



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2020 – 05:05 PM BST

PDB ID : 4WIZ
Title : Crystal structure of Grouper nervous necrosis virus-like particle at 3.6Å
Authors : Chen, N.C.; Chen, C.J.; Yoshimura, M.; Guan, H.H.; Chen, T.Y.
Deposited on : 2014-09-28
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

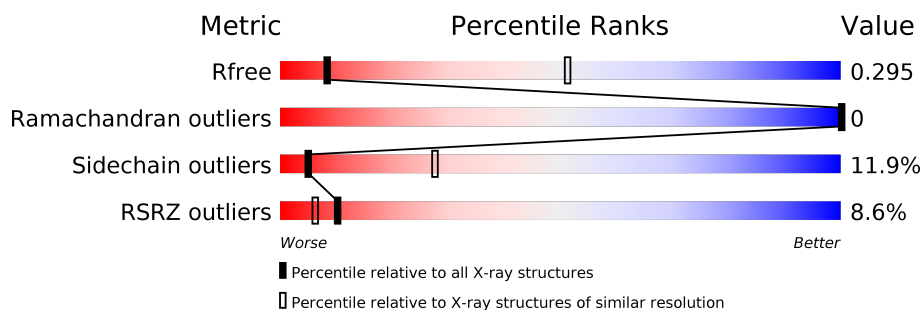
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	AA	338	
1	AB	338	
1	AC	338	
1	AD	338	
1	AE	338	
1	AF	338	
1	AG	338	

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Mol	Chain	Length	Quality of chain
1	AH	338	
1	AI	338	
1	AJ	338	
1	AK	338	
1	AL	338	
1	AM	338	
1	AN	338	
1	AO	338	
1	AP	338	
1	AQ	338	
1	AR	338	
1	AS	338	
1	AT	338	
1	AU	338	
1	AV	338	
1	AW	338	
1	AX	338	
1	AY	338	
1	AZ	338	
1	Aa	338	
1	Ab	338	
1	Ac	338	
1	Ad	338	
1	BA	338	
1	BB	338	

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Mol	Chain	Length	Quality of chain
1	BC	338	
1	BD	338	
1	BE	338	
1	BF	338	
1	BG	338	
1	BH	338	
1	BI	338	
1	BJ	338	
1	BK	338	
1	BL	338	
1	BM	338	
1	BN	338	
1	BO	338	
1	BP	338	
1	BQ	338	
1	BR	338	
1	BS	338	
1	BT	338	
1	BU	338	
1	BV	338	
1	BW	338	
1	BX	338	
1	BY	338	
1	BZ	338	
1	Ba	338	

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Mol	Chain	Length	Quality of chain
1	Bb	338	
1	Bc	338	
1	Bd	338	
1	CA	338	
1	CB	338	
1	CC	338	
1	CD	338	
1	CE	338	
1	CF	338	
1	CG	338	
1	CH	338	
1	CI	338	
1	CJ	338	
1	CK	338	
1	CL	338	
1	CM	338	
1	CN	338	
1	CO	338	
1	CP	338	
1	CQ	338	
1	CR	338	
1	CS	338	
1	CT	338	
1	CU	338	
1	CV	338	

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Mol	Chain	Length	Quality of chain
1	CW	338	
1	CX	338	
1	CY	338	
1	CZ	338	
1	Ca	338	
1	Cb	338	
1	Cc	338	
1	Cd	338	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 203250 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BA	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AA	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CA	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BB	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AB	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CB	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BC	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AC	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CC	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BD	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AD	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CD	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BE	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AE	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CE	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BF	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AF	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CF	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BG	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AG	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CG	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BH	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AH	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CH	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BI	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AI	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CI	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BJ	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AJ	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CJ	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BK	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AK	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CK	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BL	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AL	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CL	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BM	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AM	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CM	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BN	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AN	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CN	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BO	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AO	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CO	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BP	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AP	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CP	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BQ	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AQ	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CQ	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BR	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AR	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CR	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BS	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AS	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CS	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BT	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AT	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CT	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BU	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AU	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CU	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BV	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AV	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CV	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BW	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AW	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CW	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BX	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AX	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CX	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BY	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AY	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CY	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	BZ	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	AZ	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	CZ	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	Ba	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Aa	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	Ca	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	Bb	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	Ab	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	Cb	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	Bc	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	Ac	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	Cc	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			
1	Bd	286	Total	C	N	O	S	0	0	0
			2214	1401	381	425	7			
1	Ad	287	Total	C	N	O	S	0	0	0
			2218	1403	382	426	7			
1	Cd	304	Total	C	N	O	S	0	0	0
			2340	1477	406	450	7			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	214	ASN	THR	engineered mutation	UNP Q8JNX5
AA	214	ASN	THR	engineered mutation	UNP Q8JNX5
CA	214	ASN	THR	engineered mutation	UNP Q8JNX5
BB	214	ASN	THR	engineered mutation	UNP Q8JNX5
AB	214	ASN	THR	engineered mutation	UNP Q8JNX5
CB	214	ASN	THR	engineered mutation	UNP Q8JNX5
BC	214	ASN	THR	engineered mutation	UNP Q8JNX5
AC	214	ASN	THR	engineered mutation	UNP Q8JNX5
CC	214	ASN	THR	engineered mutation	UNP Q8JNX5
BD	214	ASN	THR	engineered mutation	UNP Q8JNX5
AD	214	ASN	THR	engineered mutation	UNP Q8JNX5
CD	214	ASN	THR	engineered mutation	UNP Q8JNX5
BE	214	ASN	THR	engineered mutation	UNP Q8JNX5
AE	214	ASN	THR	engineered mutation	UNP Q8JNX5
CE	214	ASN	THR	engineered mutation	UNP Q8JNX5
BF	214	ASN	THR	engineered mutation	UNP Q8JNX5
AF	214	ASN	THR	engineered mutation	UNP Q8JNX5

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Chain	Residue	Modelled	Actual	Comment	Reference
CF	214	ASN	THR	engineered mutation	UNP Q8JNX5
BG	214	ASN	THR	engineered mutation	UNP Q8JNX5
AG	214	ASN	THR	engineered mutation	UNP Q8JNX5
CG	214	ASN	THR	engineered mutation	UNP Q8JNX5
BH	214	ASN	THR	engineered mutation	UNP Q8JNX5
AH	214	ASN	THR	engineered mutation	UNP Q8JNX5
CH	214	ASN	THR	engineered mutation	UNP Q8JNX5
BI	214	ASN	THR	engineered mutation	UNP Q8JNX5
AI	214	ASN	THR	engineered mutation	UNP Q8JNX5
CI	214	ASN	THR	engineered mutation	UNP Q8JNX5
BJ	214	ASN	THR	engineered mutation	UNP Q8JNX5
AJ	214	ASN	THR	engineered mutation	UNP Q8JNX5
CJ	214	ASN	THR	engineered mutation	UNP Q8JNX5
BK	214	ASN	THR	engineered mutation	UNP Q8JNX5
AK	214	ASN	THR	engineered mutation	UNP Q8JNX5
CK	214	ASN	THR	engineered mutation	UNP Q8JNX5
BL	214	ASN	THR	engineered mutation	UNP Q8JNX5
AL	214	ASN	THR	engineered mutation	UNP Q8JNX5
CL	214	ASN	THR	engineered mutation	UNP Q8JNX5
BM	214	ASN	THR	engineered mutation	UNP Q8JNX5
AM	214	ASN	THR	engineered mutation	UNP Q8JNX5
CM	214	ASN	THR	engineered mutation	UNP Q8JNX5
BN	214	ASN	THR	engineered mutation	UNP Q8JNX5
AN	214	ASN	THR	engineered mutation	UNP Q8JNX5
CN	214	ASN	THR	engineered mutation	UNP Q8JNX5
BO	214	ASN	THR	engineered mutation	UNP Q8JNX5
AO	214	ASN	THR	engineered mutation	UNP Q8JNX5
CO	214	ASN	THR	engineered mutation	UNP Q8JNX5
BP	214	ASN	THR	engineered mutation	UNP Q8JNX5
AP	214	ASN	THR	engineered mutation	UNP Q8JNX5
CP	214	ASN	THR	engineered mutation	UNP Q8JNX5
BQ	214	ASN	THR	engineered mutation	UNP Q8JNX5
AQ	214	ASN	THR	engineered mutation	UNP Q8JNX5
CQ	214	ASN	THR	engineered mutation	UNP Q8JNX5
BR	214	ASN	THR	engineered mutation	UNP Q8JNX5
AR	214	ASN	THR	engineered mutation	UNP Q8JNX5
CR	214	ASN	THR	engineered mutation	UNP Q8JNX5
BS	214	ASN	THR	engineered mutation	UNP Q8JNX5
AS	214	ASN	THR	engineered mutation	UNP Q8JNX5
CS	214	ASN	THR	engineered mutation	UNP Q8JNX5
BT	214	ASN	THR	engineered mutation	UNP Q8JNX5
AT	214	ASN	THR	engineered mutation	UNP Q8JNX5

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Chain	Residue	Modelled	Actual	Comment	Reference
CT	214	ASN	THR	engineered mutation	UNP Q8JNX5
BU	214	ASN	THR	engineered mutation	UNP Q8JNX5
AU	214	ASN	THR	engineered mutation	UNP Q8JNX5
CU	214	ASN	THR	engineered mutation	UNP Q8JNX5
BV	214	ASN	THR	engineered mutation	UNP Q8JNX5
AV	214	ASN	THR	engineered mutation	UNP Q8JNX5
CV	214	ASN	THR	engineered mutation	UNP Q8JNX5
BW	214	ASN	THR	engineered mutation	UNP Q8JNX5
AW	214	ASN	THR	engineered mutation	UNP Q8JNX5
CW	214	ASN	THR	engineered mutation	UNP Q8JNX5
BX	214	ASN	THR	engineered mutation	UNP Q8JNX5
AX	214	ASN	THR	engineered mutation	UNP Q8JNX5
CX	214	ASN	THR	engineered mutation	UNP Q8JNX5
BY	214	ASN	THR	engineered mutation	UNP Q8JNX5
AY	214	ASN	THR	engineered mutation	UNP Q8JNX5
CY	214	ASN	THR	engineered mutation	UNP Q8JNX5
BZ	214	ASN	THR	engineered mutation	UNP Q8JNX5
AZ	214	ASN	THR	engineered mutation	UNP Q8JNX5
CZ	214	ASN	THR	engineered mutation	UNP Q8JNX5
Ba	214	ASN	THR	engineered mutation	UNP Q8JNX5
Aa	214	ASN	THR	engineered mutation	UNP Q8JNX5
Ca	214	ASN	THR	engineered mutation	UNP Q8JNX5
Bb	214	ASN	THR	engineered mutation	UNP Q8JNX5
Ab	214	ASN	THR	engineered mutation	UNP Q8JNX5
Cb	214	ASN	THR	engineered mutation	UNP Q8JNX5
Bc	214	ASN	THR	engineered mutation	UNP Q8JNX5
Ac	214	ASN	THR	engineered mutation	UNP Q8JNX5
Cc	214	ASN	THR	engineered mutation	UNP Q8JNX5
Bd	214	ASN	THR	engineered mutation	UNP Q8JNX5
Ad	214	ASN	THR	engineered mutation	UNP Q8JNX5
Cd	214	ASN	THR	engineered mutation	UNP Q8JNX5

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AP	1	Total Ca 1 1	0	0
2	BA	2	Total Ca 2 2	0	0
2	AK	1	Total Ca 1 1	0	0
2	AB	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BL	2	Total 2	Ca 2	0	0
2	Ac	1	Total 1	Ca 1	0	0
2	BE	2	Total 2	Ca 2	0	0
2	AW	1	Total 1	Ca 1	0	0
2	Bd	2	Total 2	Ca 2	0	0
2	AN	1	Total 1	Ca 1	0	0
2	BP	2	Total 2	Ca 2	0	0
2	AX	1	Total 1	Ca 1	0	0
2	BI	2	Total 2	Ca 2	0	0
2	AS	1	Total 1	Ca 1	0	0
2	BB	2	Total 2	Ca 2	0	0
2	AJ	1	Total 1	Ca 1	0	0
2	BT	2	Total 2	Ca 2	0	0
2	Ba	2	Total 2	Ca 2	0	0
2	AE	1	Total 1	Ca 1	0	0
2	BM	2	Total 2	Ca 2	0	0
2	Ab	1	Total 1	Ca 1	0	0
2	BF	2	Total 2	Ca 2	0	0
2	AV	1	Total 1	Ca 1	0	0
2	BX	2	Total 2	Ca 2	0	0
2	AA	1	Total 1	Ca 1	0	0

Continued on next page...

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BQ	2	Total 2	Ca 2	0	0
2	BJ	2	Total 2	Ca 2	0	0
2	AR	1	Total 1	Ca 1	0	0
2	BC	2	Total 2	Ca 2	0	0
2	AM	1	Total 1	Ca 1	0	0
2	BU	2	Total 2	Ca 2	0	0
2	Bb	2	Total 2	Ca 2	0	0
2	AD	1	Total 1	Ca 1	0	0
2	BN	2	Total 2	Ca 2	0	0
2	BG	2	Total 2	Ca 2	0	0
2	AI	1	Total 1	Ca 1	0	0
2	BY	2	Total 2	Ca 2	0	0
2	BR	2	Total 2	Ca 2	0	0
2	AZ	1	Total 1	Ca 1	0	0
2	Aa	1	Total 1	Ca 1	0	0
2	BK	2	Total 2	Ca 2	0	0
2	AU	1	Total 1	Ca 1	0	0
2	AL	1	Total 1	Ca 1	0	0
2	BV	2	Total 2	Ca 2	0	0
2	Bc	2	Total 2	Ca 2	0	0
2	AG	1	Total 1	Ca 1	0	0

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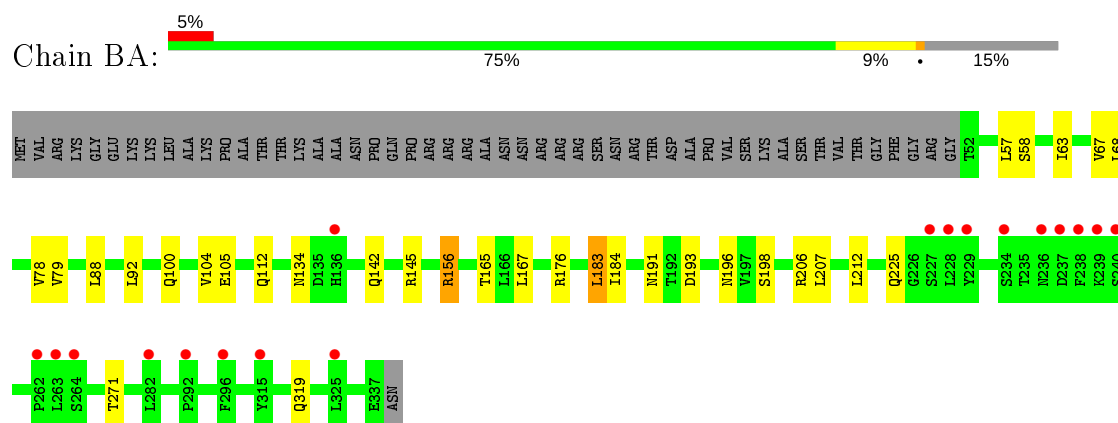
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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2	AQ	1	Total 1	Ca 1	0	0
2	Ad	1	Total 1	Ca 1	0	0
2	AH	1	Total 1	Ca 1	0	0
2	BZ	2	Total 2	Ca 2	0	0
2	AC	1	Total 1	Ca 1	0	0
2	BS	2	Total 2	Ca 2	0	0
2	BD	2	Total 2	Ca 2	0	0
2	AT	1	Total 1	Ca 1	0	0
2	AO	1	Total 1	Ca 1	0	0
2	BW	2	Total 2	Ca 2	0	0
2	AY	1	Total 1	Ca 1	0	0
2	AF	1	Total 1	Ca 1	0	0
2	BH	2	Total 2	Ca 2	0	0

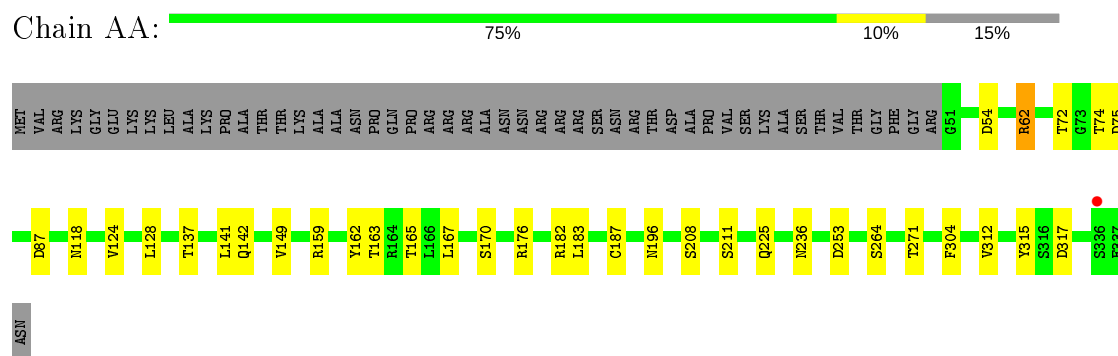
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

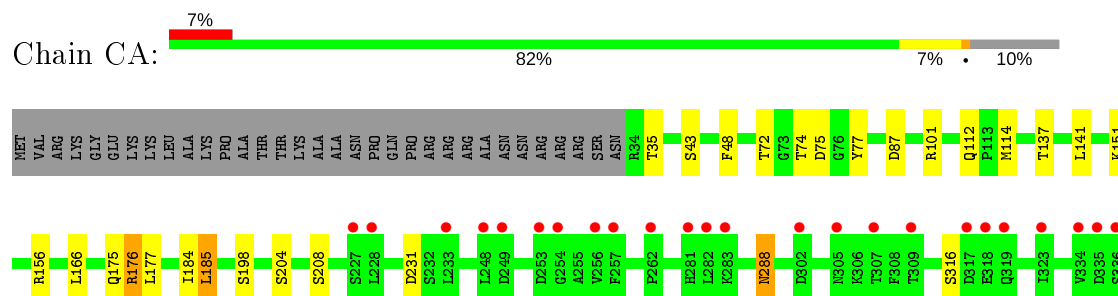
- Molecule 1: Coat protein



- Molecule 1: Coat protein



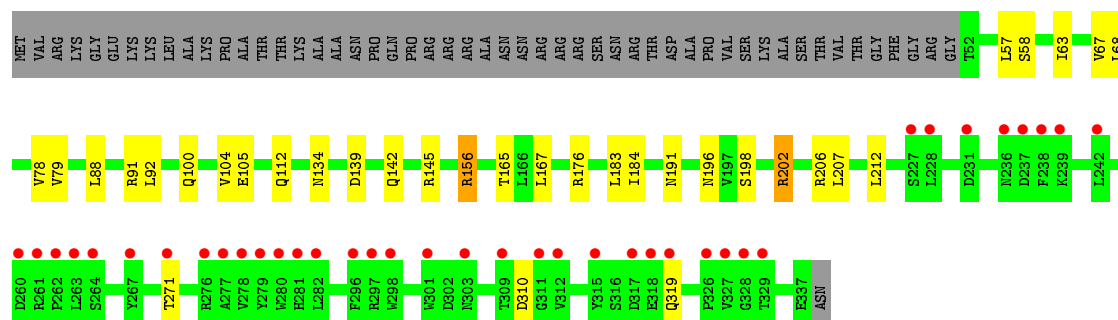
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E337
ASN

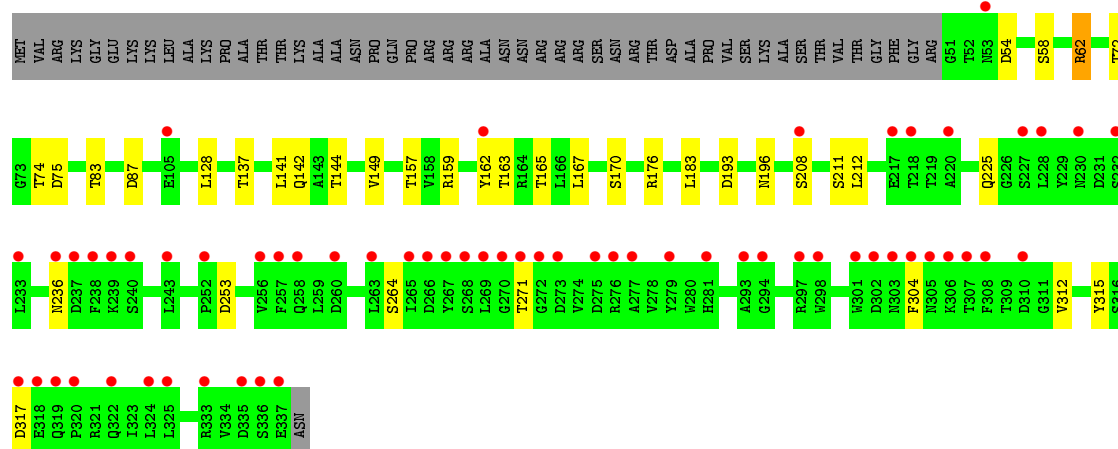
• Molecule 1: Coat protein

Chain BB: 11% 75% 9% 15%



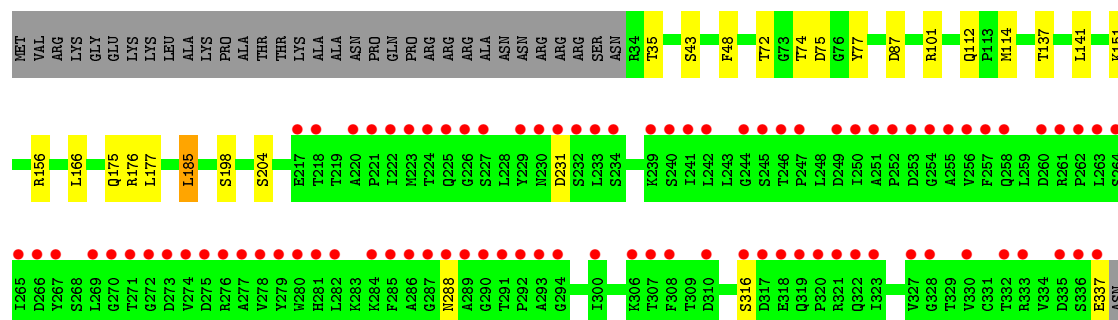
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Chain AB: 18% 74% 11% 15%

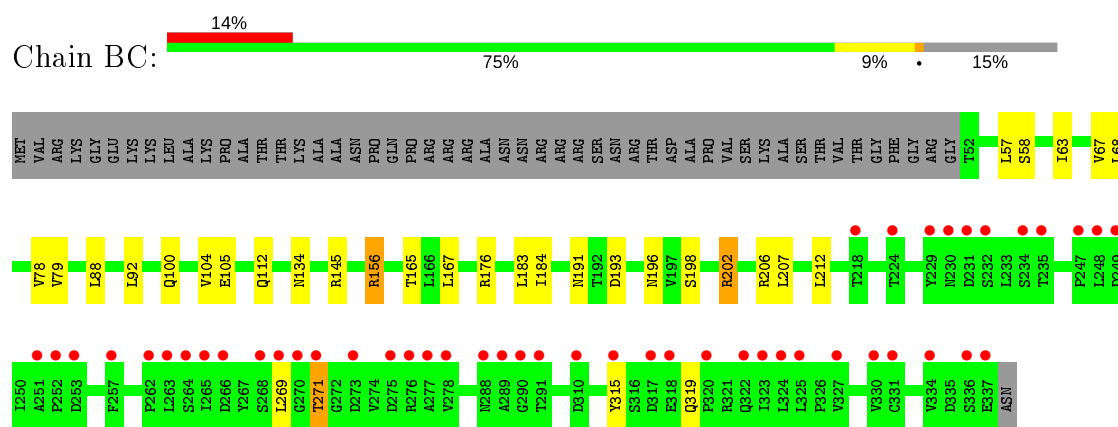


• Molecule 1: Coat protein

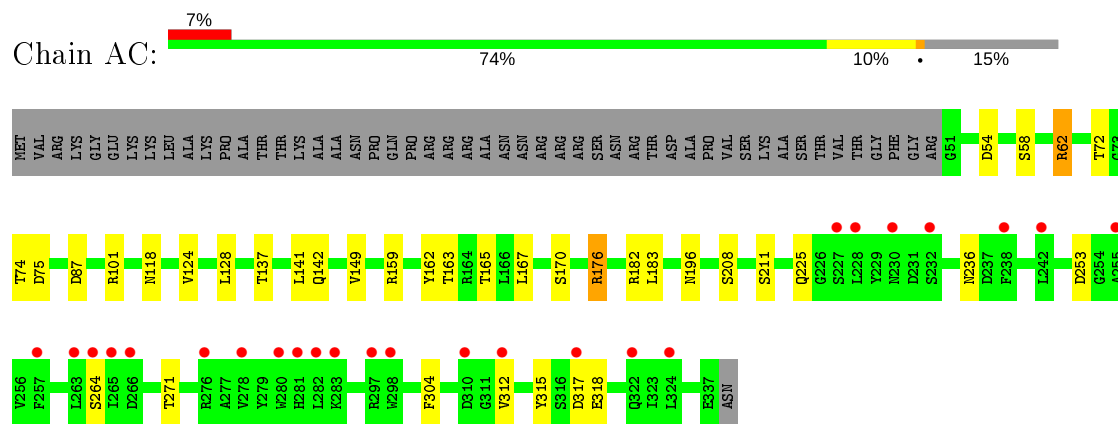
Chain CB: 26% 82% 7% 10%



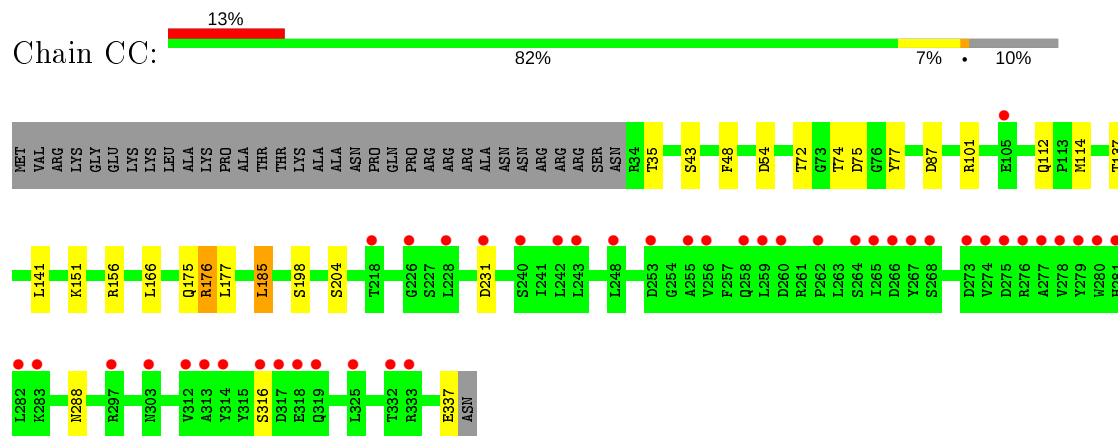
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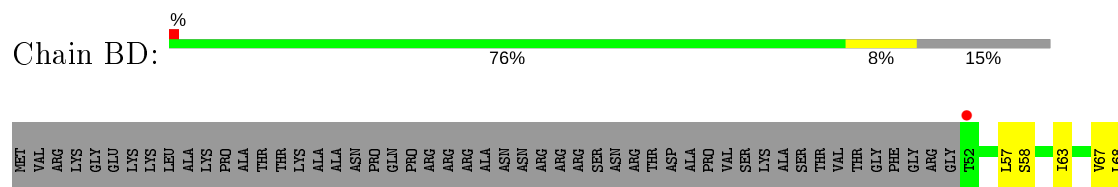
- Molecule 1: Coat protein



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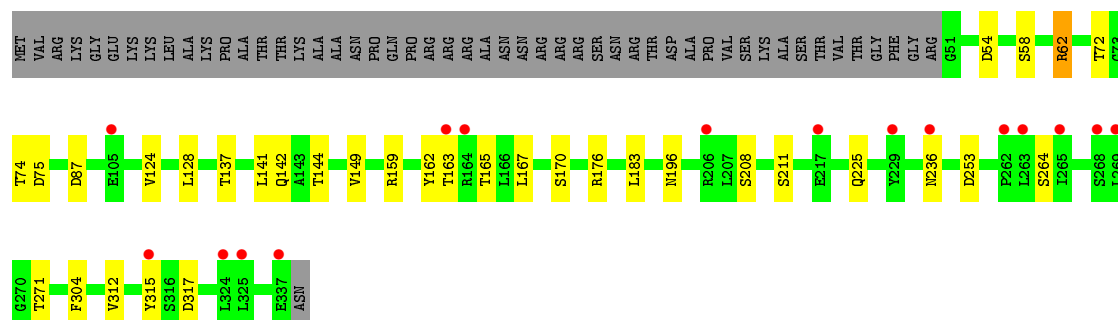
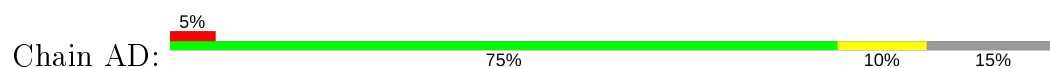


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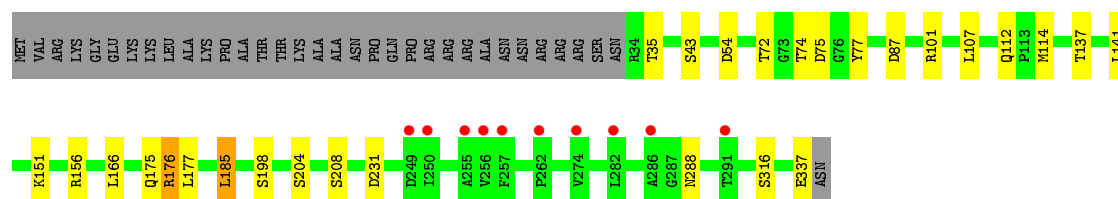
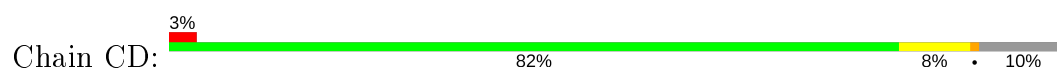




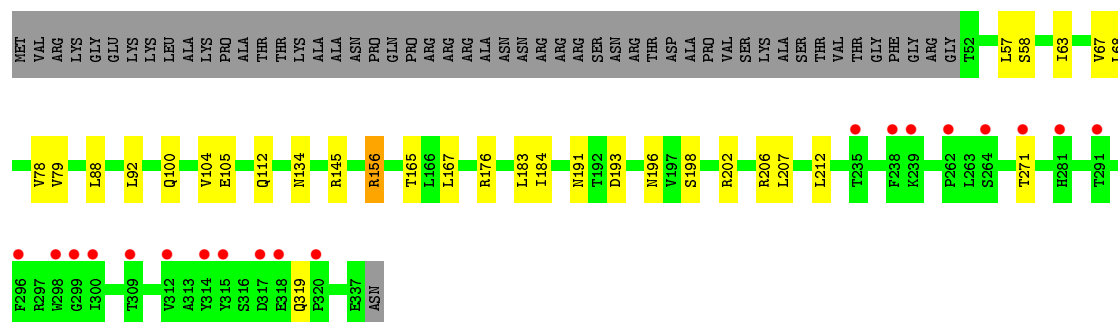
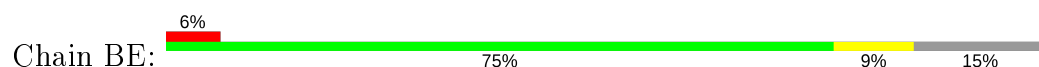
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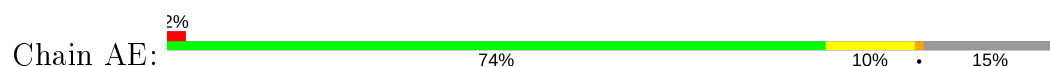
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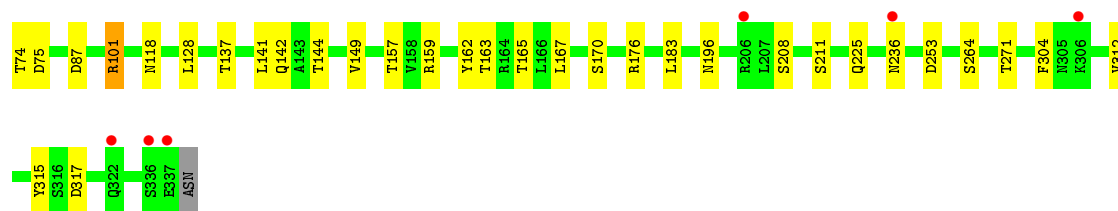


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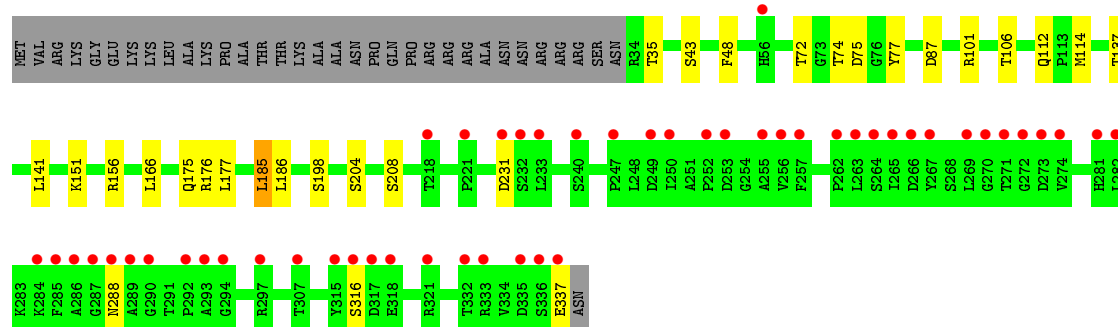
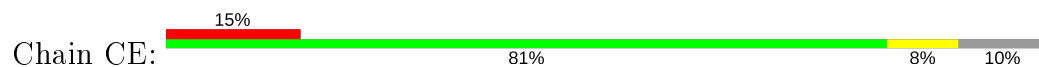


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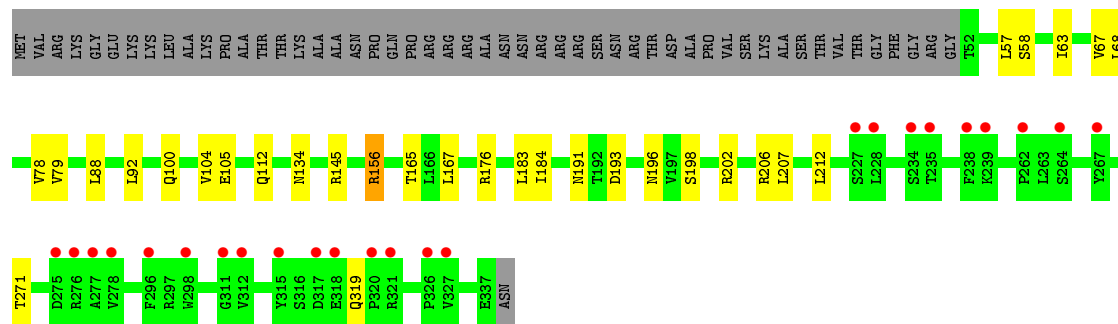
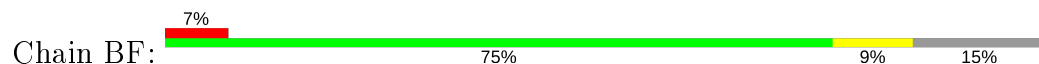




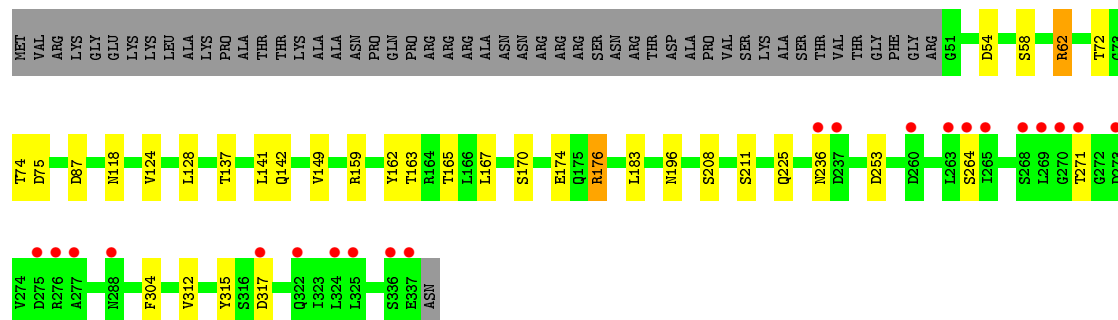
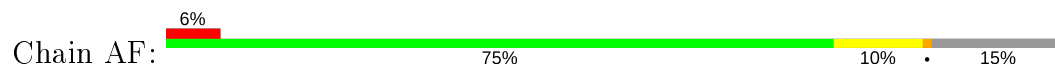
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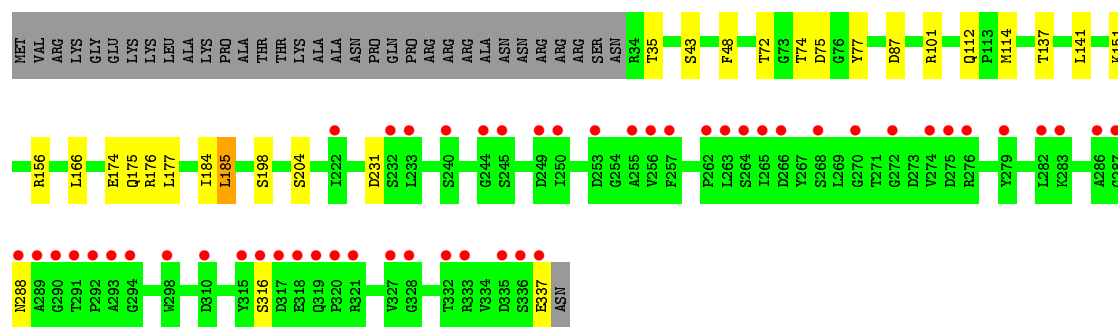


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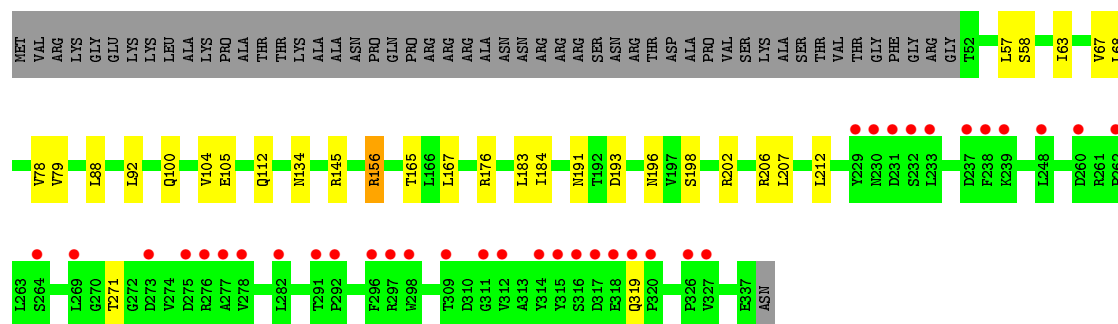
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Chain CF: 




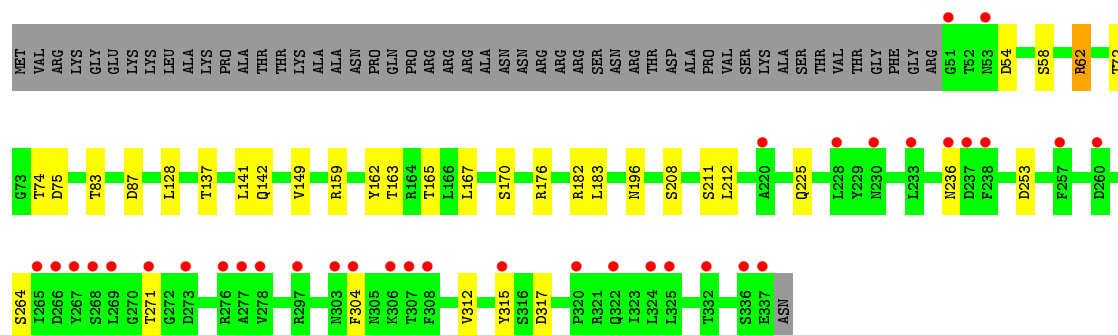
• Molecule 1: Coat protein

Chain BG: 




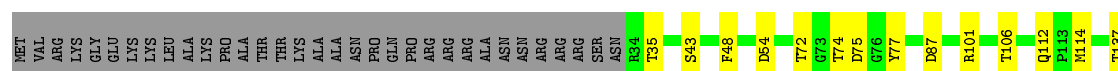
• Molecule 1: Coat protein

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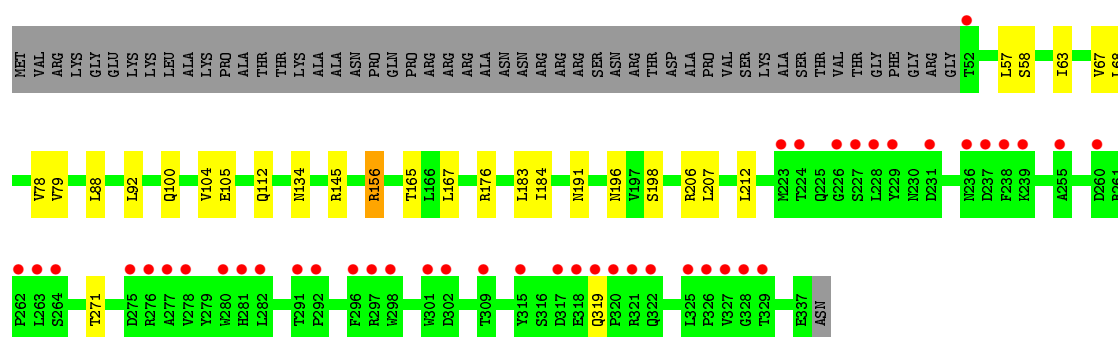
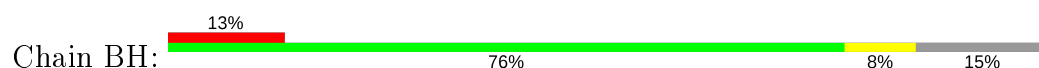
• Molecule 1: Coat protein

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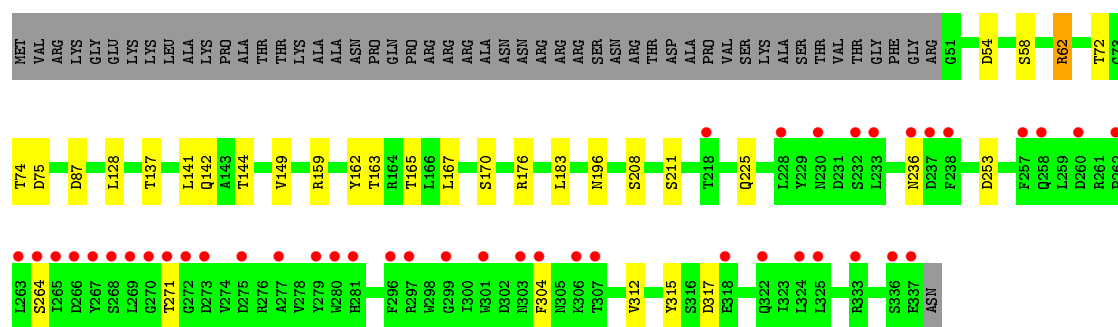
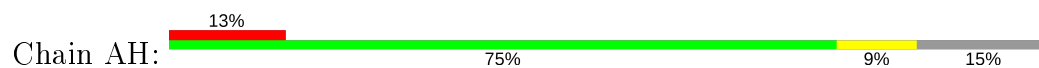




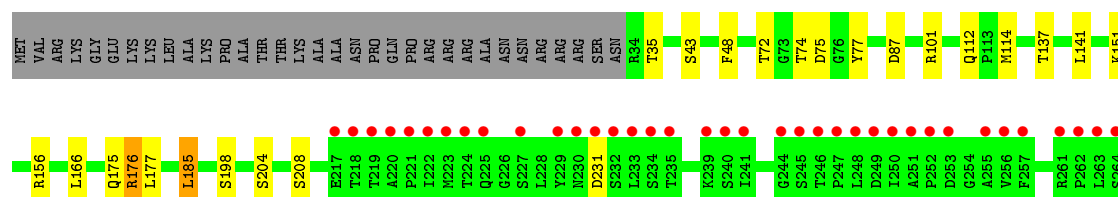
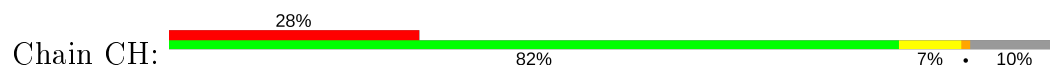
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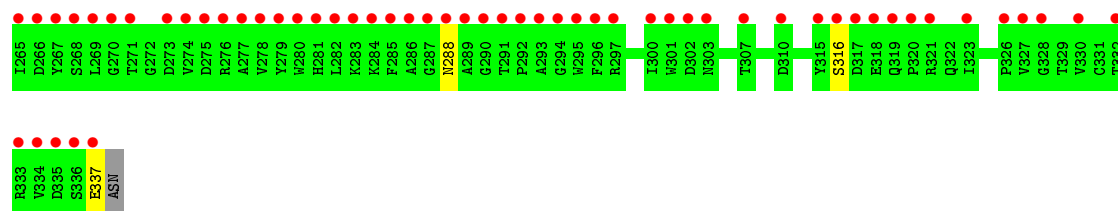


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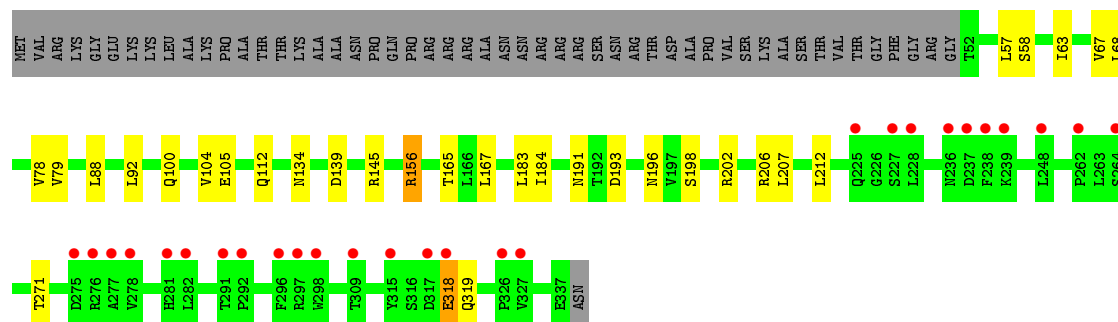
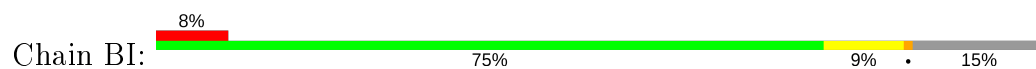


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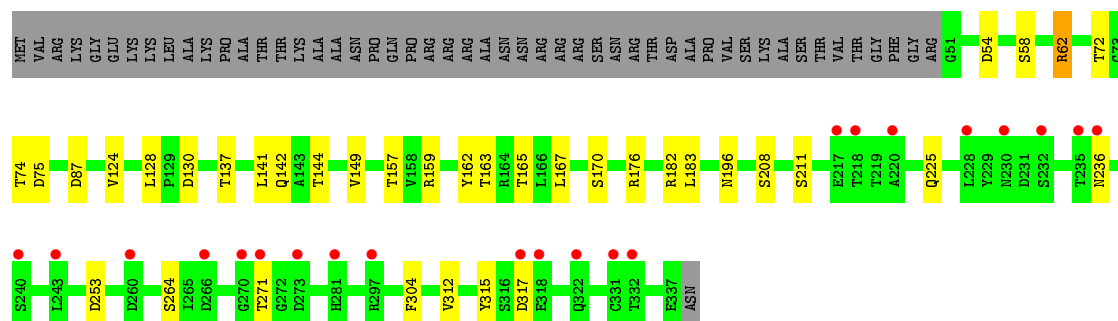
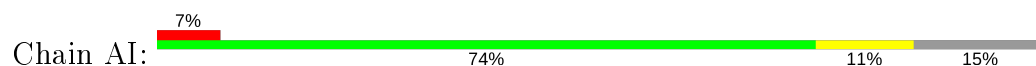




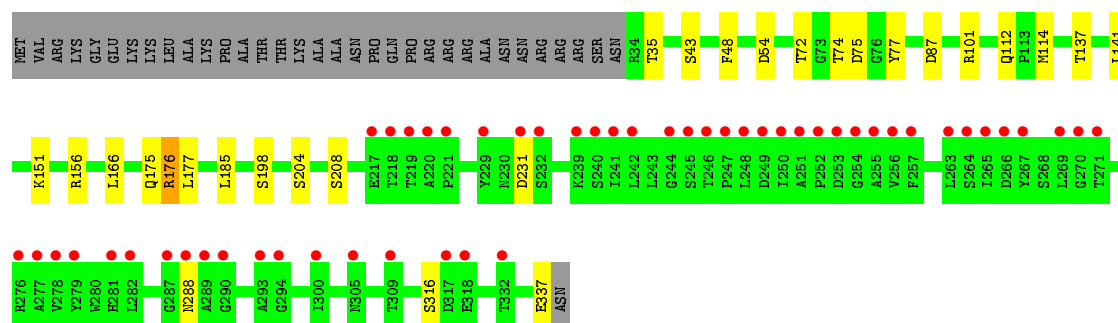
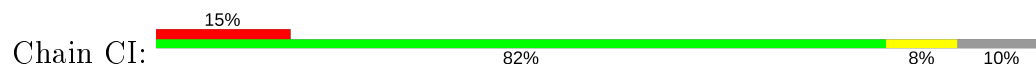
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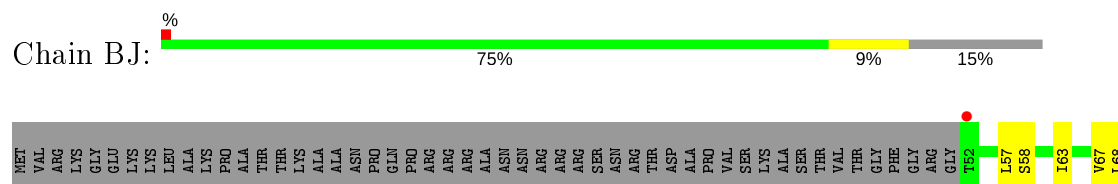
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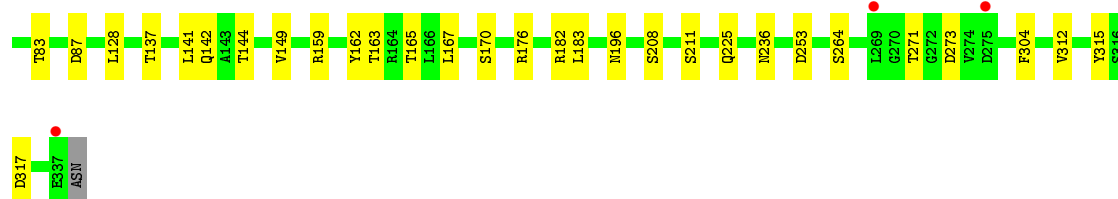
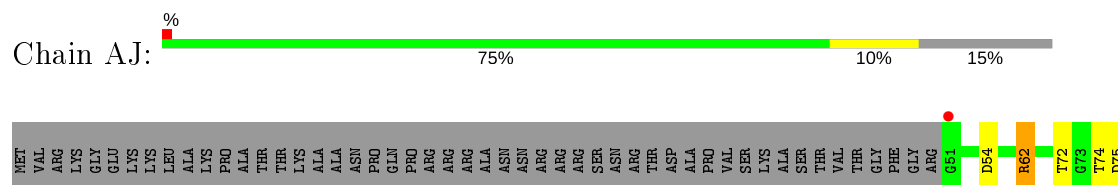
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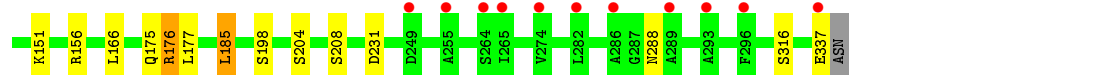
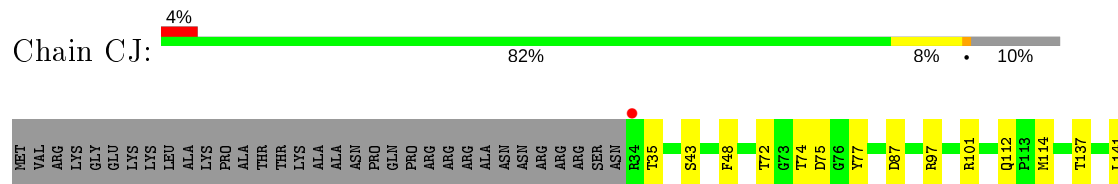
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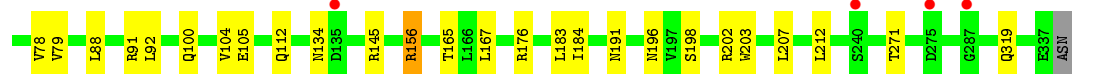
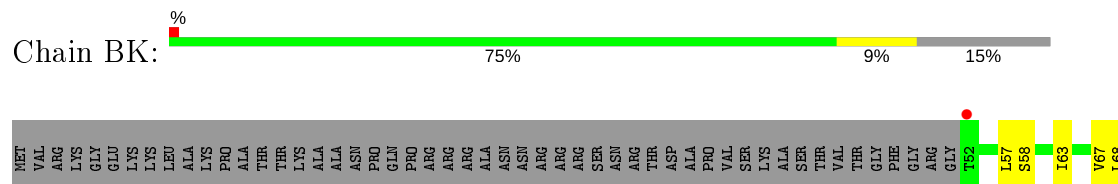
- Molecule 1: Coat protein



- Molecule 1: Coat protein

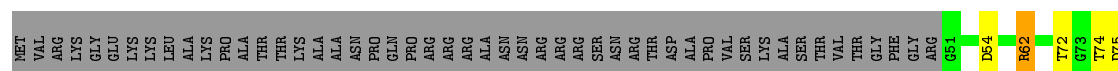


- Molecule 1: Coat protein

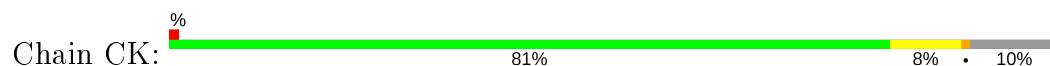


- Molecule 1: Coat protein

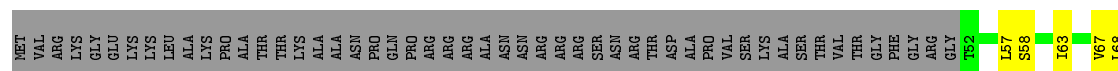




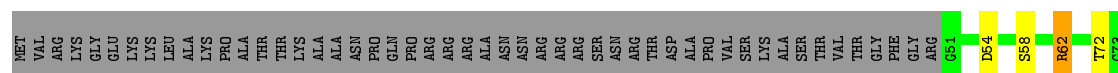
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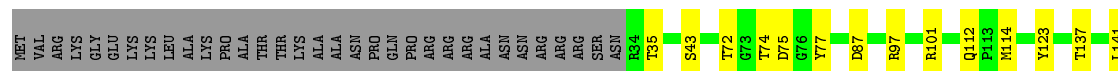
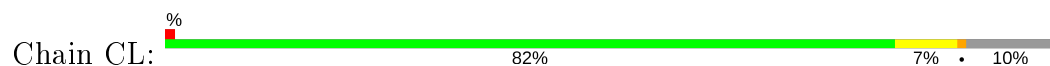
• Molecule 1: Coat protein



• Molecule 1: Coat protein

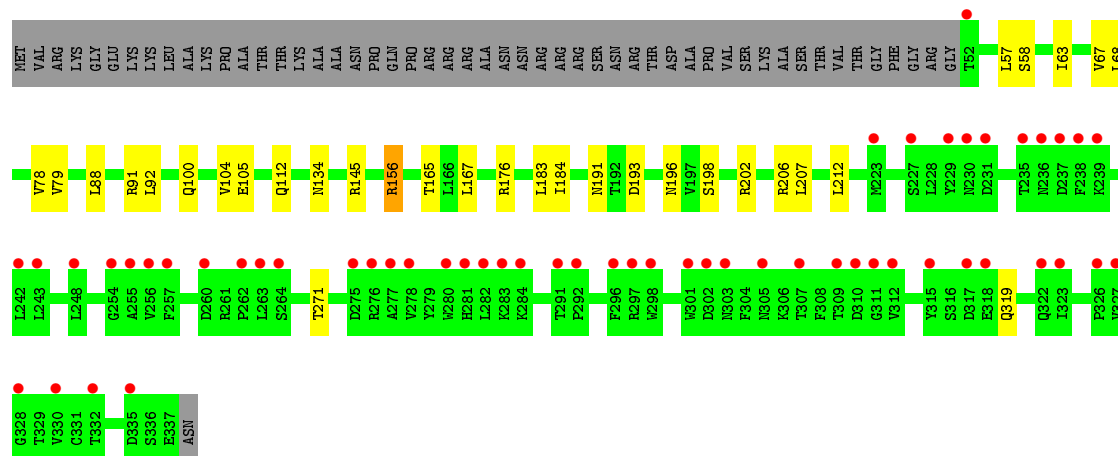
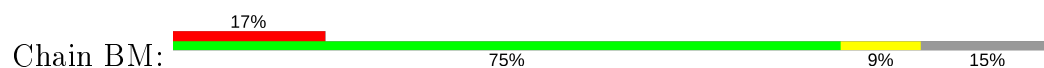


• Molecule 1: Coat protein

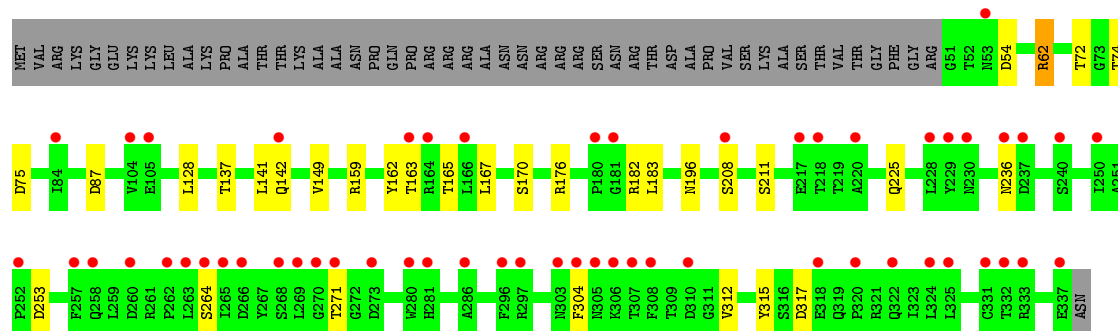
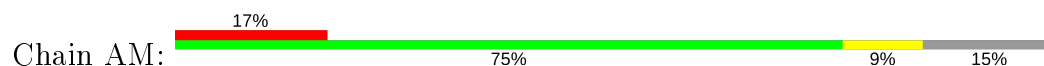




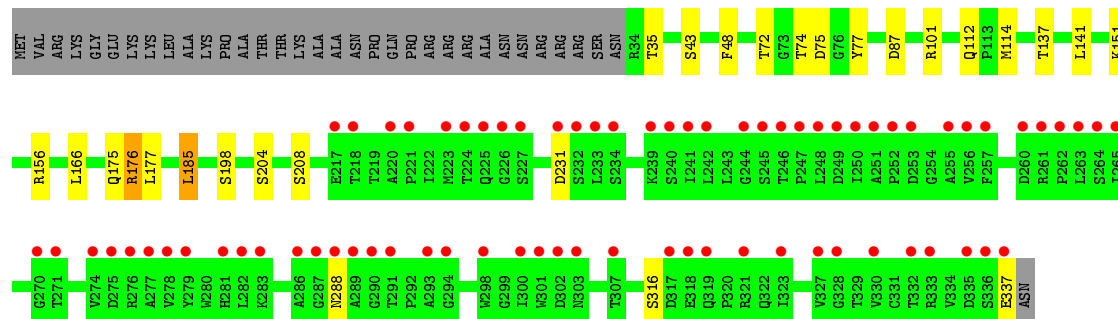
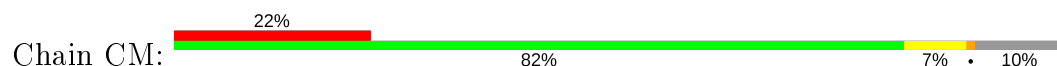
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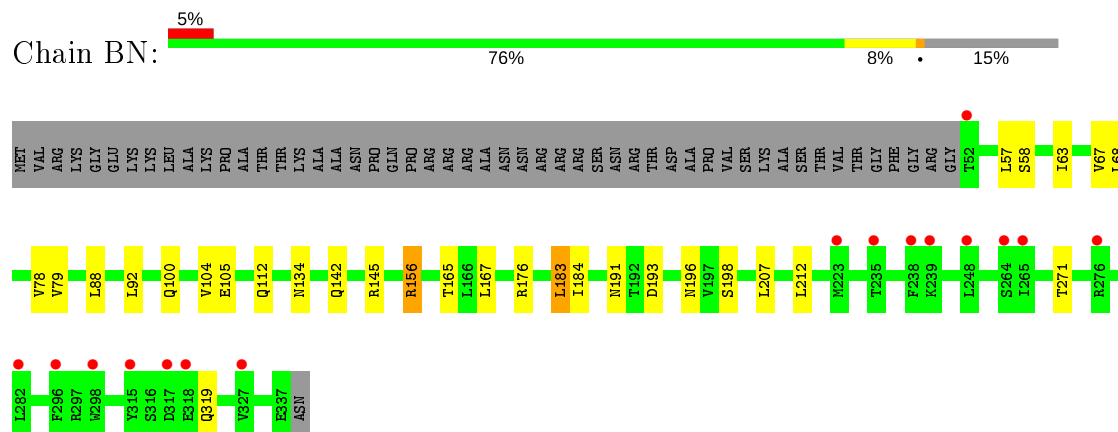
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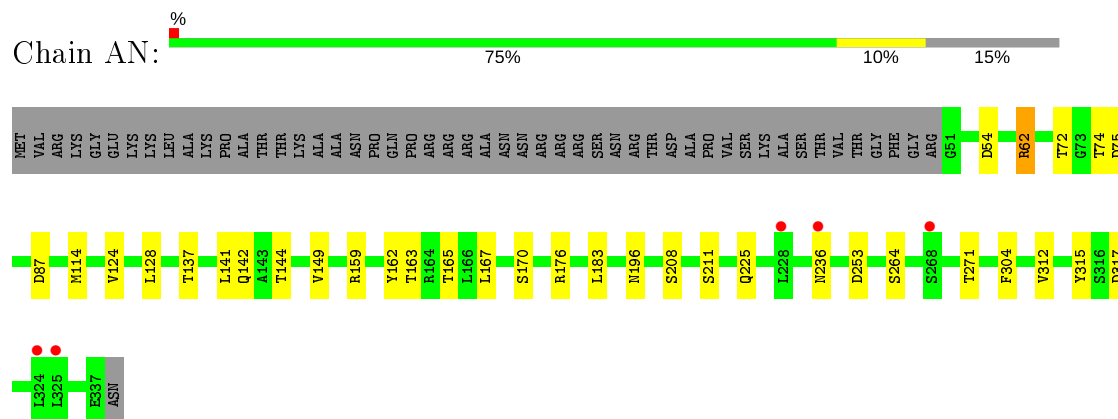
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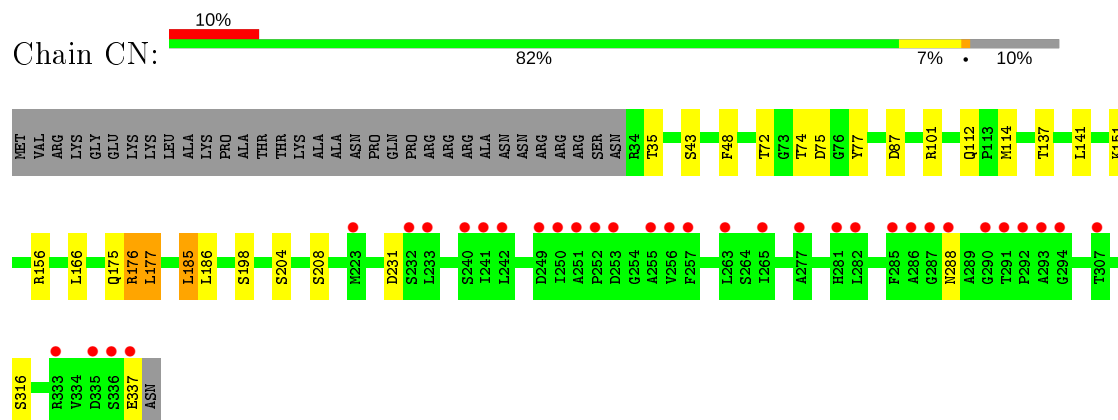
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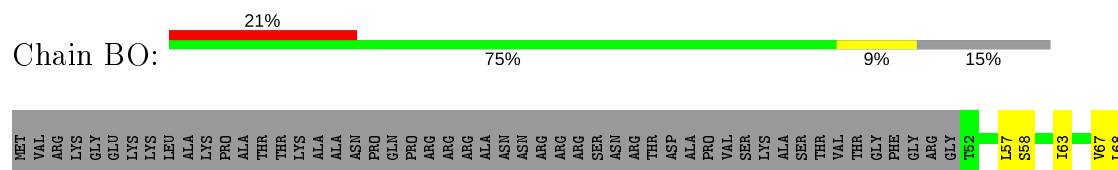
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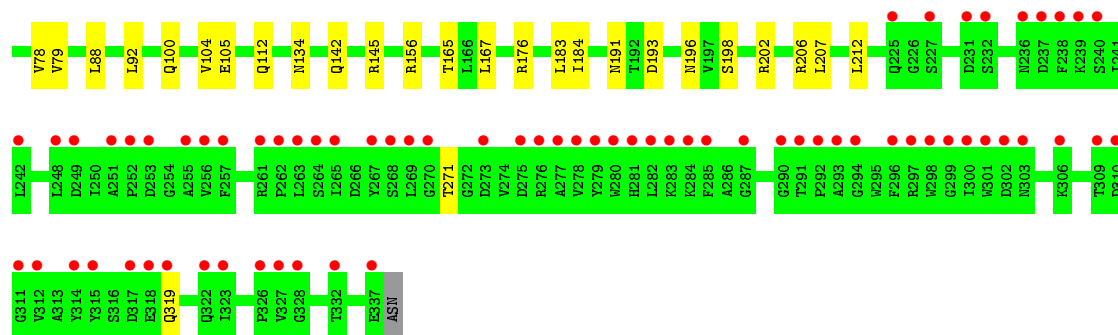


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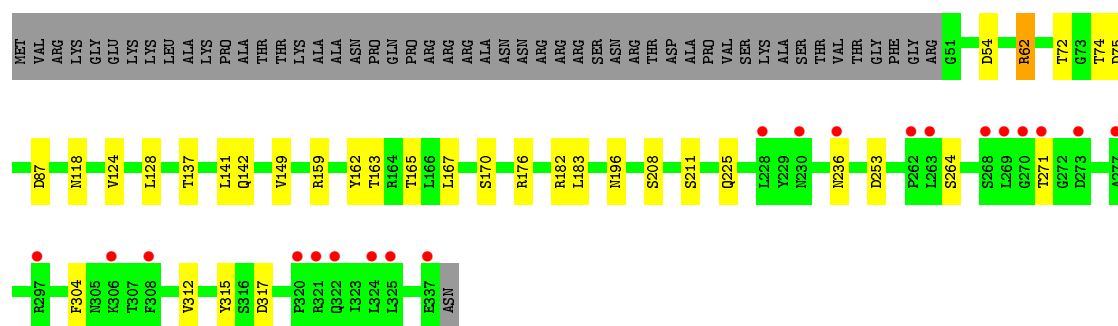
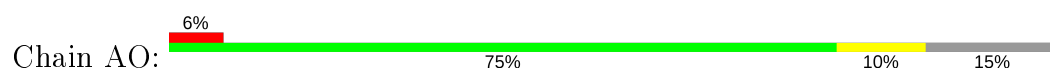


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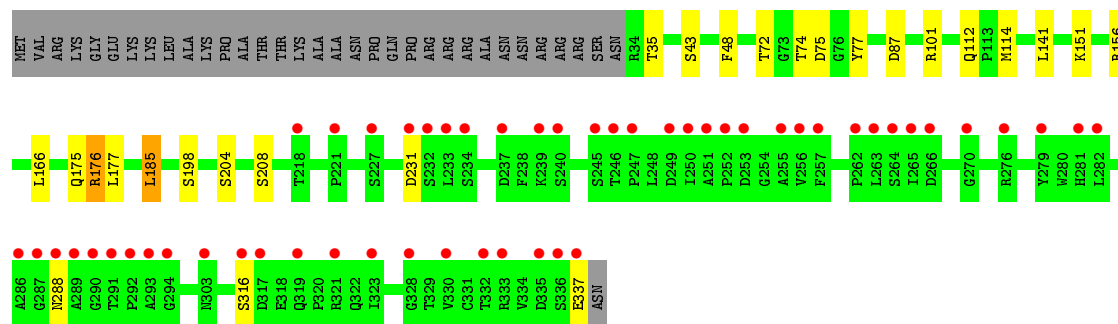
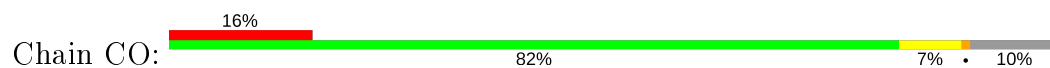




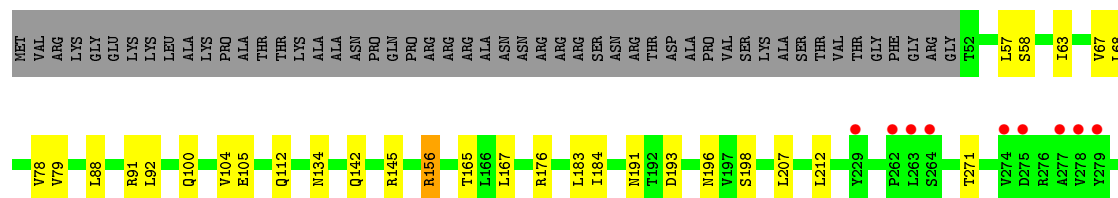
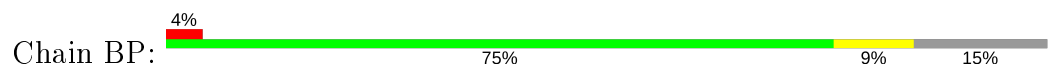
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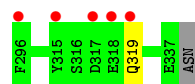


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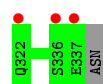
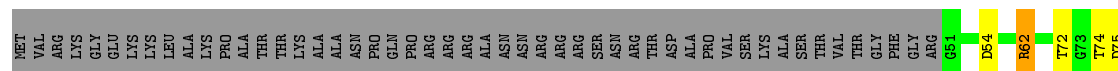
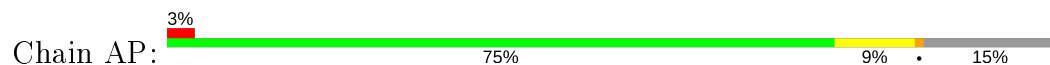


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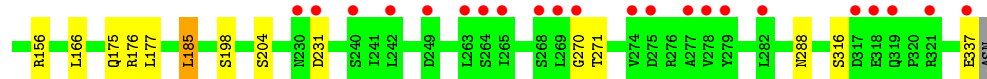
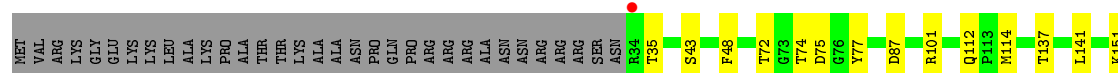
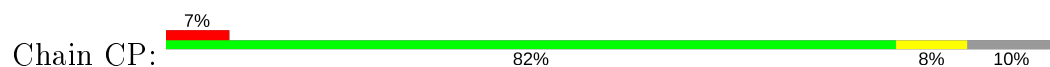




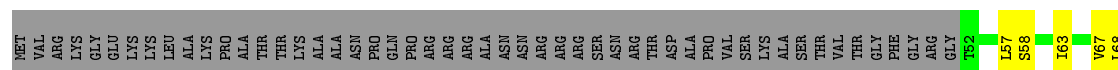
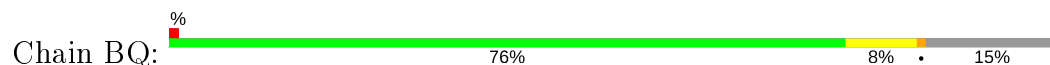
- Molecule 1: Coat protein



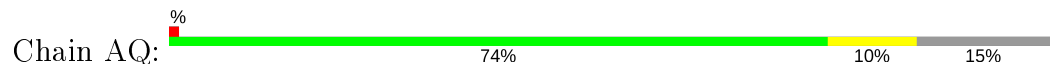
- Molecule 1: Coat protein

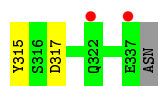


- Molecule 1: Coat protein

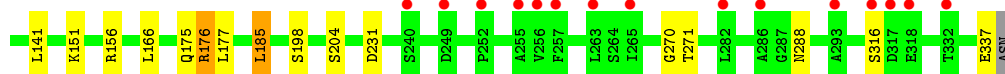
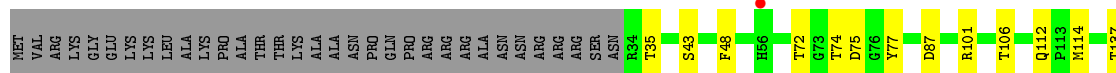
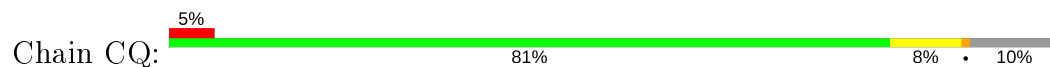


- Molecule 1: Coat protein

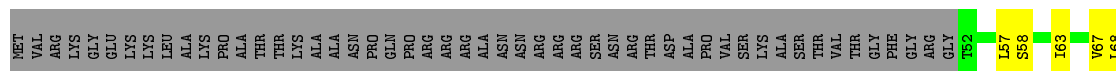
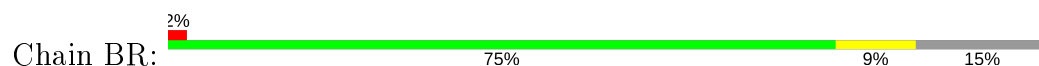




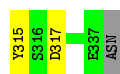
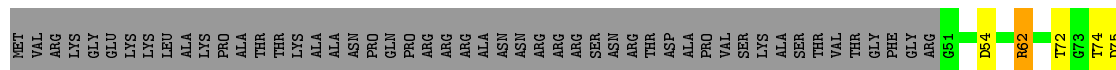
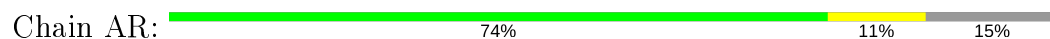
- Molecule 1: Coat protein



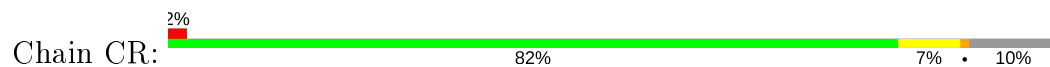
- Molecule 1: Coat protein



- Molecule 1: Coat protein

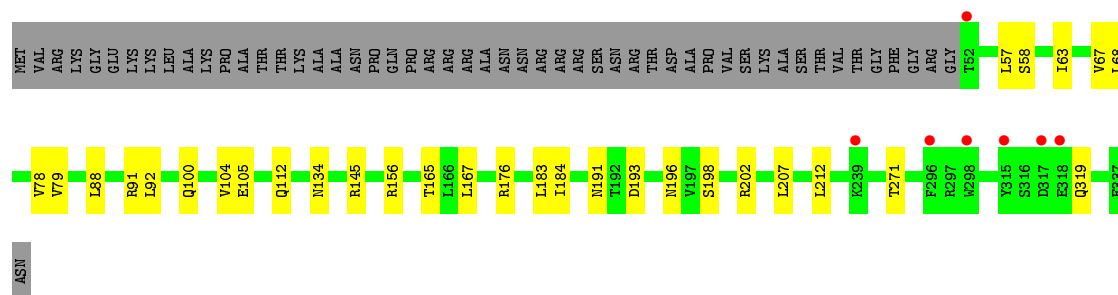
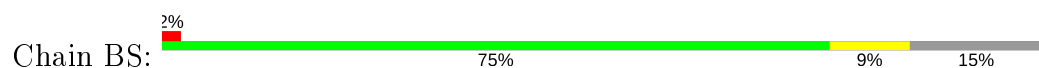


- Molecule 1: Coat protein

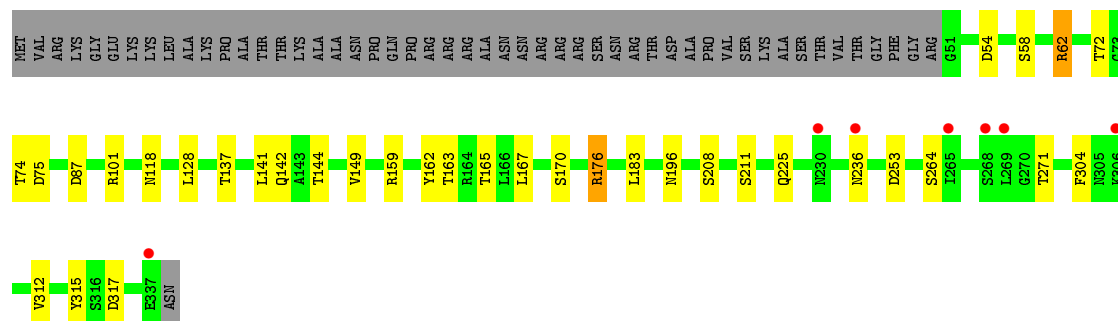
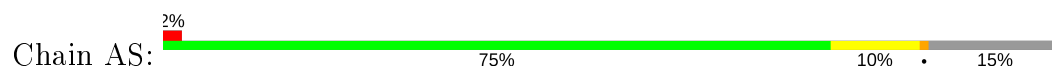




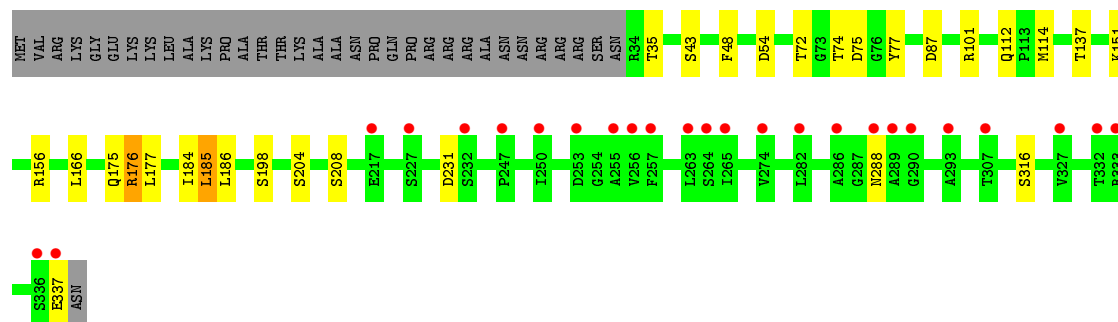
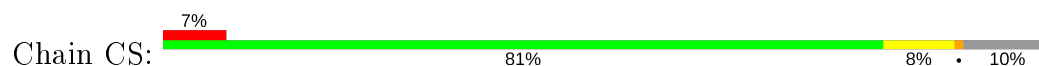
• Molecule 1: Coat protein



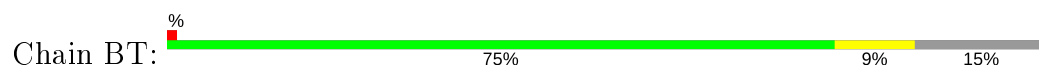
• Molecule 1: Coat protein

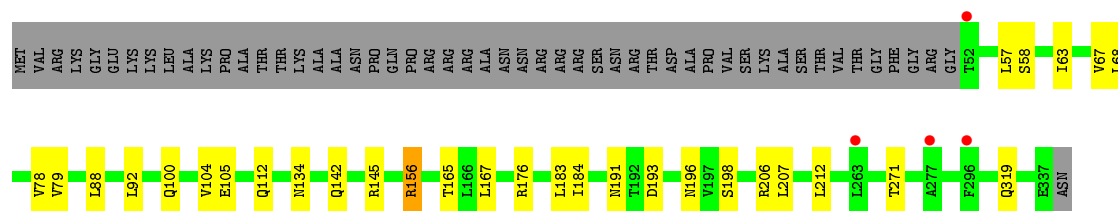


• Molecule 1: Coat protein

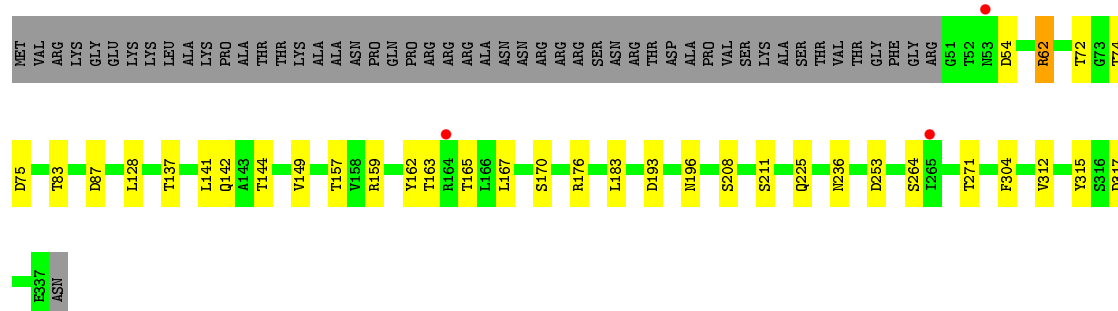
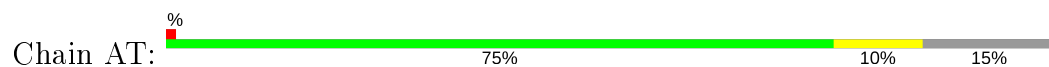


• Molecule 1: Coat protein

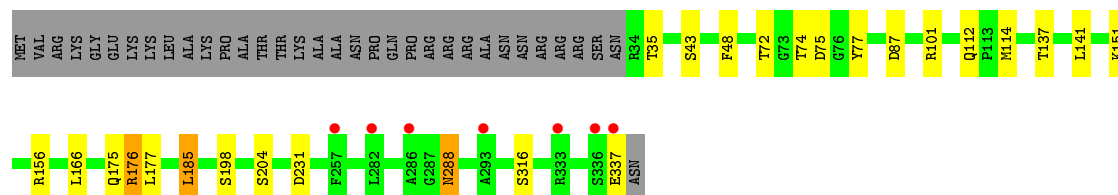
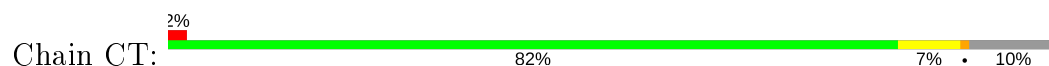




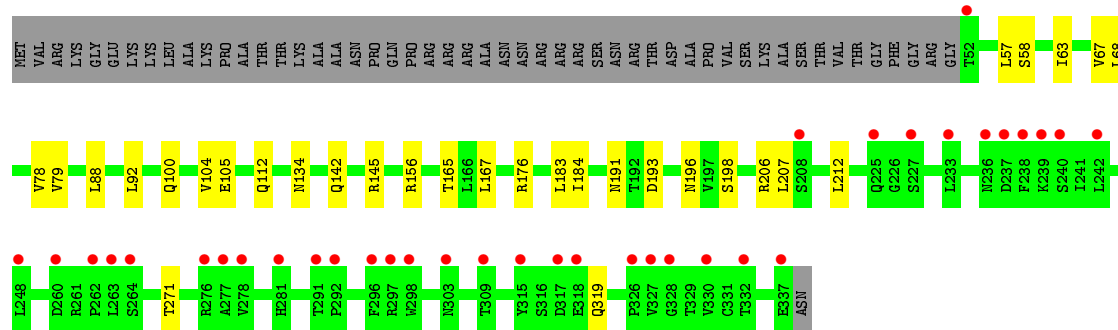
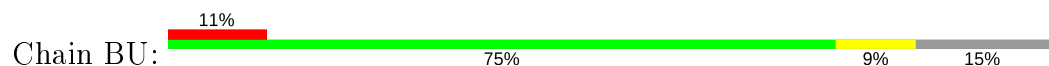
- Molecule 1: Coat protein



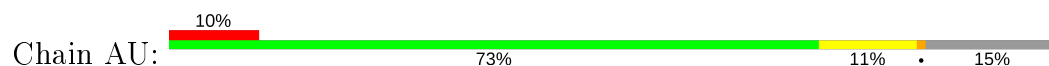
- Molecule 1: Coat protein

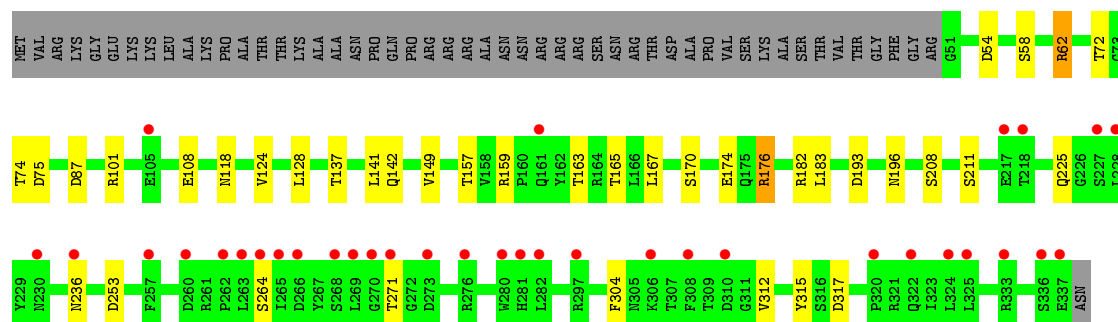


- Molecule 1: Coat protein

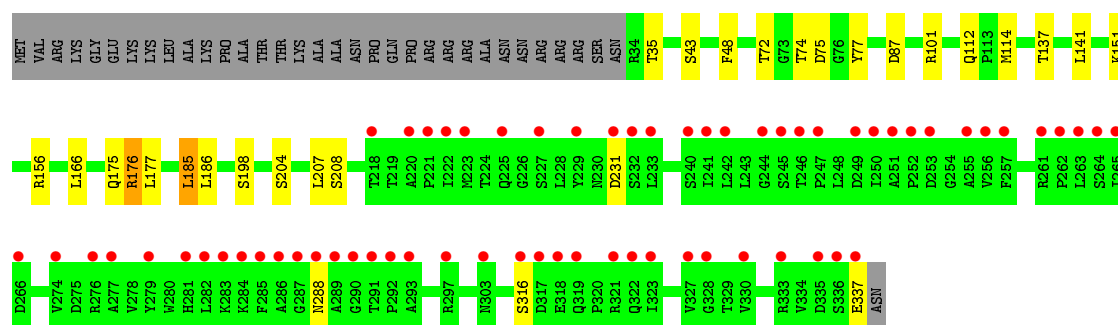
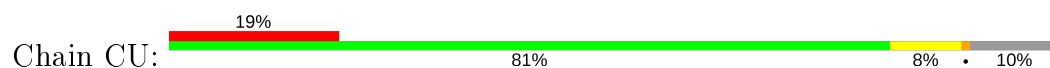


- Molecule 1: Coat protein

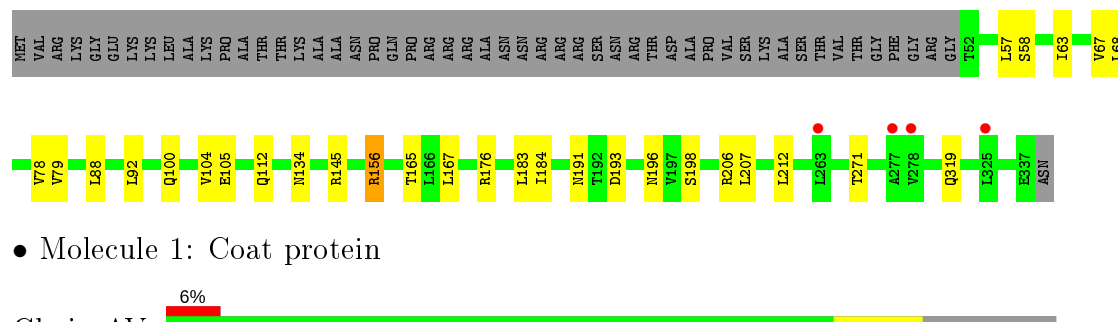
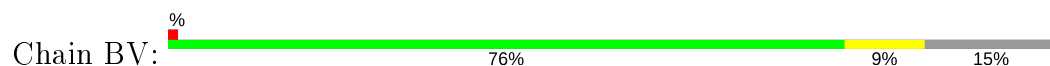




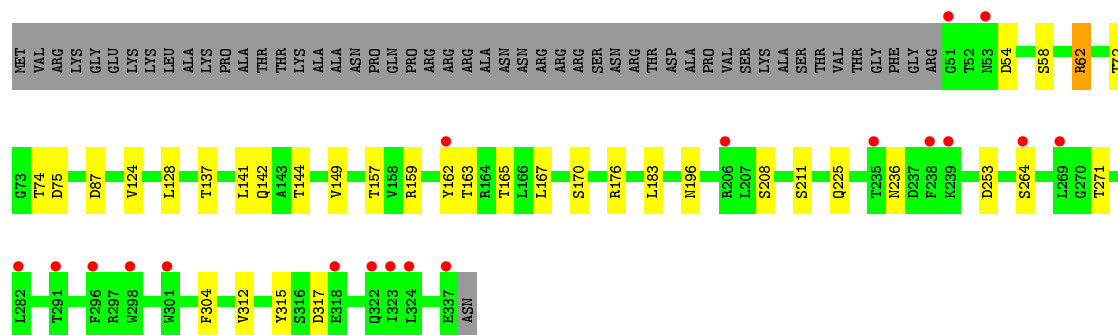
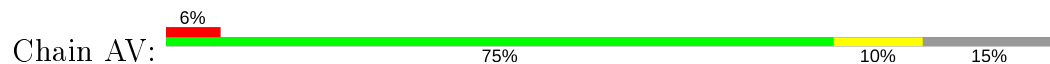
- Molecule 1: Coat protein



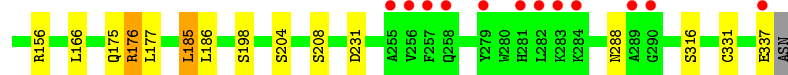
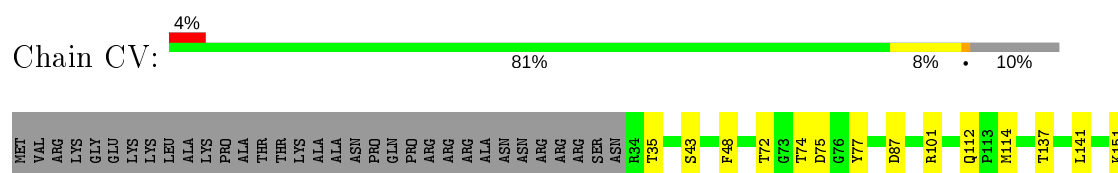
- Molecule 1: Coat protein



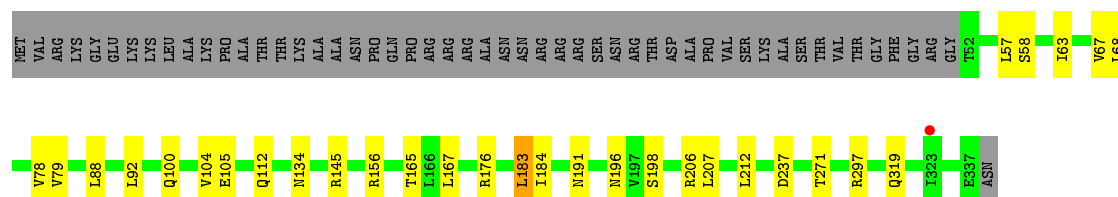
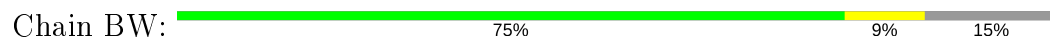
- Molecule 1: Coat protein



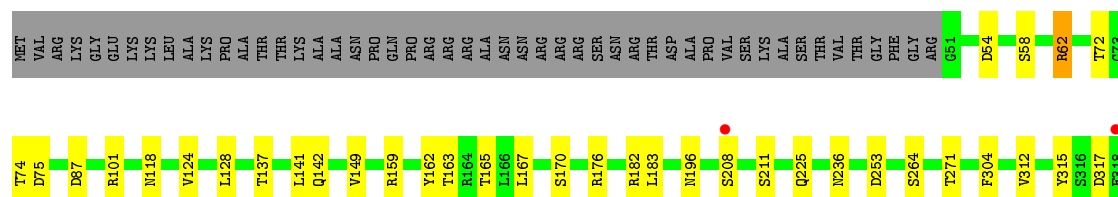
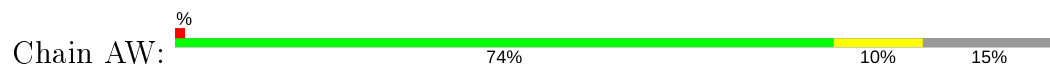
- Molecule 1: Coat protein



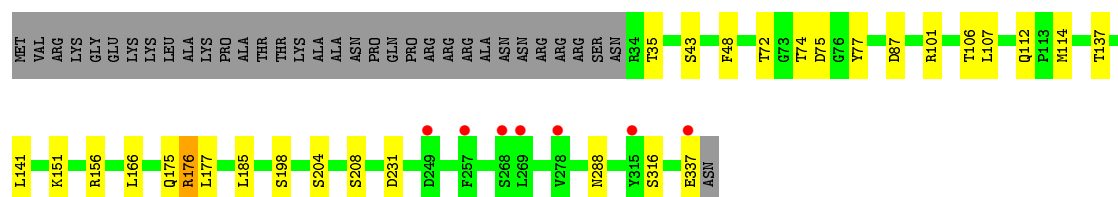
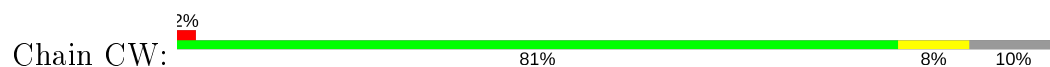
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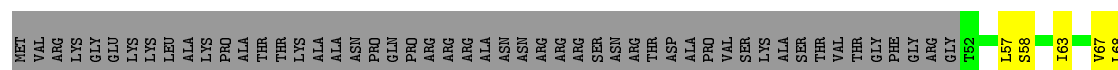
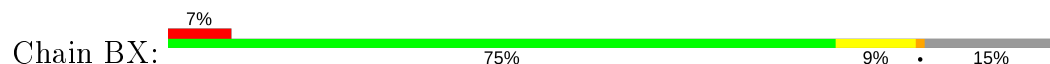
- Molecule 1: Coat protein

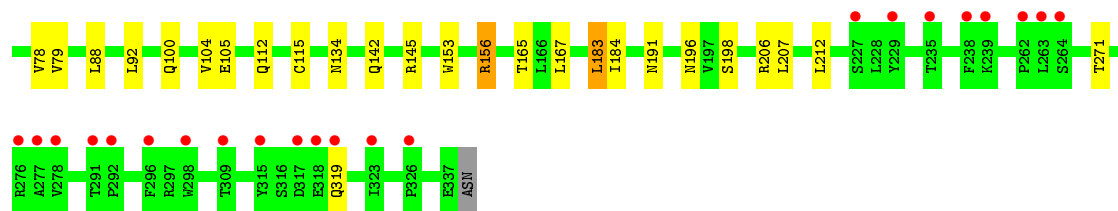


- Molecule 1: Coat protein

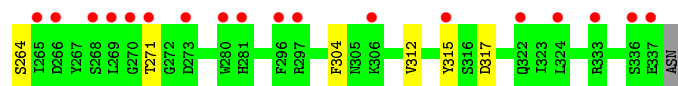
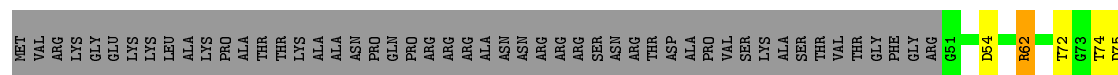
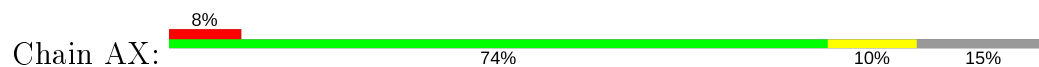


- Molecule 1: Coat protein

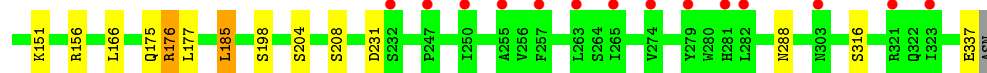
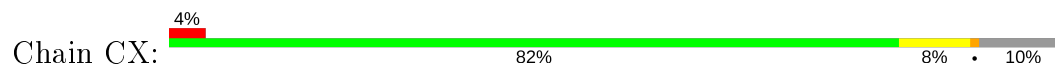




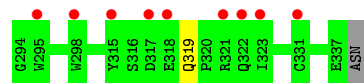
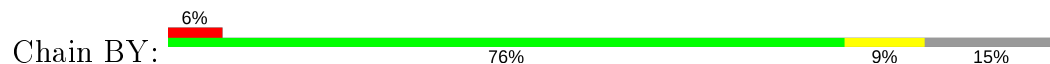
• Molecule 1: Coat protein



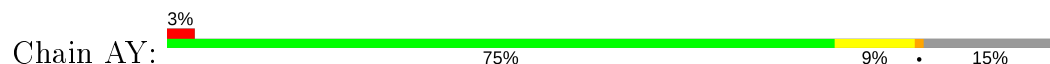
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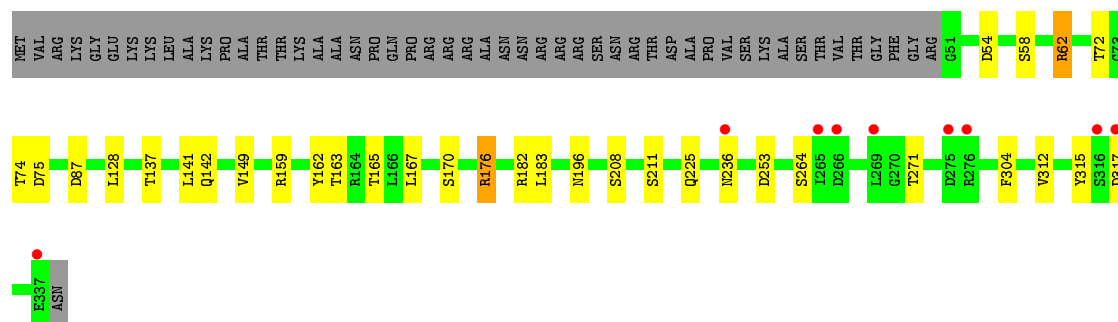


• Molecule 1: Coat protein

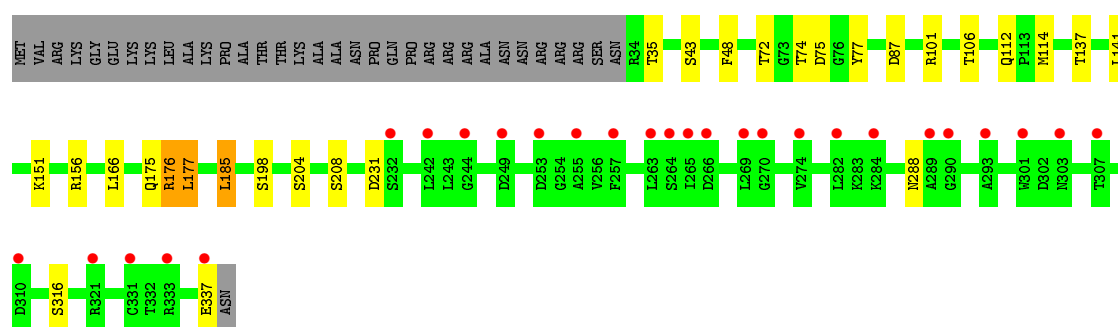
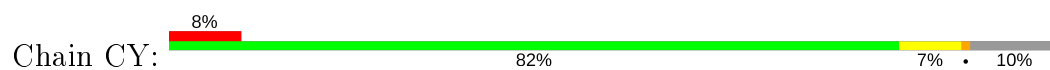


• Molecule 1: Coat protein

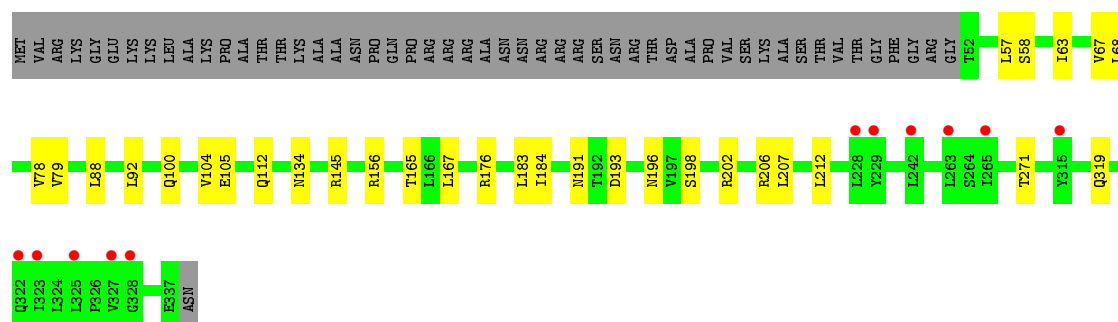
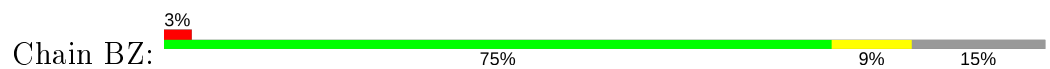




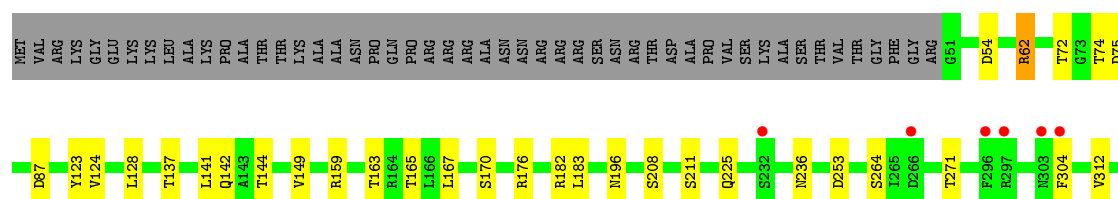
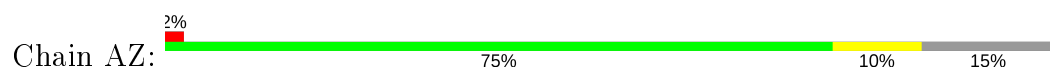
• Molecule 1: Coat protein

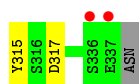


• Molecule 1: Coat protein

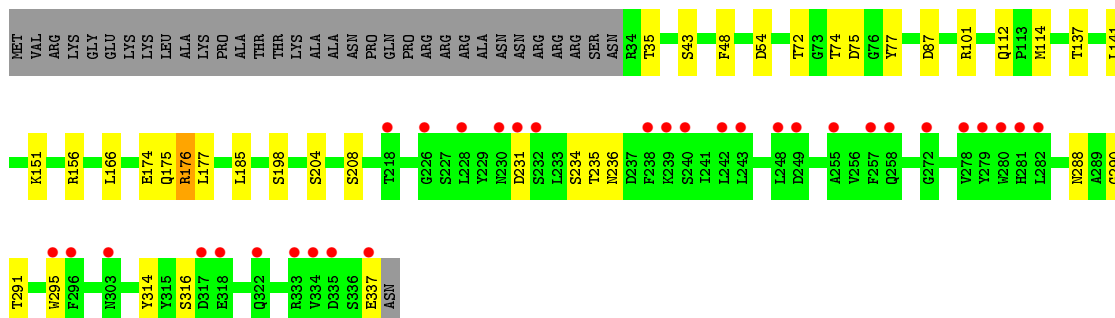
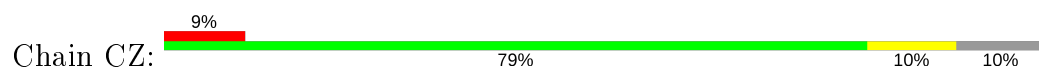


• Molecule 1: Coat protein

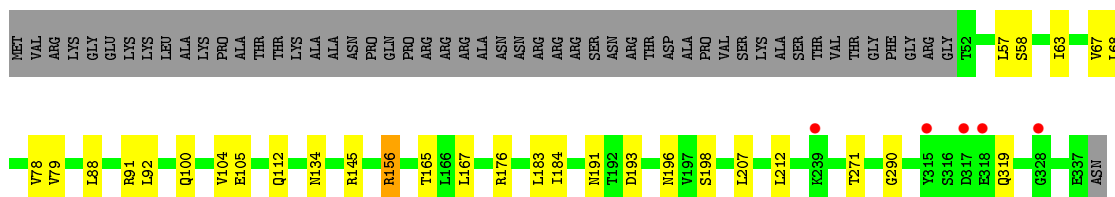
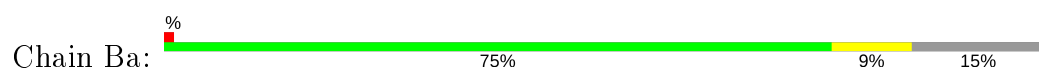




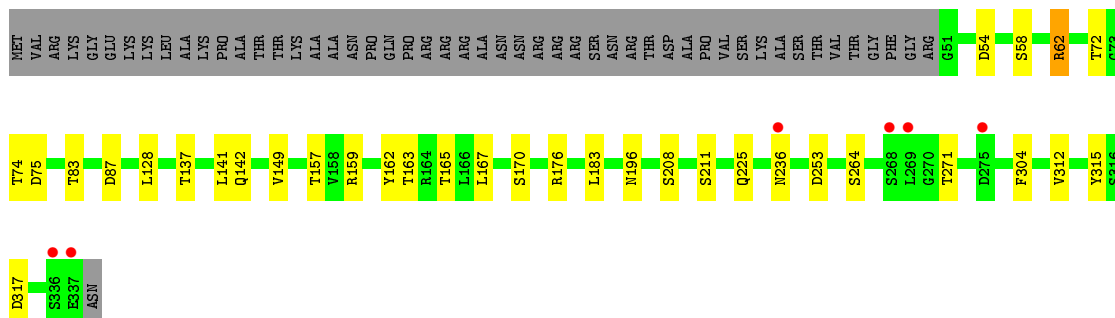
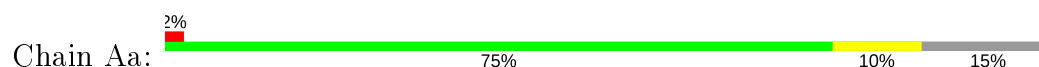
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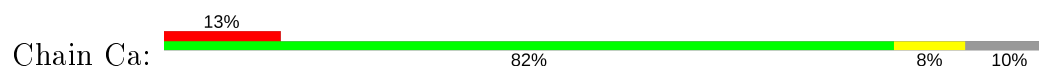
• Molecule 1: Coat protein

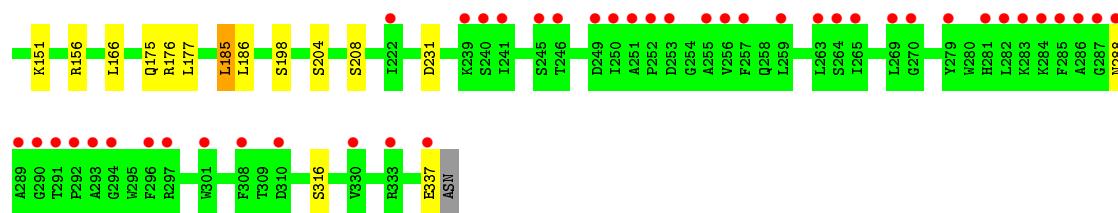


• Molecule 1: Coat protein

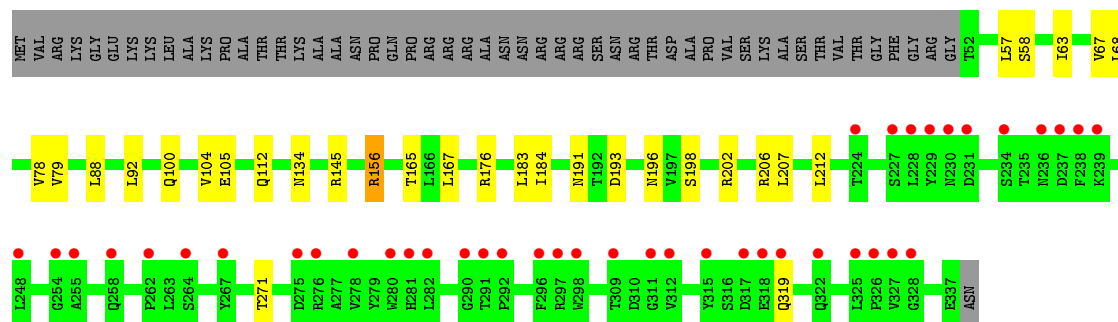
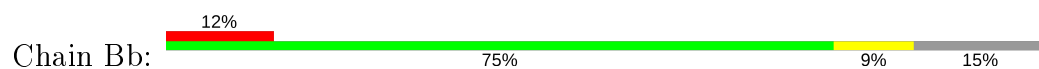


• Molecule 1: Coat protein

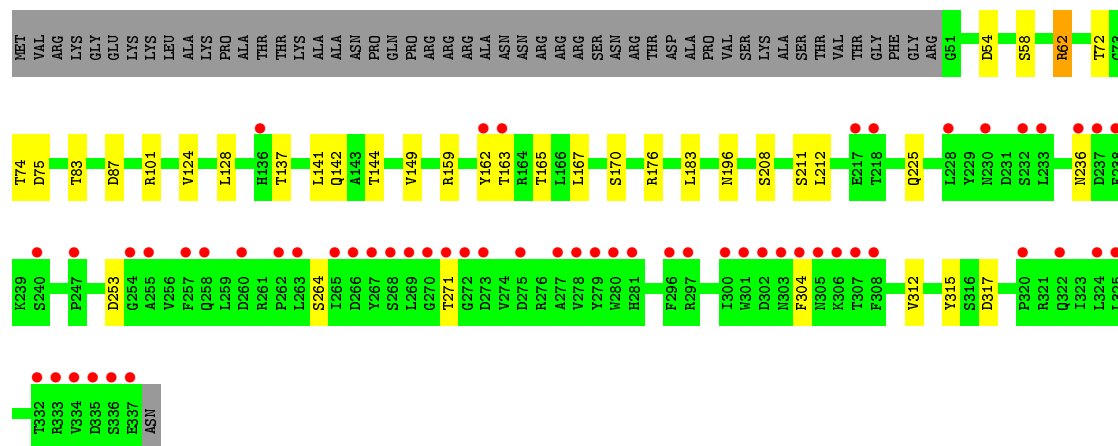
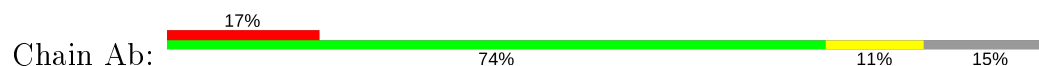




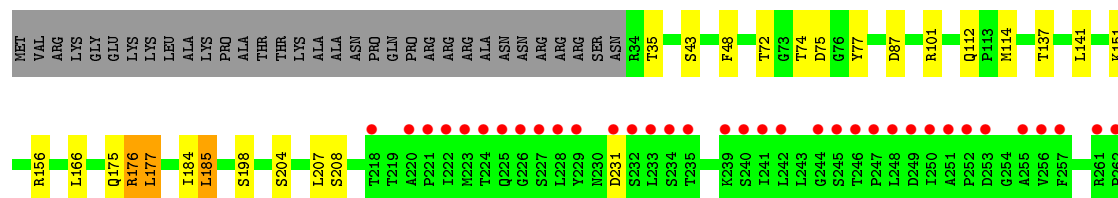
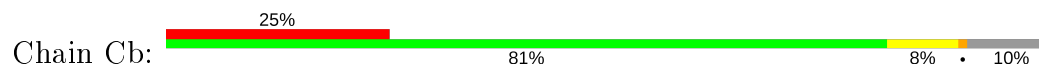
• Molecule 1: Coat protein

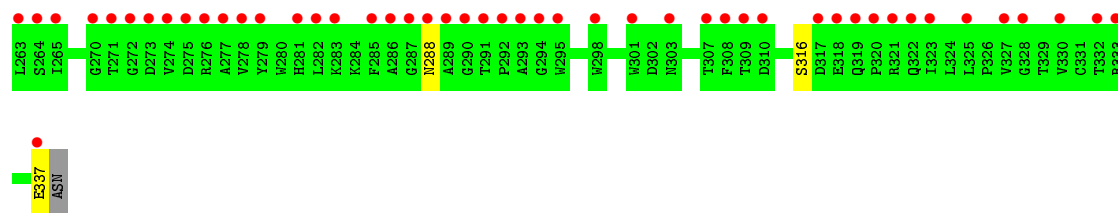


• Molecule 1: Coat protein

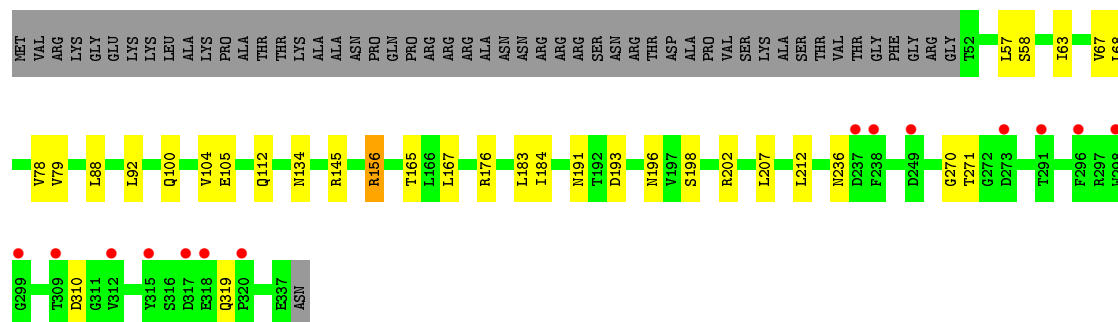
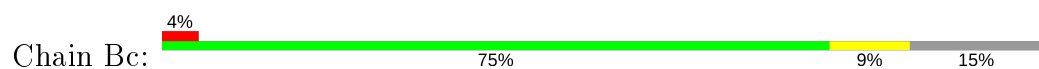


• Molecule 1: Coat protein

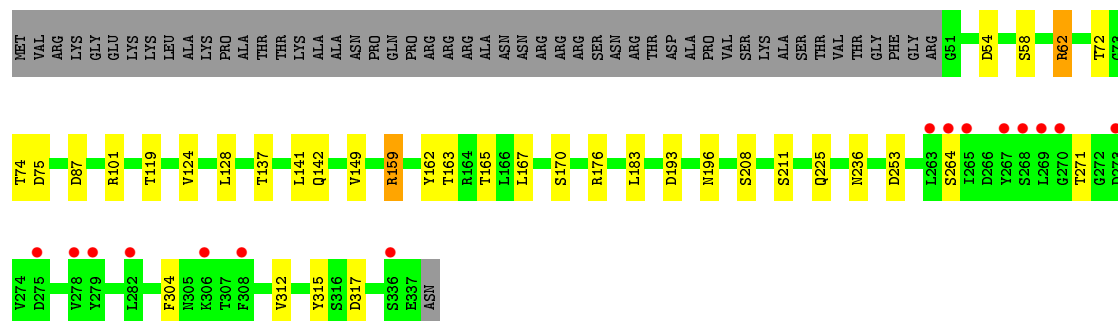
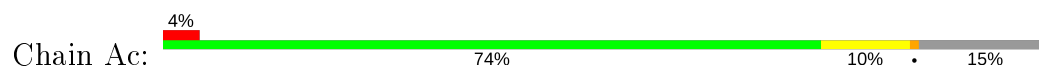




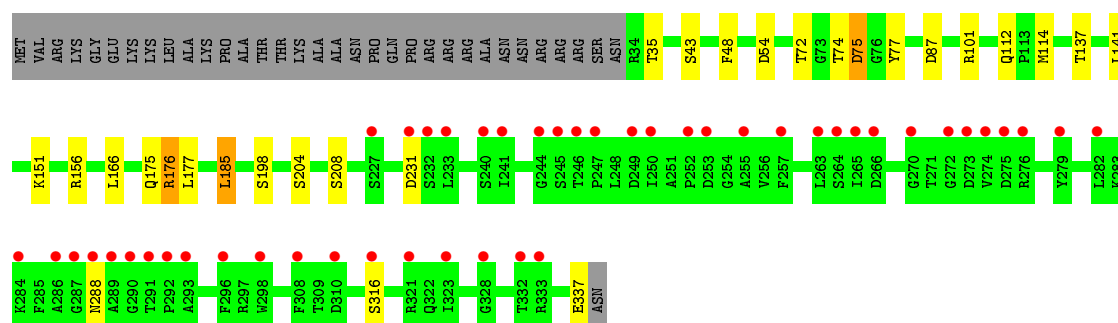
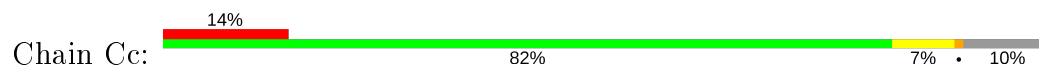
- Molecule 1: Coat protein



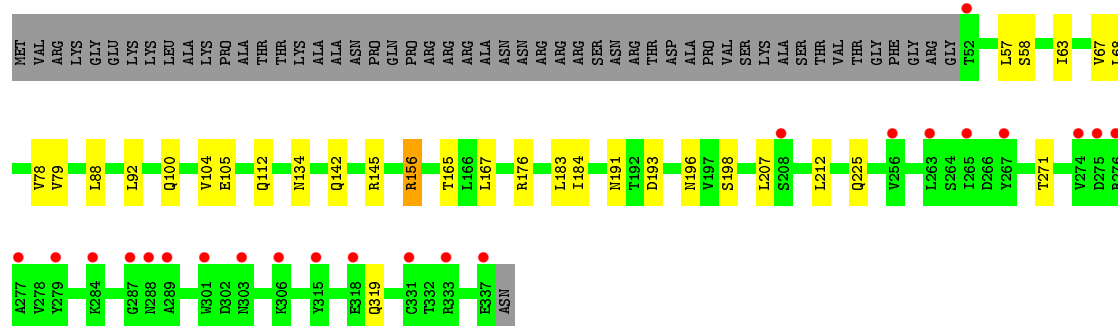
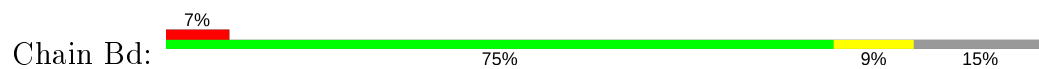
- Molecule 1: Coat protein



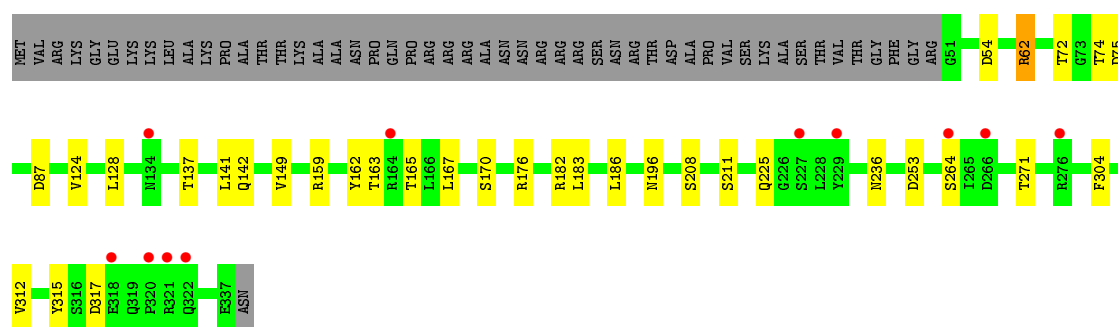
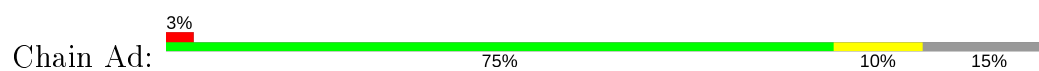
- Molecule 1: Coat protein



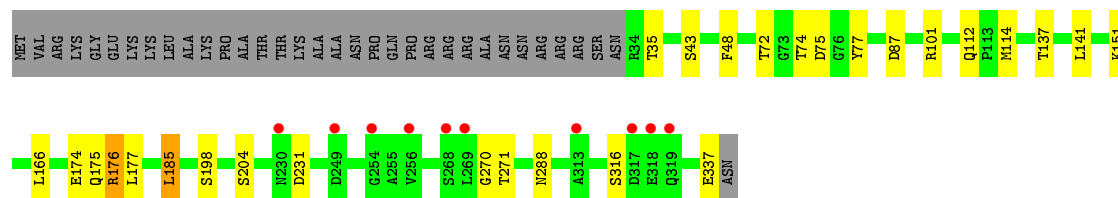
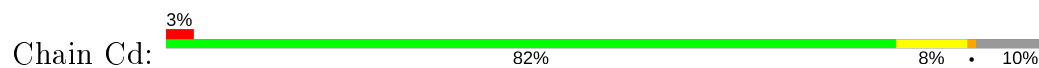
- Molecule 1: Coat protein



• Molecule 1: Coat protein



• Molecule 1: Coat protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	477.36Å 422.74Å 337.89Å 90.00° 134.03° 90.00°	Depositor
Resolution (Å)	263.91 – 3.60 263.91 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (263.91-3.60) 99.3 (263.91-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.58Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.255 , 0.297 0.255 , 0.295	Depositor DCC
R_{free} test set	27556 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	75.1	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h+2*k,-h-l 0.000 for h,-k,-h-l 0.000 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	203250	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	AA	0.71	0/2274	0.89	4/3112 (0.1%)
1	AB	0.80	0/2274	0.92	3/3112 (0.1%)
1	AC	0.79	0/2274	0.90	4/3112 (0.1%)
1	AD	0.73	0/2274	0.90	2/3112 (0.1%)
1	AE	0.75	0/2274	0.92	3/3112 (0.1%)
1	AF	0.77	1/2274 (0.0%)	0.92	3/3112 (0.1%)
1	AG	0.72	0/2274	0.89	3/3112 (0.1%)
1	AH	0.77	0/2274	0.90	2/3112 (0.1%)
1	AI	0.73	0/2274	0.89	3/3112 (0.1%)
1	AJ	0.78	0/2274	0.92	3/3112 (0.1%)
1	AK	0.92	0/2274	0.99	3/3112 (0.1%)
1	AL	0.85	0/2274	0.95	3/3112 (0.1%)
1	AM	0.72	0/2274	0.88	2/3112 (0.1%)
1	AN	0.72	0/2274	0.89	2/3112 (0.1%)
1	AO	0.76	0/2274	0.91	2/3112 (0.1%)
1	AP	0.77	0/2274	0.91	2/3112 (0.1%)
1	AQ	0.74	0/2274	0.91	4/3112 (0.1%)
1	AR	0.78	0/2274	0.91	3/3112 (0.1%)
1	AS	0.80	0/2274	0.91	2/3112 (0.1%)
1	AT	0.71	0/2274	0.89	3/3112 (0.1%)
1	AU	0.81	2/2274 (0.1%)	0.92	5/3112 (0.2%)
1	AV	0.72	0/2274	0.89	2/3112 (0.1%)
1	AW	0.80	0/2274	0.93	4/3112 (0.1%)
1	AX	0.77	0/2274	0.91	4/3112 (0.1%)
1	AY	0.78	0/2274	0.91	3/3112 (0.1%)
1	AZ	0.75	1/2274 (0.0%)	0.89	4/3112 (0.1%)
1	Aa	0.71	0/2274	0.88	2/3112 (0.1%)
1	Ab	0.78	0/2274	0.92	3/3112 (0.1%)
1	Ac	0.76	0/2274	0.92	5/3112 (0.2%)
1	Ad	0.82	0/2274	0.94	3/3112 (0.1%)
1	BA	0.76	0/2270	0.94	5/3107 (0.2%)
1	BB	0.87	0/2270	0.99	7/3107 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BC	0.77	0/2270	0.92	5/3107 (0.2%)
1	BD	0.78	0/2270	0.92	3/3107 (0.1%)
1	BE	0.79	0/2270	0.95	6/3107 (0.2%)
1	BF	0.80	0/2270	0.95	6/3107 (0.2%)
1	BG	0.80	0/2270	0.94	4/3107 (0.1%)
1	BH	0.81	0/2270	0.95	5/3107 (0.2%)
1	BI	0.79	1/2270 (0.0%)	0.93	4/3107 (0.1%)
1	BJ	0.86	0/2270	0.97	7/3107 (0.2%)
1	BK	0.92	1/2270 (0.0%)	0.98	5/3107 (0.2%)
1	BL	0.93	0/2270	0.98	8/3107 (0.3%)
1	BM	0.83	0/2270	0.95	5/3107 (0.2%)
1	BN	0.80	0/2270	0.95	5/3107 (0.2%)
1	BO	0.82	0/2270	0.96	6/3107 (0.2%)
1	BP	0.80	0/2270	0.94	5/3107 (0.2%)
1	BQ	0.80	0/2270	0.93	4/3107 (0.1%)
1	BR	0.83	0/2270	0.93	4/3107 (0.1%)
1	BS	0.85	0/2270	0.97	4/3107 (0.1%)
1	BT	0.77	0/2270	0.94	5/3107 (0.2%)
1	BU	0.84	0/2270	0.96	4/3107 (0.1%)
1	BV	0.78	0/2270	0.92	5/3107 (0.2%)
1	BW	0.87	0/2270	0.95	4/3107 (0.1%)
1	BX	0.79	1/2270 (0.0%)	0.93	4/3107 (0.1%)
1	BY	0.79	0/2270	0.92	4/3107 (0.1%)
1	BZ	0.77	0/2270	0.93	4/3107 (0.1%)
1	Ba	0.79	0/2270	0.93	4/3107 (0.1%)
1	Bb	0.85	0/2270	0.98	6/3107 (0.2%)
1	Bc	0.80	0/2270	0.93	4/3107 (0.1%)
1	Bd	0.82	0/2270	0.94	3/3107 (0.1%)
1	CA	0.72	0/2398	0.87	5/3280 (0.2%)
1	CB	0.78	0/2398	0.86	2/3280 (0.1%)
1	CC	0.84	0/2398	0.90	4/3280 (0.1%)
1	CD	0.75	0/2398	0.87	5/3280 (0.2%)
1	CE	0.79	0/2398	0.88	2/3280 (0.1%)
1	CF	0.80	1/2398 (0.0%)	0.88	3/3280 (0.1%)
1	CG	0.73	0/2398	0.86	4/3280 (0.1%)
1	CH	0.75	0/2398	0.87	3/3280 (0.1%)
1	CI	0.73	0/2398	0.86	3/3280 (0.1%)
1	CJ	0.80	0/2398	0.88	5/3280 (0.2%)
1	CK	0.94	0/2398	0.98	4/3280 (0.1%)
1	CL	0.87	1/2398 (0.0%)	0.92	4/3280 (0.1%)
1	CM	0.76	0/2398	0.88	3/3280 (0.1%)
1	CN	0.74	0/2398	0.86	4/3280 (0.1%)
1	CO	0.78	0/2398	0.89	4/3280 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CP	0.75	0/2398	0.86	2/3280 (0.1%)
1	CQ	0.77	0/2398	0.87	4/3280 (0.1%)
1	CR	0.76	0/2398	0.87	4/3280 (0.1%)
1	CS	0.82	0/2398	0.91	4/3280 (0.1%)
1	CT	0.74	0/2398	0.88	4/3280 (0.1%)
1	CU	0.81	0/2398	0.90	4/3280 (0.1%)
1	CV	0.73	0/2398	0.86	3/3280 (0.1%)
1	CW	0.81	0/2398	0.91	4/3280 (0.1%)
1	CX	0.77	0/2398	0.87	3/3280 (0.1%)
1	CY	0.78	0/2398	0.88	4/3280 (0.1%)
1	CZ	0.74	1/2398 (0.0%)	0.87	3/3280 (0.1%)
1	Ca	0.74	0/2398	0.86	2/3280 (0.1%)
1	Cb	0.79	0/2398	0.88	5/3280 (0.2%)
1	Cc	0.78	0/2398	0.88	5/3280 (0.2%)
1	Cd	0.86	1/2398 (0.0%)	0.94	4/3280 (0.1%)
All	All	0.79	11/208260 (0.0%)	0.91	346/284970 (0.1%)

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	CU	0	1
1	Cb	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BI	318	GLU	CD-OE2	7.13	1.33	1.25
1	Cd	174	GLU	CD-OE1	6.83	1.33	1.25
1	CF	174	GLU	CD-OE1	6.23	1.32	1.25
1	AF	174	GLU	CD-OE2	5.70	1.31	1.25
1	AU	108	GLU	CD-OE1	5.60	1.31	1.25
1	BK	203	TRP	CE3-CZ3	5.27	1.47	1.38
1	AU	174	GLU	CD-OE2	5.21	1.31	1.25
1	BX	115	CYS	CB-SG	-5.12	1.73	1.81
1	AZ	123	TYR	CE1-CZ	-5.12	1.31	1.38
1	CL	123	TYR	CE2-CZ	-5.04	1.31	1.38
1	CZ	174	GLU	CD-OE1	5.03	1.31	1.25

All (346) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CO	176	ARG	NE-CZ-NH2	8.79	124.70	120.30
1	AE	62	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	CT	176	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	CU	176	ARG	NE-CZ-NH2	8.25	124.42	120.30
1	CW	176	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	BO	176	ARG	NE-CZ-NH1	-7.94	116.33	120.30
1	AV	62	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	BJ	156	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	Ab	101	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	Ad	62	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	Cd	176	ARG	NE-CZ-NH2	7.51	124.05	120.30
1	BO	176	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	Ba	176	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	BJ	176	ARG	NE-CZ-NH2	7.39	123.99	120.30
1	BB	176	ARG	NE-CZ-NH1	-7.35	116.63	120.30
1	AA	62	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	BN	176	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	BT	156	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	BQ	156	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	AB	62	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	CK	176	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	BN	176	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	BL	91	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	CK	176	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	CA	176	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	CP	166	LEU	CA-CB-CG	6.91	131.19	115.30
1	BD	156	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	BJ	206	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	CZ	176	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	BK	91	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	BZ	176	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	CI	176	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	Ba	156	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	BO	206	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	CM	176	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	CQ	176	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	Ac	62	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	AH	62	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	AG	62	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	AK	182	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	AW	101	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	AF	62	ARG	NE-CZ-NH1	6.47	123.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CT	176	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	AM	182	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	AX	62	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	CI	176	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	Bd	156	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	BT	176	ARG	NE-CZ-NH1	-6.41	117.09	120.30
1	CO	166	LEU	CA-CB-CG	6.40	130.02	115.30
1	AP	176	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	CX	166	LEU	CA-CB-CG	6.37	129.95	115.30
1	BF	156	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	BK	156	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	CD	176	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	CD	166	LEU	CA-CB-CG	6.33	129.86	115.30
1	BT	176	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	CQ	166	LEU	CA-CB-CG	6.33	129.85	115.30
1	BM	156	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	CZ	166	LEU	CA-CB-CG	6.30	129.79	115.30
1	CQ	176	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	CW	176	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	Cd	176	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	BH	156	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	BJ	176	ARG	NE-CZ-NH1	-6.23	117.18	120.30
1	Cc	166	LEU	CA-CB-CG	6.23	129.62	115.30
1	Bb	206	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	CK	166	LEU	CA-CB-CG	6.22	129.60	115.30
1	BN	156	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	CB	166	LEU	CA-CB-CG	6.20	129.56	115.30
1	CG	176	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	BS	91	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	BA	156	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	BY	91	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	CF	166	LEU	CA-CB-CG	6.14	129.42	115.30
1	CW	166	LEU	CA-CB-CG	6.13	129.40	115.30
1	BK	112	GLN	N-CA-C	6.13	127.54	111.00
1	CX	185	LEU	CA-CB-CG	6.13	129.39	115.30
1	CS	166	LEU	CA-CB-CG	6.10	129.33	115.30
1	Bb	176	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	BV	176	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	CY	166	LEU	CA-CB-CG	6.09	129.31	115.30
1	BA	112	GLN	N-CA-C	6.08	127.43	111.00
1	Cd	166	LEU	CA-CB-CG	6.08	129.27	115.30
1	CC	166	LEU	CA-CB-CG	6.07	129.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BC	112	GLN	N-CA-C	6.07	127.39	111.00
1	CC	176	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	CJ	176	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	BE	176	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	Cc	176	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	BP	112	GLN	N-CA-C	6.03	127.28	111.00
1	AU	182	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	CR	166	LEU	CA-CB-CG	6.02	129.15	115.30
1	BE	156	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	BH	112	GLN	N-CA-C	6.00	127.20	111.00
1	BZ	176	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	BW	176	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	BU	206	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	BF	112	GLN	N-CA-C	5.96	127.08	111.00
1	BC	176	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	AQ	62	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	CJ	176	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	BV	112	GLN	N-CA-C	5.94	127.03	111.00
1	CS	176	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	CV	185	LEU	CA-CB-CG	5.93	128.93	115.30
1	Ab	62	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	AL	182	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	Bd	112	GLN	N-CA-C	5.92	126.99	111.00
1	BO	112	GLN	N-CA-C	5.92	126.97	111.00
1	CA	176	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	BZ	112	GLN	N-CA-C	5.90	126.92	111.00
1	BC	156	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	BW	112	GLN	N-CA-C	5.88	126.88	111.00
1	Ca	166	LEU	CA-CB-CG	5.88	128.83	115.30
1	BK	176	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	CL	166	LEU	CA-CB-CG	5.87	128.80	115.30
1	BX	206	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	BU	112	GLN	N-CA-C	5.87	126.84	111.00
1	BX	112	GLN	N-CA-C	5.87	126.83	111.00
1	CT	166	LEU	CA-CB-CG	5.86	128.78	115.30
1	BF	176	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	BI	112	GLN	N-CA-C	5.86	126.81	111.00
1	CN	176	ARG	NE-CZ-NH2	5.85	123.23	120.30
1	BN	112	GLN	N-CA-C	5.85	126.78	111.00
1	AG	62	ARG	CG-CD-NE	5.84	124.07	111.80
1	CH	166	LEU	CA-CB-CG	5.83	128.71	115.30
1	BB	112	GLN	N-CA-C	5.83	126.73	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AL	62	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	CL	97	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	AF	176	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	AU	176	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	BD	112	GLN	N-CA-C	5.82	126.71	111.00
1	AZ	62	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	CI	166	LEU	CA-CB-CG	5.81	128.66	115.30
1	Bc	176	ARG	NE-CZ-NH2	5.81	123.20	120.30
1	CU	166	LEU	CA-CB-CG	5.80	128.64	115.30
1	BR	112	GLN	N-CA-C	5.80	126.65	111.00
1	BT	206	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	CR	176	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	CJ	166	LEU	CA-CB-CG	5.78	128.60	115.30
1	AW	62	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	AU	62	ARG	CG-CD-NE	5.78	123.93	111.80
1	Cc	185	LEU	CA-CB-CG	5.77	128.56	115.30
1	CE	166	LEU	CA-CB-CG	5.76	128.56	115.30
1	BG	176	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	CM	166	LEU	CA-CB-CG	5.76	128.54	115.30
1	BM	176	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	BX	156	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	Cb	166	LEU	CA-CB-CG	5.75	128.53	115.30
1	CG	176	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	BH	176	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	CV	166	LEU	CA-CB-CG	5.73	128.47	115.30
1	BL	112	GLN	N-CA-C	5.72	126.45	111.00
1	BG	112	GLN	N-CA-C	5.72	126.44	111.00
1	BH	206	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	Ab	62	ARG	CG-CD-NE	5.71	123.79	111.80
1	AS	62	ARG	CG-CD-NE	5.71	123.79	111.80
1	CF	185	LEU	CA-CB-CG	5.70	128.40	115.30
1	BQ	112	GLN	N-CA-C	5.70	126.38	111.00
1	Cb	185	LEU	CA-CB-CG	5.70	128.40	115.30
1	BE	112	GLN	N-CA-C	5.69	126.37	111.00
1	AR	62	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	CC	176	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	Ca	185	LEU	CA-CB-CG	5.67	128.35	115.30
1	BS	112	GLN	N-CA-C	5.67	126.31	111.00
1	BY	112	GLN	N-CA-C	5.67	126.31	111.00
1	BJ	112	GLN	N-CA-C	5.66	126.28	111.00
1	Bb	156	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	BM	112	GLN	N-CA-C	5.65	126.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AI	62	ARG	CG-CD-NE	5.64	123.65	111.80
1	CA	185	LEU	CA-CB-CG	5.64	128.27	115.30
1	BB	176	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	Ba	112	GLN	N-CA-C	5.63	126.19	111.00
1	AQ	193	ASP	CB-CG-OD2	5.62	123.36	118.30
1	CE	185	LEU	CA-CB-CG	5.62	128.22	115.30
1	Bb	206	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	CY	176	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	BB	156	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	CH	176	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	BL	206	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	CN	185	LEU	CA-CB-CG	5.57	128.12	115.30
1	BL	176	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	Ac	62	ARG	CG-CD-NE	5.57	123.50	111.80
1	AG	182	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	CS	184	ILE	CG1-CB-CG2	-5.56	99.16	111.40
1	CP	185	LEU	CA-CB-CG	5.56	128.08	115.30
1	AR	193	ASP	CB-CG-OD2	5.56	123.30	118.30
1	BI	156	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	Aa	62	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	CA	166	LEU	CA-CB-CG	5.55	128.06	115.30
1	AY	62	ARG	CG-CD-NE	5.54	123.42	111.80
1	Ba	91	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	BF	176	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	BE	176	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	CK	185	LEU	CA-CB-CG	5.52	128.00	115.30
1	CU	176	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	CS	185	LEU	CA-CB-CG	5.51	127.98	115.30
1	BI	206	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	CB	185	LEU	CA-CB-CG	5.51	127.96	115.30
1	Bc	112	GLN	N-CA-C	5.50	125.85	111.00
1	BO	206	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	BG	206	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	BJ	202	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	BP	176	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	BA	176	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	Cc	176	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	BV	156	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	AD	62	ARG	CG-CD-NE	5.46	123.26	111.80
1	CJ	185	LEU	CA-CB-CG	5.45	127.84	115.30
1	BU	176	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	BJ	206	ARG	NE-CZ-NH2	-5.45	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BU	206	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	AM	62	ARG	CG-CD-NE	5.44	123.23	111.80
1	AI	182	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	BT	112	GLN	N-CA-C	5.44	125.68	111.00
1	CJ	97	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	Bc	176	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	AC	62	ARG	CG-CD-NE	5.43	123.21	111.80
1	AJ	62	ARG	CG-CD-NE	5.43	123.20	111.80
1	CD	176	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	AN	114	MET	CG-SD-CE	5.42	108.86	100.20
1	AX	62	ARG	CG-CD-NE	5.42	123.17	111.80
1	BR	156	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	BF	206	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	BL	202	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	Bb	112	GLN	N-CA-C	5.41	125.60	111.00
1	BA	206	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	BE	202	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	Bc	156	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	BO	202	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	AT	62	ARG	CG-CD-NE	5.38	123.09	111.80
1	BH	176	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	Ad	62	ARG	CG-CD-NE	5.37	123.08	111.80
1	AU	193	ASP	CB-CG-OD2	5.36	123.12	118.30
1	BZ	206	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	AA	62	ARG	CG-CD-NE	5.35	123.04	111.80
1	AB	193	ASP	CB-CG-OD2	5.35	123.12	118.30
1	BS	176	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	AO	182	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	AK	62	ARG	CG-CD-NE	5.34	123.03	111.80
1	CF	184	ILE	CG1-CB-CG2	-5.34	99.65	111.40
1	BF	206	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	BY	206	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	BB	91	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	AJ	182	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	CG	166	LEU	CA-CB-CG	5.32	127.54	115.30
1	AB	62	ARG	CG-CD-NE	5.32	122.96	111.80
1	CM	185	LEU	CA-CB-CG	5.31	127.52	115.30
1	AP	62	ARG	CG-CD-NE	5.31	122.96	111.80
1	CH	185	LEU	CA-CB-CG	5.30	127.49	115.30
1	AV	62	ARG	CG-CD-NE	5.30	122.93	111.80
1	CN	166	LEU	CA-CB-CG	5.30	127.48	115.30
1	CX	176	ARG	NE-CZ-NH1	-5.29	117.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CO	176	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	CY	185	LEU	CA-CB-CG	5.28	127.44	115.30
1	BW	206	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	AX	193	ASP	CB-CG-OD2	5.27	123.05	118.30
1	CN	177	LEU	CA-CB-CG	5.27	127.43	115.30
1	Ac	159	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	BP	156	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	AX	182	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	AT	62	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	AY	182	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	Cb	177	LEU	CA-CB-CG	5.26	127.39	115.30
1	BA	183	LEU	CA-CB-CG	5.26	127.39	115.30
1	AA	182	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	BC	202	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	AR	62	ARG	CG-CD-NE	5.25	122.83	111.80
1	AA	187	CYS	CA-CB-SG	5.25	123.44	114.00
1	BB	202	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	AN	62	ARG	CG-CD-NE	5.23	122.79	111.80
1	Cd	185	LEU	CA-CB-CG	5.23	127.34	115.30
1	CV	176	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	BI	206	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	BL	183	LEU	CA-CB-CG	5.22	127.30	115.30
1	AF	62	ARG	CG-CD-NE	5.21	122.75	111.80
1	CZ	176	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	CL	176	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	CD	107	LEU	CB-CA-C	-5.20	100.32	110.20
1	AE	101	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	AW	182	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	CD	185	LEU	CA-CB-CG	5.19	127.24	115.30
1	BL	176	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	AW	62	ARG	CG-CD-NE	5.19	122.70	111.80
1	Ac	101	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	CQ	185	LEU	CA-CB-CG	5.19	127.23	115.30
1	BY	206	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	CT	185	LEU	CA-CB-CG	5.18	127.22	115.30
1	Cb	176	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	AQ	62	ARG	CG-CD-NE	5.18	122.67	111.80
1	BW	183	LEU	CA-CB-CG	5.17	127.20	115.30
1	BR	202	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	AC	176	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	AD	62	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	BN	183	LEU	CA-CB-CG	5.16	127.17	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bb	176	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	AK	62	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	BQ	183	LEU	CA-CB-CG	5.16	127.17	115.30
1	Ad	182	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	Bd	176	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	BG	156	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	AC	62	ARG	CD-NE-CZ	5.15	130.81	123.60
1	BR	176	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	Cb	184	ILE	CG1-CB-CG2	-5.14	100.08	111.40
1	CU	185	LEU	CA-CB-CG	5.14	127.13	115.30
1	AU	62	ARG	CD-NE-CZ	5.14	130.79	123.60
1	BK	176	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	BV	206	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	BX	183	LEU	CA-CB-CG	5.13	127.09	115.30
1	AZ	182	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	AI	62	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	AY	176	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	BD	176	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	BB	206	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	BP	91	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	AC	182	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	CC	185	LEU	CA-CB-CG	5.10	127.04	115.30
1	CY	177	LEU	CA-CB-CG	5.10	127.03	115.30
1	AZ	62	ARG	CG-CD-NE	5.10	122.52	111.80
1	BC	206	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	CL	185	LEU	CA-CB-CG	5.09	127.01	115.30
1	AS	176	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	AH	62	ARG	CG-CD-NE	5.08	122.47	111.80
1	Cc	75	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	CG	185	LEU	CA-CB-CG	5.08	126.98	115.30
1	BL	193	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	BV	206	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	AT	193	ASP	CB-CG-OD2	5.06	122.85	118.30
1	BE	206	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	AJ	62	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	CO	185	LEU	CA-CB-CG	5.05	126.91	115.30
1	CR	176	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	BM	206	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	BS	202	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	CW	107	LEU	CB-CA-C	-5.04	100.62	110.20
1	CA	184	ILE	CG1-CB-CG2	-5.04	100.32	111.40
1	AQ	182	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aa	62	ARG	CG-CD-NE	5.04	122.38	111.80
1	AZ	62	ARG	CD-NE-CZ	5.03	130.65	123.60
1	AO	62	ARG	CD-NE-CZ	5.02	130.63	123.60
1	BQ	156	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	BM	91	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	CR	185	LEU	CA-CB-CG	5.01	126.81	115.30
1	BP	176	ARG	NE-CZ-NH1	-5.00	117.80	120.30
1	Ac	193	ASP	CB-CG-OD2	5.00	122.80	118.30
1	AL	62	ARG	CG-CD-NE	5.00	122.31	111.80
1	AE	62	ARG	CD-NE-CZ	5.00	130.60	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CU	207	LEU	Peptide
1	Cb	207	LEU	Peptide

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AB	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	AC	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AD	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AE	285/338 (84%)	277 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AF	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	AG	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AH	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AI	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	AJ	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AK	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AL	285/338 (84%)	275 (96%)	10 (4%)	0	100	100
1	AM	285/338 (84%)	279 (98%)	6 (2%)	0	100	100
1	AN	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AO	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AP	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	AQ	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AR	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	AS	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AT	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	AU	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AV	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AW	285/338 (84%)	275 (96%)	10 (4%)	0	100	100
1	AX	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	AY	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	AZ	285/338 (84%)	279 (98%)	6 (2%)	0	100	100
1	Aa	285/338 (84%)	278 (98%)	7 (2%)	0	100	100
1	Ab	285/338 (84%)	277 (97%)	8 (3%)	0	100	100
1	Ac	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	Ad	285/338 (84%)	276 (97%)	9 (3%)	0	100	100
1	BA	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BB	284/338 (84%)	280 (99%)	4 (1%)	0	100	100
1	BC	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BD	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BE	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BF	284/338 (84%)	280 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BG	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BH	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BI	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BJ	284/338 (84%)	280 (99%)	4 (1%)	0	100	100
1	BK	284/338 (84%)	280 (99%)	4 (1%)	0	100	100
1	BL	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BM	284/338 (84%)	280 (99%)	4 (1%)	0	100	100
1	BN	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BO	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BP	284/338 (84%)	279 (98%)	5 (2%)	0	100	100
1	BQ	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BR	284/338 (84%)	278 (98%)	6 (2%)	0	100	100
1	BS	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BT	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BU	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BV	284/338 (84%)	283 (100%)	1 (0%)	0	100	100
1	BW	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	BX	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BY	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	BZ	284/338 (84%)	280 (99%)	4 (1%)	0	100	100
1	Ba	284/338 (84%)	279 (98%)	5 (2%)	0	100	100
1	Bb	284/338 (84%)	282 (99%)	2 (1%)	0	100	100
1	Bc	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	Bd	284/338 (84%)	281 (99%)	3 (1%)	0	100	100
1	CA	302/338 (89%)	288 (95%)	14 (5%)	0	100	100
1	CB	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CC	302/338 (89%)	288 (95%)	14 (5%)	0	100	100
1	CD	302/338 (89%)	288 (95%)	14 (5%)	0	100	100
1	CE	302/338 (89%)	288 (95%)	14 (5%)	0	100	100
1	CF	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CG	302/338 (89%)	288 (95%)	14 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CH	302/338 (89%)	288 (95%)	14 (5%)	0	100	100
1	CI	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CJ	302/338 (89%)	289 (96%)	13 (4%)	0	100	100
1	CK	302/338 (89%)	286 (95%)	16 (5%)	0	100	100
1	CL	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CM	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CN	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CO	302/338 (89%)	288 (95%)	14 (5%)	0	100	100
1	CP	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CQ	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CR	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CS	302/338 (89%)	290 (96%)	12 (4%)	0	100	100
1	CT	302/338 (89%)	285 (94%)	17 (6%)	0	100	100
1	CU	302/338 (89%)	285 (94%)	17 (6%)	0	100	100
1	CV	302/338 (89%)	286 (95%)	16 (5%)	0	100	100
1	CW	302/338 (89%)	286 (95%)	16 (5%)	0	100	100
1	CX	302/338 (89%)	289 (96%)	13 (4%)	0	100	100
1	CY	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	CZ	302/338 (89%)	286 (95%)	16 (5%)	0	100	100
1	Ca	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	Cb	302/338 (89%)	287 (95%)	15 (5%)	0	100	100
1	Cc	302/338 (89%)	290 (96%)	12 (4%)	0	100	100
1	Cd	302/338 (89%)	289 (96%)	13 (4%)	0	100	100
All	All	26130/30420 (86%)	25356 (97%)	774 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	242/283 (86%)	209 (86%)	33 (14%)	3	22
1	AB	242/283 (86%)	206 (85%)	36 (15%)	3	19
1	AC	242/283 (86%)	207 (86%)	35 (14%)	3	20
1	AD	242/283 (86%)	208 (86%)	34 (14%)	3	21
1	AE	242/283 (86%)	206 (85%)	36 (15%)	3	19
1	AF	242/283 (86%)	208 (86%)	34 (14%)	3	21
1	AG	242/283 (86%)	208 (86%)	34 (14%)	3	21
1	AH	242/283 (86%)	209 (86%)	33 (14%)	3	22
1	AI	242/283 (86%)	206 (85%)	36 (15%)	3	19
1	AJ	242/283 (86%)	209 (86%)	33 (14%)	3	22
1	AK	242/283 (86%)	209 (86%)	33 (14%)	3	22
1	AL	242/283 (86%)	207 (86%)	35 (14%)	3	20
1	AM	242/283 (86%)	211 (87%)	31 (13%)	4	24
1	AN	242/283 (86%)	209 (86%)	33 (14%)	3	22
1	AO	242/283 (86%)	209 (86%)	33 (14%)	3	22
1	AP	242/283 (86%)	210 (87%)	32 (13%)	4	23
1	AQ	242/283 (86%)	208 (86%)	34 (14%)	3	21
1	AR	242/283 (86%)	205 (85%)	37 (15%)	2	18
1	AS	242/283 (86%)	207 (86%)	35 (14%)	3	20
1	AT	242/283 (86%)	208 (86%)	34 (14%)	3	21
1	AU	242/283 (86%)	207 (86%)	35 (14%)	3	20
1	AV	242/283 (86%)	207 (86%)	35 (14%)	3	20
1	AW	242/283 (86%)	208 (86%)	34 (14%)	3	21
1	AX	242/283 (86%)	208 (86%)	34 (14%)	3	21
1	AY	242/283 (86%)	210 (87%)	32 (13%)	4	23
1	AZ	242/283 (86%)	210 (87%)	32 (13%)	4	23
1	Aa	242/283 (86%)	208 (86%)	34 (14%)	3	21
1	Ab	242/283 (86%)	206 (85%)	36 (15%)	3	19
1	Ac	242/283 (86%)	208 (86%)	34 (14%)	3	21
1	Ad	242/283 (86%)	209 (86%)	33 (14%)	3	22
1	BA	242/283 (86%)	213 (88%)	29 (12%)	5	27
1	BB	242/283 (86%)	212 (88%)	30 (12%)	4	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BC	242/283 (86%)	214 (88%)	28 (12%)	5	29
1	BD	242/283 (86%)	215 (89%)	27 (11%)	6	30
1	BE	242/283 (86%)	215 (89%)	27 (11%)	6	30
1	BF	242/283 (86%)	214 (88%)	28 (12%)	5	29
1	BG	242/283 (86%)	214 (88%)	28 (12%)	5	29
1	BH	242/283 (86%)	216 (89%)	26 (11%)	6	32
1	BI	242/283 (86%)	213 (88%)	29 (12%)	5	27
1	BJ	242/283 (86%)	215 (89%)	27 (11%)	6	30
1	BK	242/283 (86%)	215 (89%)	27 (11%)	6	30
1	BL	242/283 (86%)	214 (88%)	28 (12%)	5	29
1	BM	242/283 (86%)	214 (88%)	28 (12%)	5	29
1	BN	242/283 (86%)	214 (88%)	28 (12%)	5	29
1	BO	242/283 (86%)	214 (88%)	28 (12%)	5	29
1	BP	242/283 (86%)	214 (88%)	28 (12%)	5	29
1	BQ	242/283 (86%)	215 (89%)	27 (11%)	6	30
1	BR	242/283 (86%)	215 (89%)	27 (11%)	6	30
1	BS	242/283 (86%)	215 (89%)	27 (11%)	6	30
1	BT	242/283 (86%)	214 (88%)	28 (12%)	5	29
1	BU	242/283 (86%)	214 (88%)	28 (12%)	5	29
1	BV	242/283 (86%)	215 (89%)	27 (11%)	6	30
1	BW	242/283 (86%)	216 (89%)	26 (11%)	6	32
1	BX	242/283 (86%)	215 (89%)	27 (11%)	6	30
1	BY	242/283 (86%)	215 (89%)	27 (11%)	6	30
1	BZ	242/283 (86%)	214 (88%)	28 (12%)	5	29
1	Ba	242/283 (86%)	215 (89%)	27 (11%)	6	30
1	Bb	242/283 (86%)	214 (88%)	28 (12%)	5	29
1	Bc	242/283 (86%)	213 (88%)	29 (12%)	5	27
1	Bd	242/283 (86%)	213 (88%)	29 (12%)	5	27
1	CA	255/283 (90%)	229 (90%)	26 (10%)	7	34
1	CB	255/283 (90%)	230 (90%)	25 (10%)	8	36
1	CC	255/283 (90%)	229 (90%)	26 (10%)	7	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	255/283 (90%)	229 (90%)	26 (10%)	7	34
1	CE	255/283 (90%)	227 (89%)	28 (11%)	6	31
1	CF	255/283 (90%)	230 (90%)	25 (10%)	8	36
1	CG	255/283 (90%)	226 (89%)	29 (11%)	5	29
1	CH	255/283 (90%)	229 (90%)	26 (10%)	7	34
1	CI	255/283 (90%)	228 (89%)	27 (11%)	6	32
1	CJ	255/283 (90%)	229 (90%)	26 (10%)	7	34
1	CK	255/283 (90%)	228 (89%)	27 (11%)	6	32
1	CL	255/283 (90%)	231 (91%)	24 (9%)	8	38
1	CM	255/283 (90%)	229 (90%)	26 (10%)	7	34
1	CN	255/283 (90%)	228 (89%)	27 (11%)	6	32
1	CO	255/283 (90%)	230 (90%)	25 (10%)	8	36
1	CP	255/283 (90%)	230 (90%)	25 (10%)	8	36
1	CQ	255/283 (90%)	229 (90%)	26 (10%)	7	34
1	CR	255/283 (90%)	230 (90%)	25 (10%)	8	36
1	CS	255/283 (90%)	228 (89%)	27 (11%)	6	32
1	CT	255/283 (90%)	230 (90%)	25 (10%)	8	36
1	CU	255/283 (90%)	228 (89%)	27 (11%)	6	32
1	CV	255/283 (90%)	227 (89%)	28 (11%)	6	31
1	CW	255/283 (90%)	228 (89%)	27 (11%)	6	32
1	CX	255/283 (90%)	228 (89%)	27 (11%)	6	32
1	CY	255/283 (90%)	228 (89%)	27 (11%)	6	32
1	CZ	255/283 (90%)	228 (89%)	27 (11%)	6	32
1	Ca	255/283 (90%)	228 (89%)	27 (11%)	6	32
1	Cb	255/283 (90%)	229 (90%)	26 (10%)	7	34
1	Cc	255/283 (90%)	228 (89%)	27 (11%)	6	32
1	Cd	255/283 (90%)	231 (91%)	24 (9%)	8	38
All	All	22170/25470 (87%)	19531 (88%)	2639 (12%)	5	27

All (2639) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BA	57	LEU

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Mol	Chain	Res	Type
1	BA	58	SER
1	BA	63	ILE
1	BA	67	VAL
1	BA	68	LEU
1	BA	78	VAL
1	BA	79	VAL
1	BA	88	LEU
1	BA	92	LEU
1	BA	100	GLN
1	BA	104	VAL
1	BA	105	GLU
1	BA	134	ASN
1	BA	142	GLN
1	BA	145	ARG
1	BA	156	ARG
1	BA	165	THR
1	BA	167	LEU
1	BA	183	LEU
1	BA	184	ILE
1	BA	191	ASN
1	BA	193	ASP
1	BA	196	ASN
1	BA	198	SER
1	BA	207	LEU
1	BA	212	LEU
1	BA	225	GLN
1	BA	271	THR
1	BA	319	GLN
1	AA	54	ASP
1	AA	62	ARG
1	AA	72	THR
1	AA	74	THR
1	AA	75	ASP
1	AA	87	ASP
1	AA	118	ASN
1	AA	124	VAL
1	AA	128	LEU
1	AA	137	THR
1	AA	141	LEU
1	AA	142	GLN
1	AA	149	VAL
1	AA	159	ARG

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Mol	Chain	Res	Type
1	AA	162	TYR
1	AA	163	THR
1	AA	165	THR
1	AA	167	LEU
1	AA	170	SER
1	AA	176	ARG
1	AA	183	LEU
1	AA	196	ASN
1	AA	208	SER
1	AA	211	SER
1	AA	225	GLN
1	AA	236	ASN
1	AA	253	ASP
1	AA	264	SER
1	AA	271	THR
1	AA	304	PHE
1	AA	312	VAL
1	AA	315	TYR
1	AA	317	ASP
1	CA	35	THR
1	CA	43	SER
1	CA	48	PHE
1	CA	72	THR
1	CA	74	THR
1	CA	75	ASP
1	CA	77	TYR
1	CA	87	ASP
1	CA	101	ARG
1	CA	112	GLN
1	CA	114	MET
1	CA	137	THR
1	CA	141	LEU
1	CA	151	LYS
1	CA	156	ARG
1	CA	175	GLN
1	CA	176	ARG
1	CA	177	LEU
1	CA	185	LEU
1	CA	198	SER
1	CA	204	SER
1	CA	208	SER
1	CA	231	ASP

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Mol	Chain	Res	Type
1	CA	288	ASN
1	CA	316	SER
1	CA	337	GLU
1	BB	57	LEU
1	BB	58	SER
1	BB	63	ILE
1	BB	67	VAL
1	BB	68	LEU
1	BB	78	VAL
1	BB	79	VAL
1	BB	88	LEU
1	BB	92	LEU
1	BB	100	GLN
1	BB	104	VAL
1	BB	105	GLU
1	BB	134	ASN
1	BB	139	ASP
1	BB	142	GLN
1	BB	145	ARG
1	BB	156	ARG
1	BB	165	THR
1	BB	167	LEU
1	BB	183	LEU
1	BB	184	ILE
1	BB	191	ASN
1	BB	196	ASN
1	BB	198	SER
1	BB	202	ARG
1	BB	207	LEU
1	BB	212	LEU
1	BB	271	THR
1	BB	310	ASP
1	BB	319	GLN
1	AB	54	ASP
1	AB	58	SER
1	AB	62	ARG
1	AB	72	THR
1	AB	74	THR
1	AB	75	ASP
1	AB	83	THR
1	AB	87	ASP
1	AB	128	LEU

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Mol	Chain	Res	Type
1	AB	137	THR
1	AB	141	LEU
1	AB	142	GLN
1	AB	144	THR
1	AB	149	VAL
1	AB	157	THR
1	AB	159	ARG
1	AB	162	TYR
1	AB	163	THR
1	AB	165	THR
1	AB	167	LEU
1	AB	170	SER
1	AB	176	ARG
1	AB	183	LEU
1	AB	196	ASN
1	AB	208	SER
1	AB	211	SER
1	AB	212	LEU
1	AB	225	GLN
1	AB	236	ASN
1	AB	253	ASP
1	AB	264	SER
1	AB	271	THR
1	AB	304	PHE
1	AB	312	VAL
1	AB	315	TYR
1	AB	317	ASP
1	CB	35	THR
1	CB	43	SER
1	CB	48	PHE
1	CB	72	THR
1	CB	74	THR
1	CB	75	ASP
1	CB	77	TYR
1	CB	87	ASP
1	CB	101	ARG
1	CB	112	GLN
1	CB	114	MET
1	CB	137	THR
1	CB	141	LEU
1	CB	151	LYS
1	CB	156	ARG

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Mol	Chain	Res	Type
1	CB	175	GLN
1	CB	176	ARG
1	CB	177	LEU
1	CB	185	LEU
1	CB	198	SER
1	CB	204	SER
1	CB	231	ASP
1	CB	288	ASN
1	CB	316	SER
1	CB	337	GLU
1	BC	57	LEU
1	BC	58	SER
1	BC	63	ILE
1	BC	67	VAL
1	BC	68	LEU
1	BC	78	VAL
1	BC	79	VAL
1	BC	88	LEU
1	BC	92	LEU
1	BC	100	GLN
1	BC	104	VAL
1	BC	105	GLU
1	BC	134	ASN
1	BC	145	ARG
1	BC	156	ARG
1	BC	165	THR
1	BC	167	LEU
1	BC	183	LEU
1	BC	184	ILE
1	BC	191	ASN
1	BC	193	ASP
1	BC	196	ASN
1	BC	198	SER
1	BC	202	ARG
1	BC	207	LEU
1	BC	212	LEU
1	BC	271	THR
1	BC	319	GLN
1	AC	54	ASP
1	AC	58	SER
1	AC	62	ARG
1	AC	72	THR

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Mol	Chain	Res	Type
1	AC	74	THR
1	AC	75	ASP
1	AC	87	ASP
1	AC	101	ARG
1	AC	118	ASN
1	AC	124	VAL
1	AC	128	LEU
1	AC	137	THR
1	AC	141	LEU
1	AC	142	GLN
1	AC	149	VAL
1	AC	159	ARG
1	AC	162	TYR
1	AC	163	THR
1	AC	165	THR
1	AC	167	LEU
1	AC	170	SER
1	AC	176	ARG
1	AC	183	LEU
1	AC	196	ASN
1	AC	208	SER
1	AC	211	SER
1	AC	225	GLN
1	AC	236	ASN
1	AC	253	ASP
1	AC	264	SER
1	AC	271	THR
1	AC	304	PHE
1	AC	312	VAL
1	AC	315	TYR
1	AC	317	ASP
1	CC	35	THR
1	CC	43	SER
1	CC	48	PHE
1	CC	54	ASP
1	CC	72	THR
1	CC	74	THR
1	CC	75	ASP
1	CC	77	TYR
1	CC	87	ASP
1	CC	101	ARG
1	CC	112	GLN

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Mol	Chain	Res	Type
1	CC	114	MET
1	CC	137	THR
1	CC	141	LEU
1	CC	151	LYS
1	CC	156	ARG
1	CC	175	GLN
1	CC	176	ARG
1	CC	177	LEU
1	CC	185	LEU
1	CC	198	SER
1	CC	204	SER
1	CC	231	ASP
1	CC	288	ASN
1	CC	316	SER
1	CC	337	GLU
1	BD	57	LEU
1	BD	58	SER
1	BD	63	ILE
1	BD	67	VAL
1	BD	68	LEU
1	BD	78	VAL
1	BD	79	VAL
1	BD	88	LEU
1	BD	92	LEU
1	BD	100	GLN
1	BD	104	VAL
1	BD	105	GLU
1	BD	134	ASN
1	BD	145	ARG
1	BD	156	ARG
1	BD	165	THR
1	BD	167	LEU
1	BD	183	LEU
1	BD	184	ILE
1	BD	191	ASN
1	BD	193	ASP
1	BD	196	ASN
1	BD	198	SER
1	BD	207	LEU
1	BD	212	LEU
1	BD	271	THR
1	BD	319	GLN

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Mol	Chain	Res	Type
1	AD	54	ASP
1	AD	58	SER
1	AD	62	ARG
1	AD	72	THR
1	AD	74	THR
1	AD	75	ASP
1	AD	87	ASP
1	AD	124	VAL
1	AD	128	LEU
1	AD	137	THR
1	AD	141	LEU
1	AD	142	GLN
1	AD	144	THR
1	AD	149	VAL
1	AD	159	ARG
1	AD	162	TYR
1	AD	163	THR
1	AD	165	THR
1	AD	167	LEU
1	AD	170	SER
1	AD	176	ARG
1	AD	183	LEU
1	AD	196	ASN
1	AD	208	SER
1	AD	211	SER
1	AD	225	GLN
1	AD	236	ASN
1	AD	253	ASP
1	AD	264	SER
1	AD	271	THR
1	AD	304	PHE
1	AD	312	VAL
1	AD	315	TYR
1	AD	317	ASP
1	CD	35	THR
1	CD	43	SER
1	CD	54	ASP
1	CD	72	THR
1	CD	74	THR
1	CD	75	ASP
1	CD	77	TYR
1	CD	87	ASP

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Mol	Chain	Res	Type
1	CD	101	ARG
1	CD	112	GLN
1	CD	114	MET
1	CD	137	THR
1	CD	141	LEU
1	CD	151	LYS
1	CD	156	ARG
1	CD	175	GLN
1	CD	176	ARG
1	CD	177	LEU
1	CD	185	LEU
1	CD	198	SER
1	CD	204	SER
1	CD	208	SER
1	CD	231	ASP
1	CD	288	ASN
1	CD	316	SER
1	CD	337	GLU
1	BE	57	LEU
1	BE	58	SER
1	BE	63	ILE
1	BE	67	VAL
1	BE	68	LEU
1	BE	78	VAL
1	BE	79	VAL
1	BE	88	LEU
1	BE	92	LEU
1	BE	100	GLN
1	BE	104	VAL
1	BE	105	GLU
1	BE	134	ASN
1	BE	145	ARG
1	BE	156	ARG
1	BE	165	THR
1	BE	167	LEU
1	BE	183	LEU
1	BE	184	ILE
1	BE	191	ASN
1	BE	193	ASP
1	BE	196	ASN
1	BE	198	SER
1	BE	207	LEU

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Mol	Chain	Res	Type
1	BE	212	LEU
1	BE	271	THR
1	BE	319	GLN
1	AE	54	ASP
1	AE	58	SER
1	AE	62	ARG
1	AE	72	THR
1	AE	74	THR
1	AE	75	ASP
1	AE	87	ASP
1	AE	101	ARG
1	AE	118	ASN
1	AE	128	LEU
1	AE	137	THR
1	AE	141	LEU
1	AE	142	GLN
1	AE	144	THR
1	AE	149	VAL
1	AE	157	THR
1	AE	159	ARG
1	AE	162	TYR
1	AE	163	THR
1	AE	165	THR
1	AE	167	LEU
1	AE	170	SER
1	AE	176	ARG
1	AE	183	LEU
1	AE	196	ASN
1	AE	208	SER
1	AE	211	SER
1	AE	225	GLN
1	AE	236	ASN
1	AE	253	ASP
1	AE	264	SER
1	AE	271	THR
1	AE	304	PHE
1	AE	312	VAL
1	AE	315	TYR
1	AE	317	ASP
1	CE	35	THR
1	CE	43	SER
1	CE	48	PHE

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Mol	Chain	Res	Type
1	CE	72	THR
1	CE	74	THR
1	CE	75	ASP
1	CE	77	TYR
1	CE	87	ASP
1	CE	101	ARG
1	CE	106	THR
1	CE	112	GLN
1	CE	114	MET
1	CE	137	THR
1	CE	141	LEU
1	CE	151	LYS
1	CE	156	ARG
1	CE	175	GLN
1	CE	176	ARG
1	CE	177	LEU
1	CE	185	LEU
1	CE	186	LEU
1	CE	198	SER
1	CE	204	SER
1	CE	208	SER
1	CE	231	ASP
1	CE	288	ASN
1	CE	316	SER
1	CE	337	GLU
1	BF	57	LEU
1	BF	58	SER
1	BF	63	ILE
1	BF	67	VAL
1	BF	68	LEU
1	BF	78	VAL
1	BF	79	VAL
1	BF	88	LEU
1	BF	92	LEU
1	BF	100	GLN
1	BF	104	VAL
1	BF	105	GLU
1	BF	134	ASN
1	BF	145	ARG
1	BF	156	ARG
1	BF	165	THR
1	BF	167	LEU

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Mol	Chain	Res	Type
1	BF	183	LEU
1	BF	184	ILE
1	BF	191	ASN
1	BF	193	ASP
1	BF	196	ASN
1	BF	198	SER
1	BF	202	ARG
1	BF	207	LEU
1	BF	212	LEU
1	BF	271	THR
1	BF	319	GLN
1	AF	54	ASP
1	AF	58	SER
1	AF	62	ARG
1	AF	72	THR
1	AF	74	THR
1	AF	75	ASP
1	AF	87	ASP
1	AF	118	ASN
1	AF	124	VAL
1	AF	128	LEU
1	AF	137	THR
1	AF	141	LEU
1	AF	142	GLN
1	AF	149	VAL
1	AF	159	ARG
1	AF	162	TYR
1	AF	163	THR
1	AF	165	THR
1	AF	167	LEU
1	AF	170	SER
1	AF	176	ARG
1	AF	183	LEU
1	AF	196	ASN
1	AF	208	SER
1	AF	211	SER
1	AF	225	GLN
1	AF	236	ASN
1	AF	253	ASP
1	AF	264	SER
1	AF	271	THR
1	AF	304	PHE

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Mol	Chain	Res	Type
1	AF	312	VAL
1	AF	315	TYR
1	AF	317	ASP
1	CF	35	THR
1	CF	43	SER
1	CF	48	PHE
1	CF	72	THR
1	CF	74	THR
1	CF	75	ASP
1	CF	77	TYR
1	CF	87	ASP
1	CF	101	ARG
1	CF	112	GLN
1	CF	114	MET
1	CF	137	THR
1	CF	141	LEU
1	CF	151	LYS
1	CF	156	ARG
1	CF	175	GLN
1	CF	176	ARG
1	CF	177	LEU
1	CF	185	LEU
1	CF	198	SER
1	CF	204	SER
1	CF	231	ASP
1	CF	288	ASN
1	CF	316	SER
1	CF	337	GLU
1	BG	57	LEU
1	BG	58	SER
1	BG	63	ILE
1	BG	67	VAL
1	BG	68	LEU
1	BG	78	VAL
1	BG	79	VAL
1	BG	88	LEU
1	BG	92	LEU
1	BG	100	GLN
1	BG	104	VAL
1	BG	105	GLU
1	BG	134	ASN
1	BG	145	ARG

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Mol	Chain	Res	Type
1	BG	156	ARG
1	BG	165	THR
1	BG	167	LEU
1	BG	183	LEU
1	BG	184	ILE
1	BG	191	ASN
1	BG	193	ASP
1	BG	196	ASN
1	BG	198	SER
1	BG	202	ARG
1	BG	207	LEU
1	BG	212	LEU
1	BG	271	THR
1	BG	319	GLN
1	AG	54	ASP
1	AG	58	SER
1	AG	62	ARG
1	AG	72	THR
1	AG	74	THR
1	AG	75	ASP
1	AG	83	THR
1	AG	87	ASP
1	AG	128	LEU
1	AG	137	THR
1	AG	141	LEU
1	AG	142	GLN
1	AG	149	VAL
1	AG	159	ARG
1	AG	162	TYR
1	AG	163	THR
1	AG	165	THR
1	AG	167	LEU
1	AG	170	SER
1	AG	176	ARG
1	AG	183	LEU
1	AG	196	ASN
1	AG	208	SER
1	AG	211	SER
1	AG	212	LEU
1	AG	225	GLN
1	AG	236	ASN
1	AG	253	ASP

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Mol	Chain	Res	Type
1	AG	264	SER
1	AG	271	THR
1	AG	304	PHE
1	AG	312	VAL
1	AG	315	TYR
1	AG	317	ASP
1	CG	35	THR
1	CG	43	SER
1	CG	48	PHE
1	CG	54	ASP
1	CG	72	THR
1	CG	74	THR
1	CG	75	ASP
1	CG	77	TYR
1	CG	87	ASP
1	CG	101	ARG
1	CG	106	THR
1	CG	112	GLN
1	CG	114	MET
1	CG	137	THR
1	CG	141	LEU
1	CG	151	LYS
1	CG	156	ARG
1	CG	175	GLN
1	CG	176	ARG
1	CG	177	LEU
1	CG	185	LEU
1	CG	186	LEU
1	CG	198	SER
1	CG	204	SER
1	CG	208	SER
1	CG	231	ASP
1	CG	288	ASN
1	CG	316	SER
1	CG	337	GLU
1	BH	57	LEU
1	BH	58	SER
1	BH	63	ILE
1	BH	67	VAL
1	BH	68	LEU
1	BH	78	VAL
1	BH	79	VAL

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Mol	Chain	Res	Type
1	BH	88	LEU
1	BH	92	LEU
1	BH	100	GLN
1	BH	104	VAL
1	BH	105	GLU
1	BH	134	ASN
1	BH	145	ARG
1	BH	156	ARG
1	BH	165	THR
1	BH	167	LEU
1	BH	183	LEU
1	BH	184	ILE
1	BH	191	ASN
1	BH	196	ASN
1	BH	198	SER
1	BH	207	LEU
1	BH	212	LEU
1	BH	271	THR
1	BH	319	GLN
1	AH	54	ASP
1	AH	58	SER
1	AH	62	ARG
1	AH	72	THR
1	AH	74	THR
1	AH	75	ASP
1	AH	87	ASP
1	AH	128	LEU
1	AH	137	THR
1	AH	141	LEU
1	AH	142	GLN
1	AH	144	THR
1	AH	149	VAL
1	AH	159	ARG
1	AH	162	TYR
1	AH	163	THR
1	AH	165	THR
1	AH	167	LEU
1	AH	170	SER
1	AH	176	ARG
1	AH	183	LEU
1	AH	196	ASN
1	AH	208	SER

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Mol	Chain	Res	Type
1	AH	211	SER
1	AH	225	GLN
1	AH	236	ASN
1	AH	253	ASP
1	AH	264	SER
1	AH	271	THR
1	AH	304	PHE
1	AH	312	VAL
1	AH	315	TYR
1	AH	317	ASP
1	CH	35	THR
1	CH	43	SER
1	CH	48	PHE
1	CH	72	THR
1	CH	74	THR
1	CH	75	ASP
1	CH	77	TYR
1	CH	87	ASP
1	CH	101	ARG
1	CH	112	GLN
1	CH	114	MET
1	CH	137	THR
1	CH	141	LEU
1	CH	151	LYS
1	CH	156	ARG
1	CH	175	GLN
1	CH	176	ARG
1	CH	177	LEU
1	CH	185	LEU
1	CH	198	SER
1	CH	204	SER
1	CH	208	SER
1	CH	231	ASP
1	CH	288	ASN
1	CH	316	SER
1	CH	337	GLU
1	BI	57	LEU
1	BI	58	SER
1	BI	63	ILE
1	BI	67	VAL
1	BI	68	LEU
1	BI	78	VAL

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Mol	Chain	Res	Type
1	BI	79	VAL
1	BI	88	LEU
1	BI	92	LEU
1	BI	100	GLN
1	BI	104	VAL
1	BI	105	GLU
1	BI	134	ASN
1	BI	139	ASP
1	BI	145	ARG
1	BI	156	ARG
1	BI	165	THR
1	BI	167	LEU
1	BI	183	LEU
1	BI	184	ILE
1	BI	191	ASN
1	BI	193	ASP
1	BI	196	ASN
1	BI	198	SER
1	BI	202	ARG
1	BI	207	LEU
1	BI	212	LEU
1	BI	271	THR
1	BI	319	GLN
1	AI	54	ASP
1	AI	58	SER
1	AI	62	ARG
1	AI	72	THR
1	AI	74	THR
1	AI	75	ASP
1	AI	87	ASP
1	AI	124	VAL
1	AI	128	LEU
1	AI	130	ASP
1	AI	137	THR
1	AI	141	LEU
1	AI	142	GLN
1	AI	144	THR
1	AI	149	VAL
1	AI	157	THR
1	AI	159	ARG
1	AI	162	TYR
1	AI	163	THR

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Mol	Chain	Res	Type
1	AI	165	THR
1	AI	167	LEU
1	AI	170	SER
1	AI	176	ARG
1	AI	183	LEU
1	AI	196	ASN
1	AI	208	SER
1	AI	211	SER
1	AI	225	GLN
1	AI	236	ASN
1	AI	253	ASP
1	AI	264	SER
1	AI	271	THR
1	AI	304	PHE
1	AI	312	VAL
1	AI	315	TYR
1	AI	317	ASP
1	CI	35	THR
1	CI	43	SER
1	CI	48	PHE
1	CI	54	ASP
1	CI	72	THR
1	CI	74	THR
1	CI	75	ASP
1	CI	77	TYR
1	CI	87	ASP
1	CI	101	ARG
1	CI	112	GLN
1	CI	114	MET
1	CI	137	THR
1	CI	141	LEU
1	CI	151	LYS
1	CI	156	ARG
1	CI	175	GLN
1	CI	176	ARG
1	CI	177	LEU
1	CI	185	LEU
1	CI	198	SER
1	CI	204	SER
1	CI	208	SER
1	CI	231	ASP
1	CI	288	ASN

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Mol	Chain	Res	Type
1	CI	316	SER
1	CI	337	GLU
1	BJ	57	LEU
1	BJ	58	SER
1	BJ	63	ILE
1	BJ	67	VAL
1	BJ	68	LEU
1	BJ	78	VAL
1	BJ	79	VAL
1	BJ	88	LEU
1	BJ	92	LEU
1	BJ	100	GLN
1	BJ	104	VAL
1	BJ	105	GLU
1	BJ	134	ASN
1	BJ	145	ARG
1	BJ	156	ARG
1	BJ	165	THR
1	BJ	167	LEU
1	BJ	183	LEU
1	BJ	184	ILE
1	BJ	191	ASN
1	BJ	193	ASP
1	BJ	196	ASN
1	BJ	198	SER
1	BJ	207	LEU
1	BJ	212	LEU
1	BJ	271	THR
1	BJ	319	GLN
1	AJ	54	ASP
1	AJ	62	ARG
1	AJ	72	THR
1	AJ	74	THR
1	AJ	75	ASP
1	AJ	83	THR
1	AJ	87	ASP
1	AJ	128	LEU
1	AJ	137	THR
1	AJ	141	LEU
1	AJ	142	GLN
1	AJ	144	THR
1	AJ	149	VAL

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Mol	Chain	Res	Type
1	AJ	159	ARG
1	AJ	162	TYR
1	AJ	163	THR
1	AJ	165	THR
1	AJ	167	LEU
1	AJ	170	SER
1	AJ	176	ARG
1	AJ	183	LEU
1	AJ	196	ASN
1	AJ	208	SER
1	AJ	211	SER
1	AJ	225	GLN
1	AJ	236	ASN
1	AJ	253	ASP
1	AJ	264	SER
1	AJ	271	THR
1	AJ	304	PHE
1	AJ	312	VAL
1	AJ	315	TYR
1	AJ	317	ASP
1	CJ	35	THR
1	CJ	43	SER
1	CJ	48	PHE
1	CJ	72	THR
1	CJ	74	THR
1	CJ	75	ASP
1	CJ	77	TYR
1	CJ	87	ASP
1	CJ	101	ARG
1	CJ	112	GLN
1	CJ	114	MET
1	CJ	137	THR
1	CJ	141	LEU
1	CJ	151	LYS
1	CJ	156	ARG
1	CJ	175	GLN
1	CJ	176	ARG
1	CJ	177	LEU
1	CJ	185	LEU
1	CJ	198	SER
1	CJ	204	SER
1	CJ	208	SER

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Mol	Chain	Res	Type
1	CJ	231	ASP
1	CJ	288	ASN
1	CJ	316	SER
1	CJ	337	GLU
1	BK	57	LEU
1	BK	58	SER
1	BK	63	ILE
1	BK	67	VAL
1	BK	68	LEU
1	BK	78	VAL
1	BK	79	VAL
1	BK	88	LEU
1	BK	92	LEU
1	BK	100	GLN
1	BK	104	VAL
1	BK	105	GLU
1	BK	134	ASN
1	BK	145	ARG
1	BK	156	ARG
1	BK	165	THR
1	BK	167	LEU
1	BK	183	LEU
1	BK	184	ILE
1	BK	191	ASN
1	BK	196	ASN
1	BK	198	SER
1	BK	202	ARG
1	BK	207	LEU
1	BK	212	LEU
1	BK	271	THR
1	BK	319	GLN
1	AK	54	ASP
1	AK	62	ARG
1	AK	72	THR
1	AK	74	THR
1	AK	75	ASP
1	AK	83	THR
1	AK	87	ASP
1	AK	128	LEU
1	AK	137	THR
1	AK	141	LEU
1	AK	142	GLN

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Mol	Chain	Res	Type
1	AK	144	THR
1	AK	149	VAL
1	AK	159	ARG
1	AK	162	TYR
1	AK	163	THR
1	AK	165	THR
1	AK	167	LEU
1	AK	170	SER
1	AK	176	ARG
1	AK	183	LEU
1	AK	196	ASN
1	AK	208	SER
1	AK	211	SER
1	AK	225	GLN
1	AK	236	ASN
1	AK	253	ASP
1	AK	264	SER
1	AK	271	THR
1	AK	304	PHE
1	AK	312	VAL
1	AK	315	TYR
1	AK	317	ASP
1	CK	35	THR
1	CK	43	SER
1	CK	72	THR
1	CK	74	THR
1	CK	75	ASP
1	CK	77	TYR
1	CK	81	ASP
1	CK	87	ASP
1	CK	101	ARG
1	CK	112	GLN
1	CK	114	MET
1	CK	137	THR
1	CK	141	LEU
1	CK	151	LYS
1	CK	156	ARG
1	CK	175	GLN
1	CK	176	ARG
1	CK	177	LEU
1	CK	185	LEU
1	CK	198	SER

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Mol	Chain	Res	Type
1	CK	204	SER
1	CK	208	SER
1	CK	231	ASP
1	CK	288	ASN
1	CK	296	PHE
1	CK	316	SER
1	CK	337	GLU
1	BL	57	LEU
1	BL	58	SER
1	BL	63	ILE
1	BL	67	VAL
1	BL	68	LEU
1	BL	78	VAL
1	BL	79	VAL
1	BL	88	LEU
1	BL	92	LEU
1	BL	100	GLN
1	BL	104	VAL
1	BL	105	GLU
1	BL	134	ASN
1	BL	142	GLN
1	BL	145	ARG
1	BL	156	ARG
1	BL	165	THR
1	BL	167	LEU
1	BL	183	LEU
1	BL	184	ILE
1	BL	191	ASN
1	BL	193	ASP
1	BL	196	ASN
1	BL	198	SER
1	BL	207	LEU
1	BL	212	LEU
1	BL	271	THR
1	BL	319	GLN
1	AL	54	ASP
1	AL	58	SER
1	AL	62	ARG
1	AL	72	THR
1	AL	74	THR
1	AL	75	ASP
1	AL	87	ASP

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Mol	Chain	Res	Type
1	AL	118	ASN
1	AL	124	VAL
1	AL	128	LEU
1	AL	137	THR
1	AL	141	LEU
1	AL	142	GLN
1	AL	144	THR
1	AL	149	VAL
1	AL	157	THR
1	AL	159	ARG
1	AL	163	THR
1	AL	165	THR
1	AL	167	LEU
1	AL	170	SER
1	AL	176	ARG
1	AL	183	LEU
1	AL	196	ASN
1	AL	208	SER
1	AL	211	SER
1	AL	225	GLN
1	AL	236	ASN
1	AL	253	ASP
1	AL	264	SER
1	AL	271	THR
1	AL	304	PHE
1	AL	312	VAL
1	AL	315	TYR
1	AL	317	ASP
1	CL	35	THR
1	CL	43	SER
1	CL	72	THR
1	CL	74	THR
1	CL	75	ASP
1	CL	77	TYR
1	CL	87	ASP
1	CL	101	ARG
1	CL	112	GLN
1	CL	114	MET
1	CL	137	THR
1	CL	141	LEU
1	CL	151	LYS
1	CL	156	ARG

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Mol	Chain	Res	Type
1	CL	175	GLN
1	CL	176	ARG
1	CL	177	LEU
1	CL	185	LEU
1	CL	204	SER
1	CL	208	SER
1	CL	231	ASP
1	CL	288	ASN
1	CL	316	SER
1	CL	337	GLU
1	BM	57	LEU
1	BM	58	SER
1	BM	63	ILE
1	BM	67	VAL
1	BM	68	LEU
1	BM	78	VAL
1	BM	79	VAL
1	BM	88	LEU
1	BM	92	LEU
1	BM	100	GLN
1	BM	104	VAL
1	BM	105	GLU
1	BM	134	ASN
1	BM	145	ARG
1	BM	156	ARG
1	BM	165	THR
1	BM	167	LEU
1	BM	183	LEU
1	BM	184	ILE
1	BM	191	ASN
1	BM	193	ASP
1	BM	196	ASN
1	BM	198	SER
1	BM	202	ARG
1	BM	207	LEU
1	BM	212	LEU
1	BM	271	THR
1	BM	319	GLN
1	AM	54	ASP
1	AM	62	ARG
1	AM	72	THR
1	AM	74	THR

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Mol	Chain	Res	Type
1	AM	75	ASP
1	AM	87	ASP
1	AM	128	LEU
1	AM	137	THR
1	AM	141	LEU
1	AM	142	GLN
1	AM	149	VAL
1	AM	159	ARG
1	AM	162	TYR
1	AM	163	THR
1	AM	165	THR
1	AM	167	LEU
1	AM	170	SER
1	AM	176	ARG
1	AM	183	LEU
1	AM	196	ASN
1	AM	208	SER
1	AM	211	SER
1	AM	225	GLN
1	AM	236	ASN
1	AM	253	ASP
1	AM	264	SER
1	AM	271	THR
1	AM	304	PHE
1	AM	312	VAL
1	AM	315	TYR
1	AM	317	ASP
1	CM	35	THR
1	CM	43	SER
1	CM	48	PHE
1	CM	72	THR
1	CM	74	THR
1	CM	75	ASP
1	CM	77	TYR
1	CM	87	ASP
1	CM	101	ARG
1	CM	112	GLN
1	CM	114	MET
1	CM	137	THR
1	CM	141	LEU
1	CM	151	LYS
1	CM	156	ARG

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Mol	Chain	Res	Type
1	CM	175	GLN
1	CM	176	ARG
1	CM	177	LEU
1	CM	185	LEU
1	CM	198	SER
1	CM	204	SER
1	CM	208	SER
1	CM	231	ASP
1	CM	288	ASN
1	CM	316	SER
1	CM	337	GLU
1	BN	57	LEU
1	BN	58	SER
1	BN	63	ILE
1	BN	67	VAL
1	BN	68	LEU
1	BN	78	VAL
1	BN	79	VAL
1	BN	88	LEU
1	BN	92	LEU
1	BN	100	GLN
1	BN	104	VAL
1	BN	105	GLU
1	BN	134	ASN
1	BN	142	GLN
1	BN	145	ARG
1	BN	156	ARG
1	BN	165	THR
1	BN	167	LEU
1	BN	183	LEU
1	BN	184	ILE
1	BN	191	ASN
1	BN	193	ASP
1	BN	196	ASN
1	BN	198	SER
1	BN	207	LEU
1	BN	212	LEU
1	BN	271	THR
1	BN	319	GLN
1	AN	54	ASP
1	AN	62	ARG
1	AN	72	THR

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Mol	Chain	Res	Type
1	AN	74	THR
1	AN	75	ASP
1	AN	87	ASP
1	AN	124	VAL
1	AN	128	LEU
1	AN	137	THR
1	AN	141	LEU
1	AN	142	GLN
1	AN	144	THR
1	AN	149	VAL
1	AN	159	ARG
1	AN	162	TYR
1	AN	163	THR
1	AN	165	THR
1	AN	167	LEU
1	AN	170	SER
1	AN	176	ARG
1	AN	183	LEU
1	AN	196	ASN
1	AN	208	SER
1	AN	211	SER
1	AN	225	GLN
1	AN	236	ASN
1	AN	253	ASP
1	AN	264	SER
1	AN	271	THR
1	AN	304	PHE
1	AN	312	VAL
1	AN	315	TYR
1	AN	317	ASP
1	CN	35	THR
1	CN	43	SER
1	CN	48	PHE
1	CN	72	THR
1	CN	74	THR
1	CN	75	ASP
1	CN	77	TYR
1	CN	87	ASP
1	CN	101	ARG
1	CN	112	GLN
1	CN	114	MET
1	CN	137	THR

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Mol	Chain	Res	Type
1	CN	141	LEU
1	CN	151	LYS
1	CN	156	ARG
1	CN	175	GLN
1	CN	176	ARG
1	CN	177	LEU
1	CN	185	LEU
1	CN	186	LEU
1	CN	198	SER
1	CN	204	SER
1	CN	208	SER
1	CN	231	ASP
1	CN	288	ASN
1	CN	316	SER
1	CN	337	GLU
1	BO	57	LEU
1	BO	58	SER
1	BO	63	ILE
1	BO	67	VAL
1	BO	68	LEU
1	BO	78	VAL
1	BO	79	VAL
1	BO	88	LEU
1	BO	92	LEU
1	BO	100	GLN
1	BO	104	VAL
1	BO	105	GLU
1	BO	134	ASN
1	BO	142	GLN
1	BO	145	ARG
1	BO	156	ARG
1	BO	165	THR
1	BO	167	LEU
1	BO	183	LEU
1	BO	184	ILE
1	BO	191	ASN
1	BO	193	ASP
1	BO	196	ASN
1	BO	198	SER
1	BO	207	LEU
1	BO	212	LEU
1	BO	271	THR

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Mol	Chain	Res	Type
1	BO	319	GLN
1	AO	54	ASP
1	AO	62	ARG
1	AO	72	THR
1	AO	74	THR
1	AO	75	ASP
1	AO	87	ASP
1	AO	118	ASN
1	AO	124	VAL
1	AO	128	LEU
1	AO	137	THR
1	AO	141	LEU
1	AO	142	GLN
1	AO	149	VAL
1	AO	159	ARG
1	AO	162	TYR
1	AO	163	THR
1	AO	165	THR
1	AO	167	LEU
1	AO	170	SER
1	AO	176	ARG
1	AO	183	LEU
1	AO	196	ASN
1	AO	208	SER
1	AO	211	SER
1	AO	225	GLN
1	AO	236	ASN
1	AO	253	ASP
1	AO	264	SER
1	AO	271	THR
1	AO	304	PHE
1	AO	312	VAL
1	AO	315	TYR
1	AO	317	ASP
1	CO	35	THR
1	CO	43	SER
1	CO	48	PHE
1	CO	72	THR
1	CO	74	THR
1	CO	75	ASP
1	CO	77	TYR
1	CO	87	ASP

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Mol	Chain	Res	Type
1	CO	101	ARG
1	CO	112	GLN
1	CO	114	MET
1	CO	141	LEU
1	CO	151	LYS
1	CO	156	ARG
1	CO	175	GLN
1	CO	176	ARG
1	CO	177	LEU
1	CO	185	LEU
1	CO	198	SER
1	CO	204	SER
1	CO	208	SER
1	CO	231	ASP
1	CO	288	ASN
1	CO	316	SER
1	CO	337	GLU
1	BP	57	LEU
1	BP	58	SER
1	BP	63	ILE
1	BP	67	VAL
1	BP	68	LEU
1	BP	78	VAL
1	BP	79	VAL
1	BP	88	LEU
1	BP	92	LEU
1	BP	100	GLN
1	BP	104	VAL
1	BP	105	GLU
1	BP	134	ASN
1	BP	142	GLN
1	BP	145	ARG
1	BP	156	ARG
1	BP	165	THR
1	BP	167	LEU
1	BP	183	LEU
1	BP	184	ILE
1	BP	191	ASN
1	BP	193	ASP
1	BP	196	ASN
1	BP	198	SER
1	BP	207	LEU

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Mol	Chain	Res	Type
1	BP	212	LEU
1	BP	271	THR
1	BP	319	GLN
1	AP	54	ASP
1	AP	62	ARG
1	AP	72	THR
1	AP	74	THR
1	AP	75	ASP
1	AP	87	ASP
1	AP	128	LEU
1	AP	137	THR
1	AP	141	LEU
1	AP	142	GLN
1	AP	144	THR
1	AP	149	VAL
1	AP	159	ARG
1	AP	162	TYR
1	AP	163	THR
1	AP	165	THR
1	AP	167	LEU
1	AP	170	SER
1	AP	176	ARG
1	AP	183	LEU
1	AP	196	ASN
1	AP	208	SER
1	AP	211	SER
1	AP	225	GLN
1	AP	236	ASN
1	AP	253	ASP
1	AP	264	SER
1	AP	271	THR
1	AP	304	PHE
1	AP	312	VAL
1	AP	315	TYR
1	AP	317	ASP
1	CP	35	THR
1	CP	43	SER
1	CP	48	PHE
1	CP	72	THR
1	CP	74	THR
1	CP	75	ASP
1	CP	77	TYR

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Mol	Chain	Res	Type
1	CP	87	ASP
1	CP	101	ARG
1	CP	112	GLN
1	CP	114	MET
1	CP	137	THR
1	CP	141	LEU
1	CP	151	LYS
1	CP	156	ARG
1	CP	175	GLN
1	CP	176	ARG
1	CP	177	LEU
1	CP	185	LEU
1	CP	198	SER
1	CP	204	SER
1	CP	231	ASP
1	CP	288	ASN
1	CP	316	SER
1	CP	337	GLU
1	BQ	57	LEU
1	BQ	58	SER
1	BQ	63	ILE
1	BQ	67	VAL
1	BQ	68	LEU
1	BQ	78	VAL
1	BQ	79	VAL
1	BQ	86	PRO
1	BQ	88	LEU
1	BQ	92	LEU
1	BQ	100	GLN
1	BQ	104	VAL
1	BQ	105	GLU
1	BQ	134	ASN
1	BQ	145	ARG
1	BQ	156	ARG
1	BQ	165	THR
1	BQ	167	LEU
1	BQ	183	LEU
1	BQ	184	ILE
1	BQ	191	ASN
1	BQ	196	ASN
1	BQ	198	SER
1	BQ	207	LEU

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Mol	Chain	Res	Type
1	BQ	212	LEU
1	BQ	271	THR
1	BQ	319	GLN
1	AQ	54	ASP
1	AQ	58	SER
1	AQ	62	ARG
1	AQ	72	THR
1	AQ	74	THR
1	AQ	75	ASP
1	AQ	87	ASP
1	AQ	124	VAL
1	AQ	128	LEU
1	AQ	137	THR
1	AQ	141	LEU
1	AQ	142	GLN
1	AQ	144	THR
1	AQ	149	VAL
1	AQ	159	ARG
1	AQ	162	TYR
1	AQ	163	THR
1	AQ	165	THR
1	AQ	167	LEU
1	AQ	170	SER
1	AQ	176	ARG
1	AQ	183	LEU
1	AQ	196	ASN
1	AQ	208	SER
1	AQ	211	SER
1	AQ	225	GLN
1	AQ	236	ASN
1	AQ	253	ASP
1	AQ	264	SER
1	AQ	271	THR
1	AQ	304	PHE
1	AQ	312	VAL
1	AQ	315	TYR
1	AQ	317	ASP
1	CQ	35	THR
1	CQ	43	SER
1	CQ	48	PHE
1	CQ	72	THR
1	CQ	74	THR

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Mol	Chain	Res	Type
1	CQ	75	ASP
1	CQ	77	TYR
1	CQ	87	ASP
1	CQ	101	ARG
1	CQ	106	THR
1	CQ	112	GLN
1	CQ	114	MET
1	CQ	137	THR
1	CQ	141	LEU
1	CQ	151	LYS
1	CQ	156	ARG
1	CQ	175	GLN
1	CQ	176	ARG
1	CQ	177	LEU
1	CQ	185	LEU
1	CQ	198	SER
1	CQ	204	SER
1	CQ	231	ASP
1	CQ	288	ASN
1	CQ	316	SER
1	CQ	337	GLU
1	BR	57	LEU
1	BR	58	SER
1	BR	63	ILE
1	BR	67	VAL
1	BR	68	LEU
1	BR	78	VAL
1	BR	79	VAL
1	BR	88	LEU
1	BR	92	LEU
1	BR	100	GLN
1	BR	104	VAL
1	BR	105	GLU
1	BR	134	ASN
1	BR	145	ARG
1	BR	156	ARG
1	BR	165	THR
1	BR	167	LEU
1	BR	183	LEU
1	BR	184	ILE
1	BR	191	ASN
1	BR	193	ASP

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Mol	Chain	Res	Type
1	BR	196	ASN
1	BR	198	SER
1	BR	207	LEU
1	BR	212	LEU
1	BR	271	THR
1	BR	319	GLN
1	AR	54	ASP
1	AR	62	ARG
1	AR	72	THR
1	AR	74	THR
1	AR	75	ASP
1	AR	87	ASP
1	AR	118	ASN
1	AR	128	LEU
1	AR	130	ASP
1	AR	137	THR
1	AR	141	LEU
1	AR	142	GLN
1	AR	144	THR
1	AR	149	VAL
1	AR	157	THR
1	AR	159	ARG
1	AR	162	TYR
1	AR	163	THR
1	AR	165	THR
1	AR	167	LEU
1	AR	170	SER
1	AR	176	ARG
1	AR	183	LEU
1	AR	186	LEU
1	AR	196	ASN
1	AR	208	SER
1	AR	211	SER
1	AR	212	LEU
1	AR	225	GLN
1	AR	236	ASN
1	AR	253	ASP
1	AR	264	SER
1	AR	271	THR
1	AR	304	PHE
1	AR	312	VAL
1	AR	315	TYR

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Mol	Chain	Res	Type
1	AR	317	ASP
1	CR	35	THR
1	CR	43	SER
1	CR	72	THR
1	CR	74	THR
1	CR	75	ASP
1	CR	77	TYR
1	CR	87	ASP
1	CR	101	ARG
1	CR	112	GLN
1	CR	114	MET
1	CR	137	THR
1	CR	141	LEU
1	CR	151	LYS
1	CR	156	ARG
1	CR	175	GLN
1	CR	176	ARG
1	CR	177	LEU
1	CR	185	LEU
1	CR	198	SER
1	CR	204	SER
1	CR	208	SER
1	CR	231	ASP
1	CR	288	ASN
1	CR	316	SER
1	CR	337	GLU
1	BS	57	LEU
1	BS	58	SER
1	BS	63	ILE
1	BS	67	VAL
1	BS	68	LEU
1	BS	78	VAL
1	BS	79	VAL
1	BS	88	LEU
1	BS	92	LEU
1	BS	100	GLN
1	BS	104	VAL
1	BS	105	GLU
1	BS	134	ASN
1	BS	145	ARG
1	BS	156	ARG
1	BS	165	THR

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Mol	Chain	Res	Type
1	BS	167	LEU
1	BS	183	LEU
1	BS	184	ILE
1	BS	191	ASN
1	BS	193	ASP
1	BS	196	ASN
1	BS	198	SER
1	BS	207	LEU
1	BS	212	LEU
1	BS	271	THR
1	BS	319	GLN
1	AS	54	ASP
1	AS	58	SER
1	AS	62	ARG
1	AS	72	THR
1	AS	74	THR
1	AS	75	ASP
1	AS	87	ASP
1	AS	101	ARG
1	AS	118	ASN
1	AS	128	LEU
1	AS	137	THR
1	AS	141	LEU
1	AS	142	GLN
1	AS	144	THR
1	AS	149	VAL
1	AS	159	ARG
1	AS	162	TYR
1	AS	163	THR
1	AS	165	THR
1	AS	167	LEU
1	AS	170	SER
1	AS	176	ARG
1	AS	183	LEU
1	AS	196	ASN
1	AS	208	SER
1	AS	211	SER
1	AS	225	GLN
1	AS	236	ASN
1	AS	253	ASP
1	AS	264	SER
1	AS	271	THR

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Mol	Chain	Res	Type
1	AS	304	PHE
1	AS	312	VAL
1	AS	315	TYR
1	AS	317	ASP
1	CS	35	THR
1	CS	43	SER
1	CS	48	PHE
1	CS	54	ASP
1	CS	72	THR
1	CS	74	THR
1	CS	75	ASP
1	CS	77	TYR
1	CS	87	ASP
1	CS	101	ARG
1	CS	112	GLN
1	CS	114	MET
1	CS	137	THR
1	CS	151	LYS
1	CS	156	ARG
1	CS	175	GLN
1	CS	176	ARG
1	CS	177	LEU
1	CS	185	LEU
1	CS	186	LEU
1	CS	198	SER
1	CS	204	SER
1	CS	208	SER
1	CS	231	ASP
1	CS	288	ASN
1	CS	316	SER
1	CS	337	GLU
1	BT	57	LEU
1	BT	58	SER
1	BT	63	ILE
1	BT	67	VAL
1	BT	68	LEU
1	BT	78	VAL
1	BT	79	VAL
1	BT	88	LEU
1	BT	92	LEU
1	BT	100	GLN
1	BT	104	VAL

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Mol	Chain	Res	Type
1	BT	105	GLU
1	BT	134	ASN
1	BT	142	GLN
1	BT	145	ARG
1	BT	156	ARG
1	BT	165	THR
1	BT	167	LEU
1	BT	183	LEU
1	BT	184	ILE
1	BT	191	ASN
1	BT	193	ASP
1	BT	196	ASN
1	BT	198	SER
1	BT	207	LEU
1	BT	212	LEU
1	BT	271	THR
1	BT	319	GLN
1	AT	54	ASP
1	AT	62	ARG
1	AT	72	THR
1	AT	74	THR
1	AT	75	ASP
1	AT	83	THR
1	AT	87	ASP
1	AT	128	LEU
1	AT	137	THR
1	AT	141	LEU
1	AT	142	GLN
1	AT	144	THR
1	AT	149	VAL
1	AT	157	THR
1	AT	159	ARG
1	AT	162	TYR
1	AT	163	THR
1	AT	165	THR
1	AT	167	LEU
1	AT	170	SER
1	AT	176	ARG
1	AT	183	LEU
1	AT	196	ASN
1	AT	208	SER
1	AT	211	SER

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Mol	Chain	Res	Type
1	AT	225	GLN
1	AT	236	ASN
1	AT	253	ASP
1	AT	264	SER
1	AT	271	THR
1	AT	304	PHE
1	AT	312	VAL
1	AT	315	TYR
1	AT	317	ASP
1	CT	35	THR
1	CT	43	SER
1	CT	48	PHE
1	CT	72	THR
1	CT	74	THR
1	CT	75	ASP
1	CT	77	TYR
1	CT	87	ASP
1	CT	101	ARG
1	CT	112	GLN
1	CT	114	MET
1	CT	137	THR
1	CT	141	LEU
1	CT	151	LYS
1	CT	156	ARG
1	CT	175	GLN
1	CT	176	ARG
1	CT	177	LEU
1	CT	185	LEU
1	CT	198	SER
1	CT	204	SER
1	CT	231	ASP
1	CT	288	ASN
1	CT	316	SER
1	CT	337	GLU
1	BU	57	LEU
1	BU	58	SER
1	BU	63	ILE
1	BU	67	VAL
1	BU	68	LEU
1	BU	78	VAL
1	BU	79	VAL
1	BU	88	LEU

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Mol	Chain	Res	Type
1	BU	92	LEU
1	BU	100	GLN
1	BU	104	VAL
1	BU	105	GLU
1	BU	134	ASN
1	BU	142	GLN
1	BU	145	ARG
1	BU	156	ARG
1	BU	165	THR
1	BU	167	LEU
1	BU	183	LEU
1	BU	184	ILE
1	BU	191	ASN
1	BU	193	ASP
1	BU	196	ASN
1	BU	198	SER
1	BU	207	LEU
1	BU	212	LEU
1	BU	271	THR
1	BU	319	GLN
1	AU	54	ASP
1	AU	58	SER
1	AU	62	ARG
1	AU	72	THR
1	AU	74	THR
1	AU	75	ASP
1	AU	87	ASP
1	AU	101	ARG
1	AU	118	ASN
1	AU	124	VAL
1	AU	128	LEU
1	AU	137	THR
1	AU	141	LEU
1	AU	142	GLN
1	AU	149	VAL
1	AU	157	THR
1	AU	159	ARG
1	AU	163	THR
1	AU	165	THR
1	AU	167	LEU
1	AU	170	SER
1	AU	176	ARG

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Mol	Chain	Res	Type
1	AU	183	LEU
1	AU	196	ASN
1	AU	208	SER
1	AU	211	SER
1	AU	225	GLN
1	AU	236	ASN
1	AU	253	ASP
1	AU	264	SER
1	AU	271	THR
1	AU	304	PHE
1	AU	312	VAL
1	AU	315	TYR
1	AU	317	ASP
1	CU	35	THR
1	CU	43	SER
1	CU	48	PHE
1	CU	72	THR
1	CU	74	THR
1	CU	75	ASP
1	CU	77	TYR
1	CU	87	ASP
1	CU	101	ARG
1	CU	112	GLN
1	CU	114	MET
1	CU	137	THR
1	CU	141	LEU
1	CU	151	LYS
1	CU	156	ARG
1	CU	175	GLN
1	CU	176	ARG
1	CU	177	LEU
1	CU	185	LEU
1	CU	186	LEU
1	CU	198	SER
1	CU	204	SER
1	CU	208	SER
1	CU	231	ASP
1	CU	288	ASN
1	CU	316	SER
1	CU	337	GLU
1	BV	57	LEU
1	BV	58	SER

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Mol	Chain	Res	Type
1	BV	63	ILE
1	BV	67	VAL
1	BV	68	LEU
1	BV	78	VAL
1	BV	79	VAL
1	BV	88	LEU
1	BV	92	LEU
1	BV	100	GLN
1	BV	104	VAL
1	BV	105	GLU
1	BV	134	ASN
1	BV	145	ARG
1	BV	156	ARG
1	BV	165	THR
1	BV	167	LEU
1	BV	183	LEU
1	BV	184	ILE
1	BV	191	ASN
1	BV	193	ASP
1	BV	196	ASN
1	BV	198	SER
1	BV	207	LEU
1	BV	212	LEU
1	BV	271	THR
1	BV	319	GLN
1	AV	54	ASP
1	AV	58	SER
1	AV	62	ARG
1	AV	72	THR
1	AV	74	THR
1	AV	75	ASP
1	AV	87	ASP
1	AV	124	VAL
1	AV	128	LEU
1	AV	137	THR
1	AV	141	LEU
1	AV	142	GLN
1	AV	144	THR
1	AV	149	VAL
1	AV	157	THR
1	AV	159	ARG
1	AV	162	TYR

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Mol	Chain	Res	Type
1	AV	163	THR
1	AV	165	THR
1	AV	167	LEU
1	AV	170	SER
1	AV	176	ARG
1	AV	183	LEU
1	AV	196	ASN
1	AV	208	SER
1	AV	211	SER
1	AV	225	GLN
1	AV	236	ASN
1	AV	253	ASP
1	AV	264	SER
1	AV	271	THR
1	AV	304	PHE
1	AV	312	VAL
1	AV	315	TYR
1	AV	317	ASP
1	CV	35	THR
1	CV	43	SER
1	CV	48	PHE
1	CV	72	THR
1	CV	74	THR
1	CV	75	ASP
1	CV	77	TYR
1	CV	87	ASP
1	CV	101	ARG
1	CV	112	GLN
1	CV	114	MET
1	CV	137	THR
1	CV	141	LEU
1	CV	151	LYS
1	CV	156	ARG
1	CV	175	GLN
1	CV	176	ARG
1	CV	177	LEU
1	CV	185	LEU
1	CV	186	LEU
1	CV	198	SER
1	CV	204	SER
1	CV	208	SER
1	CV	231	ASP

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Mol	Chain	Res	Type
1	CV	288	ASN
1	CV	316	SER
1	CV	331	CYS
1	CV	337	GLU
1	BW	57	LEU
1	BW	58	SER
1	BW	63	ILE
1	BW	67	VAL
1	BW	68	LEU
1	BW	78	VAL
1	BW	79	VAL
1	BW	88	LEU
1	BW	92	LEU
1	BW	100	GLN
1	BW	104	VAL
1	BW	105	GLU
1	BW	134	ASN
1	BW	145	ARG
1	BW	156	ARG
1	BW	165	THR
1	BW	167	LEU
1	BW	183	LEU
1	BW	184	ILE
1	BW	191	ASN
1	BW	196	ASN
1	BW	198	SER
1	BW	207	LEU
1	BW	212	LEU
1	BW	271	THR
1	BW	319	GLN
1	AW	54	ASP
1	AW	58	SER
1	AW	62	ARG
1	AW	72	THR
1	AW	74	THR
1	AW	75	ASP
1	AW	87	ASP
1	AW	118	ASN
1	AW	124	VAL
1	AW	128	LEU
1	AW	137	THR
1	AW	141	LEU

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Mol	Chain	Res	Type
1	AW	142	GLN
1	AW	149	VAL
1	AW	159	ARG
1	AW	162	TYR
1	AW	163	THR
1	AW	165	THR
1	AW	167	LEU
1	AW	170	SER
1	AW	176	ARG
1	AW	183	LEU
1	AW	196	ASN
1	AW	208	SER
1	AW	211	SER
1	AW	225	GLN
1	AW	236	ASN
1	AW	253	ASP
1	AW	264	SER
1	AW	271	THR
1	AW	304	PHE
1	AW	312	VAL
1	AW	315	TYR
1	AW	317	ASP
1	CW	35	THR
1	CW	43	SER
1	CW	48	PHE
1	CW	72	THR
1	CW	74	THR
1	CW	75	ASP
1	CW	77	TYR
1	CW	87	ASP
1	CW	101	ARG
1	CW	106	THR
1	CW	112	GLN
1	CW	114	MET
1	CW	137	THR
1	CW	141	LEU
1	CW	151	LYS
1	CW	156	ARG
1	CW	175	GLN
1	CW	176	ARG
1	CW	177	LEU
1	CW	185	LEU

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Mol	Chain	Res	Type
1	CW	198	SER
1	CW	204	SER
1	CW	208	SER
1	CW	231	ASP
1	CW	288	ASN
1	CW	316	SER
1	CW	337	GLU
1	BX	57	LEU
1	BX	58	SER
1	BX	63	ILE
1	BX	67	VAL
1	BX	68	LEU
1	BX	78	VAL
1	BX	79	VAL
1	BX	88	LEU
1	BX	92	LEU
1	BX	100	GLN
1	BX	104	VAL
1	BX	105	GLU
1	BX	134	ASN
1	BX	142	GLN
1	BX	145	ARG
1	BX	156	ARG
1	BX	165	THR
1	BX	167	LEU
1	BX	183	LEU
1	BX	184	ILE
1	BX	191	ASN
1	BX	196	ASN
1	BX	198	SER
1	BX	207	LEU
1	BX	212	LEU
1	BX	271	THR
1	BX	319	GLN
1	AX	54	ASP
1	AX	62	ARG
1	AX	72	THR
1	AX	74	THR
1	AX	75	ASP
1	AX	87	ASP
1	AX	118	ASN
1	AX	124	VAL

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Mol	Chain	Res	Type
1	AX	128	LEU
1	AX	137	THR
1	AX	141	LEU
1	AX	142	GLN
1	AX	144	THR
1	AX	149	VAL
1	AX	159	ARG
1	AX	162	TYR
1	AX	163	THR
1	AX	165	THR
1	AX	167	LEU
1	AX	170	SER
1	AX	176	ARG
1	AX	183	LEU
1	AX	196	ASN
1	AX	208	SER
1	AX	211	SER
1	AX	225	GLN
1	AX	236	ASN
1	AX	253	ASP
1	AX	264	SER
1	AX	271	THR
1	AX	304	PHE
1	AX	312	VAL
1	AX	315	TYR
1	AX	317	ASP
1	CX	35	THR
1	CX	43	SER
1	CX	48	PHE
1	CX	72	THR
1	CX	74	THR
1	CX	75	ASP
1	CX	77	TYR
1	CX	87	ASP
1	CX	101	ARG
1	CX	106	THR
1	CX	112	GLN
1	CX	114	MET
1	CX	137	THR
1	CX	141	LEU
1	CX	151	LYS
1	CX	156	ARG

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Mol	Chain	Res	Type
1	CX	175	GLN
1	CX	176	ARG
1	CX	177	LEU
1	CX	185	LEU
1	CX	198	SER
1	CX	204	SER
1	CX	208	SER
1	CX	231	ASP
1	CX	288	ASN
1	CX	316	SER
1	CX	337	GLU
1	BY	57	LEU
1	BY	58	SER
1	BY	63	ILE
1	BY	67	VAL
1	BY	68	LEU
1	BY	78	VAL
1	BY	79	VAL
1	BY	88	LEU
1	BY	92	LEU
1	BY	100	GLN
1	BY	104	VAL
1	BY	105	GLU
1	BY	134	ASN
1	BY	145	ARG
1	BY	156	ARG
1	BY	165	THR
1	BY	167	LEU
1	BY	183	LEU
1	BY	184	ILE
1	BY	191	ASN
1	BY	193	ASP
1	BY	196	ASN
1	BY	198	SER
1	BY	207	LEU
1	BY	212	LEU
1	BY	271	THR
1	BY	319	GLN
1	AY	54	ASP
1	AY	58	SER
1	AY	62	ARG
1	AY	72	THR

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Mol	Chain	Res	Type
1	AY	74	THR
1	AY	75	ASP
1	AY	87	ASP
1	AY	128	LEU
1	AY	137	THR
1	AY	141	LEU
1	AY	142	GLN
1	AY	149	VAL
1	AY	159	ARG
1	AY	162	TYR
1	AY	163	THR
1	AY	165	THR
1	AY	167	LEU
1	AY	170	SER
1	AY	176	ARG
1	AY	183	LEU
1	AY	196	ASN
1	AY	208	SER
1	AY	211	SER
1	AY	225	GLN
1	AY	236	ASN
1	AY	253	ASP
1	AY	264	SER
1	AY	271	THR
1	AY	304	PHE
1	AY	312	VAL
1	AY	315	TYR
1	AY	317	ASP
1	CY	35	THR
1	CY	43	SER
1	CY	48	PHE
1	CY	72	THR
1	CY	74	THR
1	CY	75	ASP
1	CY	77	TYR
1	CY	87	ASP
1	CY	101	ARG
1	CY	106	THR
1	CY	112	GLN
1	CY	114	MET
1	CY	137	THR
1	CY	141	LEU

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Mol	Chain	Res	Type
1	CY	151	LYS
1	CY	156	ARG
1	CY	175	GLN
1	CY	176	ARG
1	CY	177	LEU
1	CY	185	LEU
1	CY	198	SER
1	CY	204	SER
1	CY	208	SER
1	CY	231	ASP
1	CY	288	ASN
1	CY	316	SER
1	CY	337	GLU
1	BZ	57	LEU
1	BZ	58	SER
1	BZ	63	ILE
1	BZ	67	VAL
1	BZ	68	LEU
1	BZ	78	VAL
1	BZ	79	VAL
1	BZ	88	LEU
1	BZ	92	LEU
1	BZ	100	GLN
1	BZ	104	VAL
1	BZ	105	GLU
1	BZ	134	ASN
1	BZ	145	ARG
1	BZ	156	ARG
1	BZ	165	THR
1	BZ	167	LEU
1	BZ	183	LEU
1	BZ	184	ILE
1	BZ	191	ASN
1	BZ	193	ASP
1	BZ	196	ASN
1	BZ	198	SER
1	BZ	202	ARG
1	BZ	207	LEU
1	BZ	212	LEU
1	BZ	271	THR
1	BZ	319	GLN
1	AZ	54	ASP

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Mol	Chain	Res	Type
1	AZ	62	ARG
1	AZ	72	THR
1	AZ	74	THR
1	AZ	75	ASP
1	AZ	87	ASP
1	AZ	124	VAL
1	AZ	128	LEU
1	AZ	137	THR
1	AZ	141	LEU
1	AZ	142	GLN
1	AZ	144	THR
1	AZ	149	VAL
1	AZ	159	ARG
1	AZ	163	THR
1	AZ	165	THR
1	AZ	167	LEU
1	AZ	170	SER
1	AZ	176	ARG
1	AZ	183	LEU
1	AZ	196	ASN
1	AZ	208	SER
1	AZ	211	SER
1	AZ	225	GLN
1	AZ	236	ASN
1	AZ	253	ASP
1	AZ	264	SER
1	AZ	271	THR
1	AZ	304	PHE
1	AZ	312	VAL
1	AZ	315	TYR
1	AZ	317	ASP
1	CZ	35	THR
1	CZ	43	SER
1	CZ	48	PHE
1	CZ	54	ASP
1	CZ	72	THR
1	CZ	74	THR
1	CZ	75	ASP
1	CZ	77	TYR
1	CZ	87	ASP
1	CZ	101	ARG
1	CZ	112	GLN

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Mol	Chain	Res	Type
1	CZ	114	MET
1	CZ	137	THR
1	CZ	141	LEU
1	CZ	151	LYS
1	CZ	156	ARG
1	CZ	175	GLN
1	CZ	176	ARG
1	CZ	177	LEU
1	CZ	185	LEU
1	CZ	198	SER
1	CZ	204	SER
1	CZ	208	SER
1	CZ	231	ASP
1	CZ	288	ASN
1	CZ	316	SER
1	CZ	337	GLU
1	Ba	57	LEU
1	Ba	58	SER
1	Ba	63	ILE
1	Ba	67	VAL
1	Ba	68	LEU
1	Ba	78	VAL
1	Ba	79	VAL
1	Ba	88	LEU
1	Ba	92	LEU
1	Ba	100	GLN
1	Ba	104	VAL
1	Ba	105	GLU
1	Ba	134	ASN
1	Ba	145	ARG
1	Ba	156	ARG
1	Ba	165	THR
1	Ba	167	LEU
1	Ba	183	LEU
1	Ba	184	ILE
1	Ba	191	ASN
1	Ba	193	ASP
1	Ba	196	ASN
1	Ba	198	SER
1	Ba	207	LEU
1	Ba	212	LEU
1	Ba	271	THR

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Mol	Chain	Res	Type
1	Ba	319	GLN
1	Aa	54	ASP
1	Aa	58	SER
1	Aa	62	ARG
1	Aa	72	THR
1	Aa	74	THR
1	Aa	75	ASP
1	Aa	83	THR
1	Aa	87	ASP
1	Aa	128	LEU
1	Aa	137	THR
1	Aa	141	LEU
1	Aa	142	GLN
1	Aa	149	VAL
1	Aa	157	THR
1	Aa	159	ARG
1	Aa	162	TYR
1	Aa	163	THR
1	Aa	165	THR
1	Aa	167	LEU
1	Aa	170	SER
1	Aa	176	ARG
1	Aa	183	LEU
1	Aa	196	ASN
1	Aa	208	SER
1	Aa	211	SER
1	Aa	225	GLN
1	Aa	236	ASN
1	Aa	253	ASP
1	Aa	264	SER
1	Aa	271	THR
1	Aa	304	PHE
1	Aa	312	VAL
1	Aa	315	TYR
1	Aa	317	ASP
1	Ca	35	THR
1	Ca	43	SER
1	Ca	48	PHE
1	Ca	72	THR
1	Ca	74	THR
1	Ca	75	ASP
1	Ca	77	TYR

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Mol	Chain	Res	Type
1	Ca	87	ASP
1	Ca	101	ARG
1	Ca	112	GLN
1	Ca	114	MET
1	Ca	137	THR
1	Ca	141	LEU
1	Ca	151	LYS
1	Ca	156	ARG
1	Ca	175	GLN
1	Ca	176	ARG
1	Ca	177	LEU
1	Ca	185	LEU
1	Ca	186	LEU
1	Ca	198	SER
1	Ca	204	SER
1	Ca	208	SER
1	Ca	231	ASP
1	Ca	288	ASN
1	Ca	316	SER
1	Ca	337	GLU
1	Bb	57	LEU
1	Bb	58	SER
1	Bb	63	ILE
1	Bb	67	VAL
1	Bb	68	LEU
1	Bb	78	VAL
1	Bb	79	VAL
1	Bb	88	LEU
1	Bb	92	LEU
1	Bb	100	GLN
1	Bb	104	VAL
1	Bb	105	GLU
1	Bb	134	ASN
1	Bb	145	ARG
1	Bb	156	ARG
1	Bb	165	THR
1	Bb	167	LEU
1	Bb	183	LEU
1	Bb	184	ILE
1	Bb	191	ASN
1	Bb	193	ASP
1	Bb	196	ASN

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Mol	Chain	Res	Type
1	Bb	198	SER
1	Bb	202	ARG
1	Bb	207	LEU
1	Bb	212	LEU
1	Bb	271	THR
1	Bb	319	GLN
1	Ab	54	ASP
1	Ab	58	SER
1	Ab	62	ARG
1	Ab	72	THR
1	Ab	74	THR
1	Ab	75	ASP
1	Ab	83	THR
1	Ab	87	ASP
1	Ab	124	VAL
1	Ab	128	LEU
1	Ab	137	THR
1	Ab	141	LEU
1	Ab	142	GLN
1	Ab	144	THR
1	Ab	149	VAL
1	Ab	159	ARG
1	Ab	162	TYR
1	Ab	163	THR
1	Ab	165	THR
1	Ab	167	LEU
1	Ab	170	SER
1	Ab	176	ARG
1	Ab	183	LEU
1	Ab	196	ASN
1	Ab	208	SER
1	Ab	211	SER
1	Ab	212	LEU
1	Ab	225	GLN
1	Ab	236	ASN
1	Ab	253	ASP
1	Ab	264	SER
1	Ab	271	THR
1	Ab	304	PHE
1	Ab	312	VAL
1	Ab	315	TYR
1	Ab	317	ASP

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Mol	Chain	Res	Type
1	Cb	35	THR
1	Cb	43	SER
1	Cb	48	PHE
1	Cb	72	THR
1	Cb	74	THR
1	Cb	75	ASP
1	Cb	77	TYR
1	Cb	87	ASP
1	Cb	101	ARG
1	Cb	112	GLN
1	Cb	114	MET
1	Cb	137	THR
1	Cb	141	LEU
1	Cb	151	LYS
1	Cb	156	ARG
1	Cb	175	GLN
1	Cb	176	ARG
1	Cb	177	LEU
1	Cb	185	LEU
1	Cb	198	SER
1	Cb	204	SER
1	Cb	208	SER
1	Cb	231	ASP
1	Cb	288	ASN
1	Cb	316	SER
1	Cb	337	GLU
1	Bc	57	LEU
1	Bc	58	SER
1	Bc	63	ILE
1	Bc	67	VAL
1	Bc	68	LEU
1	Bc	78	VAL
1	Bc	79	VAL
1	Bc	88	LEU
1	Bc	92	LEU
1	Bc	100	GLN
1	Bc	104	VAL
1	Bc	105	GLU
1	Bc	134	ASN
1	Bc	145	ARG
1	Bc	156	ARG
1	Bc	165	THR

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Mol	Chain	Res	Type
1	Bc	167	LEU
1	Bc	183	LEU
1	Bc	184	ILE
1	Bc	191	ASN
1	Bc	193	ASP
1	Bc	196	ASN
1	Bc	198	SER
1	Bc	202	ARG
1	Bc	207	LEU
1	Bc	212	LEU
1	Bc	271	THR
1	Bc	310	ASP
1	Bc	319	GLN
1	Ac	54	ASP
1	Ac	58	SER
1	Ac	62	ARG
1	Ac	72	THR
1	Ac	74	THR
1	Ac	75	ASP
1	Ac	87	ASP
1	Ac	119	THR
1	Ac	124	VAL
1	Ac	128	LEU
1	Ac	137	THR
1	Ac	141	LEU
1	Ac	142	GLN
1	Ac	149	VAL
1	Ac	159	ARG
1	Ac	162	TYR
1	Ac	163	THR
1	Ac	165	THR
1	Ac	167	LEU
1	Ac	170	SER
1	Ac	176	ARG
1	Ac	183	LEU
1	Ac	196	ASN
1	Ac	208	SER
1	Ac	211	SER
1	Ac	225	GLN
1	Ac	236	ASN
1	Ac	253	ASP
1	Ac	264	SER

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Mol	Chain	Res	Type
1	Ac	271	THR
1	Ac	304	PHE
1	Ac	312	VAL
1	Ac	315	TYR
1	Ac	317	ASP
1	Cc	35	THR
1	Cc	43	SER
1	Cc	48	PHE
1	Cc	54	ASP
1	Cc	72	THR
1	Cc	74	THR
1	Cc	75	ASP
1	Cc	77	TYR
1	Cc	87	ASP
1	Cc	101	ARG
1	Cc	112	GLN
1	Cc	114	MET
1	Cc	137	THR
1	Cc	141	LEU
1	Cc	151	LYS
1	Cc	156	ARG
1	Cc	175	GLN
1	Cc	176	ARG
1	Cc	177	LEU
1	Cc	185	LEU
1	Cc	198	SER
1	Cc	204	SER
1	Cc	208	SER
1	Cc	231	ASP
1	Cc	288	ASN
1	Cc	316	SER
1	Cc	337	GLU
1	Bd	57	LEU
1	Bd	58	SER
1	Bd	63	ILE
1	Bd	67	VAL
1	Bd	68	LEU
1	Bd	78	VAL
1	Bd	79	VAL
1	Bd	88	LEU
1	Bd	92	LEU
1	Bd	100	GLN

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Mol	Chain	Res	Type
1	Bd	104	VAL
1	Bd	105	GLU
1	Bd	134	ASN
1	Bd	142	GLN
1	Bd	145	ARG
1	Bd	156	ARG
1	Bd	165	THR
1	Bd	167	LEU
1	Bd	183	LEU
1	Bd	184	ILE
1	Bd	191	ASN
1	Bd	193	ASP
1	Bd	196	ASN
1	Bd	198	SER
1	Bd	207	LEU
1	Bd	212	LEU
1	Bd	225	GLN
1	Bd	271	THR
1	Bd	319	GLN
1	Ad	54	ASP
1	Ad	62	ARG
1	Ad	72	THR
1	Ad	74	THR
1	Ad	75	ASP
1	Ad	87	ASP
1	Ad	124	VAL
1	Ad	128	LEU
1	Ad	137	THR
1	Ad	141	LEU
1	Ad	142	GLN
1	Ad	149	VAL
1	Ad	159	ARG
1	Ad	162	TYR
1	Ad	163	THR
1	Ad	165	THR
1	Ad	167	LEU
1	Ad	170	SER
1	Ad	176	ARG
1	Ad	183	LEU
1	Ad	186	LEU
1	Ad	196	ASN
1	Ad	208	SER

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Mol	Chain	Res	Type
1	Ad	211	SER
1	Ad	225	GLN
1	Ad	236	ASN
1	Ad	253	ASP
1	Ad	264	SER
1	Ad	271	THR
1	Ad	304	PHE
1	Ad	312	VAL
1	Ad	315	TYR
1	Ad	317	ASP
1	Cd	35	THR
1	Cd	43	SER
1	Cd	48	PHE
1	Cd	72	THR
1	Cd	74	THR
1	Cd	75	ASP
1	Cd	77	TYR
1	Cd	87	ASP
1	Cd	101	ARG
1	Cd	112	GLN
1	Cd	114	MET
1	Cd	137	THR
1	Cd	141	LEU
1	Cd	151	LYS
1	Cd	175	GLN
1	Cd	176	ARG
1	Cd	177	LEU
1	Cd	185	LEU
1	Cd	198	SER
1	Cd	204	SER
1	Cd	231	ASP
1	Cd	288	ASN
1	Cd	316	SER
1	Cd	337	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (487) such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	100	GLN
1	BA	142	GLN
1	BA	190	ASN
1	BA	191	ASN

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Mol	Chain	Res	Type
1	BA	196	ASN
1	BA	214	ASN
1	AA	65	GLN
1	AA	118	ASN
1	AA	134	ASN
1	AA	142	GLN
1	AA	191	ASN
1	AA	196	ASN
1	AA	225	GLN
1	AA	236	ASN
1	AA	258	GLN
1	CA	56	HIS
1	CA	112	GLN
1	CA	190	ASN
1	BB	100	GLN
1	BB	142	GLN
1	BB	190	ASN
1	BB	191	ASN
1	BB	196	ASN
1	AB	65	GLN
1	AB	118	ASN
1	AB	134	ASN
1	AB	142	GLN
1	AB	196	ASN
1	AB	236	ASN
1	AB	258	GLN
1	CB	56	HIS
1	CB	112	GLN
1	CB	190	ASN
1	BC	142	GLN
1	BC	190	ASN
1	BC	191	ASN
1	BC	196	ASN
1	AC	65	GLN
1	AC	118	ASN
1	AC	134	ASN
1	AC	142	GLN
1	AC	191	ASN
1	AC	196	ASN
1	AC	225	GLN
1	AC	236	ASN
1	AC	258	GLN

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Mol	Chain	Res	Type
1	CC	56	HIS
1	CC	112	GLN
1	CC	190	ASN
1	BD	65	GLN
1	BD	100	GLN
1	BD	142	GLN
1	BD	190	ASN
1	BD	191	ASN
1	BD	196	ASN
1	AD	65	GLN
1	AD	118	ASN
1	AD	134	ASN
1	AD	142	GLN
1	AD	191	ASN
1	AD	196	ASN
1	AD	225	GLN
1	AD	236	ASN
1	AD	258	GLN
1	CD	56	HIS
1	CD	112	GLN
1	CD	190	ASN
1	BE	100	GLN
1	BE	142	GLN
1	BE	190	ASN
1	BE	191	ASN
1	BE	196	ASN
1	AE	65	GLN
1	AE	118	ASN
1	AE	134	ASN
1	AE	142	GLN
1	AE	196	ASN
1	AE	225	GLN
1	AE	236	ASN
1	AE	258	GLN
1	CE	56	HIS
1	CE	112	GLN
1	CE	190	ASN
1	BF	100	GLN
1	BF	142	GLN
1	BF	190	ASN
1	BF	191	ASN
1	BF	196	ASN

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Mol	Chain	Res	Type
1	AF	65	GLN
1	AF	118	ASN
1	AF	134	ASN
1	AF	142	GLN
1	AF	191	ASN
1	AF	196	ASN
1	AF	225	GLN
1	AF	236	ASN
1	AF	258	GLN
1	CF	56	HIS
1	CF	112	GLN
1	CF	190	ASN
1	BG	100	GLN
1	BG	142	GLN
1	BG	190	ASN
1	BG	191	ASN
1	BG	196	ASN
1	AG	65	GLN
1	AG	118	ASN
1	AG	134	ASN
1	AG	142	GLN
1	AG	191	ASN
1	AG	196	ASN
1	AG	225	GLN
1	AG	236	ASN
1	AG	258	GLN
1	CG	56	HIS
1	CG	112	GLN
1	CG	190	ASN
1	BH	94	HIS
1	BH	100	GLN
1	BH	142	GLN
1	BH	190	ASN
1	BH	191	ASN
1	BH	196	ASN
1	AH	65	GLN
1	AH	134	ASN
1	AH	142	GLN
1	AH	191	ASN
1	AH	196	ASN
1	AH	225	GLN
1	AH	236	ASN

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Mol	Chain	Res	Type
1	AH	258	GLN
1	CH	56	HIS
1	CH	94	HIS
1	CH	112	GLN
1	CH	190	ASN
1	BI	100	GLN
1	BI	142	GLN
1	BI	190	ASN
1	BI	191	ASN
1	BI	196	ASN
1	BI	214	ASN
1	AI	65	GLN
1	AI	118	ASN
1	AI	134	ASN
1	AI	142	GLN
1	AI	196	ASN
1	AI	225	GLN
1	AI	236	ASN
1	AI	258	GLN
1	CI	56	HIS
1	CI	112	GLN
1	CI	190	ASN
1	BJ	100	GLN
1	BJ	142	GLN
1	BJ	190	ASN
1	BJ	191	ASN
1	BJ	196	ASN
1	AJ	65	GLN
1	AJ	118	ASN
1	AJ	134	ASN
1	AJ	142	GLN
1	AJ	196	ASN
1	AJ	225	GLN
1	AJ	236	ASN
1	CJ	56	HIS
1	CJ	94	HIS
1	CJ	112	GLN
1	CJ	190	ASN
1	BK	100	GLN
1	BK	190	ASN
1	BK	191	ASN
1	BK	196	ASN

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Mol	Chain	Res	Type
1	AK	65	GLN
1	AK	118	ASN
1	AK	134	ASN
1	AK	142	GLN
1	AK	191	ASN
1	AK	196	ASN
1	AK	225	GLN
1	AK	236	ASN
1	AK	258	GLN
1	CK	56	HIS
1	CK	112	GLN
1	CK	190	ASN
1	BL	100	GLN
1	BL	190	ASN
1	BL	191	ASN
1	BL	196	ASN
1	BL	214	ASN
1	AL	65	GLN
1	AL	134	ASN
1	AL	142	GLN
1	AL	196	ASN
1	AL	225	GLN
1	AL	236	ASN
1	AL	258	GLN
1	CL	56	HIS
1	CL	112	GLN
1	CL	190	ASN
1	BM	100	GLN
1	BM	142	GLN
1	BM	190	ASN
1	BM	191	ASN
1	BM	196	ASN
1	AM	65	GLN
1	AM	118	ASN
1	AM	134	ASN
1	AM	142	GLN
1	AM	196	ASN
1	AM	225	GLN
1	AM	236	ASN
1	AM	258	GLN
1	CM	56	HIS
1	CM	112	GLN

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Mol	Chain	Res	Type
1	CM	190	ASN
1	BN	100	GLN
1	BN	190	ASN
1	BN	191	ASN
1	BN	196	ASN
1	AN	65	GLN
1	AN	118	ASN
1	AN	134	ASN
1	AN	142	GLN
1	AN	196	ASN
1	AN	225	GLN
1	AN	236	ASN
1	AN	258	GLN
1	CN	56	HIS
1	CN	112	GLN
1	CN	190	ASN
1	BO	100	GLN
1	BO	142	GLN
1	BO	190	ASN
1	BO	191	ASN
1	BO	196	ASN
1	AO	65	GLN
1	AO	134	ASN
1	AO	142	GLN
1	AO	191	ASN
1	AO	196	ASN
1	AO	225	GLN
1	AO	236	ASN
1	AO	258	GLN
1	CO	56	HIS
1	CO	112	GLN
1	CO	190	ASN
1	BP	100	GLN
1	BP	142	GLN
1	BP	190	ASN
1	BP	191	ASN
1	BP	196	ASN
1	AP	65	GLN
1	AP	118	ASN
1	AP	134	ASN
1	AP	142	GLN
1	AP	196	ASN

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Mol	Chain	Res	Type
1	AP	225	GLN
1	AP	236	ASN
1	AP	258	GLN
1	CP	56	HIS
1	CP	112	GLN
1	CP	190	ASN
1	BQ	142	GLN
1	BQ	190	ASN
1	BQ	191	ASN
1	BQ	196	ASN
1	BQ	214	ASN
1	AQ	65	GLN
1	AQ	118	ASN
1	AQ	134	ASN
1	AQ	142	GLN
1	AQ	196	ASN
1	AQ	225	GLN
1	AQ	236	ASN
1	AQ	258	GLN
1	CQ	56	HIS
1	CQ	112	GLN
1	CQ	190	ASN
1	BR	100	GLN
1	BR	190	ASN
1	BR	191	ASN
1	BR	196	ASN
1	AR	65	GLN
1	AR	118	ASN
1	AR	134	ASN
1	AR	142	GLN
1	AR	196	ASN
1	AR	225	GLN
1	AR	236	ASN
1	AR	258	GLN
1	CR	56	HIS
1	CR	112	GLN
1	CR	190	ASN
1	BS	100	GLN
1	BS	190	ASN
1	BS	191	ASN
1	BS	196	ASN
1	AS	65	GLN

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Mol	Chain	Res	Type
1	AS	118	ASN
1	AS	134	ASN
1	AS	142	GLN
1	AS	196	ASN
1	AS	225	GLN
1	AS	236	ASN
1	AS	258	GLN
1	CS	56	HIS
1	CS	112	GLN
1	CS	190	ASN
1	BT	100	GLN
1	BT	190	ASN
1	BT	191	ASN
1	BT	196	ASN
1	BT	214	ASN
1	AT	65	GLN
1	AT	118	ASN
1	AT	134	ASN
1	AT	142	GLN
1	AT	196	ASN
1	AT	225	GLN
1	AT	236	ASN
1	AT	258	GLN
1	CT	56	HIS
1	CT	112	GLN
1	CT	190	ASN
1	BU	100	GLN
1	BU	142	GLN
1	BU	190	ASN
1	BU	191	ASN
1	BU	196	ASN
1	AU	65	GLN
1	AU	134	ASN
1	AU	142	GLN
1	AU	191	ASN
1	AU	196	ASN
1	AU	225	GLN
1	AU	236	ASN
1	AU	258	GLN
1	CU	56	HIS
1	CU	112	GLN
1	CU	190	ASN

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Mol	Chain	Res	Type
1	BV	142	GLN
1	BV	190	ASN
1	BV	191	ASN
1	BV	196	ASN
1	BV	214	ASN
1	AV	65	GLN
1	AV	118	ASN
1	AV	134	ASN
1	AV	142	GLN
1	AV	196	ASN
1	AV	225	GLN
1	AV	236	ASN
1	AV	258	GLN
1	CV	56	HIS
1	CV	112	GLN
1	CV	190	ASN
1	BW	100	GLN
1	BW	190	ASN
1	BW	191	ASN
1	BW	196	ASN
1	BW	214	ASN
1	AW	65	GLN
1	AW	118	ASN
1	AW	134	ASN
1	AW	142	GLN
1	AW	196	ASN
1	AW	225	GLN
1	AW	236	ASN
1	AW	258	GLN
1	CW	56	HIS
1	CW	112	GLN
1	CW	190	ASN
1	BX	100	GLN
1	BX	142	GLN
1	BX	190	ASN
1	BX	191	ASN
1	BX	196	ASN
1	AX	65	GLN
1	AX	134	ASN
1	AX	142	GLN
1	AX	196	ASN
1	AX	225	GLN

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Mol	Chain	Res	Type
1	AX	236	ASN
1	AX	258	GLN
1	CX	56	HIS
1	CX	112	GLN
1	CX	190	ASN
1	BY	100	GLN
1	BY	142	GLN
1	BY	190	ASN
1	BY	191	ASN
1	BY	196	ASN
1	BY	214	ASN
1	AY	65	GLN
1	AY	118	ASN
1	AY	134	ASN
1	AY	142	GLN
1	AY	191	ASN
1	AY	196	ASN
1	AY	225	GLN
1	AY	236	ASN
1	AY	258	GLN
1	CY	56	HIS
1	CY	112	GLN
1	CY	190	ASN
1	BZ	100	GLN
1	BZ	142	GLN
1	BZ	190	ASN
1	BZ	191	ASN
1	BZ	196	ASN
1	BZ	214	ASN
1	AZ	65	GLN
1	AZ	118	ASN
1	AZ	134	ASN
1	AZ	142	GLN
1	AZ	191	ASN
1	AZ	196	ASN
1	AZ	225	GLN
1	AZ	258	GLN
1	CZ	56	HIS
1	CZ	112	GLN
1	CZ	190	ASN
1	Ba	100	GLN
1	Ba	142	GLN

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Mol	Chain	Res	Type
1	Ba	190	ASN
1	Ba	191	ASN
1	Ba	196	ASN
1	Aa	65	GLN
1	Aa	118	ASN
1	Aa	134	ASN
1	Aa	142	GLN
1	Aa	196	ASN
1	Aa	225	GLN
1	Aa	236	ASN
1	Aa	258	GLN
1	Ca	56	HIS
1	Ca	94	HIS
1	Ca	112	GLN
1	Ca	190	ASN
1	Bb	100	GLN
1	Bb	142	GLN
1	Bb	190	ASN
1	Bb	191	ASN
1	Bb	196	ASN
1	Ab	65	GLN
1	Ab	118	ASN
1	Ab	134	ASN
1	Ab	142	GLN
1	Ab	196	ASN
1	Ab	225	GLN
1	Ab	236	ASN
1	Ab	258	GLN
1	Cb	56	HIS
1	Cb	112	GLN
1	Cb	190	ASN
1	Bc	100	GLN
1	Bc	142	GLN
1	Bc	190	ASN
1	Bc	191	ASN
1	Bc	196	ASN
1	Ac	65	GLN
1	Ac	118	ASN
1	Ac	134	ASN
1	Ac	142	GLN
1	Ac	196	ASN
1	Ac	225	GLN

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Mol	Chain	Res	Type
1	Ac	236	ASN
1	Ac	258	GLN
1	Cc	56	HIS
1	Cc	112	GLN
1	Cc	190	ASN
1	Bd	100	GLN
1	Bd	190	ASN
1	Bd	191	ASN
1	Bd	196	ASN
1	Ad	65	GLN
1	Ad	118	ASN
1	Ad	134	ASN
1	Ad	142	GLN
1	Ad	191	ASN
1	Ad	196	ASN
1	Ad	225	GLN
1	Ad	258	GLN
1	Cd	56	HIS
1	Cd	112	GLN
1	Cd	190	ASN
1	Cd	196	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 90 ligands modelled in this entry, 90 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	287/338 (84%)	-0.04	1 (0%) 94 88	44, 93, 184, 235	0
1	AB	287/338 (84%)	1.13	62 (21%) 0 0	31, 79, 239, 363	0
1	AC	287/338 (84%)	0.34	25 (8%) 10 6	32, 75, 244, 339	0
1	AD	287/338 (84%)	0.39	16 (5%) 24 14	40, 82, 155, 215	0
1	AE	287/338 (84%)	0.23	6 (2%) 63 48	44, 88, 179, 251	0
1	AF	287/338 (84%)	0.37	21 (7%) 15 9	37, 80, 176, 225	0
1	AG	287/338 (84%)	0.66	35 (12%) 4 3	42, 89, 208, 293	0
1	AH	287/338 (84%)	0.70	43 (14%) 2 1	39, 86, 244, 334	0
1	AI	287/338 (84%)	0.37	22 (7%) 13 8	38, 93, 255, 333	0
1	AJ	287/338 (84%)	0.04	4 (1%) 75 61	36, 75, 146, 223	0
1	AK	287/338 (84%)	0.03	2 (0%) 87 78	31, 63, 120, 191	0
1	AL	287/338 (84%)	0.05	1 (0%) 94 88	32, 69, 138, 194	0
1	AM	287/338 (84%)	1.11	56 (19%) 1 0	41, 91, 249, 306	0
1	AN	287/338 (84%)	-0.14	5 (1%) 70 55	41, 85, 200, 285	0
1	AO	287/338 (84%)	0.51	20 (6%) 16 9	36, 83, 203, 294	0
1	AP	287/338 (84%)	0.10	9 (3%) 49 33	41, 81, 187, 253	0
1	AQ	287/338 (84%)	0.06	5 (1%) 70 55	46, 83, 172, 212	0
1	AR	287/338 (84%)	-0.09	0 100 100	40, 77, 141, 197	0
1	AS	287/338 (84%)	-0.06	7 (2%) 59 42	28, 78, 171, 271	0
1	AT	287/338 (84%)	0.17	3 (1%) 82 70	46, 89, 169, 226	0
1	AU	287/338 (84%)	0.75	35 (12%) 4 3	32, 86, 200, 301	0
1	AV	287/338 (84%)	0.39	19 (6%) 18 10	45, 90, 183, 234	0
1	AW	287/338 (84%)	0.06	2 (0%) 87 78	37, 72, 129, 194	0
1	AX	287/338 (84%)	0.47	27 (9%) 8 4	37, 79, 185, 294	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AY	287/338 (84%)	0.12	9 (3%)	49	33	37, 77, 153, 206	0
1	AZ	287/338 (84%)	0.16	8 (2%)	53	37	39, 84, 178, 279	0
1	Aa	287/338 (84%)	-0.00	6 (2%)	63	48	41, 90, 182, 222	0
1	Ab	287/338 (84%)	1.22	57 (19%)	1	0	38, 81, 245, 357	0
1	Ac	287/338 (84%)	0.30	15 (5%)	27	17	45, 82, 169, 236	0
1	Ad	287/338 (84%)	0.32	11 (3%)	40	26	43, 77, 141, 218	0
1	BA	286/338 (84%)	0.29	18 (6%)	20	11	37, 88, 199, 239	0
1	BB	286/338 (84%)	0.77	38 (13%)	3	2	25, 71, 229, 336	0
1	BC	286/338 (84%)	0.85	48 (16%)	1	1	30, 79, 265, 341	0
1	BD	286/338 (84%)	0.04	5 (1%)	70	55	34, 79, 172, 283	0
1	BE	286/338 (84%)	0.39	19 (6%)	18	10	41, 81, 199, 285	0
1	BF	286/338 (84%)	0.32	24 (8%)	11	7	32, 75, 188, 271	0
1	BG	286/338 (84%)	0.83	36 (12%)	3	2	39, 81, 215, 307	0
1	BH	286/338 (84%)	0.85	44 (15%)	2	1	36, 78, 245, 329	0
1	BI	286/338 (84%)	0.40	27 (9%)	8	4	35, 82, 280, 360	0
1	BJ	286/338 (84%)	0.04	3 (1%)	82	70	24, 67, 162, 275	0
1	BK	286/338 (84%)	0.20	5 (1%)	70	55	27, 62, 144, 203	0
1	BL	286/338 (84%)	0.00	0	100	100	29, 66, 129, 190	0
1	BM	286/338 (84%)	1.14	56 (19%)	1	0	32, 79, 256, 365	0
1	BN	286/338 (84%)	0.13	16 (5%)	24	14	37, 80, 201, 324	0
1	BO	286/338 (84%)	1.22	70 (24%)	0	0	29, 76, 223, 315	0
1	BP	286/338 (84%)	0.18	14 (4%)	29	18	37, 81, 198, 270	0
1	BQ	286/338 (84%)	0.01	2 (0%)	87	78	35, 78, 180, 295	0
1	BR	286/338 (84%)	0.29	7 (2%)	59	42	37, 80, 149, 225	0
1	BS	286/338 (84%)	0.09	7 (2%)	59	42	27, 67, 180, 308	0
1	BT	286/338 (84%)	0.17	4 (1%)	75	61	38, 84, 176, 270	0
1	BU	286/338 (84%)	0.65	36 (12%)	3	2	32, 75, 209, 323	0
1	BV	286/338 (84%)	0.03	4 (1%)	75	61	38, 86, 183, 243	0
1	BW	286/338 (84%)	-0.05	1 (0%)	94	88	33, 66, 123, 203	0
1	BX	286/338 (84%)	0.40	22 (7%)	13	8	35, 80, 198, 263	0
1	BY	286/338 (84%)	0.54	20 (6%)	16	9	35, 78, 150, 213	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	BZ	286/338 (84%)	0.23	11 (3%) 40 26	38, 83, 195, 246	0
1	Ba	286/338 (84%)	0.09	5 (1%) 70 55	34, 81, 197, 330	0
1	Bb	286/338 (84%)	0.76	42 (14%) 2 1	30, 69, 249, 342	0
1	Bc	286/338 (84%)	0.25	14 (4%) 29 18	33, 79, 214, 279	0
1	Bd	286/338 (84%)	0.51	23 (8%) 12 7	37, 79, 168, 230	0
1	CA	304/338 (89%)	0.34	25 (8%) 11 7	40, 78, 206, 252	0
1	CB	304/338 (89%)	1.62	88 (28%) 0 0	29, 75, 282, 357	0
1	CC	304/338 (89%)	0.58	44 (14%) 2 1	28, 72, 269, 370	0
1	CD	304/338 (89%)	0.11	10 (3%) 46 31	38, 76, 190, 273	0
1	CE	304/338 (89%)	0.71	51 (16%) 1 1	34, 76, 239, 323	0
1	CF	304/338 (89%)	0.81	51 (16%) 1 1	34, 72, 234, 326	0
1	CG	304/338 (89%)	1.95	90 (29%) 0 0	39, 83, 269, 342	0
1	CH	304/338 (89%)	1.99	93 (30%) 0 0	37, 79, 323, 403	0
1	CI	304/338 (89%)	0.76	52 (17%) 1 1	34, 81, 284, 396	0
1	CJ	304/338 (89%)	0.11	12 (3%) 39 25	26, 70, 200, 287	0
1	CK	304/338 (89%)	0.14	3 (0%) 82 70	28, 64, 113, 174	0
1	CL	304/338 (89%)	0.04	2 (0%) 87 78	26, 66, 129, 190	0
1	CM	304/338 (89%)	1.38	74 (24%) 0 0	33, 75, 306, 389	0
1	CN	304/338 (89%)	0.45	33 (10%) 5 3	39, 77, 229, 320	0
1	CO	304/338 (89%)	0.89	53 (17%) 1 1	30, 74, 258, 396	0
1	CP	304/338 (89%)	0.32	23 (7%) 13 8	33, 81, 201, 288	0
1	CQ	304/338 (89%)	0.22	16 (5%) 26 16	39, 80, 187, 294	0
1	CR	304/338 (89%)	0.13	7 (2%) 60 44	34, 79, 153, 209	0
1	CS	304/338 (89%)	0.32	25 (8%) 11 7	28, 66, 226, 306	0
1	CT	304/338 (89%)	0.12	7 (2%) 60 44	37, 76, 186, 299	0
1	CU	304/338 (89%)	1.11	65 (21%) 0 0	31, 70, 249, 303	0
1	CV	304/338 (89%)	0.24	12 (3%) 39 25	41, 80, 196, 237	0
1	CW	304/338 (89%)	0.01	7 (2%) 60 44	30, 75, 137, 176	0
1	CX	304/338 (89%)	0.04	14 (4%) 32 20	39, 78, 244, 302	0
1	CY	304/338 (89%)	0.53	27 (8%) 9 5	33, 73, 176, 256	0
1	CZ	304/338 (89%)	0.39	32 (10%) 6 3	43, 82, 187, 293	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Ca	304/338 (89%)	0.71	44 (14%) 2 1	35, 78, 209, 267	0
1	Cb	304/338 (89%)	1.93	83 (27%) 0 0	30, 73, 298, 419	0
1	Cc	304/338 (89%)	0.65	47 (15%) 2 1	38, 80, 263, 325	0
1	Cd	304/338 (89%)	0.19	10 (3%) 46 31	35, 75, 137, 221	0
All	All	26310/30420 (86%)	0.45	2253 (8%) 10 6	24, 78, 223, 419	0

All (2253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Cb	232	SER	28.2
1	CG	265	ILE	22.1
1	Cb	227	SER	21.0
1	CH	337	GLU	20.1
1	BG	317	ASP	19.5
1	Cb	231	ASP	19.4
1	CH	265	ILE	18.7
1	CB	265	ILE	18.6
1	CH	293	ALA	17.5
1	Cb	265	ILE	17.3
1	CH	282	LEU	16.9
1	BM	264	SER	16.8
1	CH	286	ALA	16.6
1	Bb	318	GLU	16.4
1	CM	245	SER	16.4
1	CM	282	LEU	16.2
1	CF	293	ALA	15.7
1	Cb	249	ASP	15.7
1	Ab	306	LYS	15.5
1	Cb	294	GLY	15.2
1	CG	253	ASP	15.0
1	BH	327	VAL	15.0
1	CO	265	ILE	15.0
1	CM	265	ILE	14.8
1	CB	282	LEU	14.6
1	Cc	274	VAL	14.6
1	CH	288	ASN	14.5
1	CM	328	GLY	14.5
1	Bb	317	ASP	14.5
1	Cb	282	LEU	14.2
1	Ab	270	GLY	14.1
1	Cb	288	ASN	13.9

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Mol	Chain	Res	Type	RSRZ
1	CM	246	THR	13.8
1	Cb	241	ILE	13.8
1	CB	250	ILE	13.8
1	CG	286	ALA	13.7
1	CH	294	GLY	13.6
1	CH	336	SER	13.5
1	CG	247	PRO	13.4
1	CG	246	THR	13.4
1	CU	265	ILE	13.1
1	Cb	250	ILE	13.0
1	Ac	269	LEU	12.9
1	BC	263	LEU	12.9
1	CB	232	SER	12.8
1	Cb	286	ALA	12.6
1	CO	282	LEU	12.5
1	BM	318	GLU	12.4
1	Cb	255	ALA	12.3
1	Ab	273	ASP	12.3
1	CN	265	ILE	12.3
1	BC	264	SER	12.0
1	CG	289	ALA	12.0
1	CH	257	PHE	12.0
1	CU	232	SER	12.0
1	CI	263	LEU	11.9
1	BB	317	ASP	11.6
1	CG	293	ALA	11.6
1	CB	288	ASN	11.5
1	BG	318	GLU	11.4
1	Ab	337	GLU	11.4
1	CN	282	LEU	11.4
1	Ca	293	ALA	11.4
1	CM	256	VAL	11.4
1	CM	247	PRO	11.3
1	CG	282	LEU	11.3
1	CH	263	LEU	11.2
1	CG	232	SER	11.2
1	Cb	291	THR	11.2
1	CF	265	ILE	11.2
1	Cb	242	LEU	11.2
1	CH	289	ALA	11.2
1	AB	230	ASN	11.0
1	BM	239	LYS	11.0

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Mol	Chain	Res	Type	RSRZ
1	BB	264	SER	11.0
1	BB	318	GLU	11.0
1	CB	257	PHE	11.0
1	Bc	318	GLU	10.9
1	CH	250	ILE	10.7
1	Cb	321	ARG	10.7
1	CO	286	ALA	10.7
1	Cb	293	ALA	10.7
1	CH	262	PRO	10.7
1	BO	239	LYS	10.7
1	CM	257	PHE	10.6
1	CU	282	LEU	10.6
1	CE	265	ILE	10.6
1	CB	289	ALA	10.6
1	CG	249	ASP	10.5
1	AI	230	ASN	10.5
1	CB	321	ARG	10.5
1	CG	250	ILE	10.4
1	CO	289	ALA	10.4
1	CM	240	SER	10.4
1	CG	288	ASN	10.3
1	Ca	290	GLY	10.3
1	Cb	289	ALA	10.3
1	CO	288	ASN	10.2
1	BC	268	SER	10.2
1	Ab	303	ASN	10.1
1	Cb	263	LEU	10.0
1	CI	265	ILE	10.0
1	Cb	279	TYR	10.0
1	BO	264	SER	10.0
1	CG	274	VAL	9.9
1	Ab	304	PHE	9.9
1	Cc	232	SER	9.9
1	CH	253	ASP	9.9
1	CI	249	ASP	9.9
1	BH	318	GLU	9.9
1	BO	296	PHE	9.9
1	Ca	282	LEU	9.9
1	BO	315	TYR	9.8
1	CH	291	THR	9.8
1	CG	294	GLY	9.7
1	CH	225	GLN	9.7

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Mol	Chain	Res	Type	RSRZ
1	BO	292	PRO	9.7
1	CB	263	LEU	9.7
1	BO	318	GLU	9.6
1	BH	264	SER	9.6
1	Cc	289	ALA	9.6
1	CH	232	SER	9.6
1	CM	227	SER	9.6
1	Cb	239	LYS	9.6
1	Ab	268	SER	9.5
1	CU	293	ALA	9.5
1	BG	312	VAL	9.5
1	AB	306	LYS	9.4
1	CH	287	GLY	9.4
1	BO	291	THR	9.3
1	Cb	240	SER	9.3
1	Cb	287	GLY	9.3
1	CG	318	GLU	9.3
1	CB	291	THR	9.3
1	CM	223	MET	9.2
1	Cb	290	GLY	9.2
1	Cc	293	ALA	9.2
1	CM	294	GLY	9.2
1	Cb	223	MET	9.1
1	AM	306	LYS	9.1
1	CI	220	ALA	9.1
1	CH	249	ASP	9.1
1	BC	278	VAL	9.1
1	AH	230	ASN	9.0
1	Ab	269	LEU	9.0
1	BH	328	GLY	9.0
1	CM	249	ASP	8.9
1	BM	238	PHE	8.9
1	AB	236	ASN	8.9
1	CO	291	THR	8.9
1	CG	252	PRO	8.9
1	BG	298	TRP	8.9
1	CG	242	LEU	8.8
1	CG	279	TYR	8.8
1	CG	245	SER	8.8
1	CE	282	LEU	8.8
1	AB	322	GLN	8.8
1	CG	233	LEU	8.7

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Mol	Chain	Res	Type	RSRZ
1	BM	298	TRP	8.7
1	CB	223	MET	8.7
1	CB	251	ALA	8.6
1	CP	265	ILE	8.6
1	Cb	222	ILE	8.6
1	CM	279	TYR	8.6
1	BC	317	ASP	8.6
1	AF	269	LEU	8.6
1	Ab	271	THR	8.5
1	BB	326	PRO	8.5
1	CH	300	ILE	8.5
1	AB	268	SER	8.5
1	CH	333	ARG	8.4
1	CB	262	PRO	8.4
1	Ab	336	SER	8.4
1	BO	278	VAL	8.4
1	CX	282	LEU	8.4
1	BO	237	ASP	8.3
1	CG	255	ALA	8.3
1	AI	318	GLU	8.2
1	BE	317	ASP	8.2
1	BG	264	SER	8.2
1	CF	282	LEU	8.2
1	CH	251	ALA	8.2
1	BH	317	ASP	8.1
1	CG	285	PHE	8.1
1	CB	270	GLY	8.1
1	BH	278	VAL	8.1
1	BG	296	PHE	8.1
1	CB	256	VAL	8.1
1	BO	298	TRP	8.0
1	AB	273	ASP	8.0
1	CB	233	LEU	8.0
1	BG	276	ARG	8.0
1	CH	327	VAL	8.0
1	BH	326	PRO	8.0
1	CO	250	ILE	8.0
1	CO	279	TYR	8.0
1	CM	330	VAL	7.9
1	AG	268	SER	7.9
1	CM	241	ILE	7.8
1	CH	335	ASP	7.8

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Mol	Chain	Res	Type	RSRZ
1	CM	244	GLY	7.8
1	BO	238	PHE	7.8
1	Bb	264	SER	7.8
1	Cb	246	THR	7.8
1	BE	318	GLU	7.7
1	CM	232	SER	7.7
1	Cb	247	PRO	7.7
1	CM	327	VAL	7.7
1	CH	223	MET	7.7
1	CH	270	GLY	7.7
1	Ab	308	PHE	7.6
1	BM	317	ASP	7.6
1	BU	318	GLU	7.6
1	CU	227	SER	7.6
1	Cb	226	GLY	7.6
1	CG	241	ILE	7.6
1	BC	269	LEU	7.6
1	Cb	253	ASP	7.6
1	CI	257	PHE	7.6
1	BG	315	TYR	7.6
1	CB	249	ASP	7.6
1	CM	253	ASP	7.6
1	Cb	233	LEU	7.5
1	BO	312	VAL	7.5
1	CO	257	PHE	7.5
1	CC	279	TYR	7.5
1	CF	319	GLN	7.5
1	Cb	281	HIS	7.5
1	BI	262	PRO	7.5
1	BI	296	PHE	7.4
1	CG	287	GLY	7.4
1	CB	255	ALA	7.4
1	CO	249	ASP	7.3
1	CB	317	ASP	7.3
1	CB	287	GLY	7.3
1	CG	321	ARG	7.2
1	Ab	265	ILE	7.2
1	Cb	252	PRO	7.2
1	BB	327	VAL	7.2
1	CU	263	LEU	7.2
1	CU	292	PRO	7.2
1	AB	271	THR	7.2

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Mol	Chain	Res	Type	RSRZ
1	CH	264	SER	7.2
1	BM	315	TYR	7.2
1	CG	257	PHE	7.2
1	Ac	265	ILE	7.1
1	Cb	292	PRO	7.1
1	BB	262	PRO	7.1
1	CB	227	SER	7.1
1	CO	287	GLY	7.1
1	CA	282	LEU	7.1
1	BS	317	ASP	7.1
1	CH	221	PRO	7.1
1	CF	266	ASP	7.1
1	CH	290	GLY	7.0
1	CI	218	THR	7.0
1	CO	255	ALA	7.0
1	Cb	327	VAL	7.0
1	CH	247	PRO	7.0
1	Ab	333	ARG	7.0
1	BN	264	SER	7.0
1	Ab	272	GLY	7.0
1	AM	260	ASP	7.0
1	CU	317	ASP	7.0
1	CU	250	ILE	7.0
1	CE	293	ALA	7.0
1	CO	256	VAL	7.0
1	CF	257	PHE	7.0
1	BM	237	ASP	7.0
1	AM	269	LEU	7.0
1	BN	317	ASP	6.9
1	BM	276	ARG	6.9
1	AI	266	ASP	6.9
1	CM	293	ALA	6.9
1	Cb	274	VAL	6.9
1	Cb	333	ARG	6.9
1	CM	289	ALA	6.9
1	CG	231	ASP	6.9
1	CU	286	ALA	6.9
1	AM	325	LEU	6.9
1	CB	290	GLY	6.8
1	AO	324	LEU	6.8
1	Ab	305	ASN	6.8
1	BH	296	PHE	6.8

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Mol	Chain	Res	Type	RSRZ
1	CI	282	LEU	6.8
1	CX	265	ILE	6.8
1	AH	325	LEU	6.8
1	CB	245	SER	6.7
1	Cc	282	LEU	6.7
1	CB	240	SER	6.7
1	CM	250	ILE	6.7
1	CG	270	GLY	6.7
1	CI	294	GLY	6.7
1	CB	234	SER	6.7
1	BU	239	LYS	6.7
1	CM	263	LEU	6.7
1	BM	277	ALA	6.7
1	Bc	317	ASP	6.7
1	BB	328	GLY	6.7
1	CI	255	ALA	6.7
1	BB	228	LEU	6.7
1	CG	331	CYS	6.7
1	CU	321	ARG	6.7
1	CO	253	ASP	6.6
1	CU	262	PRO	6.6
1	Bb	315	TYR	6.6
1	BO	262	PRO	6.6
1	BH	238	PHE	6.6
1	CH	279	TYR	6.6
1	Ca	292	PRO	6.6
1	CY	232	SER	6.6
1	AF	236	ASN	6.6
1	CI	221	PRO	6.5
1	CO	263	LEU	6.6
1	CH	317	ASP	6.5
1	Bb	239	LYS	6.5
1	CU	241	ILE	6.5
1	Cc	246	THR	6.5
1	BO	236	ASN	6.5
1	CF	291	THR	6.5
1	AC	282	LEU	6.5
1	Ca	257	PHE	6.5
1	Bb	298	TRP	6.5
1	CB	231	ASP	6.5
1	CH	330	VAL	6.5
1	CI	254	GLY	6.5

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Mol	Chain	Res	Type	RSRZ
1	CG	244	GLY	6.4
1	CF	294	GLY	6.4
1	CH	227	SER	6.4
1	CG	290	GLY	6.4
1	CH	252	PRO	6.4
1	CB	225	GLN	6.4
1	CI	279	TYR	6.4
1	CH	245	SER	6.4
1	BO	317	ASP	6.4
1	CO	290	GLY	6.3
1	CG	330	VAL	6.3
1	AM	324	LEU	6.3
1	Cb	318	GLU	6.3
1	BN	318	GLU	6.3
1	Ca	249	ASP	6.3
1	AM	236	ASN	6.3
1	CG	292	PRO	6.3
1	BB	278	VAL	6.3
1	AB	260	ASP	6.3
1	BH	227	SER	6.3
1	CG	227	SER	6.3
1	Ab	218	THR	6.3
1	CE	337	GLU	6.2
1	CH	231	ASP	6.2
1	BB	296	PHE	6.2
1	CG	240	SER	6.2
1	BI	264	SER	6.2
1	BM	292	PRO	6.2
1	CO	316	SER	6.2
1	CH	240	SER	6.2
1	AB	303	ASN	6.2
1	Ab	325	LEU	6.2
1	CI	219	THR	6.2
1	CU	255	ALA	6.2
1	BP	317	ASP	6.2
1	Cc	292	PRO	6.1
1	CI	288	ASN	6.1
1	AX	337	GLU	6.1
1	BI	317	ASP	6.1
1	BY	317	ASP	6.1
1	CF	337	GLU	6.1
1	CC	317	ASP	6.1

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Mol	Chain	Res	Type	RSRZ
1	CB	318	GLU	6.1
1	CG	263	LEU	6.1
1	CI	318	GLU	6.1
1	BB	227	SER	6.1
1	CN	293	ALA	6.1
1	CE	286	ALA	6.1
1	BH	239	LYS	6.0
1	Cb	244	GLY	6.0
1	Ba	317	ASP	6.0
1	Cb	225	GLN	6.0
1	CB	337	GLU	6.0
1	AH	322	GLN	6.0
1	AI	228	LEU	6.0
1	CA	249	ASP	6.0
1	BC	249	ASP	6.0
1	CU	290	GLY	6.0
1	BH	262	PRO	6.0
1	BO	309	THR	6.0
1	BM	278	VAL	6.0
1	Cb	245	SER	6.0
1	CG	310	ASP	6.0
1	CG	333	ARG	6.0
1	CB	316	SER	6.0
1	CF	264	SER	6.0
1	BS	315	TYR	6.0
1	Cb	251	ALA	6.0
1	Ac	268	SER	6.0
1	CE	266	ASP	6.0
1	Ca	291	THR	6.0
1	AI	270	GLY	5.9
1	BB	277	ALA	5.9
1	BC	266	ASP	5.9
1	BO	297	ARG	5.9
1	CF	286	ALA	5.9
1	CB	247	PRO	5.9
1	Cb	307	THR	5.9
1	CI	248	LEU	5.9
1	Cc	264	SER	5.9
1	BI	318	GLU	5.8
1	Bb	327	VAL	5.8
1	AB	304	PHE	5.8
1	Ca	255	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	AB	307	THR	5.8
1	CI	277	ALA	5.8
1	BU	238	PHE	5.8
1	AC	298	TRP	5.8
1	CM	335	ASP	5.8
1	CB	294	GLY	5.8
1	CN	232	SER	5.8
1	CO	293	ALA	5.8
1	Cb	257	PHE	5.8
1	CU	242	LEU	5.8
1	CO	264	SER	5.8
1	Ab	307	THR	5.7
1	CY	264	SER	5.7
1	CE	287	GLY	5.7
1	CH	233	LEU	5.7
1	AE	337	GLU	5.7
1	CM	307	THR	5.7
1	CB	333	ARG	5.7
1	Ab	281	HIS	5.7
1	CF	333	ARG	5.7
1	CS	255	ALA	5.7
1	CE	289	ALA	5.6
1	BO	327	VAL	5.6
1	AO	269	LEU	5.6
1	Cb	276	ARG	5.6
1	Cb	256	VAL	5.6
1	CB	286	ALA	5.6
1	CO	251	ALA	5.6
1	CG	262	PRO	5.6
1	CE	272	GLY	5.6
1	Cb	317	ASP	5.6
1	CH	285	PHE	5.6
1	CF	287	GLY	5.6
1	CI	269	LEU	5.6
1	BM	296	PHE	5.6
1	CN	257	PHE	5.6
1	AG	307	THR	5.6
1	CH	284	LYS	5.5
1	AG	230	ASN	5.5
1	BF	239	LYS	5.5
1	CH	274	VAL	5.5
1	Bb	292	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	Cb	328	GLY	5.5
1	CG	335	ASP	5.5
1	AO	325	LEU	5.5
1	CH	283	LYS	5.5
1	CE	249	ASP	5.5
1	Ab	260	ASP	5.5
1	CM	252	PRO	5.5
1	BX	317	ASP	5.5
1	AB	232	SER	5.5
1	CU	327	VAL	5.4
1	CF	263	LEU	5.4
1	Bd	287	GLY	5.4
1	AB	305	ASN	5.4
1	BU	264	SER	5.4
1	BB	238	PHE	5.4
1	BM	297	ARG	5.4
1	AM	281	HIS	5.4
1	CF	255	ALA	5.4
1	CM	323	ILE	5.4
1	BX	264	SER	5.4
1	CP	317	ASP	5.4
1	CS	282	LEU	5.4
1	AH	260	ASP	5.4
1	AO	230	ASN	5.4
1	BU	296	PHE	5.4
1	CE	270	GLY	5.4
1	CB	271	THR	5.4
1	BU	317	ASP	5.4
1	BB	298	TRP	5.4
1	CH	281	HIS	5.4
1	AF	337	GLU	5.3
1	AU	281	HIS	5.3
1	AU	337	GLU	5.3
1	AB	269	LEU	5.3
1	BD	317	ASP	5.3
1	CU	231	ASP	5.3
1	Ca	289	ALA	5.3
1	BE	315	TYR	5.3
1	BM	291	THR	5.3
1	Bd	289	ALA	5.3
1	CB	293	ALA	5.3
1	CF	318	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	AM	337	GLU	5.3
1	CN	233	LEU	5.3
1	CG	317	ASP	5.3
1	CG	328	GLY	5.3
1	CJ	286	ALA	5.3
1	CU	287	GLY	5.3
1	CG	223	MET	5.3
1	CH	328	GLY	5.3
1	CB	281	HIS	5.2
1	CD	282	LEU	5.2
1	BF	315	TYR	5.2
1	CM	281	HIS	5.2
1	AB	270	GLY	5.2
1	AG	236	ASN	5.2
1	CH	241	ILE	5.2
1	BC	276	ARG	5.2
1	CM	333	ARG	5.2
1	BM	236	ASN	5.2
1	Cc	250	ILE	5.2
1	BX	318	GLU	5.2
1	BM	328	GLY	5.2
1	BI	227	SER	5.2
1	CU	333	ARG	5.2
1	Ba	318	GLU	5.2
1	CB	279	TYR	5.2
1	CH	222	ILE	5.2
1	CU	316	SER	5.2
1	CU	257	PHE	5.2
1	CB	246	THR	5.2
1	CG	239	LYS	5.2
1	AM	230	ASN	5.2
1	BH	277	ALA	5.2
1	CH	255	ALA	5.2
1	CC	258	GLN	5.2
1	CG	319	GLN	5.2
1	Bb	276	ARG	5.2
1	CZ	333	ARG	5.1
1	CM	248	LEU	5.1
1	CI	293	ALA	5.1
1	CH	234	SER	5.1
1	Ca	250	ILE	5.1
1	CU	328	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	AB	318	GLU	5.1
1	Ac	273	ASP	5.1
1	BO	279	TYR	5.1
1	CH	244	GLY	5.1
1	CO	232	SER	5.1
1	CB	244	GLY	5.1
1	Ab	335	ASP	5.1
1	CU	256	VAL	5.1
1	AX	265	ILE	5.1
1	Cb	323	ILE	5.1
1	AM	228	LEU	5.1
1	BS	318	GLU	5.1
1	CO	247	PRO	5.1
1	AM	297	ARG	5.1
1	AM	273	ASP	5.1
1	AO	273	ASP	5.1
1	Cb	221	PRO	5.1
1	CO	292	PRO	5.1
1	AG	306	LYS	5.1
1	CI	289	ALA	5.0
1	CF	232	SER	5.0
1	Ca	288	ASN	5.0
1	CB	253	ASP	5.0
1	AB	308	PHE	5.0
1	BA	239	LYS	5.0
1	BX	278	VAL	5.0
1	AX	268	SER	5.0
1	CG	251	ALA	5.0
1	BU	328	GLY	5.0
1	CO	252	PRO	5.0
1	BU	277	ALA	5.0
1	CB	274	VAL	5.0
1	Cd	254	GLY	5.0
1	CU	221	PRO	5.0
1	AG	266	ASP	4.9
1	CE	288	ASN	4.9
1	CB	226	GLY	4.9
1	CI	239	LYS	4.9
1	CN	250	ILE	4.9
1	CQ	282	LEU	4.9
1	CS	293	ALA	4.9
1	CM	288	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	CH	224	THR	4.9
1	BP	318	GLU	4.9
1	BO	277	ALA	4.9
1	CO	245	SER	4.9
1	Ab	277	ALA	4.9
1	CN	255	ALA	4.9
1	Bb	238	PHE	4.9
1	Ab	228	LEU	4.9
1	BC	224	THR	4.9
1	CL	269	LEU	4.9
1	CT	337	GLU	4.9
1	BC	277	ALA	4.9
1	Bb	291	THR	4.9
1	AU	306	LYS	4.8
1	Cb	319	GLN	4.8
1	CI	241	ILE	4.8
1	BF	317	ASP	4.8
1	CO	317	ASP	4.8
1	CU	252	PRO	4.8
1	CC	243	LEU	4.8
1	AC	278	VAL	4.8
1	AB	325	LEU	4.8
1	Ab	230	ASN	4.8
1	CA	256	VAL	4.8
1	AH	281	HIS	4.8
1	AB	301	TRP	4.8
1	AF	268	SER	4.8
1	BH	315	TYR	4.8
1	AD	269	LEU	4.8
1	BX	298	TRP	4.8
1	CH	218	THR	4.8
1	BC	325	LEU	4.8
1	Cb	277	ALA	4.8
1	AH	228	LEU	4.8
1	Cc	296	PHE	4.8
1	AO	322	GLN	4.8
1	AO	320	PRO	4.8
1	AC	264	SER	4.7
1	CH	316	SER	4.7
1	CG	291	THR	4.7
1	CB	335	ASP	4.7
1	AB	297	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	AH	273	ASP	4.7
1	CC	274	VAL	4.7
1	BF	318	GLU	4.7
1	BU	262	PRO	4.7
1	CF	316	SER	4.7
1	AH	279	TYR	4.7
1	CM	225	GLN	4.7
1	CG	264	SER	4.7
1	BX	291	THR	4.7
1	CJ	289	ALA	4.7
1	AB	257	PHE	4.7
1	BB	312	VAL	4.7
1	CF	274	VAL	4.7
1	BO	290	GLY	4.7
1	CB	323	ILE	4.7
1	BG	229	TYR	4.7
1	CH	323	ILE	4.7
1	AX	270	GLY	4.7
1	CC	218	THR	4.7
1	Ab	324	LEU	4.6
1	Cb	262	PRO	4.6
1	BO	255	ALA	4.6
1	Ca	240	SER	4.6
1	BO	311	GLY	4.6
1	BF	312	VAL	4.6
1	CB	292	PRO	4.6
1	CB	336	SER	4.6
1	BH	298	TRP	4.6
1	CA	281	HIS	4.6
1	CB	239	LYS	4.6
1	CM	255	ALA	4.6
1	AB	240	SER	4.6
1	BC	262	PRO	4.6
1	CF	292	PRO	4.6
1	AS	306	LYS	4.6
1	AC	232	SER	4.6
1	AD	337	GLU	4.6
1	Cc	265	ILE	4.6
1	CU	289	ALA	4.6
1	CH	235	THR	4.6
1	CO	333	ARG	4.6
1	CF	249	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	BO	284	LYS	4.6
1	AH	307	THR	4.6
1	Ad	322	GLN	4.6
1	AF	271	THR	4.6
1	BY	323	ILE	4.6
1	BU	327	VAL	4.6
1	AJ	337	GLU	4.6
1	BM	255	ALA	4.6
1	AM	220	ALA	4.6
1	CQ	249	ASP	4.6
1	Ac	306	LYS	4.5
1	BB	281	HIS	4.5
1	CG	221	PRO	4.5
1	CN	256	VAL	4.5
1	CM	251	ALA	4.5
1	CB	221	PRO	4.5
1	Cb	332	THR	4.5
1	CC	264	SER	4.5
1	CD	249	ASP	4.5
1	Bb	262	PRO	4.5
1	CU	240	SER	4.5
1	CM	262	PRO	4.5
1	AM	271	THR	4.5
1	CB	327	VAL	4.5
1	BG	275	ASP	4.5
1	AB	217	GLU	4.5
1	BO	276	ARG	4.5
1	CP	263	LEU	4.5
1	Aa	269	LEU	4.5
1	AG	269	LEU	4.5
1	CG	295	TRP	4.5
1	Cb	285	PHE	4.5
1	CI	240	SER	4.5
1	CU	291	THR	4.5
1	BH	276	ARG	4.5
1	Ab	278	VAL	4.4
1	CH	307	THR	4.4
1	AM	258	GLN	4.4
1	AB	218	THR	4.4
1	CH	319	GLN	4.4
1	Ca	256	VAL	4.4
1	AC	283	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	Bb	319	GLN	4.4
1	AB	228	LEU	4.4
1	Bd	288	ASN	4.4
1	CE	316	SER	4.4
1	CF	321	ARG	4.4
1	AH	333	ARG	4.4
1	Bb	326	PRO	4.4
1	CF	290	GLY	4.4
1	BO	227	SER	4.4
1	AU	271	THR	4.4
1	BI	237	ASP	4.4
1	BC	218	THR	4.4
1	AG	260	ASP	4.4
1	BC	265	ILE	4.4
1	CE	253	ASP	4.4
1	BH	228	LEU	4.4
1	Bb	296	PHE	4.4
1	BX	262	PRO	4.4
1	BG	239	LYS	4.4
1	CU	264	SER	4.4
1	CH	332	THR	4.3
1	AH	303	ASN	4.3
1	Ab	236	ASN	4.3
1	BB	239	LYS	4.3
1	BG	231	ASP	4.3
1	CE	274	VAL	4.3
1	CR	289	ALA	4.3
1	BG	238	PHE	4.3
1	AG	297	ARG	4.3
1	CH	271	THR	4.3
1	CP	274	VAL	4.3
1	AI	271	THR	4.3
1	CX	247	PRO	4.3
1	AG	277	ALA	4.3
1	Cc	321	ARG	4.3
1	BH	237	ASP	4.3
1	AO	228	LEU	4.3
1	Ca	294	GLY	4.3
1	BU	298	TRP	4.3
1	BB	315	TYR	4.3
1	BH	321	ARG	4.3
1	CH	318	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	BV	263	LEU	4.3
1	AU	230	ASN	4.3
1	CC	240	SER	4.3
1	BF	227	SER	4.3
1	BG	277	ALA	4.3
1	CF	279	TYR	4.3
1	BM	327	VAL	4.3
1	CS	274	VAL	4.3
1	CM	221	PRO	4.3
1	Ab	320	PRO	4.3
1	AI	218	THR	4.2
1	CU	337	GLU	4.2
1	BX	315	TYR	4.2
1	AH	265	ILE	4.2
1	CC	231	ASP	4.2
1	Cc	291	THR	4.2
1	CG	271	THR	4.2
1	CI	256	VAL	4.2
1	AO	308	PHE	4.2
1	CI	251	ALA	4.2
1	AU	268	SER	4.2
1	Ab	322	GLN	4.2
1	CB	307	THR	4.2
1	AX	322	GLN	4.2
1	BG	326	PRO	4.2
1	AG	322	GLN	4.2
1	CN	286	ALA	4.2
1	BF	298	TRP	4.2
1	CM	239	LYS	4.2
1	CG	332	THR	4.2
1	CN	249	ASP	4.2
1	Ab	217	GLU	4.2
1	CO	328	GLY	4.2
1	CM	303	ASN	4.2
1	Bd	303	ASN	4.2
1	CC	319	GLN	4.2
1	BA	227	SER	4.2
1	AU	308	PHE	4.2
1	BI	292	PRO	4.1
1	CC	228	LEU	4.1
1	CP	268	SER	4.1
1	CM	286	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	CM	318	GLU	4.1
1	CI	253	ASP	4.1
1	CU	253	ASP	4.1
1	AF	270	GLY	4.1
1	BO	301	TRP	4.1
1	CM	321	ARG	4.1
1	CU	247	PRO	4.1
1	Ca	284	LYS	4.1
1	CF	256	VAL	4.1
1	CP	279	TYR	4.1
1	AX	228	LEU	4.1
1	AG	337	GLU	4.1
1	CM	261	ARG	4.1
1	Ad	321	ARG	4.1
1	CG	284	LYS	4.1
1	CP	282	LEU	4.1
1	CA	307	THR	4.1
1	AH	337	GLU	4.1
1	CM	332	THR	4.1
1	Cb	330	VAL	4.1
1	CA	318	GLU	4.1
1	AF	275	ASP	4.1
1	BI	315	TYR	4.1
1	CX	279	TYR	4.1
1	BX	277	ALA	4.1
1	CS	227	SER	4.1
1	CH	239	LYS	4.1
1	AU	297	ARG	4.1
1	AH	263	LEU	4.0
1	AG	276	ARG	4.0
1	CS	265	ILE	4.0
1	CB	218	THR	4.0
1	BY	318	GLU	4.0
1	BP	277	ALA	4.0
1	CU	249	ASP	4.0
1	BM	312	VAL	4.0
1	CU	251	ALA	4.0
1	Cc	333	ARG	4.0
1	AH	268	SER	4.0
1	CB	284	LYS	4.0
1	AG	273	ASP	4.0
1	BU	309	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	AG	51	GLY	4.0
1	Ab	254	GLY	4.0
1	AY	269	LEU	4.0
1	BI	297	ARG	4.0
1	BF	275	ASP	4.0
1	Bb	278	VAL	4.0
1	Cc	240	SER	4.0
1	CM	337	GLU	4.0
1	AC	238	PHE	4.0
1	BE	238	PHE	4.0
1	BO	328	GLY	4.0
1	Cc	270	GLY	4.0
1	AB	266	ASP	4.0
1	Cc	316	SER	4.0
1	Cc	257	PHE	4.0
1	CU	335	ASP	4.0
1	CB	264	SER	4.0
1	AC	263	LEU	4.0
1	Ca	333	ARG	4.0
1	CA	305	ASN	4.0
1	AB	237	ASP	4.0
1	AH	269	LEU	4.0
1	AG	304	PHE	4.0
1	AH	304	PHE	3.9
1	CU	288	ASN	3.9
1	CA	233	LEU	3.9
1	BB	263	LEU	3.9
1	BR	331	CYS	3.9
1	AO	337	GLU	3.9
1	AB	324	LEU	3.9
1	AX	269	LEU	3.9
1	Cb	303	ASN	3.9
1	Cc	286	ALA	3.9
1	CE	267	TYR	3.9
1	CB	220	ALA	3.9
1	AQ	337	GLU	3.9
1	CF	335	ASP	3.9
1	AU	270	GLY	3.9
1	CU	266	ASP	3.9
1	CF	289	ALA	3.9
1	CC	332	THR	3.9
1	BY	291	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	Bb	229	TYR	3.9
1	CA	337	GLU	3.9
1	Ca	252	PRO	3.9
1	BO	257	PHE	3.9
1	CP	264	SER	3.9
1	CY	290	GLY	3.9
1	CG	225	GLN	3.9
1	CC	259	LEU	3.9
1	Ca	269	LEU	3.9
1	Ba	315	TYR	3.9
1	CG	336	SER	3.9
1	AX	271	THR	3.9
1	Ca	253	ASP	3.9
1	AI	281	HIS	3.9
1	Cc	310	ASP	3.9
1	CI	290	GLY	3.9
1	AB	337	GLU	3.9
1	CO	240	SER	3.9
1	BB	237	ASP	3.9
1	CA	257	PHE	3.9
1	AB	238	PHE	3.9
1	AU	280	TRP	3.9
1	BA	264	SER	3.9
1	CG	273	ASP	3.9
1	Cb	229	TYR	3.8
1	CG	298	TRP	3.8
1	AH	280	TRP	3.8
1	CM	274	VAL	3.8
1	CG	222	ILE	3.8
1	CY	274	VAL	3.8
1	CY	337	GLU	3.8
1	CB	229	TYR	3.8
1	CE	263	LEU	3.8
1	BF	262	PRO	3.8
1	CG	235	THR	3.8
1	AM	218	THR	3.8
1	AB	320	PRO	3.8
1	BO	326	PRO	3.8
1	AM	164	ARG	3.8
1	AX	296	PHE	3.8
1	AG	265	ILE	3.8
1	BO	242	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	BM	262	PRO	3.8
1	Ab	257	PHE	3.8
1	BH	322	GLN	3.8
1	CJ	293	ALA	3.8
1	Cb	322	GLN	3.8
1	Cc	263	LEU	3.8
1	Bc	299	GLY	3.8
1	AH	271	THR	3.8
1	AU	218	THR	3.8
1	AU	325	LEU	3.8
1	AC	242	LEU	3.8
1	CC	313	ALA	3.8
1	AU	269	LEU	3.8
1	Bb	255	ALA	3.8
1	AH	270	GLY	3.8
1	AB	252	PRO	3.8
1	BU	315	TYR	3.8
1	CM	224	THR	3.8
1	CO	332	THR	3.8
1	AM	270	GLY	3.8
1	CE	255	ALA	3.8
1	CM	287	GLY	3.7
1	CB	222	ILE	3.7
1	AH	277	ALA	3.7
1	BX	276	ARG	3.7
1	Aa	337	GLU	3.7
1	CO	281	HIS	3.7
1	CZ	278	VAL	3.7
1	Bb	231	ASP	3.7
1	CE	257	PHE	3.7
1	CU	233	LEU	3.7
1	BO	232	SER	3.7
1	BI	239	LYS	3.7
1	Cc	288	ASN	3.7
1	CB	241	ILE	3.7
1	BB	301	TRP	3.7
1	CH	266	ASP	3.7
1	AM	180	PRO	3.7
1	Bb	275	ASP	3.7
1	CE	336	SER	3.7
1	AB	276	ARG	3.7
1	AI	217	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	CH	292	PRO	3.7
1	BG	278	VAL	3.7
1	AO	263	LEU	3.7
1	CO	270	GLY	3.7
1	Ab	233	LEU	3.7
1	BX	239	LYS	3.7
1	CH	219	THR	3.7
1	CY	282	LEU	3.7
1	AM	322	GLN	3.7
1	CT	282	LEU	3.7
1	AX	297	ARG	3.7
1	AI	232	SER	3.7
1	AM	264	SER	3.7
1	AB	281	HIS	3.7
1	CF	253	ASP	3.7
1	CN	263	LEU	3.7
1	AV	296	PHE	3.7
1	CE	221	PRO	3.7
1	CC	275	ASP	3.7
1	BH	319	GLN	3.7
1	BB	311	GLY	3.7
1	Bb	311	GLY	3.7
1	CE	318	GLU	3.7
1	CF	244	GLY	3.7
1	BY	288	ASN	3.7
1	CG	234	SER	3.6
1	CG	266	ASP	3.6
1	Ad	164	ARG	3.6
1	CH	256	VAL	3.6
1	Cc	284	LYS	3.6
1	CZ	279	TYR	3.6
1	AH	324	LEU	3.6
1	BU	278	VAL	3.6
1	AM	308	PHE	3.6
1	Ca	286	ALA	3.6
1	CI	281	HIS	3.6
1	CC	325	LEU	3.6
1	Ac	267	TYR	3.6
1	AE	336	SER	3.6
1	AE	322	GLN	3.6
1	BU	242	LEU	3.6
1	Ab	258	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	AG	303	ASN	3.6
1	Bb	290	GLY	3.6
1	Cc	273	ASP	3.6
1	Ab	263	LEU	3.6
1	Cb	283	LYS	3.6
1	BH	291	THR	3.6
1	CB	252	PRO	3.6
1	AU	228	LEU	3.6
1	CU	323	ILE	3.6
1	Ab	279	TYR	3.6
1	AM	332	THR	3.6
1	CC	283	LYS	3.6
1	CB	272	GLY	3.6
1	BP	229	TYR	3.6
1	CG	281	HIS	3.6
1	BC	273	ASP	3.6
1	BF	264	SER	3.6
1	AH	306	LYS	3.6
1	CB	230	ASN	3.6
1	CE	250	ILE	3.6
1	BM	260	ASP	3.6
1	CQ	317	ASP	3.6
1	CC	268	SER	3.6
1	CZ	239	LYS	3.5
1	BH	226	GLY	3.5
1	BM	322	GLN	3.5
1	CO	337	GLU	3.5
1	CM	317	ASP	3.5
1	BU	326	PRO	3.5
1	CU	285	PHE	3.5
1	CZ	255	ALA	3.5
1	CI	271	THR	3.5
1	Bb	237	ASP	3.5
1	CI	252	PRO	3.5
1	BZ	328	GLY	3.5
1	AB	310	ASP	3.5
1	CM	277	ALA	3.5
1	Cd	269	LEU	3.5
1	CH	267	TYR	3.5
1	CW	337	GLU	3.5
1	Cc	244	GLY	3.5
1	BD	52	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	CG	307	THR	3.5
1	Cc	245	SER	3.5
1	BG	248	LEU	3.5
1	BU	237	ASP	3.5
1	BI	298	TRP	3.5
1	Cb	298	TRP	3.5
1	CC	248	LEU	3.5
1	CS	307	THR	3.5
1	CP	337	GLU	3.5
1	Cb	270	GLY	3.5
1	BC	320	PRO	3.5
1	AM	266	ASP	3.5
1	BO	249	ASP	3.5
1	BO	265	ILE	3.5
1	Ab	280	TRP	3.5
1	Cc	227	SER	3.5
1	BB	267	TYR	3.5
1	AX	336	SER	3.5
1	CI	278	VAL	3.5
1	CF	276	ARG	3.5
1	CN	241	ILE	3.5
1	AU	333	ARG	3.5
1	Cc	231	ASP	3.5
1	BK	287	GLY	3.5
1	Cb	264	SER	3.5
1	AI	236	ASN	3.5
1	Cb	228	LEU	3.5
1	CP	318	GLU	3.5
1	BH	282	LEU	3.4
1	AC	312	VAL	3.4
1	CX	257	PHE	3.4
1	Cc	290	GLY	3.4
1	AF	324	LEU	3.4
1	CG	327	VAL	3.4
1	CN	223	MET	3.4
1	Ca	283	LYS	3.4
1	Ab	301	TRP	3.4
1	Ac	278	VAL	3.4
1	CH	321	ARG	3.4
1	CP	319	GLN	3.4
1	BG	232	SER	3.4
1	AZ	232	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	AS	337	GLU	3.4
1	CZ	242	LEU	3.4
1	BG	230	ASN	3.4
1	AX	236	ASN	3.4
1	CB	224	THR	3.4
1	BO	275	ASP	3.4
1	CU	336	SER	3.4
1	AD	236	ASN	3.4
1	BH	255	ALA	3.4
1	AP	271	THR	3.4
1	BO	263	LEU	3.4
1	CO	227	SER	3.4
1	Cc	272	GLY	3.4
1	CC	276	ARG	3.4
1	BC	289	ALA	3.4
1	CJ	282	LEU	3.4
1	BM	305	ASN	3.4
1	AX	324	LEU	3.4
1	Ab	297	ARG	3.4
1	CO	303	ASN	3.4
1	Bb	280	TRP	3.4
1	CQ	318	GLU	3.4
1	Bd	279	TYR	3.4
1	BE	239	LYS	3.4
1	BX	296	PHE	3.4
1	BY	321	ARG	3.4
1	AB	258	GLN	3.4
1	Ac	275	ASP	3.4
1	Bd	277	ALA	3.4
1	AC	276	ARG	3.4
1	BB	319	GLN	3.4
1	AD	325	LEU	3.4
1	Ab	240	SER	3.4
1	AF	322	GLN	3.4
1	CH	273	ASP	3.4
1	CB	280	TRP	3.4
1	CE	285	PHE	3.4
1	CG	256	VAL	3.4
1	Cc	332	THR	3.4
1	CC	260	ASP	3.4
1	AQ	322	GLN	3.4
1	BZ	265	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	AM	257	PHE	3.4
1	CF	233	LEU	3.3
1	AC	255	ALA	3.3
1	AM	318	GLU	3.3
1	CU	261	ARG	3.3
1	CT	293	ALA	3.3
1	AV	53	ASN	3.3
1	AG	325	LEU	3.3
1	BB	329	THR	3.3
1	AX	257	PHE	3.3
1	BH	263	LEU	3.3
1	AX	273	ASP	3.3
1	Ab	275	ASP	3.3
1	BI	238	PHE	3.3
1	AM	296	PHE	3.3
1	Ab	262	PRO	3.3
1	BN	298	TRP	3.3
1	AG	237	ASP	3.3
1	CI	266	ASP	3.3
1	AE	306	LYS	3.3
1	CU	279	TYR	3.3
1	CH	275	ASP	3.3
1	Cc	253	ASP	3.3
1	BC	270	GLY	3.3
1	BF	296	PHE	3.3
1	Cb	234	SER	3.3
1	AC	310	ASP	3.3
1	CZ	243	LEU	3.3
1	CH	246	THR	3.3
1	AU	264	SER	3.3
1	BU	227	SER	3.3
1	CJ	255	ALA	3.3
1	CI	270	GLY	3.3
1	BO	337	GLU	3.3
1	BM	227	SER	3.3
1	CM	218	THR	3.3
1	BR	318	GLU	3.3
1	CW	269	LEU	3.3
1	Ac	263	LEU	3.3
1	CB	310	ASP	3.3
1	CE	335	ASP	3.3
1	AG	332	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	CP	269	LEU	3.3
1	CU	222	ILE	3.3
1	CE	294	GLY	3.3
1	BI	282	LEU	3.3
1	CG	218	THR	3.3
1	AM	280	TRP	3.3
1	BO	280	TRP	3.3
1	CE	292	PRO	3.3
1	CU	229	TYR	3.3
1	BH	301	TRP	3.2
1	CA	228	LEU	3.2
1	BN	296	PHE	3.2
1	BG	291	THR	3.2
1	Bc	298	TRP	3.2
1	AH	266	ASP	3.2
1	CV	337	GLU	3.2
1	Cc	249	ASP	3.2
1	BF	276	ARG	3.2
1	BU	292	PRO	3.2
1	BO	253	ASP	3.2
1	CH	295	TRP	3.2
1	AZ	336	SER	3.2
1	CM	226	GLY	3.2
1	BX	238	PHE	3.2
1	Bb	322	GLN	3.2
1	CE	231	ASP	3.2
1	CG	315	TYR	3.2
1	CQ	240	SER	3.2
1	Bb	328	GLY	3.2
1	Bd	315	TYR	3.2
1	CU	322	GLN	3.2
1	Cb	308	PHE	3.2
1	BC	253	ASP	3.2
1	BM	282	LEU	3.2
1	CD	286	ALA	3.2
1	CM	217	GLU	3.2
1	BH	281	HIS	3.2
1	AM	333	ARG	3.2
1	CN	333	ARG	3.2
1	AP	269	LEU	3.2
1	AU	262	PRO	3.2
1	Cb	320	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	AM	263	LEU	3.2
1	BB	260	ASP	3.2
1	CE	290	GLY	3.2
1	CZ	318	GLU	3.2
1	Bc	312	VAL	3.2
1	Ca	265	ILE	3.2
1	Bb	227	SER	3.2
1	BO	283	LYS	3.2
1	Bb	309	THR	3.2
1	AM	217	GLU	3.2
1	CI	317	ASP	3.2
1	AS	268	SER	3.2
1	Ab	266	ASP	3.2
1	BY	315	TYR	3.2
1	AP	337	GLU	3.2
1	CB	277	ALA	3.2
1	AU	320	PRO	3.2
1	CA	248	LEU	3.2
1	BM	311	GLY	3.2
1	CM	291	THR	3.2
1	CS	257	PHE	3.2
1	CG	276	ARG	3.2
1	BP	262	PRO	3.2
1	CC	262	PRO	3.1
1	CY	249	ASP	3.1
1	BF	238	PHE	3.1
1	BM	309	THR	3.1
1	Cd	313	ALA	3.1
1	CS	232	SER	3.1
1	BF	278	VAL	3.1
1	AC	297	ARG	3.1
1	Bd	52	THR	3.1
1	BH	229	TYR	3.1
1	CF	262	PRO	3.1
1	AI	260	ASP	3.1
1	Aa	236	ASN	3.1
1	BZ	315	TYR	3.1
1	CF	272	GLY	3.1
1	CI	309	THR	3.1
1	BB	261	ARG	3.1
1	CH	303	ASN	3.1
1	BG	309	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	AH	301	TRP	3.1
1	CB	276	ARG	3.1
1	BZ	229	TYR	3.1
1	BU	52	THR	3.1
1	BA	315	TYR	3.1
1	AH	237	ASP	3.1
1	Bb	267	TYR	3.1
1	Bc	273	ASP	3.1
1	BB	236	ASN	3.1
1	AB	333	ARG	3.1
1	BS	298	TRP	3.1
1	AU	263	LEU	3.1
1	AH	257	PHE	3.1
1	CE	321	ARG	3.1
1	AQ	217	GLU	3.1
1	BP	263	LEU	3.1
1	CH	277	ALA	3.1
1	AD	164	ARG	3.1
1	CB	269	LEU	3.1
1	CC	282	LEU	3.1
1	AM	163	THR	3.1
1	BC	232	SER	3.1
1	CE	256	VAL	3.1
1	CI	264	SER	3.1
1	Ac	308	PHE	3.1
1	BC	324	LEU	3.1
1	AC	280	TRP	3.1
1	Ca	337	GLU	3.1
1	CB	273	ASP	3.1
1	CZ	249	ASP	3.1
1	BC	291	THR	3.1
1	AE	236	ASN	3.1
1	BH	236	ASN	3.1
1	BM	280	TRP	3.1
1	CO	237	ASP	3.1
1	BM	303	ASN	3.1
1	AB	227	SER	3.1
1	CF	250	ILE	3.1
1	BO	319	GLN	3.0
1	BP	315	TYR	3.0
1	CP	249	ASP	3.0
1	AU	260	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	CU	276	ARG	3.0
1	BC	247	PRO	3.0
1	AB	233	LEU	3.0
1	CU	274	VAL	3.0
1	BO	310	ASP	3.0
1	CU	283	LYS	3.0
1	CH	217	GLU	3.0
1	AJ	269	LEU	3.0
1	BO	282	LEU	3.0
1	BG	297	ARG	3.0
1	CO	276	ARG	3.0
1	CC	267	TYR	3.0
1	BA	325	LEU	3.0
1	BI	291	THR	3.0
1	AY	276	ARG	3.0
1	CM	336	SER	3.0
1	CN	294	GLY	3.0
1	Ca	263	LEU	3.0
1	AT	265	ILE	3.0
1	CM	242	LEU	3.0
1	CY	269	LEU	3.0
1	Bb	297	ARG	3.0
1	Ca	281	HIS	3.0
1	BC	229	TYR	3.0
1	AN	268	SER	3.0
1	CO	233	LEU	3.0
1	CV	257	PHE	3.0
1	AH	233	LEU	3.0
1	AH	336	SER	3.0
1	AV	235	THR	3.0
1	BS	239	LYS	3.0
1	CH	269	LEU	3.0
1	Cb	218	THR	3.0
1	AM	181	GLY	3.0
1	CN	307	THR	3.0
1	CZ	337	GLU	3.0
1	CS	288	ASN	3.0
1	BB	271	THR	3.0
1	CN	288	ASN	3.0
1	AV	298	TRP	3.0
1	CX	263	LEU	3.0
1	Bc	315	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	AB	239	LYS	3.0
1	CP	270	GLY	3.0
1	CU	330	VAL	3.0
1	BM	310	ASP	3.0
1	BE	309	THR	3.0
1	BH	292	PRO	3.0
1	BX	323	ILE	3.0
1	AF	264	SER	3.0
1	Aa	336	SER	3.0
1	BG	262	PRO	3.0
1	BB	282	LEU	3.0
1	BZ	228	LEU	3.0
1	CK	315	TYR	3.0
1	BO	302	ASP	3.0
1	AU	322	GLN	3.0
1	CH	230	ASN	2.9
1	BI	276	ARG	2.9
1	AC	322	GLN	2.9
1	CM	231	ASP	2.9
1	Cb	309	THR	2.9
1	BC	230	ASN	2.9
1	CS	289	ALA	2.9
1	CB	275	ASP	2.9
1	BM	52	THR	2.9
1	AP	278	VAL	2.9
1	BM	301	TRP	2.9
1	AM	303	ASN	2.9
1	BG	233	LEU	2.9
1	BP	278	VAL	2.9
1	AG	336	SER	2.9
1	AM	320	PRO	2.9
1	AO	268	SER	2.9
1	AQ	271	THR	2.9
1	CE	333	ARG	2.9
1	CD	257	PHE	2.9
1	CT	257	PHE	2.9
1	CC	316	SER	2.9
1	CF	245	SER	2.9
1	CI	232	SER	2.9
1	AY	266	ASP	2.9
1	CY	265	ILE	2.9
1	AG	324	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	AU	324	LEU	2.9
1	CI	245	SER	2.9
1	Bc	320	PRO	2.9
1	CG	254	GLY	2.9
1	BX	235	THR	2.9
1	AB	272	GLY	2.9
1	BM	302	ASP	2.9
1	CG	296	PHE	2.9
1	BM	231	ASP	2.9
1	CM	220	ALA	2.9
1	CM	300	ILE	2.9
1	CP	277	ALA	2.9
1	Ca	245	SER	2.9
1	Cc	255	ALA	2.9
1	BO	256	VAL	2.9
1	CP	231	ASP	2.9
1	AS	230	ASN	2.9
1	CB	319	GLN	2.9
1	CH	261	ARG	2.9
1	AO	297	ARG	2.9
1	BY	322	GLN	2.9
1	AI	243	LEU	2.9
1	CY	244	GLY	2.9
1	CU	223	MET	2.9
1	CH	315	TYR	2.9
1	CO	319	GLN	2.9
1	AM	304	PHE	2.9
1	CN	291	THR	2.9
1	BA	292	PRO	2.9
1	AO	306	LYS	2.9
1	CJ	264	SER	2.9
1	Aa	268	SER	2.9
1	BU	263	LEU	2.9
1	Ab	296	PHE	2.9
1	CO	218	THR	2.8
1	AM	331	CYS	2.8
1	Bb	312	VAL	2.8
1	CB	261	ARG	2.8
1	CA	302	ASP	2.8
1	CG	267	TYR	2.8
1	CU	319	GLN	2.8
1	CG	337	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	Cc	276	ARG	2.8
1	CU	284	LYS	2.8
1	AV	264	SER	2.8
1	CZ	282	LEU	2.8
1	BY	293	ALA	2.8
1	Cb	301	TRP	2.8
1	BG	314	TYR	2.8
1	BN	327	VAL	2.8
1	CM	260	ASP	2.8
1	BI	248	LEU	2.8
1	BC	327	VAL	2.8
1	AX	281	HIS	2.8
1	Cd	317	ASP	2.8
1	BB	309	THR	2.8
1	AB	265	ILE	2.8
1	AC	257	PHE	2.8
1	AU	265	ILE	2.8
1	AU	282	LEU	2.8
1	AY	265	ILE	2.8
1	BG	327	VAL	2.8
1	Ca	287	GLY	2.8
1	AH	258	GLN	2.8
1	CM	283	LYS	2.8
1	BU	260	ASP	2.8
1	Ad	318	GLU	2.8
1	AG	320	PRO	2.8
1	CH	278	VAL	2.8
1	BU	291	THR	2.8
1	Ab	267	TYR	2.8
1	Ad	276	ARG	2.8
1	CE	284	LYS	2.8
1	CI	242	LEU	2.8
1	AB	302	ASP	2.8
1	BI	278	VAL	2.8
1	CV	279	TYR	2.8
1	CT	286	ALA	2.8
1	CY	293	ALA	2.8
1	AG	257	PHE	2.8
1	AU	105	GLU	2.8
1	Bb	281	HIS	2.8
1	CX	321	ARG	2.8
1	CZ	317	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	AS	236	ASN	2.8
1	AI	331	CYS	2.8
1	AV	239	LYS	2.8
1	CJ	296	PHE	2.8
1	Cc	241	ILE	2.8
1	AG	315	TYR	2.8
1	BG	311	GLY	2.8
1	CC	303	ASN	2.8
1	BY	239	LYS	2.8
1	Ca	264	SER	2.8
1	CN	287	GLY	2.8
1	AC	266	ASP	2.8
1	BC	288	ASN	2.8
1	CI	250	ILE	2.8
1	BO	322	GLN	2.8
1	CU	303	ASN	2.8
1	Bd	267	TYR	2.8
1	CU	244	GLY	2.8
1	CF	310	ASP	2.8
1	BZ	263	LEU	2.8
1	AB	267	TYR	2.8
1	BM	235	THR	2.8
1	BH	320	PRO	2.8
1	AO	271	THR	2.8
1	CF	270	GLY	2.8
1	Cc	287	GLY	2.8
1	BH	275	ASP	2.8
1	AY	275	ASP	2.8
1	Cd	249	ASP	2.8
1	BE	264	SER	2.7
1	BE	281	HIS	2.7
1	CH	268	SER	2.7
1	CN	290	GLY	2.8
1	Cb	248	LEU	2.8
1	CO	323	ILE	2.7
1	AC	317	ASP	2.7
1	AU	273	ASP	2.7
1	AM	53	ASN	2.7
1	CO	336	SER	2.7
1	CC	226	GLY	2.7
1	BO	248	LEU	2.7
1	AV	238	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	BB	303	ASN	2.7
1	CC	312	VAL	2.7
1	CG	303	ASN	2.7
1	CG	309	THR	2.7
1	BM	256	VAL	2.7
1	BX	326	PRO	2.7
1	AV	162	TYR	2.7
1	AS	269	LEU	2.7
1	CC	266	ASP	2.7
1	CA	227	SER	2.7
1	CM	264	SER	2.7
1	Cc	247	PRO	2.7
1	AB	53	ASN	2.7
1	BO	267	TYR	2.7
1	BO	314	TYR	2.7
1	CR	290	GLY	2.7
1	CS	290	GLY	2.7
1	CZ	295	TRP	2.7
1	Ca	251	ALA	2.7
1	Cb	273	ASP	2.7
1	CR	268	SER	2.7
1	Bb	224	THR	2.7
1	BI	236	ASN	2.7
1	CH	280	TRP	2.7
1	AM	286	ALA	2.7
1	CO	321	ARG	2.7
1	CP	275	ASP	2.7
1	AZ	304	PHE	2.7
1	Cc	275	ASP	2.7
1	AH	297	ARG	2.7
1	BC	251	ALA	2.7
1	CH	320	PRO	2.7
1	CZ	334	VAL	2.7
1	Cb	295	TRP	2.7
1	CR	337	GLU	2.7
1	CB	242	LEU	2.7
1	AB	336	SER	2.7
1	CD	250	ILE	2.7
1	CV	289	ALA	2.7
1	Cb	272	GLY	2.7
1	BU	225	GLN	2.7
1	CU	318	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	CH	334	VAL	2.7
1	BR	270	GLY	2.7
1	CY	289	ALA	2.7
1	Bd	275	ASP	2.7
1	Ad	320	PRO	2.7
1	AD	105	GLU	2.7
1	AB	162	TYR	2.7
1	CF	315	TYR	2.7
1	CB	320	PRO	2.7
1	CF	317	ASP	2.7
1	Bc	249	ASP	2.7
1	CE	233	LEU	2.7
1	AN	228	LEU	2.7
1	CZ	230	ASN	2.7
1	BO	294	GLY	2.7
1	CA	262	PRO	2.7
1	AC	228	LEU	2.7
1	AH	218	THR	2.7
1	BY	276	ARG	2.7
1	CH	229	TYR	2.7
1	BZ	322	GLN	2.7
1	CU	220	ALA	2.7
1	CA	317	ASP	2.7
1	AC	227	SER	2.7
1	CE	315	TYR	2.7
1	BT	52	THR	2.7
1	BE	320	PRO	2.7
1	BO	261	ARG	2.7
1	CB	330	VAL	2.7
1	CF	275	ASP	2.7
1	BH	260	ASP	2.7
1	CJ	337	GLU	2.7
1	BP	275	ASP	2.7
1	CA	309	THR	2.7
1	CG	277	ALA	2.7
1	CM	270	GLY	2.7
1	Ca	241	ILE	2.7
1	CG	248	LEU	2.6
1	BO	303	ASN	2.7
1	CS	253	ASP	2.6
1	CU	245	SER	2.6
1	CD	255	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	BM	283	LYS	2.6
1	Ca	222	ILE	2.6
1	AB	277	ALA	2.6
1	BC	322	GLN	2.6
1	CM	319	GLN	2.6
1	BO	306	LYS	2.6
1	AF	325	LEU	2.6
1	BI	281	HIS	2.6
1	AP	270	GLY	2.6
1	BM	248	LEU	2.6
1	CB	306	LYS	2.6
1	Ca	279	TYR	2.6
1	AM	265	ILE	2.6
1	BM	257	PHE	2.6
1	CX	281	HIS	2.6
1	CY	263	LEU	2.6
1	AD	315	TYR	2.6
1	BP	279	TYR	2.6
1	AV	337	GLU	2.6
1	CY	253	ASP	2.6
1	CZ	272	GLY	2.6
1	BR	278	VAL	2.6
1	CZ	231	ASP	2.6
1	Cb	310	ASP	2.6
1	Ac	264	SER	2.6
1	CC	105	GLU	2.6
1	BE	298	TRP	2.6
1	AI	332	THR	2.6
1	CS	263	LEU	2.6
1	Cb	220	ALA	2.6
1	CN	337	GLU	2.6
1	BH	329	THR	2.6
1	Cb	261	ARG	2.6
1	CR	283	LYS	2.6
1	CZ	232	SER	2.6
1	BE	300	ILE	2.6
1	BG	282	LEU	2.6
1	Cc	233	LEU	2.6
1	BD	303	ASN	2.6
1	CG	308	PHE	2.6
1	CG	316	SER	2.6
1	CZ	238	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	CZ	228	LEU	2.6
1	Cc	266	ASP	2.6
1	BE	271	THR	2.6
1	BE	312	VAL	2.6
1	CE	218	THR	2.6
1	CU	246	THR	2.6
1	AX	306	LYS	2.6
1	AI	273	ASP	2.6
1	BO	300	ILE	2.6
1	Cd	319	GLN	2.6
1	AF	237	ASP	2.6
1	Bb	325	LEU	2.6
1	AB	275	ASP	2.6
1	CE	247	PRO	2.6
1	BM	281	HIS	2.6
1	AU	266	ASP	2.6
1	Bc	237	ASP	2.6
1	AG	271	THR	2.6
1	Cd	318	GLU	2.6
1	CC	280	TRP	2.6
1	AI	220	ALA	2.6
1	BM	242	LEU	2.6
1	CQ	265	ILE	2.6
1	CA	254	GLY	2.6
1	CN	277	ALA	2.6
1	AM	84	ILE	2.5
1	BM	275	ASP	2.5
1	AN	325	LEU	2.5
1	AB	220	ALA	2.5
1	AF	336	SER	2.5
1	CP	240	SER	2.5
1	CF	320	PRO	2.5
1	CI	332	THR	2.5
1	CS	332	THR	2.5
1	AH	296	PHE	2.5
1	AH	318	GLU	2.5
1	CB	266	ASP	2.5
1	CC	281	HIS	2.5
1	BH	297	ARG	2.5
1	CM	290	GLY	2.5
1	BN	276	ARG	2.5
1	Cb	275	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	Ca	296	PHE	2.5
1	BU	337	GLU	2.5
1	BM	326	PRO	2.5
1	CZ	303	ASN	2.5
1	AG	233	LEU	2.5
1	CI	246	THR	2.5
1	CI	300	ILE	2.5
1	CJ	265	ILE	2.5
1	Ca	330	VAL	2.5
1	AX	333	ARG	2.5
1	AB	335	ASP	2.5
1	BC	231	ASP	2.5
1	CI	305	ASN	2.5
1	Cb	271	THR	2.5
1	Ac	270	GLY	2.5
1	Ad	227	SER	2.5
1	CA	319	GLN	2.5
1	CA	323	ILE	2.5
1	BI	228	LEU	2.5
1	AN	324	LEU	2.5
1	CZ	322	GLN	2.5
1	BU	303	ASN	2.5
1	AY	317	ASP	2.5
1	CG	229	TYR	2.5
1	AM	307	THR	2.5
1	Ab	332	THR	2.5
1	AH	238	PHE	2.5
1	AU	257	PHE	2.5
1	CG	220	ALA	2.5
1	BV	277	ALA	2.5
1	AB	319	GLN	2.5
1	BF	327	VAL	2.5
1	AZ	303	ASN	2.5
1	Ca	297	ARG	2.5
1	BQ	296	PHE	2.5
1	CC	255	ALA	2.5
1	CC	277	ALA	2.5
1	CH	326	PRO	2.5
1	BM	330	VAL	2.5
1	CV	256	VAL	2.5
1	BF	321	ARG	2.5
1	BC	271	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	CA	334	VAL	2.5
1	CQ	252	PRO	2.5
1	BO	287	GLY	2.5
1	AB	208	SER	2.5
1	CE	252	PRO	2.5
1	CJ	274	VAL	2.5
1	BX	309	THR	2.5
1	CM	276	ARG	2.5
1	CO	234	SER	2.5
1	BD	296	PHE	2.5
1	AY	337	GLU	2.5
1	BU	233	LEU	2.5
1	CY	242	LEU	2.5
1	Aa	275	ASP	2.5
1	CE	240	SER	2.5
1	CE	264	SER	2.5
1	BG	316	SER	2.5
1	CN	252	PRO	2.5
1	AX	232	SER	2.5
1	CQ	56	HIS	2.5
1	CG	224	THR	2.5
1	AG	308	PHE	2.5
1	CI	217	GLU	2.5
1	BO	281	HIS	2.5
1	CY	255	ALA	2.5
1	AH	262	PRO	2.5
1	BG	269	LEU	2.5
1	BI	277	ALA	2.5
1	Bd	331	CYS	2.5
1	BF	320	PRO	2.4
1	CH	310	ASP	2.4
1	BT	296	PHE	2.5
1	AO	236	ASN	2.4
1	BP	264	SER	2.4
1	AU	236	ASN	2.4
1	Ad	229	TYR	2.4
1	BC	336	SER	2.4
1	CV	282	LEU	2.4
1	AB	279	TYR	2.4
1	CI	231	ASP	2.4
1	CW	315	TYR	2.4
1	BN	52	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	CO	231	ASP	2.4
1	AX	237	ASP	2.4
1	BC	334	VAL	2.4
1	CE	232	SER	2.4
1	CE	281	HIS	2.4
1	CD	262	PRO	2.4
1	Cb	278	VAL	2.4
1	CB	278	VAL	2.4
1	AP	322	GLN	2.4
1	Cc	323	ILE	2.4
1	Bc	291	THR	2.4
1	Ad	266	ASP	2.4
1	BA	236	ASN	2.4
1	CT	336	SER	2.4
1	BY	295	TRP	2.4
1	AB	256	VAL	2.4
1	CZ	281	HIS	2.4
1	CN	335	ASP	2.4
1	CQ	257	PHE	2.4
1	AL	227	SER	2.4
1	AM	268	SER	2.4
1	Ca	246	THR	2.4
1	BC	330	VAL	2.4
1	AD	324	LEU	2.4
1	BZ	325	LEU	2.4
1	Cc	298	TRP	2.4
1	CS	250	ILE	2.4
1	Cc	308	PHE	2.4
1	CC	314	TYR	2.4
1	BE	235	THR	2.4
1	AH	264	SER	2.4
1	BI	275	ASP	2.4
1	CN	240	SER	2.4
1	CP	278	VAL	2.4
1	CU	218	THR	2.4
1	Ab	232	SER	2.4
1	BI	327	VAL	2.4
1	Cd	256	VAL	2.4
1	BB	297	ARG	2.4
1	AB	105	GLU	2.4
1	AP	304	PHE	2.4
1	CW	257	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	BA	262	PRO	2.4
1	CD	274	VAL	2.4
1	BC	310	ASP	2.4
1	CI	229	TYR	2.4
1	BF	235	THR	2.4
1	AU	310	ASP	2.4
1	BU	276	ARG	2.4
1	BV	325	LEU	2.4
1	BB	280	TRP	2.4
1	CG	272	GLY	2.4
1	AH	236	ASN	2.4
1	CC	318	GLU	2.4
1	BO	323	ILE	2.4
1	CV	290	GLY	2.4
1	Bb	234	SER	2.4
1	CQ	255	ALA	2.4
1	CQ	332	THR	2.4
1	CU	277	ALA	2.4
1	CO	330	VAL	2.4
1	Bb	282	LEU	2.4
1	Bd	274	VAL	2.4
1	AI	322	GLN	2.4
1	CS	337	GLU	2.4
1	BY	275	ASP	2.4
1	CZ	248	LEU	2.4
1	AM	305	ASN	2.4
1	AS	265	ILE	2.4
1	BZ	323	ILE	2.4
1	Ab	247	PRO	2.4
1	CC	333	ARG	2.4
1	AJ	275	ASP	2.4
1	BB	279	TYR	2.4
1	CG	283	LYS	2.4
1	CZ	296	PHE	2.4
1	Ac	279	TYR	2.4
1	CM	301	TRP	2.4
1	AI	240	SER	2.4
1	CL	284	LYS	2.4
1	CO	335	ASP	2.4
1	AV	323	ILE	2.3
1	Bd	337	GLU	2.3
1	AG	278	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	AV	269	LEU	2.3
1	BY	233	LEU	2.3
1	Cb	325	LEU	2.3
1	BH	52	THR	2.3
1	BR	275	ASP	2.3
1	AZ	337	GLU	2.3
1	Ab	163	THR	2.3
1	AH	299	GLY	2.3
1	CN	292	PRO	2.3
1	CO	262	PRO	2.3
1	AF	288	ASN	2.3
1	AM	240	SER	2.3
1	BO	240	SER	2.3
1	CQ	316	SER	2.3
1	CY	266	ASP	2.3
1	CY	333	ARG	2.3
1	CI	287	GLY	2.3
1	BM	307	THR	2.3
1	CU	225	GLN	2.3
1	Ab	302	ASP	2.3
1	CM	234	SER	2.3
1	AO	321	ARG	2.3
1	AU	336	SER	2.3
1	CA	335	ASP	2.3
1	CB	258	GLN	2.3
1	AF	273	ASP	2.3
1	BG	237	ASP	2.3
1	BS	52	THR	2.3
1	AV	51	GLY	2.3
1	Bd	306	LYS	2.3
1	AB	263	LEU	2.3
1	CM	275	ASP	2.3
1	BM	323	ILE	2.3
1	BN	315	TYR	2.3
1	BC	248	LEU	2.3
1	BO	269	LEU	2.3
1	BG	319	GLN	2.3
1	AG	220	ALA	2.3
1	AE	206	ARG	2.3
1	BZ	242	LEU	2.3
1	AN	236	ASN	2.3
1	Ba	239	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	Ca	259	LEU	2.3
1	BO	299	GLY	2.3
1	CU	281	HIS	2.3
1	Ab	334	VAL	2.3
1	BF	277	ALA	2.3
1	CN	251	ALA	2.3
1	BO	285	PHE	2.3
1	BG	292	PRO	2.3
1	CT	333	ARG	2.3
1	AV	206	ARG	2.3
1	BC	318	GLU	2.3
1	CD	291	THR	2.3
1	CF	283	LYS	2.3
1	CG	278	VAL	2.3
1	CH	302	ASP	2.3
1	AI	317	ASP	2.3
1	CM	271	THR	2.3
1	CB	285	PHE	2.3
1	AJ	51	GLY	2.3
1	CZ	280	TRP	2.3
1	CF	288	ASN	2.3
1	BI	326	PRO	2.3
1	AI	235	THR	2.3
1	BK	275	ASP	2.3
1	AK	105	GLU	2.3
1	BN	239	LYS	2.3
1	CY	284	LYS	2.3
1	Ab	237	ASP	2.3
1	BC	257	PHE	2.3
1	CB	322	GLN	2.3
1	CC	265	ILE	2.3
1	CX	250	ILE	2.3
1	BE	296	PHE	2.3
1	AV	301	TRP	2.3
1	CV	281	HIS	2.3
1	BA	228	LEU	2.3
1	BB	242	LEU	2.3
1	BO	225	GLN	2.3
1	CV	284	LYS	2.3
1	BF	326	PRO	2.3
1	AX	227	SER	2.3
1	CJ	249	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	BN	223	MET	2.3
1	AM	229	TYR	2.3
1	BA	238	PHE	2.3
1	BP	296	PHE	2.3
1	AW	208	SER	2.3
1	BH	280	TRP	2.3
1	CZ	218	THR	2.3
1	CP	230	ASN	2.3
1	AB	243	LEU	2.3
1	CB	300	ILE	2.3
1	CM	278	VAL	2.3
1	CM	298	TRP	2.3
1	BN	282	LEU	2.3
1	AX	315	TYR	2.3
1	Cc	279	TYR	2.3
1	BO	252	PRO	2.2
1	CY	321	ARG	2.2
1	CA	336	SER	2.2
1	BK	240	SER	2.2
1	AC	230	ASN	2.2
1	CE	269	LEU	2.2
1	CH	297	ARG	2.2
1	CN	253	ASP	2.2
1	CU	297	ARG	2.2
1	BC	252	PRO	2.2
1	BX	292	PRO	2.2
1	Cc	328	GLY	2.2
1	CG	323	ILE	2.2
1	BZ	327	VAL	2.2
1	AM	310	ASP	2.2
1	AX	266	ASP	2.2
1	Bc	238	PHE	2.2
1	BM	254	GLY	2.2
1	BM	263	LEU	2.2
1	AP	336	SER	2.2
1	AP	279	TYR	2.2
1	Ca	308	PHE	2.2
1	CZ	226	GLY	2.2
1	CC	278	VAL	2.2
1	CI	267	TYR	2.2
1	AG	53	ASN	2.2
1	CY	303	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	BC	323	ILE	2.2
1	CC	242	LEU	2.2
1	CE	273	ASP	2.2
1	BU	248	LEU	2.2
1	BY	136	HIS	2.2
1	BF	234	SER	2.2
1	BA	263	LEU	2.2
1	AC	324	LEU	2.2
1	BW	323	ILE	2.2
1	Ca	270	GLY	2.2
1	BG	320	PRO	2.2
1	CH	276	ARG	2.2
1	BN	238	PHE	2.2
1	BA	229	TYR	2.2
1	AD	268	SER	2.2
1	AG	267	TYR	2.2
1	Ac	336	SER	2.2
1	AV	318	GLU	2.2
1	CS	327	VAL	2.2
1	Bd	263	LEU	2.2
1	AF	277	ALA	2.2
1	BM	230	ASN	2.2
1	CQ	286	ALA	2.2
1	AU	161	GLN	2.2
1	BO	332	THR	2.2
1	CE	297	ARG	2.2
1	CH	296	PHE	2.2
1	BM	284	LYS	2.2
1	CV	258	GLN	2.2
1	CY	257	PHE	2.2
1	BA	237	ASP	2.2
1	BJ	315	TYR	2.2
1	BK	135	ASP	2.2
1	AF	265	ILE	2.2
1	BU	330	VAL	2.2
1	Bd	318	GLU	2.2
1	AD	229	TYR	2.2
1	CB	260	ASP	2.2
1	Cb	224	THR	2.2
1	AB	294	GLY	2.2
1	AM	250	ILE	2.2
1	CR	284	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	CS	336	SER	2.2
1	CX	274	VAL	2.2
1	BY	331	CYS	2.2
1	AX	229	TYR	2.2
1	CB	332	THR	2.2
1	AF	263	LEU	2.2
1	BP	274	VAL	2.2
1	CC	297	ARG	2.2
1	BE	299	GLY	2.2
1	CP	34	ARG	2.2
1	Cb	337	GLU	2.2
1	BC	315	TYR	2.2
1	BF	267	TYR	2.2
1	BA	282	LEU	2.2
1	Ca	301	TRP	2.2
1	AC	265	ILE	2.2
1	CB	308	PHE	2.2
1	CC	273	ASP	2.2
1	AD	163	THR	2.2
1	CS	333	ARG	2.2
1	AT	164	ARG	2.2
1	CX	255	ALA	2.2
1	Ab	255	ALA	2.2
1	CW	278	VAL	2.2
1	Ca	65	GLN	2.2
1	CA	283	LYS	2.2
1	BO	251	ALA	2.2
1	Ad	134	ASN	2.2
1	CS	264	SER	2.2
1	CP	321	ARG	2.2
1	CS	256	VAL	2.2
1	AW	318	GLU	2.2
1	Bd	333	ARG	2.2
1	AC	281	HIS	2.2
1	BH	223	MET	2.2
1	AF	260	ASP	2.2
1	AG	228	LEU	2.2
1	AH	267	TYR	2.2
1	BV	278	VAL	2.2
1	CZ	240	SER	2.2
1	AB	298	TRP	2.2
1	AO	262	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	AO	270	GLY	2.1
1	AZ	296	PHE	2.2
1	BA	240	SER	2.1
1	AA	336	SER	2.1
1	BC	275	ASP	2.1
1	AH	275	ASP	2.1
1	BI	309	THR	2.1
1	BM	229	TYR	2.1
1	AM	166	LEU	2.1
1	BT	263	LEU	2.1
1	BU	281	HIS	2.1
1	Cd	230	ASN	2.1
1	Cd	268	SER	2.1
1	CN	285	PHE	2.1
1	BY	298	TRP	2.1
1	BD	277	ALA	2.1
1	BC	331	CYS	2.1
1	BS	296	PHE	2.1
1	AO	277	ALA	2.1
1	CC	256	VAL	2.1
1	CE	271	THR	2.1
1	CE	332	THR	2.1
1	CF	336	SER	2.1
1	BU	236	ASN	2.1
1	CX	232	SER	2.1
1	BI	225	GLN	2.1
1	CX	303	ASN	2.1
1	CB	267	TYR	2.1
1	CK	269	LEU	2.1
1	CP	242	LEU	2.1
1	Cc	252	PRO	2.1
1	CC	253	ASP	2.1
1	BG	273	ASP	2.1
1	CH	301	TRP	2.1
1	CW	268	SER	2.1
1	BY	234	SER	2.1
1	CY	310	ASP	2.1
1	Ca	310	ASP	2.1
1	AD	263	LEU	2.1
1	BM	223	MET	2.1
1	CN	242	LEU	2.1
1	CQ	293	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	BR	263	LEU	2.1
1	CV	255	ALA	2.1
1	Bd	284	LYS	2.1
1	Ab	238	PHE	2.1
1	CO	239	LYS	2.1
1	AX	280	TRP	2.1
1	BA	234	SER	2.1
1	BB	276	ARG	2.1
1	AB	317	ASP	2.1
1	AH	232	SER	2.1
1	BX	227	SER	2.1
1	Bb	254	GLY	2.1
1	Bd	208	SER	2.1
1	BF	228	LEU	2.1
1	AT	53	ASN	2.1
1	BE	314	TYR	2.1
1	Bd	265	ILE	2.1
1	AB	293	ALA	2.1
1	CF	222	ILE	2.1
1	AG	238	PHE	2.1
1	BH	302	ASP	2.1
1	BN	248	LEU	2.1
1	CZ	257	PHE	2.1
1	AK	164	ARG	2.1
1	AZ	297	ARG	2.1
1	CF	240	SER	2.1
1	BH	309	THR	2.1
1	CR	257	PHE	2.1
1	CW	249	ASP	2.1
1	CX	323	ILE	2.1
1	CY	331	CYS	2.1
1	Bb	236	ASN	2.1
1	CD	256	VAL	2.1
1	CF	327	VAL	2.1
1	CJ	34	ARG	2.1
1	Bd	276	ARG	2.1
1	BT	277	ALA	2.1
1	BC	234	SER	2.1
1	CN	336	SER	2.1
1	BX	229	TYR	2.1
1	BG	260	ASP	2.1
1	CY	270	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	Bb	230	ASN	2.1
1	AM	104	VAL	2.1
1	BR	257	PHE	2.1
1	BU	240	SER	2.1
1	BC	235	THR	2.1
1	BO	273	ASP	2.1
1	CZ	335	ASP	2.1
1	CF	298	TRP	2.1
1	CG	243	LEU	2.1
1	BX	263	LEU	2.1
1	Bb	248	LEU	2.1
1	AV	322	GLN	2.1
1	AM	208	SER	2.1
1	AY	316	SER	2.1
1	Ab	136	HIS	2.1
1	BC	337	GLU	2.1
1	CF	332	THR	2.1
1	CQ	263	LEU	2.1
1	CS	286	ALA	2.1
1	AD	206	ARG	2.1
1	CB	217	GLU	2.1
1	CI	247	PRO	2.1
1	CN	281	HIS	2.1
1	BH	231	ASP	2.1
1	BK	52	THR	2.1
1	BO	270	GLY	2.1
1	CO	294	GLY	2.1
1	CS	247	PRO	2.1
1	AV	282	LEU	2.1
1	AV	291	THR	2.1
1	AV	324	LEU	2.1
1	CK	249	ASP	2.1
1	BY	135	ASP	2.1
1	Ab	162	TYR	2.1
1	AF	276	ARG	2.1
1	Ba	328	GLY	2.1
1	Bd	256	VAL	2.1
1	Ca	285	PHE	2.1
1	AD	265	ILE	2.1
1	AM	237	ASP	2.1
1	BY	235	THR	2.1
1	AX	230	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	CG	325	LEU	2.1
1	BH	325	LEU	2.1
1	CZ	258	GLN	2.1
1	Bb	258	GLN	2.1
1	CI	244	GLY	2.1
1	BA	136	HIS	2.0
1	CF	268	SER	2.0
1	AM	252	PRO	2.0
1	Ad	264	SER	2.0
1	CM	233	LEU	2.0
1	CB	254	GLY	2.0
1	CF	328	GLY	2.0
1	CV	283	LYS	2.0
1	Ca	239	LYS	2.0
1	CE	56	HIS	2.0
1	BO	268	SER	2.0
1	AU	227	SER	2.0
1	CA	253	ASP	2.0
1	BB	231	ASP	2.0
1	CE	317	ASP	2.0
1	AF	317	ASP	2.0
1	CQ	256	VAL	2.0
1	BF	311	GLY	2.0
1	BX	319	GLN	2.0
1	AY	236	ASN	2.0
1	CH	220	ALA	2.0
1	CI	276	ARG	2.0
1	AM	262	PRO	2.0
1	AQ	97	ARG	2.0
1	Ab	300	ILE	2.0
1	BE	291	THR	2.0
1	CE	307	THR	2.0
1	BH	224	THR	2.0
1	BA	296	PHE	2.0
1	CH	248	LEU	2.0
1	AZ	266	ASP	2.0
1	Ac	282	LEU	2.0
1	BC	290	GLY	2.0
1	AH	272	GLY	2.0
1	BP	319	GLN	2.0
1	AD	262	PRO	2.0
1	BE	262	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	BO	293	ALA	2.0
1	CG	268	SER	2.0
1	BU	208	SER	2.0
1	CY	301	TRP	2.0
1	BM	243	LEU	2.0
1	CB	328	GLY	2.0
1	CG	219	THR	2.0
1	CG	311	GLY	2.0
1	AM	105	GLU	2.0
1	CM	302	ASP	2.0
1	CO	266	ASP	2.0
1	BQ	317	ASP	2.0
1	BU	332	THR	2.0
1	AU	217	GLU	2.0
1	Bc	309	THR	2.0
1	AM	142	GLN	2.0
1	CE	262	PRO	2.0
1	CO	221	PRO	2.0
1	Bd	301	TRP	2.0
1	Bb	228	LEU	2.0
1	AI	297	ARG	2.0
1	BJ	52	THR	2.0
1	BN	265	ILE	2.0
1	BO	231	ASP	2.0
1	AU	276	ARG	2.0
1	CY	307	THR	2.0
1	BJ	323	ILE	2.0
1	BM	332	THR	2.0
1	BM	335	ASP	2.0
1	BN	235	THR	2.0
1	CO	246	THR	2.0
1	AX	255	ALA	2.0
1	Cb	235	THR	2.0
1	Bc	296	PHE	2.0
1	AD	217	GLU	2.0
1	CS	217	GLU	2.0
1	BU	297	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	BO	402	1/1	0.91	0.14	52,52,52,52	0
2	CA	BI	401	1/1	0.94	0.15	43,43,43,43	0
2	CA	BQ	401	1/1	0.95	0.14	32,32,32,32	0
2	CA	BN	402	1/1	0.95	0.11	50,50,50,50	0
2	CA	Ba	402	1/1	0.95	0.10	42,42,42,42	0
2	CA	BY	402	1/1	0.95	0.12	33,33,33,33	0
2	CA	BD	401	1/1	0.95	0.14	36,36,36,36	0
2	CA	BV	402	1/1	0.95	0.12	57,57,57,57	0
2	CA	BV	401	1/1	0.96	0.12	36,36,36,36	0
2	CA	BM	401	1/1	0.96	0.08	39,39,39,39	0
2	CA	BQ	402	1/1	0.96	0.12	43,43,43,43	0
2	CA	BB	402	1/1	0.96	0.12	35,35,35,35	0
2	CA	AE	401	1/1	0.96	0.18	38,38,38,38	0
2	CA	BX	401	1/1	0.97	0.14	35,35,35,35	0
2	CA	BZ	401	1/1	0.97	0.14	36,36,36,36	0
2	CA	Bb	401	1/1	0.97	0.17	24,24,24,24	0
2	CA	BJ	401	1/1	0.97	0.16	27,27,27,27	0
2	CA	BB	401	1/1	0.97	0.12	26,26,26,26	0
2	CA	AU	401	1/1	0.97	0.13	30,30,30,30	0
2	CA	BP	401	1/1	0.98	0.17	33,33,33,33	0
2	CA	BR	401	1/1	0.98	0.13	26,26,26,26	0
2	CA	Ba	401	1/1	0.98	0.19	53,53,53,53	0
2	CA	BO	401	1/1	0.98	0.18	34,34,34,34	0
2	CA	AT	401	1/1	0.98	0.12	36,36,36,36	0
2	CA	BU	402	1/1	0.98	0.15	29,29,29,29	0
2	CA	Bc	401	1/1	0.98	0.15	29,29,29,29	0
2	CA	BC	402	1/1	0.98	0.14	38,38,38,38	0
2	CA	BI	402	1/1	0.98	0.13	54,54,54,54	0
2	CA	BP	402	1/1	0.98	0.13	35,35,35,35	0
2	CA	BU	401	1/1	0.98	0.13	32,32,32,32	0
2	CA	BG	401	1/1	0.98	0.11	38,38,38,38	0
2	CA	BC	401	1/1	0.98	0.16	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	BF	401	1/1	0.98	0.16	27,27,27,27	0
2	CA	BN	401	1/1	0.98	0.17	39,39,39,39	0
2	CA	Aa	401	1/1	0.98	0.15	45,45,45,45	0
2	CA	Ab	401	1/1	0.98	0.10	38,38,38,38	0
2	CA	AC	401	1/1	0.98	0.18	28,28,28,28	0
2	CA	BG	402	1/1	0.98	0.13	54,54,54,54	0
2	CA	BT	401	1/1	0.98	0.16	19,19,19,19	0
2	CA	BL	402	1/1	0.98	0.14	34,34,34,34	0
2	CA	BL	401	1/1	0.98	0.15	24,24,24,24	0
2	CA	AK	401	1/1	0.98	0.19	36,36,36,36	0
2	CA	BK	401	1/1	0.98	0.16	22,22,22,22	0
2	CA	BZ	402	1/1	0.98	0.10	57,57,57,57	0
2	CA	AH	401	1/1	0.98	0.13	34,34,34,34	0
2	CA	BH	402	1/1	0.98	0.11	41,41,41,41	0
2	CA	AI	401	1/1	0.98	0.17	43,43,43,43	0
2	CA	Bd	402	1/1	0.98	0.12	48,48,48,48	0
2	CA	BA	402	1/1	0.98	0.13	41,41,41,41	0
2	CA	AP	401	1/1	0.98	0.12	42,42,42,42	0
2	CA	Ac	401	1/1	0.99	0.15	48,48,48,48	0
2	CA	BS	401	1/1	0.99	0.20	23,23,23,23	0
2	CA	AY	401	1/1	0.99	0.14	30,30,30,30	0
2	CA	Ad	401	1/1	0.99	0.15	42,42,42,42	0
2	CA	AJ	401	1/1	0.99	0.14	38,38,38,38	0
2	CA	BS	402	1/1	0.99	0.15	36,36,36,36	0
2	CA	AD	401	1/1	0.99	0.14	36,36,36,36	0
2	CA	AW	401	1/1	0.99	0.17	39,39,39,39	0
2	CA	BW	401	1/1	0.99	0.15	25,25,25,25	0
2	CA	BW	402	1/1	0.99	0.16	42,42,42,42	0
2	CA	BF	402	1/1	0.99	0.14	36,36,36,36	0
2	CA	BD	402	1/1	0.99	0.14	44,44,44,44	0
2	CA	BX	402	1/1	0.99	0.12	31,31,31,31	0
2	CA	BM	402	1/1	0.99	0.12	33,33,33,33	0
2	CA	Bb	402	1/1	0.99	0.16	33,33,33,33	0
2	CA	AO	401	1/1	0.99	0.16	47,47,47,47	0
2	CA	AF	401	1/1	0.99	0.18	50,50,50,50	0
2	CA	BY	401	1/1	0.99	0.12	31,31,31,31	0
2	CA	AV	401	1/1	0.99	0.15	39,39,39,39	0
2	CA	AG	401	1/1	0.99	0.11	44,44,44,44	0
2	CA	BR	402	1/1	0.99	0.10	53,53,53,53	0
2	CA	BE	402	1/1	0.99	0.18	33,33,33,33	0
2	CA	AZ	401	1/1	0.99	0.18	36,36,36,36	0
2	CA	BK	402	1/1	0.99	0.12	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	AL	401	1/1	0.99	0.15	41,41,41,41	0
2	CA	AM	401	1/1	0.99	0.12	45,45,45,45	0
2	CA	AA	401	1/1	0.99	0.15	57,57,57,57	0
2	CA	AB	401	1/1	0.99	0.14	40,40,40,40	0
2	CA	BA	401	1/1	0.99	0.16	35,35,35,35	0
2	CA	AQ	401	1/1	0.99	0.11	57,57,57,57	0
2	CA	Bd	401	1/1	0.99	0.13	37,37,37,37	0
2	CA	BT	402	1/1	0.99	0.13	42,42,42,42	0
2	CA	AX	401	1/1	0.99	0.13	38,38,38,38	0
2	CA	BH	401	1/1	0.99	0.12	34,34,34,34	0
2	CA	AN	401	1/1	0.99	0.17	42,42,42,42	0
2	CA	AS	401	1/1	0.99	0.17	27,27,27,27	0
2	CA	BE	401	1/1	0.99	0.15	35,35,35,35	0
2	CA	AR	401	1/1	0.99	0.14	40,40,40,40	0
2	CA	BJ	402	1/1	0.99	0.12	29,29,29,29	0
2	CA	Bc	402	1/1	1.00	0.16	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.