5.71	95.59	111.00
1	AU	151	SER	N-CA-C	-5.70	95.61	111.00
1	AZ	151	SER	N-CA-C	-5.70	95.60	111.00
1	DH	151	SER	N-CA-C	-5.70	95.61	111.00
1	A3	151	SER	N-CA-C	-5.70	95.61	111.00
1	A4	151	SER	N-CA-C	-5.70	95.62	111.00
1	A9	151	SER	N-CA-C	-5.70	95.62	111.00
1	Af	181	LYS	N-CA-C	-5.67	95.68	111.00
1	Ao	181	LYS	N-CA-C	-5.67	95.69	111.00
1	AQ	181	LYS	N-CA-C	-5.67	95.69	111.00
1	AU	181	LYS	N-CA-C	-5.67	95.70	111.00
1	A4	181	LYS	N-CA-C	-5.67	95.70	111.00
1	An	181	LYS	N-CA-C	-5.67	95.70	111.00
1	AB	181	LYS	N-CA-C	-5.66	95.71	111.00
1	AG	181	LYS	N-CA-C	-5.66	95.71	111.00
1	AH	181	LYS	N-CA-C	-5.66	95.71	111.00
1	A0	181	LYS	N-CA-C	-5.66	95.71	111.00
1	AS	181	LYS	N-CA-C	-5.66	95.71	111.00
1	DG	181	LYS	N-CA-C	-5.66	95.72	111.00
1	DH	181	LYS	N-CA-C	-5.66	95.72	111.00
1	AC	181	LYS	N-CA-C	-5.66	95.73	111.00
1	A6	181	LYS	N-CA-C	-5.66	95.73	111.00
1	Ah	181	LYS	N-CA-C	-5.66	95.73	111.00
1	Ae	181	LYS	N-CA-C	-5.66	95.73	111.00
1	AF	181	LYS	N-CA-C	-5.65	95.74	111.00
1	AL	181	LYS	N-CA-C	-5.65	95.74	111.00
1	AO	181	LYS	N-CA-C	-5.65	95.74	111.00
1	DJ	181	LYS	N-CA-C	-5.65	95.74	111.00
1	AN	181	LYS	N-CA-C	-5.65	95.74	111.00
1	A2	181	LYS	N-CA-C	-5.65	95.75	111.00
1	Al	181	LYS	N-CA-C	-5.65	95.74	111.00
1	DI	181	LYS	N-CA-C	-5.65	95.75	111.00
1	AI	181	LYS	N-CA-C	-5.65	95.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AK	181	LYS	N-CA-C	-5.65	95.75	111.00
1	AV	181	LYS	N-CA-C	-5.65	95.75	111.00
1	Ab	181	LYS	N-CA-C	-5.65	95.75	111.00
1	Aa	181	LYS	N-CA-C	-5.65	95.75	111.00
1	AY	181	LYS	N-CA-C	-5.64	95.76	111.00
1	A3	181	LYS	N-CA-C	-5.64	95.76	111.00
1	Aj	181	LYS	N-CA-C	-5.64	95.76	111.00
1	Ak	181	LYS	N-CA-C	-5.64	95.76	111.00
1	AP	181	LYS	N-CA-C	-5.64	95.76	111.00
1	AX	181	LYS	N-CA-C	-5.64	95.76	111.00
1	Ai	181	LYS	N-CA-C	-5.64	95.77	111.00
1	AA	181	LYS	N-CA-C	-5.64	95.77	111.00
1	AT	181	LYS	N-CA-C	-5.64	95.77	111.00
1	A9	181	LYS	N-CA-C	-5.64	95.78	111.00
1	DK	181	LYS	N-CA-C	-5.64	95.77	111.00
1	AD	181	LYS	N-CA-C	-5.64	95.78	111.00
1	AZ	181	LYS	N-CA-C	-5.64	95.78	111.00
1	DF	181	LYS	N-CA-C	-5.64	95.78	111.00
1	AM	181	LYS	N-CA-C	-5.64	95.78	111.00
1	Ac	181	LYS	N-CA-C	-5.64	95.78	111.00
1	Ad	181	LYS	N-CA-C	-5.63	95.79	111.00
1	DD	181	LYS	N-CA-C	-5.63	95.79	111.00
1	A5	181	LYS	N-CA-C	-5.63	95.79	111.00
1	Am	181	LYS	N-CA-C	-5.63	95.79	111.00
1	AE	181	LYS	N-CA-C	-5.63	95.80	111.00
1	DE	181	LYS	N-CA-C	-5.63	95.81	111.00
1	AJ	181	LYS	N-CA-C	-5.63	95.81	111.00
1	A7	181	LYS	N-CA-C	-5.63	95.81	111.00
1	AW	181	LYS	N-CA-C	-5.62	95.82	111.00
1	DC	181	LYS	N-CA-C	-5.62	95.82	111.00
1	A1	181	LYS	N-CA-C	-5.62	95.83	111.00
1	A8	181	LYS	N-CA-C	-5.62	95.83	111.00
1	Ag	181	LYS	N-CA-C	-5.62	95.84	111.00
1	AR	181	LYS	N-CA-C	-5.61	95.86	111.00
1	AV	226	PRO	N-CA-C	5.60	126.66	112.10
1	Af	226	PRO	N-CA-C	5.59	126.63	112.10
1	A1	226	PRO	N-CA-C	5.58	126.62	112.10
1	A5	226	PRO	N-CA-C	5.58	126.62	112.10
1	AC	226	PRO	N-CA-C	5.58	126.61	112.10
1	Aa	226	PRO	N-CA-C	5.58	126.61	112.10
1	Ag	226	PRO	N-CA-C	5.58	126.61	112.10
1	AQ	226	PRO	N-CA-C	5.58	126.61	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DC	226	PRO	N-CA-C	5.58	126.60	112.10
1	AX	226	PRO	N-CA-C	5.58	126.60	112.10
1	Am	226	PRO	N-CA-C	5.58	126.60	112.10
1	DI	226	PRO	N-CA-C	5.58	126.60	112.10
1	AR	226	PRO	N-CA-C	5.57	126.59	112.10
1	A0	226	PRO	N-CA-C	5.57	126.59	112.10
1	Ae	226	PRO	N-CA-C	5.57	126.59	112.10
1	DD	226	PRO	N-CA-C	5.57	126.59	112.10
1	A6	226	PRO	N-CA-C	5.57	126.58	112.10
1	A9	226	PRO	N-CA-C	5.57	126.58	112.10
1	DG	226	PRO	N-CA-C	5.57	126.58	112.10
1	AZ	226	PRO	N-CA-C	5.57	126.57	112.10
1	A3	226	PRO	N-CA-C	5.57	126.57	112.10
1	A7	226	PRO	N-CA-C	5.57	126.57	112.10
1	Ab	226	PRO	N-CA-C	5.57	126.57	112.10
1	Aj	226	PRO	N-CA-C	5.57	126.57	112.10
1	DH	226	PRO	N-CA-C	5.57	126.57	112.10
1	AF	226	PRO	N-CA-C	5.56	126.56	112.10
1	AI	226	PRO	N-CA-C	5.56	126.56	112.10
1	AL	226	PRO	N-CA-C	5.56	126.56	112.10
1	AO	226	PRO	N-CA-C	5.56	126.56	112.10
1	AA	226	PRO	N-CA-C	5.56	126.56	112.10
1	AD	226	PRO	N-CA-C	5.56	126.56	112.10
1	AP	226	PRO	N-CA-C	5.56	126.56	112.10
1	AS	226	PRO	N-CA-C	5.56	126.55	112.10
1	AH	226	PRO	N-CA-C	5.56	126.55	112.10
1	AW	226	PRO	N-CA-C	5.56	126.55	112.10
1	Al	226	PRO	N-CA-C	5.56	126.55	112.10
1	AK	226	PRO	N-CA-C	5.56	126.55	112.10
1	Ak	226	PRO	N-CA-C	5.56	126.55	112.10
1	AE	226	PRO	N-CA-C	5.55	126.54	112.10
1	AJ	226	PRO	N-CA-C	5.55	126.54	112.10
1	AM	226	PRO	N-CA-C	5.55	126.54	112.10
1	Ac	226	PRO	N-CA-C	5.55	126.54	112.10
1	A4	226	PRO	N-CA-C	5.55	126.54	112.10
1	Ao	226	PRO	N-CA-C	5.55	126.54	112.10
1	A8	226	PRO	N-CA-C	5.55	126.53	112.10
1	DE	226	PRO	N-CA-C	5.55	126.53	112.10
1	DJ	226	PRO	N-CA-C	5.55	126.54	112.10
1	AB	226	PRO	N-CA-C	5.55	126.53	112.10
1	AT	226	PRO	N-CA-C	5.55	126.53	112.10
1	AY	226	PRO	N-CA-C	5.55	126.53	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ad	226	PRO	N-CA-C	5.55	126.53	112.10
1	DK	226	PRO	N-CA-C	5.55	126.52	112.10
1	AN	226	PRO	N-CA-C	5.54	126.52	112.10
1	A2	226	PRO	N-CA-C	5.54	126.52	112.10
1	Ah	226	PRO	N-CA-C	5.54	126.51	112.10
1	DF	226	PRO	N-CA-C	5.54	126.51	112.10
1	DK	186	TRP	N-CA-C	5.54	125.96	111.00
1	AU	226	PRO	N-CA-C	5.54	126.50	112.10
3	Ci	64	VAL	CB-CA-C	-5.54	100.88	111.40
3	CR	64	VAL	CB-CA-C	-5.53	100.89	111.40
3	C4	18	VAL	CB-CA-C	-5.53	100.89	111.40
3	Cq	64	VAL	CB-CA-C	-5.53	100.89	111.40
3	C1	64	VAL	CB-CA-C	-5.53	100.89	111.40
3	Co	64	VAL	CB-CA-C	-5.53	100.89	111.40
3	Cp	64	VAL	CB-CA-C	-5.53	100.89	111.40
3	CQ	208	VAL	CB-CA-C	-5.53	100.89	111.40
1	DH	186	TRP	N-CA-C	5.53	125.93	111.00
1	AG	226	PRO	N-CA-C	5.53	126.47	112.10
1	Ai	226	PRO	N-CA-C	5.53	126.47	112.10
3	C6	64	VAL	CB-CA-C	-5.52	100.90	111.40
1	An	226	PRO	N-CA-C	5.52	126.46	112.10
3	Ct	64	VAL	CB-CA-C	-5.52	100.91	111.40
1	Aj	186	TRP	N-CA-C	5.52	125.90	111.00
3	C4	64	VAL	CB-CA-C	-5.52	100.91	111.40
3	Cj	64	VAL	CB-CA-C	-5.52	100.91	111.40
3	Cl	64	VAL	CB-CA-C	-5.52	100.92	111.40
3	CM	64	VAL	CB-CA-C	-5.52	100.92	111.40
3	Cf	64	VAL	CB-CA-C	-5.52	100.92	111.40
3	CB	64	VAL	CB-CA-C	-5.51	100.92	111.40
3	CK	64	VAL	CB-CA-C	-5.51	100.92	111.40
3	CQ	64	VAL	CB-CA-C	-5.51	100.92	111.40
3	Cn	64	VAL	CB-CA-C	-5.51	100.92	111.40
1	AH	186	TRP	N-CA-C	5.51	125.89	111.00
1	AR	186	TRP	N-CA-C	5.51	125.88	111.00
1	AS	186	TRP	N-CA-C	5.51	125.89	111.00
3	CE	64	VAL	CB-CA-C	-5.51	100.92	111.40
3	CJ	64	VAL	CB-CA-C	-5.51	100.93	111.40
3	CU	18	VAL	CB-CA-C	-5.51	100.92	111.40
3	Cd	64	VAL	CB-CA-C	-5.51	100.93	111.40
1	DG	186	TRP	N-CA-C	5.51	125.88	111.00
1	AP	186	TRP	N-CA-C	5.51	125.88	111.00
3	C1	208	VAL	CB-CA-C	-5.51	100.93	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AK	186	TRP	N-CA-C	5.51	125.88	111.00
1	AQ	186	TRP	N-CA-C	5.51	125.88	111.00
1	AU	186	TRP	N-CA-C	5.51	125.88	111.00
1	A5	186	TRP	N-CA-C	5.51	125.88	111.00
3	CR	18	VAL	CB-CA-C	-5.51	100.93	111.40
3	C3	64	VAL	CB-CA-C	-5.51	100.93	111.40
3	CL	208	VAL	CB-CA-C	-5.51	100.93	111.40
3	CU	64	VAL	CB-CA-C	-5.51	100.94	111.40
3	CW	18	VAL	CB-CA-C	-5.51	100.93	111.40
1	AX	186	TRP	N-CA-C	5.51	125.87	111.00
1	Al	186	TRP	N-CA-C	5.51	125.87	111.00
3	CA	64	VAL	CB-CA-C	-5.51	100.94	111.40
3	CJ	208	VAL	CB-CA-C	-5.51	100.94	111.40
3	Ce	208	VAL	CB-CA-C	-5.51	100.94	111.40
1	DC	186	TRP	N-CA-C	5.51	125.87	111.00
1	DJ	186	TRP	N-CA-C	5.51	125.87	111.00
1	A9	186	TRP	N-CA-C	5.50	125.86	111.00
1	Aa	186	TRP	N-CA-C	5.50	125.86	111.00
1	Ag	186	TRP	N-CA-C	5.50	125.86	111.00
1	AF	186	TRP	N-CA-C	5.50	125.86	111.00
1	AG	186	TRP	N-CA-C	5.50	125.86	111.00
1	AM	186	TRP	N-CA-C	5.50	125.86	111.00
1	A0	186	TRP	N-CA-C	5.50	125.86	111.00
3	CY	64	VAL	CB-CA-C	-5.50	100.94	111.40
3	DA	64	VAL	CB-CA-C	-5.50	100.94	111.40
1	AB	186	TRP	N-CA-C	5.50	125.86	111.00
1	AY	186	TRP	N-CA-C	5.50	125.85	111.00
1	Ad	186	TRP	N-CA-C	5.50	125.85	111.00
1	Ai	186	TRP	N-CA-C	5.50	125.86	111.00
3	CH	64	VAL	CB-CA-C	-5.50	100.95	111.40
3	Cq	18	VAL	CB-CA-C	-5.50	100.95	111.40
1	AL	186	TRP	N-CA-C	5.50	125.85	111.00
1	Ao	186	TRP	N-CA-C	5.50	125.85	111.00
3	CZ	18	VAL	CB-CA-C	-5.50	100.95	111.40
3	C7	208	VAL	CB-CA-C	-5.50	100.95	111.40
3	Ce	64	VAL	CB-CA-C	-5.50	100.95	111.40
3	Cp	208	VAL	CB-CA-C	-5.50	100.95	111.40
1	AI	186	TRP	N-CA-C	5.50	125.85	111.00
1	Am	186	TRP	N-CA-C	5.50	125.85	111.00
1	An	186	TRP	N-CA-C	5.50	125.85	111.00
3	CA	18	VAL	CB-CA-C	-5.50	100.95	111.40
3	C8	64	VAL	CB-CA-C	-5.50	100.95	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Cl	18	VAL	CB-CA-C	-5.50	100.95	111.40
3	Cv	64	VAL	CB-CA-C	-5.50	100.95	111.40
3	Cw	64	VAL	CB-CA-C	-5.50	100.95	111.40
1	AE	186	TRP	N-CA-C	5.50	125.84	111.00
1	Ak	186	TRP	N-CA-C	5.50	125.84	111.00
3	CL	64	VAL	CB-CA-C	-5.50	100.96	111.40
3	C9	18	VAL	CB-CA-C	-5.50	100.96	111.40
3	Cj	208	VAL	CB-CA-C	-5.50	100.96	111.40
3	Cu	208	VAL	CB-CA-C	-5.50	100.96	111.40
3	DB	18	VAL	CB-CA-C	-5.50	100.96	111.40
1	AC	186	TRP	N-CA-C	5.50	125.84	111.00
1	AV	186	TRP	N-CA-C	5.50	125.84	111.00
3	CB	208	VAL	CB-CA-C	-5.50	100.96	111.40
3	CF	64	VAL	CB-CA-C	-5.50	100.96	111.40
3	CO	64	VAL	CB-CA-C	-5.50	100.96	111.40
3	CV	64	VAL	CB-CA-C	-5.50	100.96	111.40
3	Cs	64	VAL	CB-CA-C	-5.50	100.96	111.40
3	Ct	18	VAL	CB-CA-C	-5.50	100.96	111.40
1	A3	186	TRP	N-CA-C	5.49	125.83	111.00
1	A8	186	TRP	N-CA-C	5.49	125.83	111.00
1	Ae	186	TRP	N-CA-C	5.49	125.83	111.00
1	Ah	186	TRP	N-CA-C	5.49	125.83	111.00
3	CZ	64	VAL	CB-CA-C	-5.49	100.96	111.40
3	C2	64	VAL	CB-CA-C	-5.49	100.96	111.40
3	Cc	18	VAL	CB-CA-C	-5.49	100.96	111.40
3	DA	18	VAL	CB-CA-C	-5.49	100.96	111.40
1	Ab	186	TRP	N-CA-C	5.49	125.83	111.00
3	CP	18	VAL	CB-CA-C	-5.49	100.97	111.40
3	C0	64	VAL	CB-CA-C	-5.49	100.97	111.40
3	Cg	64	VAL	CB-CA-C	-5.49	100.96	111.40
3	Cx	18	VAL	CB-CA-C	-5.49	100.97	111.40
1	AT	186	TRP	N-CA-C	5.49	125.83	111.00
1	A4	186	TRP	N-CA-C	5.49	125.82	111.00
3	CE	18	VAL	CB-CA-C	-5.49	100.97	111.40
3	CG	64	VAL	CB-CA-C	-5.49	100.97	111.40
3	CH	18	VAL	CB-CA-C	-5.49	100.97	111.40
3	CK	18	VAL	CB-CA-C	-5.49	100.97	111.40
3	CM	18	VAL	CB-CA-C	-5.49	100.97	111.40
3	CX	208	VAL	CB-CA-C	-5.49	100.97	111.40
3	C1	18	VAL	CB-CA-C	-5.49	100.97	111.40
3	C5	208	VAL	CB-CA-C	-5.49	100.97	111.40
3	C9	64	VAL	CB-CA-C	-5.49	100.97	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Cc	64	VAL	CB-CA-C	-5.49	100.97	111.40
3	Cf	18	VAL	CB-CA-C	-5.49	100.97	111.40
3	Ck	208	VAL	CB-CA-C	-5.49	100.97	111.40
3	Co	208	VAL	CB-CA-C	-5.49	100.97	111.40
3	Cr	208	VAL	CB-CA-C	-5.49	100.97	111.40
1	DF	186	TRP	N-CA-C	5.49	125.82	111.00
1	Ac	186	TRP	N-CA-C	5.49	125.82	111.00
3	CC	64	VAL	CB-CA-C	-5.49	100.97	111.40
3	CT	64	VAL	CB-CA-C	-5.49	100.97	111.40
3	C6	18	VAL	CB-CA-C	-5.49	100.97	111.40
3	Ch	64	VAL	CB-CA-C	-5.49	100.97	111.40
1	DI	186	TRP	N-CA-C	5.49	125.82	111.00
1	AZ	186	TRP	N-CA-C	5.49	125.81	111.00
3	CG	208	VAL	CB-CA-C	-5.49	100.97	111.40
3	CP	64	VAL	CB-CA-C	-5.49	100.97	111.40
1	AA	186	TRP	N-CA-C	5.49	125.81	111.00
1	AD	186	TRP	N-CA-C	5.49	125.81	111.00
1	AN	186	TRP	N-CA-C	5.49	125.81	111.00
1	AO	186	TRP	N-CA-C	5.49	125.81	111.00
1	A2	186	TRP	N-CA-C	5.49	125.81	111.00
1	A6	186	TRP	N-CA-C	5.49	125.81	111.00
3	CJ	18	VAL	CB-CA-C	-5.49	100.98	111.40
3	CW	208	VAL	CB-CA-C	-5.49	100.98	111.40
3	Cj	18	VAL	CB-CA-C	-5.49	100.98	111.40
1	DD	186	TRP	N-CA-C	5.49	125.81	111.00
3	CC	18	VAL	CB-CA-C	-5.48	100.98	111.40
3	CD	18	VAL	CB-CA-C	-5.48	100.98	111.40
3	CF	18	VAL	CB-CA-C	-5.48	100.98	111.40
3	CV	208	VAL	CB-CA-C	-5.48	100.98	111.40
3	Co	18	VAL	CB-CA-C	-5.48	100.98	111.40
1	AJ	186	TRP	N-CA-C	5.48	125.80	111.00
1	Af	186	TRP	N-CA-C	5.48	125.80	111.00
3	CG	18	VAL	CB-CA-C	-5.48	100.98	111.40
3	CL	18	VAL	CB-CA-C	-5.48	100.98	111.40
3	CP	208	VAL	CB-CA-C	-5.48	100.98	111.40
3	CR	208	VAL	CB-CA-C	-5.48	100.98	111.40
3	C0	208	VAL	CB-CA-C	-5.48	100.98	111.40
3	C8	18	VAL	CB-CA-C	-5.48	100.98	111.40
3	Ce	18	VAL	CB-CA-C	-5.48	100.98	111.40
3	Ck	18	VAL	CB-CA-C	-5.48	100.98	111.40
3	Cp	18	VAL	CB-CA-C	-5.48	100.98	111.40
3	Cw	18	VAL	CB-CA-C	-5.48	100.98	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	DB	64	VAL	CB-CA-C	-5.48	100.98	111.40
3	Cl	208	VAL	CB-CA-C	-5.48	100.99	111.40
3	Cu	64	VAL	CB-CA-C	-5.48	100.99	111.40
3	Cx	64	VAL	CB-CA-C	-5.48	100.99	111.40
3	C2	208	VAL	CB-CA-C	-5.48	100.99	111.40
3	Ct	208	VAL	CB-CA-C	-5.48	100.99	111.40
3	CF	208	VAL	CB-CA-C	-5.48	101.00	111.40
3	CQ	18	VAL	CB-CA-C	-5.48	100.99	111.40
3	C9	208	VAL	CB-CA-C	-5.48	100.99	111.40
3	Cf	208	VAL	CB-CA-C	-5.48	100.99	111.40
3	Ck	64	VAL	CB-CA-C	-5.48	100.99	111.40
3	Cm	18	VAL	CB-CA-C	-5.48	100.99	111.40
3	Cx	208	VAL	CB-CA-C	-5.48	100.99	111.40
3	DA	208	VAL	CB-CA-C	-5.48	100.99	111.40
1	DE	186	TRP	N-CA-C	5.48	125.79	111.00
3	CH	208	VAL	CB-CA-C	-5.48	101.00	111.40
3	C5	64	VAL	CB-CA-C	-5.48	101.00	111.40
3	Cr	64	VAL	CB-CA-C	-5.48	101.00	111.40
3	C3	18	VAL	CB-CA-C	-5.47	101.00	111.40
3	Cd	18	VAL	CB-CA-C	-5.47	101.00	111.40
3	Cg	18	VAL	CB-CA-C	-5.47	101.00	111.40
3	Ch	18	VAL	CB-CA-C	-5.47	101.00	111.40
3	Cm	64	VAL	CB-CA-C	-5.47	101.00	111.40
3	CA	208	VAL	CB-CA-C	-5.47	101.00	111.40
3	CD	64	VAL	CB-CA-C	-5.47	101.00	111.40
3	CN	18	VAL	CB-CA-C	-5.47	101.00	111.40
3	CS	64	VAL	CB-CA-C	-5.47	101.00	111.40
3	CW	64	VAL	CB-CA-C	-5.47	101.00	111.40
3	DB	208	VAL	CB-CA-C	-5.47	101.00	111.40
1	AW	186	TRP	N-CA-C	5.47	125.77	111.00
3	CI	208	VAL	CB-CA-C	-5.47	101.01	111.40
3	CX	64	VAL	CB-CA-C	-5.47	101.01	111.40
3	C7	64	VAL	CB-CA-C	-5.47	101.01	111.40
3	Cs	18	VAL	CB-CA-C	-5.47	101.01	111.40
1	A1	186	TRP	N-CA-C	5.47	125.76	111.00
3	CZ	208	VAL	CB-CA-C	-5.47	101.01	111.40
3	Cn	18	VAL	CB-CA-C	-5.47	101.01	111.40
3	CC	208	VAL	CB-CA-C	-5.47	101.01	111.40
3	CO	208	VAL	CB-CA-C	-5.47	101.01	111.40
3	C2	18	VAL	CB-CA-C	-5.47	101.01	111.40
3	C6	208	VAL	CB-CA-C	-5.47	101.02	111.40
3	Cv	18	VAL	CB-CA-C	-5.47	101.01	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	CN	208	VAL	CB-CA-C	-5.46	101.02	111.40
3	CS	18	VAL	CB-CA-C	-5.46	101.02	111.40
3	CY	18	VAL	CB-CA-C	-5.46	101.02	111.40
3	Cd	208	VAL	CB-CA-C	-5.46	101.02	111.40
3	CM	208	VAL	CB-CA-C	-5.46	101.02	111.40
3	Ci	208	VAL	CB-CA-C	-5.46	101.02	111.40
3	CD	208	VAL	CB-CA-C	-5.46	101.02	111.40
3	CX	18	VAL	CB-CA-C	-5.46	101.03	111.40
3	C5	18	VAL	CB-CA-C	-5.46	101.02	111.40
3	Cw	208	VAL	CB-CA-C	-5.46	101.02	111.40
1	A7	186	TRP	N-CA-C	5.46	125.74	111.00
3	CI	18	VAL	CB-CA-C	-5.46	101.03	111.40
3	C7	18	VAL	CB-CA-C	-5.46	101.03	111.40
3	Cr	18	VAL	CB-CA-C	-5.46	101.03	111.40
3	CO	18	VAL	CB-CA-C	-5.46	101.03	111.40
3	C4	208	VAL	CB-CA-C	-5.46	101.03	111.40
3	Cu	18	VAL	CB-CA-C	-5.46	101.03	111.40
3	CI	64	VAL	CB-CA-C	-5.45	101.04	111.40
3	CT	208	VAL	CB-CA-C	-5.45	101.04	111.40
3	CY	208	VAL	CB-CA-C	-5.45	101.04	111.40
3	CK	208	VAL	CB-CA-C	-5.45	101.04	111.40
3	CU	208	VAL	CB-CA-C	-5.45	101.04	111.40
3	CV	18	VAL	CB-CA-C	-5.45	101.04	111.40
3	Cq	208	VAL	CB-CA-C	-5.45	101.04	111.40
3	CN	64	VAL	CB-CA-C	-5.45	101.05	111.40
3	Cm	208	VAL	CB-CA-C	-5.45	101.04	111.40
3	Cv	208	VAL	CB-CA-C	-5.45	101.05	111.40
3	CB	18	VAL	CB-CA-C	-5.45	101.05	111.40
3	Cg	208	VAL	CB-CA-C	-5.45	101.05	111.40
3	Cc	208	VAL	CB-CA-C	-5.45	101.05	111.40
3	Cn	208	VAL	CB-CA-C	-5.45	101.05	111.40
3	Ci	18	VAL	CB-CA-C	-5.45	101.05	111.40
3	C8	208	VAL	CB-CA-C	-5.44	101.06	111.40
3	CE	208	VAL	CB-CA-C	-5.44	101.06	111.40
3	CT	18	VAL	CB-CA-C	-5.44	101.06	111.40
3	Cs	208	VAL	CB-CA-C	-5.44	101.06	111.40
3	C0	18	VAL	CB-CA-C	-5.43	101.08	111.40
3	C3	208	VAL	CB-CA-C	-5.43	101.08	111.40
3	CS	208	VAL	CB-CA-C	-5.43	101.09	111.40
3	Ch	208	VAL	CB-CA-C	-5.43	101.09	111.40
1	DJ	242	ASN	CB-CA-C	-5.35	99.71	110.40
1	A5	242	ASN	CB-CA-C	-5.34	99.71	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AH	242	ASN	CB-CA-C	-5.34	99.72	110.40
1	Aa	242	ASN	CB-CA-C	-5.34	99.72	110.40
1	AX	242	ASN	CB-CA-C	-5.34	99.72	110.40
1	Ag	242	ASN	CB-CA-C	-5.34	99.72	110.40
1	An	242	ASN	CB-CA-C	-5.34	99.73	110.40
1	Am	242	ASN	CB-CA-C	-5.33	99.73	110.40
1	AA	242	ASN	CB-CA-C	-5.33	99.73	110.40
1	AU	242	ASN	CB-CA-C	-5.33	99.74	110.40
1	A2	242	ASN	CB-CA-C	-5.33	99.74	110.40
1	A8	242	ASN	CB-CA-C	-5.33	99.74	110.40
1	AN	242	ASN	CB-CA-C	-5.33	99.74	110.40
1	AV	242	ASN	CB-CA-C	-5.33	99.74	110.40
1	A6	242	ASN	CB-CA-C	-5.33	99.74	110.40
1	Ac	242	ASN	CB-CA-C	-5.33	99.74	110.40
1	DF	242	ASN	CB-CA-C	-5.33	99.74	110.40
1	Ad	242	ASN	CB-CA-C	-5.33	99.75	110.40
1	DE	242	ASN	CB-CA-C	-5.33	99.75	110.40
1	A0	242	ASN	CB-CA-C	-5.32	99.75	110.40
1	A9	242	ASN	CB-CA-C	-5.32	99.75	110.40
1	Ak	242	ASN	CB-CA-C	-5.32	99.75	110.40
1	DG	242	ASN	CB-CA-C	-5.32	99.75	110.40
1	A3	242	ASN	CB-CA-C	-5.32	99.75	110.40
1	AL	242	ASN	CB-CA-C	-5.32	99.76	110.40
1	AT	242	ASN	CB-CA-C	-5.32	99.76	110.40
1	A4	242	ASN	CB-CA-C	-5.32	99.76	110.40
1	DH	242	ASN	CB-CA-C	-5.32	99.76	110.40
1	AG	242	ASN	CB-CA-C	-5.32	99.77	110.40
1	AK	242	ASN	CB-CA-C	-5.32	99.77	110.40
1	Af	242	ASN	CB-CA-C	-5.32	99.77	110.40
1	Ao	242	ASN	CB-CA-C	-5.32	99.76	110.40
1	AY	242	ASN	CB-CA-C	-5.32	99.77	110.40
1	AE	242	ASN	CB-CA-C	-5.31	99.77	110.40
1	AS	242	ASN	CB-CA-C	-5.31	99.77	110.40
1	AZ	242	ASN	CB-CA-C	-5.31	99.78	110.40
1	AB	242	ASN	CB-CA-C	-5.31	99.78	110.40
1	AC	242	ASN	CB-CA-C	-5.31	99.78	110.40
1	Aj	242	ASN	CB-CA-C	-5.31	99.78	110.40
1	DK	242	ASN	CB-CA-C	-5.31	99.78	110.40
1	AQ	242	ASN	CB-CA-C	-5.31	99.79	110.40
1	AD	242	ASN	CB-CA-C	-5.31	99.79	110.40
1	AW	242	ASN	CB-CA-C	-5.31	99.79	110.40
1	AM	242	ASN	CB-CA-C	-5.30	99.79	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AR	242	ASN	CB-CA-C	-5.30	99.79	110.40
1	A1	242	ASN	CB-CA-C	-5.30	99.79	110.40
1	Ai	242	ASN	CB-CA-C	-5.30	99.79	110.40
1	AO	242	ASN	CB-CA-C	-5.30	99.80	110.40
1	A7	242	ASN	CB-CA-C	-5.30	99.80	110.40
1	Ab	242	ASN	CB-CA-C	-5.30	99.80	110.40
1	Al	242	ASN	CB-CA-C	-5.30	99.80	110.40
1	AI	242	ASN	CB-CA-C	-5.30	99.81	110.40
1	AJ	242	ASN	CB-CA-C	-5.30	99.81	110.40
1	AP	242	ASN	CB-CA-C	-5.30	99.81	110.40
1	DC	242	ASN	CB-CA-C	-5.29	99.81	110.40
1	DI	242	ASN	CB-CA-C	-5.29	99.82	110.40
1	AF	242	ASN	CB-CA-C	-5.29	99.82	110.40
1	DD	242	ASN	CB-CA-C	-5.28	99.84	110.40
1	Ah	242	ASN	CB-CA-C	-5.27	99.86	110.40
1	Ae	242	ASN	CB-CA-C	-5.27	99.86	110.40
1	Ao	6	GLU	N-CA-C	5.25	125.17	111.00
1	A3	6	GLU	N-CA-C	5.24	125.14	111.00
1	AM	6	GLU	N-CA-C	5.24	125.13	111.00
1	AU	6	GLU	N-CA-C	5.24	125.13	111.00
1	Ac	6	GLU	N-CA-C	5.24	125.13	111.00
1	Ah	6	GLU	N-CA-C	5.24	125.14	111.00
1	A0	6	GLU	N-CA-C	5.23	125.13	111.00
1	AB	6	GLU	N-CA-C	5.23	125.13	111.00
1	AO	6	GLU	N-CA-C	5.23	125.13	111.00
1	Ai	6	GLU	N-CA-C	5.23	125.13	111.00
1	Am	6	GLU	N-CA-C	5.23	125.13	111.00
1	AP	6	GLU	N-CA-C	5.23	125.12	111.00
1	AT	6	GLU	N-CA-C	5.23	125.12	111.00
1	DI	6	GLU	N-CA-C	5.23	125.12	111.00
1	A5	6	GLU	N-CA-C	5.23	125.11	111.00
1	DJ	6	GLU	N-CA-C	5.23	125.12	111.00
1	Ae	6	GLU	N-CA-C	5.23	125.11	111.00
1	AF	6	GLU	N-CA-C	5.22	125.11	111.00
1	AS	6	GLU	N-CA-C	5.22	125.10	111.00
1	A1	6	GLU	N-CA-C	5.22	125.10	111.00
1	A4	6	GLU	N-CA-C	5.22	125.10	111.00
1	Aa	6	GLU	N-CA-C	5.22	125.10	111.00
1	DC	6	GLU	N-CA-C	5.22	125.10	111.00
1	DF	6	GLU	N-CA-C	5.22	125.10	111.00
1	DH	6	GLU	N-CA-C	5.22	125.10	111.00
1	Ag	6	GLU	N-CA-C	5.22	125.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AW	6	GLU	N-CA-C	5.22	125.09	111.00
1	AZ	6	GLU	N-CA-C	5.22	125.09	111.00
1	Af	6	GLU	N-CA-C	5.22	125.09	111.00
1	A8	6	GLU	N-CA-C	5.22	125.08	111.00
1	AC	6	GLU	N-CA-C	5.21	125.08	111.00
1	Aj	6	GLU	N-CA-C	5.21	125.08	111.00
1	Ab	6	GLU	N-CA-C	5.21	125.08	111.00
1	Ad	6	GLU	N-CA-C	5.21	125.08	111.00
1	AR	6	GLU	N-CA-C	5.21	125.07	111.00
1	DG	6	GLU	N-CA-C	5.21	125.07	111.00
1	AI	6	GLU	N-CA-C	5.21	125.07	111.00
1	A2	6	GLU	N-CA-C	5.21	125.07	111.00
1	Ak	6	GLU	N-CA-C	5.21	125.07	111.00
1	DD	6	GLU	N-CA-C	5.21	125.07	111.00
1	AH	6	GLU	N-CA-C	5.21	125.06	111.00
1	AN	6	GLU	N-CA-C	5.21	125.06	111.00
1	AQ	6	GLU	N-CA-C	5.21	125.06	111.00
1	A9	6	GLU	N-CA-C	5.21	125.06	111.00
1	DE	6	GLU	N-CA-C	5.21	125.06	111.00
1	AE	6	GLU	N-CA-C	5.21	125.06	111.00
1	AL	6	GLU	N-CA-C	5.21	125.06	111.00
1	AV	6	GLU	N-CA-C	5.21	125.06	111.00
1	AX	6	GLU	N-CA-C	5.21	125.06	111.00
1	A6	6	GLU	N-CA-C	5.21	125.06	111.00
1	A7	6	GLU	N-CA-C	5.21	125.05	111.00
1	AJ	6	GLU	N-CA-C	5.20	125.04	111.00
1	DK	6	GLU	N-CA-C	5.20	125.05	111.00
1	AT	70	ARG	N-CA-C	-5.20	96.96	111.00
1	Al	6	GLU	N-CA-C	5.20	125.04	111.00
1	AG	6	GLU	N-CA-C	5.20	125.04	111.00
1	AK	6	GLU	N-CA-C	5.20	125.04	111.00
1	AA	6	GLU	N-CA-C	5.20	125.03	111.00
1	AF	70	ARG	N-CA-C	-5.20	96.97	111.00
1	AO	70	ARG	N-CA-C	-5.20	96.97	111.00
1	Ad	70	ARG	N-CA-C	-5.20	96.97	111.00
1	DH	4	VAL	C-N-CA	5.20	133.21	122.30
1	DI	70	ARG	N-CA-C	-5.20	96.97	111.00
1	AD	6	GLU	N-CA-C	5.19	125.01	111.00
1	Ac	70	ARG	N-CA-C	-5.19	96.99	111.00
1	An	6	GLU	N-CA-C	5.19	125.01	111.00
1	A3	4	VAL	C-N-CA	5.19	133.19	122.30
1	AB	70	ARG	N-CA-C	-5.18	97.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Af	4	VAL	C-N-CA	5.18	133.19	122.30
1	AJ	70	ARG	N-CA-C	-5.18	97.01	111.00
1	AM	70	ARG	N-CA-C	-5.18	97.01	111.00
2	Bq	60	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	DF	70	ARG	N-CA-C	-5.18	97.00	111.00
1	AD	70	ARG	N-CA-C	-5.18	97.01	111.00
1	AR	70	ARG	N-CA-C	-5.18	97.01	111.00
1	A0	70	ARG	N-CA-C	-5.18	97.01	111.00
1	Af	70	ARG	N-CA-C	-5.18	97.01	111.00
1	DE	70	ARG	N-CA-C	-5.18	97.01	111.00
1	AA	70	ARG	N-CA-C	-5.18	97.01	111.00
1	AY	70	ARG	N-CA-C	-5.18	97.01	111.00
1	A8	70	ARG	N-CA-C	-5.18	97.02	111.00
1	An	4	VAL	C-N-CA	5.18	133.18	122.30
1	An	70	ARG	N-CA-C	-5.18	97.02	111.00
1	AT	4	VAL	C-N-CA	5.18	133.18	122.30
1	Ao	4	VAL	C-N-CA	5.18	133.17	122.30
1	AG	70	ARG	N-CA-C	-5.18	97.02	111.00
1	AK	4	VAL	C-N-CA	5.18	133.17	122.30
1	AY	6	GLU	N-CA-C	5.18	124.98	111.00
1	Ai	70	ARG	N-CA-C	-5.18	97.02	111.00
1	AG	62	SER	N-CA-C	5.17	124.97	111.00
1	AK	70	ARG	N-CA-C	-5.17	97.03	111.00
1	AN	70	ARG	N-CA-C	-5.17	97.03	111.00
1	A1	70	ARG	N-CA-C	-5.17	97.03	111.00
1	A9	4	VAL	C-N-CA	5.17	133.16	122.30
1	Ae	70	ARG	N-CA-C	-5.17	97.03	111.00
1	Ao	70	ARG	N-CA-C	-5.17	97.03	111.00
1	DD	70	ARG	N-CA-C	-5.17	97.03	111.00
1	AL	70	ARG	N-CA-C	-5.17	97.03	111.00
1	AW	70	ARG	N-CA-C	-5.17	97.04	111.00
1	A4	70	ARG	N-CA-C	-5.17	97.04	111.00
1	A7	70	ARG	N-CA-C	-5.17	97.04	111.00
1	Aj	70	ARG	N-CA-C	-5.17	97.03	111.00
1	Am	70	ARG	N-CA-C	-5.17	97.03	111.00
1	AL	4	VAL	C-N-CA	5.17	133.15	122.30
1	AP	70	ARG	N-CA-C	-5.17	97.05	111.00
1	Aa	70	ARG	N-CA-C	-5.17	97.05	111.00
1	Ab	70	ARG	N-CA-C	-5.17	97.05	111.00
1	AQ	4	VAL	C-N-CA	5.17	133.15	122.30
1	AV	4	VAL	C-N-CA	5.17	133.15	122.30
1	A3	70	ARG	N-CA-C	-5.17	97.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ag	70	ARG	N-CA-C	-5.17	97.05	111.00
1	DK	70	ARG	N-CA-C	-5.17	97.05	111.00
1	A0	4	VAL	C-N-CA	5.17	133.15	122.30
1	A6	70	ARG	N-CA-C	-5.17	97.06	111.00
1	AA	4	VAL	C-N-CA	5.16	133.14	122.30
1	AP	4	VAL	C-N-CA	5.16	133.14	122.30
1	AU	62	SER	N-CA-C	5.16	124.94	111.00
1	AY	4	VAL	C-N-CA	5.16	133.14	122.30
1	A9	70	ARG	N-CA-C	-5.16	97.06	111.00
2	Bb	60	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	DG	70	ARG	N-CA-C	-5.16	97.06	111.00
1	AF	4	VAL	C-N-CA	5.16	133.14	122.30
1	Ah	70	ARG	N-CA-C	-5.16	97.06	111.00
1	Ak	70	ARG	N-CA-C	-5.16	97.06	111.00
1	AB	4	VAL	C-N-CA	5.16	133.14	122.30
1	AS	70	ARG	N-CA-C	-5.16	97.07	111.00
1	AV	70	ARG	N-CA-C	-5.16	97.07	111.00
1	AW	4	VAL	C-N-CA	5.16	133.14	122.30
1	AZ	70	ARG	N-CA-C	-5.16	97.06	111.00
1	A2	70	ARG	N-CA-C	-5.16	97.07	111.00
1	Aj	4	VAL	C-N-CA	5.16	133.14	122.30
1	AE	70	ARG	N-CA-C	-5.16	97.07	111.00
1	A8	62	SER	N-CA-C	5.16	124.93	111.00
1	A9	62	SER	N-CA-C	5.16	124.93	111.00
1	DC	70	ARG	N-CA-C	-5.16	97.07	111.00
1	DG	4	VAL	C-N-CA	5.16	133.13	122.30
1	DJ	70	ARG	N-CA-C	-5.16	97.07	111.00
1	Al	70	ARG	N-CA-C	-5.16	97.08	111.00
1	DH	62	SER	N-CA-C	5.16	124.92	111.00
1	AB	62	SER	N-CA-C	5.16	124.92	111.00
1	AH	70	ARG	N-CA-C	-5.16	97.08	111.00
1	AQ	70	ARG	N-CA-C	-5.16	97.08	111.00
1	AU	70	ARG	N-CA-C	-5.16	97.08	111.00
1	A5	70	ARG	N-CA-C	-5.16	97.08	111.00
1	Ae	62	SER	N-CA-C	5.16	124.92	111.00
1	Aj	62	SER	N-CA-C	5.16	124.92	111.00
1	DC	4	VAL	C-N-CA	5.16	133.12	122.30
1	DG	62	SER	N-CA-C	5.16	124.92	111.00
1	AJ	62	SER	N-CA-C	5.15	124.92	111.00
1	AT	62	SER	N-CA-C	5.15	124.92	111.00
1	AX	70	ARG	N-CA-C	-5.15	97.08	111.00
1	AI	70	ARG	N-CA-C	-5.15	97.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AO	4	VAL	C-N-CA	5.15	133.12	122.30
1	AP	62	SER	N-CA-C	5.15	124.91	111.00
1	AZ	4	VAL	C-N-CA	5.15	133.12	122.30
1	AZ	62	SER	N-CA-C	5.15	124.91	111.00
1	AH	62	SER	N-CA-C	5.15	124.91	111.00
1	A1	62	SER	N-CA-C	5.15	124.91	111.00
1	A4	4	VAL	C-N-CA	5.15	133.12	122.30
1	Ai	62	SER	N-CA-C	5.15	124.91	111.00
2	Bl	60	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	AG	4	VAL	C-N-CA	5.15	133.11	122.30
1	AH	4	VAL	C-N-CA	5.15	133.11	122.30
1	AJ	4	VAL	C-N-CA	5.15	133.11	122.30
1	A4	62	SER	N-CA-C	5.15	124.90	111.00
1	Ak	4	VAL	C-N-CA	5.15	133.11	122.30
1	AC	70	ARG	N-CA-C	-5.15	97.10	111.00
1	AQ	62	SER	N-CA-C	5.15	124.90	111.00
1	AS	4	VAL	C-N-CA	5.15	133.11	122.30
1	DF	62	SER	N-CA-C	5.15	124.90	111.00
1	AC	4	VAL	C-N-CA	5.15	133.11	122.30
1	AU	4	VAL	C-N-CA	5.15	133.11	122.30
1	AY	62	SER	N-CA-C	5.15	124.89	111.00
1	A6	62	SER	N-CA-C	5.15	124.89	111.00
1	Ae	4	VAL	C-N-CA	5.15	133.11	122.30
1	An	62	SER	N-CA-C	5.15	124.89	111.00
1	AI	4	VAL	C-N-CA	5.14	133.10	122.30
1	A5	4	VAL	C-N-CA	5.14	133.10	122.30
1	A8	4	VAL	C-N-CA	5.14	133.10	122.30
1	DF	4	VAL	C-N-CA	5.14	133.10	122.30
1	DH	70	ARG	N-CA-C	-5.14	97.11	111.00
1	DI	62	SER	N-CA-C	5.14	124.89	111.00
1	AF	62	SER	N-CA-C	5.14	124.89	111.00
1	AI	62	SER	N-CA-C	5.14	124.89	111.00
1	AM	62	SER	N-CA-C	5.14	124.88	111.00
1	Ab	62	SER	N-CA-C	5.14	124.89	111.00
1	Ak	62	SER	N-CA-C	5.14	124.89	111.00
1	AR	4	VAL	C-N-CA	5.14	133.10	122.30
1	AX	4	VAL	C-N-CA	5.14	133.10	122.30
1	Ad	62	SER	N-CA-C	5.14	124.88	111.00
1	AD	62	SER	N-CA-C	5.14	124.88	111.00
1	Ac	4	VAL	C-N-CA	5.14	133.09	122.30
1	AR	62	SER	N-CA-C	5.14	124.87	111.00
1	AX	62	SER	N-CA-C	5.14	124.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A6	4	VAL	C-N-CA	5.14	133.09	122.30
1	Aa	4	VAL	C-N-CA	5.14	133.09	122.30
1	Al	4	VAL	C-N-CA	5.14	133.09	122.30
1	Ao	62	SER	N-CA-C	5.14	124.87	111.00
1	AA	62	SER	N-CA-C	5.13	124.86	111.00
1	AK	62	SER	N-CA-C	5.13	124.86	111.00
1	A3	62	SER	N-CA-C	5.13	124.86	111.00
1	Al	62	SER	N-CA-C	5.13	124.87	111.00
1	DJ	4	VAL	C-N-CA	5.13	133.08	122.30
1	DK	4	VAL	C-N-CA	5.13	133.08	122.30
1	Ad	4	VAL	C-N-CA	5.13	133.08	122.30
1	DC	62	SER	N-CA-C	5.13	124.86	111.00
1	Ai	4	VAL	C-N-CA	5.13	133.07	122.30
1	AO	62	SER	N-CA-C	5.13	124.84	111.00
1	A1	4	VAL	C-N-CA	5.13	133.07	122.30
1	A5	62	SER	N-CA-C	5.13	124.84	111.00
1	A7	62	SER	N-CA-C	5.13	124.84	111.00
1	Ag	62	SER	N-CA-C	5.13	124.84	111.00
1	AD	4	VAL	C-N-CA	5.12	133.06	122.30
1	AL	62	SER	N-CA-C	5.12	124.84	111.00
1	AC	62	SER	N-CA-C	5.12	124.83	111.00
1	AW	62	SER	N-CA-C	5.12	124.83	111.00
1	Af	62	SER	N-CA-C	5.12	124.84	111.00
1	DD	4	VAL	C-N-CA	5.12	133.06	122.30
1	DD	62	SER	N-CA-C	5.12	124.83	111.00
1	DK	62	SER	N-CA-C	5.12	124.83	111.00
1	AE	4	VAL	C-N-CA	5.12	133.06	122.30
1	AV	62	SER	N-CA-C	5.12	124.83	111.00
1	Ah	62	SER	N-CA-C	5.12	124.82	111.00
1	Ac	62	SER	N-CA-C	5.12	124.82	111.00
1	Am	62	SER	N-CA-C	5.12	124.82	111.00
1	AE	62	SER	N-CA-C	5.11	124.80	111.00
1	A7	4	VAL	C-N-CA	5.11	133.04	122.30
1	Aa	62	SER	N-CA-C	5.11	124.81	111.00
1	DE	62	SER	N-CA-C	5.11	124.81	111.00
1	AM	4	VAL	C-N-CA	5.11	133.03	122.30
1	AN	4	VAL	C-N-CA	5.11	133.03	122.30
1	AS	62	SER	N-CA-C	5.11	124.80	111.00
1	DJ	62	SER	N-CA-C	5.11	124.80	111.00
1	Ab	4	VAL	C-N-CA	5.11	133.03	122.30
1	DE	4	VAL	C-N-CA	5.11	133.03	122.30
1	A2	4	VAL	C-N-CA	5.11	133.02	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Ag	4	VAL	C-N-CA	5.11	133.02	122.30
1	AN	62	SER	N-CA-C	5.10	124.78	111.00
2	BQ	60	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	DI	4	VAL	C-N-CA	5.10	133.01	122.30
1	A0	62	SER	N-CA-C	5.10	124.77	111.00
1	Ah	4	VAL	C-N-CA	5.10	133.00	122.30
1	A2	62	SER	N-CA-C	5.09	124.75	111.00
1	Am	4	VAL	C-N-CA	5.09	133.00	122.30
1	A5	113	THR	N-CA-C	5.09	124.75	111.00
1	Aa	113	THR	N-CA-C	5.09	124.74	111.00
1	AI	113	THR	N-CA-C	5.08	124.72	111.00
1	AQ	113	THR	N-CA-C	5.08	124.72	111.00
2	Bl	60	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	Bs	60	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	DD	113	THR	N-CA-C	5.08	124.72	111.00
1	AA	113	THR	N-CA-C	5.08	124.71	111.00
1	AP	113	THR	N-CA-C	5.08	124.71	111.00
1	A3	113	THR	N-CA-C	5.08	124.71	111.00
1	Ak	113	THR	N-CA-C	5.08	124.71	111.00
1	DC	113	THR	N-CA-C	5.08	124.71	111.00
1	AW	113	THR	N-CA-C	5.08	124.71	111.00
2	BF	60	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	AJ	113	THR	N-CA-C	5.08	124.70	111.00
1	A4	113	THR	N-CA-C	5.08	124.70	111.00
1	Ab	113	THR	N-CA-C	5.08	124.70	111.00
2	BT	60	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	DH	113	THR	N-CA-C	5.08	124.71	111.00
1	AY	113	THR	N-CA-C	5.07	124.70	111.00
1	AC	113	THR	N-CA-C	5.07	124.69	111.00
1	A8	113	THR	N-CA-C	5.07	124.69	111.00
1	Ah	113	THR	N-CA-C	5.07	124.69	111.00
1	AV	113	THR	N-CA-C	5.07	124.68	111.00
1	AX	113	THR	N-CA-C	5.07	124.68	111.00
1	AZ	113	THR	N-CA-C	5.07	124.68	111.00
1	A0	113	THR	N-CA-C	5.07	124.68	111.00
1	An	113	THR	N-CA-C	5.07	124.68	111.00
1	AT	113	THR	N-CA-C	5.07	124.68	111.00
2	Bv	59	SER	N-CA-C	-5.07	97.32	111.00
1	AG	113	THR	N-CA-C	5.06	124.67	111.00
1	A9	113	THR	N-CA-C	5.06	124.67	111.00
1	Ag	113	THR	N-CA-C	5.06	124.67	111.00
2	BI	59	SER	N-CA-C	-5.06	97.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AK	113	THR	N-CA-C	5.06	124.67	111.00
1	AN	113	THR	N-CA-C	5.06	124.67	111.00
1	DI	113	THR	N-CA-C	5.06	124.67	111.00
1	AF	113	THR	N-CA-C	5.06	124.66	111.00
1	AL	113	THR	N-CA-C	5.06	124.66	111.00
1	AR	113	THR	N-CA-C	5.06	124.66	111.00
2	BA	59	SER	N-CA-C	-5.06	97.34	111.00
2	BQ	59	SER	N-CA-C	-5.06	97.34	111.00
2	BZ	59	SER	N-CA-C	-5.06	97.35	111.00
2	B6	59	SER	N-CA-C	-5.06	97.35	111.00
2	Bb	59	SER	N-CA-C	-5.06	97.34	111.00
1	DE	113	THR	N-CA-C	5.06	124.66	111.00
1	Ad	113	THR	N-CA-C	5.06	124.65	111.00
2	BF	59	SER	N-CA-C	-5.06	97.35	111.00
2	BK	59	SER	N-CA-C	-5.06	97.35	111.00
2	BL	59	SER	N-CA-C	-5.06	97.35	111.00
2	BW	59	SER	N-CA-C	-5.06	97.35	111.00
2	Bd	59	SER	N-CA-C	-5.06	97.35	111.00
1	AD	113	THR	N-CA-C	5.05	124.64	111.00
1	AE	113	THR	N-CA-C	5.05	124.64	111.00
1	Af	113	THR	N-CA-C	5.05	124.65	111.00
1	Ao	113	THR	N-CA-C	5.05	124.64	111.00
2	BA	60	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	BB	60	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	B0	59	SER	N-CA-C	-5.05	97.36	111.00
2	B4	60	ARG	NE-CZ-NH1	5.05	122.83	120.30
2	Bn	59	SER	N-CA-C	-5.05	97.36	111.00
2	Bu	59	SER	N-CA-C	-5.05	97.36	111.00
1	AH	113	THR	N-CA-C	5.05	124.64	111.00
2	BD	59	SER	N-CA-C	-5.05	97.36	111.00
2	B8	59	SER	N-CA-C	-5.05	97.36	111.00
2	Bj	59	SER	N-CA-C	-5.05	97.36	111.00
2	Bk	59	SER	N-CA-C	-5.05	97.36	111.00
2	Bq	59	SER	N-CA-C	-5.05	97.36	111.00
1	AO	113	THR	N-CA-C	5.05	124.63	111.00
1	A1	113	THR	N-CA-C	5.05	124.64	111.00
1	Am	113	THR	N-CA-C	5.05	124.63	111.00
2	BB	59	SER	N-CA-C	-5.05	97.37	111.00
1	AM	113	THR	N-CA-C	5.05	124.63	111.00
2	Bp	59	SER	N-CA-C	-5.05	97.37	111.00
2	Bs	59	SER	N-CA-C	-5.05	97.37	111.00
1	DF	113	THR	N-CA-C	5.05	124.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AB	113	THR	N-CA-C	5.05	124.62	111.00
1	A6	113	THR	N-CA-C	5.05	124.63	111.00
1	Aj	113	THR	N-CA-C	5.05	124.62	111.00
2	BC	59	SER	N-CA-C	-5.05	97.37	111.00
2	BM	59	SER	N-CA-C	-5.05	97.37	111.00
2	BN	59	SER	N-CA-C	-5.05	97.38	111.00
2	B2	59	SER	N-CA-C	-5.05	97.38	111.00
2	Ba	59	SER	N-CA-C	-5.05	97.37	111.00
2	Bo	59	SER	N-CA-C	-5.05	97.37	111.00
1	DG	113	THR	N-CA-C	5.05	124.62	111.00
1	DK	113	THR	N-CA-C	5.05	124.62	111.00
2	BH	59	SER	N-CA-C	-5.04	97.38	111.00
2	B4	59	SER	N-CA-C	-5.04	97.38	111.00
1	Ac	113	THR	N-CA-C	5.04	124.61	111.00
1	Ae	113	THR	N-CA-C	5.04	124.61	111.00
2	BE	60	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	Bt	59	SER	N-CA-C	-5.04	97.39	111.00
2	Bx	59	SER	N-CA-C	-5.04	97.39	111.00
1	Al	113	THR	N-CA-C	5.04	124.61	111.00
1	A2	113	THR	N-CA-C	5.04	124.61	111.00
2	BI	60	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	BN	60	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	B3	59	SER	N-CA-C	-5.04	97.39	111.00
1	Ac	71	LEU	N-CA-C	-5.04	97.40	111.00
2	BO	59	SER	N-CA-C	-5.04	97.40	111.00
2	B7	59	SER	N-CA-C	-5.04	97.40	111.00
1	Ai	113	THR	N-CA-C	5.04	124.59	111.00
2	BJ	59	SER	N-CA-C	-5.04	97.41	111.00
2	BP	59	SER	N-CA-C	-5.04	97.40	111.00
2	Be	60	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	Bf	59	SER	N-CA-C	-5.04	97.40	111.00
2	Bg	59	SER	N-CA-C	-5.04	97.40	111.00
2	Bl	59	SER	N-CA-C	-5.04	97.41	111.00
1	DJ	113	THR	N-CA-C	5.04	124.59	111.00
1	AU	113	THR	N-CA-C	5.03	124.59	111.00
2	BJ	60	ARG	NE-CZ-NH1	5.03	122.82	120.30
2	BS	59	SER	N-CA-C	-5.03	97.41	111.00
2	B5	59	SER	N-CA-C	-5.03	97.41	111.00
2	BU	59	SER	N-CA-C	-5.03	97.41	111.00
1	AS	113	THR	N-CA-C	5.03	124.58	111.00
2	B1	59	SER	N-CA-C	-5.03	97.42	111.00
2	B6	60	ARG	NE-CZ-NH1	5.03	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Bh	59	SER	N-CA-C	-5.03	97.42	111.00
2	Br	59	SER	N-CA-C	-5.03	97.42	111.00
2	BV	59	SER	N-CA-C	-5.03	97.42	111.00
2	BX	59	SER	N-CA-C	-5.03	97.42	111.00
2	BG	59	SER	N-CA-C	-5.03	97.42	111.00
2	Bq	60	ARG	NE-CZ-NH2	-5.03	117.79	120.30
2	Bi	59	SER	N-CA-C	-5.03	97.43	111.00
2	Bj	60	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A7	71	LEU	N-CA-C	-5.02	97.44	111.00
1	A7	113	THR	N-CA-C	5.02	124.56	111.00
2	BE	59	SER	N-CA-C	-5.02	97.44	111.00
2	BT	59	SER	N-CA-C	-5.02	97.44	111.00
2	Be	59	SER	N-CA-C	-5.02	97.45	111.00
2	BD	60	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	BY	59	SER	N-CA-C	-5.02	97.45	111.00
2	B9	59	SER	N-CA-C	-5.02	97.45	111.00
2	Bc	59	SER	N-CA-C	-5.02	97.45	111.00
1	AO	71	LEU	N-CA-C	-5.02	97.46	111.00
2	Bw	59	SER	N-CA-C	-5.02	97.46	111.00
1	AX	71	LEU	N-CA-C	-5.01	97.47	111.00
1	Ai	71	LEU	N-CA-C	-5.01	97.47	111.00
2	Bm	59	SER	N-CA-C	-5.01	97.47	111.00
1	Ah	71	LEU	N-CA-C	-5.01	97.48	111.00
3	Ck	178	ASN	CB-CA-C	-5.01	100.38	110.40
1	AF	71	LEU	N-CA-C	-5.01	97.48	111.00
1	AK	71	LEU	N-CA-C	-5.01	97.48	111.00
1	AS	71	LEU	N-CA-C	-5.01	97.48	111.00
1	AE	71	LEU	N-CA-C	-5.00	97.49	111.00
2	BR	59	SER	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (180) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A0	208	TYR	Sidechain
1	A1	208	TYR	Sidechain
1	A2	208	TYR	Sidechain
1	A3	208	TYR	Sidechain
1	A4	208	TYR	Sidechain
1	A5	208	TYR	Sidechain
1	A6	208	TYR	Sidechain
1	A7	208	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A8	208	TYR	Sidechain
1	A9	208	TYR	Sidechain
1	AA	208	TYR	Sidechain
1	AB	208	TYR	Sidechain
1	AC	208	TYR	Sidechain
1	AD	208	TYR	Sidechain
1	AE	208	TYR	Sidechain
1	AF	208	TYR	Sidechain
1	AG	208	TYR	Sidechain
1	AH	208	TYR	Sidechain
1	AI	208	TYR	Sidechain
1	AJ	208	TYR	Sidechain
1	AK	208	TYR	Sidechain
1	AL	208	TYR	Sidechain
1	AM	208	TYR	Sidechain
1	AN	208	TYR	Sidechain
1	AO	208	TYR	Sidechain
1	AP	208	TYR	Sidechain
1	AQ	208	TYR	Sidechain
1	AR	208	TYR	Sidechain
1	AS	208	TYR	Sidechain
1	AT	208	TYR	Sidechain
1	AU	208	TYR	Sidechain
1	AV	208	TYR	Sidechain
1	AW	208	TYR	Sidechain
1	AX	208	TYR	Sidechain
1	AY	208	TYR	Sidechain
1	AZ	208	TYR	Sidechain
1	Aa	208	TYR	Sidechain
1	Ab	208	TYR	Sidechain
1	Ac	208	TYR	Sidechain
1	Ad	208	TYR	Sidechain
1	Ae	208	TYR	Sidechain
1	Af	208	TYR	Sidechain
1	Ag	208	TYR	Sidechain
1	Ah	208	TYR	Sidechain
1	Ai	208	TYR	Sidechain
1	Aj	208	TYR	Sidechain
1	Ak	208	TYR	Sidechain
1	Al	208	TYR	Sidechain
1	Am	208	TYR	Sidechain
1	An	208	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	Ao	208	TYR	Sidechain
2	B0	177	TYR	Sidechain
2	B0	86	ASP	Mainchain
2	B1	177	TYR	Sidechain
2	B1	86	ASP	Mainchain
2	B2	177	TYR	Sidechain
2	B2	86	ASP	Mainchain
2	B3	177	TYR	Sidechain
2	B3	86	ASP	Mainchain
2	B4	177	TYR	Sidechain
2	B4	86	ASP	Mainchain
2	B5	177	TYR	Sidechain
2	B5	86	ASP	Mainchain
2	B6	177	TYR	Sidechain
2	B6	86	ASP	Mainchain
2	B7	177	TYR	Sidechain
2	B7	86	ASP	Mainchain
2	B8	177	TYR	Sidechain
2	B8	86	ASP	Mainchain
2	B9	177	TYR	Sidechain
2	B9	86	ASP	Mainchain
2	BA	177	TYR	Sidechain
2	BA	86	ASP	Mainchain
2	BB	177	TYR	Sidechain
2	BB	86	ASP	Mainchain
2	BC	177	TYR	Sidechain
2	BC	86	ASP	Mainchain
2	BD	177	TYR	Sidechain
2	BD	86	ASP	Mainchain
2	BE	177	TYR	Sidechain
2	BE	86	ASP	Mainchain
2	BF	177	TYR	Sidechain
2	BF	86	ASP	Mainchain
2	BG	177	TYR	Sidechain
2	BG	86	ASP	Mainchain
2	BH	177	TYR	Sidechain
2	BH	86	ASP	Mainchain
2	BI	177	TYR	Sidechain
2	BI	86	ASP	Mainchain
2	BJ	177	TYR	Sidechain
2	BJ	86	ASP	Mainchain
2	BK	177	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	BK	86	ASP	Mainchain
2	BL	177	TYR	Sidechain
2	BL	86	ASP	Mainchain
2	BM	177	TYR	Sidechain
2	BM	86	ASP	Mainchain
2	BN	177	TYR	Sidechain
2	BN	86	ASP	Mainchain
2	BO	177	TYR	Sidechain
2	BO	86	ASP	Mainchain
2	BP	177	TYR	Sidechain
2	BP	86	ASP	Mainchain
2	BQ	177	TYR	Sidechain
2	BQ	86	ASP	Mainchain
2	BR	177	TYR	Sidechain
2	BR	86	ASP	Mainchain
2	BS	177	TYR	Sidechain
2	BS	86	ASP	Mainchain
2	BT	177	TYR	Sidechain
2	BT	86	ASP	Mainchain
2	BU	177	TYR	Sidechain
2	BU	86	ASP	Mainchain
2	BV	177	TYR	Sidechain
2	BV	86	ASP	Mainchain
2	BW	177	TYR	Sidechain
2	BW	86	ASP	Mainchain
2	BX	177	TYR	Sidechain
2	BX	86	ASP	Mainchain
2	BY	177	TYR	Sidechain
2	BY	86	ASP	Mainchain
2	BZ	177	TYR	Sidechain
2	BZ	86	ASP	Mainchain
2	Ba	177	TYR	Sidechain
2	Ba	86	ASP	Mainchain
2	Bb	177	TYR	Sidechain
2	Bb	86	ASP	Mainchain
2	Bc	177	TYR	Sidechain
2	Bc	86	ASP	Mainchain
2	Bd	177	TYR	Sidechain
2	Bd	86	ASP	Mainchain
2	Be	177	TYR	Sidechain
2	Be	86	ASP	Mainchain
2	Bf	177	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	Bf	86	ASP	Mainchain
2	Bg	177	TYR	Sidechain
2	Bg	86	ASP	Mainchain
2	Bh	177	TYR	Sidechain
2	Bh	86	ASP	Mainchain
2	Bi	177	TYR	Sidechain
2	Bi	86	ASP	Mainchain
2	Bj	177	TYR	Sidechain
2	Bj	86	ASP	Mainchain
2	Bk	177	TYR	Sidechain
2	Bk	86	ASP	Mainchain
2	Bl	177	TYR	Sidechain
2	Bl	86	ASP	Mainchain
2	Bm	177	TYR	Sidechain
2	Bm	86	ASP	Mainchain
2	Bn	177	TYR	Sidechain
2	Bn	86	ASP	Mainchain
2	Bo	177	TYR	Sidechain
2	Bo	86	ASP	Mainchain
2	Bp	177	TYR	Sidechain
2	Bp	86	ASP	Mainchain
2	Bq	177	TYR	Sidechain
2	Bq	86	ASP	Mainchain
2	Br	177	TYR	Sidechain
2	Br	86	ASP	Mainchain
2	Bs	177	TYR	Sidechain
2	Bs	86	ASP	Mainchain
2	Bt	177	TYR	Sidechain
2	Bt	86	ASP	Mainchain
2	Bu	177	TYR	Sidechain
2	Bu	86	ASP	Mainchain
2	Bv	177	TYR	Sidechain
2	Bv	86	ASP	Mainchain
2	Bw	177	TYR	Sidechain
2	Bw	86	ASP	Mainchain
2	Bx	177	TYR	Sidechain
2	Bx	86	ASP	Mainchain
1	DC	208	TYR	Sidechain
1	DD	208	TYR	Sidechain
1	DE	208	TYR	Sidechain
1	DF	208	TYR	Sidechain
1	DG	208	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	DH	208	TYR	Sidechain
1	DI	208	TYR	Sidechain
1	DJ	208	TYR	Sidechain
1	DK	208	TYR	Sidechain

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	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	A1	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	A2	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	A3	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	A4	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	A5	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	A6	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	A7	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	A8	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	A9	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AA	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AB	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AC	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AD	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AE	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AF	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AG	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AH	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AI	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AJ	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AK	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AL	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AM	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AN	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AO	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AP	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AQ	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AR	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AS	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AT	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AU	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AV	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AW	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AX	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AY	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	AZ	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Aa	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Ab	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Ac	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Ad	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Ae	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Af	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Ag	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Ah	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Ai	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Aj	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ak	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Al	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Am	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	An	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	Ao	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	DC	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	DD	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	DE	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	DF	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	DG	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	DH	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	DI	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	DJ	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
1	DK	244/246 (99%)	206 (84%)	24 (10%)	14 (6%)	1	18
2	B0	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	B1	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	B2	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	B3	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	B4	198/200 (99%)	184 (93%)	6 (3%)	8 (4%)	3	23
2	B5	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	B6	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	B7	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	B8	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	B9	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BA	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BB	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BC	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BD	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BE	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BF	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BG	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BH	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BI	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BJ	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BK	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BL	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BM	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BN	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BO	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BP	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BQ	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BR	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BS	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BT	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BU	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BV	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BW	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BX	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BY	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	BZ	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Ba	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bb	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bc	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bd	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Be	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bf	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bg	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bh	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bi	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bj	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bk	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bl	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bm	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bn	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bo	198/200 (99%)	184 (93%)	6 (3%)	8 (4%)	3	23
2	Bp	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bq	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Br	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bs	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bt	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bu	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bv	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bw	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
2	Bx	198/200 (99%)	183 (92%)	7 (4%)	8 (4%)	3	23
3	C0	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	C1	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	C2	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	C3	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	C4	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	C5	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	C6	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	C7	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	C8	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	C9	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CA	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CB	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CC	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CD	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CE	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CF	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CG	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CH	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CI	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CJ	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CK	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CL	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CM	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CN	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CO	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CP	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CQ	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CR	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CS	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CT	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CU	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CV	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CW	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CX	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CY	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	CZ	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cc	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cd	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Ce	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cf	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cg	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Ch	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Ci	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cj	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Ck	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cl	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cm	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cn	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Co	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cp	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Cq	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cr	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cs	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Ct	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cu	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cv	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cw	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	Cx	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	DA	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
3	DB	224/226 (99%)	204 (91%)	14 (6%)	6 (3%)	5	31
All	All	39960/40320 (99%)	35582 (89%)	2698 (7%)	1680 (4%)	5	22

All (1680) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	THR
1	AA	5	GLY
1	AA	41	GLU
1	AA	202	HIS
1	AA	244	ASN
1	AB	2	THR
1	AB	5	GLY
1	AB	41	GLU
1	AB	202	HIS
1	AB	244	ASN
1	AC	2	THR
1	AC	5	GLY
1	AC	41	GLU
1	AC	202	HIS
1	AC	244	ASN
1	AD	2	THR
1	AD	5	GLY
1	AD	41	GLU
1	AD	202	HIS
1	AD	244	ASN
1	AE	2	THR
1	AE	5	GLY
1	AE	41	GLU

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Mol	Chain	Res	Type
1	AE	202	HIS
1	AE	244	ASN
1	AF	2	THR
1	AF	5	GLY
1	AF	41	GLU
1	AF	202	HIS
1	AF	244	ASN
1	AG	2	THR
1	AG	5	GLY
1	AG	41	GLU
1	AG	202	HIS
1	AG	244	ASN
1	AH	2	THR
1	AH	5	GLY
1	AH	41	GLU
1	AH	202	HIS
1	AH	244	ASN
1	AI	2	THR
1	AI	5	GLY
1	AI	41	GLU
1	AI	202	HIS
1	AI	244	ASN
1	AJ	2	THR
1	AJ	5	GLY
1	AJ	41	GLU
1	AJ	202	HIS
1	AJ	244	ASN
1	AK	2	THR
1	AK	5	GLY
1	AK	41	GLU
1	AK	202	HIS
1	AK	244	ASN
1	AL	2	THR
1	AL	5	GLY
1	AL	41	GLU
1	AL	202	HIS
1	AL	244	ASN
1	AM	2	THR
1	AM	5	GLY
1	AM	41	GLU
1	AM	202	HIS
1	AM	244	ASN

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Mol	Chain	Res	Type
1	AN	2	THR
1	AN	5	GLY
1	AN	41	GLU
1	AN	202	HIS
1	AN	244	ASN
1	AO	2	THR
1	AO	5	GLY
1	AO	41	GLU
1	AO	202	HIS
1	AO	244	ASN
1	AP	2	THR
1	AP	5	GLY
1	AP	41	GLU
1	AP	202	HIS
1	AP	244	ASN
1	AQ	2	THR
1	AQ	5	GLY
1	AQ	41	GLU
1	AQ	202	HIS
1	AQ	244	ASN
1	AR	2	THR
1	AR	5	GLY
1	AR	41	GLU
1	AR	202	HIS
1	AR	244	ASN
1	AS	2	THR
1	AS	5	GLY
1	AS	41	GLU
1	AS	202	HIS
1	AS	244	ASN
1	AT	2	THR
1	AT	5	GLY
1	AT	41	GLU
1	AT	202	HIS
1	AT	244	ASN
1	AU	2	THR
1	AU	5	GLY
1	AU	41	GLU
1	AU	202	HIS
1	AU	244	ASN
1	AV	2	THR
1	AV	5	GLY

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Mol	Chain	Res	Type
1	AV	41	GLU
1	AV	202	HIS
1	AV	244	ASN
1	AW	2	THR
1	AW	5	GLY
1	AW	41	GLU
1	AW	202	HIS
1	AW	244	ASN
1	AX	2	THR
1	AX	5	GLY
1	AX	41	GLU
1	AX	202	HIS
1	AX	244	ASN
1	AY	2	THR
1	AY	5	GLY
1	AY	41	GLU
1	AY	202	HIS
1	AY	244	ASN
1	AZ	2	THR
1	AZ	5	GLY
1	AZ	41	GLU
1	AZ	202	HIS
1	AZ	244	ASN
1	A0	2	THR
1	A0	5	GLY
1	A0	41	GLU
1	A0	202	HIS
1	A0	244	ASN
1	A1	2	THR
1	A1	5	GLY
1	A1	41	GLU
1	A1	202	HIS
1	A1	244	ASN
1	A2	2	THR
1	A2	5	GLY
1	A2	41	GLU
1	A2	202	HIS
1	A2	244	ASN
1	A3	2	THR
1	A3	5	GLY
1	A3	41	GLU
1	A3	202	HIS

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Mol	Chain	Res	Type
1	A3	244	ASN
1	A4	2	THR
1	A4	5	GLY
1	A4	41	GLU
1	A4	202	HIS
1	A4	244	ASN
1	A5	2	THR
1	A5	5	GLY
1	A5	41	GLU
1	A5	202	HIS
1	A5	244	ASN
1	A6	2	THR
1	A6	5	GLY
1	A6	41	GLU
1	A6	202	HIS
1	A6	244	ASN
1	A7	2	THR
1	A7	5	GLY
1	A7	41	GLU
1	A7	202	HIS
1	A7	244	ASN
1	A8	2	THR
1	A8	5	GLY
1	A8	41	GLU
1	A8	202	HIS
1	A8	244	ASN
1	A9	2	THR
1	A9	5	GLY
1	A9	41	GLU
1	A9	202	HIS
1	A9	244	ASN
1	Aa	2	THR
1	Aa	5	GLY
1	Aa	41	GLU
1	Aa	202	HIS
1	Aa	244	ASN
1	Ab	2	THR
1	Ab	5	GLY
1	Ab	41	GLU
1	Ab	202	HIS
1	Ab	244	ASN
1	Ac	2	THR

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Mol	Chain	Res	Type
1	Ac	5	GLY
1	Ac	41	GLU
1	Ac	202	HIS
1	Ac	244	ASN
1	Ad	2	THR
1	Ad	5	GLY
1	Ad	41	GLU
1	Ad	202	HIS
1	Ad	244	ASN
1	Ae	2	THR
1	Ae	5	GLY
1	Ae	41	GLU
1	Ae	202	HIS
1	Ae	244	ASN
1	Af	2	THR
1	Af	5	GLY
1	Af	41	GLU
1	Af	202	HIS
1	Af	244	ASN
1	Ag	2	THR
1	Ag	5	GLY
1	Ag	41	GLU
1	Ag	202	HIS
1	Ag	244	ASN
1	Ah	2	THR
1	Ah	5	GLY
1	Ah	41	GLU
1	Ah	202	HIS
1	Ah	244	ASN
1	Ai	2	THR
1	Ai	5	GLY
1	Ai	41	GLU
1	Ai	202	HIS
1	Ai	244	ASN
1	Aj	2	THR
1	Aj	5	GLY
1	Aj	41	GLU
1	Aj	202	HIS
1	Aj	244	ASN
1	Ak	2	THR
1	Ak	5	GLY
1	Ak	41	GLU

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Mol	Chain	Res	Type
1	Ak	202	HIS
1	Ak	244	ASN
1	Al	2	THR
1	Al	5	GLY
1	Al	41	GLU
1	Al	202	HIS
1	Al	244	ASN
1	Am	2	THR
1	Am	5	GLY
1	Am	41	GLU
1	Am	202	HIS
1	Am	244	ASN
1	An	2	THR
1	An	5	GLY
1	An	41	GLU
1	An	202	HIS
1	An	244	ASN
1	Ao	2	THR
1	Ao	5	GLY
1	Ao	41	GLU
1	Ao	202	HIS
1	Ao	244	ASN
2	BA	84	PRO
2	BA	85	SER
2	BA	134	HIS
2	BA	135	THR
2	BB	84	PRO
2	BB	85	SER
2	BB	134	HIS
2	BB	135	THR
2	BC	84	PRO
2	BC	85	SER
2	BC	134	HIS
2	BC	135	THR
2	BD	84	PRO
2	BD	85	SER
2	BD	134	HIS
2	BD	135	THR
2	BE	84	PRO
2	BE	85	SER
2	BE	134	HIS
2	BE	135	THR

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Mol	Chain	Res	Type
2	BF	84	PRO
2	BF	85	SER
2	BF	134	HIS
2	BF	135	THR
2	BG	84	PRO
2	BG	85	SER
2	BG	134	HIS
2	BG	135	THR
2	BH	84	PRO
2	BH	85	SER
2	BH	134	HIS
2	BH	135	THR
2	BI	84	PRO
2	BI	85	SER
2	BI	134	HIS
2	BI	135	THR
2	BJ	84	PRO
2	BJ	85	SER
2	BJ	134	HIS
2	BJ	135	THR
2	BK	84	PRO
2	BK	85	SER
2	BK	134	HIS
2	BK	135	THR
2	BL	84	PRO
2	BL	85	SER
2	BL	134	HIS
2	BL	135	THR
2	BM	84	PRO
2	BM	85	SER
2	BM	134	HIS
2	BM	135	THR
2	BN	84	PRO
2	BN	85	SER
2	BN	134	HIS
2	BN	135	THR
2	BR	84	PRO
2	BR	85	SER
2	BR	134	HIS
2	BR	135	THR
2	BO	84	PRO
2	BO	85	SER

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Mol	Chain	Res	Type
2	BO	134	HIS
2	BO	135	THR
2	BS	84	PRO
2	BS	85	SER
2	BS	134	HIS
2	BS	135	THR
2	BP	84	PRO
2	BP	85	SER
2	BP	134	HIS
2	BP	135	THR
2	BQ	84	PRO
2	BQ	85	SER
2	BQ	134	HIS
2	BQ	135	THR
2	BT	84	PRO
2	BT	85	SER
2	BT	134	HIS
2	BT	135	THR
2	BU	84	PRO
2	BU	85	SER
2	BU	134	HIS
2	BU	135	THR
2	BV	84	PRO
2	BV	85	SER
2	BV	134	HIS
2	BV	135	THR
2	BW	84	PRO
2	BW	85	SER
2	BW	134	HIS
2	BW	135	THR
2	BX	84	PRO
2	BX	85	SER
2	BX	134	HIS
2	BX	135	THR
2	BY	84	PRO
2	BY	85	SER
2	BY	134	HIS
2	BY	135	THR
2	BZ	84	PRO
2	BZ	85	SER
2	BZ	134	HIS
2	BZ	135	THR

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Mol	Chain	Res	Type
2	B0	84	PRO
2	B0	85	SER
2	B0	134	HIS
2	B0	135	THR
2	B1	84	PRO
2	B1	85	SER
2	B1	134	HIS
2	B1	135	THR
2	B2	84	PRO
2	B2	85	SER
2	B2	134	HIS
2	B2	135	THR
2	B3	84	PRO
2	B3	85	SER
2	B3	134	HIS
2	B3	135	THR
2	B4	84	PRO
2	B4	85	SER
2	B4	134	HIS
2	B4	135	THR
2	B5	84	PRO
2	B5	85	SER
2	B5	134	HIS
2	B5	135	THR
2	B6	84	PRO
2	B6	85	SER
2	B6	134	HIS
2	B6	135	THR
2	B7	84	PRO
2	B7	85	SER
2	B7	134	HIS
2	B7	135	THR
2	B8	84	PRO
2	B8	85	SER
2	B8	134	HIS
2	B8	135	THR
2	B9	84	PRO
2	B9	85	SER
2	B9	134	HIS
2	B9	135	THR
2	Ba	84	PRO
2	Ba	85	SER

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Mol	Chain	Res	Type
2	Ba	134	HIS
2	Ba	135	THR
2	Bb	84	PRO
2	Bb	85	SER
2	Bb	134	HIS
2	Bb	135	THR
2	Bc	84	PRO
2	Bc	85	SER
2	Bc	134	HIS
2	Bc	135	THR
2	Bd	84	PRO
2	Bd	85	SER
2	Bd	134	HIS
2	Bd	135	THR
2	Be	84	PRO
2	Be	85	SER
2	Be	134	HIS
2	Be	135	THR
2	Bf	84	PRO
2	Bf	85	SER
2	Bf	134	HIS
2	Bf	135	THR
2	Bg	84	PRO
2	Bg	85	SER
2	Bg	134	HIS
2	Bg	135	THR
2	Bh	84	PRO
2	Bh	85	SER
2	Bh	134	HIS
2	Bh	135	THR
2	Bi	84	PRO
2	Bi	85	SER
2	Bi	134	HIS
2	Bi	135	THR
2	Bj	84	PRO
2	Bj	85	SER
2	Bj	134	HIS
2	Bj	135	THR
2	Bk	84	PRO
2	Bk	85	SER
2	Bk	134	HIS
2	Bk	135	THR

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Mol	Chain	Res	Type
2	Bl	84	PRO
2	Bl	85	SER
2	Bl	134	HIS
2	Bl	135	THR
2	Bm	84	PRO
2	Bm	85	SER
2	Bm	134	HIS
2	Bm	135	THR
2	Bn	84	PRO
2	Bn	85	SER
2	Bn	134	HIS
2	Bn	135	THR
2	Bo	84	PRO
2	Bo	85	SER
2	Bo	134	HIS
2	Bo	135	THR
2	Bp	84	PRO
2	Bp	85	SER
2	Bp	134	HIS
2	Bp	135	THR
2	Bq	84	PRO
2	Bq	85	SER
2	Bq	134	HIS
2	Bq	135	THR
2	Br	84	PRO
2	Br	85	SER
2	Br	134	HIS
2	Br	135	THR
2	Bs	84	PRO
2	Bs	85	SER
2	Bs	134	HIS
2	Bs	135	THR
2	Bt	84	PRO
2	Bt	85	SER
2	Bt	134	HIS
2	Bt	135	THR
2	Bu	84	PRO
2	Bu	85	SER
2	Bu	134	HIS
2	Bu	135	THR
2	Bv	84	PRO
2	Bv	85	SER

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Mol	Chain	Res	Type
2	Bv	134	HIS
2	Bv	135	THR
2	Bw	84	PRO
2	Bw	85	SER
2	Bw	134	HIS
2	Bw	135	THR
2	Bx	84	PRO
2	Bx	85	SER
2	Bx	134	HIS
2	Bx	135	THR
3	CA	11	SER
3	CA	36	VAL
3	CB	11	SER
3	CB	36	VAL
3	CC	11	SER
3	CC	36	VAL
3	CD	11	SER
3	CD	36	VAL
3	CE	11	SER
3	CE	36	VAL
3	CF	11	SER
3	CF	36	VAL
3	CG	11	SER
3	CG	36	VAL
3	CH	11	SER
3	CH	36	VAL
3	CI	11	SER
3	CI	36	VAL
3	CJ	11	SER
3	CJ	36	VAL
3	CK	11	SER
3	CK	36	VAL
3	CL	11	SER
3	CL	36	VAL
3	CM	11	SER
3	CM	36	VAL
3	CN	11	SER
3	CN	36	VAL
3	CO	11	SER
3	CO	36	VAL
3	CP	11	SER
3	CP	36	VAL

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Mol	Chain	Res	Type
3	CQ	11	SER
3	CQ	36	VAL
3	CR	11	SER
3	CR	36	VAL
3	CS	11	SER
3	CS	36	VAL
3	CT	11	SER
3	CT	36	VAL
3	CU	11	SER
3	CU	36	VAL
3	CV	11	SER
3	CV	36	VAL
3	CW	11	SER
3	CW	36	VAL
3	CX	11	SER
3	CX	36	VAL
3	CY	11	SER
3	CY	36	VAL
3	CZ	11	SER
3	CZ	36	VAL
3	C0	11	SER
3	C0	36	VAL
3	C1	11	SER
3	C1	36	VAL
3	C2	11	SER
3	C2	36	VAL
3	C3	11	SER
3	C3	36	VAL
3	C4	11	SER
3	C4	36	VAL
3	C5	11	SER
3	C5	36	VAL
3	C6	11	SER
3	C6	36	VAL
3	C7	11	SER
3	C7	36	VAL
3	C8	11	SER
3	C8	36	VAL
3	C9	11	SER
3	C9	36	VAL
3	Cc	11	SER
3	Cc	36	VAL

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Mol	Chain	Res	Type
3	Cd	11	SER
3	Cd	36	VAL
3	Ce	11	SER
3	Ce	36	VAL
3	Cf	11	SER
3	Cf	36	VAL
3	Cg	11	SER
3	Cg	36	VAL
3	Ch	11	SER
3	Ch	36	VAL
3	Ci	11	SER
3	Ci	36	VAL
3	Cj	11	SER
3	Cj	36	VAL
3	Ck	11	SER
3	Ck	36	VAL
3	Cl	11	SER
3	Cl	36	VAL
3	Cm	11	SER
3	Cm	36	VAL
3	Cn	11	SER
3	Cn	36	VAL
3	Co	11	SER
3	Co	36	VAL
3	Cp	11	SER
3	Cp	36	VAL
3	Cq	11	SER
3	Cq	36	VAL
3	Cr	11	SER
3	Cr	36	VAL
3	Cs	11	SER
3	Cs	36	VAL
3	Ct	11	SER
3	Ct	36	VAL
3	Cu	11	SER
3	Cu	36	VAL
3	Cv	11	SER
3	Cv	36	VAL
3	Cw	11	SER
3	Cw	36	VAL
3	Cx	11	SER
3	Cx	36	VAL

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Mol	Chain	Res	Type
3	DA	11	SER
3	DA	36	VAL
3	DB	11	SER
3	DB	36	VAL
1	DC	2	THR
1	DC	5	GLY
1	DC	41	GLU
1	DC	202	HIS
1	DC	244	ASN
1	DD	2	THR
1	DD	5	GLY
1	DD	41	GLU
1	DD	202	HIS
1	DD	244	ASN
1	DE	2	THR
1	DE	5	GLY
1	DE	41	GLU
1	DE	202	HIS
1	DE	244	ASN
1	DF	2	THR
1	DF	5	GLY
1	DF	41	GLU
1	DF	202	HIS
1	DF	244	ASN
1	DG	2	THR
1	DG	5	GLY
1	DG	41	GLU
1	DG	202	HIS
1	DG	244	ASN
1	DH	2	THR
1	DH	5	GLY
1	DH	41	GLU
1	DH	202	HIS
1	DH	244	ASN
1	DI	2	THR
1	DI	5	GLY
1	DI	41	GLU
1	DI	202	HIS
1	DI	244	ASN
1	DJ	2	THR
1	DJ	5	GLY
1	DJ	41	GLU

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Mol	Chain	Res	Type
1	DJ	202	HIS
1	DJ	244	ASN
1	DK	2	THR
1	DK	5	GLY
1	DK	41	GLU
1	DK	202	HIS
1	DK	244	ASN
1	AA	22	VAL
1	AA	71	LEU
1	AA	147	ALA
1	AA	182	ALA
1	AA	184	TYR
1	AB	22	VAL
1	AB	71	LEU
1	AB	147	ALA
1	AB	182	ALA
1	AB	184	TYR
1	AC	22	VAL
1	AC	71	LEU
1	AC	147	ALA
1	AC	182	ALA
1	AC	184	TYR
1	AD	22	VAL
1	AD	71	LEU
1	AD	147	ALA
1	AD	182	ALA
1	AD	184	TYR
1	AE	22	VAL
1	AE	71	LEU
1	AE	147	ALA
1	AE	182	ALA
1	AE	184	TYR
1	AF	22	VAL
1	AF	71	LEU
1	AF	147	ALA
1	AF	182	ALA
1	AF	184	TYR
1	AG	22	VAL
1	AG	71	LEU
1	AG	147	ALA
1	AG	182	ALA
1	AG	184	TYR

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Mol	Chain	Res	Type
1	AH	22	VAL
1	AH	71	LEU
1	AH	147	ALA
1	AH	182	ALA
1	AH	184	TYR
1	AI	22	VAL
1	AI	71	LEU
1	AI	147	ALA
1	AI	182	ALA
1	AI	184	TYR
1	AJ	22	VAL
1	AJ	71	LEU
1	AJ	147	ALA
1	AJ	182	ALA
1	AJ	184	TYR
1	AK	22	VAL
1	AK	71	LEU
1	AK	147	ALA
1	AK	182	ALA
1	AK	184	TYR
1	AL	22	VAL
1	AL	71	LEU
1	AL	147	ALA
1	AL	182	ALA
1	AL	184	TYR
1	AM	22	VAL
1	AM	71	LEU
1	AM	147	ALA
1	AM	182	ALA
1	AM	184	TYR
1	AN	22	VAL
1	AN	71	LEU
1	AN	147	ALA
1	AN	182	ALA
1	AN	184	TYR
1	AO	22	VAL
1	AO	71	LEU
1	AO	147	ALA
1	AO	182	ALA
1	AO	184	TYR
1	AP	22	VAL
1	AP	71	LEU

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Mol	Chain	Res	Type
1	AP	147	ALA
1	AP	182	ALA
1	AP	184	TYR
1	AQ	22	VAL
1	AQ	71	LEU
1	AQ	147	ALA
1	AQ	182	ALA
1	AQ	184	TYR
1	AR	22	VAL
1	AR	71	LEU
1	AR	147	ALA
1	AR	182	ALA
1	AR	184	TYR
1	AS	22	VAL
1	AS	71	LEU
1	AS	147	ALA
1	AS	182	ALA
1	AS	184	TYR
1	AT	22	VAL
1	AT	71	LEU
1	AT	147	ALA
1	AT	182	ALA
1	AT	184	TYR
1	AU	22	VAL
1	AU	71	LEU
1	AU	147	ALA
1	AU	182	ALA
1	AU	184	TYR
1	AV	22	VAL
1	AV	71	LEU
1	AV	147	ALA
1	AV	182	ALA
1	AV	184	TYR
1	AW	22	VAL
1	AW	71	LEU
1	AW	147	ALA
1	AW	182	ALA
1	AW	184	TYR
1	AX	22	VAL
1	AX	71	LEU
1	AX	147	ALA
1	AX	182	ALA

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Mol	Chain	Res	Type
1	AX	184	TYR
1	AY	22	VAL
1	AY	71	LEU
1	AY	147	ALA
1	AY	182	ALA
1	AY	184	TYR
1	AZ	22	VAL
1	AZ	71	LEU
1	AZ	147	ALA
1	AZ	182	ALA
1	AZ	184	TYR
1	A0	22	VAL
1	A0	71	LEU
1	A0	147	ALA
1	A0	182	ALA
1	A0	184	TYR
1	A1	22	VAL
1	A1	71	LEU
1	A1	147	ALA
1	A1	182	ALA
1	A1	184	TYR
1	A2	22	VAL
1	A2	71	LEU
1	A2	147	ALA
1	A2	182	ALA
1	A2	184	TYR
1	A3	22	VAL
1	A3	71	LEU
1	A3	147	ALA
1	A3	182	ALA
1	A3	184	TYR
1	A4	22	VAL
1	A4	71	LEU
1	A4	147	ALA
1	A4	182	ALA
1	A4	184	TYR
1	A5	22	VAL
1	A5	71	LEU
1	A5	147	ALA
1	A5	182	ALA
1	A5	184	TYR
1	A6	22	VAL

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Mol	Chain	Res	Type
1	A6	71	LEU
1	A6	147	ALA
1	A6	182	ALA
1	A6	184	TYR
1	A7	22	VAL
1	A7	71	LEU
1	A7	147	ALA
1	A7	182	ALA
1	A7	184	TYR
1	A8	22	VAL
1	A8	71	LEU
1	A8	147	ALA
1	A8	182	ALA
1	A8	184	TYR
1	A9	22	VAL
1	A9	71	LEU
1	A9	147	ALA
1	A9	182	ALA
1	A9	184	TYR
1	Aa	22	VAL
1	Aa	71	LEU
1	Aa	147	ALA
1	Aa	182	ALA
1	Aa	184	TYR
1	Ab	22	VAL
1	Ab	71	LEU
1	Ab	147	ALA
1	Ab	182	ALA
1	Ab	184	TYR
1	Ac	22	VAL
1	Ac	71	LEU
1	Ac	147	ALA
1	Ac	182	ALA
1	Ac	184	TYR
1	Ad	22	VAL
1	Ad	71	LEU
1	Ad	147	ALA
1	Ad	182	ALA
1	Ad	184	TYR
1	Ae	22	VAL
1	Ae	71	LEU
1	Ae	147	ALA

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Mol	Chain	Res	Type
1	Ae	182	ALA
1	Ae	184	TYR
1	Af	22	VAL
1	Af	71	LEU
1	Af	147	ALA
1	Af	182	ALA
1	Af	184	TYR
1	Ag	22	VAL
1	Ag	71	LEU
1	Ag	147	ALA
1	Ag	182	ALA
1	Ag	184	TYR
1	Ah	22	VAL
1	Ah	71	LEU
1	Ah	147	ALA
1	Ah	182	ALA
1	Ah	184	TYR
1	Ai	22	VAL
1	Ai	71	LEU
1	Ai	147	ALA
1	Ai	182	ALA
1	Ai	184	TYR
1	Aj	22	VAL
1	Aj	71	LEU
1	Aj	147	ALA
1	Aj	182	ALA
1	Aj	184	TYR
1	Ak	22	VAL
1	Ak	71	LEU
1	Ak	147	ALA
1	Ak	182	ALA
1	Ak	184	TYR
1	Al	22	VAL
1	Al	71	LEU
1	Al	147	ALA
1	Al	182	ALA
1	Al	184	TYR
1	Am	22	VAL
1	Am	71	LEU
1	Am	147	ALA
1	Am	182	ALA
1	Am	184	TYR

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Mol	Chain	Res	Type
1	An	22	VAL
1	An	71	LEU
1	An	147	ALA
1	An	182	ALA
1	An	184	TYR
1	Ao	22	VAL
1	Ao	71	LEU
1	Ao	147	ALA
1	Ao	182	ALA
1	Ao	184	TYR
2	BA	92	GLY
2	BA	224	GLY
2	BB	92	GLY
2	BB	224	GLY
2	BC	92	GLY
2	BC	224	GLY
2	BD	92	GLY
2	BD	224	GLY
2	BE	92	GLY
2	BE	224	GLY
2	BF	92	GLY
2	BF	224	GLY
2	BG	92	GLY
2	BG	224	GLY
2	BH	92	GLY
2	BH	224	GLY
2	BI	92	GLY
2	BI	224	GLY
2	BJ	92	GLY
2	BJ	224	GLY
2	BK	92	GLY
2	BK	224	GLY
2	BL	92	GLY
2	BL	224	GLY
2	BM	92	GLY
2	BM	224	GLY
2	BN	92	GLY
2	BN	224	GLY
2	BR	92	GLY
2	BR	224	GLY
2	BO	92	GLY
2	BO	224	GLY

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Mol	Chain	Res	Type
2	BS	92	GLY
2	BS	224	GLY
2	BP	92	GLY
2	BP	224	GLY
2	BQ	92	GLY
2	BQ	224	GLY
2	BT	92	GLY
2	BT	224	GLY
2	BU	92	GLY
2	BU	224	GLY
2	BV	92	GLY
2	BV	224	GLY
2	BW	92	GLY
2	BW	224	GLY
2	BX	92	GLY
2	BX	224	GLY
2	BY	92	GLY
2	BY	224	GLY
2	BZ	92	GLY
2	BZ	224	GLY
2	B0	92	GLY
2	B0	224	GLY
2	B1	92	GLY
2	B1	224	GLY
2	B2	92	GLY
2	B2	224	GLY
2	B3	92	GLY
2	B3	224	GLY
2	B4	92	GLY
2	B4	224	GLY
2	B5	92	GLY
2	B5	224	GLY
2	B6	92	GLY
2	B6	224	GLY
2	B7	92	GLY
2	B7	224	GLY
2	B8	92	GLY
2	B8	224	GLY
2	B9	92	GLY
2	B9	224	GLY
2	Ba	92	GLY
2	Ba	224	GLY

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Mol	Chain	Res	Type
2	Bb	92	GLY
2	Bb	224	GLY
2	Bc	92	GLY
2	Bc	224	GLY
2	Bd	92	GLY
2	Bd	224	GLY
2	Be	92	GLY
2	Be	224	GLY
2	Bf	92	GLY
2	Bf	224	GLY
2	Bg	92	GLY
2	Bg	224	GLY
2	Bh	92	GLY
2	Bh	224	GLY
2	Bi	92	GLY
2	Bi	224	GLY
2	Bj	92	GLY
2	Bj	224	GLY
2	Bk	92	GLY
2	Bk	224	GLY
2	Bl	92	GLY
2	Bl	224	GLY
2	Bm	92	GLY
2	Bm	224	GLY
2	Bn	92	GLY
2	Bn	224	GLY
2	Bo	92	GLY
2	Bo	224	GLY
2	Bp	92	GLY
2	Bp	224	GLY
2	Bq	92	GLY
2	Bq	224	GLY
2	Br	92	GLY
2	Br	224	GLY
2	Bs	92	GLY
2	Bs	224	GLY
2	Bt	92	GLY
2	Bt	224	GLY
2	Bu	92	GLY
2	Bu	224	GLY
2	Bv	92	GLY
2	Bv	224	GLY

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Mol	Chain	Res	Type
2	Bw	92	GLY
2	Bw	224	GLY
2	Bx	92	GLY
2	Bx	224	GLY
3	CA	15	MET
3	CA	35	GLN
3	CA	70	ASP
3	CB	15	MET
3	CB	35	GLN
3	CB	70	ASP
3	CC	15	MET
3	CC	35	GLN
3	CC	70	ASP
3	CD	15	MET
3	CD	35	GLN
3	CD	70	ASP
3	CE	15	MET
3	CE	35	GLN
3	CE	70	ASP
3	CF	15	MET
3	CF	35	GLN
3	CF	70	ASP
3	CG	15	MET
3	CG	35	GLN
3	CG	70	ASP
3	CH	15	MET
3	CH	35	GLN
3	CH	70	ASP
3	CI	15	MET
3	CI	35	GLN
3	CI	70	ASP
3	CJ	15	MET
3	CJ	35	GLN
3	CJ	70	ASP
3	CK	15	MET
3	CK	35	GLN
3	CK	70	ASP
3	CL	15	MET
3	CL	35	GLN
3	CL	70	ASP
3	CM	15	MET
3	CM	35	GLN

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Mol	Chain	Res	Type
3	CM	70	ASP
3	CN	15	MET
3	CN	35	GLN
3	CN	70	ASP
3	CO	15	MET
3	CO	35	GLN
3	CO	70	ASP
3	CP	15	MET
3	CP	35	GLN
3	CP	70	ASP
3	CQ	15	MET
3	CQ	35	GLN
3	CQ	70	ASP
3	CR	15	MET
3	CR	35	GLN
3	CR	70	ASP
3	CS	15	MET
3	CS	35	GLN
3	CS	70	ASP
3	CT	15	MET
3	CT	35	GLN
3	CT	70	ASP
3	CU	15	MET
3	CU	35	GLN
3	CU	70	ASP
3	CV	15	MET
3	CV	35	GLN
3	CV	70	ASP
3	CW	15	MET
3	CW	35	GLN
3	CW	70	ASP
3	CX	15	MET
3	CX	35	GLN
3	CX	70	ASP
3	CY	15	MET
3	CY	35	GLN
3	CY	70	ASP
3	CZ	15	MET
3	CZ	35	GLN
3	CZ	70	ASP
3	C0	15	MET
3	C0	35	GLN

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Mol	Chain	Res	Type
3	C0	70	ASP
3	C1	15	MET
3	C1	35	GLN
3	C1	70	ASP
3	C2	15	MET
3	C2	35	GLN
3	C2	70	ASP
3	C3	15	MET
3	C3	35	GLN
3	C3	70	ASP
3	C4	15	MET
3	C4	35	GLN
3	C4	70	ASP
3	C5	15	MET
3	C5	35	GLN
3	C5	70	ASP
3	C6	15	MET
3	C6	35	GLN
3	C6	70	ASP
3	C7	15	MET
3	C7	35	GLN
3	C7	70	ASP
3	C8	15	MET
3	C8	35	GLN
3	C8	70	ASP
3	C9	15	MET
3	C9	35	GLN
3	C9	70	ASP
3	Cc	15	MET
3	Cc	35	GLN
3	Cc	70	ASP
3	Cd	15	MET
3	Cd	35	GLN
3	Cd	70	ASP
3	Ce	15	MET
3	Ce	35	GLN
3	Ce	70	ASP
3	Cf	15	MET
3	Cf	35	GLN
3	Cf	70	ASP
3	Cg	15	MET
3	Cg	35	GLN

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Mol	Chain	Res	Type
3	Cg	70	ASP
3	Ch	15	MET
3	Ch	35	GLN
3	Ch	70	ASP
3	Ci	15	MET
3	Ci	35	GLN
3	Ci	70	ASP
3	Cj	15	MET
3	Cj	35	GLN
3	Cj	70	ASP
3	Ck	15	MET
3	Ck	35	GLN
3	Ck	70	ASP
3	Cl	15	MET
3	Cl	35	GLN
3	Cl	70	ASP
3	Cm	15	MET
3	Cm	35	GLN
3	Cm	70	ASP
3	Cn	15	MET
3	Cn	35	GLN
3	Cn	70	ASP
3	Co	15	MET
3	Co	35	GLN
3	Co	70	ASP
3	Cp	15	MET
3	Cp	35	GLN
3	Cp	70	ASP
3	Cq	15	MET
3	Cq	35	GLN
3	Cq	70	ASP
3	Cr	15	MET
3	Cr	35	GLN
3	Cr	70	ASP
3	Cs	15	MET
3	Cs	35	GLN
3	Cs	70	ASP
3	Ct	15	MET
3	Ct	35	GLN
3	Ct	70	ASP
3	Cu	15	MET
3	Cu	35	GLN

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Mol	Chain	Res	Type
3	Cu	70	ASP
3	Cv	15	MET
3	Cv	35	GLN
3	Cv	70	ASP
3	Cw	15	MET
3	Cw	35	GLN
3	Cw	70	ASP
3	Cx	15	MET
3	Cx	35	GLN
3	Cx	70	ASP
3	DA	15	MET
3	DA	35	GLN
3	DA	70	ASP
3	DB	15	MET
3	DB	35	GLN
3	DB	70	ASP
1	DC	22	VAL
1	DC	71	LEU
1	DC	147	ALA
1	DC	182	ALA
1	DC	184	TYR
1	DD	22	VAL
1	DD	71	LEU
1	DD	147	ALA
1	DD	182	ALA
1	DD	184	TYR
1	DE	22	VAL
1	DE	71	LEU
1	DE	147	ALA
1	DE	182	ALA
1	DE	184	TYR
1	DF	22	VAL
1	DF	71	LEU
1	DF	147	ALA
1	DF	182	ALA
1	DF	184	TYR
1	DG	22	VAL
1	DG	71	LEU
1	DG	147	ALA
1	DG	182	ALA
1	DG	184	TYR
1	DH	22	VAL

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Mol	Chain	Res	Type
1	DH	71	LEU
1	DH	147	ALA
1	DH	182	ALA
1	DH	184	TYR
1	DI	22	VAL
1	DI	71	LEU
1	DI	147	ALA
1	DI	182	ALA
1	DI	184	TYR
1	DJ	22	VAL
1	DJ	71	LEU
1	DJ	147	ALA
1	DJ	182	ALA
1	DJ	184	TYR
1	DK	22	VAL
1	DK	71	LEU
1	DK	147	ALA
1	DK	182	ALA
1	DK	184	TYR
1	AA	3	ASN
1	AB	3	ASN
1	AC	3	ASN
1	AD	3	ASN
1	AE	3	ASN
1	AF	3	ASN
1	AG	3	ASN
1	AH	3	ASN
1	AI	3	ASN
1	AJ	3	ASN
1	AK	3	ASN
1	AL	3	ASN
1	AM	3	ASN
1	AN	3	ASN
1	AO	3	ASN
1	AP	3	ASN
1	AQ	3	ASN
1	AR	3	ASN
1	AS	3	ASN
1	AT	3	ASN
1	AU	3	ASN
1	AV	3	ASN
1	AW	3	ASN

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Mol	Chain	Res	Type
1	AX	3	ASN
1	AY	3	ASN
1	AZ	3	ASN
1	A0	3	ASN
1	A1	3	ASN
1	A2	3	ASN
1	A3	3	ASN
1	A4	3	ASN
1	A5	3	ASN
1	A6	3	ASN
1	A7	3	ASN
1	A8	3	ASN
1	A9	3	ASN
1	Aa	3	ASN
1	Ab	3	ASN
1	Ac	3	ASN
1	Ad	3	ASN
1	Ae	3	ASN
1	Af	3	ASN
1	Ag	3	ASN
1	Ah	3	ASN
1	Ai	3	ASN
1	Aj	3	ASN
1	Ak	3	ASN
1	Al	3	ASN
1	Am	3	ASN
1	An	3	ASN
1	Ao	3	ASN
1	DC	3	ASN
1	DD	3	ASN
1	DE	3	ASN
1	DF	3	ASN
1	DG	3	ASN
1	DH	3	ASN
1	DI	3	ASN
1	DJ	3	ASN
1	DK	3	ASN
1	AA	187	LEU
1	AA	208	TYR
1	AB	187	LEU
1	AB	208	TYR
1	AC	187	LEU

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Mol	Chain	Res	Type
1	AC	208	TYR
1	AD	187	LEU
1	AD	208	TYR
1	AE	187	LEU
1	AE	208	TYR
1	AF	187	LEU
1	AF	208	TYR
1	AG	187	LEU
1	AG	208	TYR
1	AH	187	LEU
1	AH	208	TYR
1	AI	187	LEU
1	AI	208	TYR
1	AJ	187	LEU
1	AJ	208	TYR
1	AK	187	LEU
1	AK	208	TYR
1	AL	187	LEU
1	AL	208	TYR
1	AM	187	LEU
1	AM	208	TYR
1	AN	187	LEU
1	AN	208	TYR
1	AO	187	LEU
1	AO	208	TYR
1	AP	187	LEU
1	AP	208	TYR
1	AQ	187	LEU
1	AQ	208	TYR
1	AR	187	LEU
1	AR	208	TYR
1	AS	187	LEU
1	AS	208	TYR
1	AT	187	LEU
1	AT	208	TYR
1	AU	187	LEU
1	AU	208	TYR
1	AV	187	LEU
1	AV	208	TYR
1	AW	187	LEU
1	AW	208	TYR
1	AX	187	LEU

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Mol	Chain	Res	Type
1	AX	208	TYR
1	AY	187	LEU
1	AY	208	TYR
1	AZ	187	LEU
1	AZ	208	TYR
1	A0	187	LEU
1	A0	208	TYR
1	A1	187	LEU
1	A1	208	TYR
1	A2	187	LEU
1	A2	208	TYR
1	A3	187	LEU
1	A3	208	TYR
1	A4	187	LEU
1	A4	208	TYR
1	A5	187	LEU
1	A5	208	TYR
1	A6	187	LEU
1	A6	208	TYR
1	A7	187	LEU
1	A7	208	TYR
1	A8	187	LEU
1	A8	208	TYR
1	A9	187	LEU
1	A9	208	TYR
1	Aa	187	LEU
1	Aa	208	TYR
1	Ab	187	LEU
1	Ab	208	TYR
1	Ac	187	LEU
1	Ac	208	TYR
1	Ad	187	LEU
1	Ad	208	TYR
1	Ae	187	LEU
1	Ae	208	TYR
1	Af	187	LEU
1	Af	208	TYR
1	Ag	187	LEU
1	Ag	208	TYR
1	Ah	187	LEU
1	Ah	208	TYR
1	Ai	187	LEU

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Mol	Chain	Res	Type
1	Ai	208	TYR
1	Aj	187	LEU
1	Aj	208	TYR
1	Ak	187	LEU
1	Ak	208	TYR
1	Al	187	LEU
1	Al	208	TYR
1	Am	187	LEU
1	Am	208	TYR
1	An	187	LEU
1	An	208	TYR
1	Ao	187	LEU
1	Ao	208	TYR
2	BA	149	ALA
2	BB	149	ALA
2	BC	149	ALA
2	BD	149	ALA
2	BE	149	ALA
2	BF	149	ALA
2	BG	149	ALA
2	BH	149	ALA
2	BI	149	ALA
2	BJ	149	ALA
2	BK	149	ALA
2	BL	149	ALA
2	BM	149	ALA
2	BN	149	ALA
2	BR	149	ALA
2	BO	149	ALA
2	BS	149	ALA
2	BP	149	ALA
2	BQ	149	ALA
2	BT	149	ALA
2	BU	149	ALA
2	BV	149	ALA
2	BW	149	ALA
2	BX	149	ALA
2	BY	149	ALA
2	BZ	149	ALA
2	B0	149	ALA
2	B1	149	ALA
2	B2	149	ALA

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Mol	Chain	Res	Type
2	B3	149	ALA
2	B4	149	ALA
2	B5	149	ALA
2	B6	149	ALA
2	B7	149	ALA
2	B8	149	ALA
2	B9	149	ALA
2	Ba	149	ALA
2	Bb	149	ALA
2	Bc	149	ALA
2	Bd	149	ALA
2	Be	149	ALA
2	Bf	149	ALA
2	Bg	149	ALA
2	Bh	149	ALA
2	Bi	149	ALA
2	Bj	149	ALA
2	Bk	149	ALA
2	Bl	149	ALA
2	Bm	149	ALA
2	Bn	149	ALA
2	Bo	149	ALA
2	Bp	149	ALA
2	Bq	149	ALA
2	Br	149	ALA
2	Bs	149	ALA
2	Bt	149	ALA
2	Bu	149	ALA
2	Bv	149	ALA
2	Bw	149	ALA
2	Bx	149	ALA
3	CA	131	ALA
3	CB	131	ALA
3	CC	131	ALA
3	CD	131	ALA
3	CE	131	ALA
3	CF	131	ALA
3	CG	131	ALA
3	CH	131	ALA
3	CI	131	ALA
3	CJ	131	ALA
3	CK	131	ALA

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Mol	Chain	Res	Type
3	CL	131	ALA
3	CM	131	ALA
3	CN	131	ALA
3	CO	131	ALA
3	CP	131	ALA
3	CQ	131	ALA
3	CR	131	ALA
3	CS	131	ALA
3	CT	131	ALA
3	CU	131	ALA
3	CV	131	ALA
3	CW	131	ALA
3	CX	131	ALA
3	CY	131	ALA
3	CZ	131	ALA
3	C0	131	ALA
3	C1	131	ALA
3	C2	131	ALA
3	C3	131	ALA
3	C4	131	ALA
3	C5	131	ALA
3	C6	131	ALA
3	C7	131	ALA
3	C8	131	ALA
3	C9	131	ALA
3	Cc	131	ALA
3	Cd	131	ALA
3	Ce	131	ALA
3	Cf	131	ALA
3	Cg	131	ALA
3	Ch	131	ALA
3	Ci	131	ALA
3	Cj	131	ALA
3	Ck	131	ALA
3	Cl	131	ALA
3	Cm	131	ALA
3	Cn	131	ALA
3	Co	131	ALA
3	Cp	131	ALA
3	Cq	131	ALA
3	Cr	131	ALA
3	Cs	131	ALA

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Mol	Chain	Res	Type
3	Ct	131	ALA
3	Cu	131	ALA
3	Cv	131	ALA
3	Cw	131	ALA
3	Cx	131	ALA
3	DA	131	ALA
3	DB	131	ALA
1	DC	187	LEU
1	DC	208	TYR
1	DD	187	LEU
1	DD	208	TYR
1	DE	187	LEU
1	DE	208	TYR
1	DF	187	LEU
1	DF	208	TYR
1	DG	187	LEU
1	DG	208	TYR
1	DH	187	LEU
1	DH	208	TYR
1	DI	187	LEU
1	DI	208	TYR
1	DJ	187	LEU
1	DJ	208	TYR
1	DK	187	LEU
1	DK	208	TYR
2	BA	60	ARG
2	BB	60	ARG
2	BC	60	ARG
2	BD	60	ARG
2	BE	60	ARG
2	BF	60	ARG
2	BG	60	ARG
2	BH	60	ARG
2	BI	60	ARG
2	BJ	60	ARG
2	BK	60	ARG
2	BL	60	ARG
2	BM	60	ARG
2	BN	60	ARG
2	BR	60	ARG
2	BO	60	ARG
2	BS	60	ARG

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Mol	Chain	Res	Type
2	BP	60	ARG
2	BQ	60	ARG
2	BT	60	ARG
2	BU	60	ARG
2	BV	60	ARG
2	BW	60	ARG
2	BX	60	ARG
2	BY	60	ARG
2	BZ	60	ARG
2	B0	60	ARG
2	B1	60	ARG
2	B2	60	ARG
2	B3	60	ARG
2	B4	60	ARG
2	B5	60	ARG
2	B6	60	ARG
2	B7	60	ARG
2	B8	60	ARG
2	B9	60	ARG
2	Ba	60	ARG
2	Bb	60	ARG
2	Bc	60	ARG
2	Bd	60	ARG
2	Be	60	ARG
2	Bf	60	ARG
2	Bg	60	ARG
2	Bh	60	ARG
2	Bi	60	ARG
2	Bj	60	ARG
2	Bk	60	ARG
2	Bl	60	ARG
2	Bm	60	ARG
2	Bn	60	ARG
2	Bo	60	ARG
2	Bp	60	ARG
2	Bq	60	ARG
2	Br	60	ARG
2	Bs	60	ARG
2	Bt	60	ARG
2	Bu	60	ARG
2	Bv	60	ARG
2	Bw	60	ARG

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Mol	Chain	Res	Type
2	Bx	60	ARG
1	Ac	226	PRO
1	AA	226	PRO
1	AB	226	PRO
1	AC	226	PRO
1	AD	226	PRO
1	AE	226	PRO
1	AF	226	PRO
1	AG	226	PRO
1	AH	226	PRO
1	AI	226	PRO
1	AJ	226	PRO
1	AK	226	PRO
1	AL	226	PRO
1	AM	226	PRO
1	AN	226	PRO
1	AO	226	PRO
1	AP	226	PRO
1	AQ	226	PRO
1	AR	226	PRO
1	AS	226	PRO
1	AT	226	PRO
1	AU	226	PRO
1	AV	226	PRO
1	AW	226	PRO
1	AX	226	PRO
1	AY	226	PRO
1	AZ	226	PRO
1	A0	226	PRO
1	A1	226	PRO
1	A2	226	PRO
1	A3	226	PRO
1	A4	226	PRO
1	A5	226	PRO
1	A6	226	PRO
1	A7	226	PRO
1	A8	226	PRO
1	A9	226	PRO
1	Aa	226	PRO
1	Ab	226	PRO
1	Ad	226	PRO
1	Ae	226	PRO

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Mol	Chain	Res	Type
1	Af	226	PRO
1	Ag	226	PRO
1	Ah	226	PRO
1	Ai	226	PRO
1	Aj	226	PRO
1	Ak	226	PRO
1	Al	226	PRO
1	Am	226	PRO
1	An	226	PRO
1	Ao	226	PRO
1	DC	226	PRO
1	DD	226	PRO
1	DE	226	PRO
1	DF	226	PRO
1	DG	226	PRO
1	DH	226	PRO
1	DI	226	PRO
1	DJ	226	PRO
1	DK	226	PRO

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	208/208 (100%)	184 (88%)	24 (12%)	5 21
1	A1	208/208 (100%)	184 (88%)	24 (12%)	5 21
1	A2	208/208 (100%)	184 (88%)	24 (12%)	5 21
1	A3	208/208 (100%)	184 (88%)	24 (12%)	5 21
1	A4	208/208 (100%)	184 (88%)	24 (12%)	5 21
1	A5	208/208 (100%)	184 (88%)	24 (12%)	5 21
1	A6	208/208 (100%)	184 (88%)	24 (12%)	5 21
1	A7	208/208 (100%)	184 (88%)	24 (12%)	5 21
1	A8	208/208 (100%)	184 (88%)	24 (12%)	5 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A9	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AA	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AB	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AC	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AD	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AE	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AF	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AG	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AH	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AI	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AJ	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AK	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AL	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AM	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AN	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AO	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AP	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AQ	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AR	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AS	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AT	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AU	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AV	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AW	208/208 (100%)	183 (88%)	25 (12%)	5	20
1	AX	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AY	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	AZ	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	Aa	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	Ab	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	Ac	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	Ad	208/208 (100%)	184 (88%)	24 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ae	208/208 (100%)	183 (88%)	25 (12%)	5	20
1	Af	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	Ag	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	Ah	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	Ai	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	Aj	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	Ak	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	Al	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	Am	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	An	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	Ao	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	DC	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	DD	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	DE	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	DF	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	DG	208/208 (100%)	183 (88%)	25 (12%)	5	20
1	DH	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	DI	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	DJ	208/208 (100%)	184 (88%)	24 (12%)	5	21
1	DK	208/208 (100%)	184 (88%)	24 (12%)	5	21
2	B0	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	B1	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	B2	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	B3	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	B4	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	B5	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	B6	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	B7	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	B8	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	B9	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BA	176/176 (100%)	150 (85%)	26 (15%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BB	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BC	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BD	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BE	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BF	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BG	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BH	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BI	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BJ	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BK	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BL	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BM	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BN	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BO	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BP	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BQ	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BR	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BS	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BT	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BU	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BV	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BW	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BX	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BY	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	BZ	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	Ba	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	Bb	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	Bc	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	Bd	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	Be	176/176 (100%)	150 (85%)	26 (15%)	3	15
2	Bf	176/176 (100%)	150 (85%)	26 (15%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	Bg	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bh	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bi	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bj	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bk	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bl	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bm	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bn	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bo	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bp	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bq	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Br	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bs	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bt	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bu	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bv	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bw	176/176 (100%)	150 (85%)	26 (15%)	3 15
2	Bx	176/176 (100%)	150 (85%)	26 (15%)	3 15
3	C0	190/190 (100%)	150 (79%)	40 (21%)	1 6
3	C1	190/190 (100%)	150 (79%)	40 (21%)	1 6
3	C2	190/190 (100%)	150 (79%)	40 (21%)	1 6
3	C3	190/190 (100%)	150 (79%)	40 (21%)	1 6
3	C4	190/190 (100%)	150 (79%)	40 (21%)	1 6
3	C5	190/190 (100%)	150 (79%)	40 (21%)	1 6
3	C6	190/190 (100%)	150 (79%)	40 (21%)	1 6
3	C7	190/190 (100%)	150 (79%)	40 (21%)	1 6
3	C8	190/190 (100%)	150 (79%)	40 (21%)	1 6
3	C9	190/190 (100%)	150 (79%)	40 (21%)	1 6
3	CA	190/190 (100%)	150 (79%)	40 (21%)	1 6
3	CB	190/190 (100%)	150 (79%)	40 (21%)	1 6
3	CC	190/190 (100%)	150 (79%)	40 (21%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CD	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CE	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CF	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CG	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CH	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CI	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CJ	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CK	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CL	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CM	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CN	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CO	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CP	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CQ	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CR	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CS	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CT	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CU	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CV	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CW	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CX	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CY	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	CZ	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cc	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cd	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Ce	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cf	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cg	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Ch	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Ci	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cj	190/190 (100%)	150 (79%)	40 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Ck	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cl	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cm	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cn	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Co	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cp	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cq	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cr	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cs	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Ct	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cu	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cv	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cw	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	Cx	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	DA	190/190 (100%)	150 (79%)	40 (21%)	1	6
3	DB	190/190 (100%)	150 (79%)	40 (21%)	1	6
All	All	34440/34440 (100%)	29037 (84%)	5403 (16%)	5	14

All (5403) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	4	VAL
1	AA	28	THR
1	AA	36	ARG
1	AA	39	ASP
1	AA	40	VAL
1	AA	42	THR
1	AA	45	LEU
1	AA	49	THR
1	AA	62	SER
1	AA	71	LEU
1	AA	113	THR
1	AA	120	GLN
1	AA	150	ARG
1	AA	158	VAL
1	AA	163	MET

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Mol	Chain	Res	Type
1	AA	166	VAL
1	AA	187	LEU
1	AA	196	LEU
1	AA	198	THR
1	AA	203	ASP
1	AA	209	LEU
1	AA	226	PRO
1	AA	237	HIS
1	AA	246	GLN
1	AB	4	VAL
1	AB	28	THR
1	AB	36	ARG
1	AB	39	ASP
1	AB	40	VAL
1	AB	42	THR
1	AB	45	LEU
1	AB	49	THR
1	AB	62	SER
1	AB	71	LEU
1	AB	113	THR
1	AB	120	GLN
1	AB	150	ARG
1	AB	158	VAL
1	AB	163	MET
1	AB	166	VAL
1	AB	187	LEU
1	AB	196	LEU
1	AB	198	THR
1	AB	203	ASP
1	AB	209	LEU
1	AB	226	PRO
1	AB	237	HIS
1	AB	246	GLN
1	AC	4	VAL
1	AC	28	THR
1	AC	36	ARG
1	AC	39	ASP
1	AC	40	VAL
1	AC	42	THR
1	AC	45	LEU
1	AC	49	THR
1	AC	62	SER

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Mol	Chain	Res	Type
1	AC	71	LEU
1	AC	113	THR
1	AC	120	GLN
1	AC	150	ARG
1	AC	158	VAL
1	AC	163	MET
1	AC	166	VAL
1	AC	187	LEU
1	AC	196	LEU
1	AC	198	THR
1	AC	203	ASP
1	AC	209	LEU
1	AC	226	PRO
1	AC	237	HIS
1	AC	246	GLN
1	AD	4	VAL
1	AD	28	THR
1	AD	36	ARG
1	AD	39	ASP
1	AD	40	VAL
1	AD	42	THR
1	AD	45	LEU
1	AD	49	THR
1	AD	62	SER
1	AD	71	LEU
1	AD	113	THR
1	AD	120	GLN
1	AD	150	ARG
1	AD	158	VAL
1	AD	163	MET
1	AD	166	VAL
1	AD	187	LEU
1	AD	196	LEU
1	AD	198	THR
1	AD	203	ASP
1	AD	209	LEU
1	AD	226	PRO
1	AD	237	HIS
1	AD	246	GLN
1	AE	4	VAL
1	AE	28	THR
1	AE	36	ARG

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Mol	Chain	Res	Type
1	AE	39	ASP
1	AE	40	VAL
1	AE	42	THR
1	AE	45	LEU
1	AE	49	THR
1	AE	62	SER
1	AE	71	LEU
1	AE	113	THR
1	AE	120	GLN
1	AE	150	ARG
1	AE	158	VAL
1	AE	163	MET
1	AE	166	VAL
1	AE	187	LEU
1	AE	196	LEU
1	AE	198	THR
1	AE	203	ASP
1	AE	209	LEU
1	AE	226	PRO
1	AE	237	HIS
1	AE	246	GLN
1	AF	4	VAL
1	AF	28	THR
1	AF	36	ARG
1	AF	39	ASP
1	AF	40	VAL
1	AF	42	THR
1	AF	45	LEU
1	AF	49	THR
1	AF	62	SER
1	AF	71	LEU
1	AF	113	THR
1	AF	120	GLN
1	AF	150	ARG
1	AF	158	VAL
1	AF	163	MET
1	AF	166	VAL
1	AF	187	LEU
1	AF	196	LEU
1	AF	198	THR
1	AF	203	ASP
1	AF	209	LEU

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Mol	Chain	Res	Type
1	AF	226	PRO
1	AF	237	HIS
1	AF	246	GLN
1	AG	4	VAL
1	AG	28	THR
1	AG	36	ARG
1	AG	39	ASP
1	AG	40	VAL
1	AG	42	THR
1	AG	45	LEU
1	AG	49	THR
1	AG	62	SER
1	AG	71	LEU
1	AG	113	THR
1	AG	120	GLN
1	AG	150	ARG
1	AG	158	VAL
1	AG	163	MET
1	AG	166	VAL
1	AG	187	LEU
1	AG	196	LEU
1	AG	198	THR
1	AG	203	ASP
1	AG	209	LEU
1	AG	226	PRO
1	AG	237	HIS
1	AG	246	GLN
1	AH	4	VAL
1	AH	28	THR
1	AH	36	ARG
1	AH	39	ASP
1	AH	40	VAL
1	AH	42	THR
1	AH	45	LEU
1	AH	49	THR
1	AH	62	SER
1	AH	71	LEU
1	AH	113	THR
1	AH	120	GLN
1	AH	150	ARG
1	AH	158	VAL
1	AH	163	MET

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Continued from previous page...

Mol	Chain	Res	Type
1	AH	166	VAL
1	AH	187	LEU
1	AH	196	LEU
1	AH	198	THR
1	AH	203	ASP
1	AH	209	LEU
1	AH	226	PRO
1	AH	237	HIS
1	AH	246	GLN
1	AI	4	VAL
1	AI	28	THR
1	AI	36	ARG
1	AI	39	ASP
1	AI	40	VAL
1	AI	42	THR
1	AI	45	LEU
1	AI	49	THR
1	AI	62	SER
1	AI	71	LEU
1	AI	113	THR
1	AI	120	GLN
1	AI	150	ARG
1	AI	158	VAL
1	AI	163	MET
1	AI	166	VAL
1	AI	187	LEU
1	AI	196	LEU
1	AI	198	THR
1	AI	203	ASP
1	AI	209	LEU
1	AI	226	PRO
1	AI	237	HIS
1	AI	246	GLN
1	AJ	4	VAL
1	AJ	28	THR
1	AJ	36	ARG
1	AJ	39	ASP
1	AJ	40	VAL
1	AJ	42	THR
1	AJ	45	LEU
1	AJ	49	THR
1	AJ	62	SER

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Continued from previous page...

Mol	Chain	Res	Type
1	AJ	71	LEU
1	AJ	113	THR
1	AJ	120	GLN
1	AJ	150	ARG
1	AJ	158	VAL
1	AJ	163	MET
1	AJ	166	VAL
1	AJ	187	LEU
1	AJ	196	LEU
1	AJ	198	THR
1	AJ	203	ASP
1	AJ	209	LEU
1	AJ	226	PRO
1	AJ	237	HIS
1	AJ	246	GLN
1	AK	4	VAL
1	AK	28	THR
1	AK	36	ARG
1	AK	39	ASP
1	AK	40	VAL
1	AK	42	THR
1	AK	45	LEU
1	AK	49	THR
1	AK	62	SER
1	AK	71	LEU
1	AK	113	THR
1	AK	120	GLN
1	AK	150	ARG
1	AK	158	VAL
1	AK	163	MET
1	AK	166	VAL
1	AK	187	LEU
1	AK	196	LEU
1	AK	198	THR
1	AK	203	ASP
1	AK	209	LEU
1	AK	226	PRO
1	AK	237	HIS
1	AK	246	GLN
1	AL	4	VAL
1	AL	28	THR
1	AL	36	ARG

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Mol	Chain	Res	Type
1	AL	39	ASP
1	AL	40	VAL
1	AL	42	THR
1	AL	45	LEU
1	AL	49	THR
1	AL	62	SER
1	AL	71	LEU
1	AL	113	THR
1	AL	120	GLN
1	AL	150	ARG
1	AL	158	VAL
1	AL	163	MET
1	AL	166	VAL
1	AL	187	LEU
1	AL	196	LEU
1	AL	198	THR
1	AL	203	ASP
1	AL	209	LEU
1	AL	226	PRO
1	AL	237	HIS
1	AL	246	GLN
1	AM	4	VAL
1	AM	28	THR
1	AM	36	ARG
1	AM	39	ASP
1	AM	40	VAL
1	AM	42	THR
1	AM	45	LEU
1	AM	49	THR
1	AM	62	SER
1	AM	71	LEU
1	AM	113	THR
1	AM	120	GLN
1	AM	150	ARG
1	AM	158	VAL
1	AM	163	MET
1	AM	166	VAL
1	AM	187	LEU
1	AM	196	LEU
1	AM	198	THR
1	AM	203	ASP
1	AM	209	LEU

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Mol	Chain	Res	Type
1	AM	226	PRO
1	AM	237	HIS
1	AM	246	GLN
1	AN	4	VAL
1	AN	28	THR
1	AN	36	ARG
1	AN	39	ASP
1	AN	40	VAL
1	AN	42	THR
1	AN	45	LEU
1	AN	49	THR
1	AN	62	SER
1	AN	71	LEU
1	AN	113	THR
1	AN	120	GLN
1	AN	150	ARG
1	AN	158	VAL
1	AN	163	MET
1	AN	166	VAL
1	AN	187	LEU
1	AN	196	LEU
1	AN	198	THR
1	AN	203	ASP
1	AN	209	LEU
1	AN	226	PRO
1	AN	237	HIS
1	AN	246	GLN
1	AO	4	VAL
1	AO	28	THR
1	AO	36	ARG
1	AO	39	ASP
1	AO	40	VAL
1	AO	42	THR
1	AO	45	LEU
1	AO	49	THR
1	AO	62	SER
1	AO	71	LEU
1	AO	113	THR
1	AO	120	GLN
1	AO	150	ARG
1	AO	158	VAL
1	AO	163	MET

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Mol	Chain	Res	Type
1	AO	166	VAL
1	AO	187	LEU
1	AO	196	LEU
1	AO	198	THR
1	AO	203	ASP
1	AO	209	LEU
1	AO	226	PRO
1	AO	237	HIS
1	AO	246	GLN
1	AP	4	VAL
1	AP	28	THR
1	AP	36	ARG
1	AP	39	ASP
1	AP	40	VAL
1	AP	42	THR
1	AP	45	LEU
1	AP	49	THR
1	AP	62	SER
1	AP	71	LEU
1	AP	113	THR
1	AP	120	GLN
1	AP	150	ARG
1	AP	158	VAL
1	AP	163	MET
1	AP	166	VAL
1	AP	187	LEU
1	AP	196	LEU
1	AP	198	THR
1	AP	203	ASP
1	AP	209	LEU
1	AP	226	PRO
1	AP	237	HIS
1	AP	246	GLN
1	AQ	4	VAL
1	AQ	28	THR
1	AQ	36	ARG
1	AQ	39	ASP
1	AQ	40	VAL
1	AQ	42	THR
1	AQ	45	LEU
1	AQ	49	THR
1	AQ	62	SER

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Mol	Chain	Res	Type
1	AQ	71	LEU
1	AQ	113	THR
1	AQ	120	GLN
1	AQ	150	ARG
1	AQ	158	VAL
1	AQ	163	MET
1	AQ	166	VAL
1	AQ	187	LEU
1	AQ	196	LEU
1	AQ	198	THR
1	AQ	203	ASP
1	AQ	209	LEU
1	AQ	226	PRO
1	AQ	237	HIS
1	AQ	246	GLN
1	AR	4	VAL
1	AR	28	THR
1	AR	36	ARG
1	AR	39	ASP
1	AR	40	VAL
1	AR	42	THR
1	AR	45	LEU
1	AR	49	THR
1	AR	62	SER
1	AR	71	LEU
1	AR	113	THR
1	AR	120	GLN
1	AR	150	ARG
1	AR	158	VAL
1	AR	163	MET
1	AR	166	VAL
1	AR	187	LEU
1	AR	196	LEU
1	AR	198	THR
1	AR	203	ASP
1	AR	209	LEU
1	AR	226	PRO
1	AR	237	HIS
1	AR	246	GLN
1	AS	4	VAL
1	AS	28	THR
1	AS	36	ARG

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Mol	Chain	Res	Type
1	AS	39	ASP
1	AS	40	VAL
1	AS	42	THR
1	AS	45	LEU
1	AS	49	THR
1	AS	62	SER
1	AS	71	LEU
1	AS	113	THR
1	AS	120	GLN
1	AS	150	ARG
1	AS	158	VAL
1	AS	163	MET
1	AS	166	VAL
1	AS	187	LEU
1	AS	196	LEU
1	AS	198	THR
1	AS	203	ASP
1	AS	209	LEU
1	AS	226	PRO
1	AS	237	HIS
1	AS	246	GLN
1	AT	4	VAL
1	AT	28	THR
1	AT	36	ARG
1	AT	39	ASP
1	AT	40	VAL
1	AT	42	THR
1	AT	45	LEU
1	AT	49	THR
1	AT	62	SER
1	AT	71	LEU
1	AT	113	THR
1	AT	120	GLN
1	AT	150	ARG
1	AT	158	VAL
1	AT	163	MET
1	AT	166	VAL
1	AT	187	LEU
1	AT	196	LEU
1	AT	198	THR
1	AT	203	ASP
1	AT	209	LEU

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Mol	Chain	Res	Type
1	AT	226	PRO
1	AT	237	HIS
1	AT	246	GLN
1	AU	4	VAL
1	AU	28	THR
1	AU	36	ARG
1	AU	39	ASP
1	AU	40	VAL
1	AU	42	THR
1	AU	45	LEU
1	AU	49	THR
1	AU	62	SER
1	AU	71	LEU
1	AU	113	THR
1	AU	120	GLN
1	AU	150	ARG
1	AU	158	VAL
1	AU	163	MET
1	AU	166	VAL
1	AU	187	LEU
1	AU	196	LEU
1	AU	198	THR
1	AU	203	ASP
1	AU	209	LEU
1	AU	226	PRO
1	AU	237	HIS
1	AU	246	GLN
1	AV	4	VAL
1	AV	28	THR
1	AV	36	ARG
1	AV	39	ASP
1	AV	40	VAL
1	AV	42	THR
1	AV	45	LEU
1	AV	49	THR
1	AV	62	SER
1	AV	71	LEU
1	AV	113	THR
1	AV	120	GLN
1	AV	150	ARG
1	AV	158	VAL
1	AV	163	MET

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Continued from previous page...

Mol	Chain	Res	Type
1	AV	166	VAL
1	AV	187	LEU
1	AV	196	LEU
1	AV	198	THR
1	AV	203	ASP
1	AV	209	LEU
1	AV	226	PRO
1	AV	237	HIS
1	AV	246	GLN
1	AW	4	VAL
1	AW	28	THR
1	AW	36	ARG
1	AW	39	ASP
1	AW	40	VAL
1	AW	42	THR
1	AW	45	LEU
1	AW	49	THR
1	AW	62	SER
1	AW	71	LEU
1	AW	113	THR
1	AW	120	GLN
1	AW	150	ARG
1	AW	158	VAL
1	AW	163	MET
1	AW	166	VAL
1	AW	187	LEU
1	AW	196	LEU
1	AW	198	THR
1	AW	203	ASP
1	AW	209	LEU
1	AW	223	PRO
1	AW	226	PRO
1	AW	237	HIS
1	AW	246	GLN
1	AX	4	VAL
1	AX	28	THR
1	AX	36	ARG
1	AX	39	ASP
1	AX	40	VAL
1	AX	42	THR
1	AX	45	LEU
1	AX	49	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AX	62	SER
1	AX	71	LEU
1	AX	113	THR
1	AX	120	GLN
1	AX	150	ARG
1	AX	158	VAL
1	AX	163	MET
1	AX	166	VAL
1	AX	187	LEU
1	AX	196	LEU
1	AX	198	THR
1	AX	203	ASP
1	AX	209	LEU
1	AX	226	PRO
1	AX	237	HIS
1	AX	246	GLN
1	AY	4	VAL
1	AY	28	THR
1	AY	36	ARG
1	AY	39	ASP
1	AY	40	VAL
1	AY	42	THR
1	AY	45	LEU
1	AY	49	THR
1	AY	62	SER
1	AY	71	LEU
1	AY	113	THR
1	AY	120	GLN
1	AY	150	ARG
1	AY	158	VAL
1	AY	163	MET
1	AY	166	VAL
1	AY	187	LEU
1	AY	196	LEU
1	AY	198	THR
1	AY	203	ASP
1	AY	209	LEU
1	AY	226	PRO
1	AY	237	HIS
1	AY	246	GLN
1	AZ	4	VAL
1	AZ	28	THR

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Mol	Chain	Res	Type
1	AZ	36	ARG
1	AZ	39	ASP
1	AZ	40	VAL
1	AZ	42	THR
1	AZ	45	LEU
1	AZ	49	THR
1	AZ	62	SER
1	AZ	71	LEU
1	AZ	113	THR
1	AZ	120	GLN
1	AZ	150	ARG
1	AZ	158	VAL
1	AZ	163	MET
1	AZ	166	VAL
1	AZ	187	LEU
1	AZ	196	LEU
1	AZ	198	THR
1	AZ	203	ASP
1	AZ	209	LEU
1	AZ	226	PRO
1	AZ	237	HIS
1	AZ	246	GLN
1	A0	4	VAL
1	A0	28	THR
1	A0	36	ARG
1	A0	39	ASP
1	A0	40	VAL
1	A0	42	THR
1	A0	45	LEU
1	A0	49	THR
1	A0	62	SER
1	A0	71	LEU
1	A0	113	THR
1	A0	120	GLN
1	A0	150	ARG
1	A0	158	VAL
1	A0	163	MET
1	A0	166	VAL
1	A0	187	LEU
1	A0	196	LEU
1	A0	198	THR
1	A0	203	ASP

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Mol	Chain	Res	Type
1	A0	209	LEU
1	A0	226	PRO
1	A0	237	HIS
1	A0	246	GLN
1	A1	4	VAL
1	A1	28	THR
1	A1	36	ARG
1	A1	39	ASP
1	A1	40	VAL
1	A1	42	THR
1	A1	45	LEU
1	A1	49	THR
1	A1	62	SER
1	A1	71	LEU
1	A1	113	THR
1	A1	120	GLN
1	A1	150	ARG
1	A1	158	VAL
1	A1	163	MET
1	A1	166	VAL
1	A1	187	LEU
1	A1	196	LEU
1	A1	198	THR
1	A1	203	ASP
1	A1	209	LEU
1	A1	226	PRO
1	A1	237	HIS
1	A1	246	GLN
1	A2	4	VAL
1	A2	28	THR
1	A2	36	ARG
1	A2	39	ASP
1	A2	40	VAL
1	A2	42	THR
1	A2	45	LEU
1	A2	49	THR
1	A2	62	SER
1	A2	71	LEU
1	A2	113	THR
1	A2	120	GLN
1	A2	150	ARG
1	A2	158	VAL

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Mol	Chain	Res	Type
1	A2	163	MET
1	A2	166	VAL
1	A2	187	LEU
1	A2	196	LEU
1	A2	198	THR
1	A2	203	ASP
1	A2	209	LEU
1	A2	226	PRO
1	A2	237	HIS
1	A2	246	GLN
1	A3	4	VAL
1	A3	28	THR
1	A3	36	ARG
1	A3	39	ASP
1	A3	40	VAL
1	A3	42	THR
1	A3	45	LEU
1	A3	49	THR
1	A3	62	SER
1	A3	71	LEU
1	A3	113	THR
1	A3	120	GLN
1	A3	150	ARG
1	A3	158	VAL
1	A3	163	MET
1	A3	166	VAL
1	A3	187	LEU
1	A3	196	LEU
1	A3	198	THR
1	A3	203	ASP
1	A3	209	LEU
1	A3	226	PRO
1	A3	237	HIS
1	A3	246	GLN
1	A4	4	VAL
1	A4	28	THR
1	A4	36	ARG
1	A4	39	ASP
1	A4	40	VAL
1	A4	42	THR
1	A4	45	LEU
1	A4	49	THR

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Mol	Chain	Res	Type
1	A4	62	SER
1	A4	71	LEU
1	A4	113	THR
1	A4	120	GLN
1	A4	150	ARG
1	A4	158	VAL
1	A4	163	MET
1	A4	166	VAL
1	A4	187	LEU
1	A4	196	LEU
1	A4	198	THR
1	A4	203	ASP
1	A4	209	LEU
1	A4	226	PRO
1	A4	237	HIS
1	A4	246	GLN
1	A5	4	VAL
1	A5	28	THR
1	A5	36	ARG
1	A5	39	ASP
1	A5	40	VAL
1	A5	42	THR
1	A5	45	LEU
1	A5	49	THR
1	A5	62	SER
1	A5	71	LEU
1	A5	113	THR
1	A5	120	GLN
1	A5	150	ARG
1	A5	158	VAL
1	A5	163	MET
1	A5	166	VAL
1	A5	187	LEU
1	A5	196	LEU
1	A5	198	THR
1	A5	203	ASP
1	A5	209	LEU
1	A5	226	PRO
1	A5	237	HIS
1	A5	246	GLN
1	A6	4	VAL
1	A6	28	THR

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Mol	Chain	Res	Type
1	A6	36	ARG
1	A6	39	ASP
1	A6	40	VAL
1	A6	42	THR
1	A6	45	LEU
1	A6	49	THR
1	A6	62	SER
1	A6	71	LEU
1	A6	113	THR
1	A6	120	GLN
1	A6	150	ARG
1	A6	158	VAL
1	A6	163	MET
1	A6	166	VAL
1	A6	187	LEU
1	A6	196	LEU
1	A6	198	THR
1	A6	203	ASP
1	A6	209	LEU
1	A6	226	PRO
1	A6	237	HIS
1	A6	246	GLN
1	A7	4	VAL
1	A7	28	THR
1	A7	36	ARG
1	A7	39	ASP
1	A7	40	VAL
1	A7	42	THR
1	A7	45	LEU
1	A7	49	THR
1	A7	62	SER
1	A7	71	LEU
1	A7	113	THR
1	A7	120	GLN
1	A7	150	ARG
1	A7	158	VAL
1	A7	163	MET
1	A7	166	VAL
1	A7	187	LEU
1	A7	196	LEU
1	A7	198	THR
1	A7	203	ASP

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Mol	Chain	Res	Type
1	A7	209	LEU
1	A7	226	PRO
1	A7	237	HIS
1	A7	246	GLN
1	A8	4	VAL
1	A8	28	THR
1	A8	36	ARG
1	A8	39	ASP
1	A8	40	VAL
1	A8	42	THR
1	A8	45	LEU
1	A8	49	THR
1	A8	62	SER
1	A8	71	LEU
1	A8	113	THR
1	A8	120	GLN
1	A8	150	ARG
1	A8	158	VAL
1	A8	163	MET
1	A8	166	VAL
1	A8	187	LEU
1	A8	196	LEU
1	A8	198	THR
1	A8	203	ASP
1	A8	209	LEU
1	A8	226	PRO
1	A8	237	HIS
1	A8	246	GLN
1	A9	4	VAL
1	A9	28	THR
1	A9	36	ARG
1	A9	39	ASP
1	A9	40	VAL
1	A9	42	THR
1	A9	45	LEU
1	A9	49	THR
1	A9	62	SER
1	A9	71	LEU
1	A9	113	THR
1	A9	120	GLN
1	A9	150	ARG
1	A9	158	VAL

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Mol	Chain	Res	Type
1	A9	163	MET
1	A9	166	VAL
1	A9	187	LEU
1	A9	196	LEU
1	A9	198	THR
1	A9	203	ASP
1	A9	209	LEU
1	A9	226	PRO
1	A9	237	HIS
1	A9	246	GLN
1	Aa	4	VAL
1	Aa	28	THR
1	Aa	36	ARG
1	Aa	39	ASP
1	Aa	40	VAL
1	Aa	42	THR
1	Aa	45	LEU
1	Aa	49	THR
1	Aa	62	SER
1	Aa	71	LEU
1	Aa	113	THR
1	Aa	120	GLN
1	Aa	150	ARG
1	Aa	158	VAL
1	Aa	163	MET
1	Aa	166	VAL
1	Aa	187	LEU
1	Aa	196	LEU
1	Aa	198	THR
1	Aa	203	ASP
1	Aa	209	LEU
1	Aa	226	PRO
1	Aa	237	HIS
1	Aa	246	GLN
1	Ab	4	VAL
1	Ab	28	THR
1	Ab	36	ARG
1	Ab	39	ASP
1	Ab	40	VAL
1	Ab	42	THR
1	Ab	45	LEU
1	Ab	49	THR

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Mol	Chain	Res	Type
1	Ab	62	SER
1	Ab	71	LEU
1	Ab	113	THR
1	Ab	120	GLN
1	Ab	150	ARG
1	Ab	158	VAL
1	Ab	163	MET
1	Ab	166	VAL
1	Ab	187	LEU
1	Ab	196	LEU
1	Ab	198	THR
1	Ab	203	ASP
1	Ab	209	LEU
1	Ab	226	PRO
1	Ab	237	HIS
1	Ab	246	GLN
1	Ac	4	VAL
1	Ac	28	THR
1	Ac	36	ARG
1	Ac	39	ASP
1	Ac	40	VAL
1	Ac	42	THR
1	Ac	45	LEU
1	Ac	49	THR
1	Ac	62	SER
1	Ac	71	LEU
1	Ac	113	THR
1	Ac	120	GLN
1	Ac	150	ARG
1	Ac	158	VAL
1	Ac	163	MET
1	Ac	166	VAL
1	Ac	187	LEU
1	Ac	196	LEU
1	Ac	198	THR
1	Ac	203	ASP
1	Ac	209	LEU
1	Ac	226	PRO
1	Ac	237	HIS
1	Ac	246	GLN
1	Ad	4	VAL
1	Ad	28	THR

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Mol	Chain	Res	Type
1	Ad	36	ARG
1	Ad	39	ASP
1	Ad	40	VAL
1	Ad	42	THR
1	Ad	45	LEU
1	Ad	49	THR
1	Ad	62	SER
1	Ad	71	LEU
1	Ad	113	THR
1	Ad	120	GLN
1	Ad	150	ARG
1	Ad	158	VAL
1	Ad	163	MET
1	Ad	166	VAL
1	Ad	187	LEU
1	Ad	196	LEU
1	Ad	198	THR
1	Ad	203	ASP
1	Ad	209	LEU
1	Ad	226	PRO
1	Ad	237	HIS
1	Ad	246	GLN
1	Ae	4	VAL
1	Ae	28	THR
1	Ae	36	ARG
1	Ae	39	ASP
1	Ae	40	VAL
1	Ae	42	THR
1	Ae	45	LEU
1	Ae	49	THR
1	Ae	62	SER
1	Ae	71	LEU
1	Ae	113	THR
1	Ae	120	GLN
1	Ae	150	ARG
1	Ae	158	VAL
1	Ae	163	MET
1	Ae	166	VAL
1	Ae	187	LEU
1	Ae	196	LEU
1	Ae	198	THR
1	Ae	203	ASP

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Mol	Chain	Res	Type
1	Ae	209	LEU
1	Ae	223	PRO
1	Ae	226	PRO
1	Ae	237	HIS
1	Ae	246	GLN
1	Af	4	VAL
1	Af	28	THR
1	Af	36	ARG
1	Af	39	ASP
1	Af	40	VAL
1	Af	42	THR
1	Af	45	LEU
1	Af	49	THR
1	Af	62	SER
1	Af	71	LEU
1	Af	113	THR
1	Af	120	GLN
1	Af	150	ARG
1	Af	158	VAL
1	Af	163	MET
1	Af	166	VAL
1	Af	187	LEU
1	Af	196	LEU
1	Af	198	THR
1	Af	203	ASP
1	Af	209	LEU
1	Af	226	PRO
1	Af	237	HIS
1	Af	246	GLN
1	Ag	4	VAL
1	Ag	28	THR
1	Ag	36	ARG
1	Ag	39	ASP
1	Ag	40	VAL
1	Ag	42	THR
1	Ag	45	LEU
1	Ag	49	THR
1	Ag	62	SER
1	Ag	71	LEU
1	Ag	113	THR
1	Ag	120	GLN
1	Ag	150	ARG

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Mol	Chain	Res	Type
1	Ag	158	VAL
1	Ag	163	MET
1	Ag	166	VAL
1	Ag	187	LEU
1	Ag	196	LEU
1	Ag	198	THR
1	Ag	203	ASP
1	Ag	209	LEU
1	Ag	226	PRO
1	Ag	237	HIS
1	Ag	246	GLN
1	Ah	4	VAL
1	Ah	28	THR
1	Ah	36	ARG
1	Ah	39	ASP
1	Ah	40	VAL
1	Ah	42	THR
1	Ah	45	LEU
1	Ah	49	THR
1	Ah	62	SER
1	Ah	71	LEU
1	Ah	113	THR
1	Ah	120	GLN
1	Ah	150	ARG
1	Ah	158	VAL
1	Ah	163	MET
1	Ah	166	VAL
1	Ah	187	LEU
1	Ah	196	LEU
1	Ah	198	THR
1	Ah	203	ASP
1	Ah	209	LEU
1	Ah	226	PRO
1	Ah	237	HIS
1	Ah	246	GLN
1	Ai	4	VAL
1	Ai	28	THR
1	Ai	36	ARG
1	Ai	39	ASP
1	Ai	40	VAL
1	Ai	42	THR
1	Ai	45	LEU

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Mol	Chain	Res	Type
1	Ai	49	THR
1	Ai	62	SER
1	Ai	71	LEU
1	Ai	113	THR
1	Ai	120	GLN
1	Ai	150	ARG
1	Ai	158	VAL
1	Ai	163	MET
1	Ai	166	VAL
1	Ai	187	LEU
1	Ai	196	LEU
1	Ai	198	THR
1	Ai	203	ASP
1	Ai	209	LEU
1	Ai	226	PRO
1	Ai	237	HIS
1	Ai	246	GLN
1	Aj	4	VAL
1	Aj	28	THR
1	Aj	36	ARG
1	Aj	39	ASP
1	Aj	40	VAL
1	Aj	42	THR
1	Aj	45	LEU
1	Aj	49	THR
1	Aj	62	SER
1	Aj	71	LEU
1	Aj	113	THR
1	Aj	120	GLN
1	Aj	150	ARG
1	Aj	158	VAL
1	Aj	163	MET
1	Aj	166	VAL
1	Aj	187	LEU
1	Aj	196	LEU
1	Aj	198	THR
1	Aj	203	ASP
1	Aj	209	LEU
1	Aj	226	PRO
1	Aj	237	HIS
1	Aj	246	GLN
1	Ak	4	VAL

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Mol	Chain	Res	Type
1	Ak	28	THR
1	Ak	36	ARG
1	Ak	39	ASP
1	Ak	40	VAL
1	Ak	42	THR
1	Ak	45	LEU
1	Ak	49	THR
1	Ak	62	SER
1	Ak	71	LEU
1	Ak	113	THR
1	Ak	120	GLN
1	Ak	150	ARG
1	Ak	158	VAL
1	Ak	163	MET
1	Ak	166	VAL
1	Ak	187	LEU
1	Ak	196	LEU
1	Ak	198	THR
1	Ak	203	ASP
1	Ak	209	LEU
1	Ak	226	PRO
1	Ak	237	HIS
1	Ak	246	GLN
1	Al	4	VAL
1	Al	28	THR
1	Al	36	ARG
1	Al	39	ASP
1	Al	40	VAL
1	Al	42	THR
1	Al	45	LEU
1	Al	49	THR
1	Al	62	SER
1	Al	71	LEU
1	Al	113	THR
1	Al	120	GLN
1	Al	150	ARG
1	Al	158	VAL
1	Al	163	MET
1	Al	166	VAL
1	Al	187	LEU
1	Al	196	LEU
1	Al	198	THR

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Mol	Chain	Res	Type
1	Al	203	ASP
1	Al	209	LEU
1	Al	226	PRO
1	Al	237	HIS
1	Al	246	GLN
1	Am	4	VAL
1	Am	28	THR
1	Am	36	ARG
1	Am	39	ASP
1	Am	40	VAL
1	Am	42	THR
1	Am	45	LEU
1	Am	49	THR
1	Am	62	SER
1	Am	71	LEU
1	Am	113	THR
1	Am	120	GLN
1	Am	150	ARG
1	Am	158	VAL
1	Am	163	MET
1	Am	166	VAL
1	Am	187	LEU
1	Am	196	LEU
1	Am	198	THR
1	Am	203	ASP
1	Am	209	LEU
1	Am	226	PRO
1	Am	237	HIS
1	Am	246	GLN
1	An	4	VAL
1	An	28	THR
1	An	36	ARG
1	An	39	ASP
1	An	40	VAL
1	An	42	THR
1	An	45	LEU
1	An	49	THR
1	An	62	SER
1	An	71	LEU
1	An	113	THR
1	An	120	GLN
1	An	150	ARG

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Mol	Chain	Res	Type
1	An	158	VAL
1	An	163	MET
1	An	166	VAL
1	An	187	LEU
1	An	196	LEU
1	An	198	THR
1	An	203	ASP
1	An	209	LEU
1	An	226	PRO
1	An	237	HIS
1	An	246	GLN
1	Ao	4	VAL
1	Ao	28	THR
1	Ao	36	ARG
1	Ao	39	ASP
1	Ao	40	VAL
1	Ao	42	THR
1	Ao	45	LEU
1	Ao	49	THR
1	Ao	62	SER
1	Ao	71	LEU
1	Ao	113	THR
1	Ao	120	GLN
1	Ao	150	ARG
1	Ao	158	VAL
1	Ao	163	MET
1	Ao	166	VAL
1	Ao	187	LEU
1	Ao	196	LEU
1	Ao	198	THR
1	Ao	203	ASP
1	Ao	209	LEU
1	Ao	226	PRO
1	Ao	237	HIS
1	Ao	246	GLN
2	BA	45	SER
2	BA	49	ASP
2	BA	53	ARG
2	BA	58	LEU
2	BA	70	PRO
2	BA	73	GLN
2	BA	86	ASP

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Mol	Chain	Res	Type
2	BA	88	LEU
2	BA	93	SER
2	BA	110	VAL
2	BA	114	VAL
2	BA	126	VAL
2	BA	135	THR
2	BA	136	HIS
2	BA	145	LEU
2	BA	146	GLU
2	BA	156	SER
2	BA	157	VAL
2	BA	161	GLN
2	BA	166	ARG
2	BA	167	THR
2	BA	168	ASN
2	BA	193	THR
2	BA	194	ILE
2	BA	197	LEU
2	BA	212	THR
2	BB	45	SER
2	BB	49	ASP
2	BB	53	ARG
2	BB	58	LEU
2	BB	70	PRO
2	BB	73	GLN
2	BB	86	ASP
2	BB	88	LEU
2	BB	93	SER
2	BB	110	VAL
2	BB	114	VAL
2	BB	126	VAL
2	BB	135	THR
2	BB	136	HIS
2	BB	145	LEU
2	BB	146	GLU
2	BB	156	SER
2	BB	157	VAL
2	BB	161	GLN
2	BB	166	ARG
2	BB	167	THR
2	BB	168	ASN
2	BB	193	THR

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Mol	Chain	Res	Type
2	BB	194	ILE
2	BB	197	LEU
2	BB	212	THR
2	BC	45	SER
2	BC	49	ASP
2	BC	53	ARG
2	BC	58	LEU
2	BC	70	PRO
2	BC	73	GLN
2	BC	86	ASP
2	BC	88	LEU
2	BC	93	SER
2	BC	110	VAL
2	BC	114	VAL
2	BC	126	VAL
2	BC	135	THR
2	BC	136	HIS
2	BC	145	LEU
2	BC	146	GLU
2	BC	156	SER
2	BC	157	VAL
2	BC	161	GLN
2	BC	166	ARG
2	BC	167	THR
2	BC	168	ASN
2	BC	193	THR
2	BC	194	ILE
2	BC	197	LEU
2	BC	212	THR
2	BD	45	SER
2	BD	49	ASP
2	BD	53	ARG
2	BD	58	LEU
2	BD	70	PRO
2	BD	73	GLN
2	BD	86	ASP
2	BD	88	LEU
2	BD	93	SER
2	BD	110	VAL
2	BD	114	VAL
2	BD	126	VAL
2	BD	135	THR

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Mol	Chain	Res	Type
2	BD	136	HIS
2	BD	145	LEU
2	BD	146	GLU
2	BD	156	SER
2	BD	157	VAL
2	BD	161	GLN
2	BD	166	ARG
2	BD	167	THR
2	BD	168	ASN
2	BD	193	THR
2	BD	194	ILE
2	BD	197	LEU
2	BD	212	THR
2	BE	45	SER
2	BE	49	ASP
2	BE	53	ARG
2	BE	58	LEU
2	BE	70	PRO
2	BE	73	GLN
2	BE	86	ASP
2	BE	88	LEU
2	BE	93	SER
2	BE	110	VAL
2	BE	114	VAL
2	BE	126	VAL
2	BE	135	THR
2	BE	136	HIS
2	BE	145	LEU
2	BE	146	GLU
2	BE	156	SER
2	BE	157	VAL
2	BE	161	GLN
2	BE	166	ARG
2	BE	167	THR
2	BE	168	ASN
2	BE	193	THR
2	BE	194	ILE
2	BE	197	LEU
2	BE	212	THR
2	BF	45	SER
2	BF	49	ASP
2	BF	53	ARG

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Mol	Chain	Res	Type
2	BF	58	LEU
2	BF	70	PRO
2	BF	73	GLN
2	BF	86	ASP
2	BF	88	LEU
2	BF	93	SER
2	BF	110	VAL
2	BF	114	VAL
2	BF	126	VAL
2	BF	135	THR
2	BF	136	HIS
2	BF	145	LEU
2	BF	146	GLU
2	BF	156	SER
2	BF	157	VAL
2	BF	161	GLN
2	BF	166	ARG
2	BF	167	THR
2	BF	168	ASN
2	BF	193	THR
2	BF	194	ILE
2	BF	197	LEU
2	BF	212	THR
2	BG	45	SER
2	BG	49	ASP
2	BG	53	ARG
2	BG	58	LEU
2	BG	70	PRO
2	BG	73	GLN
2	BG	86	ASP
2	BG	88	LEU
2	BG	93	SER
2	BG	110	VAL
2	BG	114	VAL
2	BG	126	VAL
2	BG	135	THR
2	BG	136	HIS
2	BG	145	LEU
2	BG	146	GLU
2	BG	156	SER
2	BG	157	VAL
2	BG	161	GLN

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Mol	Chain	Res	Type
2	BG	166	ARG
2	BG	167	THR
2	BG	168	ASN
2	BG	193	THR
2	BG	194	ILE
2	BG	197	LEU
2	BG	212	THR
2	BH	45	SER
2	BH	49	ASP
2	BH	53	ARG
2	BH	58	LEU
2	BH	70	PRO
2	BH	73	GLN
2	BH	86	ASP
2	BH	88	LEU
2	BH	93	SER
2	BH	110	VAL
2	BH	114	VAL
2	BH	126	VAL
2	BH	135	THR
2	BH	136	HIS
2	BH	145	LEU
2	BH	146	GLU
2	BH	156	SER
2	BH	157	VAL
2	BH	161	GLN
2	BH	166	ARG
2	BH	167	THR
2	BH	168	ASN
2	BH	193	THR
2	BH	194	ILE
2	BH	197	LEU
2	BH	212	THR
2	BI	45	SER
2	BI	49	ASP
2	BI	53	ARG
2	BI	58	LEU
2	BI	70	PRO
2	BI	73	GLN
2	BI	86	ASP
2	BI	88	LEU
2	BI	93	SER

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Mol	Chain	Res	Type
2	BI	110	VAL
2	BI	114	VAL
2	BI	126	VAL
2	BI	135	THR
2	BI	136	HIS
2	BI	145	LEU
2	BI	146	GLU
2	BI	156	SER
2	BI	157	VAL
2	BI	161	GLN
2	BI	166	ARG
2	BI	167	THR
2	BI	168	ASN
2	BI	193	THR
2	BI	194	ILE
2	BI	197	LEU
2	BI	212	THR
2	BJ	45	SER
2	BJ	49	ASP
2	BJ	53	ARG
2	BJ	58	LEU
2	BJ	70	PRO
2	BJ	73	GLN
2	BJ	86	ASP
2	BJ	88	LEU
2	BJ	93	SER
2	BJ	110	VAL
2	BJ	114	VAL
2	BJ	126	VAL
2	BJ	135	THR
2	BJ	136	HIS
2	BJ	145	LEU
2	BJ	146	GLU
2	BJ	156	SER
2	BJ	157	VAL
2	BJ	161	GLN
2	BJ	166	ARG
2	BJ	167	THR
2	BJ	168	ASN
2	BJ	193	THR
2	BJ	194	ILE
2	BJ	197	LEU

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Mol	Chain	Res	Type
2	BJ	212	THR
2	BK	45	SER
2	BK	49	ASP
2	BK	53	ARG
2	BK	58	LEU
2	BK	70	PRO
2	BK	73	GLN
2	BK	86	ASP
2	BK	88	LEU
2	BK	93	SER
2	BK	110	VAL
2	BK	114	VAL
2	BK	126	VAL
2	BK	135	THR
2	BK	136	HIS
2	BK	145	LEU
2	BK	146	GLU
2	BK	156	SER
2	BK	157	VAL
2	BK	161	GLN
2	BK	166	ARG
2	BK	167	THR
2	BK	168	ASN
2	BK	193	THR
2	BK	194	ILE
2	BK	197	LEU
2	BK	212	THR
2	BL	45	SER
2	BL	49	ASP
2	BL	53	ARG
2	BL	58	LEU
2	BL	70	PRO
2	BL	73	GLN
2	BL	86	ASP
2	BL	88	LEU
2	BL	93	SER
2	BL	110	VAL
2	BL	114	VAL
2	BL	126	VAL
2	BL	135	THR
2	BL	136	HIS
2	BL	145	LEU

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Mol	Chain	Res	Type
2	BL	146	GLU
2	BL	156	SER
2	BL	157	VAL
2	BL	161	GLN
2	BL	166	ARG
2	BL	167	THR
2	BL	168	ASN
2	BL	193	THR
2	BL	194	ILE
2	BL	197	LEU
2	BL	212	THR
2	BM	45	SER
2	BM	49	ASP
2	BM	53	ARG
2	BM	58	LEU
2	BM	70	PRO
2	BM	73	GLN
2	BM	86	ASP
2	BM	88	LEU
2	BM	93	SER
2	BM	110	VAL
2	BM	114	VAL
2	BM	126	VAL
2	BM	135	THR
2	BM	136	HIS
2	BM	145	LEU
2	BM	146	GLU
2	BM	156	SER
2	BM	157	VAL
2	BM	161	GLN
2	BM	166	ARG
2	BM	167	THR
2	BM	168	ASN
2	BM	193	THR
2	BM	194	ILE
2	BM	197	LEU
2	BM	212	THR
2	BN	45	SER
2	BN	49	ASP
2	BN	53	ARG
2	BN	58	LEU
2	BN	70	PRO

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Mol	Chain	Res	Type
2	BN	73	GLN
2	BN	86	ASP
2	BN	88	LEU
2	BN	93	SER
2	BN	110	VAL
2	BN	114	VAL
2	BN	126	VAL
2	BN	135	THR
2	BN	136	HIS
2	BN	145	LEU
2	BN	146	GLU
2	BN	156	SER
2	BN	157	VAL
2	BN	161	GLN
2	BN	166	ARG
2	BN	167	THR
2	BN	168	ASN
2	BN	193	THR
2	BN	194	ILE
2	BN	197	LEU
2	BN	212	THR
2	BR	45	SER
2	BR	49	ASP
2	BR	53	ARG
2	BR	58	LEU
2	BR	70	PRO
2	BR	73	GLN
2	BR	86	ASP
2	BR	88	LEU
2	BR	93	SER
2	BR	110	VAL
2	BR	114	VAL
2	BR	126	VAL
2	BR	135	THR
2	BR	136	HIS
2	BR	145	LEU
2	BR	146	GLU
2	BR	156	SER
2	BR	157	VAL
2	BR	161	GLN
2	BR	166	ARG
2	BR	167	THR

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Mol	Chain	Res	Type
2	BR	168	ASN
2	BR	193	THR
2	BR	194	ILE
2	BR	197	LEU
2	BR	212	THR
2	BO	45	SER
2	BO	49	ASP
2	BO	53	ARG
2	BO	58	LEU
2	BO	70	PRO
2	BO	73	GLN
2	BO	86	ASP
2	BO	88	LEU
2	BO	93	SER
2	BO	110	VAL
2	BO	114	VAL
2	BO	126	VAL
2	BO	135	THR
2	BO	136	HIS
2	BO	145	LEU
2	BO	146	GLU
2	BO	156	SER
2	BO	157	VAL
2	BO	161	GLN
2	BO	166	ARG
2	BO	167	THR
2	BO	168	ASN
2	BO	193	THR
2	BO	194	ILE
2	BO	197	LEU
2	BO	212	THR
2	BS	45	SER
2	BS	49	ASP
2	BS	53	ARG
2	BS	58	LEU
2	BS	70	PRO
2	BS	73	GLN
2	BS	86	ASP
2	BS	88	LEU
2	BS	93	SER
2	BS	110	VAL
2	BS	114	VAL

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Mol	Chain	Res	Type
2	BS	126	VAL
2	BS	135	THR
2	BS	136	HIS
2	BS	145	LEU
2	BS	146	GLU
2	BS	156	SER
2	BS	157	VAL
2	BS	161	GLN
2	BS	166	ARG
2	BS	167	THR
2	BS	168	ASN
2	BS	193	THR
2	BS	194	ILE
2	BS	197	LEU
2	BS	212	THR
2	BP	45	SER
2	BP	49	ASP
2	BP	53	ARG
2	BP	58	LEU
2	BP	70	PRO
2	BP	73	GLN
2	BP	86	ASP
2	BP	88	LEU
2	BP	93	SER
2	BP	110	VAL
2	BP	114	VAL
2	BP	126	VAL
2	BP	135	THR
2	BP	136	HIS
2	BP	145	LEU
2	BP	146	GLU
2	BP	156	SER
2	BP	157	VAL
2	BP	161	GLN
2	BP	166	ARG
2	BP	167	THR
2	BP	168	ASN
2	BP	193	THR
2	BP	194	ILE
2	BP	197	LEU
2	BP	212	THR
2	BQ	45	SER

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Mol	Chain	Res	Type
2	BQ	49	ASP
2	BQ	53	ARG
2	BQ	58	LEU
2	BQ	70	PRO
2	BQ	73	GLN
2	BQ	86	ASP
2	BQ	88	LEU
2	BQ	93	SER
2	BQ	110	VAL
2	BQ	114	VAL
2	BQ	126	VAL
2	BQ	135	THR
2	BQ	136	HIS
2	BQ	145	LEU
2	BQ	146	GLU
2	BQ	156	SER
2	BQ	157	VAL
2	BQ	161	GLN
2	BQ	166	ARG
2	BQ	167	THR
2	BQ	168	ASN
2	BQ	193	THR
2	BQ	194	ILE
2	BQ	197	LEU
2	BQ	212	THR
2	BT	45	SER
2	BT	49	ASP
2	BT	53	ARG
2	BT	58	LEU
2	BT	70	PRO
2	BT	73	GLN
2	BT	86	ASP
2	BT	88	LEU
2	BT	93	SER
2	BT	110	VAL
2	BT	114	VAL
2	BT	126	VAL
2	BT	135	THR
2	BT	136	HIS
2	BT	145	LEU
2	BT	146	GLU
2	BT	156	SER

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Mol	Chain	Res	Type
2	BT	157	VAL
2	BT	161	GLN
2	BT	166	ARG
2	BT	167	THR
2	BT	168	ASN
2	BT	193	THR
2	BT	194	ILE
2	BT	197	LEU
2	BT	212	THR
2	BU	45	SER
2	BU	49	ASP
2	BU	53	ARG
2	BU	58	LEU
2	BU	70	PRO
2	BU	73	GLN
2	BU	86	ASP
2	BU	88	LEU
2	BU	93	SER
2	BU	110	VAL
2	BU	114	VAL
2	BU	126	VAL
2	BU	135	THR
2	BU	136	HIS
2	BU	145	LEU
2	BU	146	GLU
2	BU	156	SER
2	BU	157	VAL
2	BU	161	GLN
2	BU	166	ARG
2	BU	167	THR
2	BU	168	ASN
2	BU	193	THR
2	BU	194	ILE
2	BU	197	LEU
2	BU	212	THR
2	BV	45	SER
2	BV	49	ASP
2	BV	53	ARG
2	BV	58	LEU
2	BV	70	PRO
2	BV	73	GLN
2	BV	86	ASP

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Mol	Chain	Res	Type
2	BV	88	LEU
2	BV	93	SER
2	BV	110	VAL
2	BV	114	VAL
2	BV	126	VAL
2	BV	135	THR
2	BV	136	HIS
2	BV	145	LEU
2	BV	146	GLU
2	BV	156	SER
2	BV	157	VAL
2	BV	161	GLN
2	BV	166	ARG
2	BV	167	THR
2	BV	168	ASN
2	BV	193	THR
2	BV	194	ILE
2	BV	197	LEU
2	BV	212	THR
2	BW	45	SER
2	BW	49	ASP
2	BW	53	ARG
2	BW	58	LEU
2	BW	70	PRO
2	BW	73	GLN
2	BW	86	ASP
2	BW	88	LEU
2	BW	93	SER
2	BW	110	VAL
2	BW	114	VAL
2	BW	126	VAL
2	BW	135	THR
2	BW	136	HIS
2	BW	145	LEU
2	BW	146	GLU
2	BW	156	SER
2	BW	157	VAL
2	BW	161	GLN
2	BW	166	ARG
2	BW	167	THR
2	BW	168	ASN
2	BW	193	THR

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Mol	Chain	Res	Type
2	BW	194	ILE
2	BW	197	LEU
2	BW	212	THR
2	BX	45	SER
2	BX	49	ASP
2	BX	53	ARG
2	BX	58	LEU
2	BX	70	PRO
2	BX	73	GLN
2	BX	86	ASP
2	BX	88	LEU
2	BX	93	SER
2	BX	110	VAL
2	BX	114	VAL
2	BX	126	VAL
2	BX	135	THR
2	BX	136	HIS
2	BX	145	LEU
2	BX	146	GLU
2	BX	156	SER
2	BX	157	VAL
2	BX	161	GLN
2	BX	166	ARG
2	BX	167	THR
2	BX	168	ASN
2	BX	193	THR
2	BX	194	ILE
2	BX	197	LEU
2	BX	212	THR
2	BY	45	SER
2	BY	49	ASP
2	BY	53	ARG
2	BY	58	LEU
2	BY	70	PRO
2	BY	73	GLN
2	BY	86	ASP
2	BY	88	LEU
2	BY	93	SER
2	BY	110	VAL
2	BY	114	VAL
2	BY	126	VAL
2	BY	135	THR

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Mol	Chain	Res	Type
2	BY	136	HIS
2	BY	145	LEU
2	BY	146	GLU
2	BY	156	SER
2	BY	157	VAL
2	BY	161	GLN
2	BY	166	ARG
2	BY	167	THR
2	BY	168	ASN
2	BY	193	THR
2	BY	194	ILE
2	BY	197	LEU
2	BY	212	THR
2	BZ	45	SER
2	BZ	49	ASP
2	BZ	53	ARG
2	BZ	58	LEU
2	BZ	70	PRO
2	BZ	73	GLN
2	BZ	86	ASP
2	BZ	88	LEU
2	BZ	93	SER
2	BZ	110	VAL
2	BZ	114	VAL
2	BZ	126	VAL
2	BZ	135	THR
2	BZ	136	HIS
2	BZ	145	LEU
2	BZ	146	GLU
2	BZ	156	SER
2	BZ	157	VAL
2	BZ	161	GLN
2	BZ	166	ARG
2	BZ	167	THR
2	BZ	168	ASN
2	BZ	193	THR
2	BZ	194	ILE
2	BZ	197	LEU
2	BZ	212	THR
2	B0	45	SER
2	B0	49	ASP
2	B0	53	ARG

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Mol	Chain	Res	Type
2	B0	58	LEU
2	B0	70	PRO
2	B0	73	GLN
2	B0	86	ASP
2	B0	88	LEU
2	B0	93	SER
2	B0	110	VAL
2	B0	114	VAL
2	B0	126	VAL
2	B0	135	THR
2	B0	136	HIS
2	B0	145	LEU
2	B0	146	GLU
2	B0	156	SER
2	B0	157	VAL
2	B0	161	GLN
2	B0	166	ARG
2	B0	167	THR
2	B0	168	ASN
2	B0	193	THR
2	B0	194	ILE
2	B0	197	LEU
2	B0	212	THR
2	B1	45	SER
2	B1	49	ASP
2	B1	53	ARG
2	B1	58	LEU
2	B1	70	PRO
2	B1	73	GLN
2	B1	86	ASP
2	B1	88	LEU
2	B1	93	SER
2	B1	110	VAL
2	B1	114	VAL
2	B1	126	VAL
2	B1	135	THR
2	B1	136	HIS
2	B1	145	LEU
2	B1	146	GLU
2	B1	156	SER
2	B1	157	VAL
2	B1	161	GLN

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Mol	Chain	Res	Type
2	B1	166	ARG
2	B1	167	THR
2	B1	168	ASN
2	B1	193	THR
2	B1	194	ILE
2	B1	197	LEU
2	B1	212	THR
2	B2	45	SER
2	B2	49	ASP
2	B2	53	ARG
2	B2	58	LEU
2	B2	70	PRO
2	B2	73	GLN
2	B2	86	ASP
2	B2	88	LEU
2	B2	93	SER
2	B2	110	VAL
2	B2	114	VAL
2	B2	126	VAL
2	B2	135	THR
2	B2	136	HIS
2	B2	145	LEU
2	B2	146	GLU
2	B2	156	SER
2	B2	157	VAL
2	B2	161	GLN
2	B2	166	ARG
2	B2	167	THR
2	B2	168	ASN
2	B2	193	THR
2	B2	194	ILE
2	B2	197	LEU
2	B2	212	THR
2	B3	45	SER
2	B3	49	ASP
2	B3	53	ARG
2	B3	58	LEU
2	B3	70	PRO
2	B3	73	GLN
2	B3	86	ASP
2	B3	88	LEU
2	B3	93	SER

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Mol	Chain	Res	Type
2	B3	110	VAL
2	B3	114	VAL
2	B3	126	VAL
2	B3	135	THR
2	B3	136	HIS
2	B3	145	LEU
2	B3	146	GLU
2	B3	156	SER
2	B3	157	VAL
2	B3	161	GLN
2	B3	166	ARG
2	B3	167	THR
2	B3	168	ASN
2	B3	193	THR
2	B3	194	ILE
2	B3	197	LEU
2	B3	212	THR
2	B4	45	SER
2	B4	49	ASP
2	B4	53	ARG
2	B4	58	LEU
2	B4	70	PRO
2	B4	73	GLN
2	B4	86	ASP
2	B4	88	LEU
2	B4	93	SER
2	B4	110	VAL
2	B4	114	VAL
2	B4	126	VAL
2	B4	135	THR
2	B4	136	HIS
2	B4	145	LEU
2	B4	146	GLU
2	B4	156	SER
2	B4	157	VAL
2	B4	161	GLN
2	B4	166	ARG
2	B4	167	THR
2	B4	168	ASN
2	B4	193	THR
2	B4	194	ILE
2	B4	197	LEU

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Mol	Chain	Res	Type
2	B4	212	THR
2	B5	45	SER
2	B5	49	ASP
2	B5	53	ARG
2	B5	58	LEU
2	B5	70	PRO
2	B5	73	GLN
2	B5	86	ASP
2	B5	88	LEU
2	B5	93	SER
2	B5	110	VAL
2	B5	114	VAL
2	B5	126	VAL
2	B5	135	THR
2	B5	136	HIS
2	B5	145	LEU
2	B5	146	GLU
2	B5	156	SER
2	B5	157	VAL
2	B5	161	GLN
2	B5	166	ARG
2	B5	167	THR
2	B5	168	ASN
2	B5	193	THR
2	B5	194	ILE
2	B5	197	LEU
2	B5	212	THR
2	B6	45	SER
2	B6	49	ASP
2	B6	53	ARG
2	B6	58	LEU
2	B6	70	PRO
2	B6	73	GLN
2	B6	86	ASP
2	B6	88	LEU
2	B6	93	SER
2	B6	110	VAL
2	B6	114	VAL
2	B6	126	VAL
2	B6	135	THR
2	B6	136	HIS
2	B6	145	LEU

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Mol	Chain	Res	Type
2	B6	146	GLU
2	B6	156	SER
2	B6	157	VAL
2	B6	161	GLN
2	B6	166	ARG
2	B6	167	THR
2	B6	168	ASN
2	B6	193	THR
2	B6	194	ILE
2	B6	197	LEU
2	B6	212	THR
2	B7	45	SER
2	B7	49	ASP
2	B7	53	ARG
2	B7	58	LEU
2	B7	70	PRO
2	B7	73	GLN
2	B7	86	ASP
2	B7	88	LEU
2	B7	93	SER
2	B7	110	VAL
2	B7	114	VAL
2	B7	126	VAL
2	B7	135	THR
2	B7	136	HIS
2	B7	145	LEU
2	B7	146	GLU
2	B7	156	SER
2	B7	157	VAL
2	B7	161	GLN
2	B7	166	ARG
2	B7	167	THR
2	B7	168	ASN
2	B7	193	THR
2	B7	194	ILE
2	B7	197	LEU
2	B7	212	THR
2	B8	45	SER
2	B8	49	ASP
2	B8	53	ARG
2	B8	58	LEU
2	B8	70	PRO

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Mol	Chain	Res	Type
2	B8	73	GLN
2	B8	86	ASP
2	B8	88	LEU
2	B8	93	SER
2	B8	110	VAL
2	B8	114	VAL
2	B8	126	VAL
2	B8	135	THR
2	B8	136	HIS
2	B8	145	LEU
2	B8	146	GLU
2	B8	156	SER
2	B8	157	VAL
2	B8	161	GLN
2	B8	166	ARG
2	B8	167	THR
2	B8	168	ASN
2	B8	193	THR
2	B8	194	ILE
2	B8	197	LEU
2	B8	212	THR
2	B9	45	SER
2	B9	49	ASP
2	B9	53	ARG
2	B9	58	LEU
2	B9	70	PRO
2	B9	73	GLN
2	B9	86	ASP
2	B9	88	LEU
2	B9	93	SER
2	B9	110	VAL
2	B9	114	VAL
2	B9	126	VAL
2	B9	135	THR
2	B9	136	HIS
2	B9	145	LEU
2	B9	146	GLU
2	B9	156	SER
2	B9	157	VAL
2	B9	161	GLN
2	B9	166	ARG
2	B9	167	THR

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Mol	Chain	Res	Type
2	B9	168	ASN
2	B9	193	THR
2	B9	194	ILE
2	B9	197	LEU
2	B9	212	THR
2	Ba	45	SER
2	Ba	49	ASP
2	Ba	53	ARG
2	Ba	58	LEU
2	Ba	70	PRO
2	Ba	73	GLN
2	Ba	86	ASP
2	Ba	88	LEU
2	Ba	93	SER
2	Ba	110	VAL
2	Ba	114	VAL
2	Ba	126	VAL
2	Ba	135	THR
2	Ba	136	HIS
2	Ba	145	LEU
2	Ba	146	GLU
2	Ba	156	SER
2	Ba	157	VAL
2	Ba	161	GLN
2	Ba	166	ARG
2	Ba	167	THR
2	Ba	168	ASN
2	Ba	193	THR
2	Ba	194	ILE
2	Ba	197	LEU
2	Ba	212	THR
2	Bb	45	SER
2	Bb	49	ASP
2	Bb	53	ARG
2	Bb	58	LEU
2	Bb	70	PRO
2	Bb	73	GLN
2	Bb	86	ASP
2	Bb	88	LEU
2	Bb	93	SER
2	Bb	110	VAL
2	Bb	114	VAL

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Mol	Chain	Res	Type
2	Bb	126	VAL
2	Bb	135	THR
2	Bb	136	HIS
2	Bb	145	LEU
2	Bb	146	GLU
2	Bb	156	SER
2	Bb	157	VAL
2	Bb	161	GLN
2	Bb	166	ARG
2	Bb	167	THR
2	Bb	168	ASN
2	Bb	193	THR
2	Bb	194	ILE
2	Bb	197	LEU
2	Bb	212	THR
2	Bc	45	SER
2	Bc	49	ASP
2	Bc	53	ARG
2	Bc	58	LEU
2	Bc	70	PRO
2	Bc	73	GLN
2	Bc	86	ASP
2	Bc	88	LEU
2	Bc	93	SER
2	Bc	110	VAL
2	Bc	114	VAL
2	Bc	126	VAL
2	Bc	135	THR
2	Bc	136	HIS
2	Bc	145	LEU
2	Bc	146	GLU
2	Bc	156	SER
2	Bc	157	VAL
2	Bc	161	GLN
2	Bc	166	ARG
2	Bc	167	THR
2	Bc	168	ASN
2	Bc	193	THR
2	Bc	194	ILE
2	Bc	197	LEU
2	Bc	212	THR
2	Bd	45	SER

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Mol	Chain	Res	Type
2	Bd	49	ASP
2	Bd	53	ARG
2	Bd	58	LEU
2	Bd	70	PRO
2	Bd	73	GLN
2	Bd	86	ASP
2	Bd	88	LEU
2	Bd	93	SER
2	Bd	110	VAL
2	Bd	114	VAL
2	Bd	126	VAL
2	Bd	135	THR
2	Bd	136	HIS
2	Bd	145	LEU
2	Bd	146	GLU
2	Bd	156	SER
2	Bd	157	VAL
2	Bd	161	GLN
2	Bd	166	ARG
2	Bd	167	THR
2	Bd	168	ASN
2	Bd	193	THR
2	Bd	194	ILE
2	Bd	197	LEU
2	Bd	212	THR
2	Be	45	SER
2	Be	49	ASP
2	Be	53	ARG
2	Be	58	LEU
2	Be	70	PRO
2	Be	73	GLN
2	Be	86	ASP
2	Be	88	LEU
2	Be	93	SER
2	Be	110	VAL
2	Be	114	VAL
2	Be	126	VAL
2	Be	135	THR
2	Be	136	HIS
2	Be	145	LEU
2	Be	146	GLU
2	Be	156	SER

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Mol	Chain	Res	Type
2	Be	157	VAL
2	Be	161	GLN
2	Be	166	ARG
2	Be	167	THR
2	Be	168	ASN
2	Be	193	THR
2	Be	194	ILE
2	Be	197	LEU
2	Be	212	THR
2	Bf	45	SER
2	Bf	49	ASP
2	Bf	53	ARG
2	Bf	58	LEU
2	Bf	70	PRO
2	Bf	73	GLN
2	Bf	86	ASP
2	Bf	88	LEU
2	Bf	93	SER
2	Bf	110	VAL
2	Bf	114	VAL
2	Bf	126	VAL
2	Bf	135	THR
2	Bf	136	HIS
2	Bf	145	LEU
2	Bf	146	GLU
2	Bf	156	SER
2	Bf	157	VAL
2	Bf	161	GLN
2	Bf	166	ARG
2	Bf	167	THR
2	Bf	168	ASN
2	Bf	193	THR
2	Bf	194	ILE
2	Bf	197	LEU
2	Bf	212	THR
2	Bg	45	SER
2	Bg	49	ASP
2	Bg	53	ARG
2	Bg	58	LEU
2	Bg	70	PRO
2	Bg	73	GLN
2	Bg	86	ASP

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Mol	Chain	Res	Type
2	Bg	88	LEU
2	Bg	93	SER
2	Bg	110	VAL
2	Bg	114	VAL
2	Bg	126	VAL
2	Bg	135	THR
2	Bg	136	HIS
2	Bg	145	LEU
2	Bg	146	GLU
2	Bg	156	SER
2	Bg	157	VAL
2	Bg	161	GLN
2	Bg	166	ARG
2	Bg	167	THR
2	Bg	168	ASN
2	Bg	193	THR
2	Bg	194	ILE
2	Bg	197	LEU
2	Bg	212	THR
2	Bh	45	SER
2	Bh	49	ASP
2	Bh	53	ARG
2	Bh	58	LEU
2	Bh	70	PRO
2	Bh	73	GLN
2	Bh	86	ASP
2	Bh	88	LEU
2	Bh	93	SER
2	Bh	110	VAL
2	Bh	114	VAL
2	Bh	126	VAL
2	Bh	135	THR
2	Bh	136	HIS
2	Bh	145	LEU
2	Bh	146	GLU
2	Bh	156	SER
2	Bh	157	VAL
2	Bh	161	GLN
2	Bh	166	ARG
2	Bh	167	THR
2	Bh	168	ASN
2	Bh	193	THR

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Mol	Chain	Res	Type
2	Bh	194	ILE
2	Bh	197	LEU
2	Bh	212	THR
2	Bi	45	SER
2	Bi	49	ASP
2	Bi	53	ARG
2	Bi	58	LEU
2	Bi	70	PRO
2	Bi	73	GLN
2	Bi	86	ASP
2	Bi	88	LEU
2	Bi	93	SER
2	Bi	110	VAL
2	Bi	114	VAL
2	Bi	126	VAL
2	Bi	135	THR
2	Bi	136	HIS
2	Bi	145	LEU
2	Bi	146	GLU
2	Bi	156	SER
2	Bi	157	VAL
2	Bi	161	GLN
2	Bi	166	ARG
2	Bi	167	THR
2	Bi	168	ASN
2	Bi	193	THR
2	Bi	194	ILE
2	Bi	197	LEU
2	Bi	212	THR
2	Bj	45	SER
2	Bj	49	ASP
2	Bj	53	ARG
2	Bj	58	LEU
2	Bj	70	PRO
2	Bj	73	GLN
2	Bj	86	ASP
2	Bj	88	LEU
2	Bj	93	SER
2	Bj	110	VAL
2	Bj	114	VAL
2	Bj	126	VAL
2	Bj	135	THR

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Mol	Chain	Res	Type
2	Bj	136	HIS
2	Bj	145	LEU
2	Bj	146	GLU
2	Bj	156	SER
2	Bj	157	VAL
2	Bj	161	GLN
2	Bj	166	ARG
2	Bj	167	THR
2	Bj	168	ASN
2	Bj	193	THR
2	Bj	194	ILE
2	Bj	197	LEU
2	Bj	212	THR
2	Bk	45	SER
2	Bk	49	ASP
2	Bk	53	ARG
2	Bk	58	LEU
2	Bk	70	PRO
2	Bk	73	GLN
2	Bk	86	ASP
2	Bk	88	LEU
2	Bk	93	SER
2	Bk	110	VAL
2	Bk	114	VAL
2	Bk	126	VAL
2	Bk	135	THR
2	Bk	136	HIS
2	Bk	145	LEU
2	Bk	146	GLU
2	Bk	156	SER
2	Bk	157	VAL
2	Bk	161	GLN
2	Bk	166	ARG
2	Bk	167	THR
2	Bk	168	ASN
2	Bk	193	THR
2	Bk	194	ILE
2	Bk	197	LEU
2	Bk	212	THR
2	Bl	45	SER
2	Bl	49	ASP
2	Bl	53	ARG

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Mol	Chain	Res	Type
2	Bl	58	LEU
2	Bl	70	PRO
2	Bl	73	GLN
2	Bl	86	ASP
2	Bl	88	LEU
2	Bl	93	SER
2	Bl	110	VAL
2	Bl	114	VAL
2	Bl	126	VAL
2	Bl	135	THR
2	Bl	136	HIS
2	Bl	145	LEU
2	Bl	146	GLU
2	Bl	156	SER
2	Bl	157	VAL
2	Bl	161	GLN
2	Bl	166	ARG
2	Bl	167	THR
2	Bl	168	ASN
2	Bl	193	THR
2	Bl	194	ILE
2	Bl	197	LEU
2	Bl	212	THR
2	Bm	45	SER
2	Bm	49	ASP
2	Bm	53	ARG
2	Bm	58	LEU
2	Bm	70	PRO
2	Bm	73	GLN
2	Bm	86	ASP
2	Bm	88	LEU
2	Bm	93	SER
2	Bm	110	VAL
2	Bm	114	VAL
2	Bm	126	VAL
2	Bm	135	THR
2	Bm	136	HIS
2	Bm	145	LEU
2	Bm	146	GLU
2	Bm	156	SER
2	Bm	157	VAL
2	Bm	161	GLN

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Mol	Chain	Res	Type
2	Bm	166	ARG
2	Bm	167	THR
2	Bm	168	ASN
2	Bm	193	THR
2	Bm	194	ILE
2	Bm	197	LEU
2	Bm	212	THR
2	Bn	45	SER
2	Bn	49	ASP
2	Bn	53	ARG
2	Bn	58	LEU
2	Bn	70	PRO
2	Bn	73	GLN
2	Bn	86	ASP
2	Bn	88	LEU
2	Bn	93	SER
2	Bn	110	VAL
2	Bn	114	VAL
2	Bn	126	VAL
2	Bn	135	THR
2	Bn	136	HIS
2	Bn	145	LEU
2	Bn	146	GLU
2	Bn	156	SER
2	Bn	157	VAL
2	Bn	161	GLN
2	Bn	166	ARG
2	Bn	167	THR
2	Bn	168	ASN
2	Bn	193	THR
2	Bn	194	ILE
2	Bn	197	LEU
2	Bn	212	THR
2	Bo	45	SER
2	Bo	49	ASP
2	Bo	53	ARG
2	Bo	58	LEU
2	Bo	70	PRO
2	Bo	73	GLN
2	Bo	86	ASP
2	Bo	88	LEU
2	Bo	93	SER

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Mol	Chain	Res	Type
2	Bo	110	VAL
2	Bo	114	VAL
2	Bo	126	VAL
2	Bo	135	THR
2	Bo	136	HIS
2	Bo	145	LEU
2	Bo	146	GLU
2	Bo	156	SER
2	Bo	157	VAL
2	Bo	161	GLN
2	Bo	166	ARG
2	Bo	167	THR
2	Bo	168	ASN
2	Bo	193	THR
2	Bo	194	ILE
2	Bo	197	LEU
2	Bo	212	THR
2	Bp	45	SER
2	Bp	49	ASP
2	Bp	53	ARG
2	Bp	58	LEU
2	Bp	70	PRO
2	Bp	73	GLN
2	Bp	86	ASP
2	Bp	88	LEU
2	Bp	93	SER
2	Bp	110	VAL
2	Bp	114	VAL
2	Bp	126	VAL
2	Bp	135	THR
2	Bp	136	HIS
2	Bp	145	LEU
2	Bp	146	GLU
2	Bp	156	SER
2	Bp	157	VAL
2	Bp	161	GLN
2	Bp	166	ARG
2	Bp	167	THR
2	Bp	168	ASN
2	Bp	193	THR
2	Bp	194	ILE
2	Bp	197	LEU

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Mol	Chain	Res	Type
2	Bp	212	THR
2	Bq	45	SER
2	Bq	49	ASP
2	Bq	53	ARG
2	Bq	58	LEU
2	Bq	70	PRO
2	Bq	73	GLN
2	Bq	86	ASP
2	Bq	88	LEU
2	Bq	93	SER
2	Bq	110	VAL
2	Bq	114	VAL
2	Bq	126	VAL
2	Bq	135	THR
2	Bq	136	HIS
2	Bq	145	LEU
2	Bq	146	GLU
2	Bq	156	SER
2	Bq	157	VAL
2	Bq	161	GLN
2	Bq	166	ARG
2	Bq	167	THR
2	Bq	168	ASN
2	Bq	193	THR
2	Bq	194	ILE
2	Bq	197	LEU
2	Bq	212	THR
2	Br	45	SER
2	Br	49	ASP
2	Br	53	ARG
2	Br	58	LEU
2	Br	70	PRO
2	Br	73	GLN
2	Br	86	ASP
2	Br	88	LEU
2	Br	93	SER
2	Br	110	VAL
2	Br	114	VAL
2	Br	126	VAL
2	Br	135	THR
2	Br	136	HIS
2	Br	145	LEU

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Mol	Chain	Res	Type
2	Br	146	GLU
2	Br	156	SER
2	Br	157	VAL
2	Br	161	GLN
2	Br	166	ARG
2	Br	167	THR
2	Br	168	ASN
2	Br	193	THR
2	Br	194	ILE
2	Br	197	LEU
2	Br	212	THR
2	Bs	45	SER
2	Bs	49	ASP
2	Bs	53	ARG
2	Bs	58	LEU
2	Bs	70	PRO
2	Bs	73	GLN
2	Bs	86	ASP
2	Bs	88	LEU
2	Bs	93	SER
2	Bs	110	VAL
2	Bs	114	VAL
2	Bs	126	VAL
2	Bs	135	THR
2	Bs	136	HIS
2	Bs	145	LEU
2	Bs	146	GLU
2	Bs	156	SER
2	Bs	157	VAL
2	Bs	161	GLN
2	Bs	166	ARG
2	Bs	167	THR
2	Bs	168	ASN
2	Bs	193	THR
2	Bs	194	ILE
2	Bs	197	LEU
2	Bs	212	THR
2	Bt	45	SER
2	Bt	49	ASP
2	Bt	53	ARG
2	Bt	58	LEU
2	Bt	70	PRO

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Mol	Chain	Res	Type
2	Bt	73	GLN
2	Bt	86	ASP
2	Bt	88	LEU
2	Bt	93	SER
2	Bt	110	VAL
2	Bt	114	VAL
2	Bt	126	VAL
2	Bt	135	THR
2	Bt	136	HIS
2	Bt	145	LEU
2	Bt	146	GLU
2	Bt	156	SER
2	Bt	157	VAL
2	Bt	161	GLN
2	Bt	166	ARG
2	Bt	167	THR
2	Bt	168	ASN
2	Bt	193	THR
2	Bt	194	ILE
2	Bt	197	LEU
2	Bt	212	THR
2	Bu	45	SER
2	Bu	49	ASP
2	Bu	53	ARG
2	Bu	58	LEU
2	Bu	70	PRO
2	Bu	73	GLN
2	Bu	86	ASP
2	Bu	88	LEU
2	Bu	93	SER
2	Bu	110	VAL
2	Bu	114	VAL
2	Bu	126	VAL
2	Bu	135	THR
2	Bu	136	HIS
2	Bu	145	LEU
2	Bu	146	GLU
2	Bu	156	SER
2	Bu	157	VAL
2	Bu	161	GLN
2	Bu	166	ARG
2	Bu	167	THR

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Mol	Chain	Res	Type
2	Bu	168	ASN
2	Bu	193	THR
2	Bu	194	ILE
2	Bu	197	LEU
2	Bu	212	THR
2	Bv	45	SER
2	Bv	49	ASP
2	Bv	53	ARG
2	Bv	58	LEU
2	Bv	70	PRO
2	Bv	73	GLN
2	Bv	86	ASP
2	Bv	88	LEU
2	Bv	93	SER
2	Bv	110	VAL
2	Bv	114	VAL
2	Bv	126	VAL
2	Bv	135	THR
2	Bv	136	HIS
2	Bv	145	LEU
2	Bv	146	GLU
2	Bv	156	SER
2	Bv	157	VAL
2	Bv	161	GLN
2	Bv	166	ARG
2	Bv	167	THR
2	Bv	168	ASN
2	Bv	193	THR
2	Bv	194	ILE
2	Bv	197	LEU
2	Bv	212	THR
2	Bw	45	SER
2	Bw	49	ASP
2	Bw	53	ARG
2	Bw	58	LEU
2	Bw	70	PRO
2	Bw	73	GLN
2	Bw	86	ASP
2	Bw	88	LEU
2	Bw	93	SER
2	Bw	110	VAL
2	Bw	114	VAL

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Mol	Chain	Res	Type
2	Bw	126	VAL
2	Bw	135	THR
2	Bw	136	HIS
2	Bw	145	LEU
2	Bw	146	GLU
2	Bw	156	SER
2	Bw	157	VAL
2	Bw	161	GLN
2	Bw	166	ARG
2	Bw	167	THR
2	Bw	168	ASN
2	Bw	193	THR
2	Bw	194	ILE
2	Bw	197	LEU
2	Bw	212	THR
2	Bx	45	SER
2	Bx	49	ASP
2	Bx	53	ARG
2	Bx	58	LEU
2	Bx	70	PRO
2	Bx	73	GLN
2	Bx	86	ASP
2	Bx	88	LEU
2	Bx	93	SER
2	Bx	110	VAL
2	Bx	114	VAL
2	Bx	126	VAL
2	Bx	135	THR
2	Bx	136	HIS
2	Bx	145	LEU
2	Bx	146	GLU
2	Bx	156	SER
2	Bx	157	VAL
2	Bx	161	GLN
2	Bx	166	ARG
2	Bx	167	THR
2	Bx	168	ASN
2	Bx	193	THR
2	Bx	194	ILE
2	Bx	197	LEU
2	Bx	212	THR
3	CA	5	VAL

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Mol	Chain	Res	Type
3	CA	8	VAL
3	CA	11	SER
3	CA	16	SER
3	CA	18	VAL
3	CA	23	THR
3	CA	31	VAL
3	CA	35	GLN
3	CA	36	VAL
3	CA	42	ASN
3	CA	50	THR
3	CA	56	ILE
3	CA	59	LYS
3	CA	64	VAL
3	CA	73	LEU
3	CA	76	MET
3	CA	77	ASP
3	CA	80	LEU
3	CA	93	LEU
3	CA	116	THR
3	CA	122	VAL
3	CA	129	SER
3	CA	135	ARG
3	CA	139	MET
3	CA	151	ASN
3	CA	157	ASN
3	CA	161	SER
3	CA	175	THR
3	CA	176	VAL
3	CA	178	ASN
3	CA	179	VAL
3	CA	183	LEU
3	CA	188	LEU
3	CA	192	THR
3	CA	194	THR
3	CA	196	ILE
3	CA	206	VAL
3	CA	208	VAL
3	CA	216	LEU
3	CA	217	ARG
3	CB	5	VAL
3	CB	8	VAL
3	CB	11	SER

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Mol	Chain	Res	Type
3	CB	16	SER
3	CB	18	VAL
3	CB	23	THR
3	CB	31	VAL
3	CB	35	GLN
3	CB	36	VAL
3	CB	42	ASN
3	CB	50	THR
3	CB	56	ILE
3	CB	59	LYS
3	CB	64	VAL
3	CB	73	LEU
3	CB	76	MET
3	CB	77	ASP
3	CB	80	LEU
3	CB	93	LEU
3	CB	116	THR
3	CB	122	VAL
3	CB	129	SER
3	CB	135	ARG
3	CB	139	MET
3	CB	151	ASN
3	CB	157	ASN
3	CB	161	SER
3	CB	175	THR
3	CB	176	VAL
3	CB	178	ASN
3	CB	179	VAL
3	CB	183	LEU
3	CB	188	LEU
3	CB	192	THR
3	CB	194	THR
3	CB	196	ILE
3	CB	206	VAL
3	CB	208	VAL
3	CB	216	LEU
3	CB	217	ARG
3	CC	5	VAL
3	CC	8	VAL
3	CC	11	SER
3	CC	16	SER
3	CC	18	VAL

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Mol	Chain	Res	Type
3	CC	23	THR
3	CC	31	VAL
3	CC	35	GLN
3	CC	36	VAL
3	CC	42	ASN
3	CC	50	THR
3	CC	56	ILE
3	CC	59	LYS
3	CC	64	VAL
3	CC	73	LEU
3	CC	76	MET
3	CC	77	ASP
3	CC	80	LEU
3	CC	93	LEU
3	CC	116	THR
3	CC	122	VAL
3	CC	129	SER
3	CC	135	ARG
3	CC	139	MET
3	CC	151	ASN
3	CC	157	ASN
3	CC	161	SER
3	CC	175	THR
3	CC	176	VAL
3	CC	178	ASN
3	CC	179	VAL
3	CC	183	LEU
3	CC	188	LEU
3	CC	192	THR
3	CC	194	THR
3	CC	196	ILE
3	CC	206	VAL
3	CC	208	VAL
3	CC	216	LEU
3	CC	217	ARG
3	CD	5	VAL
3	CD	8	VAL
3	CD	11	SER
3	CD	16	SER
3	CD	18	VAL
3	CD	23	THR
3	CD	31	VAL

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Mol	Chain	Res	Type
3	CD	35	GLN
3	CD	36	VAL
3	CD	42	ASN
3	CD	50	THR
3	CD	56	ILE
3	CD	59	LYS
3	CD	64	VAL
3	CD	73	LEU
3	CD	76	MET
3	CD	77	ASP
3	CD	80	LEU
3	CD	93	LEU
3	CD	116	THR
3	CD	122	VAL
3	CD	129	SER
3	CD	135	ARG
3	CD	139	MET
3	CD	151	ASN
3	CD	157	ASN
3	CD	161	SER
3	CD	175	THR
3	CD	176	VAL
3	CD	178	ASN
3	CD	179	VAL
3	CD	183	LEU
3	CD	188	LEU
3	CD	192	THR
3	CD	194	THR
3	CD	196	ILE
3	CD	206	VAL
3	CD	208	VAL
3	CD	216	LEU
3	CD	217	ARG
3	CE	5	VAL
3	CE	8	VAL
3	CE	11	SER
3	CE	16	SER
3	CE	18	VAL
3	CE	23	THR
3	CE	31	VAL
3	CE	35	GLN
3	CE	36	VAL

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Mol	Chain	Res	Type
3	CE	42	ASN
3	CE	50	THR
3	CE	56	ILE
3	CE	59	LYS
3	CE	64	VAL
3	CE	73	LEU
3	CE	76	MET
3	CE	77	ASP
3	CE	80	LEU
3	CE	93	LEU
3	CE	116	THR
3	CE	122	VAL
3	CE	129	SER
3	CE	135	ARG
3	CE	139	MET
3	CE	151	ASN
3	CE	157	ASN
3	CE	161	SER
3	CE	175	THR
3	CE	176	VAL
3	CE	178	ASN
3	CE	179	VAL
3	CE	183	LEU
3	CE	188	LEU
3	CE	192	THR
3	CE	194	THR
3	CE	196	ILE
3	CE	206	VAL
3	CE	208	VAL
3	CE	216	LEU
3	CE	217	ARG
3	CF	5	VAL
3	CF	8	VAL
3	CF	11	SER
3	CF	16	SER
3	CF	18	VAL
3	CF	23	THR
3	CF	31	VAL
3	CF	35	GLN
3	CF	36	VAL
3	CF	42	ASN
3	CF	50	THR

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Mol	Chain	Res	Type
3	CF	56	ILE
3	CF	59	LYS
3	CF	64	VAL
3	CF	73	LEU
3	CF	76	MET
3	CF	77	ASP
3	CF	80	LEU
3	CF	93	LEU
3	CF	116	THR
3	CF	122	VAL
3	CF	129	SER
3	CF	135	ARG
3	CF	139	MET
3	CF	151	ASN
3	CF	157	ASN
3	CF	161	SER
3	CF	175	THR
3	CF	176	VAL
3	CF	178	ASN
3	CF	179	VAL
3	CF	183	LEU
3	CF	188	LEU
3	CF	192	THR
3	CF	194	THR
3	CF	196	ILE
3	CF	206	VAL
3	CF	208	VAL
3	CF	216	LEU
3	CF	217	ARG
3	CG	5	VAL
3	CG	8	VAL
3	CG	11	SER
3	CG	16	SER
3	CG	18	VAL
3	CG	23	THR
3	CG	31	VAL
3	CG	35	GLN
3	CG	36	VAL
3	CG	42	ASN
3	CG	50	THR
3	CG	56	ILE
3	CG	59	LYS

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Mol	Chain	Res	Type
3	CG	64	VAL
3	CG	73	LEU
3	CG	76	MET
3	CG	77	ASP
3	CG	80	LEU
3	CG	93	LEU
3	CG	116	THR
3	CG	122	VAL
3	CG	129	SER
3	CG	135	ARG
3	CG	139	MET
3	CG	151	ASN
3	CG	157	ASN
3	CG	161	SER
3	CG	175	THR
3	CG	176	VAL
3	CG	178	ASN
3	CG	179	VAL
3	CG	183	LEU
3	CG	188	LEU
3	CG	192	THR
3	CG	194	THR
3	CG	196	ILE
3	CG	206	VAL
3	CG	208	VAL
3	CG	216	LEU
3	CG	217	ARG
3	CH	5	VAL
3	CH	8	VAL
3	CH	11	SER
3	CH	16	SER
3	CH	18	VAL
3	CH	23	THR
3	CH	31	VAL
3	CH	35	GLN
3	CH	36	VAL
3	CH	42	ASN
3	CH	50	THR
3	CH	56	ILE
3	CH	59	LYS
3	CH	64	VAL
3	CH	73	LEU

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Mol	Chain	Res	Type
3	CH	76	MET
3	CH	77	ASP
3	CH	80	LEU
3	CH	93	LEU
3	CH	116	THR
3	CH	122	VAL
3	CH	129	SER
3	CH	135	ARG
3	CH	139	MET
3	CH	151	ASN
3	CH	157	ASN
3	CH	161	SER
3	CH	175	THR
3	CH	176	VAL
3	CH	178	ASN
3	CH	179	VAL
3	CH	183	LEU
3	CH	188	LEU
3	CH	192	THR
3	CH	194	THR
3	CH	196	ILE
3	CH	206	VAL
3	CH	208	VAL
3	CH	216	LEU
3	CH	217	ARG
3	CI	5	VAL
3	CI	8	VAL
3	CI	11	SER
3	CI	16	SER
3	CI	18	VAL
3	CI	23	THR
3	CI	31	VAL
3	CI	35	GLN
3	CI	36	VAL
3	CI	42	ASN
3	CI	50	THR
3	CI	56	ILE
3	CI	59	LYS
3	CI	64	VAL
3	CI	73	LEU
3	CI	76	MET
3	CI	77	ASP

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Mol	Chain	Res	Type
3	CI	80	LEU
3	CI	93	LEU
3	CI	116	THR
3	CI	122	VAL
3	CI	129	SER
3	CI	135	ARG
3	CI	139	MET
3	CI	151	ASN
3	CI	157	ASN
3	CI	161	SER
3	CI	175	THR
3	CI	176	VAL
3	CI	178	ASN
3	CI	179	VAL
3	CI	183	LEU
3	CI	188	LEU
3	CI	192	THR
3	CI	194	THR
3	CI	196	ILE
3	CI	206	VAL
3	CI	208	VAL
3	CI	216	LEU
3	CI	217	ARG
3	CJ	5	VAL
3	CJ	8	VAL
3	CJ	11	SER
3	CJ	16	SER
3	CJ	18	VAL
3	CJ	23	THR
3	CJ	31	VAL
3	CJ	35	GLN
3	CJ	36	VAL
3	CJ	42	ASN
3	CJ	50	THR
3	CJ	56	ILE
3	CJ	59	LYS
3	CJ	64	VAL
3	CJ	73	LEU
3	CJ	76	MET
3	CJ	77	ASP
3	CJ	80	LEU
3	CJ	93	LEU

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Mol	Chain	Res	Type
3	CJ	116	THR
3	CJ	122	VAL
3	CJ	129	SER
3	CJ	135	ARG
3	CJ	139	MET
3	CJ	151	ASN
3	CJ	157	ASN
3	CJ	161	SER
3	CJ	175	THR
3	CJ	176	VAL
3	CJ	178	ASN
3	CJ	179	VAL
3	CJ	183	LEU
3	CJ	188	LEU
3	CJ	192	THR
3	CJ	194	THR
3	CJ	196	ILE
3	CJ	206	VAL
3	CJ	208	VAL
3	CJ	216	LEU
3	CJ	217	ARG
3	CK	5	VAL
3	CK	8	VAL
3	CK	11	SER
3	CK	16	SER
3	CK	18	VAL
3	CK	23	THR
3	CK	31	VAL
3	CK	35	GLN
3	CK	36	VAL
3	CK	42	ASN
3	CK	50	THR
3	CK	56	ILE
3	CK	59	LYS
3	CK	64	VAL
3	CK	73	LEU
3	CK	76	MET
3	CK	77	ASP
3	CK	80	LEU
3	CK	93	LEU
3	CK	116	THR
3	CK	122	VAL

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Mol	Chain	Res	Type
3	CK	129	SER
3	CK	135	ARG
3	CK	139	MET
3	CK	151	ASN
3	CK	157	ASN
3	CK	161	SER
3	CK	175	THR
3	CK	176	VAL
3	CK	178	ASN
3	CK	179	VAL
3	CK	183	LEU
3	CK	188	LEU
3	CK	192	THR
3	CK	194	THR
3	CK	196	ILE
3	CK	206	VAL
3	CK	208	VAL
3	CK	216	LEU
3	CK	217	ARG
3	CL	5	VAL
3	CL	8	VAL
3	CL	11	SER
3	CL	16	SER
3	CL	18	VAL
3	CL	23	THR
3	CL	31	VAL
3	CL	35	GLN
3	CL	36	VAL
3	CL	42	ASN
3	CL	50	THR
3	CL	56	ILE
3	CL	59	LYS
3	CL	64	VAL
3	CL	73	LEU
3	CL	76	MET
3	CL	77	ASP
3	CL	80	LEU
3	CL	93	LEU
3	CL	116	THR
3	CL	122	VAL
3	CL	129	SER
3	CL	135	ARG

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Mol	Chain	Res	Type
3	CL	139	MET
3	CL	151	ASN
3	CL	157	ASN
3	CL	161	SER
3	CL	175	THR
3	CL	176	VAL
3	CL	178	ASN
3	CL	179	VAL
3	CL	183	LEU
3	CL	188	LEU
3	CL	192	THR
3	CL	194	THR
3	CL	196	ILE
3	CL	206	VAL
3	CL	208	VAL
3	CL	216	LEU
3	CL	217	ARG
3	CM	5	VAL
3	CM	8	VAL
3	CM	11	SER
3	CM	16	SER
3	CM	18	VAL
3	CM	23	THR
3	CM	31	VAL
3	CM	35	GLN
3	CM	36	VAL
3	CM	42	ASN
3	CM	50	THR
3	CM	56	ILE
3	CM	59	LYS
3	CM	64	VAL
3	CM	73	LEU
3	CM	76	MET
3	CM	77	ASP
3	CM	80	LEU
3	CM	93	LEU
3	CM	116	THR
3	CM	122	VAL
3	CM	129	SER
3	CM	135	ARG
3	CM	139	MET
3	CM	151	ASN

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Mol	Chain	Res	Type
3	CM	157	ASN
3	CM	161	SER
3	CM	175	THR
3	CM	176	VAL
3	CM	178	ASN
3	CM	179	VAL
3	CM	183	LEU
3	CM	188	LEU
3	CM	192	THR
3	CM	194	THR
3	CM	196	ILE
3	CM	206	VAL
3	CM	208	VAL
3	CM	216	LEU
3	CM	217	ARG
3	CN	5	VAL
3	CN	8	VAL
3	CN	11	SER
3	CN	16	SER
3	CN	18	VAL
3	CN	23	THR
3	CN	31	VAL
3	CN	35	GLN
3	CN	36	VAL
3	CN	42	ASN
3	CN	50	THR
3	CN	56	ILE
3	CN	59	LYS
3	CN	64	VAL
3	CN	73	LEU
3	CN	76	MET
3	CN	77	ASP
3	CN	80	LEU
3	CN	93	LEU
3	CN	116	THR
3	CN	122	VAL
3	CN	129	SER
3	CN	135	ARG
3	CN	139	MET
3	CN	151	ASN
3	CN	157	ASN
3	CN	161	SER

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Mol	Chain	Res	Type
3	CN	175	THR
3	CN	176	VAL
3	CN	178	ASN
3	CN	179	VAL
3	CN	183	LEU
3	CN	188	LEU
3	CN	192	THR
3	CN	194	THR
3	CN	196	ILE
3	CN	206	VAL
3	CN	208	VAL
3	CN	216	LEU
3	CN	217	ARG
3	CO	5	VAL
3	CO	8	VAL
3	CO	11	SER
3	CO	16	SER
3	CO	18	VAL
3	CO	23	THR
3	CO	31	VAL
3	CO	35	GLN
3	CO	36	VAL
3	CO	42	ASN
3	CO	50	THR
3	CO	56	ILE
3	CO	59	LYS
3	CO	64	VAL
3	CO	73	LEU
3	CO	76	MET
3	CO	77	ASP
3	CO	80	LEU
3	CO	93	LEU
3	CO	116	THR
3	CO	122	VAL
3	CO	129	SER
3	CO	135	ARG
3	CO	139	MET
3	CO	151	ASN
3	CO	157	ASN
3	CO	161	SER
3	CO	175	THR
3	CO	176	VAL

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Mol	Chain	Res	Type
3	CO	178	ASN
3	CO	179	VAL
3	CO	183	LEU
3	CO	188	LEU
3	CO	192	THR
3	CO	194	THR
3	CO	196	ILE
3	CO	206	VAL
3	CO	208	VAL
3	CO	216	LEU
3	CO	217	ARG
3	CP	5	VAL
3	CP	8	VAL
3	CP	11	SER
3	CP	16	SER
3	CP	18	VAL
3	CP	23	THR
3	CP	31	VAL
3	CP	35	GLN
3	CP	36	VAL
3	CP	42	ASN
3	CP	50	THR
3	CP	56	ILE
3	CP	59	LYS
3	CP	64	VAL
3	CP	73	LEU
3	CP	76	MET
3	CP	77	ASP
3	CP	80	LEU
3	CP	93	LEU
3	CP	116	THR
3	CP	122	VAL
3	CP	129	SER
3	CP	135	ARG
3	CP	139	MET
3	CP	151	ASN
3	CP	157	ASN
3	CP	161	SER
3	CP	175	THR
3	CP	176	VAL
3	CP	178	ASN
3	CP	179	VAL

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Mol	Chain	Res	Type
3	CP	183	LEU
3	CP	188	LEU
3	CP	192	THR
3	CP	194	THR
3	CP	196	ILE
3	CP	206	VAL
3	CP	208	VAL
3	CP	216	LEU
3	CP	217	ARG
3	CQ	5	VAL
3	CQ	8	VAL
3	CQ	11	SER
3	CQ	16	SER
3	CQ	18	VAL
3	CQ	23	THR
3	CQ	31	VAL
3	CQ	35	GLN
3	CQ	36	VAL
3	CQ	42	ASN
3	CQ	50	THR
3	CQ	56	ILE
3	CQ	59	LYS
3	CQ	64	VAL
3	CQ	73	LEU
3	CQ	76	MET
3	CQ	77	ASP
3	CQ	80	LEU
3	CQ	93	LEU
3	CQ	116	THR
3	CQ	122	VAL
3	CQ	129	SER
3	CQ	135	ARG
3	CQ	139	MET
3	CQ	151	ASN
3	CQ	157	ASN
3	CQ	161	SER
3	CQ	175	THR
3	CQ	176	VAL
3	CQ	178	ASN
3	CQ	179	VAL
3	CQ	183	LEU
3	CQ	188	LEU

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Mol	Chain	Res	Type
3	CQ	192	THR
3	CQ	194	THR
3	CQ	196	ILE
3	CQ	206	VAL
3	CQ	208	VAL
3	CQ	216	LEU
3	CQ	217	ARG
3	CR	5	VAL
3	CR	8	VAL
3	CR	11	SER
3	CR	16	SER
3	CR	18	VAL
3	CR	23	THR
3	CR	31	VAL
3	CR	35	GLN
3	CR	36	VAL
3	CR	42	ASN
3	CR	50	THR
3	CR	56	ILE
3	CR	59	LYS
3	CR	64	VAL
3	CR	73	LEU
3	CR	76	MET
3	CR	77	ASP
3	CR	80	LEU
3	CR	93	LEU
3	CR	116	THR
3	CR	122	VAL
3	CR	129	SER
3	CR	135	ARG
3	CR	139	MET
3	CR	151	ASN
3	CR	157	ASN
3	CR	161	SER
3	CR	175	THR
3	CR	176	VAL
3	CR	178	ASN
3	CR	179	VAL
3	CR	183	LEU
3	CR	188	LEU
3	CR	192	THR
3	CR	194	THR

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Mol	Chain	Res	Type
3	CR	196	ILE
3	CR	206	VAL
3	CR	208	VAL
3	CR	216	LEU
3	CR	217	ARG
3	CS	5	VAL
3	CS	8	VAL
3	CS	11	SER
3	CS	16	SER
3	CS	18	VAL
3	CS	23	THR
3	CS	31	VAL
3	CS	35	GLN
3	CS	36	VAL
3	CS	42	ASN
3	CS	50	THR
3	CS	56	ILE
3	CS	59	LYS
3	CS	64	VAL
3	CS	73	LEU
3	CS	76	MET
3	CS	77	ASP
3	CS	80	LEU
3	CS	93	LEU
3	CS	116	THR
3	CS	122	VAL
3	CS	129	SER
3	CS	135	ARG
3	CS	139	MET
3	CS	151	ASN
3	CS	157	ASN
3	CS	161	SER
3	CS	175	THR
3	CS	176	VAL
3	CS	178	ASN
3	CS	179	VAL
3	CS	183	LEU
3	CS	188	LEU
3	CS	192	THR
3	CS	194	THR
3	CS	196	ILE
3	CS	206	VAL

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Mol	Chain	Res	Type
3	CS	208	VAL
3	CS	216	LEU
3	CS	217	ARG
3	CT	5	VAL
3	CT	8	VAL
3	CT	11	SER
3	CT	16	SER
3	CT	18	VAL
3	CT	23	THR
3	CT	31	VAL
3	CT	35	GLN
3	CT	36	VAL
3	CT	42	ASN
3	CT	50	THR
3	CT	56	ILE
3	CT	59	LYS
3	CT	64	VAL
3	CT	73	LEU
3	CT	76	MET
3	CT	77	ASP
3	CT	80	LEU
3	CT	93	LEU
3	CT	116	THR
3	CT	122	VAL
3	CT	129	SER
3	CT	135	ARG
3	CT	139	MET
3	CT	151	ASN
3	CT	157	ASN
3	CT	161	SER
3	CT	175	THR
3	CT	176	VAL
3	CT	178	ASN
3	CT	179	VAL
3	CT	183	LEU
3	CT	188	LEU
3	CT	192	THR
3	CT	194	THR
3	CT	196	ILE
3	CT	206	VAL
3	CT	208	VAL
3	CT	216	LEU

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Mol	Chain	Res	Type
3	CT	217	ARG
3	CU	5	VAL
3	CU	8	VAL
3	CU	11	SER
3	CU	16	SER
3	CU	18	VAL
3	CU	23	THR
3	CU	31	VAL
3	CU	35	GLN
3	CU	36	VAL
3	CU	42	ASN
3	CU	50	THR
3	CU	56	ILE
3	CU	59	LYS
3	CU	64	VAL
3	CU	73	LEU
3	CU	76	MET
3	CU	77	ASP
3	CU	80	LEU
3	CU	93	LEU
3	CU	116	THR
3	CU	122	VAL
3	CU	129	SER
3	CU	135	ARG
3	CU	139	MET
3	CU	151	ASN
3	CU	157	ASN
3	CU	161	SER
3	CU	175	THR
3	CU	176	VAL
3	CU	178	ASN
3	CU	179	VAL
3	CU	183	LEU
3	CU	188	LEU
3	CU	192	THR
3	CU	194	THR
3	CU	196	ILE
3	CU	206	VAL
3	CU	208	VAL
3	CU	216	LEU
3	CU	217	ARG
3	CV	5	VAL

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Mol	Chain	Res	Type
3	CV	8	VAL
3	CV	11	SER
3	CV	16	SER
3	CV	18	VAL
3	CV	23	THR
3	CV	31	VAL
3	CV	35	GLN
3	CV	36	VAL
3	CV	42	ASN
3	CV	50	THR
3	CV	56	ILE
3	CV	59	LYS
3	CV	64	VAL
3	CV	73	LEU
3	CV	76	MET
3	CV	77	ASP
3	CV	80	LEU
3	CV	93	LEU
3	CV	116	THR
3	CV	122	VAL
3	CV	129	SER
3	CV	135	ARG
3	CV	139	MET
3	CV	151	ASN
3	CV	157	ASN
3	CV	161	SER
3	CV	175	THR
3	CV	176	VAL
3	CV	178	ASN
3	CV	179	VAL
3	CV	183	LEU
3	CV	188	LEU
3	CV	192	THR
3	CV	194	THR
3	CV	196	ILE
3	CV	206	VAL
3	CV	208	VAL
3	CV	216	LEU
3	CV	217	ARG
3	CW	5	VAL
3	CW	8	VAL
3	CW	11	SER

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Mol	Chain	Res	Type
3	CW	16	SER
3	CW	18	VAL
3	CW	23	THR
3	CW	31	VAL
3	CW	35	GLN
3	CW	36	VAL
3	CW	42	ASN
3	CW	50	THR
3	CW	56	ILE
3	CW	59	LYS
3	CW	64	VAL
3	CW	73	LEU
3	CW	76	MET
3	CW	77	ASP
3	CW	80	LEU
3	CW	93	LEU
3	CW	116	THR
3	CW	122	VAL
3	CW	129	SER
3	CW	135	ARG
3	CW	139	MET
3	CW	151	ASN
3	CW	157	ASN
3	CW	161	SER
3	CW	175	THR
3	CW	176	VAL
3	CW	178	ASN
3	CW	179	VAL
3	CW	183	LEU
3	CW	188	LEU
3	CW	192	THR
3	CW	194	THR
3	CW	196	ILE
3	CW	206	VAL
3	CW	208	VAL
3	CW	216	LEU
3	CW	217	ARG
3	CX	5	VAL
3	CX	8	VAL
3	CX	11	SER
3	CX	16	SER
3	CX	18	VAL

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Mol	Chain	Res	Type
3	CX	23	THR
3	CX	31	VAL
3	CX	35	GLN
3	CX	36	VAL
3	CX	42	ASN
3	CX	50	THR
3	CX	56	ILE
3	CX	59	LYS
3	CX	64	VAL
3	CX	73	LEU
3	CX	76	MET
3	CX	77	ASP
3	CX	80	LEU
3	CX	93	LEU
3	CX	116	THR
3	CX	122	VAL
3	CX	129	SER
3	CX	135	ARG
3	CX	139	MET
3	CX	151	ASN
3	CX	157	ASN
3	CX	161	SER
3	CX	175	THR
3	CX	176	VAL
3	CX	178	ASN
3	CX	179	VAL
3	CX	183	LEU
3	CX	188	LEU
3	CX	192	THR
3	CX	194	THR
3	CX	196	ILE
3	CX	206	VAL
3	CX	208	VAL
3	CX	216	LEU
3	CX	217	ARG
3	CY	5	VAL
3	CY	8	VAL
3	CY	11	SER
3	CY	16	SER
3	CY	18	VAL
3	CY	23	THR
3	CY	31	VAL

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Mol	Chain	Res	Type
3	CY	35	GLN
3	CY	36	VAL
3	CY	42	ASN
3	CY	50	THR
3	CY	56	ILE
3	CY	59	LYS
3	CY	64	VAL
3	CY	73	LEU
3	CY	76	MET
3	CY	77	ASP
3	CY	80	LEU
3	CY	93	LEU
3	CY	116	THR
3	CY	122	VAL
3	CY	129	SER
3	CY	135	ARG
3	CY	139	MET
3	CY	151	ASN
3	CY	157	ASN
3	CY	161	SER
3	CY	175	THR
3	CY	176	VAL
3	CY	178	ASN
3	CY	179	VAL
3	CY	183	LEU
3	CY	188	LEU
3	CY	192	THR
3	CY	194	THR
3	CY	196	ILE
3	CY	206	VAL
3	CY	208	VAL
3	CY	216	LEU
3	CY	217	ARG
3	CZ	5	VAL
3	CZ	8	VAL
3	CZ	11	SER
3	CZ	16	SER
3	CZ	18	VAL
3	CZ	23	THR
3	CZ	31	VAL
3	CZ	35	GLN
3	CZ	36	VAL

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Mol	Chain	Res	Type
3	CZ	42	ASN
3	CZ	50	THR
3	CZ	56	ILE
3	CZ	59	LYS
3	CZ	64	VAL
3	CZ	73	LEU
3	CZ	76	MET
3	CZ	77	ASP
3	CZ	80	LEU
3	CZ	93	LEU
3	CZ	116	THR
3	CZ	122	VAL
3	CZ	129	SER
3	CZ	135	ARG
3	CZ	139	MET
3	CZ	151	ASN
3	CZ	157	ASN
3	CZ	161	SER
3	CZ	175	THR
3	CZ	176	VAL
3	CZ	178	ASN
3	CZ	179	VAL
3	CZ	183	LEU
3	CZ	188	LEU
3	CZ	192	THR
3	CZ	194	THR
3	CZ	196	ILE
3	CZ	206	VAL
3	CZ	208	VAL
3	CZ	216	LEU
3	CZ	217	ARG
3	C0	5	VAL
3	C0	8	VAL
3	C0	11	SER
3	C0	16	SER
3	C0	18	VAL
3	C0	23	THR
3	C0	31	VAL
3	C0	35	GLN
3	C0	36	VAL
3	C0	42	ASN
3	C0	50	THR

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Mol	Chain	Res	Type
3	C0	56	ILE
3	C0	59	LYS
3	C0	64	VAL
3	C0	73	LEU
3	C0	76	MET
3	C0	77	ASP
3	C0	80	LEU
3	C0	93	LEU
3	C0	116	THR
3	C0	122	VAL
3	C0	129	SER
3	C0	135	ARG
3	C0	139	MET
3	C0	151	ASN
3	C0	157	ASN
3	C0	161	SER
3	C0	175	THR
3	C0	176	VAL
3	C0	178	ASN
3	C0	179	VAL
3	C0	183	LEU
3	C0	188	LEU
3	C0	192	THR
3	C0	194	THR
3	C0	196	ILE
3	C0	206	VAL
3	C0	208	VAL
3	C0	216	LEU
3	C0	217	ARG
3	C1	5	VAL
3	C1	8	VAL
3	C1	11	SER
3	C1	16	SER
3	C1	18	VAL
3	C1	23	THR
3	C1	31	VAL
3	C1	35	GLN
3	C1	36	VAL
3	C1	42	ASN
3	C1	50	THR
3	C1	56	ILE
3	C1	59	LYS

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Mol	Chain	Res	Type
3	C1	64	VAL
3	C1	73	LEU
3	C1	76	MET
3	C1	77	ASP
3	C1	80	LEU
3	C1	93	LEU
3	C1	116	THR
3	C1	122	VAL
3	C1	129	SER
3	C1	135	ARG
3	C1	139	MET
3	C1	151	ASN
3	C1	157	ASN
3	C1	161	SER
3	C1	175	THR
3	C1	176	VAL
3	C1	178	ASN
3	C1	179	VAL
3	C1	183	LEU
3	C1	188	LEU
3	C1	192	THR
3	C1	194	THR
3	C1	196	ILE
3	C1	206	VAL
3	C1	208	VAL
3	C1	216	LEU
3	C1	217	ARG
3	C2	5	VAL
3	C2	8	VAL
3	C2	11	SER
3	C2	16	SER
3	C2	18	VAL
3	C2	23	THR
3	C2	31	VAL
3	C2	35	GLN
3	C2	36	VAL
3	C2	42	ASN
3	C2	50	THR
3	C2	56	ILE
3	C2	59	LYS
3	C2	64	VAL
3	C2	73	LEU

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Mol	Chain	Res	Type
3	C2	76	MET
3	C2	77	ASP
3	C2	80	LEU
3	C2	93	LEU
3	C2	116	THR
3	C2	122	VAL
3	C2	129	SER
3	C2	135	ARG
3	C2	139	MET
3	C2	151	ASN
3	C2	157	ASN
3	C2	161	SER
3	C2	175	THR
3	C2	176	VAL
3	C2	178	ASN
3	C2	179	VAL
3	C2	183	LEU
3	C2	188	LEU
3	C2	192	THR
3	C2	194	THR
3	C2	196	ILE
3	C2	206	VAL
3	C2	208	VAL
3	C2	216	LEU
3	C2	217	ARG
3	C3	5	VAL
3	C3	8	VAL
3	C3	11	SER
3	C3	16	SER
3	C3	18	VAL
3	C3	23	THR
3	C3	31	VAL
3	C3	35	GLN
3	C3	36	VAL
3	C3	42	ASN
3	C3	50	THR
3	C3	56	ILE
3	C3	59	LYS
3	C3	64	VAL
3	C3	73	LEU
3	C3	76	MET
3	C3	77	ASP

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Mol	Chain	Res	Type
3	C3	80	LEU
3	C3	93	LEU
3	C3	116	THR
3	C3	122	VAL
3	C3	129	SER
3	C3	135	ARG
3	C3	139	MET
3	C3	151	ASN
3	C3	157	ASN
3	C3	161	SER
3	C3	175	THR
3	C3	176	VAL
3	C3	178	ASN
3	C3	179	VAL
3	C3	183	LEU
3	C3	188	LEU
3	C3	192	THR
3	C3	194	THR
3	C3	196	ILE
3	C3	206	VAL
3	C3	208	VAL
3	C3	216	LEU
3	C3	217	ARG
3	C4	5	VAL
3	C4	8	VAL
3	C4	11	SER
3	C4	16	SER
3	C4	18	VAL
3	C4	23	THR
3	C4	31	VAL
3	C4	35	GLN
3	C4	36	VAL
3	C4	42	ASN
3	C4	50	THR
3	C4	56	ILE
3	C4	59	LYS
3	C4	64	VAL
3	C4	73	LEU
3	C4	76	MET
3	C4	77	ASP
3	C4	80	LEU
3	C4	93	LEU

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Mol	Chain	Res	Type
3	C4	116	THR
3	C4	122	VAL
3	C4	129	SER
3	C4	135	ARG
3	C4	139	MET
3	C4	151	ASN
3	C4	157	ASN
3	C4	161	SER
3	C4	175	THR
3	C4	176	VAL
3	C4	178	ASN
3	C4	179	VAL
3	C4	183	LEU
3	C4	188	LEU
3	C4	192	THR
3	C4	194	THR
3	C4	196	ILE
3	C4	206	VAL
3	C4	208	VAL
3	C4	216	LEU
3	C4	217	ARG
3	C5	5	VAL
3	C5	8	VAL
3	C5	11	SER
3	C5	16	SER
3	C5	18	VAL
3	C5	23	THR
3	C5	31	VAL
3	C5	35	GLN
3	C5	36	VAL
3	C5	42	ASN
3	C5	50	THR
3	C5	56	ILE
3	C5	59	LYS
3	C5	64	VAL
3	C5	73	LEU
3	C5	76	MET
3	C5	77	ASP
3	C5	80	LEU
3	C5	93	LEU
3	C5	116	THR
3	C5	122	VAL

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Mol	Chain	Res	Type
3	C5	129	SER
3	C5	135	ARG
3	C5	139	MET
3	C5	151	ASN
3	C5	157	ASN
3	C5	161	SER
3	C5	175	THR
3	C5	176	VAL
3	C5	178	ASN
3	C5	179	VAL
3	C5	183	LEU
3	C5	188	LEU
3	C5	192	THR
3	C5	194	THR
3	C5	196	ILE
3	C5	206	VAL
3	C5	208	VAL
3	C5	216	LEU
3	C5	217	ARG
3	C6	5	VAL
3	C6	8	VAL
3	C6	11	SER
3	C6	16	SER
3	C6	18	VAL
3	C6	23	THR
3	C6	31	VAL
3	C6	35	GLN
3	C6	36	VAL
3	C6	42	ASN
3	C6	50	THR
3	C6	56	ILE
3	C6	59	LYS
3	C6	64	VAL
3	C6	73	LEU
3	C6	76	MET
3	C6	77	ASP
3	C6	80	LEU
3	C6	93	LEU
3	C6	116	THR
3	C6	122	VAL
3	C6	129	SER
3	C6	135	ARG

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Mol	Chain	Res	Type
3	C6	139	MET
3	C6	151	ASN
3	C6	157	ASN
3	C6	161	SER
3	C6	175	THR
3	C6	176	VAL
3	C6	178	ASN
3	C6	179	VAL
3	C6	183	LEU
3	C6	188	LEU
3	C6	192	THR
3	C6	194	THR
3	C6	196	ILE
3	C6	206	VAL
3	C6	208	VAL
3	C6	216	LEU
3	C6	217	ARG
3	C7	5	VAL
3	C7	8	VAL
3	C7	11	SER
3	C7	16	SER
3	C7	18	VAL
3	C7	23	THR
3	C7	31	VAL
3	C7	35	GLN
3	C7	36	VAL
3	C7	42	ASN
3	C7	50	THR
3	C7	56	ILE
3	C7	59	LYS
3	C7	64	VAL
3	C7	73	LEU
3	C7	76	MET
3	C7	77	ASP
3	C7	80	LEU
3	C7	93	LEU
3	C7	116	THR
3	C7	122	VAL
3	C7	129	SER
3	C7	135	ARG
3	C7	139	MET
3	C7	151	ASN

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Mol	Chain	Res	Type
3	C7	157	ASN
3	C7	161	SER
3	C7	175	THR
3	C7	176	VAL
3	C7	178	ASN
3	C7	179	VAL
3	C7	183	LEU
3	C7	188	LEU
3	C7	192	THR
3	C7	194	THR
3	C7	196	ILE
3	C7	206	VAL
3	C7	208	VAL
3	C7	216	LEU
3	C7	217	ARG
3	C8	5	VAL
3	C8	8	VAL
3	C8	11	SER
3	C8	16	SER
3	C8	18	VAL
3	C8	23	THR
3	C8	31	VAL
3	C8	35	GLN
3	C8	36	VAL
3	C8	42	ASN
3	C8	50	THR
3	C8	56	ILE
3	C8	59	LYS
3	C8	64	VAL
3	C8	73	LEU
3	C8	76	MET
3	C8	77	ASP
3	C8	80	LEU
3	C8	93	LEU
3	C8	116	THR
3	C8	122	VAL
3	C8	129	SER
3	C8	135	ARG
3	C8	139	MET
3	C8	151	ASN
3	C8	157	ASN
3	C8	161	SER

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Mol	Chain	Res	Type
3	C8	175	THR
3	C8	176	VAL
3	C8	178	ASN
3	C8	179	VAL
3	C8	183	LEU
3	C8	188	LEU
3	C8	192	THR
3	C8	194	THR
3	C8	196	ILE
3	C8	206	VAL
3	C8	208	VAL
3	C8	216	LEU
3	C8	217	ARG
3	C9	5	VAL
3	C9	8	VAL
3	C9	11	SER
3	C9	16	SER
3	C9	18	VAL
3	C9	23	THR
3	C9	31	VAL
3	C9	35	GLN
3	C9	36	VAL
3	C9	42	ASN
3	C9	50	THR
3	C9	56	ILE
3	C9	59	LYS
3	C9	64	VAL
3	C9	73	LEU
3	C9	76	MET
3	C9	77	ASP
3	C9	80	LEU
3	C9	93	LEU
3	C9	116	THR
3	C9	122	VAL
3	C9	129	SER
3	C9	135	ARG
3	C9	139	MET
3	C9	151	ASN
3	C9	157	ASN
3	C9	161	SER
3	C9	175	THR
3	C9	176	VAL

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Mol	Chain	Res	Type
3	C9	178	ASN
3	C9	179	VAL
3	C9	183	LEU
3	C9	188	LEU
3	C9	192	THR
3	C9	194	THR
3	C9	196	ILE
3	C9	206	VAL
3	C9	208	VAL
3	C9	216	LEU
3	C9	217	ARG
3	Cc	5	VAL
3	Cc	8	VAL
3	Cc	11	SER
3	Cc	16	SER
3	Cc	18	VAL
3	Cc	23	THR
3	Cc	31	VAL
3	Cc	35	GLN
3	Cc	36	VAL
3	Cc	42	ASN
3	Cc	50	THR
3	Cc	56	ILE
3	Cc	59	LYS
3	Cc	64	VAL
3	Cc	73	LEU
3	Cc	76	MET
3	Cc	77	ASP
3	Cc	80	LEU
3	Cc	93	LEU
3	Cc	116	THR
3	Cc	122	VAL
3	Cc	129	SER
3	Cc	135	ARG
3	Cc	139	MET
3	Cc	151	ASN
3	Cc	157	ASN
3	Cc	161	SER
3	Cc	175	THR
3	Cc	176	VAL
3	Cc	178	ASN
3	Cc	179	VAL

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Mol	Chain	Res	Type
3	Cc	183	LEU
3	Cc	188	LEU
3	Cc	192	THR
3	Cc	194	THR
3	Cc	196	ILE
3	Cc	206	VAL
3	Cc	208	VAL
3	Cc	216	LEU
3	Cc	217	ARG
3	Cd	5	VAL
3	Cd	8	VAL
3	Cd	11	SER
3	Cd	16	SER
3	Cd	18	VAL
3	Cd	23	THR
3	Cd	31	VAL
3	Cd	35	GLN
3	Cd	36	VAL
3	Cd	42	ASN
3	Cd	50	THR
3	Cd	56	ILE
3	Cd	59	LYS
3	Cd	64	VAL
3	Cd	73	LEU
3	Cd	76	MET
3	Cd	77	ASP
3	Cd	80	LEU
3	Cd	93	LEU
3	Cd	116	THR
3	Cd	122	VAL
3	Cd	129	SER
3	Cd	135	ARG
3	Cd	139	MET
3	Cd	151	ASN
3	Cd	157	ASN
3	Cd	161	SER
3	Cd	175	THR
3	Cd	176	VAL
3	Cd	178	ASN
3	Cd	179	VAL
3	Cd	183	LEU
3	Cd	188	LEU

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Mol	Chain	Res	Type
3	Cd	192	THR
3	Cd	194	THR
3	Cd	196	ILE
3	Cd	206	VAL
3	Cd	208	VAL
3	Cd	216	LEU
3	Cd	217	ARG
3	Ce	5	VAL
3	Ce	8	VAL
3	Ce	11	SER
3	Ce	16	SER
3	Ce	18	VAL
3	Ce	23	THR
3	Ce	31	VAL
3	Ce	35	GLN
3	Ce	36	VAL
3	Ce	42	ASN
3	Ce	50	THR
3	Ce	56	ILE
3	Ce	59	LYS
3	Ce	64	VAL
3	Ce	73	LEU
3	Ce	76	MET
3	Ce	77	ASP
3	Ce	80	LEU
3	Ce	93	LEU
3	Ce	116	THR
3	Ce	122	VAL
3	Ce	129	SER
3	Ce	135	ARG
3	Ce	139	MET
3	Ce	151	ASN
3	Ce	157	ASN
3	Ce	161	SER
3	Ce	175	THR
3	Ce	176	VAL
3	Ce	178	ASN
3	Ce	179	VAL
3	Ce	183	LEU
3	Ce	188	LEU
3	Ce	192	THR
3	Ce	194	THR

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Mol	Chain	Res	Type
3	Ce	196	ILE
3	Ce	206	VAL
3	Ce	208	VAL
3	Ce	216	LEU
3	Ce	217	ARG
3	Cf	5	VAL
3	Cf	8	VAL
3	Cf	11	SER
3	Cf	16	SER
3	Cf	18	VAL
3	Cf	23	THR
3	Cf	31	VAL
3	Cf	35	GLN
3	Cf	36	VAL
3	Cf	42	ASN
3	Cf	50	THR
3	Cf	56	ILE
3	Cf	59	LYS
3	Cf	64	VAL
3	Cf	73	LEU
3	Cf	76	MET
3	Cf	77	ASP
3	Cf	80	LEU
3	Cf	93	LEU
3	Cf	116	THR
3	Cf	122	VAL
3	Cf	129	SER
3	Cf	135	ARG
3	Cf	139	MET
3	Cf	151	ASN
3	Cf	157	ASN
3	Cf	161	SER
3	Cf	175	THR
3	Cf	176	VAL
3	Cf	178	ASN
3	Cf	179	VAL
3	Cf	183	LEU
3	Cf	188	LEU
3	Cf	192	THR
3	Cf	194	THR
3	Cf	196	ILE
3	Cf	206	VAL

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Mol	Chain	Res	Type
3	Cf	208	VAL
3	Cf	216	LEU
3	Cf	217	ARG
3	Cg	5	VAL
3	Cg	8	VAL
3	Cg	11	SER
3	Cg	16	SER
3	Cg	18	VAL
3	Cg	23	THR
3	Cg	31	VAL
3	Cg	35	GLN
3	Cg	36	VAL
3	Cg	42	ASN
3	Cg	50	THR
3	Cg	56	ILE
3	Cg	59	LYS
3	Cg	64	VAL
3	Cg	73	LEU
3	Cg	76	MET
3	Cg	77	ASP
3	Cg	80	LEU
3	Cg	93	LEU
3	Cg	116	THR
3	Cg	122	VAL
3	Cg	129	SER
3	Cg	135	ARG
3	Cg	139	MET
3	Cg	151	ASN
3	Cg	157	ASN
3	Cg	161	SER
3	Cg	175	THR
3	Cg	176	VAL
3	Cg	178	ASN
3	Cg	179	VAL
3	Cg	183	LEU
3	Cg	188	LEU
3	Cg	192	THR
3	Cg	194	THR
3	Cg	196	ILE
3	Cg	206	VAL
3	Cg	208	VAL
3	Cg	216	LEU

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Mol	Chain	Res	Type
3	Cg	217	ARG
3	Ch	5	VAL
3	Ch	8	VAL
3	Ch	11	SER
3	Ch	16	SER
3	Ch	18	VAL
3	Ch	23	THR
3	Ch	31	VAL
3	Ch	35	GLN
3	Ch	36	VAL
3	Ch	42	ASN
3	Ch	50	THR
3	Ch	56	ILE
3	Ch	59	LYS
3	Ch	64	VAL
3	Ch	73	LEU
3	Ch	76	MET
3	Ch	77	ASP
3	Ch	80	LEU
3	Ch	93	LEU
3	Ch	116	THR
3	Ch	122	VAL
3	Ch	129	SER
3	Ch	135	ARG
3	Ch	139	MET
3	Ch	151	ASN
3	Ch	157	ASN
3	Ch	161	SER
3	Ch	175	THR
3	Ch	176	VAL
3	Ch	178	ASN
3	Ch	179	VAL
3	Ch	183	LEU
3	Ch	188	LEU
3	Ch	192	THR
3	Ch	194	THR
3	Ch	196	ILE
3	Ch	206	VAL
3	Ch	208	VAL
3	Ch	216	LEU
3	Ch	217	ARG
3	Ci	5	VAL

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Mol	Chain	Res	Type
3	Ci	8	VAL
3	Ci	11	SER
3	Ci	16	SER
3	Ci	18	VAL
3	Ci	23	THR
3	Ci	31	VAL
3	Ci	35	GLN
3	Ci	36	VAL
3	Ci	42	ASN
3	Ci	50	THR
3	Ci	56	ILE
3	Ci	59	LYS
3	Ci	64	VAL
3	Ci	73	LEU
3	Ci	76	MET
3	Ci	77	ASP
3	Ci	80	LEU
3	Ci	93	LEU
3	Ci	116	THR
3	Ci	122	VAL
3	Ci	129	SER
3	Ci	135	ARG
3	Ci	139	MET
3	Ci	151	ASN
3	Ci	157	ASN
3	Ci	161	SER
3	Ci	175	THR
3	Ci	176	VAL
3	Ci	178	ASN
3	Ci	179	VAL
3	Ci	183	LEU
3	Ci	188	LEU
3	Ci	192	THR
3	Ci	194	THR
3	Ci	196	ILE
3	Ci	206	VAL
3	Ci	208	VAL
3	Ci	216	LEU
3	Ci	217	ARG
3	Cj	5	VAL
3	Cj	8	VAL
3	Cj	11	SER

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Mol	Chain	Res	Type
3	Cj	16	SER
3	Cj	18	VAL
3	Cj	23	THR
3	Cj	31	VAL
3	Cj	35	GLN
3	Cj	36	VAL
3	Cj	42	ASN
3	Cj	50	THR
3	Cj	56	ILE
3	Cj	59	LYS
3	Cj	64	VAL
3	Cj	73	LEU
3	Cj	76	MET
3	Cj	77	ASP
3	Cj	80	LEU
3	Cj	93	LEU
3	Cj	116	THR
3	Cj	122	VAL
3	Cj	129	SER
3	Cj	135	ARG
3	Cj	139	MET
3	Cj	151	ASN
3	Cj	157	ASN
3	Cj	161	SER
3	Cj	175	THR
3	Cj	176	VAL
3	Cj	178	ASN
3	Cj	179	VAL
3	Cj	183	LEU
3	Cj	188	LEU
3	Cj	192	THR
3	Cj	194	THR
3	Cj	196	ILE
3	Cj	206	VAL
3	Cj	208	VAL
3	Cj	216	LEU
3	Cj	217	ARG
3	Ck	5	VAL
3	Ck	8	VAL
3	Ck	11	SER
3	Ck	16	SER
3	Ck	18	VAL

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Mol	Chain	Res	Type
3	Ck	23	THR
3	Ck	31	VAL
3	Ck	35	GLN
3	Ck	36	VAL
3	Ck	42	ASN
3	Ck	50	THR
3	Ck	56	ILE
3	Ck	59	LYS
3	Ck	64	VAL
3	Ck	73	LEU
3	Ck	76	MET
3	Ck	77	ASP
3	Ck	80	LEU
3	Ck	93	LEU
3	Ck	116	THR
3	Ck	122	VAL
3	Ck	129	SER
3	Ck	135	ARG
3	Ck	139	MET
3	Ck	151	ASN
3	Ck	157	ASN
3	Ck	161	SER
3	Ck	175	THR
3	Ck	176	VAL
3	Ck	178	ASN
3	Ck	179	VAL
3	Ck	183	LEU
3	Ck	188	LEU
3	Ck	192	THR
3	Ck	194	THR
3	Ck	196	ILE
3	Ck	206	VAL
3	Ck	208	VAL
3	Ck	216	LEU
3	Ck	217	ARG
3	Cl	5	VAL
3	Cl	8	VAL
3	Cl	11	SER
3	Cl	16	SER
3	Cl	18	VAL
3	Cl	23	THR
3	Cl	31	VAL

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Mol	Chain	Res	Type
3	Cl	35	GLN
3	Cl	36	VAL
3	Cl	42	ASN
3	Cl	50	THR
3	Cl	56	ILE
3	Cl	59	LYS
3	Cl	64	VAL
3	Cl	73	LEU
3	Cl	76	MET
3	Cl	77	ASP
3	Cl	80	LEU
3	Cl	93	LEU
3	Cl	116	THR
3	Cl	122	VAL
3	Cl	129	SER
3	Cl	135	ARG
3	Cl	139	MET
3	Cl	151	ASN
3	Cl	157	ASN
3	Cl	161	SER
3	Cl	175	THR
3	Cl	176	VAL
3	Cl	178	ASN
3	Cl	179	VAL
3	Cl	183	LEU
3	Cl	188	LEU
3	Cl	192	THR
3	Cl	194	THR
3	Cl	196	ILE
3	Cl	206	VAL
3	Cl	208	VAL
3	Cl	216	LEU
3	Cl	217	ARG
3	Cm	5	VAL
3	Cm	8	VAL
3	Cm	11	SER
3	Cm	16	SER
3	Cm	18	VAL
3	Cm	23	THR
3	Cm	31	VAL
3	Cm	35	GLN
3	Cm	36	VAL

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Mol	Chain	Res	Type
3	Cm	42	ASN
3	Cm	50	THR
3	Cm	56	ILE
3	Cm	59	LYS
3	Cm	64	VAL
3	Cm	73	LEU
3	Cm	76	MET
3	Cm	77	ASP
3	Cm	80	LEU
3	Cm	93	LEU
3	Cm	116	THR
3	Cm	122	VAL
3	Cm	129	SER
3	Cm	135	ARG
3	Cm	139	MET
3	Cm	151	ASN
3	Cm	157	ASN
3	Cm	161	SER
3	Cm	175	THR
3	Cm	176	VAL
3	Cm	178	ASN
3	Cm	179	VAL
3	Cm	183	LEU
3	Cm	188	LEU
3	Cm	192	THR
3	Cm	194	THR
3	Cm	196	ILE
3	Cm	206	VAL
3	Cm	208	VAL
3	Cm	216	LEU
3	Cm	217	ARG
3	Cn	5	VAL
3	Cn	8	VAL
3	Cn	11	SER
3	Cn	16	SER
3	Cn	18	VAL
3	Cn	23	THR
3	Cn	31	VAL
3	Cn	35	GLN
3	Cn	36	VAL
3	Cn	42	ASN
3	Cn	50	THR

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Mol	Chain	Res	Type
3	Cn	56	ILE
3	Cn	59	LYS
3	Cn	64	VAL
3	Cn	73	LEU
3	Cn	76	MET
3	Cn	77	ASP
3	Cn	80	LEU
3	Cn	93	LEU
3	Cn	116	THR
3	Cn	122	VAL
3	Cn	129	SER
3	Cn	135	ARG
3	Cn	139	MET
3	Cn	151	ASN
3	Cn	157	ASN
3	Cn	161	SER
3	Cn	175	THR
3	Cn	176	VAL
3	Cn	178	ASN
3	Cn	179	VAL
3	Cn	183	LEU
3	Cn	188	LEU
3	Cn	192	THR
3	Cn	194	THR
3	Cn	196	ILE
3	Cn	206	VAL
3	Cn	208	VAL
3	Cn	216	LEU
3	Cn	217	ARG
3	Co	5	VAL
3	Co	8	VAL
3	Co	11	SER
3	Co	16	SER
3	Co	18	VAL
3	Co	23	THR
3	Co	31	VAL
3	Co	35	GLN
3	Co	36	VAL
3	Co	42	ASN
3	Co	50	THR
3	Co	56	ILE
3	Co	59	LYS

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Mol	Chain	Res	Type
3	Co	64	VAL
3	Co	73	LEU
3	Co	76	MET
3	Co	77	ASP
3	Co	80	LEU
3	Co	93	LEU
3	Co	116	THR
3	Co	122	VAL
3	Co	129	SER
3	Co	135	ARG
3	Co	139	MET
3	Co	151	ASN
3	Co	157	ASN
3	Co	161	SER
3	Co	175	THR
3	Co	176	VAL
3	Co	178	ASN
3	Co	179	VAL
3	Co	183	LEU
3	Co	188	LEU
3	Co	192	THR
3	Co	194	THR
3	Co	196	ILE
3	Co	206	VAL
3	Co	208	VAL
3	Co	216	LEU
3	Co	217	ARG
3	Cp	5	VAL
3	Cp	8	VAL
3	Cp	11	SER
3	Cp	16	SER
3	Cp	18	VAL
3	Cp	23	THR
3	Cp	31	VAL
3	Cp	35	GLN
3	Cp	36	VAL
3	Cp	42	ASN
3	Cp	50	THR
3	Cp	56	ILE
3	Cp	59	LYS
3	Cp	64	VAL
3	Cp	73	LEU

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Mol	Chain	Res	Type
3	Cp	76	MET
3	Cp	77	ASP
3	Cp	80	LEU
3	Cp	93	LEU
3	Cp	116	THR
3	Cp	122	VAL
3	Cp	129	SER
3	Cp	135	ARG
3	Cp	139	MET
3	Cp	151	ASN
3	Cp	157	ASN
3	Cp	161	SER
3	Cp	175	THR
3	Cp	176	VAL
3	Cp	178	ASN
3	Cp	179	VAL
3	Cp	183	LEU
3	Cp	188	LEU
3	Cp	192	THR
3	Cp	194	THR
3	Cp	196	ILE
3	Cp	206	VAL
3	Cp	208	VAL
3	Cp	216	LEU
3	Cp	217	ARG
3	Cq	5	VAL
3	Cq	8	VAL
3	Cq	11	SER
3	Cq	16	SER
3	Cq	18	VAL
3	Cq	23	THR
3	Cq	31	VAL
3	Cq	35	GLN
3	Cq	36	VAL
3	Cq	42	ASN
3	Cq	50	THR
3	Cq	56	ILE
3	Cq	59	LYS
3	Cq	64	VAL
3	Cq	73	LEU
3	Cq	76	MET
3	Cq	77	ASP

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Mol	Chain	Res	Type
3	Cq	80	LEU
3	Cq	93	LEU
3	Cq	116	THR
3	Cq	122	VAL
3	Cq	129	SER
3	Cq	135	ARG
3	Cq	139	MET
3	Cq	151	ASN
3	Cq	157	ASN
3	Cq	161	SER
3	Cq	175	THR
3	Cq	176	VAL
3	Cq	178	ASN
3	Cq	179	VAL
3	Cq	183	LEU
3	Cq	188	LEU
3	Cq	192	THR
3	Cq	194	THR
3	Cq	196	ILE
3	Cq	206	VAL
3	Cq	208	VAL
3	Cq	216	LEU
3	Cq	217	ARG
3	Cr	5	VAL
3	Cr	8	VAL
3	Cr	11	SER
3	Cr	16	SER
3	Cr	18	VAL
3	Cr	23	THR
3	Cr	31	VAL
3	Cr	35	GLN
3	Cr	36	VAL
3	Cr	42	ASN
3	Cr	50	THR
3	Cr	56	ILE
3	Cr	59	LYS
3	Cr	64	VAL
3	Cr	73	LEU
3	Cr	76	MET
3	Cr	77	ASP
3	Cr	80	LEU
3	Cr	93	LEU

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Mol	Chain	Res	Type
3	Cr	116	THR
3	Cr	122	VAL
3	Cr	129	SER
3	Cr	135	ARG
3	Cr	139	MET
3	Cr	151	ASN
3	Cr	157	ASN
3	Cr	161	SER
3	Cr	175	THR
3	Cr	176	VAL
3	Cr	178	ASN
3	Cr	179	VAL
3	Cr	183	LEU
3	Cr	188	LEU
3	Cr	192	THR
3	Cr	194	THR
3	Cr	196	ILE
3	Cr	206	VAL
3	Cr	208	VAL
3	Cr	216	LEU
3	Cr	217	ARG
3	Cs	5	VAL
3	Cs	8	VAL
3	Cs	11	SER
3	Cs	16	SER
3	Cs	18	VAL
3	Cs	23	THR
3	Cs	31	VAL
3	Cs	35	GLN
3	Cs	36	VAL
3	Cs	42	ASN
3	Cs	50	THR
3	Cs	56	ILE
3	Cs	59	LYS
3	Cs	64	VAL
3	Cs	73	LEU
3	Cs	76	MET
3	Cs	77	ASP
3	Cs	80	LEU
3	Cs	93	LEU
3	Cs	116	THR
3	Cs	122	VAL

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Mol	Chain	Res	Type
3	Cs	129	SER
3	Cs	135	ARG
3	Cs	139	MET
3	Cs	151	ASN
3	Cs	157	ASN
3	Cs	161	SER
3	Cs	175	THR
3	Cs	176	VAL
3	Cs	178	ASN
3	Cs	179	VAL
3	Cs	183	LEU
3	Cs	188	LEU
3	Cs	192	THR
3	Cs	194	THR
3	Cs	196	ILE
3	Cs	206	VAL
3	Cs	208	VAL
3	Cs	216	LEU
3	Cs	217	ARG
3	Ct	5	VAL
3	Ct	8	VAL
3	Ct	11	SER
3	Ct	16	SER
3	Ct	18	VAL
3	Ct	23	THR
3	Ct	31	VAL
3	Ct	35	GLN
3	Ct	36	VAL
3	Ct	42	ASN
3	Ct	50	THR
3	Ct	56	ILE
3	Ct	59	LYS
3	Ct	64	VAL
3	Ct	73	LEU
3	Ct	76	MET
3	Ct	77	ASP
3	Ct	80	LEU
3	Ct	93	LEU
3	Ct	116	THR
3	Ct	122	VAL
3	Ct	129	SER
3	Ct	135	ARG

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Mol	Chain	Res	Type
3	Ct	139	MET
3	Ct	151	ASN
3	Ct	157	ASN
3	Ct	161	SER
3	Ct	175	THR
3	Ct	176	VAL
3	Ct	178	ASN
3	Ct	179	VAL
3	Ct	183	LEU
3	Ct	188	LEU
3	Ct	192	THR
3	Ct	194	THR
3	Ct	196	ILE
3	Ct	206	VAL
3	Ct	208	VAL
3	Ct	216	LEU
3	Ct	217	ARG
3	Cu	5	VAL
3	Cu	8	VAL
3	Cu	11	SER
3	Cu	16	SER
3	Cu	18	VAL
3	Cu	23	THR
3	Cu	31	VAL
3	Cu	35	GLN
3	Cu	36	VAL
3	Cu	42	ASN
3	Cu	50	THR
3	Cu	56	ILE
3	Cu	59	LYS
3	Cu	64	VAL
3	Cu	73	LEU
3	Cu	76	MET
3	Cu	77	ASP
3	Cu	80	LEU
3	Cu	93	LEU
3	Cu	116	THR
3	Cu	122	VAL
3	Cu	129	SER
3	Cu	135	ARG
3	Cu	139	MET
3	Cu	151	ASN

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Mol	Chain	Res	Type
3	Cu	157	ASN
3	Cu	161	SER
3	Cu	175	THR
3	Cu	176	VAL
3	Cu	178	ASN
3	Cu	179	VAL
3	Cu	183	LEU
3	Cu	188	LEU
3	Cu	192	THR
3	Cu	194	THR
3	Cu	196	ILE
3	Cu	206	VAL
3	Cu	208	VAL
3	Cu	216	LEU
3	Cu	217	ARG
3	Cv	5	VAL
3	Cv	8	VAL
3	Cv	11	SER
3	Cv	16	SER
3	Cv	18	VAL
3	Cv	23	THR
3	Cv	31	VAL
3	Cv	35	GLN
3	Cv	36	VAL
3	Cv	42	ASN
3	Cv	50	THR
3	Cv	56	ILE
3	Cv	59	LYS
3	Cv	64	VAL
3	Cv	73	LEU
3	Cv	76	MET
3	Cv	77	ASP
3	Cv	80	LEU
3	Cv	93	LEU
3	Cv	116	THR
3	Cv	122	VAL
3	Cv	129	SER
3	Cv	135	ARG
3	Cv	139	MET
3	Cv	151	ASN
3	Cv	157	ASN
3	Cv	161	SER

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Mol	Chain	Res	Type
3	Cv	175	THR
3	Cv	176	VAL
3	Cv	178	ASN
3	Cv	179	VAL
3	Cv	183	LEU
3	Cv	188	LEU
3	Cv	192	THR
3	Cv	194	THR
3	Cv	196	ILE
3	Cv	206	VAL
3	Cv	208	VAL
3	Cv	216	LEU
3	Cv	217	ARG
3	Cw	5	VAL
3	Cw	8	VAL
3	Cw	11	SER
3	Cw	16	SER
3	Cw	18	VAL
3	Cw	23	THR
3	Cw	31	VAL
3	Cw	35	GLN
3	Cw	36	VAL
3	Cw	42	ASN
3	Cw	50	THR
3	Cw	56	ILE
3	Cw	59	LYS
3	Cw	64	VAL
3	Cw	73	LEU
3	Cw	76	MET
3	Cw	77	ASP
3	Cw	80	LEU
3	Cw	93	LEU
3	Cw	116	THR
3	Cw	122	VAL
3	Cw	129	SER
3	Cw	135	ARG
3	Cw	139	MET
3	Cw	151	ASN
3	Cw	157	ASN
3	Cw	161	SER
3	Cw	175	THR
3	Cw	176	VAL

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Mol	Chain	Res	Type
3	Cw	178	ASN
3	Cw	179	VAL
3	Cw	183	LEU
3	Cw	188	LEU
3	Cw	192	THR
3	Cw	194	THR
3	Cw	196	ILE
3	Cw	206	VAL
3	Cw	208	VAL
3	Cw	216	LEU
3	Cw	217	ARG
3	Cx	5	VAL
3	Cx	8	VAL
3	Cx	11	SER
3	Cx	16	SER
3	Cx	18	VAL
3	Cx	23	THR
3	Cx	31	VAL
3	Cx	35	GLN
3	Cx	36	VAL
3	Cx	42	ASN
3	Cx	50	THR
3	Cx	56	ILE
3	Cx	59	LYS
3	Cx	64	VAL
3	Cx	73	LEU
3	Cx	76	MET
3	Cx	77	ASP
3	Cx	80	LEU
3	Cx	93	LEU
3	Cx	116	THR
3	Cx	122	VAL
3	Cx	129	SER
3	Cx	135	ARG
3	Cx	139	MET
3	Cx	151	ASN
3	Cx	157	ASN
3	Cx	161	SER
3	Cx	175	THR
3	Cx	176	VAL
3	Cx	178	ASN
3	Cx	179	VAL

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Mol	Chain	Res	Type
3	Cx	183	LEU
3	Cx	188	LEU
3	Cx	192	THR
3	Cx	194	THR
3	Cx	196	ILE
3	Cx	206	VAL
3	Cx	208	VAL
3	Cx	216	LEU
3	Cx	217	ARG
3	DA	5	VAL
3	DA	8	VAL
3	DA	11	SER
3	DA	16	SER
3	DA	18	VAL
3	DA	23	THR
3	DA	31	VAL
3	DA	35	GLN
3	DA	36	VAL
3	DA	42	ASN
3	DA	50	THR
3	DA	56	ILE
3	DA	59	LYS
3	DA	64	VAL
3	DA	73	LEU
3	DA	76	MET
3	DA	77	ASP
3	DA	80	LEU
3	DA	93	LEU
3	DA	116	THR
3	DA	122	VAL
3	DA	129	SER
3	DA	135	ARG
3	DA	139	MET
3	DA	151	ASN
3	DA	157	ASN
3	DA	161	SER
3	DA	175	THR
3	DA	176	VAL
3	DA	178	ASN
3	DA	179	VAL
3	DA	183	LEU
3	DA	188	LEU

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Mol	Chain	Res	Type
3	DA	192	THR
3	DA	194	THR
3	DA	196	ILE
3	DA	206	VAL
3	DA	208	VAL
3	DA	216	LEU
3	DA	217	ARG
3	DB	5	VAL
3	DB	8	VAL
3	DB	11	SER
3	DB	16	SER
3	DB	18	VAL
3	DB	23	THR
3	DB	31	VAL
3	DB	35	GLN
3	DB	36	VAL
3	DB	42	ASN
3	DB	50	THR
3	DB	56	ILE
3	DB	59	LYS
3	DB	64	VAL
3	DB	73	LEU
3	DB	76	MET
3	DB	77	ASP
3	DB	80	LEU
3	DB	93	LEU
3	DB	116	THR
3	DB	122	VAL
3	DB	129	SER
3	DB	135	ARG
3	DB	139	MET
3	DB	151	ASN
3	DB	157	ASN
3	DB	161	SER
3	DB	175	THR
3	DB	176	VAL
3	DB	178	ASN
3	DB	179	VAL
3	DB	183	LEU
3	DB	188	LEU
3	DB	192	THR
3	DB	194	THR

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Mol	Chain	Res	Type
3	DB	196	ILE
3	DB	206	VAL
3	DB	208	VAL
3	DB	216	LEU
3	DB	217	ARG
1	DC	4	VAL
1	DC	28	THR
1	DC	36	ARG
1	DC	39	ASP
1	DC	40	VAL
1	DC	42	THR
1	DC	45	LEU
1	DC	49	THR
1	DC	62	SER
1	DC	71	LEU
1	DC	113	THR
1	DC	120	GLN
1	DC	150	ARG
1	DC	158	VAL
1	DC	163	MET
1	DC	166	VAL
1	DC	187	LEU
1	DC	196	LEU
1	DC	198	THR
1	DC	203	ASP
1	DC	209	LEU
1	DC	226	PRO
1	DC	237	HIS
1	DC	246	GLN
1	DD	4	VAL
1	DD	28	THR
1	DD	36	ARG
1	DD	39	ASP
1	DD	40	VAL
1	DD	42	THR
1	DD	45	LEU
1	DD	49	THR
1	DD	62	SER
1	DD	71	LEU
1	DD	113	THR
1	DD	120	GLN
1	DD	150	ARG

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Mol	Chain	Res	Type
1	DD	158	VAL
1	DD	163	MET
1	DD	166	VAL
1	DD	187	LEU
1	DD	196	LEU
1	DD	198	THR
1	DD	203	ASP
1	DD	209	LEU
1	DD	226	PRO
1	DD	237	HIS
1	DD	246	GLN
1	DE	4	VAL
1	DE	28	THR
1	DE	36	ARG
1	DE	39	ASP
1	DE	40	VAL
1	DE	42	THR
1	DE	45	LEU
1	DE	49	THR
1	DE	62	SER
1	DE	71	LEU
1	DE	113	THR
1	DE	120	GLN
1	DE	150	ARG
1	DE	158	VAL
1	DE	163	MET
1	DE	166	VAL
1	DE	187	LEU
1	DE	196	LEU
1	DE	198	THR
1	DE	203	ASP
1	DE	209	LEU
1	DE	226	PRO
1	DE	237	HIS
1	DE	246	GLN
1	DF	4	VAL
1	DF	28	THR
1	DF	36	ARG
1	DF	39	ASP
1	DF	40	VAL
1	DF	42	THR
1	DF	45	LEU

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Mol	Chain	Res	Type
1	DF	49	THR
1	DF	62	SER
1	DF	71	LEU
1	DF	113	THR
1	DF	120	GLN
1	DF	150	ARG
1	DF	158	VAL
1	DF	163	MET
1	DF	166	VAL
1	DF	187	LEU
1	DF	196	LEU
1	DF	198	THR
1	DF	203	ASP
1	DF	209	LEU
1	DF	226	PRO
1	DF	237	HIS
1	DF	246	GLN
1	DG	4	VAL
1	DG	28	THR
1	DG	36	ARG
1	DG	39	ASP
1	DG	40	VAL
1	DG	42	THR
1	DG	45	LEU
1	DG	49	THR
1	DG	62	SER
1	DG	71	LEU
1	DG	113	THR
1	DG	120	GLN
1	DG	150	ARG
1	DG	158	VAL
1	DG	163	MET
1	DG	166	VAL
1	DG	187	LEU
1	DG	196	LEU
1	DG	198	THR
1	DG	203	ASP
1	DG	209	LEU
1	DG	223	PRO
1	DG	226	PRO
1	DG	237	HIS
1	DG	246	GLN

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Mol	Chain	Res	Type
1	DH	4	VAL
1	DH	28	THR
1	DH	36	ARG
1	DH	39	ASP
1	DH	40	VAL
1	DH	42	THR
1	DH	45	LEU
1	DH	49	THR
1	DH	62	SER
1	DH	71	LEU
1	DH	113	THR
1	DH	120	GLN
1	DH	150	ARG
1	DH	158	VAL
1	DH	163	MET
1	DH	166	VAL
1	DH	187	LEU
1	DH	196	LEU
1	DH	198	THR
1	DH	203	ASP
1	DH	209	LEU
1	DH	226	PRO
1	DH	237	HIS
1	DH	246	GLN
1	DI	4	VAL
1	DI	28	THR
1	DI	36	ARG
1	DI	39	ASP
1	DI	40	VAL
1	DI	42	THR
1	DI	45	LEU
1	DI	49	THR
1	DI	62	SER
1	DI	71	LEU
1	DI	113	THR
1	DI	120	GLN
1	DI	150	ARG
1	DI	158	VAL
1	DI	163	MET
1	DI	166	VAL
1	DI	187	LEU
1	DI	196	LEU

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Mol	Chain	Res	Type
1	DI	198	THR
1	DI	203	ASP
1	DI	209	LEU
1	DI	226	PRO
1	DI	237	HIS
1	DI	246	GLN
1	DJ	4	VAL
1	DJ	28	THR
1	DJ	36	ARG
1	DJ	39	ASP
1	DJ	40	VAL
1	DJ	42	THR
1	DJ	45	LEU
1	DJ	49	THR
1	DJ	62	SER
1	DJ	71	LEU
1	DJ	113	THR
1	DJ	120	GLN
1	DJ	150	ARG
1	DJ	158	VAL
1	DJ	163	MET
1	DJ	166	VAL
1	DJ	187	LEU
1	DJ	196	LEU
1	DJ	198	THR
1	DJ	203	ASP
1	DJ	209	LEU
1	DJ	226	PRO
1	DJ	237	HIS
1	DJ	246	GLN
1	DK	4	VAL
1	DK	28	THR
1	DK	36	ARG
1	DK	39	ASP
1	DK	40	VAL
1	DK	42	THR
1	DK	45	LEU
1	DK	49	THR
1	DK	62	SER
1	DK	71	LEU
1	DK	113	THR
1	DK	120	GLN

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Mol	Chain	Res	Type
1	DK	150	ARG
1	DK	158	VAL
1	DK	163	MET
1	DK	166	VAL
1	DK	187	LEU
1	DK	196	LEU
1	DK	198	THR
1	DK	203	ASP
1	DK	209	LEU
1	DK	226	PRO
1	DK	237	HIS
1	DK	246	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1200) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	47	ASN
1	AA	87	GLN
1	AA	191	HIS
1	AA	217	ASN
1	AA	242	ASN
1	AA	246	GLN
1	AB	47	ASN
1	AB	87	GLN
1	AB	191	HIS
1	AB	217	ASN
1	AB	242	ASN
1	AB	246	GLN
1	AC	47	ASN
1	AC	87	GLN
1	AC	191	HIS
1	AC	217	ASN
1	AC	242	ASN
1	AC	246	GLN
1	AD	47	ASN
1	AD	87	GLN
1	AD	191	HIS
1	AD	217	ASN
1	AD	242	ASN
1	AD	246	GLN
1	AE	47	ASN
1	AE	87	GLN

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Mol	Chain	Res	Type
1	AE	191	HIS
1	AE	217	ASN
1	AE	242	ASN
1	AE	246	GLN
1	AF	47	ASN
1	AF	87	GLN
1	AF	191	HIS
1	AF	217	ASN
1	AF	242	ASN
1	AF	246	GLN
1	AG	47	ASN
1	AG	87	GLN
1	AG	191	HIS
1	AG	217	ASN
1	AG	242	ASN
1	AG	246	GLN
1	AH	47	ASN
1	AH	87	GLN
1	AH	191	HIS
1	AH	217	ASN
1	AH	242	ASN
1	AH	246	GLN
1	AI	47	ASN
1	AI	87	GLN
1	AI	191	HIS
1	AI	217	ASN
1	AI	242	ASN
1	AI	246	GLN
1	AJ	47	ASN
1	AJ	87	GLN
1	AJ	191	HIS
1	AJ	217	ASN
1	AJ	242	ASN
1	AJ	246	GLN
1	AK	47	ASN
1	AK	87	GLN
1	AK	191	HIS
1	AK	217	ASN
1	AK	242	ASN
1	AK	246	GLN
1	AL	47	ASN
1	AL	87	GLN

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Mol	Chain	Res	Type
1	AL	191	HIS
1	AL	217	ASN
1	AL	242	ASN
1	AL	246	GLN
1	AM	47	ASN
1	AM	87	GLN
1	AM	191	HIS
1	AM	217	ASN
1	AM	242	ASN
1	AM	246	GLN
1	AN	47	ASN
1	AN	87	GLN
1	AN	191	HIS
1	AN	217	ASN
1	AN	242	ASN
1	AN	246	GLN
1	AO	47	ASN
1	AO	87	GLN
1	AO	191	HIS
1	AO	217	ASN
1	AO	242	ASN
1	AO	246	GLN
1	AP	47	ASN
1	AP	87	GLN
1	AP	191	HIS
1	AP	217	ASN
1	AP	242	ASN
1	AP	246	GLN
1	AQ	47	ASN
1	AQ	87	GLN
1	AQ	191	HIS
1	AQ	217	ASN
1	AQ	242	ASN
1	AQ	246	GLN
1	AR	47	ASN
1	AR	87	GLN
1	AR	191	HIS
1	AR	217	ASN
1	AR	242	ASN
1	AR	246	GLN
1	AS	47	ASN
1	AS	87	GLN

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Mol	Chain	Res	Type
1	AS	191	HIS
1	AS	217	ASN
1	AS	242	ASN
1	AS	246	GLN
1	AT	47	ASN
1	AT	87	GLN
1	AT	191	HIS
1	AT	217	ASN
1	AT	242	ASN
1	AT	246	GLN
1	AU	47	ASN
1	AU	87	GLN
1	AU	191	HIS
1	AU	217	ASN
1	AU	242	ASN
1	AU	246	GLN
1	AV	47	ASN
1	AV	87	GLN
1	AV	191	HIS
1	AV	217	ASN
1	AV	242	ASN
1	AV	246	GLN
1	AW	47	ASN
1	AW	87	GLN
1	AW	191	HIS
1	AW	217	ASN
1	AW	242	ASN
1	AW	246	GLN
1	AX	47	ASN
1	AX	87	GLN
1	AX	191	HIS
1	AX	217	ASN
1	AX	242	ASN
1	AX	246	GLN
1	AY	47	ASN
1	AY	87	GLN
1	AY	191	HIS
1	AY	217	ASN
1	AY	242	ASN
1	AY	246	GLN
1	AZ	47	ASN
1	AZ	87	GLN

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Mol	Chain	Res	Type
1	AZ	191	HIS
1	AZ	217	ASN
1	AZ	242	ASN
1	AZ	246	GLN
1	A0	47	ASN
1	A0	87	GLN
1	A0	191	HIS
1	A0	217	ASN
1	A0	242	ASN
1	A0	246	GLN
1	A1	47	ASN
1	A1	87	GLN
1	A1	191	HIS
1	A1	217	ASN
1	A1	242	ASN
1	A1	246	GLN
1	A2	47	ASN
1	A2	87	GLN
1	A2	191	HIS
1	A2	217	ASN
1	A2	242	ASN
1	A2	246	GLN
1	A3	47	ASN
1	A3	87	GLN
1	A3	191	HIS
1	A3	217	ASN
1	A3	242	ASN
1	A3	246	GLN
1	A4	47	ASN
1	A4	87	GLN
1	A4	191	HIS
1	A4	217	ASN
1	A4	242	ASN
1	A4	246	GLN
1	A5	47	ASN
1	A5	87	GLN
1	A5	191	HIS
1	A5	217	ASN
1	A5	242	ASN
1	A5	246	GLN
1	A6	47	ASN
1	A6	87	GLN

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Mol	Chain	Res	Type
1	A6	191	HIS
1	A6	217	ASN
1	A6	242	ASN
1	A6	246	GLN
1	A7	47	ASN
1	A7	87	GLN
1	A7	191	HIS
1	A7	217	ASN
1	A7	242	ASN
1	A7	246	GLN
1	A8	47	ASN
1	A8	87	GLN
1	A8	191	HIS
1	A8	217	ASN
1	A8	242	ASN
1	A8	246	GLN
1	A9	47	ASN
1	A9	87	GLN
1	A9	191	HIS
1	A9	217	ASN
1	A9	242	ASN
1	A9	246	GLN
1	Aa	47	ASN
1	Aa	87	GLN
1	Aa	191	HIS
1	Aa	217	ASN
1	Aa	242	ASN
1	Aa	246	GLN
1	Ab	47	ASN
1	Ab	87	GLN
1	Ab	191	HIS
1	Ab	217	ASN
1	Ab	242	ASN
1	Ab	246	GLN
1	Ac	47	ASN
1	Ac	87	GLN
1	Ac	191	HIS
1	Ac	217	ASN
1	Ac	242	ASN
1	Ac	246	GLN
1	Ad	47	ASN
1	Ad	87	GLN

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Mol	Chain	Res	Type
1	Ad	191	HIS
1	Ad	217	ASN
1	Ad	242	ASN
1	Ad	246	GLN
1	Ae	47	ASN
1	Ae	87	GLN
1	Ae	191	HIS
1	Ae	217	ASN
1	Ae	242	ASN
1	Ae	246	GLN
1	Af	47	ASN
1	Af	87	GLN
1	Af	191	HIS
1	Af	217	ASN
1	Af	242	ASN
1	Af	246	GLN
1	Ag	47	ASN
1	Ag	87	GLN
1	Ag	191	HIS
1	Ag	217	ASN
1	Ag	242	ASN
1	Ag	246	GLN
1	Ah	47	ASN
1	Ah	87	GLN
1	Ah	191	HIS
1	Ah	217	ASN
1	Ah	242	ASN
1	Ah	246	GLN
1	Ai	47	ASN
1	Ai	87	GLN
1	Ai	191	HIS
1	Ai	217	ASN
1	Ai	242	ASN
1	Ai	246	GLN
1	Aj	47	ASN
1	Aj	87	GLN
1	Aj	191	HIS
1	Aj	217	ASN
1	Aj	242	ASN
1	Aj	246	GLN
1	Ak	47	ASN
1	Ak	87	GLN

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Mol	Chain	Res	Type
1	Ak	191	HIS
1	Ak	217	ASN
1	Ak	242	ASN
1	Ak	246	GLN
1	Al	47	ASN
1	Al	87	GLN
1	Al	191	HIS
1	Al	217	ASN
1	Al	242	ASN
1	Al	246	GLN
1	Am	47	ASN
1	Am	87	GLN
1	Am	191	HIS
1	Am	217	ASN
1	Am	242	ASN
1	Am	246	GLN
1	An	47	ASN
1	An	87	GLN
1	An	191	HIS
1	An	217	ASN
1	An	242	ASN
1	An	246	GLN
1	Ao	47	ASN
1	Ao	87	GLN
1	Ao	191	HIS
1	Ao	217	ASN
1	Ao	242	ASN
1	Ao	246	GLN
2	BA	73	GLN
2	BA	77	HIS
2	BA	95	HIS
2	BA	101	HIS
2	BA	134	HIS
2	BA	136	HIS
2	BA	168	ASN
2	BA	190	ASN
2	BB	73	GLN
2	BB	77	HIS
2	BB	95	HIS
2	BB	101	HIS
2	BB	134	HIS
2	BB	136	HIS

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Mol	Chain	Res	Type
2	BB	168	ASN
2	BB	190	ASN
2	BC	73	GLN
2	BC	77	HIS
2	BC	95	HIS
2	BC	101	HIS
2	BC	134	HIS
2	BC	136	HIS
2	BC	168	ASN
2	BC	190	ASN
2	BD	73	GLN
2	BD	77	HIS
2	BD	95	HIS
2	BD	101	HIS
2	BD	134	HIS
2	BD	136	HIS
2	BD	168	ASN
2	BD	190	ASN
2	BE	73	GLN
2	BE	77	HIS
2	BE	95	HIS
2	BE	101	HIS
2	BE	134	HIS
2	BE	136	HIS
2	BE	168	ASN
2	BE	190	ASN
2	BF	73	GLN
2	BF	77	HIS
2	BF	95	HIS
2	BF	101	HIS
2	BF	134	HIS
2	BF	136	HIS
2	BF	168	ASN
2	BF	190	ASN
2	BG	73	GLN
2	BG	77	HIS
2	BG	95	HIS
2	BG	101	HIS
2	BG	134	HIS
2	BG	136	HIS
2	BG	168	ASN
2	BG	190	ASN

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Mol	Chain	Res	Type
2	BH	73	GLN
2	BH	77	HIS
2	BH	95	HIS
2	BH	101	HIS
2	BH	134	HIS
2	BH	136	HIS
2	BH	168	ASN
2	BH	190	ASN
2	BI	73	GLN
2	BI	77	HIS
2	BI	95	HIS
2	BI	101	HIS
2	BI	134	HIS
2	BI	136	HIS
2	BI	168	ASN
2	BI	190	ASN
2	BJ	73	GLN
2	BJ	77	HIS
2	BJ	95	HIS
2	BJ	101	HIS
2	BJ	134	HIS
2	BJ	136	HIS
2	BJ	168	ASN
2	BJ	190	ASN
2	BK	73	GLN
2	BK	77	HIS
2	BK	95	HIS
2	BK	101	HIS
2	BK	134	HIS
2	BK	136	HIS
2	BK	168	ASN
2	BK	190	ASN
2	BL	73	GLN
2	BL	77	HIS
2	BL	95	HIS
2	BL	101	HIS
2	BL	134	HIS
2	BL	136	HIS
2	BL	168	ASN
2	BL	190	ASN
2	BM	73	GLN
2	BM	77	HIS

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Mol	Chain	Res	Type
2	BM	95	HIS
2	BM	101	HIS
2	BM	134	HIS
2	BM	136	HIS
2	BM	168	ASN
2	BM	190	ASN
2	BN	73	GLN
2	BN	77	HIS
2	BN	95	HIS
2	BN	101	HIS
2	BN	134	HIS
2	BN	136	HIS
2	BN	168	ASN
2	BN	190	ASN
2	BR	73	GLN
2	BR	77	HIS
2	BR	95	HIS
2	BR	101	HIS
2	BR	134	HIS
2	BR	136	HIS
2	BR	168	ASN
2	BR	190	ASN
2	BO	73	GLN
2	BO	77	HIS
2	BO	95	HIS
2	BO	101	HIS
2	BO	134	HIS
2	BO	136	HIS
2	BO	168	ASN
2	BO	190	ASN
2	BS	73	GLN
2	BS	77	HIS
2	BS	95	HIS
2	BS	101	HIS
2	BS	134	HIS
2	BS	136	HIS
2	BS	168	ASN
2	BS	190	ASN
2	BP	73	GLN
2	BP	77	HIS
2	BP	95	HIS
2	BP	101	HIS

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Mol	Chain	Res	Type
2	BP	134	HIS
2	BP	136	HIS
2	BP	168	ASN
2	BP	190	ASN
2	BQ	73	GLN
2	BQ	77	HIS
2	BQ	95	HIS
2	BQ	101	HIS
2	BQ	134	HIS
2	BQ	136	HIS
2	BQ	168	ASN
2	BQ	190	ASN
2	BT	73	GLN
2	BT	77	HIS
2	BT	95	HIS
2	BT	101	HIS
2	BT	134	HIS
2	BT	136	HIS
2	BT	168	ASN
2	BT	190	ASN
2	BU	73	GLN
2	BU	77	HIS
2	BU	95	HIS
2	BU	101	HIS
2	BU	134	HIS
2	BU	136	HIS
2	BU	168	ASN
2	BU	190	ASN
2	BV	73	GLN
2	BV	77	HIS
2	BV	95	HIS
2	BV	101	HIS
2	BV	134	HIS
2	BV	136	HIS
2	BV	168	ASN
2	BV	190	ASN
2	BW	73	GLN
2	BW	77	HIS
2	BW	95	HIS
2	BW	101	HIS
2	BW	134	HIS
2	BW	136	HIS

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Mol	Chain	Res	Type
2	BW	168	ASN
2	BW	190	ASN
2	BX	73	GLN
2	BX	77	HIS
2	BX	95	HIS
2	BX	101	HIS
2	BX	134	HIS
2	BX	136	HIS
2	BX	168	ASN
2	BX	190	ASN
2	BY	73	GLN
2	BY	77	HIS
2	BY	95	HIS
2	BY	101	HIS
2	BY	134	HIS
2	BY	136	HIS
2	BY	168	ASN
2	BY	190	ASN
2	BZ	73	GLN
2	BZ	77	HIS
2	BZ	95	HIS
2	BZ	101	HIS
2	BZ	134	HIS
2	BZ	136	HIS
2	BZ	168	ASN
2	BZ	190	ASN
2	B0	73	GLN
2	B0	77	HIS
2	B0	95	HIS
2	B0	101	HIS
2	B0	134	HIS
2	B0	136	HIS
2	B0	168	ASN
2	B0	190	ASN
2	B1	73	GLN
2	B1	77	HIS
2	B1	95	HIS
2	B1	101	HIS
2	B1	134	HIS
2	B1	136	HIS
2	B1	168	ASN
2	B1	190	ASN

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Mol	Chain	Res	Type
2	B2	73	GLN
2	B2	77	HIS
2	B2	95	HIS
2	B2	101	HIS
2	B2	134	HIS
2	B2	136	HIS
2	B2	168	ASN
2	B2	190	ASN
2	B3	73	GLN
2	B3	77	HIS
2	B3	95	HIS
2	B3	101	HIS
2	B3	134	HIS
2	B3	136	HIS
2	B3	168	ASN
2	B3	190	ASN
2	B4	73	GLN
2	B4	77	HIS
2	B4	95	HIS
2	B4	101	HIS
2	B4	134	HIS
2	B4	136	HIS
2	B4	168	ASN
2	B4	190	ASN
2	B5	73	GLN
2	B5	77	HIS
2	B5	95	HIS
2	B5	101	HIS
2	B5	134	HIS
2	B5	136	HIS
2	B5	168	ASN
2	B5	190	ASN
2	B6	73	GLN
2	B6	77	HIS
2	B6	95	HIS
2	B6	101	HIS
2	B6	134	HIS
2	B6	136	HIS
2	B6	168	ASN
2	B6	190	ASN
2	B7	73	GLN
2	B7	77	HIS

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Mol	Chain	Res	Type
2	B7	95	HIS
2	B7	101	HIS
2	B7	134	HIS
2	B7	136	HIS
2	B7	168	ASN
2	B7	190	ASN
2	B8	73	GLN
2	B8	77	HIS
2	B8	95	HIS
2	B8	101	HIS
2	B8	134	HIS
2	B8	136	HIS
2	B8	168	ASN
2	B8	190	ASN
2	B9	73	GLN
2	B9	77	HIS
2	B9	95	HIS
2	B9	101	HIS
2	B9	134	HIS
2	B9	136	HIS
2	B9	168	ASN
2	B9	190	ASN
2	Ba	73	GLN
2	Ba	77	HIS
2	Ba	95	HIS
2	Ba	101	HIS
2	Ba	134	HIS
2	Ba	136	HIS
2	Ba	168	ASN
2	Ba	190	ASN
2	Bb	73	GLN
2	Bb	77	HIS
2	Bb	95	HIS
2	Bb	101	HIS
2	Bb	134	HIS
2	Bb	136	HIS
2	Bb	168	ASN
2	Bb	190	ASN
2	Bc	73	GLN
2	Bc	77	HIS
2	Bc	95	HIS
2	Bc	101	HIS

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Mol	Chain	Res	Type
2	Bc	134	HIS
2	Bc	136	HIS
2	Bc	168	ASN
2	Bc	190	ASN
2	Bd	73	GLN
2	Bd	77	HIS
2	Bd	95	HIS
2	Bd	101	HIS
2	Bd	134	HIS
2	Bd	136	HIS
2	Bd	168	ASN
2	Bd	190	ASN
2	Be	73	GLN
2	Be	77	HIS
2	Be	95	HIS
2	Be	101	HIS
2	Be	134	HIS
2	Be	136	HIS
2	Be	168	ASN
2	Be	190	ASN
2	Bf	73	GLN
2	Bf	77	HIS
2	Bf	95	HIS
2	Bf	101	HIS
2	Bf	134	HIS
2	Bf	136	HIS
2	Bf	168	ASN
2	Bf	190	ASN
2	Bg	73	GLN
2	Bg	77	HIS
2	Bg	95	HIS
2	Bg	101	HIS
2	Bg	134	HIS
2	Bg	136	HIS
2	Bg	168	ASN
2	Bg	190	ASN
2	Bh	73	GLN
2	Bh	77	HIS
2	Bh	95	HIS
2	Bh	101	HIS
2	Bh	134	HIS
2	Bh	136	HIS

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Mol	Chain	Res	Type
2	Bh	168	ASN
2	Bh	190	ASN
2	Bi	73	GLN
2	Bi	77	HIS
2	Bi	95	HIS
2	Bi	101	HIS
2	Bi	134	HIS
2	Bi	136	HIS
2	Bi	168	ASN
2	Bi	190	ASN
2	Bj	73	GLN
2	Bj	77	HIS
2	Bj	95	HIS
2	Bj	101	HIS
2	Bj	134	HIS
2	Bj	136	HIS
2	Bj	168	ASN
2	Bj	190	ASN
2	Bk	73	GLN
2	Bk	77	HIS
2	Bk	95	HIS
2	Bk	101	HIS
2	Bk	134	HIS
2	Bk	136	HIS
2	Bk	168	ASN
2	Bk	190	ASN
2	Bl	73	GLN
2	Bl	77	HIS
2	Bl	95	HIS
2	Bl	101	HIS
2	Bl	134	HIS
2	Bl	136	HIS
2	Bl	168	ASN
2	Bl	190	ASN
2	Bm	73	GLN
2	Bm	77	HIS
2	Bm	95	HIS
2	Bm	101	HIS
2	Bm	134	HIS
2	Bm	136	HIS
2	Bm	168	ASN
2	Bm	190	ASN

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Mol	Chain	Res	Type
2	Bn	73	GLN
2	Bn	77	HIS
2	Bn	95	HIS
2	Bn	101	HIS
2	Bn	134	HIS
2	Bn	136	HIS
2	Bn	168	ASN
2	Bn	190	ASN
2	Bo	73	GLN
2	Bo	77	HIS
2	Bo	95	HIS
2	Bo	101	HIS
2	Bo	134	HIS
2	Bo	136	HIS
2	Bo	168	ASN
2	Bo	190	ASN
2	Bp	73	GLN
2	Bp	77	HIS
2	Bp	95	HIS
2	Bp	101	HIS
2	Bp	134	HIS
2	Bp	136	HIS
2	Bp	168	ASN
2	Bp	190	ASN
2	Bq	73	GLN
2	Bq	77	HIS
2	Bq	95	HIS
2	Bq	101	HIS
2	Bq	134	HIS
2	Bq	136	HIS
2	Bq	168	ASN
2	Bq	190	ASN
2	Br	73	GLN
2	Br	77	HIS
2	Br	95	HIS
2	Br	101	HIS
2	Br	134	HIS
2	Br	136	HIS
2	Br	168	ASN
2	Br	190	ASN
2	Bs	73	GLN
2	Bs	77	HIS

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Mol	Chain	Res	Type
2	Bs	95	HIS
2	Bs	101	HIS
2	Bs	134	HIS
2	Bs	136	HIS
2	Bs	168	ASN
2	Bs	190	ASN
2	Bt	73	GLN
2	Bt	77	HIS
2	Bt	95	HIS
2	Bt	101	HIS
2	Bt	134	HIS
2	Bt	136	HIS
2	Bt	168	ASN
2	Bt	190	ASN
2	Bu	73	GLN
2	Bu	77	HIS
2	Bu	95	HIS
2	Bu	101	HIS
2	Bu	134	HIS
2	Bu	136	HIS
2	Bu	168	ASN
2	Bu	190	ASN
2	Bv	73	GLN
2	Bv	77	HIS
2	Bv	95	HIS
2	Bv	101	HIS
2	Bv	134	HIS
2	Bv	136	HIS
2	Bv	168	ASN
2	Bv	190	ASN
2	Bw	73	GLN
2	Bw	77	HIS
2	Bw	95	HIS
2	Bw	101	HIS
2	Bw	134	HIS
2	Bw	136	HIS
2	Bw	168	ASN
2	Bw	190	ASN
2	Bx	73	GLN
2	Bx	77	HIS
2	Bx	95	HIS
2	Bx	101	HIS

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Mol	Chain	Res	Type
2	Bx	134	HIS
2	Bx	136	HIS
2	Bx	168	ASN
2	Bx	190	ASN
3	CA	35	GLN
3	CA	42	ASN
3	CA	75	GLN
3	CA	157	ASN
3	CA	178	ASN
3	CA	184	GLN
3	CB	35	GLN
3	CB	42	ASN
3	CB	75	GLN
3	CB	157	ASN
3	CB	178	ASN
3	CB	184	GLN
3	CC	35	GLN
3	CC	42	ASN
3	CC	75	GLN
3	CC	157	ASN
3	CC	178	ASN
3	CC	184	GLN
3	CD	35	GLN
3	CD	42	ASN
3	CD	75	GLN
3	CD	157	ASN
3	CD	178	ASN
3	CD	184	GLN
3	CE	35	GLN
3	CE	42	ASN
3	CE	75	GLN
3	CE	157	ASN
3	CE	178	ASN
3	CE	184	GLN
3	CF	35	GLN
3	CF	42	ASN
3	CF	75	GLN
3	CF	157	ASN
3	CF	178	ASN
3	CF	184	GLN
3	CG	35	GLN
3	CG	42	ASN

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Mol	Chain	Res	Type
3	CG	75	GLN
3	CG	157	ASN
3	CG	178	ASN
3	CG	184	GLN
3	CH	35	GLN
3	CH	42	ASN
3	CH	75	GLN
3	CH	157	ASN
3	CH	178	ASN
3	CH	184	GLN
3	CI	35	GLN
3	CI	42	ASN
3	CI	75	GLN
3	CI	157	ASN
3	CI	178	ASN
3	CI	184	GLN
3	CJ	35	GLN
3	CJ	42	ASN
3	CJ	75	GLN
3	CJ	157	ASN
3	CJ	178	ASN
3	CJ	184	GLN
3	CK	35	GLN
3	CK	42	ASN
3	CK	75	GLN
3	CK	157	ASN
3	CK	178	ASN
3	CK	184	GLN
3	CL	35	GLN
3	CL	42	ASN
3	CL	75	GLN
3	CL	157	ASN
3	CL	178	ASN
3	CL	184	GLN
3	CM	35	GLN
3	CM	42	ASN
3	CM	75	GLN
3	CM	157	ASN
3	CM	178	ASN
3	CM	184	GLN
3	CN	35	GLN
3	CN	42	ASN

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Mol	Chain	Res	Type
3	CN	75	GLN
3	CN	157	ASN
3	CN	178	ASN
3	CN	184	GLN
3	CO	35	GLN
3	CO	42	ASN
3	CO	75	GLN
3	CO	157	ASN
3	CO	178	ASN
3	CO	184	GLN
3	CP	35	GLN
3	CP	42	ASN
3	CP	75	GLN
3	CP	157	ASN
3	CP	178	ASN
3	CP	184	GLN
3	CQ	35	GLN
3	CQ	42	ASN
3	CQ	75	GLN
3	CQ	157	ASN
3	CQ	178	ASN
3	CQ	184	GLN
3	CR	35	GLN
3	CR	42	ASN
3	CR	75	GLN
3	CR	157	ASN
3	CR	178	ASN
3	CR	184	GLN
3	CS	35	GLN
3	CS	42	ASN
3	CS	75	GLN
3	CS	157	ASN
3	CS	178	ASN
3	CS	184	GLN
3	CT	35	GLN
3	CT	42	ASN
3	CT	75	GLN
3	CT	157	ASN
3	CT	178	ASN
3	CT	184	GLN
3	CU	35	GLN
3	CU	42	ASN

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Mol	Chain	Res	Type
3	CU	75	GLN
3	CU	157	ASN
3	CU	178	ASN
3	CU	184	GLN
3	CV	35	GLN
3	CV	42	ASN
3	CV	75	GLN
3	CV	157	ASN
3	CV	178	ASN
3	CV	184	GLN
3	CW	35	GLN
3	CW	42	ASN
3	CW	75	GLN
3	CW	157	ASN
3	CW	178	ASN
3	CW	184	GLN
3	CX	35	GLN
3	CX	42	ASN
3	CX	75	GLN
3	CX	157	ASN
3	CX	178	ASN
3	CX	184	GLN
3	CY	35	GLN
3	CY	42	ASN
3	CY	75	GLN
3	CY	157	ASN
3	CY	178	ASN
3	CY	184	GLN
3	CZ	35	GLN
3	CZ	42	ASN
3	CZ	75	GLN
3	CZ	157	ASN
3	CZ	178	ASN
3	CZ	184	GLN
3	C0	35	GLN
3	C0	42	ASN
3	C0	75	GLN
3	C0	157	ASN
3	C0	178	ASN
3	C0	184	GLN
3	C1	35	GLN
3	C1	42	ASN

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Mol	Chain	Res	Type
3	C1	75	GLN
3	C1	157	ASN
3	C1	178	ASN
3	C1	184	GLN
3	C2	35	GLN
3	C2	42	ASN
3	C2	75	GLN
3	C2	157	ASN
3	C2	178	ASN
3	C2	184	GLN
3	C3	35	GLN
3	C3	42	ASN
3	C3	75	GLN
3	C3	157	ASN
3	C3	178	ASN
3	C3	184	GLN
3	C4	35	GLN
3	C4	42	ASN
3	C4	75	GLN
3	C4	157	ASN
3	C4	178	ASN
3	C4	184	GLN
3	C5	35	GLN
3	C5	42	ASN
3	C5	75	GLN
3	C5	157	ASN
3	C5	178	ASN
3	C5	184	GLN
3	C6	35	GLN
3	C6	42	ASN
3	C6	75	GLN
3	C6	157	ASN
3	C6	178	ASN
3	C6	184	GLN
3	C7	35	GLN
3	C7	42	ASN
3	C7	75	GLN
3	C7	157	ASN
3	C7	178	ASN
3	C7	184	GLN
3	C8	35	GLN
3	C8	42	ASN

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Mol	Chain	Res	Type
3	C8	75	GLN
3	C8	157	ASN
3	C8	178	ASN
3	C8	184	GLN
3	C9	35	GLN
3	C9	42	ASN
3	C9	75	GLN
3	C9	157	ASN
3	C9	178	ASN
3	C9	184	GLN
3	Cc	35	GLN
3	Cc	42	ASN
3	Cc	75	GLN
3	Cc	157	ASN
3	Cc	178	ASN
3	Cc	184	GLN
3	Cd	35	GLN
3	Cd	42	ASN
3	Cd	75	GLN
3	Cd	157	ASN
3	Cd	178	ASN
3	Cd	184	GLN
3	Ce	35	GLN
3	Ce	42	ASN
3	Ce	75	GLN
3	Ce	157	ASN
3	Ce	178	ASN
3	Ce	184	GLN
3	Cf	35	GLN
3	Cf	42	ASN
3	Cf	75	GLN
3	Cf	157	ASN
3	Cf	178	ASN
3	Cf	184	GLN
3	Cg	35	GLN
3	Cg	42	ASN
3	Cg	75	GLN
3	Cg	157	ASN
3	Cg	178	ASN
3	Cg	184	GLN
3	Ch	35	GLN
3	Ch	42	ASN

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Mol	Chain	Res	Type
3	Ch	75	GLN
3	Ch	157	ASN
3	Ch	178	ASN
3	Ch	184	GLN
3	Ci	35	GLN
3	Ci	42	ASN
3	Ci	75	GLN
3	Ci	157	ASN
3	Ci	178	ASN
3	Ci	184	GLN
3	Cj	35	GLN
3	Cj	42	ASN
3	Cj	75	GLN
3	Cj	157	ASN
3	Cj	178	ASN
3	Cj	184	GLN
3	Ck	35	GLN
3	Ck	42	ASN
3	Ck	75	GLN
3	Ck	157	ASN
3	Ck	178	ASN
3	Ck	184	GLN
3	Cl	35	GLN
3	Cl	42	ASN
3	Cl	75	GLN
3	Cl	157	ASN
3	Cl	178	ASN
3	Cl	184	GLN
3	Cm	35	GLN
3	Cm	42	ASN
3	Cm	75	GLN
3	Cm	157	ASN
3	Cm	178	ASN
3	Cm	184	GLN
3	Cn	35	GLN
3	Cn	42	ASN
3	Cn	75	GLN
3	Cn	157	ASN
3	Cn	178	ASN
3	Cn	184	GLN
3	Co	35	GLN
3	Co	42	ASN

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Mol	Chain	Res	Type
3	Co	75	GLN
3	Co	157	ASN
3	Co	178	ASN
3	Co	184	GLN
3	Cp	35	GLN
3	Cp	42	ASN
3	Cp	75	GLN
3	Cp	157	ASN
3	Cp	178	ASN
3	Cp	184	GLN
3	Cq	35	GLN
3	Cq	42	ASN
3	Cq	75	GLN
3	Cq	157	ASN
3	Cq	178	ASN
3	Cq	184	GLN
3	Cr	35	GLN
3	Cr	42	ASN
3	Cr	75	GLN
3	Cr	157	ASN
3	Cr	178	ASN
3	Cr	184	GLN
3	Cs	35	GLN
3	Cs	42	ASN
3	Cs	75	GLN
3	Cs	157	ASN
3	Cs	178	ASN
3	Cs	184	GLN
3	Ct	35	GLN
3	Ct	42	ASN
3	Ct	75	GLN
3	Ct	157	ASN
3	Ct	178	ASN
3	Ct	184	GLN
3	Cu	35	GLN
3	Cu	42	ASN
3	Cu	75	GLN
3	Cu	157	ASN
3	Cu	178	ASN
3	Cu	184	GLN
3	Cv	35	GLN
3	Cv	42	ASN

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Mol	Chain	Res	Type
3	Cv	75	GLN
3	Cv	157	ASN
3	Cv	178	ASN
3	Cv	184	GLN
3	Cw	35	GLN
3	Cw	42	ASN
3	Cw	75	GLN
3	Cw	157	ASN
3	Cw	178	ASN
3	Cw	184	GLN
3	Cx	35	GLN
3	Cx	42	ASN
3	Cx	75	GLN
3	Cx	157	ASN
3	Cx	178	ASN
3	Cx	184	GLN
3	DA	35	GLN
3	DA	42	ASN
3	DA	75	GLN
3	DA	157	ASN
3	DA	178	ASN
3	DA	184	GLN
3	DB	35	GLN
3	DB	42	ASN
3	DB	75	GLN
3	DB	157	ASN
3	DB	178	ASN
3	DB	184	GLN
1	DC	47	ASN
1	DC	87	GLN
1	DC	191	HIS
1	DC	217	ASN
1	DC	242	ASN
1	DC	246	GLN
1	DD	47	ASN
1	DD	87	GLN
1	DD	191	HIS
1	DD	217	ASN
1	DD	242	ASN
1	DD	246	GLN
1	DE	47	ASN
1	DE	87	GLN

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Mol	Chain	Res	Type
1	DE	191	HIS
1	DE	217	ASN
1	DE	242	ASN
1	DE	246	GLN
1	DF	47	ASN
1	DF	87	GLN
1	DF	191	HIS
1	DF	217	ASN
1	DF	242	ASN
1	DF	246	GLN
1	DG	47	ASN
1	DG	87	GLN
1	DG	191	HIS
1	DG	217	ASN
1	DG	242	ASN
1	DG	246	GLN
1	DH	47	ASN
1	DH	87	GLN
1	DH	191	HIS
1	DH	217	ASN
1	DH	242	ASN
1	DH	246	GLN
1	DI	47	ASN
1	DI	87	GLN
1	DI	191	HIS
1	DI	217	ASN
1	DI	242	ASN
1	DI	246	GLN
1	DJ	47	ASN
1	DJ	87	GLN
1	DJ	191	HIS
1	DJ	217	ASN
1	DJ	242	ASN
1	DJ	246	GLN
1	DK	47	ASN
1	DK	87	GLN
1	DK	191	HIS
1	DK	217	ASN
1	DK	242	ASN
1	DK	246	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

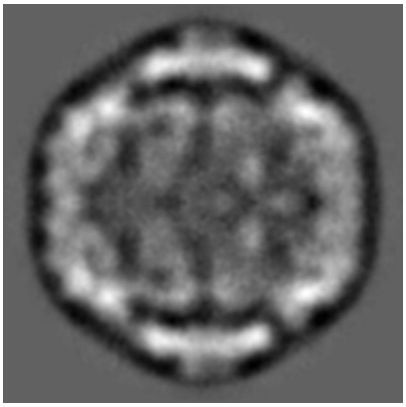
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2390. These allow visual inspection of the internal detail of the map and identification of artifacts.

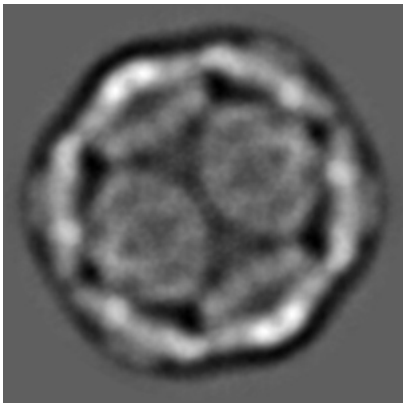
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



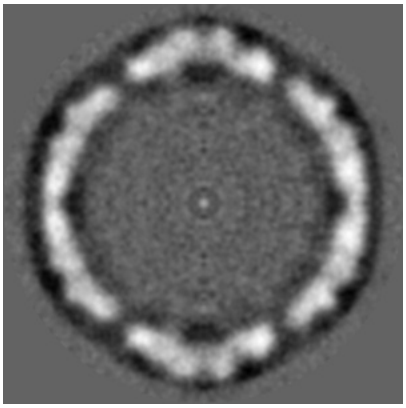
Y

Z

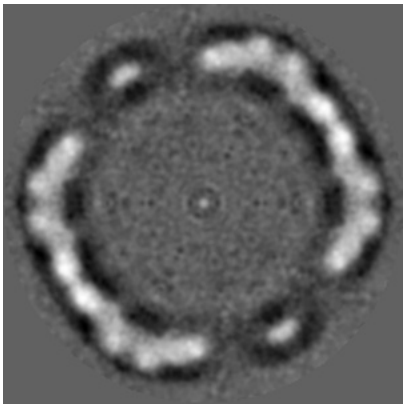
The images above show the map projected in three orthogonal directions.

6.2 Central slices

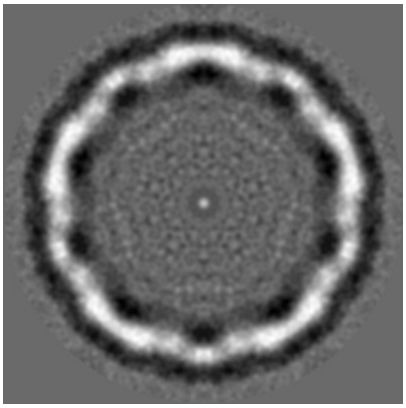
6.2.1 Primary map



X Index: 120



Y Index: 120

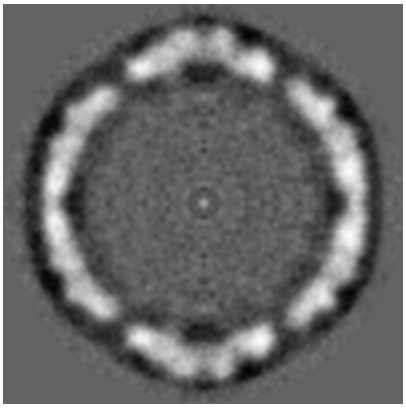


Z Index: 120

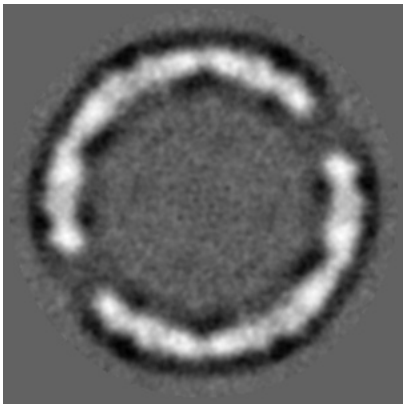
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

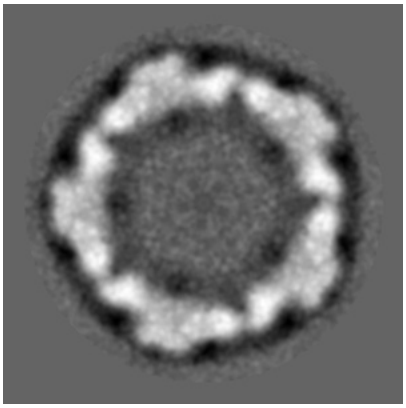
6.3.1 Primary map



X Index: 120



Y Index: 92

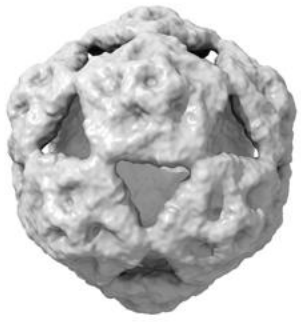


Z Index: 67

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 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

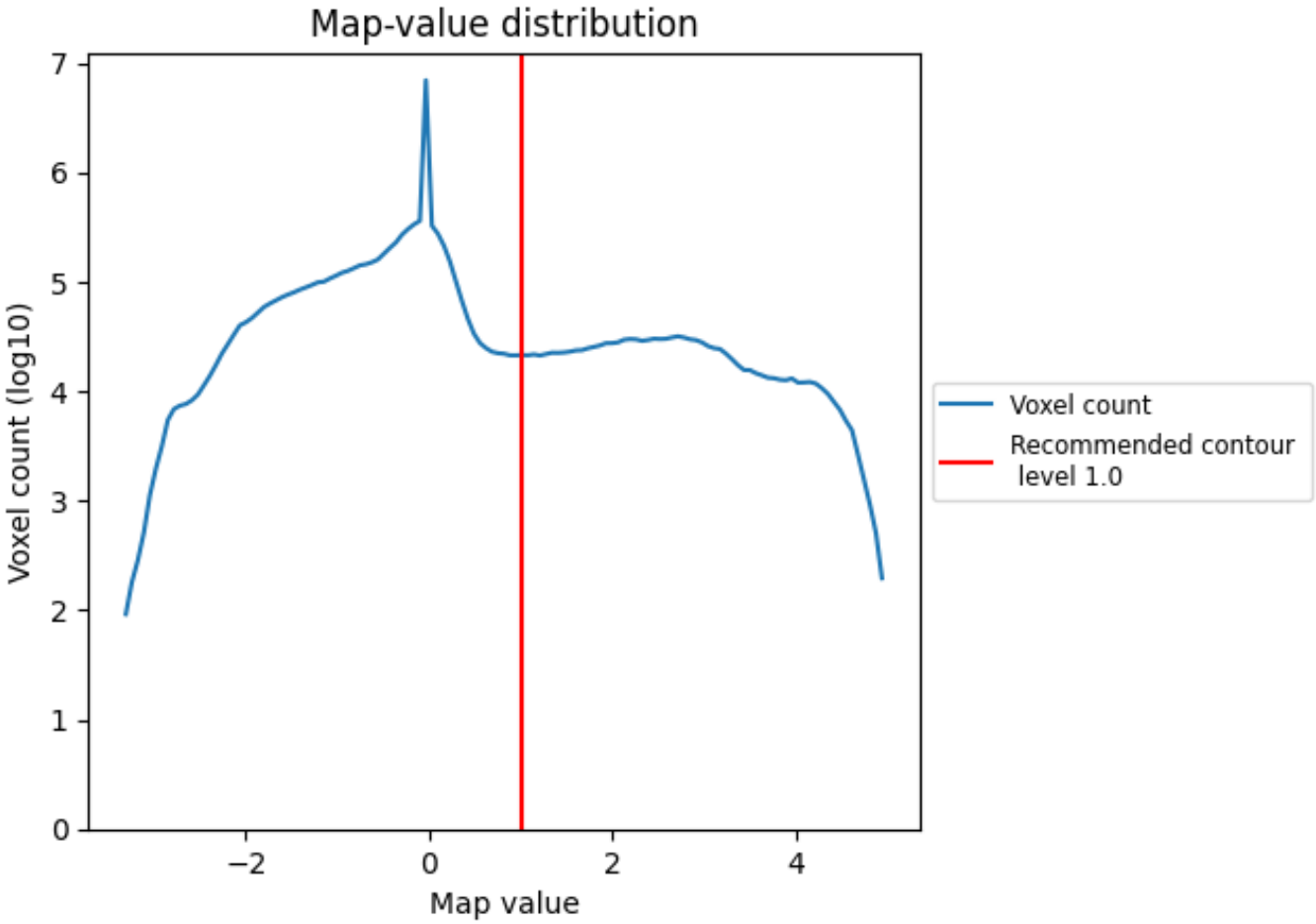
6.5 Mask visualisation (i)

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

7 Map analysis

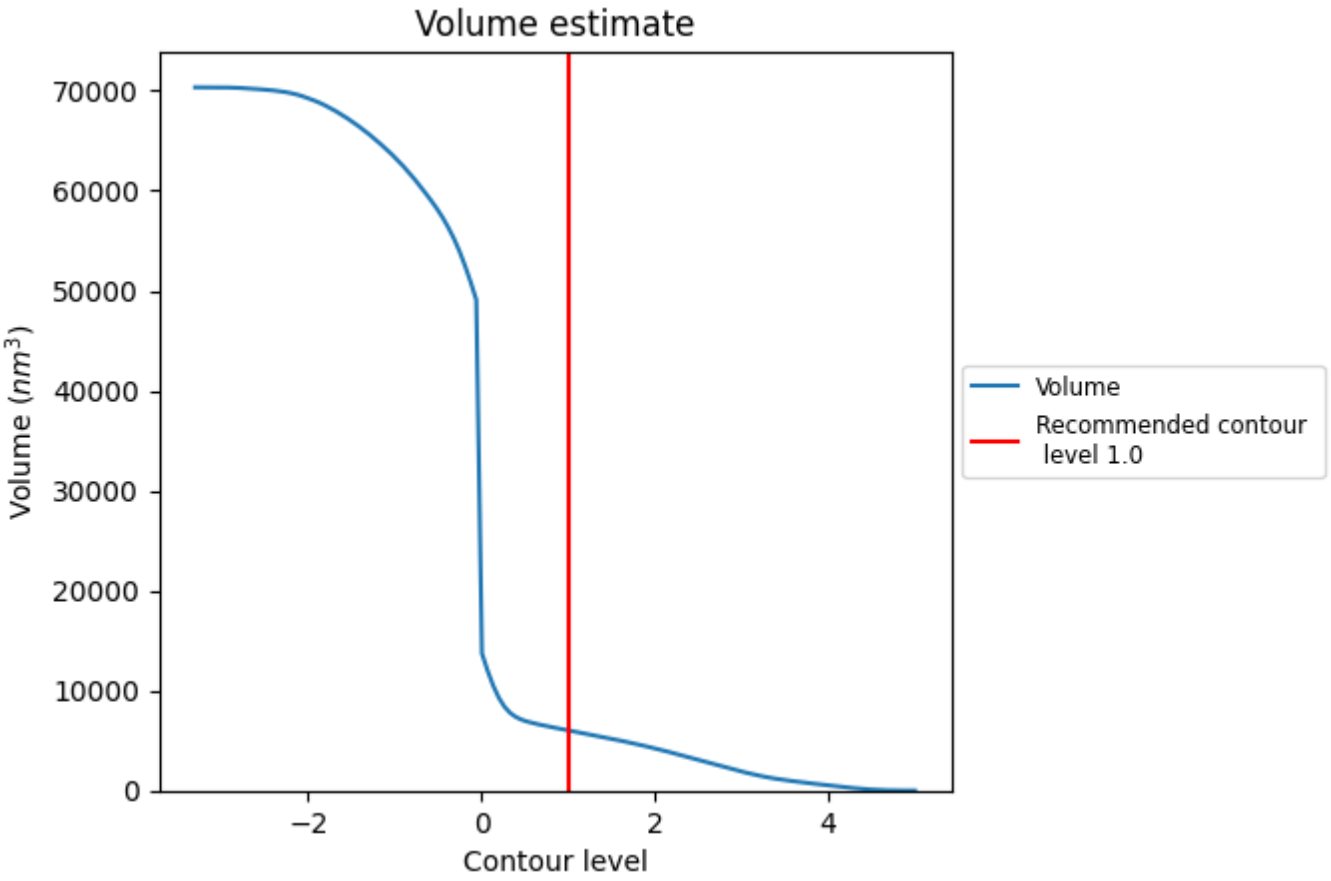
This section contains the results of statistical analysis of the map.

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.

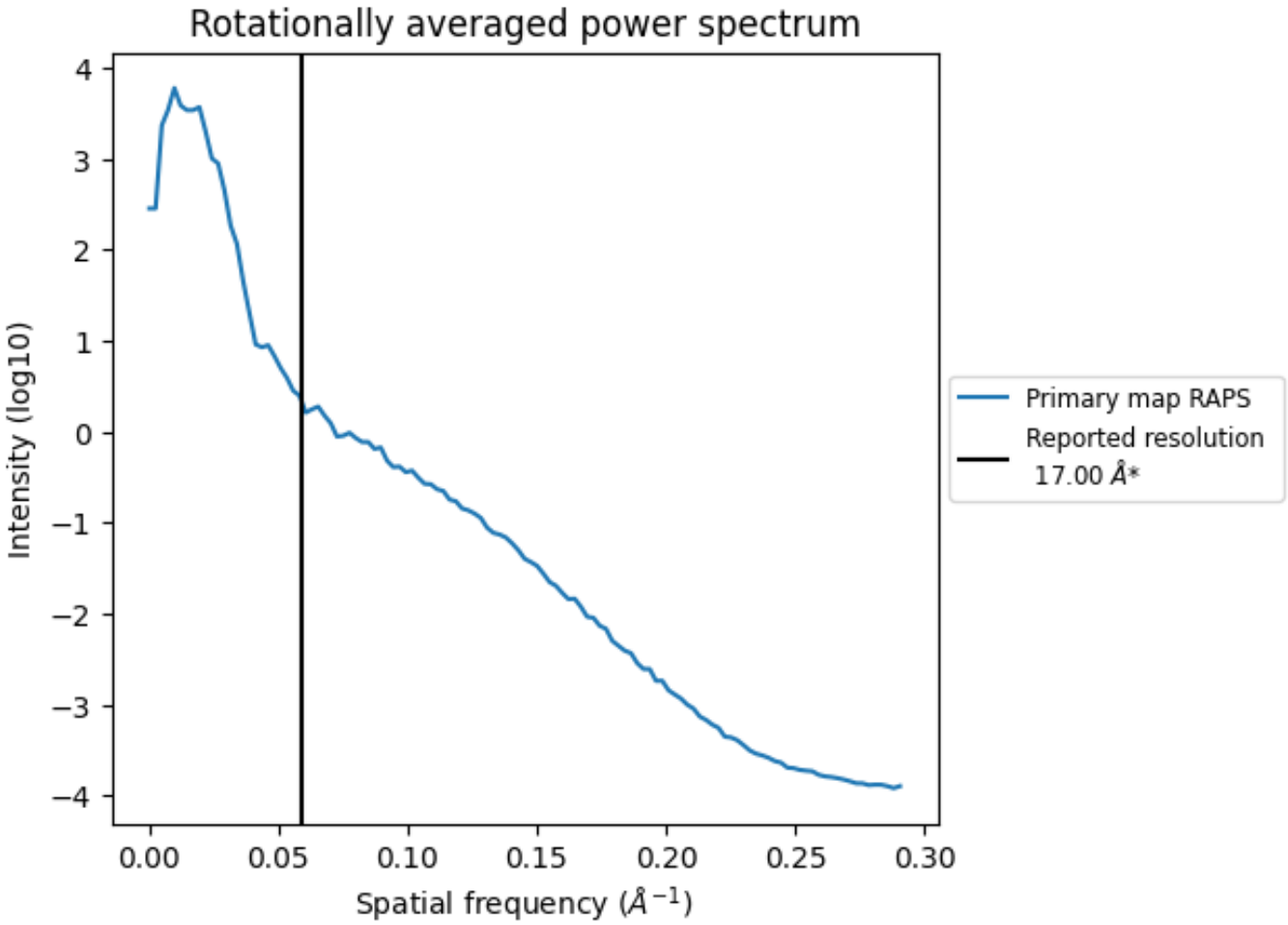
7.2 Volume estimate



The volume at the recommended contour level is 6027 nm^3; this corresponds to an approximate mass of 5444 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 0.059 Å^{-1}

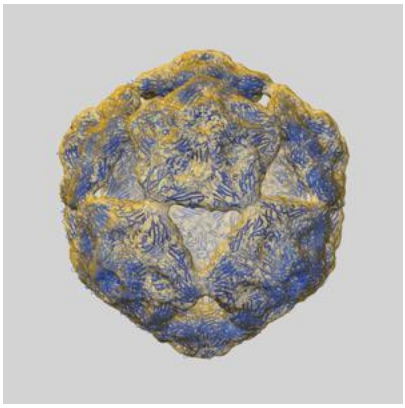
8 Fourier-Shell correlation

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

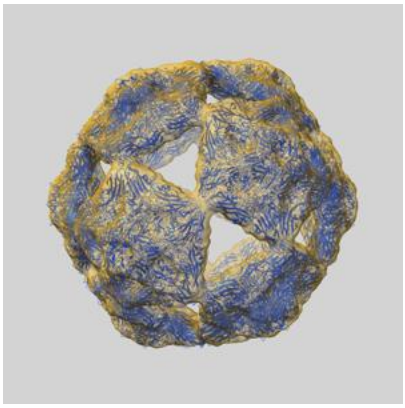
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2390 and PDB model 4CTG. Per-residue inclusion information can be found in section 3 on page 21.

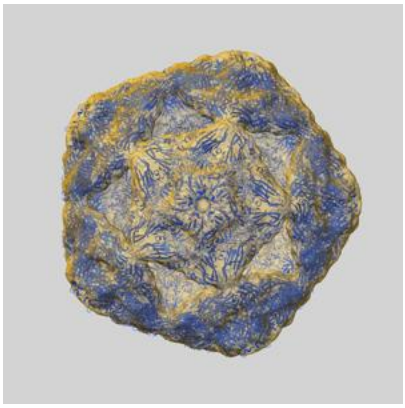
9.1 Map-model overlay



X



Y



Z

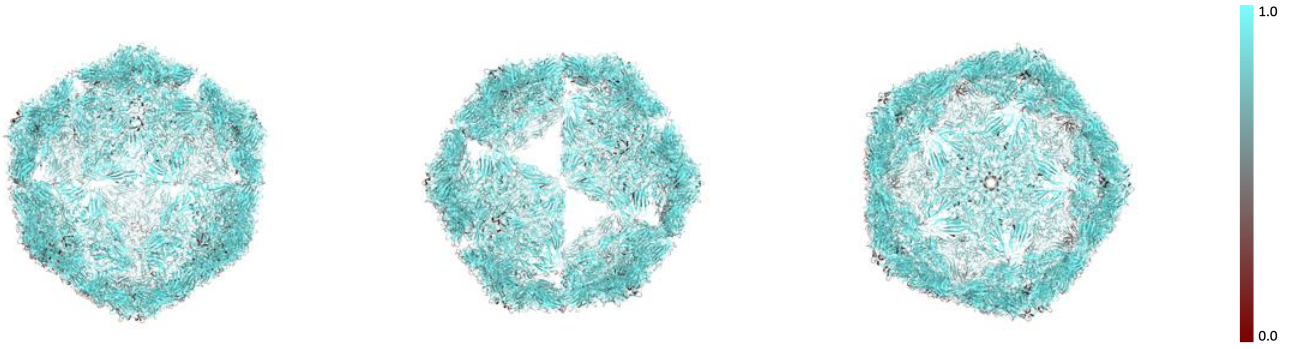
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

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.

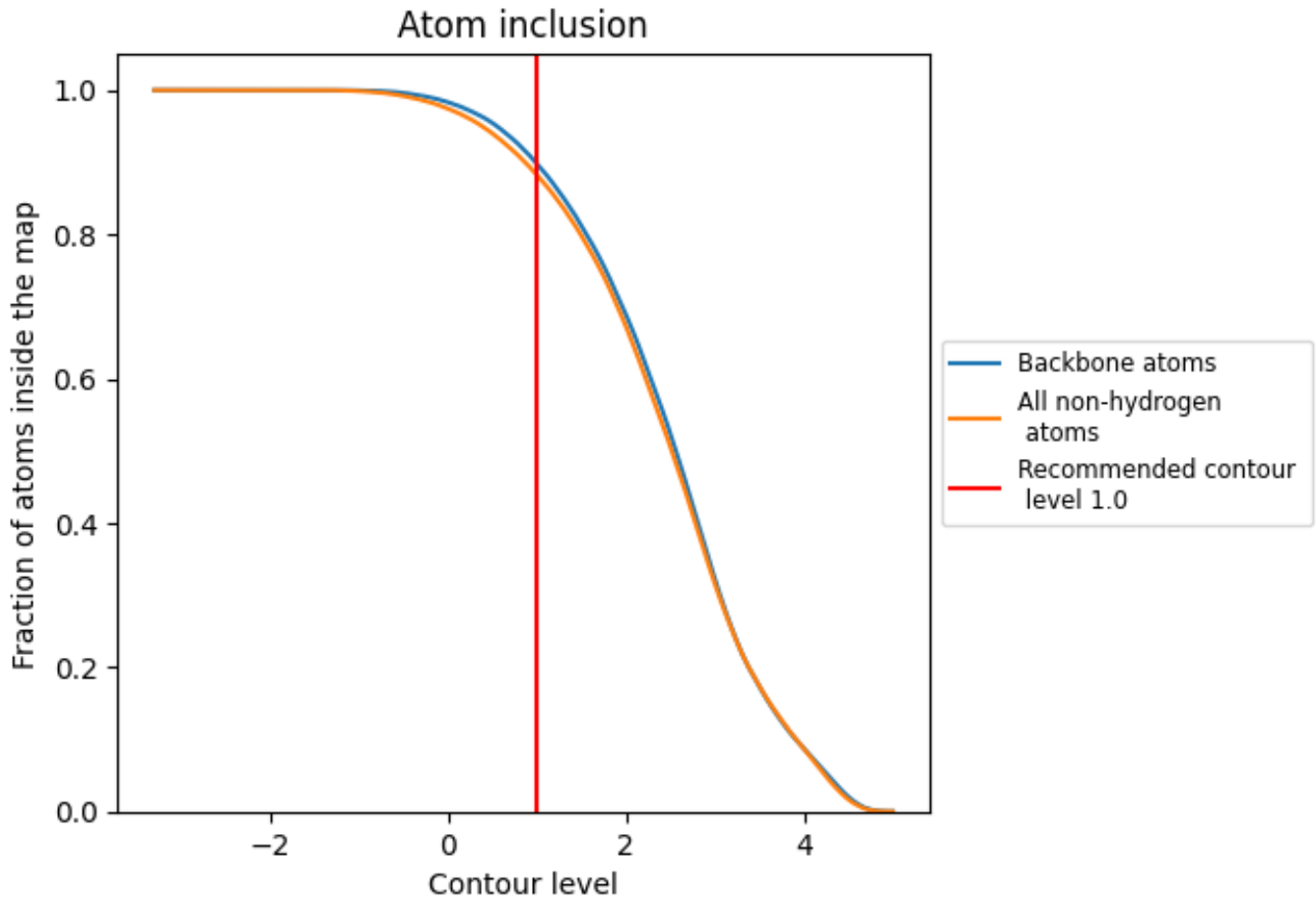
9.3 Atom inclusion mapped to coordinate model



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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8822	0.0570
A0	0.8794	0.0570
A1	0.8836	0.0500
A2	0.8878	0.0590
A3	0.8820	0.0530
A4	0.8947	0.0510
A5	0.8947	0.0550
A6	0.8847	0.0570
A7	0.8979	0.0490
A8	0.8593	0.0490
A9	0.8677	0.0510
AA	0.8942	0.0520
AB	0.9079	0.0500
AC	0.8815	0.0650
AD	0.8794	0.0530
AE	0.8921	0.0580
AF	0.8767	0.0470
AG	0.8884	0.0520
AH	0.8582	0.0570
AI	0.8608	0.0520
AJ	0.8730	0.0490
AK	0.8952	0.0510
AL	0.8799	0.0570
AM	0.8735	0.0610
AN	0.9042	0.0460
AO	0.8841	0.0470
AP	0.9053	0.0490
AQ	0.8683	0.0600
AR	0.8693	0.0520
AS	0.8841	0.0520
AT	0.8762	0.0500
AU	0.8741	0.0510
AV	0.8513	0.0560
AW	0.8608	0.0530
AX	0.8587	0.0540

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Chain	Atom inclusion	Q-score
AY	0.8984	0.0520
AZ	0.9037	0.0490
Aa	0.8519	0.0540
Ab	0.8513	0.0510
Ac	0.8624	0.0540
Ad	0.8783	0.0460
Ae	0.9021	0.0480
Af	0.8725	0.0620
Ag	0.8709	0.0570
Ah	0.8921	0.0510
Ai	0.8931	0.0460
Aj	0.8974	0.0480
Ak	0.8672	0.0550
Al	0.8704	0.0440
Am	0.8693	0.0530
An	0.8698	0.0470
Ao	0.8831	0.0480
B0	0.9008	0.0710
B1	0.9080	0.0710
B2	0.9185	0.0670
B3	0.8871	0.0720
B4	0.9087	0.0640
B5	0.8943	0.0730
B6	0.9022	0.0690
B7	0.8995	0.0750
B8	0.9217	0.0700
B9	0.9185	0.0640
BA	0.9224	0.0590
BB	0.9139	0.0690
BC	0.8943	0.0720
BD	0.9250	0.0640
BE	0.8891	0.0700
BF	0.9315	0.0620
BG	0.9217	0.0680
BH	0.8982	0.0610
BI	0.9289	0.0670
BJ	0.9041	0.0670
BK	0.9335	0.0600
BL	0.9269	0.0630
BM	0.8950	0.0680
BN	0.9106	0.0650
BO	0.9328	0.0620

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Chain	Atom inclusion	Q-score
BP	0.9008	0.0700
BQ	0.9341	0.0700
BR	0.9119	0.0720
BS	0.9198	0.0660
BT	0.8963	0.0650
BU	0.9237	0.0640
BV	0.9139	0.0680
BW	0.9028	0.0650
BX	0.9263	0.0670
BY	0.8950	0.0680
BZ	0.9172	0.0670
Ba	0.8917	0.0660
Bb	0.9067	0.0680
Bc	0.9100	0.0650
Bd	0.9289	0.0620
Be	0.9250	0.0680
Bf	0.9008	0.0680
Bg	0.9256	0.0680
Bh	0.9093	0.0730
Bi	0.9289	0.0630
Bj	0.9132	0.0670
Bk	0.9191	0.0720
Bl	0.9348	0.0690
Bm	0.8956	0.0660
Bn	0.9315	0.0670
Bo	0.9243	0.0670
Bp	0.8891	0.0690
Bq	0.9139	0.0710
Br	0.9100	0.0720
Bs	0.8982	0.0730
Bt	0.8943	0.0710
Bu	0.9237	0.0650
Bv	0.9204	0.0710
Bw	0.9230	0.0680
Bx	0.9087	0.0710
C0	0.8388	0.0540
C1	0.8524	0.0460
C2	0.8477	0.0500
C3	0.8524	0.0470
C4	0.8471	0.0510
C5	0.8424	0.0510
C6	0.8471	0.0460

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Chain	Atom inclusion	Q-score
C7	0.8501	0.0450
C8	0.8383	0.0540
C9	0.8689	0.0590
CA	0.8489	0.0560
CB	0.8406	0.0540
CC	0.8630	0.0410
CD	0.8583	0.0480
CE	0.8442	0.0460
CF	0.8784	0.0550
CG	0.8548	0.0520
CH	0.8625	0.0500
CI	0.8843	0.0550
CJ	0.8412	0.0460
CK	0.8713	0.0510
CL	0.8560	0.0540
CM	0.8554	0.0450
CN	0.8719	0.0470
CO	0.8412	0.0470
CP	0.8660	0.0550
CQ	0.8518	0.0480
CR	0.8719	0.0480
CS	0.8808	0.0520
CT	0.8442	0.0480
CU	0.8689	0.0600
CV	0.8471	0.0540
CW	0.8672	0.0560
CX	0.8790	0.0610
CY	0.8459	0.0500
CZ	0.8412	0.0530
Cc	0.8636	0.0560
Cd	0.8453	0.0540
Ce	0.8666	0.0580
Cf	0.8489	0.0560
Cg	0.8654	0.0490
Ch	0.8743	0.0520
Ci	0.8424	0.0490
Cj	0.8630	0.0570
Ck	0.8436	0.0490
Cl	0.8784	0.0530
Cm	0.8825	0.0540
Cn	0.8571	0.0460
Co	0.8819	0.0620

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Chain	Atom inclusion	Q-score
Cp	0.8566	0.0570
Cq	0.8560	0.0520
Cr	0.8802	0.0610
Cs	0.8406	0.0510
Ct	0.8436	0.0510
Cu	0.8613	0.0450
Cv	0.8548	0.0570
Cw	0.8442	0.0580
Cx	0.8619	0.0490
DA	0.8571	0.0590
DB	0.8518	0.0560
DC	0.8571	0.0560
DD	0.8561	0.0530
DE	0.8772	0.0530
DF	0.8958	0.0520
DG	0.8820	0.0630
DH	0.8852	0.0460
DI	0.9074	0.0490
DJ	0.8788	0.0530
DK	0.8772	0.0540