



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:11 am BST

PDB ID : 4V98
Title : The 8S snRNP Assembly Intermediate
Authors : Grimm, C.; Pelz, J.P.; Schindelin, H.; Diederichs, K.; Kuper, J.; Kisker, C.
Deposited on : 2012-05-15
Resolution : 3.10 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

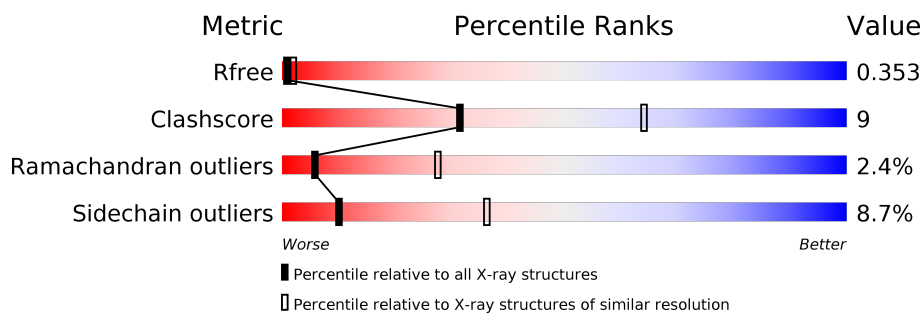
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	AA	119	
1	AI	119	
1	AQ	119	
1	AY	119	
1	Ag	119	
1	Ao	119	
1	Aw	119	


























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Mol	Chain	Length	Quality of chain
1	BA	119	
1	BI	119	
1	BQ	119	
1	BY	119	
1	Bg	119	
1	Bo	119	
1	Bw	119	
1	CA	119	
1	CI	119	
1	CQ	119	
1	CY	119	
1	Cg	119	
1	Co	119	
2	AB	118	
2	AJ	118	
2	AR	118	
2	AZ	118	
2	Ah	118	
2	Ap	118	
2	Ax	118	
2	BB	118	
2	BJ	118	
2	BR	118	
2	BZ	118	
2	Bh	118	















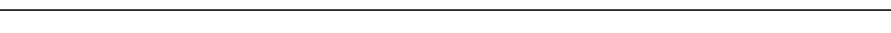




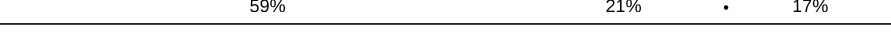





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Mol	Chain	Length	Quality of chain
2	Bp	118	
2	Bx	118	
2	CB	118	
2	CJ	118	
2	CR	118	
2	CZ	118	
2	Ch	118	
2	Cp	118	
3	AC	92	
3	AK	92	
3	AS	92	
3	Aa	92	
3	Ai	92	
3	Aq	92	
3	Ay	92	
3	BC	92	
3	BK	92	
3	BS	92	
3	Ba	92	
3	Bi	92	
3	Bq	92	
3	By	92	
3	CC	92	
3	CK	92	
3	CS	92	

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Mol	Chain	Length	Quality of chain
3	Ca	92	
3	Ci	92	
3	Cq	92	
4	AD	86	
4	AL	86	
4	AT	86	
4	Ab	86	
4	Aj	86	
4	Ar	86	
4	Az	86	
4	BD	86	
4	BL	86	
4	BT	86	
4	Bb	86	
4	Bj	86	
4	Br	86	
4	Bz	86	
4	CD	86	
4	CL	86	
4	CT	86	
4	Cb	86	
4	Cj	86	
4	Cr	86	
5	A1	124	
5	AE	124	


























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Mol	Chain	Length	Quality of chain
5	AM	124	9% . . 86%
5	AU	124	10% . . 86%
5	Ac	124	11% . . 86%
5	Ak	124	12% . . 86%
5	As	124	11% . . 86%
5	B1	124	10% . . 86%
5	BE	124	9% . . 86%
5	BM	124	9% . . 86%
5	BU	124	10% . . 86%
5	Bc	124	11% . . 86%
5	Bk	124	10% . 86%
5	Bs	124	11% . 86%
5	CE	124	10% . . 86%
5	CM	124	10% . . 86%
5	CU	124	10% . 86%
5	Cc	124	12% . . 86%
5	Ck	124	10% . 86%
5	Cs	124	9% . . 86%
6	A2	247	56% 26% . . 13%
6	AF	247	51% 30% 5% . 13%
6	AN	247	51% 30% 5% . 13%
6	AV	247	52% 29% 5% . 13%
6	Ad	247	74% 12% . 13%
6	Al	247	73% 13% . 13%
6	At	247	71% 15% . 13%


























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Mol	Chain	Length	Quality of chain
6	B2	247	
6	BF	247	
6	BN	247	
6	BV	247	
6	Bd	247	
6	Bl	247	
6	Bt	247	
6	CF	247	
6	CN	247	
6	CV	247	
6	Cd	247	
6	Cl	247	
6	Ct	247	
7	A3	186	
7	AG	186	
7	AO	186	
7	AW	186	
7	Ae	186	
7	Am	186	
7	Au	186	
7	B3	186	
7	BG	186	
7	BO	186	
7	BW	186	
7	Be	186	

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Mol	Chain	Length	Quality of chain
7	Bm	186	
7	Bu	186	
7	CG	186	
7	CO	186	
7	CW	186	
7	Ce	186	
7	Cm	186	
7	Cu	186	
8	A4	76	
8	AH	76	
8	AP	76	
8	AX	76	
8	Af	76	
8	An	76	
8	Av	76	
8	B4	76	
8	BH	76	
8	BP	76	
8	BX	76	
8	Bf	76	
8	Bn	76	
8	Bv	76	
8	CH	76	
8	CP	76	
8	CX	76	

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Mol	Chain	Length	Quality of chain
8	Cf	76	<div><div></div><div>88%</div><div></div><div>•</div><div>8%</div></div>
8	Cn	76	<div><div></div><div>88%</div><div></div><div>•</div><div>8%</div></div>
8	Cv	76	<div><div></div><div>88%</div><div></div><div>•</div><div>8%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 121990 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 Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AI	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	AA	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	AQ	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	AY	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Ag	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Ao	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Aw	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	BA	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	BI	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	BQ	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	BY	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Bg	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Bo	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Bw	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	CA	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	CI	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CQ	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	CY	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Cg	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			
1	Co	82	Total	C	N	O	S	0	0	0
			648	413	113	119	3			

- Molecule 2 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AJ	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	AB	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	AR	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	AZ	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Ah	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Ap	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Ax	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	BB	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	BJ	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	BR	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	BZ	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Bh	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Bp	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Bx	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	CB	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CJ	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	CR	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	CZ	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Ch	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			
2	Cp	100	Total	C	N	O	S	0	0	0
			807	505	146	150	6			

- Molecule 3 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AK	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	AC	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	AS	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Aa	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Ai	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Aq	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Ay	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	BC	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	BK	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	BS	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Ba	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Bi	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Bq	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	By	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CC	77	Total 638	C 405	N 113	O 115	S 5	0	0	0
3	CK	77	Total 638	C 405	N 113	O 115	S 5	0	0	0
3	CS	77	Total 638	C 405	N 113	O 115	S 5	0	0	0
3	Ca	77	Total 638	C 405	N 113	O 115	S 5	0	0	0
3	Ci	77	Total 638	C 405	N 113	O 115	S 5	0	0	0
3	Cq	77	Total 638	C 405	N 113	O 115	S 5	0	0	0

- Molecule 4 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AL	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	AD	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	AT	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Ab	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Aj	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Ar	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Az	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	BD	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	BL	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	BT	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Bb	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Bj	71	Total 556	C 358	N 92	O 101	S 5	0	0	0
4	Br	71	Total 556	C 358	N 92	O 101	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Bz	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			
4	CD	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			
4	CL	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			
4	CT	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			
4	Cb	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			
4	Cj	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			
4	Cr	71	Total	C	N	O	S	0	0	0
			556	358	92	101	5			

- Molecule 5 is a protein called LD23602p.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AM	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	AE	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	AU	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	Ac	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	Ak	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	As	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	A1	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	BE	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	BM	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	BU	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	Bc	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	Bk	17	Total	C	N	O	0	0	0
			133	85	19	29			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Bs	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	B1	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	CE	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	CM	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	CU	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	Cc	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	Ck	17	Total	C	N	O	0	0	0
			133	85	19	29			
5	Cs	17	Total	C	N	O	0	0	0
			133	85	19	29			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AM	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
AM	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
AE	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
AE	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
AU	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
AU	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
Ac	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
Ac	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
Ak	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
Ak	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
As	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
As	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
A1	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
A1	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
BE	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
BE	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
BM	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
BM	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
BU	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
BU	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
Bc	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
Bc	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
Bk	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74

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Chain	Residue	Modelled	Actual	Comment	Reference
Bk	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
Bs	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
Bs	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
B1	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
B1	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
CE	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
CE	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
CM	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
CM	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
CU	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
CU	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
Cc	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
Cc	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
Ck	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
Ck	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74
Cs	6991	GLY	-	EXPRESSION TAG	UNP Q9VV74
Cs	6992	ALA	-	EXPRESSION TAG	UNP Q9VV74

- Molecule 6 is a protein called CG10419.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AN	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	AF	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	AV	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Ad	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Al	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	At	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	A2	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	BF	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	BN	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	BV	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Bd	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B1	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Bt	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	B2	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	CF	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	CN	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	CV	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Cd	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Cl	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			
6	Ct	216	Total	C	N	O	S	0	0	0
			1787	1138	309	331	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	7969	GLY	-	EXPRESSION TAG	UNP Q9VVDX0
AN	7970	ALA	-	EXPRESSION TAG	UNP Q9VVDX0
AF	7969	GLY	-	EXPRESSION TAG	UNP Q9VVDX0
AF	7970	ALA	-	EXPRESSION TAG	UNP Q9VVDX0
AV	7969	GLY	-	EXPRESSION TAG	UNP Q9VVDX0
AV	7970	ALA	-	EXPRESSION TAG	UNP Q9VVDX0
Ad	7969	GLY	-	EXPRESSION TAG	UNP Q9VVDX0
Ad	7970	ALA	-	EXPRESSION TAG	UNP Q9VVDX0
Al	7969	GLY	-	EXPRESSION TAG	UNP Q9VVDX0
Al	7970	ALA	-	EXPRESSION TAG	UNP Q9VVDX0
At	7969	GLY	-	EXPRESSION TAG	UNP Q9VVDX0
At	7970	ALA	-	EXPRESSION TAG	UNP Q9VVDX0
A2	7969	GLY	-	EXPRESSION TAG	UNP Q9VVDX0
A2	7970	ALA	-	EXPRESSION TAG	UNP Q9VVDX0
BF	7969	GLY	-	EXPRESSION TAG	UNP Q9VVDX0
BF	7970	ALA	-	EXPRESSION TAG	UNP Q9VVDX0
BN	7969	GLY	-	EXPRESSION TAG	UNP Q9VVDX0
BN	7970	ALA	-	EXPRESSION TAG	UNP Q9VVDX0
BV	7969	GLY	-	EXPRESSION TAG	UNP Q9VVDX0
BV	7970	ALA	-	EXPRESSION TAG	UNP Q9VVDX0
Bd	7969	GLY	-	EXPRESSION TAG	UNP Q9VVDX0

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Chain	Residue	Modelled	Actual	Comment	Reference
Bd	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
Bl	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
Bl	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
Bt	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
Bt	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
B2	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
B2	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
CF	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
CF	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
CN	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
CN	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
CV	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
CV	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
Cd	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
Cd	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
Cl	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
Cl	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
Ct	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
Ct	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0

- Molecule 7 is a protein called Icln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AO	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	AG	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	AW	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Ae	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Am	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Au	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	A3	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	BG	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	BO	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	BW	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Be	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Bm	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Bu	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	B3	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	CG	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	CO	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	CW	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Ce	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Cm	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			
7	Cu	127	Total	C	N	O	S	0	0	0
			984	626	161	188	9			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AO	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AO	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AO	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AO	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AO	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AG	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AG	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AG	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AG	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AG	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AG	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AW	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AW	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AW	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AW	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AW	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
AW	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Ae	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1

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Chain	Residue	Modelled	Actual	Comment	Reference
Ae	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Ae	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Ae	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Ae	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Ae	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Am	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Am	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Am	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Am	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Am	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Am	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Au	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Au	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Au	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Au	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Au	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Au	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
A3	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
A3	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
A3	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
A3	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
A3	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
A3	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BG	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BG	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BG	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BG	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BG	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BG	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BO	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BO	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BO	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BO	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BO	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BO	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BW	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BW	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BW	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BW	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BW	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
BW	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Be	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1

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Chain	Residue	Modelled	Actual	Comment	Reference
Be	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Be	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Be	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Be	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Be	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Bm	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Bm	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Bm	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Bm	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Bm	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Bm	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Bu	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Bu	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Bu	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Bu	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Bu	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Bu	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
B3	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
B3	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
B3	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
B3	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
B3	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
B3	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CG	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CG	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CG	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CG	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CG	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CG	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CO	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CO	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CO	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CO	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CO	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CO	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CW	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CW	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CW	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CW	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CW	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
CW	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Ce	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1

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Chain	Residue	Modelled	Actual	Comment	Reference
Ce	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Ce	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Ce	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Ce	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Ce	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Cm	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Cm	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Cm	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Cm	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Cm	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Cm	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Cu	6180	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Cu	6181	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Cu	6182	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Cu	6183	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Cu	6184	HIS	-	EXPRESSION TAG	UNP Q9U3W1
Cu	6185	HIS	-	EXPRESSION TAG	UNP Q9U3W1

- Molecule 8 is a protein called Small nuclear ribonucleoprotein G.

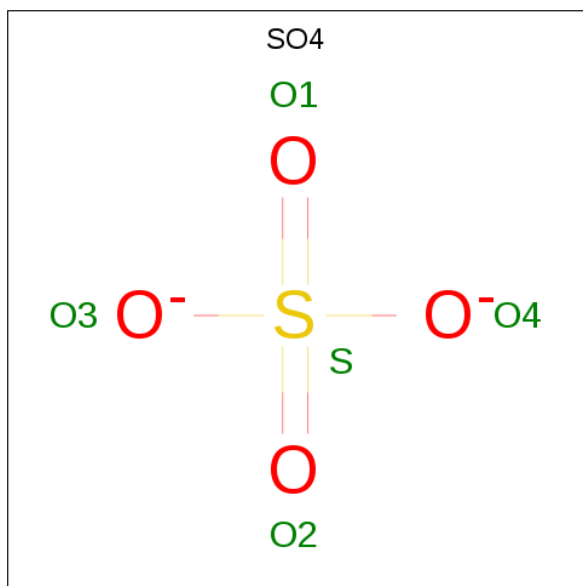
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AP	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	AH	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	AX	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Af	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	An	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Av	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	A4	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	BH	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	BP	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	BX	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Bf	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	Bn	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Bv	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	B4	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	CH	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	CP	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	CX	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Cf	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Cn	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Cv	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	Ad	1	Total	O	S	0	0
			5	4	1		
9	At	1	Total	O	S	0	0
			5	4	1		

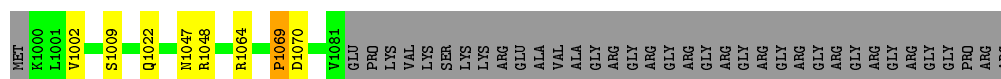
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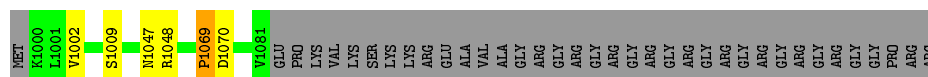
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A2	1	Total	O	S	0	0
			5	4	1		
9	BF	1	Total	O	S	0	0
			5	4	1		
9	BV	1	Total	O	S	0	0
			5	4	1		
9	Bd	1	Total	O	S	0	0
			5	4	1		
9	Bt	1	Total	O	S	0	0
			5	4	1		
9	B2	1	Total	O	S	0	0
			5	4	1		
9	CF	1	Total	O	S	0	0
			5	4	1		
9	Cl	1	Total	O	S	0	0
			5	4	1		

- Molecule 1: Small nuclear ribonucleoprotein Sm D1

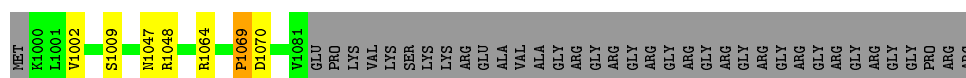




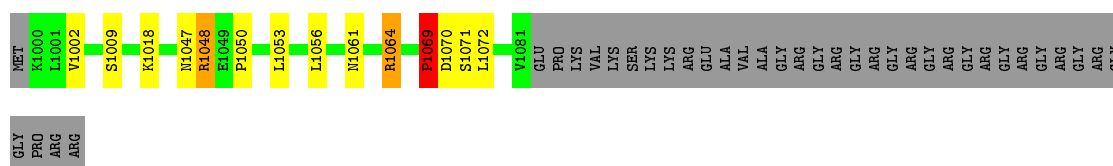
- Molecule 1: Small nuclear ribonucleoprotein Sm D1



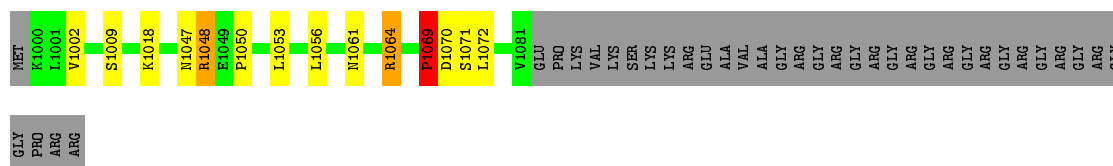
- Molecule 1: Small nuclear ribonucleoprotein Sm D1



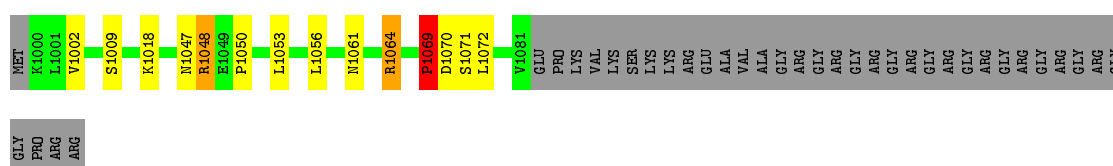
- Molecule 1: Small nuclear ribonucleoprotein Sm D1



- Molecule 1: Small nuclear ribonucleoprotein Sm D1



- Molecule 1: Small nuclear ribonucleoprotein Sm D1



- Molecule 1: Small nuclear ribonucleoprotein Sm D1



MT	SR	LEU	LEU	ASN	LVS	P2000	T2019	S2023	Q2027	Q2034	N2038	G2039	R2040	N2041	N2042	R2043	R2048	V2049	R2054	L2060	E2065	M2066	V2067	P2070	PRQ	LVS	GLY	LVS	GLY	LVS	LVS	LVS	SR	LVS	P2071	K2074	R2075	Z2076	Y2077	T2089	V2090	Z2091	L2092	T2097
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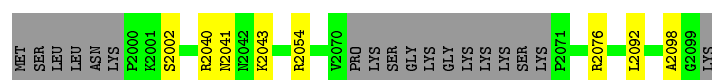
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain AZ: 69% 15% 15%



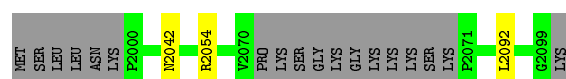
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Ah: 78% 7% 15%



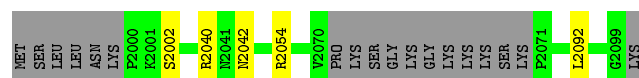
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Ap: 82% 15%



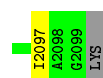
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Ax: 81% 15%



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain BB: 65% 18% 15%



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

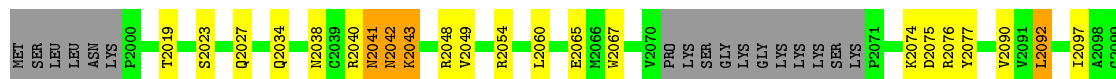
Chain BJ: 65% 17% 15%





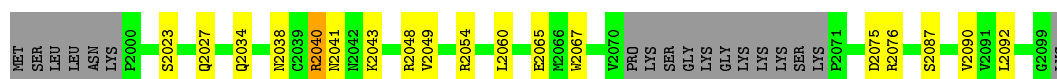
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain BR: 66% 15% 15%



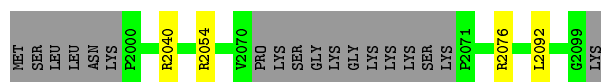
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain BZ: 69% 14% 15%



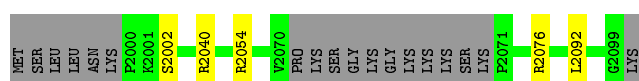
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Bh: 81% 15%



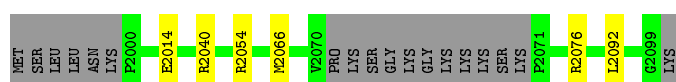
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Bp: 81% 15%



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Bx: 80% 5% 15%



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

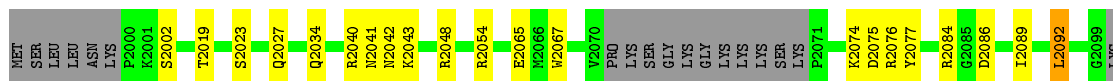
Chain CB: 68% 14% 15%



LYS

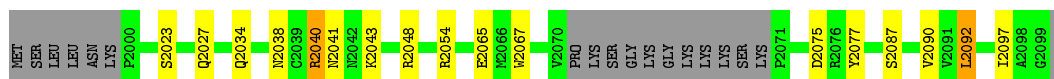
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain CJ: 



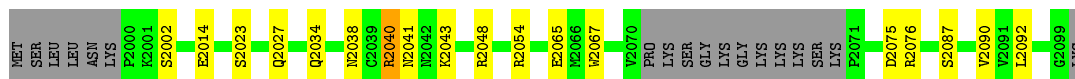
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain CR: 




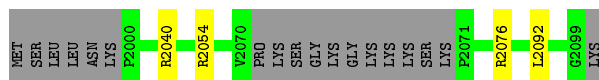
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain CZ: 




- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Ch: 



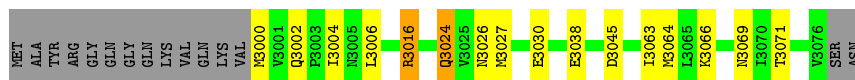
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Cp: 



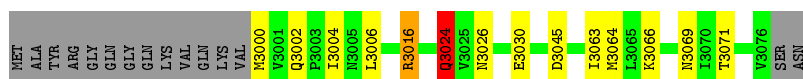
- Molecule 3: Small nuclear ribonucleoprotein E

Chain AK: 

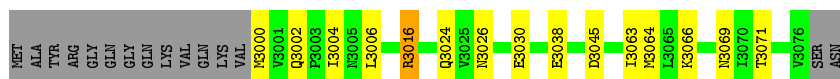


- Molecule 3: Small nuclear ribonucleoprotein E

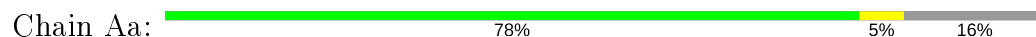
Chain AC: 



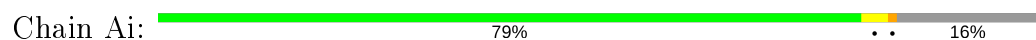
- Molecule 3: Small nuclear ribonucleoprotein E



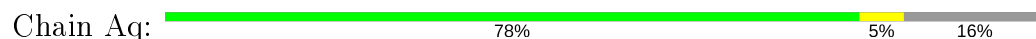
- Molecule 3: Small nuclear ribonucleoprotein E



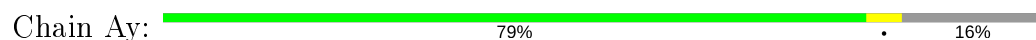
- Molecule 3: Small nuclear ribonucleoprotein E



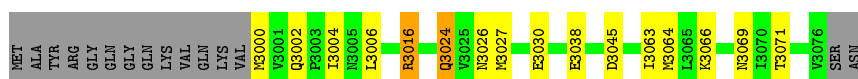
- Molecule 3: Small nuclear ribonucleoprotein E



- Molecule 3: Small nuclear ribonucleoprotein E



- Molecule 3: Small nuclear ribonucleoprotein E



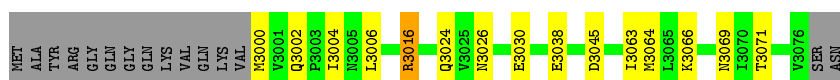
- Molecule 3: Small nuclear ribonucleoprotein E

Chain BK:  66% 15% 16%




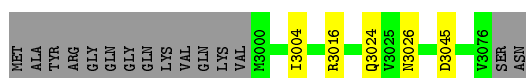
- Molecule 3: Small nuclear ribonucleoprotein E

Chain BS:  67% 15% 16%




- Molecule 3: Small nuclear ribonucleoprotein E

Chain Ba:  78% 5% 16%




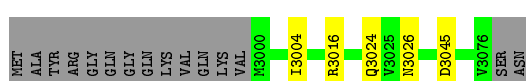
- Molecule 3: Small nuclear ribonucleoprotein E

Chain Bi:  78% 5% 16%




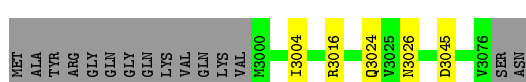
- Molecule 3: Small nuclear ribonucleoprotein E

Chain Bq:  78% 5% 16%



- Molecule 3: Small nuclear ribonucleoprotein E

Chain By:  78% 5% 16%



- Molecule 3: Small nuclear ribonucleoprotein E

Chain CC:  67% 14% 16%



- Molecule 3: Small nuclear ribonucleoprotein E

Chain CK:  67% 14% 16%




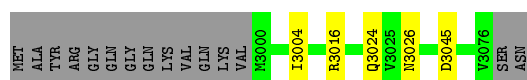
- Molecule 3: Small nuclear ribonucleoprotein E

Chain CS:  67% 14% 16%




- Molecule 3: Small nuclear ribonucleoprotein E

Chain Ca:  78% 5% 16%




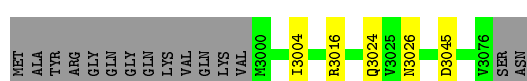
- Molecule 3: Small nuclear ribonucleoprotein E

Chain Ci:  78% 5% 16%



- Molecule 3: Small nuclear ribonucleoprotein E

Chain Cq:  78% 5% 16%



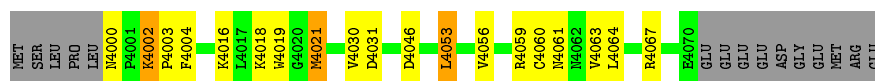
- Molecule 4: Small nuclear ribonucleoprotein F

Chain AL:  59% 21% 17%



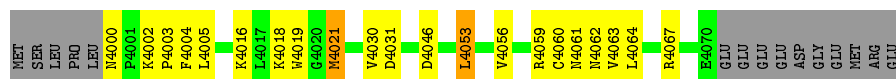
- Molecule 4: Small nuclear ribonucleoprotein F

Chain AD:  60% 19% 17%




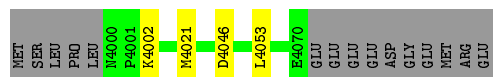
- Molecule 4: Small nuclear ribonucleoprotein F

Chain AT:  58% 22% 17%




- Molecule 4: Small nuclear ribonucleoprotein F

Chain Ab:  78% 5% 17%




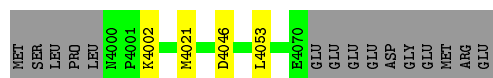
- Molecule 4: Small nuclear ribonucleoprotein F

Chain Aj:  78% 5% 17%




- Molecule 4: Small nuclear ribonucleoprotein F

Chain Ar:  78% 5% 17%



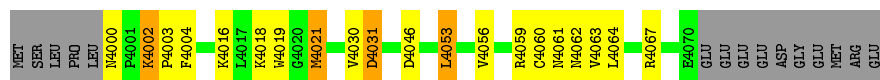
- Molecule 4: Small nuclear ribonucleoprotein F

Chain Az:  79% 1% 17%



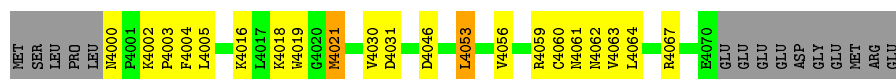
- Molecule 4: Small nuclear ribonucleoprotein F

Chain BD:  59% 19% 5% 17%



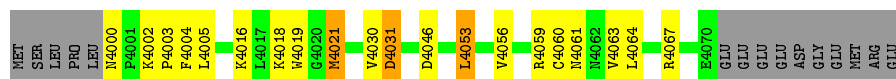
- Molecule 4: Small nuclear ribonucleoprotein F

Chain BL:  58% 22% 17%




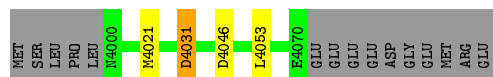
- Molecule 4: Small nuclear ribonucleoprotein F

Chain BT:  59% 20% 17%




- Molecule 4: Small nuclear ribonucleoprotein F

Chain Bb:  78% 17%




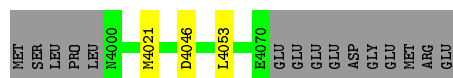
- Molecule 4: Small nuclear ribonucleoprotein F

Chain Bj:  77% 6% 17%




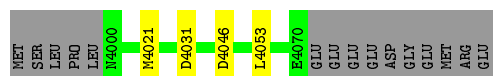
- Molecule 4: Small nuclear ribonucleoprotein F

Chain Br:  79% 17%



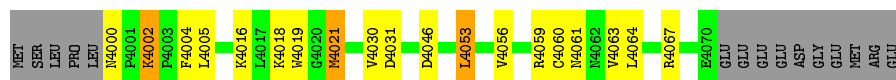
- Molecule 4: Small nuclear ribonucleoprotein F

Chain Bz:  78% 5% 17%



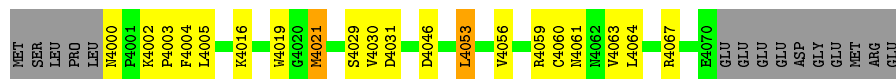
- Molecule 4: Small nuclear ribonucleoprotein F

Chain CD:  60% 19% 17%



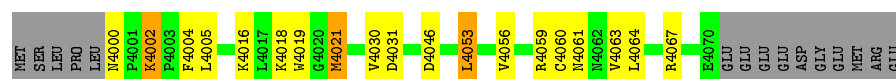
- Molecule 4: Small nuclear ribonucleoprotein F

Chain CL:  59% 21% 17%

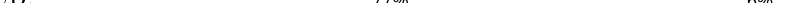


- Molecule 4: Small nuclear ribonucleoprotein F

Chain CT: 

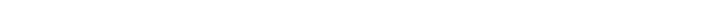


- Molecule 4: Small nuclear ribonucleoprotein F

Chain Cb:  77% 6% 17%

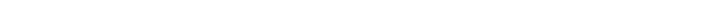


- Molecule 4: Small nuclear ribonucleoprotein F

Chain Cj:  78% 5% 17%



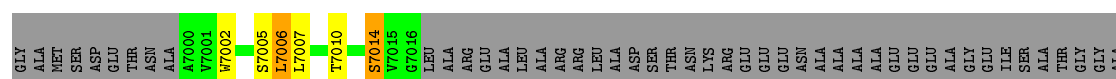
- Molecule 4: Small nuclear ribonucleoprotein F

Chain Cr:  78% 5% 17%



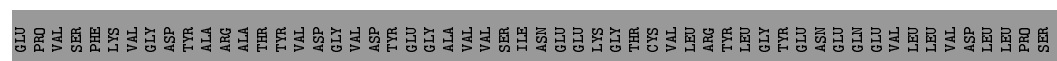
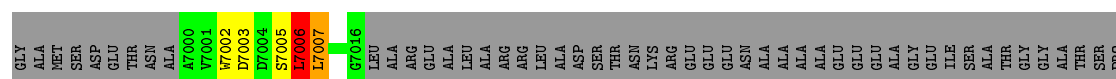
- Molecule 5: LD23602p

Chain AM: 9% . . 86%



- Molecule 5: LD23602p

Chain AE: 10% ... 86%



- Molecule 5: LD23602p

Chain AU:  10% 22% 86%

GLY	ALA	THR	ASP	THR	ASN	ALA	A7000	A7001	A7002	A7003	A7004	A7005	A7006	A7009	S7014	V7015	G7016	LEU	ALA	ARG	GLU	ALA	ALA	LEU	VAL	ALA	ALA	VAL	ARG	ILE	ASN	LEU	LEU	ASP	GLY	THR	ASN	LYS	VAL	ARG	GLU	GLU	TYR	ASN	ALA	ALA	ALA	ALA	GLN	GLU	GLU	ALA	VAL	LEU	LEU	VAL	ILE	ASP	SER	LEU	THR	GLY	GLY	ALA
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THR	SER	PRO	GLU	SER	PRO	VAL	SER	PHE	LYS	VAL	GLY	ASP	TYR	ALA	ARG	ALA	THR	TYR	VAL	ASP	GLY	VAL	ASP	LEU	TYR	ALA	GLU	GLY	VAL	VAL	SER	ARG	ILE	ASN	GLU	LYS	VAL	ARG	GLU	TYR	LEU	ASN	GLY	TYR	ALA	ALA	ALA	GLN	GLU	VAL	VAL	VAL	ILE	VAL	LEU	LEU	ASP	ALA	THR	LEU	PRO	GLY	SER	TRP
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• Molecule 5: LD23602p

Chain BM:  9% 86%

GLY	ALA	THR	ASP	THR	ASN	ALA	A7000	A7001	A7002	S7005	L7006	L7007	Y7011	S7014	V7015	G7016	LEU	ALA	ARG	GLU	ALA	LEU	VAL	VAL	ALA	VAL	ARG	ARG	ILE	ASN	GLU	LYS	VAL	ARG	GLU	TYR	LEU	ASN	GLY	TYR	ALA	ALA	ALA	GLN	GLU	GLU	ALA	VAL	VAL	ILE	GLY	GLU	SER	ALA	THR	GLY	SER	GLY	ALA
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THR	SER	PRO	GLU	SER	PRO	VAL	SER	PHE	LYS	VAL	GLY	ASP	TYR	ALA	ARG	ALA	THR	TYR	VAL	ASP	GLY	VAL	ASP	LEU	TYR	ALA	GLU	GLY	VAL	VAL	SER	ARG	ILE	ASN	GLU	LYS	VAL	ARG	GLU	TYR	LEU	ASN	GLY	TYR	ALA	ALA	ALA	GLN	GLU	VAL	VAL	VAL	ILE	VAL	LEU	LEU	ASP	ALA	THR	LEU	PRO	GLY	SER	TRP
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• Molecule 5: LD23602p

Chain BU:  10% 86%

GLY	ALA	THR	ASP	THR	ASN	ALA	A7000	A7001	A7002	S7005	L7006	L7007	G7016	LEU	ALA	ARG	GLU	ALA	LEU	VAL	ARG	GLU	ALA	LEU	VAL	VAL	ALA	VAL	ARG	ILE	ASN	GLU	LYS	VAL	ARG	GLU	TYR	LEU	ASN	GLY	TYR	ALA	ALA	ALA	GLN	GLU	GLU	ALA	VAL	VAL	ILE	SER	ALA	THR	GLY	GLY	ALA	THR	SER	PRO	GLU
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PRO	VAL	SER	PHE	LYS	VAL	GLY	ASP	TYR	THR	ALA	ARG	ALA	THR	VAL	ASP	GLY	VAL	ASP	GLY	VAL	ASP	LEU	TYR	ALA	GLU	GLY	VAL	VAL	SER	ILE	ASN	GLU	LYS	VAL	ARG	GLU	TYR	LEU	ASN	GLY	TYR	ALA	ALA	ALA	GLN	GLU	VAL	VAL	ILE	VAL	ASP	ALA	THR	GLY	GLY	ALA	THR	SER	PRO	GLU
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• Molecule 5: LD23602p

Chain Bc:  11% 86%

GLY	ALA	THR	ASP	THR	ASN	ALA	A7000	A7001	A7002	L7006	L7007	G7016	LEU	ALA	ARG	GLU	ALA	LEU	VAL	ARG	GLU	ALA	LEU	VAL	VAL	ALA	VAL	ARG	ILE	ASN	GLU	LYS	VAL	ARG	GLU	TYR	LEU	ASN	GLY	TYR	ALA	ALA	ALA	GLN	GLU	GLU	ALA	VAL	VAL	ILE	SER	ALA	THR	GLY	GLY	ALA	THR	SER	PRO	GLU	PRO
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VAL	SER	PHE	LYS	VAL	GLY	ASP	TYR	THR	ALA	ARG	ALA	THR	VAL	ASP	GLY	VAL	ASP	GLY	VAL	ASP	LEU	TYR	ALA	GLU	GLY	VAL	VAL	VAL	SER	ILE	ASN	GLU	LYS	VAL	ARG	GLU	TYR	LEU	ASN	GLY	TYR	ALA	ALA	ALA	GLN	GLU	VAL	VAL	ILE	VAL	ASP	ALA	THR	GLY	GLY	ALA	THR	SER	PRO	GLU	PRO
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• Molecule 5: LD23602p

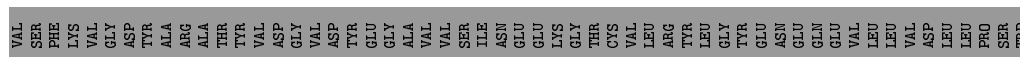
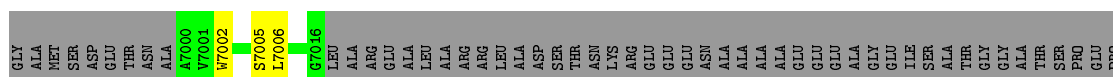
Chain Bk:  10% 86%

GLY	ALA	THR	ASP	THR	ASN	ALA	A7000	A7001	A7002	S7005	L7006	G7016	LEU	ALA	ARG	GLU	ALA	LEU	VAL	ARG	GLU	ALA	LEU	VAL	VAL	ALA	VAL	ARG	ILE	ASN	GLU	LYS	VAL	ARG	GLU	TYR	LEU	ASN	GLY	TYR	ALA	ALA	ALA	GLN	GLU	GLU	ALA	VAL	VAL	ILE	SER	ALA	THR	GLY	GLY	ALA	THR	SER	PRO	GLU	PRO
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VAL	SER	PHE	LYS	VAL	GLY	ASP	TYR	THR	ALA	ARG	ALA	THR	VAL	ASP	GLY	VAL	ASP	GLY	VAL	ASP	LEU	TYR	ALA	GLU	GLY	VAL	VAL	VAL	SER	ILE	ASN	GLU	LYS	VAL	ARG	GLU	TYR	LEU	ASN	GLY	TYR	ALA	ALA	ALA	GLN	GLU	VAL	VAL	ILE	VAL	ASP	ALA	THR	GLY	GLY	ALA	THR	SER	PRO	GLU	PRO
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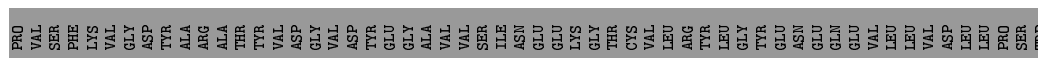
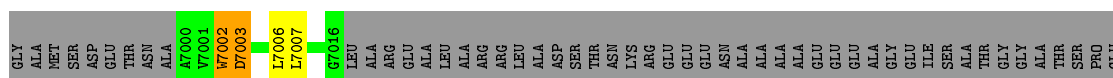
• Molecule 5: LD23602p

Chain Bs:  11% 86%



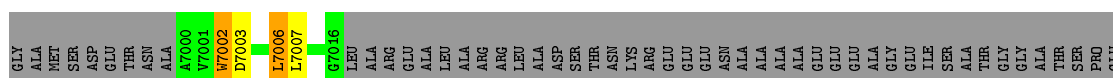
• Molecule 5: LD23602p

Chain B1:  10% .. 86%



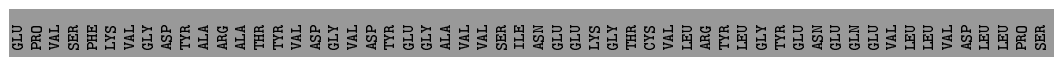
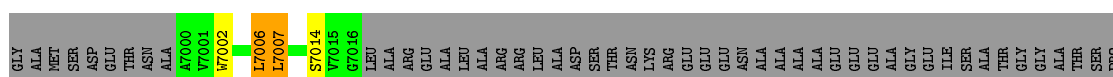
• Molecule 5: LD23602p

Chain CE:  10% .. 86%



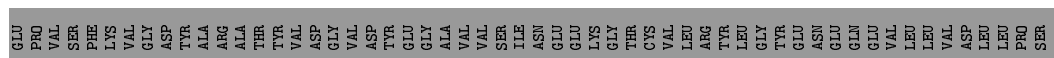
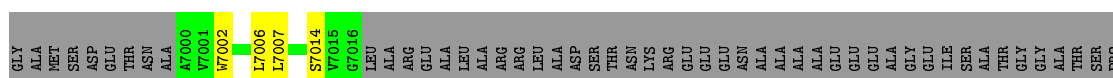
• Molecule 5: LD23602p

Chain CM:  10% .. 86%



• Molecule 5: LD23602p

Chain CU:  10% . 86%

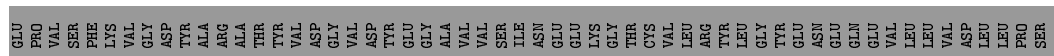


• Molecule 5: LD23602p

Chain Cc:  12% .. 86%



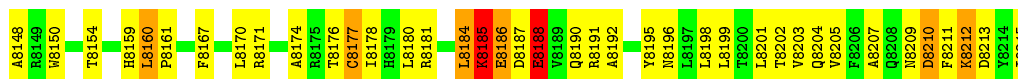
Chain Ck:  10% 86%



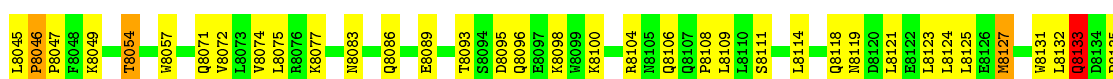
Chain Cs: 9% 2% 1% 88%

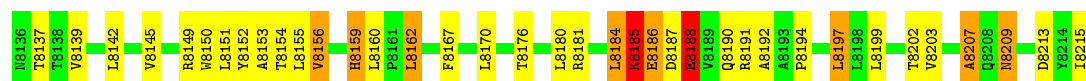


Chain AN:  51% 30% 5% 13%

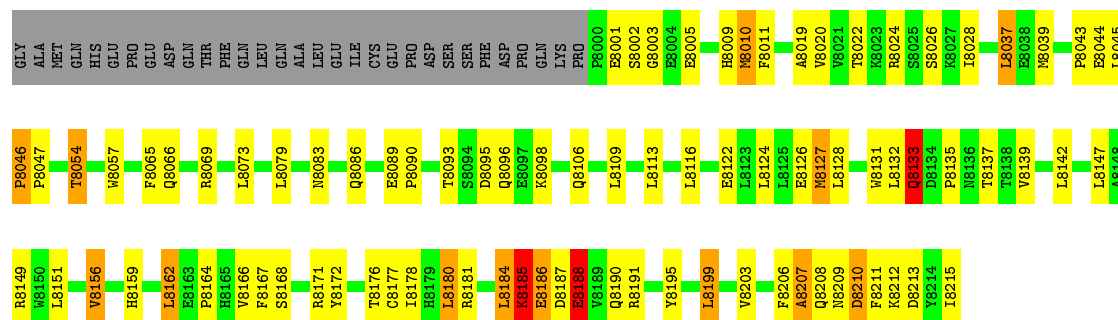


Chain AF:  51% 30% 5% • 13%

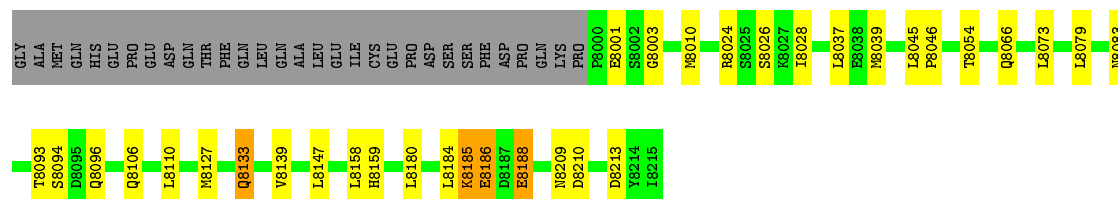




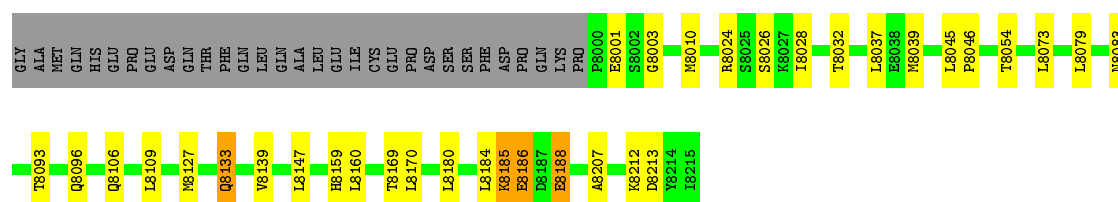
• Molecule 6: CG10419



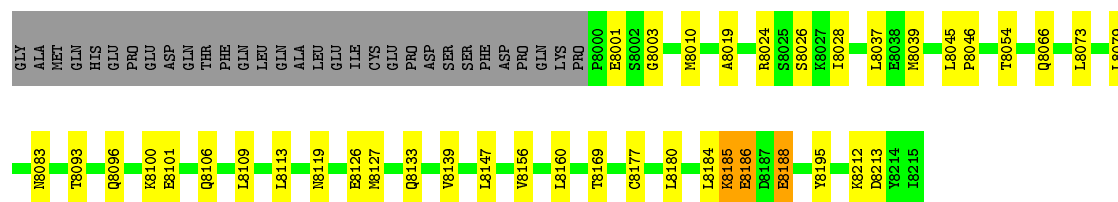
• Molecule 6: CG10419



• Molecule 6: CG10419

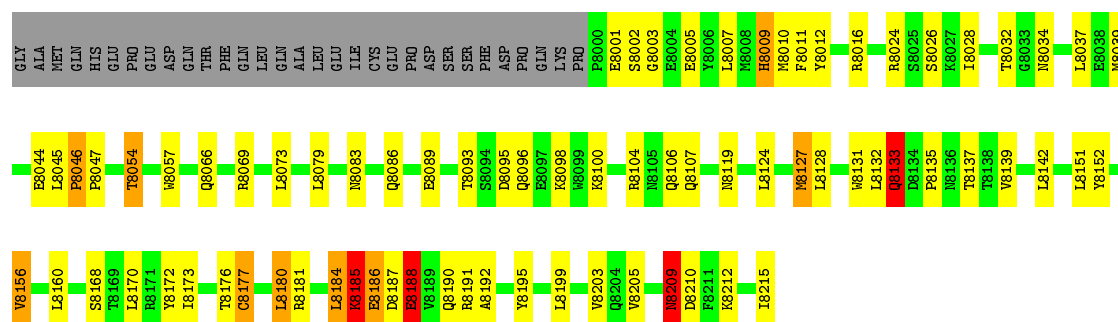


• Molecule 6: CG10419



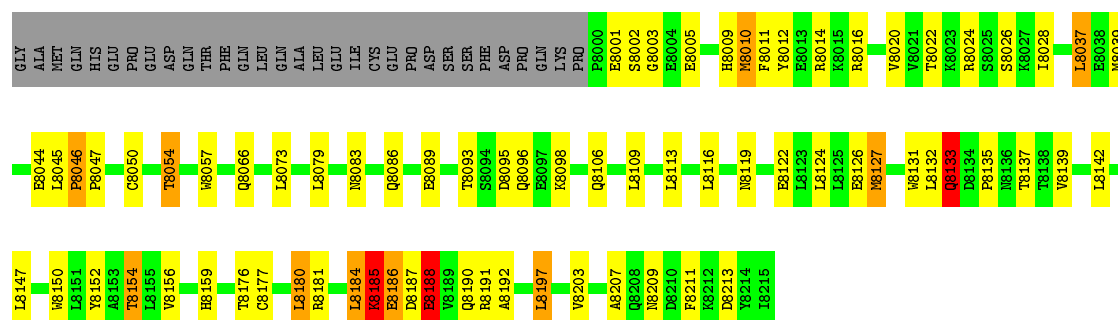
• Molecule 6: CG10419

Chain A2: 



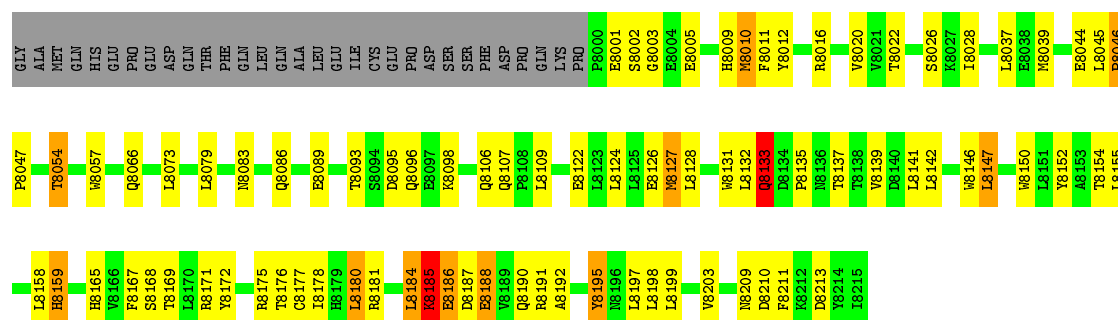
• Molecule 6: CG10419

Chain BF: 



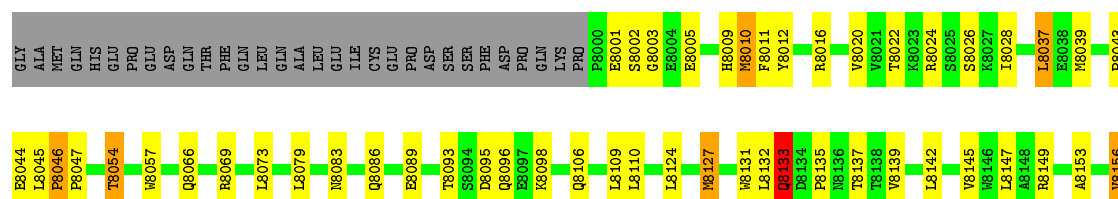
• Molecule 6: CG10419

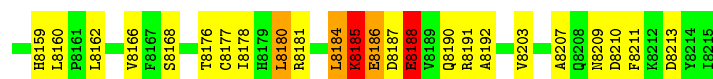
Chain BN: 



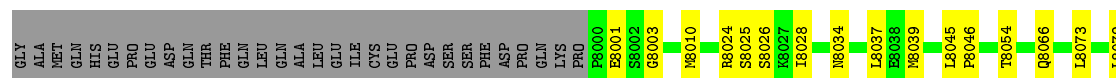
• Molecule 6: CG10419

Chain BV: 

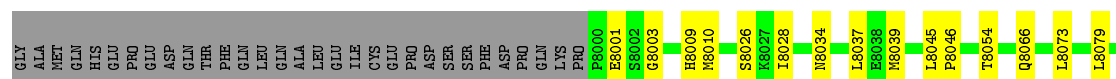




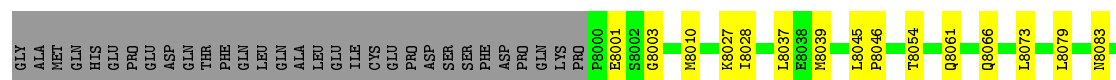
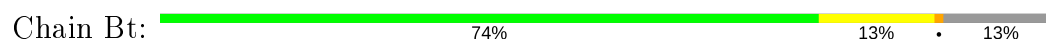
• Molecule 6: CG10419



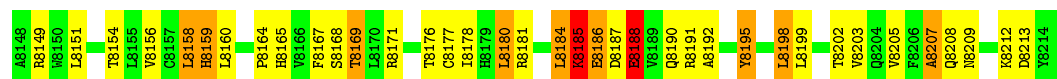
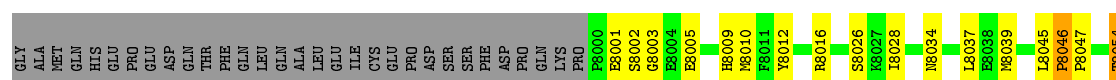
• Molecule 6: CG10419



• Molecule 6: CG10419

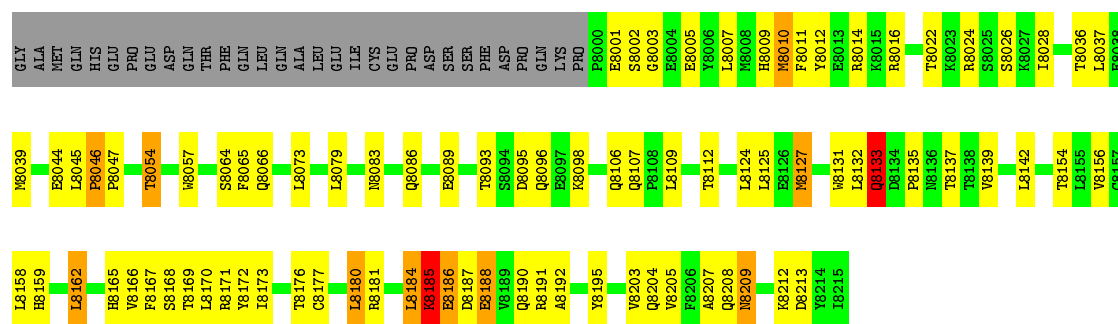


• Molecule 6: CG10419



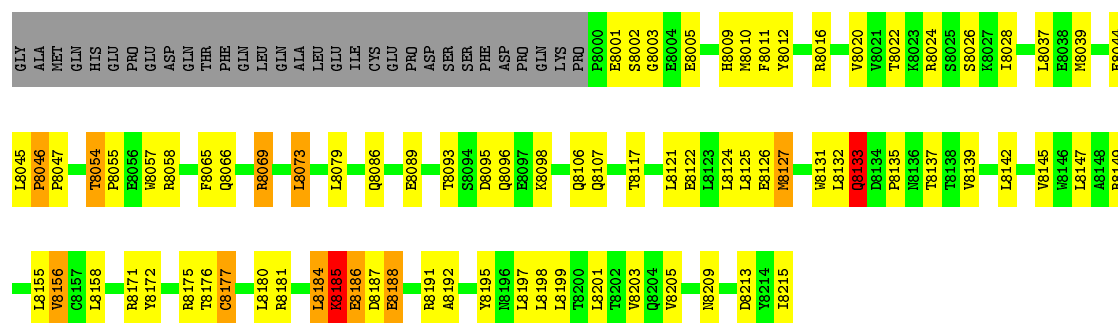
• Molecule 6: CG10419

Chain CF: 



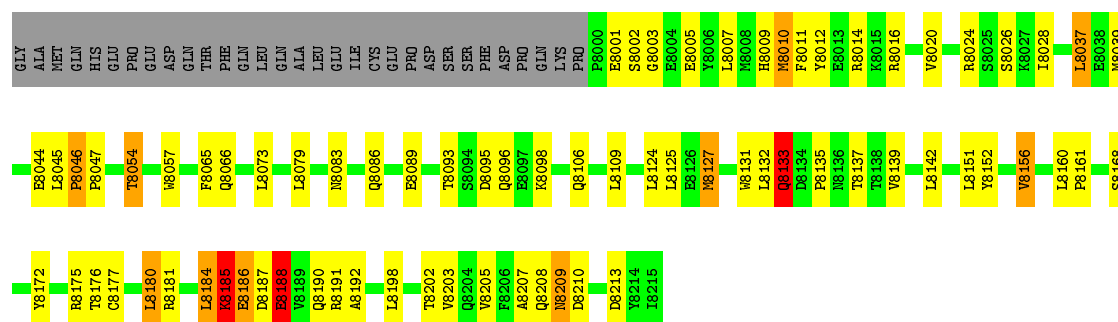
• Molecule 6: CG10419

Chain CN: 



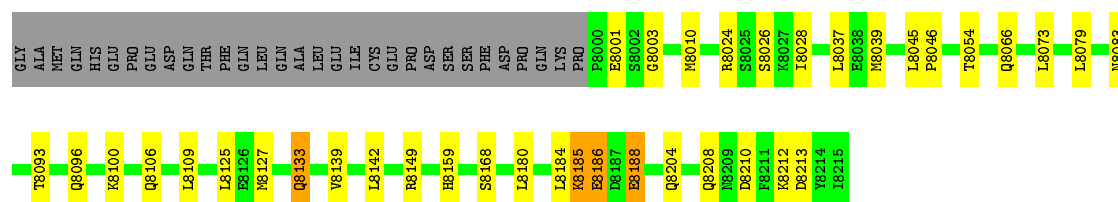
• Molecule 6: CG10419

Chain CV: 

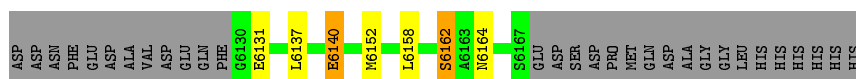


• Molecule 6: CG10419

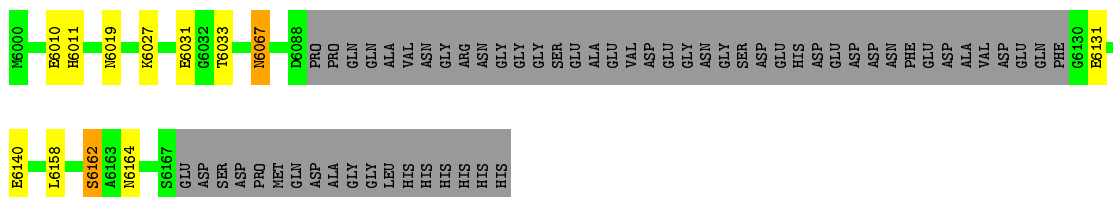
Chain Cd: 



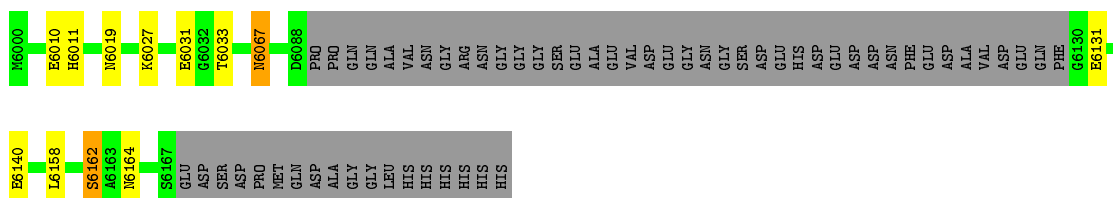
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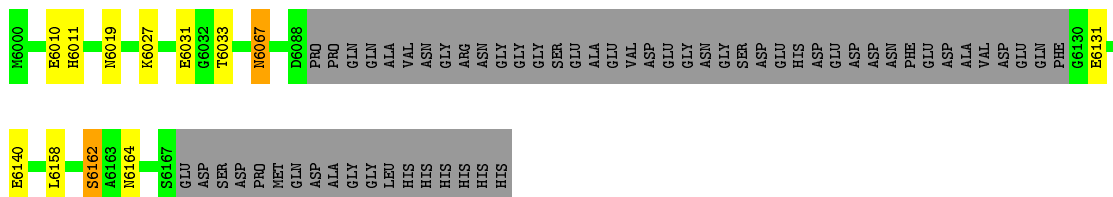
- Molecule 7: Icn



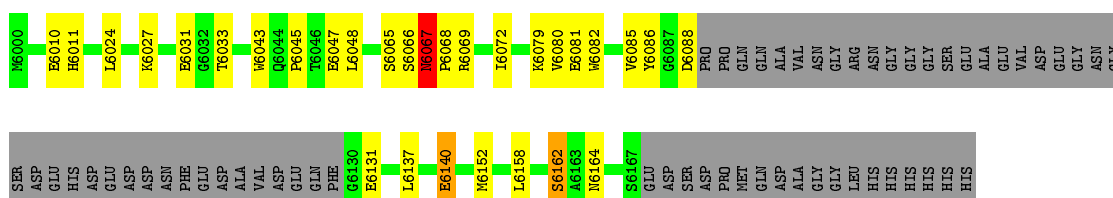
- Molecule 7: Icn



- Molecule 7: Icn

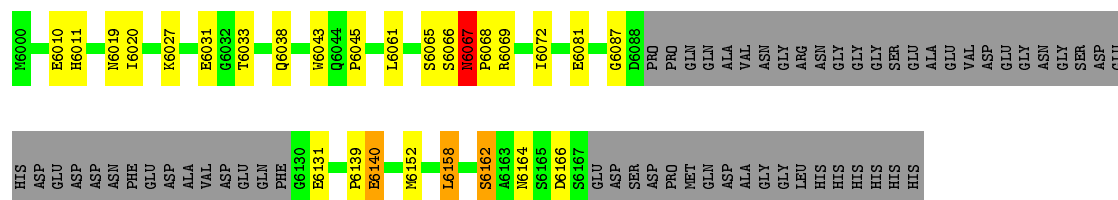


- Molecule 7: Icn

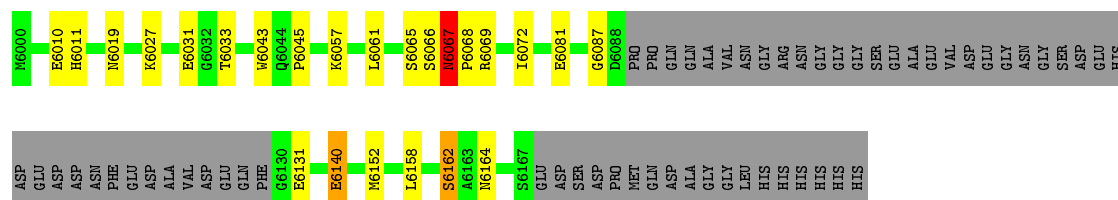


- Molecule 7: Icn

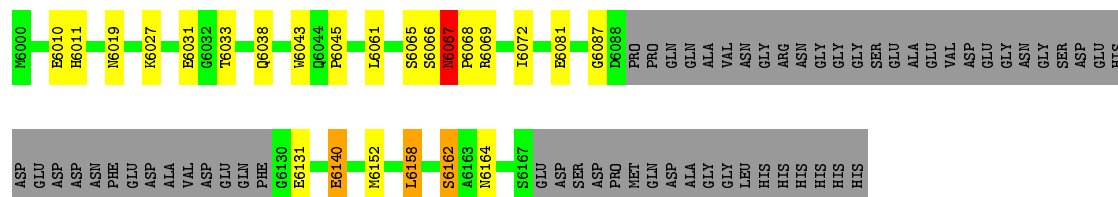




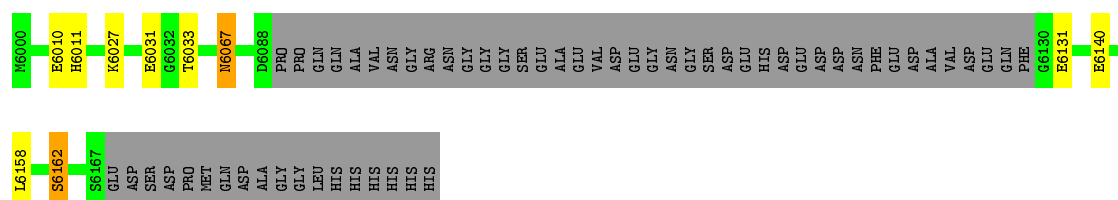
• Molecule 7: Icln



• Molecule 7: Icln



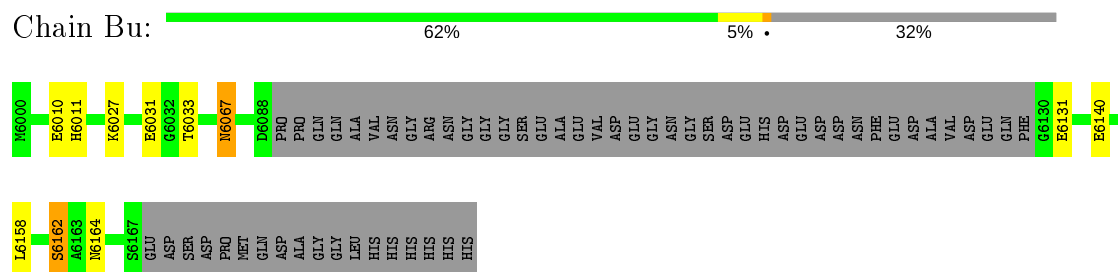
• Molecule 7: Icln



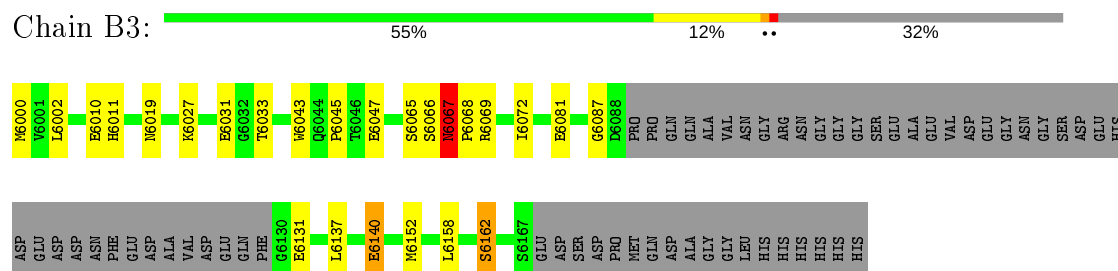
• Molecule 7: Icln



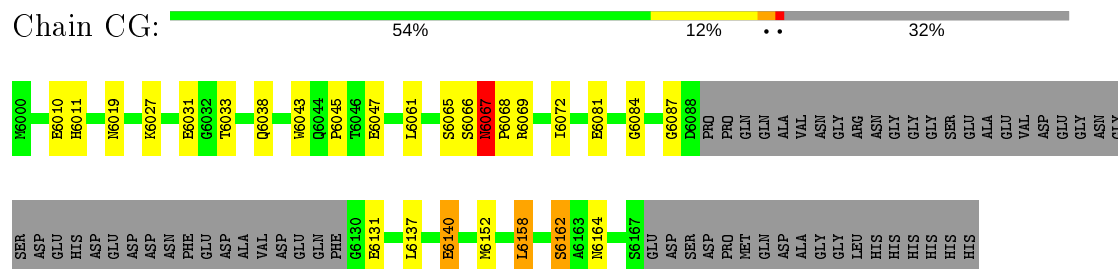
• Molecule 7: Icln



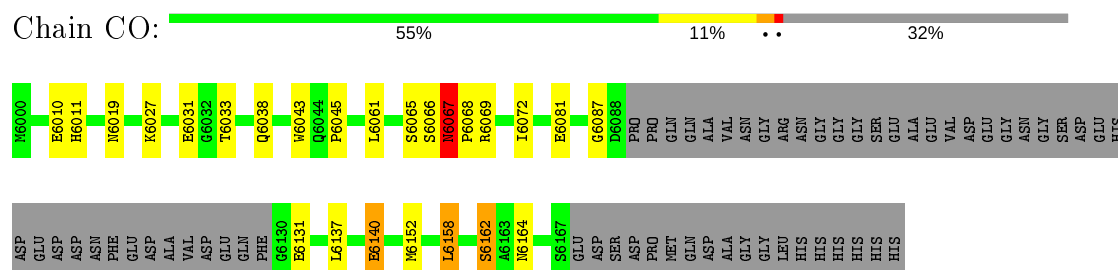
- Molecule 7: Icln



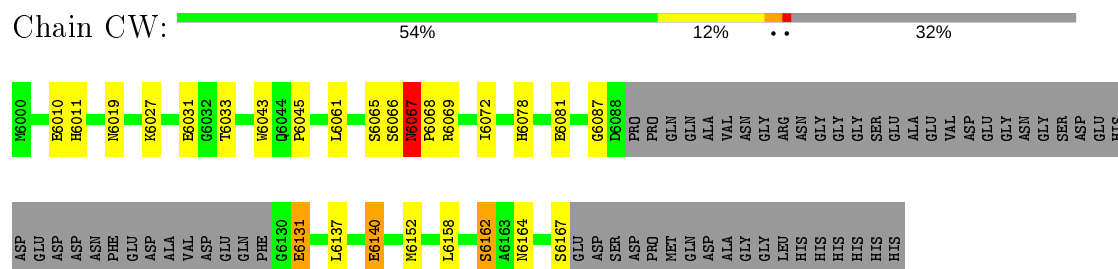
- Molecule 7: Icln



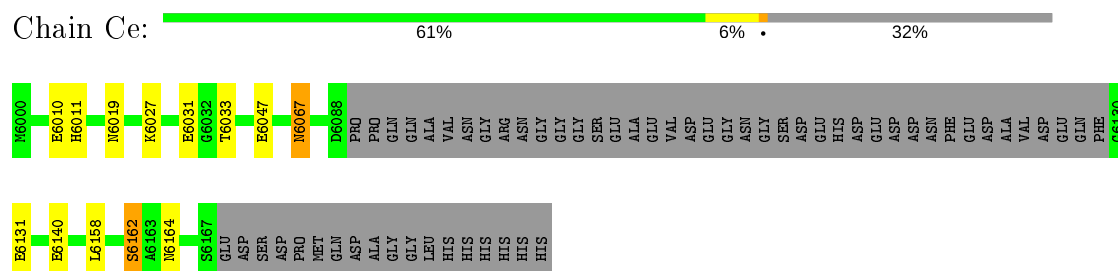
- Molecule 7: Icln



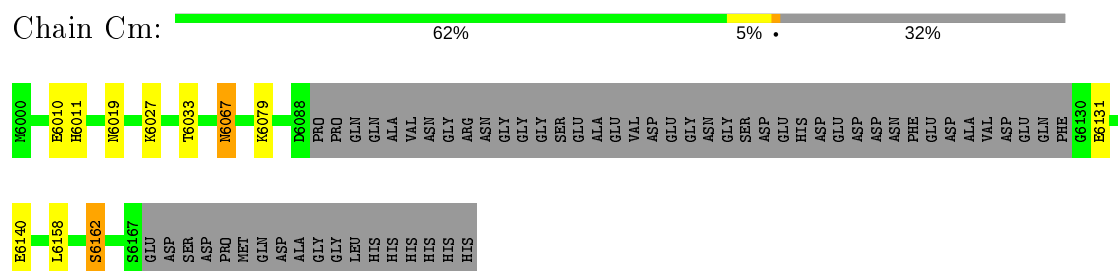
- Molecule 7: Icln



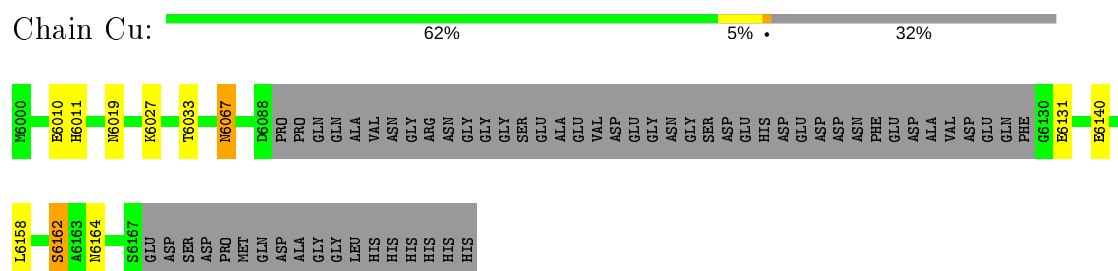
- Molecule 7: Icln



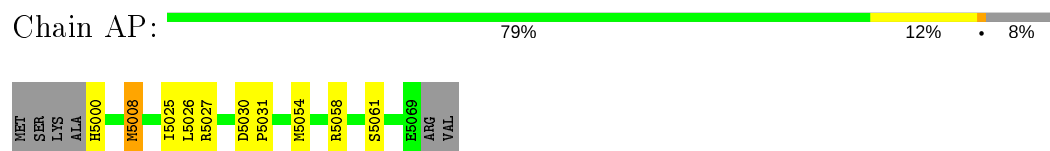
- Molecule 7: Icln



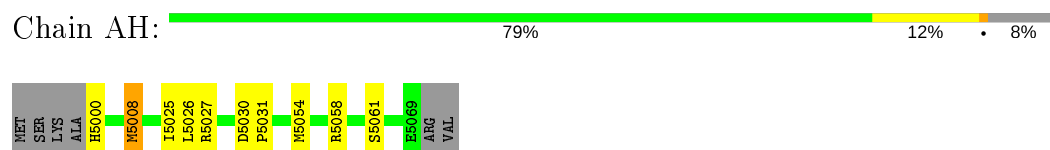
- Molecule 7: Icln



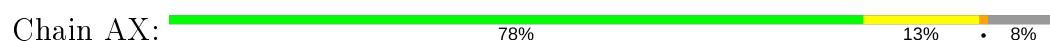
- Molecule 8: Small nuclear ribonucleoprotein G



- Molecule 8: Small nuclear ribonucleoprotein G



- Molecule 8: Small nuclear ribonucleoprotein G





- Molecule 8: Small nuclear ribonucleoprotein G

Chain Af: 88% 8%



- Molecule 8: Small nuclear ribonucleoprotein G

Chain An: 88% 8%



- Molecule 8: Small nuclear ribonucleoprotein G

Chain Av: 88% 8%



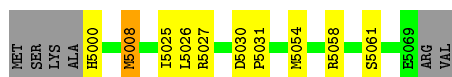
- Molecule 8: Small nuclear ribonucleoprotein G

Chain A4: 79% 12% 8%



- Molecule 8: Small nuclear ribonucleoprotein G

Chain BH: 79% 12% 8%



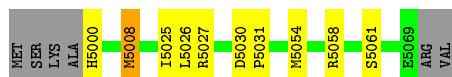
- Molecule 8: Small nuclear ribonucleoprotein G

Chain BP: 78% 13% 8%

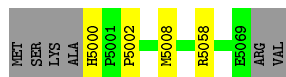
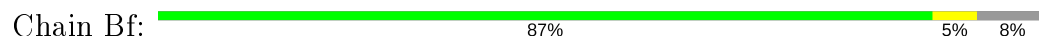


- Molecule 8: Small nuclear ribonucleoprotein G

Chain BX: 79% 12% 8%



- Molecule 8: Small nuclear ribonucleoprotein G



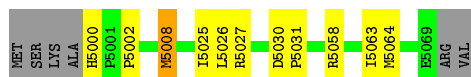
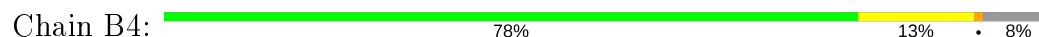
- Molecule 8: Small nuclear ribonucleoprotein G



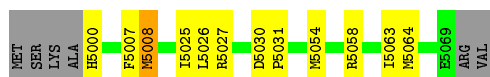
- Molecule 8: Small nuclear ribonucleoprotein G



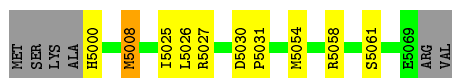
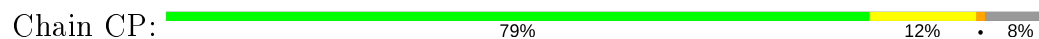
- Molecule 8: Small nuclear ribonucleoprotein G



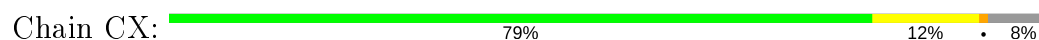
- Molecule 8: Small nuclear ribonucleoprotein G



- Molecule 8: Small nuclear ribonucleoprotein G

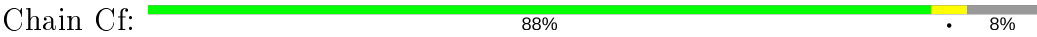


- Molecule 8: Small nuclear ribonucleoprotein G

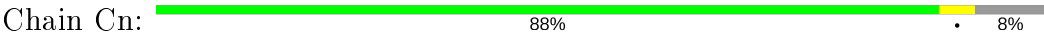




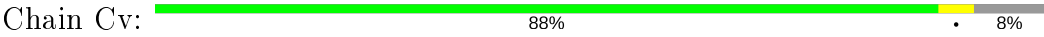
• Molecule 8: Small nuclear ribonucleoprotein G



• Molecule 8: Small nuclear ribonucleoprotein G



• Molecule 8: Small nuclear ribonucleoprotein G



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	150.93Å 356.81Å 230.75Å 90.00° 97.31° 90.00°	Depositor
Resolution (Å)	59.47 – 3.10 59.47 – 3.10	Depositor EDS
% Data completeness (in resolution range)	64.6 (59.47-3.10) 64.6 (59.47-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.232 , 0.256 0.348 , 0.353	Depositor DCC
R_{free} test set	2901 reflections (1.03%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 76.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	121990	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 77.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.7504e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4

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	0.51	0/656	0.75	1/888 (0.1%)
1	AI	0.51	0/656	0.74	1/888 (0.1%)
1	AQ	0.49	0/656	0.76	1/888 (0.1%)
1	AY	0.49	0/656	0.75	1/888 (0.1%)
1	Ag	0.49	0/656	0.74	1/888 (0.1%)
1	Ao	0.51	0/656	0.75	1/888 (0.1%)
1	Aw	0.46	0/656	0.74	1/888 (0.1%)
1	BA	0.45	0/656	0.73	1/888 (0.1%)
1	BI	0.46	0/656	0.72	1/888 (0.1%)
1	BQ	0.46	0/656	0.73	1/888 (0.1%)
1	BY	0.50	0/656	0.74	1/888 (0.1%)
1	Bg	0.46	0/656	0.74	1/888 (0.1%)
1	Bo	0.48	0/656	0.73	1/888 (0.1%)
1	Bw	0.52	0/656	0.75	1/888 (0.1%)
1	CA	0.47	0/656	0.74	1/888 (0.1%)
1	CI	0.46	0/656	0.70	1/888 (0.1%)
1	CQ	0.49	0/656	0.75	1/888 (0.1%)
1	CY	0.53	0/656	0.76	1/888 (0.1%)
1	Cg	0.45	0/656	0.73	1/888 (0.1%)
1	Co	0.45	0/656	0.71	1/888 (0.1%)
2	AB	0.52	0/817	0.70	0/1096
2	AJ	0.50	0/817	0.70	0/1096
2	AR	0.48	0/817	0.69	0/1096
2	AZ	0.47	0/817	0.68	0/1096
2	Ah	0.47	0/817	0.68	0/1096
2	Ap	0.47	0/817	0.67	0/1096
2	Ax	0.48	0/817	0.69	0/1096
2	BB	0.42	0/817	0.64	0/1096
2	BJ	0.44	0/817	0.68	0/1096
2	BR	0.45	0/817	0.68	0/1096
2	BZ	0.50	0/817	0.70	0/1096
2	Bh	0.46	0/817	0.68	0/1096

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Bp	0.46	0/817	0.68	0/1096
2	Bx	0.49	0/817	0.70	0/1096
2	CB	0.45	0/817	0.68	0/1096
2	CJ	0.44	0/817	0.68	0/1096
2	CR	0.46	0/817	0.68	0/1096
2	CZ	0.47	0/817	0.68	0/1096
2	Ch	0.45	0/817	0.67	0/1096
2	Cp	0.46	0/817	0.69	0/1096
3	AC	0.43	0/646	0.75	1/867 (0.1%)
3	AK	0.46	0/646	0.76	1/867 (0.1%)
3	AS	0.44	0/646	0.75	1/867 (0.1%)
3	Aa	0.40	0/646	0.74	1/867 (0.1%)
3	Ai	0.41	0/646	0.74	1/867 (0.1%)
3	Aq	0.43	0/646	0.74	1/867 (0.1%)
3	Ay	0.42	0/646	0.74	1/867 (0.1%)
3	BC	0.41	0/646	0.74	1/867 (0.1%)
3	BK	0.39	0/646	0.73	1/867 (0.1%)
3	BS	0.40	0/646	0.74	1/867 (0.1%)
3	Ba	0.41	0/646	0.74	1/867 (0.1%)
3	Bi	0.38	0/646	0.73	1/867 (0.1%)
3	Bq	0.37	0/646	0.73	1/867 (0.1%)
3	By	0.46	0/646	0.75	1/867 (0.1%)
3	CC	0.40	0/646	0.74	1/867 (0.1%)
3	CK	0.38	0/646	0.74	1/867 (0.1%)
3	CS	0.41	0/646	0.74	1/867 (0.1%)
3	Ca	0.41	0/646	0.74	1/867 (0.1%)
3	Ci	0.39	0/646	0.73	1/867 (0.1%)
3	Cq	0.37	0/646	0.73	1/867 (0.1%)
4	AD	0.39	0/567	0.65	0/765
4	AL	0.39	0/567	0.65	0/765
4	AT	0.40	0/567	0.64	0/765
4	Ab	0.40	0/567	0.64	0/765
4	Aj	0.39	0/567	0.64	0/765
4	Ar	0.39	0/567	0.67	0/765
4	Az	0.38	0/567	0.64	0/765
4	BD	0.38	0/567	0.65	0/765
4	BL	0.37	0/567	0.64	0/765
4	BT	0.37	0/567	0.64	0/765
4	Bb	0.40	0/567	0.68	1/765 (0.1%)
4	Bj	0.39	0/567	0.67	1/765 (0.1%)
4	Br	0.37	0/567	0.64	0/765
4	Bz	0.40	0/567	0.66	0/765
4	CD	0.38	0/567	0.68	0/765

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	CL	0.37	0/567	0.66	0/765
4	CT	0.38	0/567	0.64	0/765
4	Cb	0.40	0/567	0.69	1/765 (0.1%)
4	Cj	0.38	0/567	0.64	0/765
4	Cr	0.37	0/567	0.63	0/765
5	A1	0.65	0/135	0.90	0/184
5	AE	0.57	0/135	0.88	0/184
5	AM	0.63	0/135	0.89	0/184
5	AU	0.56	0/135	0.83	0/184
5	Ac	0.64	0/135	0.94	0/184
5	Ak	0.64	0/135	0.91	0/184
5	As	0.55	0/135	0.87	0/184
5	B1	0.60	0/135	0.88	0/184
5	BE	0.59	0/135	0.81	0/184
5	BM	0.59	0/135	0.86	0/184
5	BU	0.54	0/135	0.83	0/184
5	Bc	0.60	0/135	0.88	0/184
5	Bk	0.63	0/135	0.86	0/184
5	Bs	0.57	0/135	0.89	0/184
5	CE	0.66	0/135	0.92	0/184
5	CM	0.61	0/135	0.89	0/184
5	CU	0.67	0/135	0.90	0/184
5	Cc	0.69	0/135	0.94	0/184
5	Ck	0.64	0/135	0.89	0/184
5	Cs	0.58	0/135	0.86	0/184
6	A2	0.56	0/1830	0.88	2/2489 (0.1%)
6	AF	0.58	0/1830	0.89	2/2489 (0.1%)
6	AN	0.60	0/1830	0.91	2/2489 (0.1%)
6	AV	0.56	0/1830	0.87	2/2489 (0.1%)
6	Ad	0.53	0/1830	0.86	2/2489 (0.1%)
6	Al	0.58	0/1830	0.89	2/2489 (0.1%)
6	At	0.60	0/1830	0.89	2/2489 (0.1%)
6	B2	0.58	0/1830	0.89	2/2489 (0.1%)
6	BF	0.50	0/1830	0.84	2/2489 (0.1%)
6	BN	0.52	0/1830	0.83	2/2489 (0.1%)
6	BV	0.52	0/1830	0.85	2/2489 (0.1%)
6	Bd	0.56	0/1830	0.88	2/2489 (0.1%)
6	Bl	0.54	0/1830	0.86	2/2489 (0.1%)
6	Bt	0.55	0/1830	0.86	2/2489 (0.1%)
6	CF	0.54	0/1830	0.86	2/2489 (0.1%)
6	CN	0.52	0/1830	0.84	2/2489 (0.1%)
6	CV	0.54	0/1830	0.85	2/2489 (0.1%)
6	Cd	0.56	0/1830	0.90	3/2489 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	Cl	0.54	0/1830	0.86	2/2489 (0.1%)
6	Ct	0.53	0/1830	0.86	2/2489 (0.1%)
7	A3	0.46	0/1008	0.74	0/1373
7	AG	0.57	0/1008	0.76	0/1373
7	AO	0.55	0/1008	0.75	0/1373
7	AW	0.53	0/1008	0.75	0/1373
7	Ae	0.47	0/1008	0.72	0/1373
7	Am	0.57	0/1008	0.75	0/1373
7	Au	0.55	0/1008	0.75	0/1373
7	B3	0.53	0/1008	0.75	0/1373
7	BG	0.52	0/1008	0.74	0/1373
7	BO	0.50	0/1008	0.76	1/1373 (0.1%)
7	BW	0.54	0/1008	0.75	0/1373
7	Be	0.54	0/1008	0.75	0/1373
7	Bm	0.49	0/1008	0.72	0/1373
7	Bu	0.51	0/1008	0.75	0/1373
7	CG	0.53	0/1008	0.75	0/1373
7	CO	0.49	0/1008	0.73	0/1373
7	CW	0.55	0/1008	0.75	0/1373
7	Ce	0.57	0/1008	0.76	0/1373
7	Cm	0.49	0/1008	0.74	0/1373
7	Cu	0.48	0/1008	0.74	0/1373
8	A4	0.40	0/551	0.72	0/737
8	AH	0.42	0/551	0.73	0/737
8	AP	0.42	0/551	0.73	0/737
8	AX	0.42	0/551	0.73	0/737
8	Af	0.39	0/551	0.72	0/737
8	An	0.42	0/551	0.73	0/737
8	Av	0.41	0/551	0.73	0/737
8	B4	0.47	0/551	0.75	0/737
8	BH	0.40	0/551	0.72	0/737
8	BP	0.40	0/551	0.71	0/737
8	BX	0.40	0/551	0.69	0/737
8	Bf	0.44	0/551	0.74	0/737
8	Bn	0.40	0/551	0.74	0/737
8	Bv	0.42	0/551	0.73	0/737
8	CH	0.44	0/551	0.73	0/737
8	CP	0.41	0/551	0.73	0/737
8	CX	0.44	0/551	0.74	0/737
8	Cf	0.45	0/551	0.74	0/737
8	Cn	0.39	0/551	0.72	0/737
8	Cv	0.39	0/551	0.72	0/737
All	All	0.49	0/124200	0.77	85/167980 (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
7	A3	0	1
7	AG	0	1
7	AO	0	1
7	AW	0	1
7	Ae	0	1
7	Am	0	1
7	Au	0	1
7	B3	0	1
7	BG	0	1
7	BO	0	1
7	BW	0	1
7	Be	0	1
7	Bm	0	1
7	Bu	0	1
7	CG	0	1
7	CO	0	1
7	CW	0	1
7	Ce	0	1
7	Cm	0	1
7	Cu	0	1
All	All	0	20

There are no bond length outliers.

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AN	8185	LYS	C-N-CA	7.12	139.50	121.70
6	AF	8185	LYS	C-N-CA	7.10	139.44	121.70
6	A2	8185	LYS	C-N-CA	7.08	139.40	121.70
6	Bd	8185	LYS	C-N-CA	7.07	139.36	121.70
6	Cd	8185	LYS	C-N-CA	7.06	139.34	121.70
6	Ct	8185	LYS	C-N-CA	7.01	139.22	121.70
6	Cl	8185	LYS	C-N-CA	7.01	139.22	121.70
6	Al	8185	LYS	C-N-CA	7.01	139.21	121.70
6	At	8185	LYS	C-N-CA	7.01	139.22	121.70
6	BF	8185	LYS	C-N-CA	7.00	139.19	121.70
6	CV	8185	LYS	C-N-CA	6.99	139.18	121.70
6	BN	8185	LYS	C-N-CA	6.99	139.17	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AV	8185	LYS	C-N-CA	6.98	139.16	121.70
6	B2	8185	LYS	C-N-CA	6.98	139.16	121.70
6	Ad	8185	LYS	C-N-CA	6.98	139.15	121.70
6	CF	8185	LYS	C-N-CA	6.97	139.12	121.70
6	Bl	8185	LYS	C-N-CA	6.95	139.08	121.70
6	CN	8185	LYS	C-N-CA	6.95	139.07	121.70
6	Bt	8185	LYS	C-N-CA	6.94	139.04	121.70
6	BV	8185	LYS	C-N-CA	6.92	139.00	121.70
6	AN	8045	LEU	N-CA-C	6.54	128.66	111.00
1	CY	1069	PRO	N-CA-C	6.32	128.54	112.10
1	CQ	1069	PRO	N-CA-C	6.29	128.44	112.10
1	Bg	1069	PRO	N-CA-C	6.28	128.42	112.10
1	BY	1069	PRO	N-CA-C	6.25	128.34	112.10
1	Ao	1069	PRO	N-CA-C	6.24	128.32	112.10
1	Bw	1069	PRO	N-CA-C	6.22	128.28	112.10
1	AA	1069	PRO	N-CA-C	6.17	128.14	112.10
1	Bo	1069	PRO	N-CA-C	6.11	127.97	112.10
1	CA	1069	PRO	N-CA-C	6.10	127.97	112.10
1	BI	1069	PRO	N-CA-C	6.10	127.95	112.10
1	BQ	1069	PRO	N-CA-C	6.07	127.88	112.10
6	CN	8045	LEU	N-CA-C	6.07	127.38	111.00
1	AI	1069	PRO	N-CA-C	6.06	127.86	112.10
1	AQ	1069	PRO	N-CA-C	6.05	127.84	112.10
1	Cg	1069	PRO	N-CA-C	6.03	127.79	112.10
3	Bq	3024	GLN	N-CA-C	6.01	127.24	111.00
1	AY	1069	PRO	N-CA-C	6.01	127.72	112.10
1	Co	1069	PRO	N-CA-C	6.00	127.71	112.10
1	Ag	1069	PRO	N-CA-C	6.00	127.69	112.10
1	BA	1069	PRO	N-CA-C	5.98	127.65	112.10
6	A2	8045	LEU	N-CA-C	5.98	127.14	111.00
6	Cl	8045	LEU	N-CA-C	5.96	127.10	111.00
6	AV	8045	LEU	N-CA-C	5.96	127.08	111.00
6	Ct	8045	LEU	N-CA-C	5.95	127.07	111.00
6	Al	8045	LEU	N-CA-C	5.95	127.06	111.00
6	CV	8045	LEU	N-CA-C	5.95	127.06	111.00
6	BN	8045	LEU	N-CA-C	5.93	127.02	111.00
6	Cd	8045	LEU	N-CA-C	5.93	127.01	111.00
6	Bd	8045	LEU	N-CA-C	5.92	126.98	111.00
6	At	8045	LEU	N-CA-C	5.92	126.97	111.00
6	BF	8045	LEU	N-CA-C	5.90	126.94	111.00
6	BV	8045	LEU	N-CA-C	5.88	126.88	111.00
6	CF	8045	LEU	N-CA-C	5.87	126.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Ay	3024	GLN	N-CA-C	5.85	126.79	111.00
3	Ai	3024	GLN	N-CA-C	5.84	126.77	111.00
3	AK	3024	GLN	N-CA-C	5.84	126.76	111.00
1	Aw	1069	PRO	N-CA-C	5.84	127.28	112.10
6	Bl	8045	LEU	N-CA-C	5.83	126.75	111.00
3	CK	3024	GLN	N-CA-C	5.83	126.75	111.00
6	Ad	8045	LEU	N-CA-C	5.82	126.72	111.00
3	By	3024	GLN	N-CA-C	5.82	126.73	111.00
3	BC	3024	GLN	N-CA-C	5.82	126.70	111.00
3	AS	3024	GLN	N-CA-C	5.80	126.66	111.00
6	Bt	8045	LEU	N-CA-C	5.80	126.66	111.00
3	Aa	3024	GLN	N-CA-C	5.79	126.64	111.00
3	Aq	3024	GLN	N-CA-C	5.79	126.64	111.00
3	CC	3024	GLN	N-CA-C	5.79	126.64	111.00
6	AF	8045	LEU	N-CA-C	5.78	126.61	111.00
3	BS	3024	GLN	N-CA-C	5.78	126.59	111.00
3	BK	3024	GLN	N-CA-C	5.77	126.59	111.00
3	Cq	3024	GLN	N-CA-C	5.76	126.56	111.00
3	Ba	3024	GLN	N-CA-C	5.76	126.54	111.00
3	Ca	3024	GLN	N-CA-C	5.70	126.39	111.00
3	CS	3024	GLN	N-CA-C	5.70	126.39	111.00
3	Bi	3024	GLN	N-CA-C	5.66	126.27	111.00
3	AC	3024	GLN	N-CA-C	5.64	126.24	111.00
3	Ci	3024	GLN	N-CA-C	5.63	126.20	111.00
6	B2	8045	LEU	N-CA-C	5.54	125.95	111.00
4	Cb	4031	ASP	N-CA-CB	-5.47	100.75	110.60
1	CI	1069	PRO	N-CA-C	5.35	126.01	112.10
7	BO	6057	LYS	CB-CG-CD	5.30	125.37	111.60
6	Cd	8208	GLN	C-N-CA	5.15	134.58	121.70
4	Bb	4031	ASP	N-CA-CB	-5.04	101.52	110.60
4	Bj	4031	ASP	N-CA-CB	-5.03	101.55	110.60

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A3	6067	ASN	Mainchain
7	AG	6067	ASN	Mainchain
7	AO	6067	ASN	Mainchain
7	AW	6067	ASN	Mainchain
7	Ae	6067	ASN	Mainchain
7	Am	6067	ASN	Mainchain

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Mol	Chain	Res	Type	Group
7	Au	6067	ASN	Mainchain
7	B3	6067	ASN	Mainchain
7	BG	6067	ASN	Mainchain
7	BO	6067	ASN	Mainchain
7	BW	6067	ASN	Mainchain
7	Be	6067	ASN	Mainchain
7	Bm	6067	ASN	Mainchain
7	Bu	6067	ASN	Mainchain
7	CG	6067	ASN	Mainchain
7	CO	6067	ASN	Mainchain
7	CW	6067	ASN	Mainchain
7	Ce	6067	ASN	Mainchain
7	Cm	6067	ASN	Mainchain
7	Cu	6067	ASN	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	648	0	690	6	0
1	AI	648	0	690	10	0
1	AQ	648	0	690	10	0
1	AY	648	0	690	7	0
1	Ag	648	0	690	0	0
1	Ao	648	0	690	0	0
1	Aw	648	0	690	0	0
1	BA	648	0	690	10	0
1	BI	648	0	690	9	0
1	BQ	648	0	690	11	0
1	BY	648	0	690	6	0
1	Bg	648	0	690	0	0
1	Bo	648	0	690	0	0
1	Bw	648	0	690	0	0
1	CA	648	0	690	8	0
1	CI	648	0	690	10	0
1	CQ	648	0	690	10	0
1	CY	648	0	690	8	0
1	Cg	648	0	690	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Co	648	0	690	0	0
2	AB	807	0	833	13	0
2	AJ	807	0	833	18	0
2	AR	807	0	833	19	0
2	AZ	807	0	833	9	0
2	Ah	807	0	833	0	0
2	Ap	807	0	833	0	0
2	Ax	807	0	833	0	0
2	BB	807	0	833	19	0
2	BJ	807	0	833	16	0
2	BR	807	0	833	16	0
2	BZ	807	0	833	9	0
2	Bh	807	0	833	0	0
2	Bp	807	0	833	0	0
2	Bx	807	0	833	0	0
2	CB	807	0	833	16	0
2	CJ	807	0	833	18	0
2	CR	807	0	833	15	0
2	CZ	807	0	833	8	0
2	Ch	807	0	833	0	0
2	Cp	807	0	833	0	0
3	AC	638	0	657	13	0
3	AK	638	0	657	15	0
3	AS	638	0	657	13	0
3	Aa	638	0	657	0	0
3	Ai	638	0	657	0	0
3	Aq	638	0	657	0	0
3	Ay	638	0	657	0	0
3	BC	638	0	657	13	0
3	BK	638	0	657	15	0
3	BS	638	0	657	13	0
3	Ba	638	0	657	0	0
3	Bi	638	0	657	0	0
3	Bq	638	0	657	0	0
3	By	638	0	657	0	0
3	CC	638	0	657	12	0
3	CK	638	0	657	12	0
3	CS	638	0	657	13	0
3	Ca	638	0	657	0	0
3	Ci	638	0	657	0	0
3	Cq	638	0	657	0	0
4	AD	556	0	561	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AL	556	0	561	17	0
4	AT	556	0	561	17	0
4	Ab	556	0	561	0	0
4	Aj	556	0	561	0	0
4	Ar	556	0	561	0	0
4	Az	556	0	561	0	0
4	BD	556	0	561	18	0
4	BL	556	0	561	17	0
4	BT	556	0	561	15	0
4	Bb	556	0	561	0	0
4	Bj	556	0	561	0	0
4	Br	556	0	561	0	0
4	Bz	556	0	561	0	0
4	CD	556	0	561	14	0
4	CL	556	0	561	15	0
4	CT	556	0	561	16	0
4	Cb	556	0	561	0	0
4	Cj	556	0	561	0	0
4	Cr	556	0	561	0	0
5	A1	133	0	123	0	0
5	AE	133	0	123	2	0
5	AM	133	0	123	2	0
5	AU	133	0	123	2	0
5	Ac	133	0	123	0	0
5	Ak	133	0	123	0	0
5	As	133	0	123	0	0
5	B1	133	0	123	1	0
5	BE	133	0	123	2	0
5	BM	133	0	123	2	0
5	BU	133	0	123	1	0
5	Bc	133	0	123	0	0
5	Bk	133	0	123	0	0
5	Bs	133	0	123	0	0
5	CE	133	0	123	1	0
5	CM	133	0	123	2	0
5	CU	133	0	123	0	0
5	Cc	133	0	123	0	0
5	Ck	133	0	123	0	0
5	Cs	133	0	123	0	0
6	A2	1787	0	1779	37	0
6	AF	1787	0	1779	51	0
6	AN	1787	0	1779	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AV	1787	0	1779	55	0
6	Ad	1787	0	1779	0	0
6	Al	1787	0	1779	0	0
6	At	1787	0	1779	0	0
6	B2	1787	0	1779	40	0
6	BF	1787	0	1779	45	0
6	BN	1787	0	1779	50	0
6	BV	1787	0	1779	45	0
6	Bd	1787	0	1779	0	0
6	Bl	1787	0	1779	0	0
6	Bt	1787	0	1779	0	0
6	CF	1787	0	1779	46	0
6	CN	1787	0	1779	48	0
6	CV	1787	0	1779	39	0
6	Cd	1787	0	1779	0	0
6	Cl	1787	0	1779	0	0
6	Ct	1787	0	1779	0	0
7	A3	984	0	943	19	0
7	AG	984	0	943	21	0
7	AO	984	0	943	19	0
7	AW	984	0	943	19	0
7	Ae	984	0	943	0	0
7	Am	984	0	943	0	0
7	Au	984	0	943	0	0
7	B3	984	0	943	18	0
7	BG	984	0	943	20	0
7	BO	984	0	943	19	0
7	BW	984	0	943	17	0
7	Be	984	0	943	0	0
7	Bm	984	0	943	0	0
7	Bu	984	0	943	0	0
7	CG	984	0	943	22	0
7	CO	984	0	943	19	0
7	CW	984	0	943	22	0
7	Ce	984	0	943	0	0
7	Cm	984	0	943	0	0
7	Cu	984	0	943	0	0
8	A4	544	0	563	6	0
8	AH	544	0	563	7	0
8	AP	544	0	563	7	0
8	AX	544	0	563	8	0
8	Af	544	0	563	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	An	544	0	563	0	0
8	Av	544	0	563	0	0
8	B4	544	0	563	4	0
8	BH	544	0	563	7	0
8	BP	544	0	563	9	0
8	BX	544	0	563	7	0
8	Bf	544	0	563	0	0
8	Bn	544	0	563	0	0
8	Bv	544	0	563	0	0
8	CH	544	0	563	8	0
8	CP	544	0	563	7	0
8	CX	544	0	563	7	0
8	Cf	544	0	563	0	0
8	Cn	544	0	563	0	0
8	Cv	544	0	563	0	0
9	A2	5	0	0	0	0
9	Ad	5	0	0	0	0
9	At	5	0	0	0	0
9	B2	5	0	0	0	0
9	BF	5	0	0	0	0
9	BV	5	0	0	0	0
9	Bd	5	0	0	0	0
9	Bt	5	0	0	0	0
9	CF	5	0	0	0	0
9	Cl	5	0	0	0	0
All	All	121990	0	122980	1154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AR:2043:LYS:HG2	2:AR:2067:TRP:HB3	1.49	0.94
7:AO:6067:ASN:HB2	7:AO:6068:PRO:HD3	1.49	0.92
2:AR:2092:LEU:HD23	4:AT:4056:VAL:HG22	1.51	0.91
7:CG:6067:ASN:HB2	7:CG:6068:PRO:HD3	1.50	0.91
2:AB:2092:LEU:HD23	4:AD:4056:VAL:HG22	1.51	0.91
2:BR:2092:LEU:HD23	4:BT:4056:VAL:HG22	1.51	0.91
2:CB:2092:LEU:HD23	4:CD:4056:VAL:HG22	1.51	0.91
7:AG:6067:ASN:HB2	7:AG:6068:PRO:HD3	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AJ:2092:LEU:HD23	4:AL:4056:VAL:HG22	1.52	0.90
2:BJ:2092:LEU:HD23	4:BL:4056:VAL:HG22	1.52	0.90
2:CJ:2092:LEU:HD23	4:CL:4056:VAL:HG22	1.52	0.90
2:CR:2092:LEU:HD23	4:CT:4056:VAL:HG22	1.51	0.90
7:AW:6067:ASN:HB2	7:AW:6068:PRO:HD3	1.51	0.89
7:CO:6067:ASN:HB2	7:CO:6068:PRO:HD3	1.51	0.89
7:B3:6067:ASN:HB2	7:B3:6068:PRO:HD3	1.52	0.89
7:CW:6067:ASN:HB2	7:CW:6068:PRO:HD3	1.52	0.89
7:A3:6067:ASN:HB2	7:A3:6068:PRO:HD3	1.53	0.89
7:BW:6067:ASN:HB2	7:BW:6068:PRO:HD3	1.53	0.88
7:BG:6067:ASN:HB2	7:BG:6068:PRO:HD3	1.53	0.88
2:BB:2092:LEU:HD23	4:BD:4056:VAL:HG22	1.53	0.87
7:BO:6067:ASN:HB2	7:BO:6068:PRO:HD3	1.54	0.87
4:CL:4060:CYS:O	4:CL:4063:VAL:HG12	1.76	0.85
7:CG:6067:ASN:HB2	7:CG:6068:PRO:CD	2.07	0.84
2:BR:2043:LYS:HG2	2:BR:2067:TRP:HB3	1.59	0.84
6:CV:8185:LYS:H	6:CV:8187:ASP:HB2	1.43	0.84
7:AO:6067:ASN:HB2	7:AO:6068:PRO:CD	2.07	0.84
6:B2:8203:VAL:HG13	6:B2:8209:ASN:HA	1.59	0.83
7:B3:6067:ASN:HB2	7:B3:6068:PRO:CD	2.08	0.83
7:CO:6067:ASN:HB2	7:CO:6068:PRO:CD	2.08	0.83
7:AG:6067:ASN:HB2	7:AG:6068:PRO:CD	2.08	0.83
6:AF:8185:LYS:H	6:AF:8187:ASP:HB2	1.44	0.83
7:CW:6067:ASN:HB2	7:CW:6068:PRO:CD	2.09	0.83
6:AV:8185:LYS:H	6:AV:8187:ASP:HB2	1.44	0.82
3:CK:3066:LYS:HG3	4:CL:4063:VAL:HG13	1.61	0.82
6:CF:8185:LYS:H	6:CF:8187:ASP:HB2	1.44	0.82
7:AW:6067:ASN:HB2	7:AW:6068:PRO:CD	2.09	0.82
7:A3:6067:ASN:HB2	7:A3:6068:PRO:CD	2.09	0.81
7:BW:6067:ASN:HB2	7:BW:6068:PRO:CD	2.09	0.81
6:BF:8185:LYS:H	6:BF:8187:ASP:HB2	1.44	0.81
6:BV:8185:LYS:H	6:BV:8187:ASP:HB2	1.44	0.81
6:CN:8185:LYS:H	6:CN:8187:ASP:HB2	1.46	0.81
6:AN:8185:LYS:H	6:AN:8187:ASP:HB2	1.45	0.81
7:BO:6067:ASN:HB2	7:BO:6068:PRO:CD	2.10	0.81
7:BG:6067:ASN:HB2	7:BG:6068:PRO:CD	2.11	0.81
2:BJ:2043:LYS:HG2	2:BJ:2067:TRP:HB3	1.62	0.81
2:AB:2077:TYR:CE2	6:AF:8209:ASN:HB2	2.16	0.80
6:A2:8185:LYS:H	6:A2:8187:ASP:HB2	1.45	0.80
6:B2:8185:LYS:H	6:B2:8187:ASP:HB2	1.45	0.80
6:BN:8185:LYS:H	6:BN:8187:ASP:HB2	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CG:6067:ASN:CB	7:CG:6068:PRO:HD3	2.12	0.80
7:AG:6067:ASN:CB	7:AG:6068:PRO:HD3	2.12	0.79
7:CW:6067:ASN:CB	7:CW:6068:PRO:HD3	2.13	0.79
7:B3:6067:ASN:CB	7:B3:6068:PRO:HD3	2.12	0.79
7:AO:6067:ASN:CB	7:AO:6068:PRO:HD3	2.12	0.78
2:BB:2043:LYS:HG2	2:BB:2067:TRP:HB3	1.66	0.78
7:CO:6067:ASN:CB	7:CO:6068:PRO:HD3	2.14	0.78
7:AW:6067:ASN:CB	7:AW:6068:PRO:HD3	2.12	0.78
6:BN:8177:CYS:HB2	6:BN:8195:TYR:HB3	1.67	0.77
7:BG:6067:ASN:CB	7:BG:6068:PRO:HD3	2.14	0.75
7:BW:6067:ASN:CB	7:BW:6068:PRO:HD3	2.15	0.75
7:A3:6067:ASN:CB	7:A3:6068:PRO:HD3	2.16	0.75
4:BD:4060:CYS:O	4:BD:4063:VAL:HG12	1.87	0.74
7:BO:6067:ASN:CB	7:BO:6068:PRO:HD3	2.16	0.74
6:CN:8133:GLN:HG3	6:CN:8176:THR:HG21	1.70	0.74
6:CF:8203:VAL:HG13	6:CF:8209:ASN:HA	1.71	0.73
1:BQ:1050:PRO:HG3	6:BV:8159:HIS:CB	2.19	0.72
1:BI:1056:LEU:HD11	7:BO:6061:LEU:HD13	1.70	0.72
4:BT:4060:CYS:O	4:BT:4063:VAL:HG12	1.88	0.72
4:AT:4060:CYS:O	4:AT:4063:VAL:HG12	1.89	0.72
6:B2:8142:LEU:HG	6:B2:8191:ARG:HA	1.71	0.72
2:AZ:2043:LYS:HG2	2:AZ:2067:TRP:HB3	1.72	0.72
1:BA:1056:LEU:HD11	7:BG:6061:LEU:HD13	1.71	0.72
4:CT:4060:CYS:O	4:CT:4063:VAL:HG12	1.89	0.72
6:AV:8203:VAL:HG13	6:AV:8209:ASN:HA	1.72	0.71
6:B2:8184:LEU:HD22	6:B2:8192:ALA:HB2	1.71	0.71
1:AQ:1050:PRO:HG3	6:AV:8159:HIS:HB2	1.72	0.71
1:BQ:1056:LEU:HD11	7:BW:6061:LEU:HD13	1.71	0.71
6:AV:8167:PHE:O	6:AV:8171:ARG:HG3	1.90	0.71
4:BL:4060:CYS:O	4:BL:4063:VAL:HG12	1.90	0.71
4:CD:4060:CYS:O	4:CD:4063:VAL:HG12	1.90	0.71
6:BN:8142:LEU:HG	6:BN:8191:ARG:HA	1.72	0.70
7:AG:6068:PRO:HD2	7:AG:6069:ARG:H	1.57	0.70
1:AQ:1056:LEU:HD11	7:AW:6061:LEU:HD13	1.73	0.70
1:AA:1056:LEU:HD11	7:AG:6061:LEU:HD13	1.74	0.70
6:A2:8142:LEU:HG	6:A2:8191:ARG:HA	1.74	0.70
1:AI:1050:PRO:HG3	6:AN:8159:HIS:CB	2.22	0.69
7:CG:6068:PRO:HD2	7:CG:6069:ARG:H	1.56	0.69
2:BJ:2077:TYR:CE2	6:BN:8209:ASN:HB2	2.27	0.69
2:BJ:2040:ARG:HE	4:BL:4019:TRP:HZ2	1.38	0.69
1:BQ:1050:PRO:HG3	6:BV:8159:HIS:HB3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CI:1056:LEU:HD11	7:CO:6061:LEU:HD13	1.75	0.69
1:AI:1056:LEU:HD11	7:AO:6061:LEU:HD13	1.73	0.69
7:CW:6068:PRO:HD2	7:CW:6069:ARG:H	1.57	0.69
7:BG:6072:ILE:HD12	7:BG:6152:MET:HE2	1.75	0.69
5:BM:7014:SER:HB3	6:BN:8197:LEU:HD11	1.74	0.69
1:BY:1064:ARG:HD3	2:BZ:2041:ASN:HB3	1.73	0.69
6:AN:8142:LEU:HG	6:AN:8191:ARG:HA	1.75	0.69
6:BF:8142:LEU:HG	6:BF:8191:ARG:HA	1.74	0.69
2:CR:2043:LYS:HG2	2:CR:2067:TRP:HB3	1.75	0.69
7:AO:6068:PRO:HD2	7:AO:6069:ARG:H	1.56	0.68
6:CN:8142:LEU:HG	6:CN:8191:ARG:HA	1.75	0.68
7:B3:6068:PRO:HD2	7:B3:6069:ARG:H	1.58	0.68
5:CM:7014:SER:HB3	6:CN:8197:LEU:HD11	1.74	0.68
6:CN:8184:LEU:HD22	6:CN:8192:ALA:HB2	1.75	0.68
1:CQ:1056:LEU:HD11	7:CW:6061:LEU:HD13	1.76	0.68
6:AF:8160:LEU:H	6:AF:8160:LEU:HD12	1.58	0.68
2:CB:2043:LYS:HG2	2:CB:2067:TRP:HB3	1.74	0.68
1:CA:1056:LEU:HD11	7:CG:6061:LEU:HD13	1.76	0.68
3:CK:3016:ARG:HE	3:CK:3030:GLU:HG2	1.58	0.68
6:B2:8124:LEU:HA	6:B2:8127:MET:HE2	1.76	0.67
6:CV:8142:LEU:HG	6:CV:8191:ARG:HA	1.75	0.67
7:AW:6068:PRO:HD2	7:AW:6069:ARG:H	1.57	0.67
6:BV:8142:LEU:HG	6:BV:8191:ARG:HA	1.75	0.67
7:BW:6068:PRO:HD2	7:BW:6069:ARG:H	1.58	0.67
3:AC:3016:ARG:HE	3:AC:3030:GLU:HG2	1.59	0.67
4:AD:4060:CYS:O	4:AD:4063:VAL:HG12	1.94	0.67
6:AF:8145:VAL:HG22	6:AF:8149:ARG:HD2	1.77	0.67
6:CF:8142:LEU:HG	6:CF:8191:ARG:HA	1.75	0.67
3:CK:3016:ARG:NE	3:CK:3030:GLU:HG2	2.09	0.67
7:BO:6068:PRO:HD2	7:BO:6069:ARG:H	1.59	0.67
7:CO:6068:PRO:HD2	7:CO:6069:ARG:H	1.60	0.67
6:AF:8142:LEU:HG	6:AF:8191:ARG:HA	1.76	0.66
3:AK:3016:ARG:HE	3:AK:3030:GLU:HG2	1.58	0.66
6:AN:8178:ILE:HG13	6:AN:8199:LEU:HD21	1.77	0.66
3:BK:3066:LYS:HG3	4:BL:4063:VAL:HG13	1.77	0.66
6:AN:8209:ASN:C	6:AN:8211:PHE:H	1.99	0.66
3:CC:3016:ARG:HE	3:CC:3030:GLU:HG2	1.61	0.66
7:BG:6068:PRO:HD2	7:BG:6069:ARG:H	1.59	0.66
1:AY:1064:ARG:HD3	2:AZ:2041:ASN:HB3	1.77	0.66
2:CB:2040:ARG:HE	4:CD:4019:TRP:HZ2	1.44	0.66
6:A2:8152:TYR:O	6:A2:8156:VAL:HG12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:3016:ARG:NE	3:AC:3030:GLU:HG2	2.10	0.66
3:CC:3016:ARG:NE	3:CC:3030:GLU:HG2	2.11	0.66
6:CV:8203:VAL:O	6:CV:8207:ALA:HA	1.96	0.66
3:BK:3016:ARG:NE	3:BK:3030:GLU:HG2	2.11	0.65
3:CS:3016:ARG:NE	3:CS:3030:GLU:HG2	2.12	0.65
3:AK:3016:ARG:NE	3:AK:3030:GLU:HG2	2.10	0.65
3:BC:3016:ARG:HE	3:BC:3030:GLU:HG2	1.60	0.65
3:BC:3016:ARG:NE	3:BC:3030:GLU:HG2	2.10	0.65
3:CS:3016:ARG:HE	3:CS:3030:GLU:HG2	1.62	0.65
1:AA:1050:PRO:HG3	6:AF:8159:HIS:HB2	1.78	0.65
3:BK:3016:ARG:HE	3:BK:3030:GLU:HG2	1.60	0.65
3:BS:3016:ARG:NE	3:BS:3030:GLU:HG2	2.11	0.65
7:AO:6067:ASN:CB	7:AO:6068:PRO:CD	2.73	0.65
3:BS:3066:LYS:HG3	4:BT:4063:VAL:HG13	1.79	0.65
7:BW:6069:ARG:NH2	7:BW:6140:GLU:O	2.30	0.65
6:B2:8154:THR:O	6:B2:8158:LEU:HG	1.97	0.65
3:AS:3016:ARG:HE	3:AS:3030:GLU:HG2	1.61	0.64
3:AS:3066:LYS:HG3	4:AT:4063:VAL:HG13	1.79	0.64
7:A3:6068:PRO:HD2	7:A3:6069:ARG:H	1.60	0.64
7:AG:6069:ARG:NH2	7:AG:6140:GLU:O	2.31	0.64
6:BV:8160:LEU:HG	6:BV:8162:LEU:HD13	1.79	0.64
7:B3:6067:ASN:CB	7:B3:6068:PRO:CD	2.72	0.64
2:CB:2077:TYR:CE2	6:CF:8209:ASN:HB2	2.32	0.64
7:AW:6067:ASN:CB	7:AW:6068:PRO:CD	2.73	0.64
3:BS:3016:ARG:HE	3:BS:3030:GLU:HG2	1.61	0.64
3:AS:3016:ARG:NE	3:AS:3030:GLU:HG2	2.11	0.64
1:BQ:1064:ARG:HD3	2:BR:2041:ASN:HB3	1.79	0.64
1:AA:1064:ARG:HD3	2:AB:2041:ASN:HB3	1.79	0.64
4:AL:4060:CYS:O	4:AL:4063:VAL:HG12	1.97	0.64
2:AJ:2043:LYS:HG2	2:AJ:2067:TRP:HB3	1.80	0.64
6:BF:8203:VAL:HG13	6:BF:8209:ASN:HA	1.79	0.64
7:AG:6067:ASN:CB	7:AG:6068:PRO:CD	2.72	0.64
4:AT:4031:ASP:HA	6:AV:8020:VAL:HG22	1.79	0.63
6:AV:8142:LEU:HG	6:AV:8191:ARG:HA	1.80	0.63
3:CC:3066:LYS:HG3	4:CD:4063:VAL:HG13	1.80	0.63
6:AV:8164:PRO:HA	6:AV:8167:PHE:HD1	1.63	0.63
6:A2:8199:LEU:O	6:A2:8203:VAL:HG23	1.99	0.63
3:BC:3066:LYS:HG3	4:BD:4063:VAL:HG13	1.79	0.63
8:BP:5030:ASP:HB2	8:BP:5031:PRO:CD	2.29	0.63
8:BX:5030:ASP:HB2	8:BX:5031:PRO:CD	2.29	0.63
8:BH:5030:ASP:HB2	8:BH:5031:PRO:CD	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BI:1050:PRO:HG3	6:BN:8159:HIS:HB2	1.80	0.63
7:AW:6069:ARG:NH2	7:AW:6140:GLU:O	2.31	0.63
7:BG:6067:ASN:CB	7:BG:6068:PRO:CD	2.75	0.63
6:AF:8203:VAL:O	6:AF:8207:ALA:HA	1.99	0.62
7:A3:6067:ASN:CB	7:A3:6068:PRO:CD	2.76	0.62
7:BW:6067:ASN:CB	7:BW:6068:PRO:CD	2.75	0.62
8:A4:5030:ASP:HB2	8:A4:5031:PRO:CD	2.29	0.62
2:BB:2040:ARG:HE	4:BD:4019:TRP:HZ2	1.45	0.62
2:CZ:2043:LYS:HG2	2:CZ:2067:TRP:HB3	1.81	0.62
1:AI:1064:ARG:HD3	2:AJ:2041:ASN:HB3	1.81	0.62
1:AI:1050:PRO:HG3	6:AN:8159:HIS:HB3	1.79	0.62
6:AN:8177:CYS:HB2	6:AN:8195:TYR:HB3	1.80	0.62
6:CV:8152:TYR:O	6:CV:8156:VAL:HG12	1.99	0.62
3:BC:3000:MET:CE	3:BC:3002:GLN:HE22	2.13	0.62
3:CS:3000:MET:CE	3:CS:3002:GLN:HE22	2.12	0.62
3:CK:3000:MET:CE	3:CK:3002:GLN:HE22	2.13	0.62
8:AH:5030:ASP:HB2	8:AH:5031:PRO:CD	2.30	0.61
3:AK:3000:MET:CE	3:AK:3002:GLN:HE22	2.13	0.61
3:AC:3000:MET:CE	3:AC:3002:GLN:HE22	2.13	0.61
7:BO:6069:ARG:NH2	7:BO:6140:GLU:O	2.33	0.61
3:CC:3000:MET:CE	3:CC:3002:GLN:HE22	2.13	0.61
4:CT:4031:ASP:HA	6:CV:8020:VAL:HG22	1.82	0.61
8:AP:5030:ASP:HB2	8:AP:5031:PRO:CD	2.30	0.61
7:BO:6067:ASN:CB	7:BO:6068:PRO:CD	2.76	0.61
1:AQ:1050:PRO:HG3	6:AV:8159:HIS:CB	2.30	0.61
2:BB:2077:TYR:CE2	6:BF:8209:ASN:HB2	2.35	0.61
7:CW:6069:ARG:NH2	7:CW:6140:GLU:O	2.34	0.61
7:CG:6069:ARG:NH2	7:CG:6140:GLU:O	2.34	0.61
8:CH:5030:ASP:HB2	8:CH:5031:PRO:CD	2.30	0.61
8:CX:5030:ASP:HB2	8:CX:5031:PRO:CD	2.30	0.61
6:AV:8128:LEU:HD22	6:AV:8151:LEU:HG	1.82	0.61
8:AX:5030:ASP:HB2	8:AX:5031:PRO:CD	2.30	0.61
2:CJ:2077:TYR:CE2	6:CN:8209:ASN:HB2	2.36	0.61
8:CP:5030:ASP:HB2	8:CP:5031:PRO:CD	2.30	0.61
7:AO:6069:ARG:NH2	7:AO:6140:GLU:O	2.34	0.60
7:BG:6069:ARG:NH2	7:BG:6140:GLU:O	2.34	0.60
7:A3:6069:ARG:NH2	7:A3:6140:GLU:O	2.34	0.60
3:BS:3000:MET:CE	3:BS:3002:GLN:HE22	2.14	0.60
7:AG:6018:ASN:HD22	7:AG:6019:ASN:HB2	1.66	0.60
3:AS:3000:MET:CE	3:AS:3002:GLN:HE22	2.14	0.60
7:AW:6072:ILE:HD12	7:AW:6152:MET:HE2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CS:3066:LYS:HG3	4:CT:4063:VAL:HG13	1.83	0.60
6:AN:8146:TRP:O	6:AN:8150:TRP:HD1	1.85	0.60
3:BK:3000:MET:CE	3:BK:3002:GLN:HE22	2.15	0.60
6:B2:8203:VAL:O	6:B2:8207:ALA:HA	2.01	0.60
6:CN:8065:PHE:CE2	6:CN:8205:VAL:HG11	2.37	0.60
7:CW:6067:ASN:CB	7:CW:6068:PRO:CD	2.74	0.60
6:AF:8152:TYR:O	6:AF:8156:VAL:HG12	2.01	0.60
6:AV:8124:LEU:HA	6:AV:8127:MET:HE2	1.84	0.60
1:BI:1064:ARG:HD3	2:BJ:2041:ASN:HB3	1.84	0.60
6:BV:8124:LEU:HA	6:BV:8127:MET:HE2	1.84	0.60
7:CG:6067:ASN:CB	7:CG:6068:PRO:CD	2.73	0.60
2:AR:2043:LYS:HG2	2:AR:2067:TRP:CB	2.28	0.60
6:B2:8133:GLN:HG3	6:B2:8176:THR:HG21	1.83	0.60
6:BN:8124:LEU:HA	6:BN:8127:MET:HE2	1.84	0.60
7:CW:6072:ILE:HD12	7:CW:6152:MET:HE2	1.84	0.60
6:AN:8167:PHE:O	6:AN:8171:ARG:HG3	2.03	0.59
1:BI:1048:ARG:HG3	1:BI:1048:ARG:HH11	1.66	0.59
7:B3:6069:ARG:NH2	7:B3:6140:GLU:O	2.36	0.59
1:AY:1069:PRO:O	1:AY:1071:SER:N	2.33	0.59
7:CO:6067:ASN:CB	7:CO:6068:PRO:CD	2.74	0.59
7:B3:6068:PRO:CD	7:B3:6069:ARG:H	2.15	0.59
7:CG:6068:PRO:CD	7:CG:6069:ARG:H	2.14	0.59
6:CN:8054:THR:HG23	6:CN:8057:TRP:CB	2.33	0.59
1:AI:1024:HIS:HB3	6:AN:8161:PRO:HD3	1.85	0.58
7:CG:6072:ILE:HD12	7:CG:6152:MET:HE2	1.84	0.58
1:CY:1048:ARG:HG3	1:CY:1048:ARG:HH11	1.66	0.58
6:AV:8177:CYS:HA	6:AV:8180:LEU:HB2	1.85	0.58
7:CO:6069:ARG:NH2	7:CO:6140:GLU:O	2.36	0.58
6:AN:8124:LEU:HA	6:AN:8127:MET:HE2	1.86	0.58
6:CV:8124:LEU:HA	6:CV:8127:MET:HE2	1.84	0.58
7:CW:6068:PRO:CD	7:CW:6069:ARG:H	2.15	0.58
7:AG:6072:ILE:HD12	7:AG:6152:MET:HE2	1.85	0.58
7:AO:6068:PRO:CD	7:AO:6069:ARG:H	2.14	0.58
1:BY:1048:ARG:HH11	1:BY:1048:ARG:HG3	1.68	0.58
6:AN:8095:ASP:HB3	6:AN:8098:LYS:HB2	1.86	0.58
6:AN:8133:GLN:HG3	6:AN:8176:THR:HG21	1.85	0.58
7:AW:6068:PRO:CD	7:AW:6069:ARG:H	2.14	0.57
7:BW:6068:PRO:CD	7:BW:6069:ARG:H	2.15	0.57
6:AN:8100:LYS:HD3	6:AN:8104:ARG:CZ	2.34	0.57
6:AF:8095:ASP:HB3	6:AF:8098:LYS:HB2	1.87	0.57
8:B4:5008:MET:O	8:B4:5026:LEU:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:1069:PRO:O	1:AI:1071:SER:N	2.36	0.57
1:AQ:1069:PRO:O	1:AQ:1071:SER:N	2.36	0.57
1:BQ:1069:PRO:O	1:BQ:1071:SER:N	2.35	0.57
6:A2:8095:ASP:HB3	6:A2:8098:LYS:HB2	1.87	0.57
3:AK:3066:LYS:HG3	4:AL:4063:VAL:HG13	1.86	0.57
6:AV:8203:VAL:O	6:AV:8207:ALA:HA	2.05	0.57
6:B2:8065:PHE:CE2	6:B2:8205:VAL:HG11	2.40	0.57
1:BA:1048:ARG:HG3	1:BA:1048:ARG:HH11	1.70	0.57
7:CO:6072:ILE:HD12	7:CO:6152:MET:HE2	1.86	0.57
6:B2:8095:ASP:HB3	6:B2:8098:LYS:HB2	1.87	0.57
7:BO:6068:PRO:CD	7:BO:6069:ARG:H	2.16	0.57
7:A3:6072:ILE:HD12	7:A3:6152:MET:HE2	1.86	0.56
6:CF:8133:GLN:HG3	6:CF:8176:THR:HG21	1.87	0.56
1:CQ:1048:ARG:HH11	1:CQ:1048:ARG:HG3	1.70	0.56
2:CR:2040:ARG:HE	4:CT:4019:TRP:HZ2	1.51	0.56
3:AC:3066:LYS:HG3	4:AD:4063:VAL:HG13	1.87	0.56
1:BA:1050:PRO:HG3	6:BF:8159:HIS:HB2	1.86	0.56
7:BG:6068:PRO:CD	7:BG:6069:ARG:H	2.16	0.56
1:BQ:1048:ARG:HH11	1:BQ:1048:ARG:HG3	1.70	0.56
6:BV:8095:ASP:HB3	6:BV:8098:LYS:HB2	1.87	0.56
1:CA:1069:PRO:O	1:CA:1071:SER:N	2.35	0.56
6:CN:8095:ASP:HB3	6:CN:8098:LYS:HB2	1.87	0.56
1:CY:1069:PRO:O	1:CY:1071:SER:N	2.35	0.56
6:AF:8199:LEU:O	6:AF:8203:VAL:HG23	2.05	0.56
1:CA:1048:ARG:HG3	1:CA:1048:ARG:HH11	1.69	0.56
1:CQ:1069:PRO:O	1:CQ:1071:SER:N	2.36	0.56
7:AO:6066:SER:HA	7:AO:6069:ARG:O	2.06	0.56
6:BF:8095:ASP:HB3	6:BF:8098:LYS:HB2	1.88	0.56
6:BF:8150:TRP:O	6:BF:8154:THR:OG1	2.23	0.56
6:BN:8095:ASP:HB3	6:BN:8098:LYS:HB2	1.88	0.56
7:BO:6081:GLU:H	8:BP:5064:MET:HE1	1.71	0.56
6:A2:8168:SER:O	6:A2:8172:TYR:HD2	1.89	0.56
7:A3:6066:SER:HA	7:A3:6069:ARG:O	2.06	0.56
1:AQ:1048:ARG:HH11	1:AQ:1048:ARG:HG3	1.70	0.56
6:AV:8095:ASP:HB3	6:AV:8098:LYS:HB2	1.88	0.56
6:CF:8095:ASP:HB3	6:CF:8098:LYS:HB2	1.88	0.56
2:AZ:2064:LYS:HE3	2:AZ:2075:ASP:OD2	2.06	0.56
7:BG:6066:SER:HA	7:BG:6069:ARG:O	2.06	0.56
6:BN:8155:LEU:HA	6:BN:8158:LEU:HD12	1.87	0.55
6:CF:8167:PHE:O	6:CF:8171:ARG:HG3	2.06	0.55
7:AG:6066:SER:HA	7:AG:6069:ARG:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CI:1048:ARG:HH11	1:CI:1048:ARG:HG3	1.71	0.55
4:CL:4031:ASP:HA	6:CN:8020:VAL:HG22	1.88	0.55
3:CS:3000:MET:HE2	3:CS:3002:GLN:HE22	1.71	0.55
6:CV:8095:ASP:HB3	6:CV:8098:LYS:HB2	1.88	0.55
6:CV:8203:VAL:HG13	6:CV:8209:ASN:HA	1.87	0.55
6:AF:8181:ARG:O	6:AF:8184:LEU:HB2	2.06	0.55
7:A3:6068:PRO:CD	7:A3:6069:ARG:H	2.17	0.55
2:AR:2097:ILE:HG22	6:AV:8037:LEU:HB3	1.88	0.55
8:A4:5008:MET:O	8:A4:5026:LEU:HB3	2.07	0.55
2:CR:2097:ILE:HG22	6:CV:8037:LEU:HB3	1.88	0.55
8:CP:5008:MET:O	8:CP:5026:LEU:HB3	2.07	0.55
7:AO:6072:ILE:HD12	7:AO:6152:MET:HE2	1.88	0.55
1:BA:1069:PRO:O	1:BA:1071:SER:N	2.38	0.55
8:BH:5008:MET:O	8:BH:5026:LEU:HB3	2.07	0.55
7:BO:6066:SER:HA	7:BO:6069:ARG:O	2.06	0.55
1:AQ:1064:ARG:HD3	2:AR:2041:ASN:HB3	1.89	0.55
6:BN:8141:LEU:HD12	6:BN:8195:TYR:CD1	2.42	0.55
1:BY:1069:PRO:O	1:BY:1071:SER:N	2.36	0.55
6:CV:8133:GLN:HG3	6:CV:8176:THR:HG21	1.89	0.55
7:AG:6068:PRO:CD	7:AG:6069:ARG:H	2.14	0.55
7:B3:6066:SER:HA	7:B3:6069:ARG:O	2.07	0.55
7:CO:6066:SER:HA	7:CO:6069:ARG:O	2.06	0.55
6:AN:8160:LEU:HD23	6:AN:8161:PRO:HA	1.89	0.54
7:BW:6066:SER:HA	7:BW:6069:ARG:O	2.07	0.54
1:CY:1064:ARG:HD3	2:CZ:2041:ASN:HB3	1.89	0.54
1:AA:1069:PRO:O	1:AA:1071:SER:N	2.37	0.54
7:B3:6072:ILE:HD12	7:B3:6152:MET:HE2	1.88	0.54
1:BI:1048:ARG:HG3	1:BI:1048:ARG:NH1	2.21	0.54
6:AN:8181:ARG:HA	6:AN:8184:LEU:CD1	2.37	0.54
8:BP:5008:MET:O	8:BP:5026:LEU:HB3	2.08	0.54
7:CW:6066:SER:HA	7:CW:6069:ARG:O	2.07	0.54
6:A2:8199:LEU:HB2	6:A2:8215:ILE:HD13	1.89	0.54
6:AV:8209:ASN:C	6:AV:8211:PHE:H	2.11	0.54
8:B4:5030:ASP:HB2	8:B4:5031:PRO:CD	2.36	0.54
6:BF:8184:LEU:HD22	6:BF:8192:ALA:HB2	1.88	0.54
2:BJ:2023:SER:O	2:BJ:2027:GLN:HG3	2.08	0.54
6:AV:8113:LEU:HD13	6:AV:8116:LEU:HD12	1.90	0.54
6:B2:8046:PRO:HB2	6:B2:8047:PRO:HD2	1.90	0.54
7:CG:6066:SER:HA	7:CG:6069:ARG:O	2.07	0.54
6:AN:8054:THR:HG23	6:AN:8057:TRP:HB2	1.90	0.54
8:CX:5008:MET:O	8:CX:5026:LEU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A3:6081:GLU:OE1	7:A3:6088:ASP:HB2	2.07	0.54
2:AJ:2097:ILE:HG22	6:AN:8037:LEU:HB3	1.90	0.54
6:AV:8168:SER:O	6:AV:8172:TYR:HD2	1.91	0.54
2:BB:2023:SER:O	2:BB:2027:GLN:HG3	2.08	0.54
6:BN:8133:GLN:HG3	6:BN:8176:THR:HG21	1.88	0.54
8:CH:5008:MET:O	8:CH:5026:LEU:HB3	2.08	0.54
6:A2:8184:LEU:HD22	6:A2:8192:ALA:HB2	1.88	0.54
7:BO:6081:GLU:H	8:BP:5064:MET:CE	2.21	0.54
2:BR:2023:SER:O	2:BR:2027:GLN:HG3	2.08	0.53
7:BW:6072:ILE:HD12	7:BW:6152:MET:HE2	1.89	0.53
2:AB:2040:ARG:C	2:AB:2042:ASN:H	2.11	0.53
2:BB:2027:GLN:OE1	2:BB:2093:ARG:HD3	2.09	0.53
1:BI:1069:PRO:O	1:BI:1071:SER:N	2.37	0.53
2:CJ:2040:ARG:HE	4:CL:4019:TRP:HZ2	1.54	0.53
7:AW:6066:SER:HA	7:AW:6069:ARG:O	2.08	0.53
8:AX:5008:MET:O	8:AX:5026:LEU:HB3	2.08	0.53
4:BD:4031:ASP:HA	6:BF:8020:VAL:HG22	1.90	0.53
2:CJ:2065:GLU:O	2:CJ:2075:ASP:HA	2.08	0.53
6:AV:8046:PRO:HB2	6:AV:8047:PRO:HD2	1.90	0.53
6:B2:8203:VAL:CG1	6:B2:8209:ASN:HA	2.33	0.53
6:AF:8046:PRO:HB2	6:AF:8047:PRO:HD2	1.89	0.53
2:AR:2040:ARG:HE	4:AT:4019:TRP:HZ2	1.56	0.53
4:BL:4031:ASP:HA	6:BN:8020:VAL:HG22	1.90	0.53
6:A2:8133:GLN:HG3	6:A2:8176:THR:HG21	1.90	0.53
2:AJ:2077:TYR:CD1	6:AN:8210:ASP:HB3	2.43	0.53
6:BF:8124:LEU:HA	6:BF:8127:MET:HE2	1.91	0.53
6:CF:8124:LEU:HA	6:CF:8127:MET:HE2	1.89	0.53
2:CR:2034:GLN:HG2	2:CR:2048:ARG:HG3	1.90	0.53
6:CV:8185:LYS:N	6:CV:8187:ASP:HB2	2.20	0.53
1:CY:1048:ARG:HG3	1:CY:1048:ARG:NH1	2.24	0.53
6:A2:8054:THR:HG23	6:A2:8057:TRP:HB2	1.91	0.53
6:AV:8054:THR:HG23	6:AV:8057:TRP:HB2	1.90	0.53
8:BX:5008:MET:O	8:BX:5026:LEU:HB3	2.08	0.53
2:CB:2034:GLN:HG2	2:CB:2048:ARG:HG3	1.91	0.53
1:CQ:1064:ARG:HD3	2:CR:2041:ASN:HB3	1.90	0.53
4:BT:4031:ASP:HA	6:BV:8020:VAL:HG22	1.91	0.53
1:CI:1069:PRO:O	1:CI:1071:SER:N	2.39	0.53
2:CJ:2034:GLN:HG2	2:CJ:2048:ARG:HG3	1.91	0.53
6:AF:8184:LEU:HD22	6:AF:8192:ALA:HB2	1.90	0.53
2:AJ:2023:SER:O	2:AJ:2027:GLN:HG3	2.09	0.53
4:AT:4019:TRP:HB2	4:AT:4021:MET:SD	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AV:8171:ARG:NH1	6:AV:8208:GLN:OE1	2.40	0.53
6:BF:8046:PRO:HB2	6:BF:8047:PRO:HD2	1.91	0.53
6:BV:8153:ALA:O	6:BV:8156:VAL:HG13	2.09	0.53
6:BV:8203:VAL:HG13	6:BV:8209:ASN:HA	1.90	0.53
7:A3:6047:GLU:HA	6:BF:8054:THR:HB	1.91	0.52
3:AK:3000:MET:HE2	3:AK:3002:GLN:HE22	1.73	0.52
2:AZ:2023:SER:O	2:AZ:2027:GLN:HG3	2.09	0.52
2:BZ:2023:SER:O	2:BZ:2027:GLN:HG3	2.09	0.52
3:CC:3000:MET:HE2	3:CC:3002:GLN:HE22	1.74	0.52
2:CJ:2077:TYR:HE2	6:CN:8209:ASN:HB2	1.73	0.52
6:A2:8046:PRO:HB2	6:A2:8047:PRO:HD2	1.91	0.52
6:BF:8133:GLN:HG3	6:BF:8176:THR:HG21	1.90	0.52
2:CJ:2023:SER:O	2:CJ:2027:GLN:HG3	2.08	0.52
6:CV:8184:LEU:HD22	6:CV:8192:ALA:HB2	1.90	0.52
2:BB:2065:GLU:O	2:BB:2075:ASP:HA	2.08	0.52
6:AF:8054:THR:HG23	6:AF:8057:TRP:HB2	1.89	0.52
8:AH:5008:MET:O	8:AH:5026:LEU:HB3	2.09	0.52
8:AP:5008:MET:O	8:AP:5026:LEU:HB3	2.09	0.52
5:AU:7005:SER:O	5:AU:7008:VAL:HG22	2.10	0.52
2:CB:2065:GLU:O	2:CB:2075:ASP:HA	2.08	0.52
2:CZ:2034:GLN:HG2	2:CZ:2048:ARG:HG3	1.91	0.52
3:BK:3024:GLN:NE2	3:BK:3027:MET:HB3	2.25	0.52
6:BN:8165:HIS:O	6:BN:8169:THR:HG23	2.10	0.52
2:BR:2043:LYS:HG2	2:BR:2067:TRP:CB	2.33	0.52
6:CF:8131:TRP:O	6:CF:8135:PRO:HG3	2.10	0.52
3:CK:3000:MET:HE2	3:CK:3002:GLN:HE22	1.74	0.52
2:BB:2034:GLN:HG2	2:BB:2048:ARG:HG3	1.91	0.52
6:BN:8184:LEU:HD22	6:BN:8192:ALA:HB2	1.90	0.52
6:CN:8155:LEU:HA	6:CN:8158:LEU:HD12	1.92	0.52
4:AL:4019:TRP:HB2	4:AL:4021:MET:SD	2.50	0.52
2:BJ:2065:GLU:O	2:BJ:2075:ASP:HA	2.09	0.52
6:BN:8203:VAL:HG13	6:BN:8209:ASN:HA	1.92	0.52
6:CF:8170:LEU:HA	6:CF:8173:ILE:HD12	1.91	0.52
3:BC:3000:MET:HE2	3:BC:3002:GLN:HE22	1.74	0.52
6:CN:8054:THR:HG23	6:CN:8057:TRP:HB3	1.92	0.52
6:CN:8145:VAL:HG22	6:CN:8149:ARG:HD2	1.92	0.52
6:AN:8046:PRO:HB2	6:AN:8047:PRO:HD2	1.92	0.52
6:AN:8181:ARG:O	6:AN:8184:LEU:HB2	2.09	0.52
6:B2:8185:LYS:N	6:B2:8187:ASP:HB2	2.22	0.52
6:BV:8054:THR:HG23	6:BV:8057:TRP:HB2	1.91	0.52
6:CN:8054:THR:HG23	6:CN:8057:TRP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A2:8044:GLU:HA	6:A2:8044:GLU:OE1	2.10	0.52
2:AB:2023:SER:O	2:AB:2027:GLN:HG3	2.09	0.52
6:AF:8135:PRO:C	6:AF:8137:THR:H	2.13	0.52
2:AJ:2034:GLN:HG2	2:AJ:2048:ARG:HG3	1.92	0.52
6:CF:8185:LYS:N	6:CF:8187:ASP:HB2	2.21	0.52
1:CI:1049:GLU:OE2	6:CN:8117:THR:HB	2.10	0.52
7:A3:6048:LEU:HD22	6:BF:8050:CYS:HA	1.92	0.51
5:AE:7005:SER:O	5:AE:7007:LEU:N	2.43	0.51
6:AN:8135:PRO:C	6:AN:8137:THR:H	2.12	0.51
2:BR:2034:GLN:HG2	2:BR:2048:ARG:HG3	1.93	0.51
6:CN:8199:LEU:HB2	6:CN:8215:ILE:HD13	1.91	0.51
6:AF:8072:VAL:HG13	6:AF:8114:LEU:HD21	1.91	0.51
6:AN:8131:TRP:O	6:AN:8135:PRO:HG3	2.10	0.51
2:AR:2023:SER:O	2:AR:2027:GLN:HG3	2.10	0.51
6:AV:8135:PRO:C	6:AV:8137:THR:H	2.13	0.51
2:CB:2096:LEU:HB3	6:CF:8036:THR:HG22	1.91	0.51
6:CF:8184:LEU:HD22	6:CF:8192:ALA:HB2	1.91	0.51
6:CN:8046:PRO:HB2	6:CN:8047:PRO:HD2	1.91	0.51
6:CN:8203:VAL:HG13	6:CN:8209:ASN:HA	1.92	0.51
6:A2:8128:LEU:HD22	6:A2:8151:LEU:HG	1.93	0.51
2:CJ:2075:ASP:O	6:CN:8171:ARG:HD3	2.11	0.51
2:AB:2034:GLN:HG2	2:AB:2048:ARG:HG3	1.92	0.51
4:CT:4019:TRP:HB2	4:CT:4021:MET:SD	2.51	0.51
4:CD:4019:TRP:HB2	4:CD:4021:MET:SD	2.51	0.51
4:BD:4019:TRP:HB2	4:BD:4021:MET:SD	2.51	0.51
2:BR:2074:LYS:HD3	6:BV:8168:SER:OG	2.11	0.51
6:CN:8124:LEU:HA	6:CN:8127:MET:HE2	1.91	0.51
2:CZ:2043:LYS:HE2	2:CZ:2067:TRP:CD2	2.46	0.51
2:BB:2097:ILE:HG22	6:BF:8037:LEU:HB3	1.93	0.51
6:BV:8203:VAL:HG22	6:BV:8211:PHE:HB2	1.92	0.51
2:BZ:2065:GLU:O	2:BZ:2075:ASP:HA	2.11	0.51
1:CA:1048:ARG:HG3	1:CA:1048:ARG:NH1	2.26	0.51
6:CF:8054:THR:HG23	6:CF:8057:TRP:HB2	1.93	0.51
7:AO:6043:TRP:CZ3	7:AO:6045:PRO:HG3	2.46	0.51
6:AV:8188:GLU:CD	6:AV:8190:GLN:HB2	2.31	0.51
3:BC:3063:ILE:HG22	4:BD:4067:ARG:HB3	1.93	0.51
2:BR:2040:ARG:C	2:BR:2042:ASN:H	2.14	0.51
6:BV:8133:GLN:HG3	6:BV:8176:THR:HG21	1.92	0.51
6:CF:8162:LEU:HD23	6:CF:8166:VAL:HB	1.92	0.51
2:AB:2043:LYS:HD3	2:AB:2067:TRP:CE3	2.46	0.51
7:AG:6043:TRP:CZ3	7:AG:6045:PRO:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AR:2077:TYR:CD1	6:AV:8210:ASP:HB3	2.46	0.50
6:BV:8046:PRO:HB2	6:BV:8047:PRO:HD2	1.92	0.50
6:BV:8177:CYS:HA	6:BV:8180:LEU:HB2	1.92	0.50
1:CQ:1053:LEU:CD2	7:CW:6065:SER:HB2	2.41	0.50
6:CV:8046:PRO:HB2	6:CV:8047:PRO:HD2	1.91	0.50
2:BJ:2034:GLN:HG2	2:BJ:2048:ARG:HG3	1.93	0.50
2:CB:2075:ASP:O	6:CF:8171:ARG:HD3	2.12	0.50
2:CR:2023:SER:O	2:CR:2027:GLN:HG3	2.10	0.50
2:AR:2092:LEU:HD22	4:AT:4053:LEU:HG	1.93	0.50
2:AZ:2065:GLU:O	2:AZ:2075:ASP:HA	2.11	0.50
3:BK:3063:ILE:HG22	4:BL:4067:ARG:HB3	1.93	0.50
6:CF:8177:CYS:HA	6:CF:8180:LEU:HB2	1.93	0.50
6:A2:8135:PRO:C	6:A2:8137:THR:H	2.13	0.50
6:AN:8184:LEU:HD22	6:AN:8192:ALA:HB2	1.91	0.50
3:AS:3063:ILE:HG22	4:AT:4067:ARG:HB3	1.93	0.50
1:AY:1048:ARG:HG3	1:AY:1048:ARG:HH11	1.76	0.50
6:BV:8145:VAL:HG22	6:BV:8149:ARG:HD2	1.94	0.50
1:BY:1048:ARG:NH1	1:BY:1048:ARG:HG3	2.26	0.50
6:A2:8177:CYS:HB2	6:A2:8195:TYR:HD1	1.76	0.50
4:AD:4019:TRP:HB2	4:AD:4021:MET:SD	2.50	0.50
4:AL:4002:LYS:HB2	4:AL:4003:PRO:HD3	1.93	0.50
3:AS:3000:MET:HE2	3:AS:3002:GLN:HE22	1.75	0.50
2:AZ:2040:ARG:HA	2:AZ:2089:ILE:HD11	1.93	0.50
2:CB:2023:SER:O	2:CB:2027:GLN:HG3	2.10	0.50
3:CC:3063:ILE:HG22	4:CD:4067:ARG:HB3	1.93	0.50
3:AC:3063:ILE:HG22	4:AD:4067:ARG:HB3	1.94	0.50
6:AV:8177:CYS:HB2	6:AV:8195:TYR:HB3	1.94	0.50
6:B2:8177:CYS:HA	6:B2:8180:LEU:HB2	1.93	0.50
2:BR:2097:ILE:HG22	6:BV:8037:LEU:HB3	1.93	0.50
3:CK:3063:ILE:HG22	4:CL:4067:ARG:HB3	1.93	0.50
2:AR:2074:LYS:HD3	6:AV:8168:SER:OG	2.11	0.50
2:BB:2040:ARG:NH1	7:BG:6166:ASP:O	2.44	0.50
6:CN:8184:LEU:HD23	6:CN:8187:ASP:HB3	1.94	0.50
2:CR:2065:GLU:O	2:CR:2075:ASP:HA	2.10	0.50
3:CS:3063:ILE:HG22	4:CT:4067:ARG:HB3	1.93	0.50
4:BL:4019:TRP:HB2	4:BL:4021:MET:SD	2.52	0.50
6:BN:8131:TRP:O	6:BN:8135:PRO:HG3	2.12	0.50
3:BS:3063:ILE:HG22	4:BT:4067:ARG:HB3	1.93	0.50
6:BV:8184:LEU:HD22	6:BV:8192:ALA:HB2	1.92	0.50
2:BZ:2034:GLN:HG2	2:BZ:2048:ARG:HG3	1.93	0.50
3:AC:3000:MET:HE2	3:AC:3002:GLN:HE22	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BR:2065:GLU:O	2:BR:2075:ASP:HA	2.11	0.50
4:BT:4019:TRP:HB2	4:BT:4021:MET:SD	2.52	0.50
6:BV:8131:TRP:O	6:BV:8135:PRO:HG3	2.12	0.50
6:BV:8135:PRO:C	6:BV:8137:THR:H	2.13	0.50
1:CY:1018:LYS:HA	1:CY:1064:ARG:HD2	1.93	0.50
1:AA:1053:LEU:CD2	7:AG:6065:SER:HB2	2.42	0.49
2:AJ:2065:GLU:O	2:AJ:2075:ASP:HA	2.12	0.49
2:AJ:2040:ARG:HA	2:AJ:2089:ILE:HD11	1.93	0.49
6:AV:8065:PHE:CE1	6:AV:8156:VAL:HG12	2.47	0.49
6:B2:8131:TRP:O	6:B2:8135:PRO:HG3	2.11	0.49
2:BJ:2043:LYS:HG2	2:BJ:2067:TRP:CB	2.37	0.49
6:CF:8046:PRO:HB2	6:CF:8047:PRO:HD2	1.92	0.49
7:CG:6081:GLU:HA	7:CG:6087:GLY:HA3	1.94	0.49
6:CN:8135:PRO:C	6:CN:8137:THR:H	2.15	0.49
6:CF:8135:PRO:C	6:CF:8137:THR:H	2.16	0.49
6:A2:8131:TRP:O	6:A2:8135:PRO:HG3	2.12	0.49
6:A2:8177:CYS:HA	6:A2:8180:LEU:HB2	1.93	0.49
7:A3:6043:TRP:CZ3	7:A3:6045:PRO:HG3	2.47	0.49
7:B3:6081:GLU:HA	7:B3:6087:GLY:HA3	1.94	0.49
2:CZ:2023:SER:O	2:CZ:2027:GLN:HG3	2.11	0.49
2:AZ:2034:GLN:HG2	2:AZ:2048:ARG:HG3	1.94	0.49
7:B3:6066:SER:O	7:B3:6067:ASN:O	2.30	0.49
5:BE:7005:SER:HB3	5:BE:7009:LYS:HG3	1.93	0.49
6:BN:8046:PRO:HB2	6:BN:8047:PRO:HD2	1.94	0.49
1:CI:1048:ARG:NH1	1:CI:1048:ARG:HG3	2.27	0.49
7:CO:6081:GLU:HA	7:CO:6087:GLY:HA3	1.95	0.49
6:CV:8131:TRP:O	6:CV:8135:PRO:HG3	2.13	0.49
6:AN:8181:ARG:HA	6:AN:8184:LEU:HD12	1.95	0.49
3:AS:3038:GLU:HB3	6:AV:8011:PHE:HE1	1.78	0.49
6:AV:8131:TRP:O	6:AV:8135:PRO:HG3	2.13	0.49
6:BF:8131:TRP:O	6:BF:8135:PRO:HG3	2.12	0.49
2:BZ:2043:LYS:HG2	2:BZ:2067:TRP:HB3	1.95	0.49
2:CJ:2040:ARG:C	2:CJ:2042:ASN:H	2.15	0.49
2:CJ:2092:LEU:HD22	4:CL:4053:LEU:HG	1.95	0.49
6:A2:8132:LEU:O	6:A2:8135:PRO:HD3	2.13	0.49
3:AK:3063:ILE:HG22	4:AL:4067:ARG:HB3	1.94	0.49
6:AN:8044:GLU:HA	6:AN:8044:GLU:OE1	2.13	0.49
6:AV:8181:ARG:O	6:AV:8184:LEU:HB2	2.13	0.49
7:BW:6066:SER:O	7:BW:6067:ASN:O	2.31	0.49
6:CV:8135:PRO:C	6:CV:8137:THR:H	2.16	0.49
2:AB:2065:GLU:O	2:AB:2075:ASP:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BK:3000:MET:HE2	3:BK:3002:GLN:HE22	1.77	0.49
1:BQ:1053:LEU:CD2	7:BW:6065:SER:HB2	2.43	0.49
1:CQ:1048:ARG:HG3	1:CQ:1048:ARG:NH1	2.27	0.49
1:AI:1050:PRO:HG3	6:AN:8159:HIS:HB2	1.93	0.49
7:AO:6081:GLU:HA	7:AO:6087:GLY:HA3	1.95	0.49
6:AV:8209:ASN:HB3	6:AV:8212:LYS:HE3	1.95	0.49
7:AW:6081:GLU:HA	7:AW:6087:GLY:HA3	1.95	0.49
6:BF:8203:VAL:O	6:BF:8207:ALA:HA	2.13	0.49
1:BQ:1048:ARG:NH1	1:BQ:1048:ARG:HG3	2.27	0.49
2:CJ:2040:ARG:HA	2:CJ:2089:ILE:HD11	1.94	0.49
6:A2:8181:ARG:O	6:A2:8184:LEU:HB2	2.13	0.49
3:BS:3000:MET:HE2	3:BS:3002:GLN:HE22	1.77	0.49
6:BV:8209:ASN:C	6:BV:8211:PHE:H	2.15	0.49
6:CN:8177:CYS:HA	6:CN:8180:LEU:HB2	1.95	0.49
6:CV:8054:THR:HG23	6:CV:8057:TRP:HB2	1.94	0.49
6:AF:8188:GLU:CD	6:AF:8190:GLN:HB2	2.33	0.48
2:AR:2034:GLN:HG2	2:AR:2048:ARG:HG3	1.95	0.48
1:BA:1048:ARG:HG3	1:BA:1048:ARG:NH1	2.26	0.48
6:BN:8054:THR:HG23	6:BN:8057:TRP:HB2	1.94	0.48
2:BR:2077:TYR:CD1	6:BV:8210:ASP:HB3	2.47	0.48
7:CO:6068:PRO:CD	7:CO:6069:ARG:H	2.17	0.48
6:AF:8108:PRO:HB2	6:AF:8153:ALA:CB	2.43	0.48
6:AF:8131:TRP:O	6:AF:8135:PRO:HG3	2.13	0.48
2:AR:2065:GLU:O	2:AR:2075:ASP:HA	2.12	0.48
7:AW:6043:TRP:CZ3	7:AW:6045:PRO:HG3	2.48	0.48
2:BJ:2092:LEU:HD22	4:BL:4053:LEU:HG	1.95	0.48
1:BA:1064:ARG:HD3	2:BB:2041:ASN:HB3	1.95	0.48
4:BD:4000:ASN:ND2	6:BF:8010:MET:HB2	2.27	0.48
3:BK:3038:GLU:HB3	6:BN:8011:PHE:HE1	1.78	0.48
7:BO:6081:GLU:HA	7:BO:6087:GLY:HA3	1.95	0.48
7:A3:6082:TRP:N	7:A3:6086:TYR:O	2.38	0.48
6:AV:8199:LEU:HB2	6:AV:8215:ILE:HD13	1.95	0.48
7:B3:6043:TRP:CZ3	7:B3:6045:PRO:HG3	2.48	0.48
6:BF:8044:GLU:HA	6:BF:8044:GLU:OE1	2.13	0.48
6:BV:8044:GLU:OE1	6:BV:8044:GLU:HA	2.13	0.48
6:CV:8132:LEU:O	6:CV:8135:PRO:HD3	2.14	0.48
1:AI:1053:LEU:CD2	7:AO:6065:SER:HB2	2.44	0.48
6:AV:8188:GLU:OE2	6:AV:8190:GLN:HB2	2.11	0.48
6:AF:8132:LEU:O	6:AF:8135:PRO:HD3	2.14	0.48
7:BO:6043:TRP:CZ3	7:BO:6045:PRO:HG3	2.48	0.48
6:CN:8131:TRP:O	6:CN:8135:PRO:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AE:7003:ASP:O	5:AE:7006:LEU:HB2	2.13	0.48
6:BF:8054:THR:HG23	6:BF:8057:TRP:HB2	1.95	0.48
6:BF:8113:LEU:HD13	6:BF:8116:LEU:HD12	1.96	0.48
7:BG:6043:TRP:CZ3	7:BG:6045:PRO:HG3	2.49	0.48
8:BX:5030:ASP:HB2	8:BX:5031:PRO:HD2	1.96	0.48
6:AF:8044:GLU:OE1	6:AF:8044:GLU:HA	2.13	0.48
6:AF:8185:LYS:N	6:AF:8187:ASP:HB2	2.21	0.48
6:AV:8133:GLN:HG3	6:AV:8176:THR:HG21	1.96	0.48
4:AL:4016:LYS:HG2	4:AL:4064:LEU:HD23	1.96	0.48
6:B2:8054:THR:HG23	6:B2:8057:TRP:HB2	1.95	0.48
6:B2:8132:LEU:O	6:B2:8135:PRO:HD3	2.14	0.48
6:B2:8184:LEU:HD23	6:B2:8187:ASP:HB3	1.95	0.48
1:CA:1053:LEU:CD2	7:CG:6065:SER:HB2	2.44	0.48
6:AF:8160:LEU:HA	6:AF:8162:LEU:HD13	1.96	0.48
4:BD:4016:LYS:HG2	4:BD:4064:LEU:HD23	1.96	0.48
7:CO:6066:SER:O	7:CO:6067:ASN:O	2.32	0.48
4:CT:4000:ASN:ND2	6:CV:8010:MET:HB2	2.29	0.48
6:CF:8168:SER:HA	6:CF:8171:ARG:HD3	1.96	0.47
1:CI:1053:LEU:CD2	7:CO:6065:SER:HB2	2.43	0.47
1:AQ:1048:ARG:NH1	1:AQ:1048:ARG:HG3	2.27	0.47
6:B2:8181:ARG:O	6:B2:8184:LEU:HB2	2.14	0.47
6:BF:8177:CYS:HA	6:BF:8180:LEU:HB2	1.95	0.47
2:BR:2092:LEU:HD22	4:BT:4053:LEU:HG	1.96	0.47
7:BW:6043:TRP:CZ3	7:BW:6045:PRO:HG3	2.49	0.47
6:CV:8177:CYS:HA	6:CV:8180:LEU:HB2	1.96	0.47
4:AT:4016:LYS:HG2	4:AT:4064:LEU:HD23	1.96	0.47
2:BB:2043:LYS:HG2	2:BB:2067:TRP:CB	2.39	0.47
4:CD:4000:ASN:ND2	6:CF:8010:MET:HB2	2.30	0.47
7:CW:6081:GLU:HA	7:CW:6087:GLY:HA3	1.97	0.47
6:AN:8201:LEU:HD22	6:AN:8205:VAL:HG21	1.95	0.47
6:B2:8135:PRO:C	6:B2:8137:THR:H	2.16	0.47
6:BN:8177:CYS:HA	6:BN:8180:LEU:HB2	1.95	0.47
6:CF:8168:SER:O	6:CF:8172:TYR:HD2	1.96	0.47
4:AD:4016:LYS:HG2	4:AD:4064:LEU:HD23	1.97	0.47
6:BV:8181:ARG:O	6:BV:8184:LEU:HB2	2.15	0.47
2:BB:2092:LEU:HD22	4:BD:4053:LEU:HG	1.97	0.47
8:BH:5030:ASP:HB2	8:BH:5031:PRO:HD2	1.97	0.47
6:BN:8044:GLU:HA	6:BN:8044:GLU:OE1	2.15	0.47
6:BN:8135:PRO:C	6:BN:8137:THR:H	2.16	0.47
6:BV:8188:GLU:CD	6:BV:8190:GLN:HB2	2.35	0.47
6:CF:8132:LEU:O	6:CF:8135:PRO:HD3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CV:8065:PHE:CE2	6:CV:8205:VAL:HG11	2.50	0.47
6:AF:8194:PRO:O	6:AF:8197:LEU:HB3	2.14	0.47
8:AP:5030:ASP:HB2	8:AP:5031:PRO:HD2	1.97	0.47
1:AQ:1053:LEU:CD2	7:AW:6065:SER:HB2	2.45	0.47
6:BN:8167:PHE:O	6:BN:8171:ARG:HG3	2.14	0.47
6:CV:8044:GLU:OE1	6:CV:8044:GLU:HA	2.15	0.47
8:A4:5030:ASP:HB2	8:A4:5031:PRO:HD2	1.97	0.47
6:AF:8181:ARG:HA	6:AF:8184:LEU:CD1	2.45	0.47
3:AK:3064:MET:HB2	4:AL:4004:PHE:CD2	2.50	0.47
7:AO:6068:PRO:CD	7:AO:6069:ARG:N	2.78	0.47
3:BS:3038:GLU:HB3	6:BV:8011:PHE:HE1	1.80	0.47
2:CB:2092:LEU:HD22	4:CD:4053:LEU:HG	1.97	0.47
7:AG:6081:GLU:HA	7:AG:6087:GLY:HA3	1.97	0.47
6:AN:8132:LEU:O	6:AN:8135:PRO:HD3	2.15	0.47
6:BF:8135:PRO:C	6:BF:8137:THR:H	2.17	0.47
4:BL:4016:LYS:HG2	4:BL:4064:LEU:HD23	1.97	0.47
7:A3:6066:SER:O	7:A3:6067:ASN:O	2.33	0.47
1:AI:1064:ARG:NH2	2:AJ:2040:ARG:HB3	2.29	0.47
6:CF:8181:ARG:O	6:CF:8184:LEU:HB2	2.15	0.47
6:CF:8188:GLU:CD	6:CF:8190:GLN:HB2	2.35	0.47
7:CG:6081:GLU:O	8:CH:5064:MET:HE1	2.15	0.47
6:CN:8044:GLU:HA	6:CN:8044:GLU:OE1	2.15	0.47
3:AC:3064:MET:HB2	4:AD:4004:PHE:CD2	2.50	0.47
6:AV:8066:GLN:HE22	6:AV:8069:ARG:HH11	1.63	0.47
6:AV:8185:LYS:N	6:AV:8187:ASP:HB2	2.22	0.47
7:AW:6066:SER:O	7:AW:6067:ASN:O	2.33	0.47
3:BC:3064:MET:HB2	4:BD:4004:PHE:CD2	2.50	0.47
6:BF:8181:ARG:O	6:BF:8184:LEU:HB2	2.15	0.47
6:BF:8188:GLU:CD	6:BF:8190:GLN:HB2	2.35	0.47
1:BI:1053:LEU:CD2	7:BO:6065:SER:HB2	2.45	0.47
6:BN:8184:LEU:HD23	6:BN:8187:ASP:HB3	1.96	0.47
6:CF:8002:SER:H	6:CF:8005:GLU:HB2	1.80	0.47
6:CV:8002:SER:H	6:CV:8005:GLU:HB2	1.80	0.47
6:AN:8141:LEU:HD22	6:AN:8148:ALA:HB2	1.96	0.46
2:AR:2077:TYR:CE2	6:AV:8209:ASN:HB2	2.50	0.46
3:BS:3064:MET:HB2	4:BT:4004:PHE:CD2	2.50	0.46
4:BT:4016:LYS:HG2	4:BT:4064:LEU:HD23	1.97	0.46
7:BW:6081:GLU:HA	7:BW:6087:GLY:HA3	1.97	0.46
4:CL:4019:TRP:HB2	4:CL:4021:MET:SD	2.55	0.46
6:CN:8132:LEU:O	6:CN:8135:PRO:HD3	2.15	0.46
7:A3:6024:LEU:HD13	7:A3:6080:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:6081:GLU:HA	7:BG:6087:GLY:HA3	1.97	0.46
6:BN:8181:ARG:O	6:BN:8184:LEU:HB2	2.15	0.46
3:CK:3064:MET:HB2	4:CL:4004:PHE:CD2	2.50	0.46
3:CS:3064:MET:HB2	4:CT:4004:PHE:CD2	2.49	0.46
7:CW:6066:SER:O	7:CW:6067:ASN:O	2.33	0.46
2:CZ:2065:GLU:O	2:CZ:2075:ASP:HA	2.14	0.46
6:AN:8188:GLU:CD	6:AN:8190:GLN:HB2	2.36	0.46
6:BF:8184:LEU:HD23	6:BF:8187:ASP:HB3	1.96	0.46
3:CC:3064:MET:HB2	4:CD:4004:PHE:CD2	2.50	0.46
6:CF:8184:LEU:HD23	6:CF:8187:ASP:HB3	1.97	0.46
7:CO:6043:TRP:CZ3	7:CO:6045:PRO:HG3	2.50	0.46
4:CT:4016:LYS:HG2	4:CT:4064:LEU:HD23	1.96	0.46
6:AF:8002:SER:H	6:AF:8005:GLU:HB2	1.80	0.46
6:AN:8002:SER:H	6:AN:8005:GLU:HB2	1.80	0.46
3:BK:3064:MET:HB2	4:BL:4004:PHE:CD2	2.51	0.46
5:BU:7005:SER:O	5:BU:7007:LEU:N	2.48	0.46
6:CF:8171:ARG:NH1	6:CF:8208:GLN:OE1	2.49	0.46
6:BF:8152:TYR:HD1	6:BF:8197:LEU:HD21	1.80	0.46
7:CG:6065:SER:OG	7:CG:6066:SER:N	2.48	0.46
4:AT:4059:ARG:HD3	4:AT:4061:ASN:OD1	2.16	0.46
6:BN:8195:TYR:HA	6:BN:8198:LEU:HD12	1.97	0.46
7:BO:6066:SER:O	7:BO:6067:ASN:O	2.34	0.46
2:CB:2040:ARG:HB2	2:CB:2087:SER:O	2.16	0.46
7:CG:6043:TRP:CZ3	7:CG:6045:PRO:HG3	2.51	0.46
6:CN:8127:MET:HG2	6:CN:8131:TRP:CZ2	2.51	0.46
6:AV:8044:GLU:OE1	6:AV:8044:GLU:HA	2.15	0.46
6:BN:8203:VAL:HG22	6:BN:8211:PHE:HB2	1.98	0.46
7:CG:6068:PRO:CD	7:CG:6069:ARG:N	2.79	0.46
2:CR:2038:ASN:HB2	2:CR:2090:VAL:HG22	1.98	0.46
6:AF:8127:MET:HG2	6:AF:8131:TRP:CZ2	2.51	0.46
2:AJ:2092:LEU:HD22	4:AL:4053:LEU:HG	1.97	0.46
8:AX:5030:ASP:HB2	8:AX:5031:PRO:HD2	1.98	0.46
6:BF:8002:SER:H	6:BF:8005:GLU:HB2	1.80	0.46
6:BV:8086:GLN:O	6:BV:8089:GLU:HB2	2.15	0.46
4:CD:4016:LYS:HG2	4:CD:4064:LEU:HD23	1.97	0.46
3:CC:3038:GLU:HB3	6:CF:8011:PHE:HE1	1.81	0.46
6:CV:8184:LEU:HD23	6:CV:8187:ASP:HB3	1.98	0.46
6:A2:8002:SER:H	6:A2:8005:GLU:HB2	1.81	0.46
7:AG:6068:PRO:CD	7:AG:6069:ARG:N	2.78	0.46
2:AJ:2043:LYS:HD3	2:AJ:2067:TRP:CE3	2.51	0.46
7:AW:6068:PRO:CD	7:AW:6069:ARG:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BV:8185:LYS:N	6:BV:8187:ASP:HB2	2.22	0.46
6:CF:8203:VAL:O	6:CF:8207:ALA:HA	2.15	0.46
7:CG:6066:SER:O	7:CG:6067:ASN:O	2.34	0.46
6:CV:8181:ARG:O	6:CV:8184:LEU:HB2	2.16	0.46
7:CW:6068:PRO:CD	7:CW:6069:ARG:N	2.79	0.46
2:AB:2092:LEU:HD22	4:AD:4053:LEU:HG	1.98	0.46
8:AH:5030:ASP:HB2	8:AH:5031:PRO:HD2	1.97	0.46
6:AN:8203:VAL:HG22	6:AN:8211:PHE:HB2	1.97	0.46
3:AS:3064:MET:HB2	4:AT:4004:PHE:CD2	2.51	0.46
6:AV:8002:SER:H	6:AV:8005:GLU:HB2	1.81	0.46
6:BV:8184:LEU:HD23	6:BV:8187:ASP:HB3	1.97	0.46
2:CZ:2038:ASN:HB2	2:CZ:2090:VAL:HG22	1.98	0.46
6:AF:8184:LEU:HD23	6:AF:8187:ASP:HB3	1.98	0.45
6:AN:8185:LYS:N	6:AN:8187:ASP:HB2	2.22	0.45
6:AV:8132:LEU:O	6:AV:8135:PRO:HD3	2.16	0.45
6:BN:8168:SER:HA	6:BN:8171:ARG:HD3	1.99	0.45
3:CS:3038:GLU:HB3	6:CV:8011:PHE:HE1	1.82	0.45
3:AC:3024:GLN:HE21	3:AC:3024:GLN:HB2	1.56	0.45
6:AN:8184:LEU:HD23	6:AN:8187:ASP:HB3	1.98	0.45
7:B3:6000:MET:HG3	7:B3:6002:LEU:HD13	1.98	0.45
7:B3:6065:SER:OG	7:B3:6066:SER:N	2.49	0.45
7:BO:6065:SER:OG	7:BO:6066:SER:N	2.49	0.45
6:CF:8086:GLN:O	6:CF:8089:GLU:HB2	2.16	0.45
6:CN:8181:ARG:O	6:CN:8184:LEU:HB2	2.17	0.45
3:CS:3000:MET:CE	3:CS:3002:GLN:NE2	2.79	0.45
6:A2:8007:LEU:HG	6:A2:8011:PHE:CE1	2.52	0.45
6:AN:8146:TRP:O	6:AN:8150:TRP:CD1	2.67	0.45
6:B2:8145:VAL:HG22	6:B2:8149:ARG:HD2	1.98	0.45
6:BF:8185:LYS:N	6:BF:8187:ASP:HB2	2.22	0.45
7:BW:6068:PRO:CD	7:BW:6069:ARG:N	2.79	0.45
6:CF:8184:LEU:HD21	6:CF:8191:ARG:HB3	1.98	0.45
4:CL:4016:LYS:HG2	4:CL:4064:LEU:HD23	1.98	0.45
2:CR:2092:LEU:HD22	4:CT:4053:LEU:HG	1.98	0.45
3:CS:3006:LEU:HD11	8:CX:5054:MET:HG2	1.98	0.45
6:A2:8066:GLN:HE22	6:A2:8205:VAL:HG13	1.82	0.45
3:AK:3000:MET:CE	3:AK:3002:GLN:NE2	2.80	0.45
4:AL:4059:ARG:HD3	4:AL:4061:ASN:OD1	2.16	0.45
2:CB:2038:ASN:HB2	2:CB:2090:VAL:HG22	1.98	0.45
3:CC:3006:LEU:HD11	8:CH:5054:MET:HG2	1.98	0.45
6:CN:8197:LEU:O	6:CN:8201:LEU:HG	2.16	0.45
2:BJ:2077:TYR:CD1	6:BN:8210:ASP:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BK:3024:GLN:HE22	3:BK:3027:MET:CE	2.29	0.45
4:BT:4059:ARG:HD3	4:BT:4061:ASN:OD1	2.16	0.45
7:CW:6043:TRP:CZ3	7:CW:6045:PRO:HG3	2.51	0.45
8:CX:5030:ASP:HB2	8:CX:5031:PRO:HD2	1.97	0.45
6:A2:8185:LYS:N	6:A2:8187:ASP:HB2	2.22	0.45
6:AF:8133:GLN:HG3	6:AF:8176:THR:HG21	1.97	0.45
7:AG:6066:SER:O	7:AG:6067:ASN:O	2.35	0.45
6:B2:8002:SER:H	6:B2:8005:GLU:HB2	1.81	0.45
6:B2:8209:ASN:HD22	6:B2:8212:LYS:HE3	1.82	0.45
6:BN:8185:LYS:N	6:BN:8187:ASP:HB2	2.22	0.45
8:BP:5030:ASP:HB2	8:BP:5031:PRO:HD2	1.97	0.45
6:BV:8002:SER:H	6:BV:8005:GLU:HB2	1.82	0.45
8:CH:5030:ASP:HB2	8:CH:5031:PRO:HD2	1.97	0.45
4:AT:4000:ASN:ND2	6:AV:8010:MET:HB2	2.32	0.45
6:B2:8188:GLU:CD	6:B2:8190:GLN:HB2	2.37	0.45
4:BL:4059:ARG:HD3	4:BL:4061:ASN:OD1	2.16	0.45
6:BN:8172:TYR:HA	6:BN:8175:ARG:HD2	1.98	0.45
1:BQ:1050:PRO:HG3	6:BV:8159:HIS:HB2	1.96	0.45
6:CF:8065:PHE:CE2	6:CF:8205:VAL:HG11	2.52	0.45
6:CN:8086:GLN:O	6:CN:8089:GLU:HB2	2.16	0.45
6:CN:8185:LYS:N	6:CN:8187:ASP:HB2	2.23	0.45
7:CW:6065:SER:OG	7:CW:6066:SER:N	2.49	0.45
1:CY:1018:LYS:HD3	1:CY:1064:ARG:NH2	2.31	0.45
6:AN:8174:ALA:HB2	6:AN:8202:THR:HG21	1.97	0.45
7:AO:6066:SER:O	7:AO:6067:ASN:O	2.35	0.45
3:BK:3069:ASN:OD1	4:BL:4018:LYS:HG2	2.17	0.45
6:CN:8195:TYR:HA	6:CN:8198:LEU:HD12	1.99	0.45
6:A2:8069:ARG:HA	6:A2:8156:VAL:HG23	1.99	0.45
6:BN:8002:SER:H	6:BN:8005:GLU:HB2	1.81	0.45
6:BN:8132:LEU:O	6:BN:8135:PRO:HD3	2.17	0.45
2:CB:2043:LYS:HE2	2:CB:2067:TRP:CD2	2.51	0.45
6:CF:8127:MET:HG2	6:CF:8131:TRP:CZ2	2.52	0.45
3:CK:3006:LEU:HD11	8:CP:5054:MET:HG2	1.98	0.45
2:CR:2092:LEU:CD2	4:CT:4056:VAL:HG22	2.37	0.45
6:A2:8127:MET:HE3	6:A2:8131:TRP:CH2	2.51	0.45
6:A2:8184:LEU:HD23	6:A2:8187:ASP:HB3	1.98	0.45
8:B4:5025:ILE:HG21	8:B4:5027:ARG:CZ	2.47	0.45
4:BT:4000:ASN:ND2	6:BV:8010:MET:HB2	2.31	0.45
7:BW:6065:SER:OG	7:BW:6066:SER:N	2.50	0.45
3:CK:3038:GLU:HB3	6:CN:8011:PHE:HE1	1.82	0.45
6:AF:8181:ARG:HA	6:AF:8184:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AN:8211:PHE:O	6:AN:8213:ASP:N	2.50	0.44
6:AV:8178:ILE:HG13	6:AV:8199:LEU:HD21	1.99	0.44
2:AB:2092:LEU:CD2	4:AD:4056:VAL:HG22	2.36	0.44
6:AF:8049:LYS:HG3	7:CG:6084:GLY:HA3	1.98	0.44
7:AG:6065:SER:OG	7:AG:6066:SER:N	2.50	0.44
7:AO:6065:SER:OG	7:AO:6066:SER:N	2.50	0.44
7:BO:6072:ILE:HG21	7:BO:6152:MET:CE	2.48	0.44
3:BS:3006:LEU:HD11	8:BX:5054:MET:HG2	1.99	0.44
5:CM:7007:LEU:HD11	6:CN:8156:VAL:HG21	2.00	0.44
7:BG:6068:PRO:HD2	7:BG:6069:ARG:N	2.31	0.44
2:BZ:2040:ARG:HB2	2:BZ:2087:SER:O	2.18	0.44
2:BZ:2038:ASN:HB2	2:BZ:2090:VAL:HG22	1.98	0.44
6:CN:8002:SER:H	6:CN:8005:GLU:HB2	1.82	0.44
7:A3:6068:PRO:CD	7:A3:6069:ARG:N	2.81	0.44
6:AF:8124:LEU:HA	6:AF:8127:MET:HE2	1.99	0.44
6:AF:8155:LEU:HD21	6:AF:8170:LEU:HD13	1.99	0.44
3:AS:3069:ASN:OD1	4:AT:4018:LYS:HG2	2.18	0.44
6:B2:8195:TYR:HA	6:B2:8198:LEU:HD12	1.99	0.44
7:B3:6068:PRO:HD2	7:B3:6069:ARG:N	2.30	0.44
7:BG:6068:PRO:CD	7:BG:6069:ARG:N	2.80	0.44
3:BC:3006:LEU:HD11	8:BH:5054:MET:HG2	2.00	0.44
3:BK:3006:LEU:HD11	8:BP:5054:MET:HG2	1.99	0.44
3:CC:3000:MET:CE	3:CC:3002:GLN:NE2	2.80	0.44
8:CP:5030:ASP:HB2	8:CP:5031:PRO:HD2	1.97	0.44
3:CS:3000:MET:HE2	3:CS:3002:GLN:NE2	2.32	0.44
6:A2:8160:LEU:HD12	6:A2:8160:LEU:H	1.82	0.44
7:A3:6065:SER:OG	7:A3:6066:SER:N	2.50	0.44
6:AV:8122:GLU:O	6:AV:8126:GLU:HG2	2.17	0.44
6:BF:8132:LEU:O	6:BF:8135:PRO:HD3	2.18	0.44
8:BH:5025:ILE:HG21	8:BH:5027:ARG:CZ	2.48	0.44
6:BV:8132:LEU:O	6:BV:8135:PRO:HD3	2.18	0.44
6:A2:8170:LEU:HA	6:A2:8173:ILE:HD12	2.00	0.44
2:BB:2038:ASN:HB2	2:BB:2090:VAL:HG22	1.99	0.44
3:BC:3038:GLU:HB3	6:BF:8011:PHE:HE1	1.83	0.44
6:BN:8146:TRP:O	6:BN:8150:TRP:HB2	2.16	0.44
1:BY:1064:ARG:NH2	2:BZ:2040:ARG:HB3	2.33	0.44
2:CJ:2019:THR:O	6:CN:8022:THR:HG21	2.17	0.44
4:BL:4000:ASN:ND2	6:BN:8010:MET:HB2	2.32	0.44
6:BV:8184:LEU:HD21	6:BV:8191:ARG:HB3	2.00	0.44
4:CL:4029:SER:HB2	6:CN:8022:THR:HG22	2.00	0.44
7:CO:6038:GLN:HG2	7:CO:6158:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CR:2043:LYS:HG2	2:CR:2067:TRP:CB	2.46	0.44
8:A4:5025:ILE:HG21	8:A4:5027:ARG:CZ	2.48	0.44
6:AF:8086:GLN:O	6:AF:8089:GLU:HB2	2.17	0.44
6:AN:8086:GLN:O	6:AN:8089:GLU:HB2	2.17	0.44
6:AN:8167:PHE:O	6:AN:8170:LEU:HB3	2.18	0.44
3:AS:3006:LEU:HD11	8:AX:5054:MET:HG2	2.00	0.44
6:BN:8188:GLU:CD	6:BN:8190:GLN:HB2	2.38	0.44
7:BO:6068:PRO:CD	7:BO:6069:ARG:N	2.80	0.44
4:CD:4059:ARG:HD3	4:CD:4061:ASN:OD1	2.18	0.44
6:CV:8188:GLU:CD	6:CV:8190:GLN:HB2	2.38	0.44
8:CX:5025:ILE:HG21	8:CX:5027:ARG:CZ	2.48	0.44
4:AD:4000:ASN:ND2	6:AF:8010:MET:HB2	2.33	0.44
6:AF:8108:PRO:HB3	6:AF:8150:TRP:CD2	2.53	0.44
6:AF:8118:GLN:HA	6:AF:8121:LEU:HD12	1.99	0.44
7:AG:6018:ASN:HD22	7:AG:6018:ASN:C	2.21	0.44
6:AV:8184:LEU:HD21	6:AV:8191:ARG:HB3	2.00	0.44
7:B3:6068:PRO:CD	7:B3:6069:ARG:N	2.79	0.44
1:BA:1053:LEU:CD2	7:BG:6065:SER:HB2	2.48	0.44
4:AD:4002:LYS:HG3	6:AF:8014:ARG:CB	2.48	0.43
6:AN:8209:ASN:HB3	6:AN:8212:LYS:HE3	1.99	0.43
3:AS:3000:MET:CE	3:AS:3002:GLN:NE2	2.81	0.43
6:BF:8086:GLN:O	6:BF:8089:GLU:HB2	2.18	0.43
2:BJ:2038:ASN:HB2	2:BJ:2090:VAL:HG22	1.99	0.43
4:BL:4005:LEU:HD23	4:BL:4030:VAL:HG11	2.00	0.43
3:CK:3000:MET:CE	3:CK:3002:GLN:NE2	2.80	0.43
4:CL:4059:ARG:HD3	4:CL:4061:ASN:OD1	2.18	0.43
6:CV:8086:GLN:O	6:CV:8089:GLU:HB2	2.18	0.43
6:CV:8127:MET:HG2	6:CV:8131:TRP:CZ2	2.53	0.43
3:AK:3071:THR:HG23	8:AP:5061:SER:HB3	2.00	0.43
2:AR:2049:VAL:HA	2:AR:2060:LEU:HD23	2.01	0.43
2:AZ:2049:VAL:HA	2:AZ:2060:LEU:HD23	2.00	0.43
6:BF:8127:MET:HG2	6:BF:8131:TRP:CZ2	2.53	0.43
6:BV:8188:GLU:OE2	6:BV:8190:GLN:HB2	2.18	0.43
6:CV:8184:LEU:HD21	6:CV:8191:ARG:HB3	1.99	0.43
6:A2:8188:GLU:CD	6:A2:8190:GLN:HB2	2.39	0.43
6:AF:8203:VAL:HG13	6:AF:8209:ASN:HA	2.00	0.43
6:AV:8184:LEU:HD23	6:AV:8187:ASP:HB3	1.99	0.43
7:BG:6065:SER:OG	7:BG:6066:SER:N	2.51	0.43
8:BP:5025:ILE:HG21	8:BP:5027:ARG:CZ	2.49	0.43
3:BS:3069:ASN:OD1	4:BT:4018:LYS:HG2	2.19	0.43
8:CH:5025:ILE:HG21	8:CH:5027:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CO:6068:PRO:CD	7:CO:6069:ARG:N	2.81	0.43
8:CP:5025:ILE:HG21	8:CP:5027:ARG:CZ	2.49	0.43
7:CW:6078:HIS:CD2	8:CX:5063:ILE:HG23	2.53	0.43
4:AD:4059:ARG:HD3	4:AD:4061:ASN:OD1	2.17	0.43
6:AF:8046:PRO:HB2	6:AF:8047:PRO:CD	2.48	0.43
2:AB:2077:TYR:HE2	6:AF:8209:ASN:HB2	1.71	0.43
4:AL:4031:ASP:HA	6:AN:8020:VAL:HG22	2.01	0.43
4:AT:4030:VAL:HG12	4:AT:4031:ASP:N	2.34	0.43
8:AX:5025:ILE:HG21	8:AX:5027:ARG:CZ	2.49	0.43
1:AY:1018:LYS:HE2	1:AY:1061:ASN:O	2.18	0.43
6:B2:8005:GLU:O	6:B2:8009:HIS:ND1	2.52	0.43
6:B2:8086:GLN:O	6:B2:8089:GLU:HB2	2.18	0.43
3:BC:3069:ASN:OD1	4:BD:4018:LYS:HG2	2.19	0.43
4:BD:4059:ARG:HD3	4:BD:4061:ASN:OD1	2.17	0.43
7:BG:6066:SER:O	7:BG:6067:ASN:O	2.37	0.43
4:BT:4030:VAL:HG12	4:BT:4031:ASP:N	2.34	0.43
6:AN:8127:MET:HG2	6:AN:8131:TRP:CZ2	2.53	0.43
8:AP:5025:ILE:HG21	8:AP:5027:ARG:CZ	2.49	0.43
7:B3:6000:MET:HG3	7:B3:6002:LEU:CD1	2.48	0.43
6:BN:8127:MET:HG2	6:BN:8131:TRP:CZ2	2.53	0.43
2:BR:2043:LYS:CG	2:BR:2067:TRP:HB3	2.40	0.43
6:CF:8044:GLU:HA	6:CF:8044:GLU:OE1	2.18	0.43
1:CI:1064:ARG:HD3	2:CJ:2041:ASN:HB3	2.00	0.43
3:AC:3006:LEU:HD11	8:AH:5054:MET:HG2	2.00	0.43
6:AV:8206:PHE:O	6:AV:8208:GLN:HG2	2.19	0.43
6:BV:8127:MET:HG2	6:BV:8131:TRP:CZ2	2.53	0.43
8:BX:5025:ILE:HG21	8:BX:5027:ARG:CZ	2.49	0.43
3:AS:3038:GLU:HB3	6:AV:8011:PHE:CE1	2.53	0.43
6:AV:8086:GLN:O	6:AV:8089:GLU:HB2	2.18	0.43
7:AW:6152:MET:HE3	7:AW:6152:MET:HB2	1.91	0.43
6:B2:8046:PRO:HB2	6:B2:8047:PRO:CD	2.49	0.43
6:B2:8127:MET:HG2	6:B2:8131:TRP:CZ2	2.54	0.43
1:CI:1064:ARG:NH2	2:CJ:2040:ARG:HB3	2.34	0.43
6:CN:8121:LEU:HD13	6:CN:8158:LEU:HA	1.99	0.43
8:AP:5008:MET:O	8:AP:5026:LEU:O	2.37	0.43
6:AV:8005:GLU:O	6:AV:8009:HIS:ND1	2.52	0.43
6:AV:8127:MET:HG2	6:AV:8131:TRP:CZ2	2.53	0.43
1:AY:1048:ARG:HG3	1:AY:1048:ARG:NH1	2.32	0.43
4:BD:4030:VAL:HG12	4:BD:4031:ASP:N	2.34	0.43
2:BR:2019:THR:O	6:BV:8022:THR:HG21	2.19	0.43
6:CF:8188:GLU:OE1	6:CF:8190:GLN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CV:8172:TYR:HA	6:CV:8175:ARG:HD2	2.01	0.43
6:AF:8188:GLU:OE2	6:AF:8190:GLN:HB2	2.18	0.43
8:AH:5008:MET:O	8:AH:5026:LEU:O	2.37	0.43
8:AH:5025:ILE:HG21	8:AH:5027:ARG:CZ	2.49	0.43
3:AK:3038:GLU:HB3	6:AN:8011:PHE:HE1	1.84	0.43
1:CI:1069:PRO:HD2	1:CI:1072:LEU:HD22	2.01	0.43
4:CT:4002:LYS:HG3	6:CV:8014:ARG:HB3	2.01	0.43
6:A2:8005:GLU:O	6:A2:8009:HIS:ND1	2.52	0.43
4:AD:4030:VAL:HG12	4:AD:4031:ASP:N	2.33	0.43
3:AK:3069:ASN:OD1	4:AL:4018:LYS:HG2	2.19	0.43
2:AR:2019:THR:O	6:AV:8022:THR:HG21	2.19	0.43
6:B2:8165:HIS:O	6:B2:8169:THR:HG23	2.19	0.43
6:BF:8152:TYR:CD1	6:BF:8197:LEU:HD21	2.54	0.43
6:BF:8209:ASN:C	6:BF:8211:PHE:H	2.21	0.43
3:BK:3038:GLU:HB3	6:BN:8011:PHE:CE1	2.54	0.43
2:BJ:2019:THR:O	6:BN:8022:THR:HG21	2.19	0.43
2:BR:2038:ASN:HB2	2:BR:2090:VAL:HG22	2.00	0.43
7:CO:6065:SER:OG	7:CO:6066:SER:N	2.52	0.43
8:A4:5008:MET:O	8:A4:5026:LEU:O	2.37	0.42
6:BF:8122:GLU:O	6:BF:8126:GLU:HG2	2.19	0.42
6:BV:8005:GLU:O	6:BV:8009:HIS:ND1	2.52	0.42
7:CG:6152:MET:HB2	7:CG:6152:MET:HE3	1.93	0.42
2:CJ:2075:ASP:OD1	6:CN:8175:ARG:NH2	2.52	0.42
6:CN:8005:GLU:O	6:CN:8009:HIS:ND1	2.52	0.42
6:CN:8055:PRO:HA	6:CN:8058:ARG:HB2	2.02	0.42
6:AN:8209:ASN:C	6:AN:8211:PHE:N	2.69	0.42
4:AT:4000:ASN:O	4:AT:4003:PRO:HD2	2.19	0.42
6:B2:8159:HIS:ND1	6:B2:8159:HIS:N	2.67	0.42
3:BC:3024:GLN:HE22	3:BC:3027:MET:CE	2.32	0.42
1:CA:1001:LEU:HD23	1:CA:1001:LEU:HA	1.83	0.42
2:CB:2019:THR:O	6:CF:8022:THR:HG21	2.19	0.42
6:A2:8086:GLN:O	6:A2:8089:GLU:HB2	2.18	0.42
7:AG:6068:PRO:HD2	7:AG:6069:ARG:N	2.29	0.42
4:AL:4030:VAL:HG12	4:AL:4031:ASP:N	2.35	0.42
6:BN:8086:GLN:O	6:BN:8089:GLU:HB2	2.18	0.42
1:BQ:1018:LYS:HE2	1:BQ:1061:ASN:O	2.19	0.42
6:CF:8005:GLU:O	6:CF:8009:HIS:ND1	2.52	0.42
7:CG:6038:GLN:HG2	7:CG:6158:LEU:HD23	2.01	0.42
1:CQ:1018:LYS:HA	1:CQ:1064:ARG:HD2	2.02	0.42
2:CR:2043:LYS:HE2	2:CR:2067:TRP:CD2	2.54	0.42
4:CT:4059:ARG:HD3	4:CT:4061:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CV:8005:GLU:O	6:CV:8009:HIS:ND1	2.52	0.42
7:CW:6152:MET:HE3	7:CW:6152:MET:HB2	1.90	0.42
6:A2:8046:PRO:HB2	6:A2:8047:PRO:CD	2.50	0.42
7:AG:6018:ASN:ND2	7:AG:6019:ASN:HB2	2.31	0.42
2:AJ:2040:ARG:C	2:AJ:2042:ASN:H	2.22	0.42
1:BA:1064:ARG:NH2	2:BB:2040:ARG:HB3	2.35	0.42
6:BV:8203:VAL:O	6:BV:8207:ALA:HA	2.19	0.42
4:CL:4005:LEU:HD23	4:CL:4030:VAL:HG11	2.01	0.42
2:CR:2040:ARG:HB2	2:CR:2087:SER:O	2.20	0.42
3:AC:3000:MET:CE	3:AC:3002:GLN:NE2	2.80	0.42
6:AF:8188:GLU:OE1	6:AF:8190:GLN:HB2	2.19	0.42
6:AN:8046:PRO:HB2	6:AN:8047:PRO:CD	2.50	0.42
4:BD:4002:LYS:HG3	6:BF:8014:ARG:CB	2.50	0.42
6:BF:8005:GLU:O	6:BF:8009:HIS:ND1	2.52	0.42
8:BH:5008:MET:O	8:BH:5026:LEU:O	2.38	0.42
6:AN:8012:TYR:O	6:AN:8016:ARG:HG2	2.20	0.42
1:AY:1001:LEU:HD23	1:AY:1001:LEU:HA	1.86	0.42
6:B2:8171:ARG:NH1	6:B2:8208:GLN:OE1	2.52	0.42
3:BC:3000:MET:CE	3:BC:3002:GLN:NE2	2.80	0.42
6:BF:8188:GLU:OE1	6:BF:8190:GLN:HB2	2.19	0.42
4:BL:4030:VAL:HG12	4:BL:4031:ASP:N	2.35	0.42
7:CO:6072:ILE:HB	7:CO:6137:LEU:HB2	2.00	0.42
6:A2:8124:LEU:HD12	6:A2:8127:MET:CE	2.49	0.42
2:AB:2016:GLU:OE1	6:AF:8020:VAL:HG11	2.19	0.42
3:AK:3006:LEU:HD11	8:AP:5054:MET:HG2	2.02	0.42
6:AN:8005:GLU:O	6:AN:8009:HIS:ND1	2.53	0.42
7:AW:6065:SER:OG	7:AW:6066:SER:N	2.52	0.42
6:B2:8113:LEU:HA	6:B2:8116:LEU:HD12	2.00	0.42
6:BV:8043:PRO:HB2	6:BV:8178:ILE:HG21	2.01	0.42
4:CL:4030:VAL:HG12	4:CL:4031:ASP:N	2.35	0.42
3:AK:3024:GLN:HE22	3:AK:3027:MET:CE	2.32	0.42
4:AL:4000:ASN:O	4:AL:4003:PRO:HD2	2.20	0.42
6:AN:8141:LEU:HD12	6:AN:8195:TYR:CD1	2.54	0.42
4:AT:4005:LEU:HD23	4:AT:4030:VAL:HG11	2.02	0.42
6:AV:8046:PRO:HB2	6:AV:8047:PRO:CD	2.50	0.42
8:AX:5008:MET:O	8:AX:5026:LEU:O	2.38	0.42
5:B1:7002:TRP:HB2	5:B1:7003:ASP:H	1.60	0.42
6:BN:8012:TYR:O	6:BN:8016:ARG:HG2	2.20	0.42
4:BT:4005:LEU:HD23	4:BT:4030:VAL:HG11	2.02	0.42
7:CO:6152:MET:HE3	7:CO:6152:MET:HB2	1.94	0.42
3:AC:3069:ASN:OD1	4:AD:4018:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:3071:THR:HG23	8:AH:5061:SER:HB3	2.01	0.42
1:AI:1018:LYS:HE2	1:AI:1061:ASN:O	2.20	0.42
7:AW:6081:GLU:HB2	8:AX:5064:MET:HE1	2.02	0.42
6:B2:8012:TYR:O	6:B2:8016:ARG:HG2	2.20	0.42
3:BC:3071:THR:HG23	8:BH:5061:SER:HB3	2.02	0.42
6:BN:8005:GLU:O	6:BN:8009:HIS:ND1	2.53	0.42
3:BS:3038:GLU:HB3	6:BV:8011:PHE:CE1	2.55	0.42
2:CJ:2043:LYS:HD3	2:CJ:2067:TRP:CD2	2.55	0.42
8:BX:5008:MET:O	8:BX:5026:LEU:O	2.38	0.42
3:BS:3071:THR:HG23	8:BX:5061:SER:HB3	2.02	0.42
6:CF:8154:THR:O	6:CF:8158:LEU:HG	2.20	0.42
8:A4:5063:ILE:HG22	8:A4:5064:MET:HG3	2.02	0.41
6:AF:8012:TYR:O	6:AF:8016:ARG:HG2	2.20	0.41
6:AF:8071:GLN:O	6:AF:8074:VAL:HB	2.20	0.41
6:BN:8178:ILE:HG13	6:BN:8199:LEU:HD21	2.02	0.41
1:BQ:1069:PRO:HD2	1:BQ:1072:LEU:HD22	2.02	0.41
6:BV:8012:TYR:O	6:BV:8016:ARG:HG2	2.20	0.41
1:CA:1069:PRO:HD2	1:CA:1072:LEU:HD22	2.02	0.41
2:CB:2067:TRP:CE2	2:CB:2074:LYS:HB2	2.55	0.41
6:CF:8012:TYR:O	6:CF:8016:ARG:HG2	2.20	0.41
3:CK:3071:THR:HG23	8:CP:5061:SER:HB3	2.01	0.41
6:A2:8100:LYS:HD3	6:A2:8104:ARG:CZ	2.50	0.41
7:A3:6072:ILE:HB	7:A3:6137:LEU:HB2	2.03	0.41
7:AW:6072:ILE:HB	7:AW:6137:LEU:HB2	2.03	0.41
6:B2:8168:SER:HA	6:B2:8171:ARG:HD3	2.01	0.41
6:BF:8046:PRO:HB2	6:BF:8047:PRO:CD	2.50	0.41
2:BJ:2049:VAL:HA	2:BJ:2060:LEU:HD23	2.03	0.41
8:BP:5008:MET:O	8:BP:5026:LEU:O	2.38	0.41
3:CC:3069:ASN:OD1	4:CD:4018:LYS:HG2	2.18	0.41
3:CK:3024:GLN:HE22	3:CK:3027:MET:CE	2.33	0.41
2:CZ:2040:ARG:HB2	2:CZ:2087:SER:O	2.20	0.41
6:AN:8007:LEU:HG	6:AN:8011:PHE:CE1	2.55	0.41
6:AN:8196:ASN:HA	6:AN:8215:ILE:HD11	2.02	0.41
2:AR:2038:ASN:HB2	2:AR:2090:VAL:HG22	2.01	0.41
1:AY:1069:PRO:HD2	1:AY:1072:LEU:HD22	2.02	0.41
2:AZ:2038:ASN:HB2	2:AZ:2090:VAL:HG22	2.01	0.41
6:B2:8167:PHE:O	6:B2:8171:ARG:HG3	2.20	0.41
4:BD:4002:LYS:HG3	6:BF:8014:ARG:HB3	2.01	0.41
3:BK:3000:MET:CE	3:BK:3002:GLN:NE2	2.82	0.41
6:BN:8209:ASN:C	6:BN:8211:PHE:H	2.24	0.41
3:CC:3024:GLN:HE22	3:CC:3027:MET:CE	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CN:8046:PRO:HB2	6:CN:8047:PRO:CD	2.50	0.41
6:CN:8172:TYR:CD2	6:CN:8175:ARG:NH1	2.88	0.41
2:AR:2040:ARG:HA	2:AR:2089:ILE:HD11	2.02	0.41
2:BJ:2077:TYR:HE2	6:BN:8209:ASN:HB2	1.80	0.41
1:CQ:1001:LEU:HA	1:CQ:1001:LEU:HD23	1.85	0.41
6:CV:8188:GLU:OE1	6:CV:8190:GLN:HB2	2.20	0.41
4:AD:4000:ASN:O	4:AD:4003:PRO:HD2	2.20	0.41
6:AF:8005:GLU:O	6:AF:8009:HIS:ND1	2.53	0.41
2:AJ:2049:VAL:HA	2:AJ:2060:LEU:HD23	2.03	0.41
6:AN:8188:GLU:OE2	6:AN:8190:GLN:HB2	2.20	0.41
6:AN:8203:VAL:O	6:AN:8207:ALA:HA	2.21	0.41
6:BN:8122:GLU:O	6:BN:8126:GLU:HG2	2.20	0.41
7:CG:6072:ILE:HB	7:CG:6137:LEU:HB2	2.02	0.41
7:CW:6078:HIS:HA	7:CW:6131:GLU:O	2.20	0.41
2:AB:2049:VAL:HA	2:AB:2060:LEU:HD23	2.03	0.41
6:B2:8184:LEU:HD21	6:B2:8191:ARG:HB3	2.03	0.41
1:BA:1069:PRO:HD2	1:BA:1072:LEU:HD22	2.02	0.41
2:BR:2049:VAL:HA	2:BR:2060:LEU:HD23	2.03	0.41
1:CA:1050:PRO:HG3	6:CF:8159:HIS:HB2	2.03	0.41
8:CH:5063:ILE:HG22	8:CH:5064:MET:HG3	2.03	0.41
6:CN:8122:GLU:O	6:CN:8126:GLU:HG2	2.21	0.41
6:CN:8184:LEU:HD21	6:CN:8191:ARG:HB3	2.02	0.41
4:CT:4005:LEU:HD23	4:CT:4030:VAL:HG11	2.02	0.41
6:CV:8012:TYR:O	6:CV:8016:ARG:HG2	2.21	0.41
6:CV:8168:SER:O	6:CV:8172:TYR:HD2	2.03	0.41
6:BF:8184:LEU:HD21	6:BF:8191:ARG:HB3	2.03	0.41
2:BJ:2089:ILE:HA	4:BL:4062:ASN:ND2	2.36	0.41
4:BT:4000:ASN:O	4:BT:4003:PRO:HD2	2.21	0.41
1:CY:1069:PRO:HD2	1:CY:1072:LEU:HD22	2.02	0.41
2:AJ:2038:ASN:HB2	2:AJ:2090:VAL:HG22	2.01	0.41
6:AN:8201:LEU:CD2	6:AN:8205:VAL:HG21	2.50	0.41
4:BL:4000:ASN:O	4:BL:4003:PRO:HD2	2.21	0.41
6:BN:8184:LEU:HD21	6:BN:8191:ARG:HB3	2.03	0.41
4:CD:4005:LEU:HD23	4:CD:4030:VAL:HG11	2.03	0.41
1:CI:1018:LYS:HE2	1:CI:1061:ASN:O	2.21	0.41
6:CV:8202:THR:HG22	6:CV:8208:GLN:HB2	2.02	0.41
5:BM:7011:TYR:HB2	6:BN:8152:TYR:CD2	2.55	0.41
7:BO:6072:ILE:HG21	7:BO:6152:MET:HE2	2.03	0.41
7:AO:6038:GLN:HG2	7:AO:6158:LEU:HD23	2.02	0.41
6:AV:8054:THR:HG23	6:AV:8057:TRP:CB	2.51	0.41
2:BB:2019:THR:O	6:BF:8022:THR:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CF:8209:ASN:O	6:CF:8212:LYS:HB2	2.21	0.41
7:CG:6068:PRO:HD2	7:CG:6069:ARG:N	2.29	0.41
6:CN:8012:TYR:O	6:CN:8016:ARG:HG2	2.21	0.41
4:CD:4002:LYS:HG3	6:CF:8014:ARG:HB3	2.03	0.41
6:AF:8100:LYS:HD3	6:AF:8104:ARG:CZ	2.51	0.41
6:BN:8128:LEU:HD23	6:BN:8147:LEU:HD23	2.02	0.41
6:A2:8209:ASN:HB3	6:A2:8212:LYS:HE3	2.03	0.41
1:AA:1018:LYS:HE2	1:AA:1061:ASN:O	2.21	0.41
6:AF:8054:THR:HG23	6:AF:8057:TRP:CB	2.50	0.41
3:AK:3000:MET:HE2	3:AK:3002:GLN:NE2	2.34	0.41
2:AJ:2092:LEU:CD2	4:AL:4056:VAL:HG22	2.38	0.41
5:AM:7005:SER:O	5:AM:7007:LEU:N	2.53	0.41
4:AL:4000:ASN:ND2	6:AN:8010:MET:HB2	2.36	0.41
6:A2:8184:LEU:HD21	6:A2:8191:ARG:HB3	2.03	0.41
6:AF:8162:LEU:HB2	6:AF:8167:PHE:CE1	2.56	0.41
5:AM:7010:THR:O	5:AM:7014:SER:HB2	2.21	0.41
3:AS:3071:THR:HG23	8:AX:5061:SER:HB3	2.03	0.41
6:B2:8100:LYS:HD3	6:B2:8104:ARG:CZ	2.51	0.41
2:BB:2049:VAL:HA	2:BB:2060:LEU:HD23	2.03	0.41
6:CF:8007:LEU:HG	6:CF:8011:PHE:CE1	2.55	0.41
8:CH:5007:PHE:O	8:CH:5008:MET:O	2.39	0.41
2:CJ:2084:ARG:NH2	2:CJ:2086:ASP:OD2	2.54	0.41
6:CN:8069:ARG:O	6:CN:8073:LEU:HD12	2.20	0.41
8:CP:5008:MET:O	8:CP:5026:LEU:O	2.38	0.41
6:B2:8188:GLU:OE1	6:B2:8190:GLN:HB2	2.20	0.41
3:AC:3016:ARG:CD	3:AC:3030:GLU:HG2	2.52	0.40
6:B2:8178:ILE:HG13	6:B2:8199:LEU:HD21	2.03	0.40
4:BD:4000:ASN:O	4:BD:4003:PRO:HD2	2.21	0.40
1:BI:1018:LYS:HE2	1:BI:1061:ASN:O	2.21	0.40
3:CS:3024:GLN:HE22	3:CS:3027:MET:CE	2.34	0.40
1:BI:1069:PRO:HD2	1:BI:1072:LEU:HD22	2.03	0.40
2:CJ:2067:TRP:CE2	2:CJ:2074:LYS:HB2	2.56	0.40
4:CL:4000:ASN:O	4:CL:4003:PRO:HD2	2.21	0.40
7:AG:6038:GLN:HG2	7:AG:6158:LEU:HD23	2.04	0.40
3:AK:3016:ARG:CD	3:AK:3030:GLU:HG2	2.51	0.40
7:AO:6072:ILE:HB	7:AO:6137:LEU:HB2	2.04	0.40
1:AQ:1069:PRO:HD2	1:AQ:1072:LEU:HD22	2.04	0.40
8:B4:5063:ILE:HG22	8:B4:5064:MET:HG3	2.04	0.40
6:BN:8188:GLU:OE1	6:BN:8190:GLN:HB2	2.21	0.40
3:BS:3000:MET:CE	3:BS:3002:GLN:NE2	2.81	0.40
6:BV:8162:LEU:HG	6:BV:8166:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CW:6068:PRO:HD2	7:CW:6069:ARG:N	2.29	0.40
6:AV:8090:PRO:HG3	6:CF:8112:THR:HG23	2.03	0.40
1:CQ:1064:ARG:HH22	7:CW:6167:SER:C	2.24	0.40
6:CV:8007:LEU:HG	6:CV:8011:PHE:CE1	2.55	0.40
1:CQ:1044:THR:OG1	6:CV:8161:PRO:HD2	2.22	0.40
1:CY:1001:LEU:HA	1:CY:1001:LEU:HD23	1.86	0.40
2:AJ:2016:GLU:OE1	6:AN:8020:VAL:HG11	2.21	0.40
6:AN:8215:ILE:HA	6:AN:8215:ILE:HD12	1.93	0.40
2:AR:2089:ILE:HA	4:AT:4062:ASN:ND2	2.36	0.40
5:AU:7002:TRP:HB2	5:AU:7003:ASP:H	1.66	0.40
6:BF:8012:TYR:O	6:BF:8016:ARG:HG2	2.22	0.40
7:BG:6038:GLN:HG2	7:BG:6158:LEU:HD23	2.03	0.40
1:BY:1069:PRO:HD2	1:BY:1072:LEU:HD22	2.03	0.40
6:CF:8188:GLU:OE2	6:CF:8190:GLN:HB2	2.21	0.40
3:CS:3069:ASN:OD1	4:CT:4018:LYS:HG2	2.20	0.40
7:BW:6038:GLN:HG2	7:BW:6158:LEU:HD23	2.02	0.40
8:CX:5008:MET:O	8:CX:5026:LEU:O	2.38	0.40
6:A2:8012:TYR:O	6:A2:8016:ARG:HG2	2.21	0.40
4:AD:4002:LYS:HG3	6:AF:8014:ARG:HB3	2.02	0.40
2:AJ:2089:ILE:HA	4:AL:4062:ASN:ND2	2.37	0.40
7:AO:6152:MET:HB2	7:AO:6152:MET:HE3	1.91	0.40
6:AV:8162:LEU:HG	6:AV:8166:VAL:HG11	2.04	0.40
7:B3:6072:ILE:HB	7:B3:6137:LEU:HB2	2.03	0.40
2:BB:2067:TRP:CE2	2:BB:2074:LYS:HB2	2.56	0.40
6:BF:8188:GLU:OE2	6:BF:8190:GLN:HB2	2.22	0.40
7:BG:6020:ILE:CD1	7:BG:6139:PRO:HB3	2.52	0.40
3:BK:3071:THR:HG23	8:BP:5061:SER:HB3	2.04	0.40
5:CE:7002:TRP:HB2	5:CE:7003:ASP:H	1.68	0.40
2:CB:2043:LYS:HG3	2:CB:2043:LYS:H	1.72	0.40
1:AQ:1018:LYS:HE2	1:AQ:1061:ASN:O	2.22	0.40
2:AR:2067:TRP:CE2	2:AR:2074:LYS:HB2	2.56	0.40
6:AV:8043:PRO:HB2	6:AV:8178:ILE:HG21	2.03	0.40
1:BA:1018:LYS:HE2	1:BA:1061:ASN:O	2.21	0.40
2:BB:2089:ILE:HA	4:BD:4062:ASN:ND2	2.37	0.40
2:BZ:2049:VAL:HA	2:BZ:2060:LEU:HD23	2.03	0.40
2:CR:2077:TYR:CD1	6:CV:8210:ASP:HB3	2.57	0.40
7:CW:6072:ILE:HB	7:CW:6137:LEU:HB2	2.03	0.40
5:BE:7002:TRP:HB2	5:BE:7003:ASP:H	1.67	0.40
6:BV:8069:ARG:NH2	6:BV:8160:LEU:HD11	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	AI	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	AQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	AY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	Ag	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	Ao	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	5	27
1	Aw	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	5	27
1	BA	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	BI	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	5	27
1	BQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	BY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	Bg	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	Bo	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	Bw	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	CA	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	CI	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	CQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	CY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	Cg	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
1	Co	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	5	27
2	AB	96/118 (81%)	92 (96%)	4 (4%)	0	100	100
2	AJ	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	AR	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	AZ	96/118 (81%)	92 (96%)	4 (4%)	0	100	100
2	Ah	96/118 (81%)	90 (94%)	3 (3%)	3 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Ap	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	Ax	96/118 (81%)	92 (96%)	3 (3%)	1 (1%)	15	49
2	BB	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	BJ	96/118 (81%)	90 (94%)	4 (4%)	2 (2%)	7	30
2	BR	96/118 (81%)	90 (94%)	4 (4%)	2 (2%)	7	30
2	BZ	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	Bh	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	Bp	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	Bx	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	CB	96/118 (81%)	90 (94%)	5 (5%)	1 (1%)	15	49
2	CJ	96/118 (81%)	89 (93%)	7 (7%)	0	100	100
2	CR	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	CZ	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	Ch	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	Cp	96/118 (81%)	89 (93%)	7 (7%)	0	100	100
3	AC	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	AK	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	AS	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Aa	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Ai	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Aq	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Ay	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	BC	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	BK	75/92 (82%)	74 (99%)	1 (1%)	0	100	100
3	BS	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Ba	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Bi	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Bq	75/92 (82%)	74 (99%)	1 (1%)	0	100	100
3	By	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	CC	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	CK	75/92 (82%)	73 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CS	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Ca	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Ci	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
3	Cq	75/92 (82%)	73 (97%)	2 (3%)	0	100	100
4	AD	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	AL	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	AT	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
4	Ab	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Aj	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
4	Ar	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Az	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	BD	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
4	BL	69/86 (80%)	67 (97%)	2 (3%)	0	100	100
4	BT	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Bb	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Bj	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Br	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Bz	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	CD	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	CL	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	CT	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Cb	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Cj	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
4	Cr	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
5	A1	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	7
5	AE	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	7
5	AM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	7
5	AU	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	7
5	Ac	15/124 (12%)	9 (60%)	5 (33%)	1 (7%)	1	7
5	Ak	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	7
5	As	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B1	15/124 (12%)	10 (67%)	3 (20%)	2 (13%)	0	1
5	BE	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	7
5	BM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	7
5	BU	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	7
5	Bc	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	7
5	Bk	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	7
5	Bs	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	7
5	CE	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	7
5	CM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	7
5	CU	15/124 (12%)	10 (67%)	5 (33%)	0	100	100
5	Cc	15/124 (12%)	9 (60%)	5 (33%)	1 (7%)	1	7
5	Ck	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	7
5	Cs	15/124 (12%)	10 (67%)	2 (13%)	3 (20%)	0	0
6	A2	214/247 (87%)	187 (87%)	17 (8%)	10 (5%)	2	14
6	AF	214/247 (87%)	182 (85%)	22 (10%)	10 (5%)	2	14
6	AN	214/247 (87%)	174 (81%)	31 (14%)	9 (4%)	3	16
6	AV	214/247 (87%)	182 (85%)	21 (10%)	11 (5%)	2	13
6	Ad	214/247 (87%)	183 (86%)	20 (9%)	11 (5%)	2	13
6	Al	214/247 (87%)	183 (86%)	21 (10%)	10 (5%)	2	14
6	At	214/247 (87%)	182 (85%)	21 (10%)	11 (5%)	2	13
6	B2	214/247 (87%)	179 (84%)	23 (11%)	12 (6%)	2	11
6	BF	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	3	19
6	BN	214/247 (87%)	185 (86%)	22 (10%)	7 (3%)	4	21
6	BV	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	3	19
6	Bd	214/247 (87%)	185 (86%)	19 (9%)	10 (5%)	2	14
6	Bl	214/247 (87%)	186 (87%)	18 (8%)	10 (5%)	2	14
6	Bt	214/247 (87%)	181 (85%)	27 (13%)	6 (3%)	5	25
6	CF	214/247 (87%)	187 (87%)	19 (9%)	8 (4%)	3	19
6	CN	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	3	19
6	CV	214/247 (87%)	182 (85%)	24 (11%)	8 (4%)	3	19
6	Cd	214/247 (87%)	185 (86%)	19 (9%)	10 (5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Cl	214/247 (87%)	186 (87%)	19 (9%)	9 (4%)	3	16
6	Ct	214/247 (87%)	178 (83%)	26 (12%)	10 (5%)	2	14
7	A3	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	AG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	AO	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	AW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	Ae	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	Am	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	Au	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	B3	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	6	27
7	BG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	BO	123/186 (66%)	115 (94%)	4 (3%)	4 (3%)	4	21
7	BW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	Be	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	6	27
7	Bm	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	6	27
7	Bu	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	CG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	CO	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	CW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	Ce	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
7	Cm	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	6	27
7	Cu	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	4	21
8	A4	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	AH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	AP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	AX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	Af	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	An	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	Av	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	B4	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	BH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	BP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	BX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	Bf	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	Bn	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	Bv	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	CH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	CP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	CX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	Cf	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	Cn	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
8	Cv	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	10	39
All	All	14800/20960 (71%)	13553 (92%)	894 (6%)	353 (2%)	6	27

All (353) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AM	7006	LEU
6	AN	8028	ILE
6	AN	8185	LYS
6	AN	8186	GLU
6	AN	8212	LYS
7	AO	6162	SER
8	AP	5008	MET
5	AE	7006	LEU
6	AF	8028	ILE
6	AF	8185	LYS
6	AF	8186	GLU
7	AG	6162	SER
8	AH	5008	MET
5	AU	7006	LEU
6	AV	8028	ILE
6	AV	8185	LYS
6	AV	8186	GLU
7	AW	6011	HIS
8	AX	5008	MET
5	Ac	7006	LEU
6	Ad	8028	ILE
6	Ad	8185	LYS

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Mol	Chain	Res	Type
6	Ad	8209	ASN
7	Ae	6011	HIS
8	Af	5008	MET
5	Ak	7006	LEU
6	Al	8028	ILE
6	Al	8185	LYS
6	Al	8186	GLU
7	Am	6011	HIS
8	An	5008	MET
5	As	7006	LEU
6	At	8028	ILE
6	At	8185	LYS
6	At	8186	GLU
6	At	8212	LYS
7	Au	6011	HIS
8	Av	5008	MET
5	A1	7006	LEU
6	A2	8028	ILE
6	A2	8185	LYS
8	A4	5008	MET
2	Ax	2042	ASN
5	BE	7006	LEU
6	BF	8185	LYS
7	BG	6011	HIS
8	BH	5008	MET
5	BM	7006	LEU
6	BN	8028	ILE
6	BN	8185	LYS
7	BO	6164	ASN
8	BP	5008	MET
5	BU	7006	LEU
6	BV	8028	ILE
6	BV	8185	LYS
7	BW	6011	HIS
8	BX	5008	MET
5	Bc	7006	LEU
6	Bd	8133	GLN
6	Bd	8185	LYS
6	Bd	8186	GLU
8	Bf	5008	MET
6	Bl	8034	ASN
6	Bl	8185	LYS

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Mol	Chain	Res	Type
8	Bn	5008	MET
5	Bs	7006	LEU
6	Bt	8185	LYS
6	Bt	8186	GLU
8	Bv	5008	MET
5	B1	7006	LEU
6	B2	8133	GLN
6	B2	8185	LYS
6	B2	8186	GLU
8	B4	5008	MET
5	CE	7006	LEU
6	CF	8185	LYS
6	CF	8186	GLU
8	CH	5008	MET
5	CM	7006	LEU
6	CN	8028	ILE
6	CN	8185	LYS
8	CP	5008	MET
6	CV	8185	LYS
6	CV	8186	GLU
8	CX	5008	MET
5	Cc	7006	LEU
6	Cd	8185	LYS
6	Cd	8186	GLU
7	Ce	6011	HIS
8	Cf	5008	MET
5	Ck	7006	LEU
6	Cl	8185	LYS
6	Cl	8186	GLU
7	Cm	6011	HIS
8	Cn	5008	MET
5	Cs	7002	TRP
5	Cs	7006	LEU
8	Cv	5008	MET
1	AI	1070	ASP
6	AN	8133	GLN
7	AO	6011	HIS
1	AA	1070	ASP
6	AF	8133	GLN
6	AF	8207	ALA
7	AG	6011	HIS
1	AQ	1070	ASP

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Mol	Chain	Res	Type
6	AV	8026	SER
6	AV	8133	GLN
6	AV	8207	ALA
7	AW	6162	SER
1	AY	1070	ASP
6	Ad	8026	SER
6	Ad	8133	GLN
6	Ad	8186	GLU
7	Ae	6162	SER
1	Ag	1070	ASP
6	Al	8133	GLN
7	Am	6162	SER
7	Am	6164	ASN
1	Ao	1070	ASP
6	At	8026	SER
6	At	8133	GLN
7	Au	6162	SER
6	A2	8026	SER
6	A2	8133	GLN
6	A2	8186	GLU
6	A2	8209	ASN
7	A3	6011	HIS
7	A3	6162	SER
1	Aw	1070	ASP
1	BA	1070	ASP
6	BF	8026	SER
6	BF	8028	ILE
6	BF	8133	GLN
6	BF	8186	GLU
7	BG	6162	SER
1	BI	1070	ASP
2	BJ	2043	LYS
6	BN	8133	GLN
6	BN	8186	GLU
7	BO	6011	HIS
7	BO	6162	SER
1	BQ	1070	ASP
6	BV	8133	GLN
6	BV	8186	GLU
7	BW	6162	SER
1	BY	1070	ASP
6	Bd	8028	ILE

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Mol	Chain	Res	Type
6	Bd	8034	ASN
7	Be	6011	HIS
1	Bg	1070	ASP
6	Bl	8028	ILE
6	Bl	8133	GLN
6	Bl	8186	GLU
7	Bm	6011	HIS
7	Bm	6162	SER
1	Bo	1070	ASP
6	Bt	8028	ILE
6	Bt	8133	GLN
7	Bu	6011	HIS
7	Bu	6162	SER
6	B2	8028	ILE
6	B2	8158	LEU
7	B3	6011	HIS
7	B3	6162	SER
1	Bw	1070	ASP
1	CA	1070	ASP
2	CB	2043	LYS
6	CF	8026	SER
6	CF	8028	ILE
6	CF	8133	GLN
7	CG	6011	HIS
7	CG	6162	SER
6	CN	8026	SER
6	CN	8133	GLN
6	CN	8186	GLU
7	CO	6011	HIS
7	CO	6162	SER
7	CO	6164	ASN
1	CQ	1070	ASP
6	CV	8028	ILE
6	CV	8133	GLN
7	CW	6011	HIS
7	CW	6162	SER
1	CY	1070	ASP
6	Cd	8028	ILE
6	Cd	8133	GLN
7	Ce	6162	SER
1	Cg	1070	ASP
6	Cl	8028	ILE

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Mol	Chain	Res	Type
6	Cl	8133	GLN
6	Cl	8212	LYS
7	Cm	6162	SER
1	Co	1070	ASP
6	Ct	8028	ILE
6	Ct	8185	LYS
6	Ct	8186	GLU
7	Cu	6011	HIS
7	Cu	6162	SER
7	Cu	6164	ASN
6	AN	8003	GLY
6	AN	8026	SER
6	AF	8026	SER
6	Ad	8158	LEU
6	Al	8026	SER
6	Al	8212	LYS
6	At	8113	LEU
7	A3	6164	ASN
6	BV	8026	SER
6	Bd	8026	SER
7	Be	6162	SER
6	Bl	8026	SER
6	Bl	8209	ASN
6	B2	8026	SER
6	B2	8034	ASN
6	CF	8209	ASN
6	CV	8026	SER
6	Cd	8026	SER
6	Cd	8212	LYS
6	Cl	8026	SER
5	Cs	7001	VAL
6	Ct	8026	SER
6	Ct	8133	GLN
6	AF	8046	PRO
6	AF	8209	ASN
7	AG	6164	ASN
6	AV	8019	ALA
6	AV	8046	PRO
7	AW	6164	ASN
6	Ad	8003	GLY
6	Ad	8046	PRO
6	Ad	8110	LEU

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Mol	Chain	Res	Type
7	Ae	6164	ASN
2	Ah	2098	ALA
6	Al	8003	GLY
6	Al	8207	ALA
6	At	8046	PRO
7	Au	6067	ASN
7	Au	6164	ASN
6	A2	8003	GLY
6	A2	8034	ASN
6	BF	8003	GLY
7	BG	6164	ASN
2	BJ	2098	ALA
6	BN	8003	GLY
2	BR	2041	ASN
6	BV	8003	GLY
7	BW	6164	ASN
6	Bd	8046	PRO
7	Be	6067	ASN
6	Bt	8046	PRO
7	Bu	6067	ASN
5	B1	7003	ASP
6	B2	8046	PRO
7	B3	6067	ASN
7	CG	6067	ASN
7	CG	6164	ASN
1	CI	1069	PRO
1	CI	1070	ASP
7	CO	6067	ASN
7	CW	6067	ASN
7	Ce	6067	ASN
7	Ce	6164	ASN
7	Cm	6067	ASN
6	Ct	8036	THR
6	Ct	8046	PRO
6	AN	8188	GLU
7	AO	6067	ASN
7	AO	6164	ASN
6	AF	8003	GLY
6	AF	8188	GLU
7	AG	6067	ASN
6	AV	8003	GLY
6	AV	8188	GLU

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Mol	Chain	Res	Type
7	AW	6067	ASN
6	Ad	8188	GLU
7	Ae	6067	ASN
2	Ah	2041	ASN
2	Ah	2043	LYS
6	Al	8188	GLU
7	Am	6067	ASN
6	At	8003	GLY
6	At	8019	ALA
6	A2	8188	GLU
7	A3	6067	ASN
1	BA	1069	PRO
7	BG	6067	ASN
1	BI	1069	PRO
6	BN	8026	SER
6	BN	8046	PRO
7	BO	6067	ASN
2	BR	2043	LYS
7	BW	6067	ASN
6	Bd	8025	SER
6	Bl	8003	GLY
7	Bm	6067	ASN
6	Bt	8003	GLY
7	Bu	6164	ASN
6	B2	8207	ALA
1	CA	1069	PRO
6	CN	8003	GLY
6	CN	8046	PRO
7	CW	6164	ASN
6	Cd	8210	ASP
6	Cl	8003	GLY
6	Cl	8188	GLU
7	Cu	6067	ASN
1	AI	1069	PRO
6	AN	8046	PRO
1	AA	1069	PRO
1	AQ	1069	PRO
6	AV	8210	ASP
1	Ao	1069	PRO
6	At	8188	GLU
1	Aw	1069	PRO
6	BF	8188	GLU

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Mol	Chain	Res	Type
1	BQ	1069	PRO
6	BV	8046	PRO
6	BV	8188	GLU
6	Bd	8003	GLY
6	Bd	8188	GLU
6	Bl	8188	GLU
6	B2	8188	GLU
6	CF	8003	GLY
6	CN	8188	GLU
1	CQ	1069	PRO
6	CV	8003	GLY
6	CV	8188	GLU
1	CY	1069	PRO
6	Cd	8188	GLU
1	Cg	1069	PRO
6	Ct	8003	GLY
6	Ct	8188	GLU
6	Ct	8204	GLN
1	AY	1069	PRO
1	Ag	1069	PRO
6	BF	8046	PRO
1	BY	1069	PRO
1	Bo	1069	PRO
6	B2	8164	PRO
1	Bw	1069	PRO
6	CF	8046	PRO
6	Cd	8003	GLY
6	Cd	8046	PRO
1	Co	1069	PRO
6	Al	8046	PRO
1	Bg	1069	PRO
6	A2	8046	PRO
6	Cl	8046	PRO
6	Bl	8046	PRO
6	B2	8003	GLY
6	CV	8046	PRO
5	Bk	7001	VAL

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	77/101 (76%)	70 (91%)	7 (9%)	9	33
1	AI	77/101 (76%)	72 (94%)	5 (6%)	17	47
1	AQ	77/101 (76%)	72 (94%)	5 (6%)	17	47
1	AY	77/101 (76%)	71 (92%)	6 (8%)	12	40
1	Ag	77/101 (76%)	71 (92%)	6 (8%)	12	40
1	Ao	77/101 (76%)	73 (95%)	4 (5%)	23	55
1	Aw	77/101 (76%)	72 (94%)	5 (6%)	17	47
1	BA	77/101 (76%)	72 (94%)	5 (6%)	17	47
1	BI	77/101 (76%)	72 (94%)	5 (6%)	17	47
1	BQ	77/101 (76%)	72 (94%)	5 (6%)	17	47
1	BY	77/101 (76%)	72 (94%)	5 (6%)	17	47
1	Bg	77/101 (76%)	72 (94%)	5 (6%)	17	47
1	Bo	77/101 (76%)	71 (92%)	6 (8%)	12	40
1	Bw	77/101 (76%)	71 (92%)	6 (8%)	12	40
1	CA	77/101 (76%)	72 (94%)	5 (6%)	17	47
1	CI	77/101 (76%)	72 (94%)	5 (6%)	17	47
1	CQ	77/101 (76%)	71 (92%)	6 (8%)	12	40
1	CY	77/101 (76%)	71 (92%)	6 (8%)	12	40
1	Cg	77/101 (76%)	71 (92%)	6 (8%)	12	40
1	Co	77/101 (76%)	73 (95%)	4 (5%)	23	55
2	AB	94/110 (86%)	90 (96%)	4 (4%)	29	62
2	AJ	94/110 (86%)	92 (98%)	2 (2%)	53	79
2	AR	94/110 (86%)	91 (97%)	3 (3%)	39	69
2	AZ	94/110 (86%)	90 (96%)	4 (4%)	29	62
2	Ah	94/110 (86%)	89 (95%)	5 (5%)	22	54
2	Ap	94/110 (86%)	91 (97%)	3 (3%)	39	69
2	Ax	94/110 (86%)	90 (96%)	4 (4%)	29	62
2	BB	94/110 (86%)	90 (96%)	4 (4%)	29	62
2	BJ	94/110 (86%)	88 (94%)	6 (6%)	17	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BR	94/110 (86%)	90 (96%)	4 (4%)	29	62
2	BZ	94/110 (86%)	90 (96%)	4 (4%)	29	62
2	Bh	94/110 (86%)	90 (96%)	4 (4%)	29	62
2	Bp	94/110 (86%)	89 (95%)	5 (5%)	22	54
2	Bx	94/110 (86%)	88 (94%)	6 (6%)	17	48
2	CB	94/110 (86%)	89 (95%)	5 (5%)	22	54
2	CJ	94/110 (86%)	90 (96%)	4 (4%)	29	62
2	CR	94/110 (86%)	91 (97%)	3 (3%)	39	69
2	CZ	94/110 (86%)	88 (94%)	6 (6%)	17	48
2	Ch	94/110 (86%)	90 (96%)	4 (4%)	29	62
2	Cp	94/110 (86%)	89 (95%)	5 (5%)	22	54
3	AC	72/84 (86%)	67 (93%)	5 (7%)	15	45
3	AK	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	AS	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	Aa	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	Ai	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	Aq	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	Ay	72/84 (86%)	69 (96%)	3 (4%)	30	62
3	BC	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	BK	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	BS	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	Ba	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	Bi	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	Bq	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	By	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	CC	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	CK	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	CS	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	Ca	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	Ci	72/84 (86%)	68 (94%)	4 (6%)	21	52
3	Cq	72/84 (86%)	68 (94%)	4 (6%)	21	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	AL	60/74 (81%)	57 (95%)	3 (5%)	24	57
4	AT	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	Ab	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	Aj	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	Ar	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	Az	60/74 (81%)	57 (95%)	3 (5%)	24	57
4	BD	60/74 (81%)	55 (92%)	5 (8%)	11	38
4	BL	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	BT	60/74 (81%)	55 (92%)	5 (8%)	11	38
4	Bb	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	Bj	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	Br	60/74 (81%)	57 (95%)	3 (5%)	24	57
4	Bz	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	CD	60/74 (81%)	55 (92%)	5 (8%)	11	38
4	CL	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	CT	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	Cb	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	Cj	60/74 (81%)	56 (93%)	4 (7%)	16	46
4	Cr	60/74 (81%)	56 (93%)	4 (7%)	16	46
5	A1	15/97 (16%)	11 (73%)	4 (27%)	0	1
5	AE	15/97 (16%)	12 (80%)	3 (20%)	1	5
5	AM	15/97 (16%)	12 (80%)	3 (20%)	1	5
5	AU	15/97 (16%)	13 (87%)	2 (13%)	4	16
5	Ac	15/97 (16%)	12 (80%)	3 (20%)	1	5
5	Ak	15/97 (16%)	13 (87%)	2 (13%)	4	16
5	As	15/97 (16%)	12 (80%)	3 (20%)	1	5
5	B1	15/97 (16%)	13 (87%)	2 (13%)	4	16
5	BE	15/97 (16%)	11 (73%)	4 (27%)	0	1
5	BM	15/97 (16%)	11 (73%)	4 (27%)	0	1
5	BU	15/97 (16%)	12 (80%)	3 (20%)	1	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Bc	15/97 (16%)	12 (80%)	3 (20%)	1	5
5	Bk	15/97 (16%)	12 (80%)	3 (20%)	1	5
5	Bs	15/97 (16%)	13 (87%)	2 (13%)	4	16
5	CE	15/97 (16%)	12 (80%)	3 (20%)	1	5
5	CM	15/97 (16%)	12 (80%)	3 (20%)	1	5
5	CU	15/97 (16%)	11 (73%)	4 (27%)	0	1
5	Cc	15/97 (16%)	13 (87%)	2 (13%)	4	16
5	Ck	15/97 (16%)	12 (80%)	3 (20%)	1	5
5	Cs	15/97 (16%)	10 (67%)	5 (33%)	0	0
6	A2	203/231 (88%)	176 (87%)	27 (13%)	4	16
6	AF	203/231 (88%)	170 (84%)	33 (16%)	2	10
6	AN	203/231 (88%)	171 (84%)	32 (16%)	2	11
6	AV	203/231 (88%)	177 (87%)	26 (13%)	4	18
6	Ad	203/231 (88%)	178 (88%)	25 (12%)	4	19
6	Al	203/231 (88%)	176 (87%)	27 (13%)	4	16
6	At	203/231 (88%)	172 (85%)	31 (15%)	2	12
6	B2	203/231 (88%)	169 (83%)	34 (17%)	2	9
6	BF	203/231 (88%)	176 (87%)	27 (13%)	4	16
6	BN	203/231 (88%)	177 (87%)	26 (13%)	4	18
6	BV	203/231 (88%)	178 (88%)	25 (12%)	4	19
6	Bd	203/231 (88%)	176 (87%)	27 (13%)	4	16
6	Bl	203/231 (88%)	175 (86%)	28 (14%)	3	16
6	Bt	203/231 (88%)	174 (86%)	29 (14%)	3	14
6	CF	203/231 (88%)	172 (85%)	31 (15%)	2	12
6	CN	203/231 (88%)	178 (88%)	25 (12%)	4	19
6	CV	203/231 (88%)	175 (86%)	28 (14%)	3	16
6	Cd	203/231 (88%)	174 (86%)	29 (14%)	3	14
6	Cl	203/231 (88%)	172 (85%)	31 (15%)	2	12
6	Ct	203/231 (88%)	174 (86%)	29 (14%)	3	14
7	A3	108/159 (68%)	98 (91%)	10 (9%)	9	32
7	AG	108/159 (68%)	98 (91%)	10 (9%)	9	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AO	108/159 (68%)	99 (92%)	9 (8%)	11	38
7	AW	108/159 (68%)	99 (92%)	9 (8%)	11	38
7	Ae	108/159 (68%)	99 (92%)	9 (8%)	11	38
7	Am	108/159 (68%)	99 (92%)	9 (8%)	11	38
7	Au	108/159 (68%)	99 (92%)	9 (8%)	11	38
7	B3	108/159 (68%)	98 (91%)	10 (9%)	9	32
7	BG	108/159 (68%)	99 (92%)	9 (8%)	11	38
7	BO	108/159 (68%)	99 (92%)	9 (8%)	11	38
7	BW	108/159 (68%)	99 (92%)	9 (8%)	11	38
7	Be	108/159 (68%)	100 (93%)	8 (7%)	13	42
7	Bm	108/159 (68%)	100 (93%)	8 (7%)	13	42
7	Bu	108/159 (68%)	100 (93%)	8 (7%)	13	42
7	CG	108/159 (68%)	98 (91%)	10 (9%)	9	32
7	CO	108/159 (68%)	99 (92%)	9 (8%)	11	38
7	CW	108/159 (68%)	99 (92%)	9 (8%)	11	38
7	Ce	108/159 (68%)	98 (91%)	10 (9%)	9	32
7	Cm	108/159 (68%)	99 (92%)	9 (8%)	11	38
7	Cu	108/159 (68%)	100 (93%)	8 (7%)	13	42
8	A4	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	AH	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	AP	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	AX	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	Af	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	An	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	Av	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	B4	61/66 (92%)	58 (95%)	3 (5%)	25	57
8	BH	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	BP	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	BX	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	Bf	61/66 (92%)	58 (95%)	3 (5%)	25	57
8	Bn	61/66 (92%)	59 (97%)	2 (3%)	38	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Bv	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	CH	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	CP	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	CX	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	Cf	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	Cn	61/66 (92%)	59 (97%)	2 (3%)	38	69
8	Cv	61/66 (92%)	59 (97%)	2 (3%)	38	69
All	All	13800/18440 (75%)	12594 (91%)	1206 (9%)	10	36

All (1206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AI	1002	VAL
1	AI	1009	SER
1	AI	1047	ASN
1	AI	1048	ARG
1	AI	1064	ARG
2	AJ	2054	ARG
2	AJ	2092	LEU
3	AK	3004	ILE
3	AK	3016	ARG
3	AK	3026	ASN
3	AK	3045	ASP
4	AL	4021	MET
4	AL	4046	ASP
4	AL	4053	LEU
5	AM	7002	TRP
5	AM	7006	LEU
5	AM	7014	SER
6	AN	8001	GLU
6	AN	8009	HIS
6	AN	8010	MET
6	AN	8024	ARG
6	AN	8032	THR
6	AN	8037	LEU
6	AN	8039	MET
6	AN	8054	THR
6	AN	8066	GLN
6	AN	8073	LEU
6	AN	8079	LEU

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Mol	Chain	Res	Type
6	AN	8083	ASN
6	AN	8093	THR
6	AN	8096	GLN
6	AN	8106	GLN
6	AN	8109	LEU
6	AN	8113	LEU
6	AN	8117	THR
6	AN	8127	MET
6	AN	8133	GLN
6	AN	8139	VAL
6	AN	8147	LEU
6	AN	8154	THR
6	AN	8160	LEU
6	AN	8177	CYS
6	AN	8180	LEU
6	AN	8184	LEU
6	AN	8186	GLU
6	AN	8188	GLU
6	AN	8198	LEU
6	AN	8204	GLN
6	AN	8210	ASP
7	AO	6010	GLU
7	AO	6019	ASN
7	AO	6027	LYS
7	AO	6031	GLU
7	AO	6033	THR
7	AO	6131	GLU
7	AO	6140	GLU
7	AO	6158	LEU
7	AO	6162	SER
8	AP	5000	HIS
8	AP	5058	ARG
1	AA	1002	VAL
1	AA	1009	SER
1	AA	1042	LYS
1	AA	1046	LYS
1	AA	1047	ASN
1	AA	1048	ARG
1	AA	1064	ARG
2	AB	2040	ARG
2	AB	2054	ARG
2	AB	2076	ARG

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Mol	Chain	Res	Type
2	AB	2092	LEU
3	AC	3004	ILE
3	AC	3016	ARG
3	AC	3024	GLN
3	AC	3026	ASN
3	AC	3045	ASP
4	AD	4002	LYS
4	AD	4021	MET
4	AD	4046	ASP
4	AD	4053	LEU
5	AE	7002	TRP
5	AE	7006	LEU
5	AE	7007	LEU
6	AF	8001	GLU
6	AF	8010	MET
6	AF	8024	ARG
6	AF	8037	LEU
6	AF	8039	MET
6	AF	8054	THR
6	AF	8075	LEU
6	AF	8077	LYS
6	AF	8083	ASN
6	AF	8093	THR
6	AF	8096	GLN
6	AF	8106	GLN
6	AF	8109	LEU
6	AF	8111	SER
6	AF	8119	ASN
6	AF	8123	LEU
6	AF	8125	LEU
6	AF	8127	MET
6	AF	8133	GLN
6	AF	8139	VAL
6	AF	8151	LEU
6	AF	8154	THR
6	AF	8156	VAL
6	AF	8159	HIS
6	AF	8162	LEU
6	AF	8180	LEU
6	AF	8184	LEU
6	AF	8186	GLU
6	AF	8188	GLU

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Mol	Chain	Res	Type
6	AF	8197	LEU
6	AF	8202	THR
6	AF	8213	ASP
6	AF	8215	ILE
7	AG	6010	GLU
7	AG	6018	ASN
7	AG	6019	ASN
7	AG	6027	LYS
7	AG	6031	GLU
7	AG	6033	THR
7	AG	6131	GLU
7	AG	6140	GLU
7	AG	6158	LEU
7	AG	6162	SER
8	AH	5000	HIS
8	AH	5058	ARG
1	AQ	1002	VAL
1	AQ	1009	SER
1	AQ	1046	LYS
1	AQ	1047	ASN
1	AQ	1048	ARG
2	AR	2054	ARG
2	AR	2076	ARG
2	AR	2092	LEU
3	AS	3004	ILE
3	AS	3016	ARG
3	AS	3026	ASN
3	AS	3045	ASP
4	AT	4002	LYS
4	AT	4021	MET
4	AT	4046	ASP
4	AT	4053	LEU
5	AU	7002	TRP
5	AU	7006	LEU
6	AV	8001	GLU
6	AV	8010	MET
6	AV	8024	ARG
6	AV	8037	LEU
6	AV	8039	MET
6	AV	8054	THR
6	AV	8073	LEU
6	AV	8079	LEU

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Mol	Chain	Res	Type
6	AV	8083	ASN
6	AV	8093	THR
6	AV	8096	GLN
6	AV	8106	GLN
6	AV	8109	LEU
6	AV	8127	MET
6	AV	8133	GLN
6	AV	8139	VAL
6	AV	8147	LEU
6	AV	8149	ARG
6	AV	8156	VAL
6	AV	8162	LEU
6	AV	8180	LEU
6	AV	8184	LEU
6	AV	8186	GLU
6	AV	8188	GLU
6	AV	8199	LEU
6	AV	8213	ASP
7	AW	6010	GLU
7	AW	6019	ASN
7	AW	6027	LYS
7	AW	6031	GLU
7	AW	6033	THR
7	AW	6131	GLU
7	AW	6140	GLU
7	AW	6158	LEU
7	AW	6162	SER
8	AX	5000	HIS
8	AX	5058	ARG
1	AY	1002	VAL
1	AY	1009	SER
1	AY	1046	LYS
1	AY	1047	ASN
1	AY	1048	ARG
1	AY	1064	ARG
2	AZ	2040	ARG
2	AZ	2054	ARG
2	AZ	2076	ARG
2	AZ	2092	LEU
3	Aa	3004	ILE
3	Aa	3016	ARG
3	Aa	3026	ASN

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Mol	Chain	Res	Type
3	Aa	3045	ASP
4	Ab	4002	LYS
4	Ab	4021	MET
4	Ab	4046	ASP
4	Ab	4053	LEU
5	Ac	7002	TRP
5	Ac	7006	LEU
5	Ac	7007	LEU
6	Ad	8001	GLU
6	Ad	8010	MET
6	Ad	8024	ARG
6	Ad	8037	LEU
6	Ad	8039	MET
6	Ad	8054	THR
6	Ad	8066	GLN
6	Ad	8073	LEU
6	Ad	8079	LEU
6	Ad	8083	ASN
6	Ad	8093	THR
6	Ad	8094	SER
6	Ad	8096	GLN
6	Ad	8106	GLN
6	Ad	8127	MET
6	Ad	8133	GLN
6	Ad	8139	VAL
6	Ad	8147	LEU
6	Ad	8159	HIS
6	Ad	8180	LEU
6	Ad	8184	LEU
6	Ad	8186	GLU
6	Ad	8188	GLU
6	Ad	8210	ASP
6	Ad	8213	ASP
7	Ae	6010	GLU
7	Ae	6019	ASN
7	Ae	6027	LYS
7	Ae	6031	GLU
7	Ae	6033	THR
7	Ae	6131	GLU
7	Ae	6140	GLU
7	Ae	6158	LEU
7	Ae	6162	SER

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Mol	Chain	Res	Type
8	Af	5000	HIS
8	Af	5058	ARG
1	Ag	1002	VAL
1	Ag	1009	SER
1	Ag	1022	GLN
1	Ag	1047	ASN
1	Ag	1048	ARG
1	Ag	1064	ARG
2	Ah	2002	SER
2	Ah	2040	ARG
2	Ah	2054	ARG
2	Ah	2076	ARG
2	Ah	2092	LEU
3	Ai	3004	ILE
3	Ai	3016	ARG
3	Ai	3024	GLN
3	Ai	3045	ASP
4	Aj	4002	LYS
4	Aj	4021	MET
4	Aj	4046	ASP
4	Aj	4053	LEU
5	Ak	7002	TRP
5	Ak	7006	LEU
6	Al	8001	GLU
6	Al	8010	MET
6	Al	8024	ARG
6	Al	8032	THR
6	Al	8037	LEU
6	Al	8039	MET
6	Al	8054	THR
6	Al	8073	LEU
6	Al	8079	LEU
6	Al	8083	ASN
6	Al	8093	THR
6	Al	8096	GLN
6	Al	8106	GLN
6	Al	8109	LEU
6	Al	8127	MET
6	Al	8133	GLN
6	Al	8139	VAL
6	Al	8147	LEU
6	Al	8159	HIS

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Mol	Chain	Res	Type
6	Al	8160	LEU
6	Al	8169	THR
6	Al	8170	LEU
6	Al	8180	LEU
6	Al	8184	LEU
6	Al	8186	GLU
6	Al	8188	GLU
6	Al	8213	ASP
7	Am	6010	GLU
7	Am	6019	ASN
7	Am	6027	LYS
7	Am	6031	GLU
7	Am	6033	THR
7	Am	6131	GLU
7	Am	6140	GLU
7	Am	6158	LEU
7	Am	6162	SER
8	An	5000	HIS
8	An	5058	ARG
1	Ao	1002	VAL
1	Ao	1009	SER
1	Ao	1047	ASN
1	Ao	1048	ARG
2	Ap	2042	ASN
2	Ap	2054	ARG
2	Ap	2092	LEU
3	Aq	3004	ILE
3	Aq	3016	ARG
3	Aq	3026	ASN
3	Aq	3045	ASP
4	Ar	4002	LYS
4	Ar	4021	MET
4	Ar	4046	ASP
4	Ar	4053	LEU
5	As	7002	TRP
5	As	7006	LEU
5	As	7007	LEU
6	At	8001	GLU
6	At	8010	MET
6	At	8024	ARG
6	At	8037	LEU
6	At	8039	MET

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Mol	Chain	Res	Type
6	At	8054	THR
6	At	8066	GLN
6	At	8073	LEU
6	At	8079	LEU
6	At	8083	ASN
6	At	8093	THR
6	At	8096	GLN
6	At	8100	LYS
6	At	8101	GLU
6	At	8106	GLN
6	At	8109	LEU
6	At	8119	ASN
6	At	8126	GLU
6	At	8127	MET
6	At	8139	VAL
6	At	8147	LEU
6	At	8156	VAL
6	At	8160	LEU
6	At	8169	THR
6	At	8177	CYS
6	At	8180	LEU
6	At	8184	LEU
6	At	8186	GLU
6	At	8188	GLU
6	At	8195	TYR
6	At	8213	ASP
7	Au	6010	GLU
7	Au	6019	ASN
7	Au	6027	LYS
7	Au	6031	GLU
7	Au	6033	THR
7	Au	6131	GLU
7	Au	6140	GLU
7	Au	6158	LEU
7	Au	6162	SER
8	Av	5000	HIS
8	Av	5058	ARG
5	A1	7002	TRP
5	A1	7006	LEU
5	A1	7007	LEU
5	A1	7014	SER
6	A2	8001	GLU

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Mol	Chain	Res	Type
6	A2	8009	HIS
6	A2	8010	MET
6	A2	8024	ARG
6	A2	8032	THR
6	A2	8037	LEU
6	A2	8039	MET
6	A2	8054	THR
6	A2	8073	LEU
6	A2	8079	LEU
6	A2	8083	ASN
6	A2	8093	THR
6	A2	8096	GLN
6	A2	8106	GLN
6	A2	8107	GLN
6	A2	8119	ASN
6	A2	8127	MET
6	A2	8133	GLN
6	A2	8139	VAL
6	A2	8156	VAL
6	A2	8177	CYS
6	A2	8180	LEU
6	A2	8184	LEU
6	A2	8186	GLU
6	A2	8188	GLU
6	A2	8209	ASN
6	A2	8210	ASP
7	A3	6010	GLU
7	A3	6027	LYS
7	A3	6031	GLU
7	A3	6033	THR
7	A3	6079	LYS
7	A3	6085	VAL
7	A3	6131	GLU
7	A3	6140	GLU
7	A3	6158	LEU
7	A3	6162	SER
8	A4	5000	HIS
8	A4	5058	ARG
1	Aw	1002	VAL
1	Aw	1009	SER
1	Aw	1047	ASN
1	Aw	1048	ARG

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Mol	Chain	Res	Type
1	Aw	1064	ARG
2	Ax	2002	SER
2	Ax	2040	ARG
2	Ax	2054	ARG
2	Ax	2092	LEU
3	Ay	3016	ARG
3	Ay	3026	ASN
3	Ay	3045	ASP
4	Az	4021	MET
4	Az	4046	ASP
4	Az	4053	LEU
1	BA	1002	VAL
1	BA	1009	SER
1	BA	1047	ASN
1	BA	1048	ARG
1	BA	1064	ARG
2	BB	2002	SER
2	BB	2040	ARG
2	BB	2054	ARG
2	BB	2092	LEU
3	BC	3004	ILE
3	BC	3016	ARG
3	BC	3026	ASN
3	BC	3045	ASP
4	BD	4002	LYS
4	BD	4021	MET
4	BD	4031	ASP
4	BD	4046	ASP
4	BD	4053	LEU
5	BE	7002	TRP
5	BE	7005	SER
5	BE	7006	LEU
5	BE	7014	SER
6	BF	8001	GLU
6	BF	8010	MET
6	BF	8024	ARG
6	BF	8037	LEU
6	BF	8039	MET
6	BF	8054	THR
6	BF	8066	GLN
6	BF	8073	LEU
6	BF	8079	LEU

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Mol	Chain	Res	Type
6	BF	8083	ASN
6	BF	8093	THR
6	BF	8096	GLN
6	BF	8106	GLN
6	BF	8109	LEU
6	BF	8119	ASN
6	BF	8127	MET
6	BF	8133	GLN
6	BF	8139	VAL
6	BF	8147	LEU
6	BF	8154	THR
6	BF	8156	VAL
6	BF	8180	LEU
6	BF	8184	LEU
6	BF	8186	GLU
6	BF	8188	GLU
6	BF	8197	LEU
6	BF	8213	ASP
7	BG	6010	GLU
7	BG	6019	ASN
7	BG	6027	LYS
7	BG	6031	GLU
7	BG	6033	THR
7	BG	6131	GLU
7	BG	6140	GLU
7	BG	6158	LEU
7	BG	6162	SER
8	BH	5000	HIS
8	BH	5058	ARG
1	BI	1002	VAL
1	BI	1009	SER
1	BI	1047	ASN
1	BI	1048	ARG
1	BI	1064	ARG
2	BJ	2002	SER
2	BJ	2040	ARG
2	BJ	2042	ASN
2	BJ	2054	ARG
2	BJ	2076	ARG
2	BJ	2092	LEU
3	BK	3004	ILE
3	BK	3016	ARG

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Mol	Chain	Res	Type
3	BK	3026	ASN
3	BK	3045	ASP
4	BL	4002	LYS
4	BL	4021	MET
4	BL	4046	ASP
4	BL	4053	LEU
5	BM	7002	TRP
5	BM	7005	SER
5	BM	7006	LEU
5	BM	7007	LEU
6	BN	8001	GLU
6	BN	8010	MET
6	BN	8037	LEU
6	BN	8039	MET
6	BN	8054	THR
6	BN	8066	GLN
6	BN	8073	LEU
6	BN	8079	LEU
6	BN	8083	ASN
6	BN	8093	THR
6	BN	8096	GLN
6	BN	8106	GLN
6	BN	8107	GLN
6	BN	8109	LEU
6	BN	8127	MET
6	BN	8133	GLN
6	BN	8139	VAL
6	BN	8147	LEU
6	BN	8154	THR
6	BN	8159	HIS
6	BN	8180	LEU
6	BN	8184	LEU
6	BN	8186	GLU
6	BN	8188	GLU
6	BN	8195	TYR
6	BN	8213	ASP
7	BO	6010	GLU
7	BO	6019	ASN
7	BO	6027	LYS
7	BO	6031	GLU
7	BO	6033	THR
7	BO	6131	GLU

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Mol	Chain	Res	Type
7	BO	6140	GLU
7	BO	6158	LEU
7	BO	6162	SER
8	BP	5000	HIS
8	BP	5058	ARG
1	BQ	1002	VAL
1	BQ	1009	SER
1	BQ	1047	ASN
1	BQ	1048	ARG
1	BQ	1064	ARG
2	BR	2042	ASN
2	BR	2054	ARG
2	BR	2076	ARG
2	BR	2092	LEU
3	BS	3004	ILE
3	BS	3016	ARG
3	BS	3026	ASN
3	BS	3045	ASP
4	BT	4002	LYS
4	BT	4021	MET
4	BT	4031	ASP
4	BT	4046	ASP
4	BT	4053	LEU
5	BU	7002	TRP
5	BU	7006	LEU
5	BU	7007	LEU
6	BV	8001	GLU
6	BV	8010	MET
6	BV	8024	ARG
6	BV	8037	LEU
6	BV	8039	MET
6	BV	8054	THR
6	BV	8066	GLN
6	BV	8073	LEU
6	BV	8079	LEU
6	BV	8083	ASN
6	BV	8093	THR
6	BV	8096	GLN
6	BV	8106	GLN
6	BV	8109	LEU
6	BV	8110	LEU
6	BV	8127	MET

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Mol	Chain	Res	Type
6	BV	8133	GLN
6	BV	8139	VAL
6	BV	8147	LEU
6	BV	8156	VAL
6	BV	8180	LEU
6	BV	8184	LEU
6	BV	8186	GLU
6	BV	8188	GLU
6	BV	8213	ASP
7	BW	6010	GLU
7	BW	6019	ASN
7	BW	6027	LYS
7	BW	6031	GLU
7	BW	6033	THR
7	BW	6131	GLU
7	BW	6140	GLU
7	BW	6158	LEU
7	BW	6162	SER
8	BX	5000	HIS
8	BX	5058	ARG
1	BY	1002	VAL
1	BY	1009	SER
1	BY	1047	ASN
1	BY	1048	ARG
1	BY	1064	ARG
2	BZ	2040	ARG
2	BZ	2054	ARG
2	BZ	2076	ARG
2	BZ	2092	LEU
3	Ba	3004	ILE
3	Ba	3016	ARG
3	Ba	3026	ASN
3	Ba	3045	ASP
4	Bb	4021	MET
4	Bb	4031	ASP
4	Bb	4046	ASP
4	Bb	4053	LEU
5	Bc	7002	TRP
5	Bc	7006	LEU
5	Bc	7007	LEU
6	Bd	8001	GLU
6	Bd	8010	MET

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Mol	Chain	Res	Type
6	Bd	8024	ARG
6	Bd	8037	LEU
6	Bd	8039	MET
6	Bd	8054	THR
6	Bd	8066	GLN
6	Bd	8073	LEU
6	Bd	8079	LEU
6	Bd	8083	ASN
6	Bd	8093	THR
6	Bd	8096	GLN
6	Bd	8101	GLU
6	Bd	8106	GLN
6	Bd	8109	LEU
6	Bd	8125	LEU
6	Bd	8127	MET
6	Bd	8133	GLN
6	Bd	8145	VAL
6	Bd	8147	LEU
6	Bd	8156	VAL
6	Bd	8180	LEU
6	Bd	8184	LEU
6	Bd	8186	GLU
6	Bd	8188	GLU
6	Bd	8195	TYR
6	Bd	8213	ASP
7	Be	6010	GLU
7	Be	6027	LYS
7	Be	6031	GLU
7	Be	6033	THR
7	Be	6131	GLU
7	Be	6140	GLU
7	Be	6158	LEU
7	Be	6162	SER
8	Bf	5000	HIS
8	Bf	5002	PRO
8	Bf	5058	ARG
1	Bg	1002	VAL
1	Bg	1009	SER
1	Bg	1047	ASN
1	Bg	1048	ARG
1	Bg	1064	ARG
2	Bh	2040	ARG

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Mol	Chain	Res	Type
2	Bh	2054	ARG
2	Bh	2076	ARG
2	Bh	2092	LEU
3	Bi	3004	ILE
3	Bi	3016	ARG
3	Bi	3026	ASN
3	Bi	3045	ASP
4	Bj	4002	LYS
4	Bj	4021	MET
4	Bj	4046	ASP
4	Bj	4053	LEU
5	Bk	7002	TRP
5	Bk	7005	SER
5	Bk	7006	LEU
6	Bl	8001	GLU
6	Bl	8009	HIS
6	Bl	8010	MET
6	Bl	8037	LEU
6	Bl	8039	MET
6	Bl	8054	THR
6	Bl	8066	GLN
6	Bl	8073	LEU
6	Bl	8079	LEU
6	Bl	8083	ASN
6	Bl	8093	THR
6	Bl	8096	GLN
6	Bl	8106	GLN
6	Bl	8110	LEU
6	Bl	8127	MET
6	Bl	8133	GLN
6	Bl	8139	VAL
6	Bl	8147	LEU
6	Bl	8154	THR
6	Bl	8162	LEU
6	Bl	8169	THR
6	Bl	8173	ILE
6	Bl	8180	LEU
6	Bl	8184	LEU
6	Bl	8186	GLU
6	Bl	8188	GLU
6	Bl	8195	TYR
6	Bl	8213	ASP

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Mol	Chain	Res	Type
7	Bm	6010	GLU
7	Bm	6027	LYS
7	Bm	6031	GLU
7	Bm	6033	THR
7	Bm	6131	GLU
7	Bm	6140	GLU
7	Bm	6158	LEU
7	Bm	6162	SER
8	Bn	5000	HIS
8	Bn	5058	ARG
1	Bo	1002	VAL
1	Bo	1009	SER
1	Bo	1047	ASN
1	Bo	1048	ARG
1	Bo	1049	GLU
1	Bo	1064	ARG
2	Bp	2002	SER
2	Bp	2040	ARG
2	Bp	2054	ARG
2	Bp	2076	ARG
2	Bp	2092	LEU
3	Bq	3004	ILE
3	Bq	3016	ARG
3	Bq	3026	ASN
3	Bq	3045	ASP
4	Br	4021	MET
4	Br	4046	ASP
4	Br	4053	LEU
5	Bs	7002	TRP
5	Bs	7005	SER
6	Bt	8001	GLU
6	Bt	8010	MET
6	Bt	8027	LYS
6	Bt	8037	LEU
6	Bt	8039	MET
6	Bt	8054	THR
6	Bt	8061	GLN
6	Bt	8066	GLN
6	Bt	8073	LEU
6	Bt	8079	LEU
6	Bt	8083	ASN
6	Bt	8093	THR

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Mol	Chain	Res	Type
6	Bt	8096	GLN
6	Bt	8106	GLN
6	Bt	8107	GLN
6	Bt	8109	LEU
6	Bt	8113	LEU
6	Bt	8127	MET
6	Bt	8133	GLN
6	Bt	8139	VAL
6	Bt	8147	LEU
6	Bt	8149	ARG
6	Bt	8159	HIS
6	Bt	8180	LEU
6	Bt	8184	LEU
6	Bt	8186	GLU
6	Bt	8188	GLU
6	Bt	8195	TYR
6	Bt	8213	ASP
7	Bu	6010	GLU
7	Bu	6027	LYS
7	Bu	6031	GLU
7	Bu	6033	THR
7	Bu	6131	GLU
7	Bu	6140	GLU
7	Bu	6158	LEU
7	Bu	6162	SER
8	Bv	5000	HIS
8	Bv	5058	ARG
5	B1	7002	TRP
5	B1	7007	LEU
6	B2	8001	GLU
6	B2	8010	MET
6	B2	8037	LEU
6	B2	8039	MET
6	B2	8054	THR
6	B2	8061	GLN
6	B2	8066	GLN
6	B2	8073	LEU
6	B2	8079	LEU
6	B2	8083	ASN
6	B2	8093	THR
6	B2	8096	GLN
6	B2	8106	GLN

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Mol	Chain	Res	Type
6	B2	8109	LEU
6	B2	8117	THR
6	B2	8119	ASN
6	B2	8125	LEU
6	B2	8127	MET
6	B2	8133	GLN
6	B2	8139	VAL
6	B2	8147	LEU
6	B2	8151	LEU
6	B2	8156	VAL
6	B2	8159	HIS
6	B2	8160	LEU
6	B2	8169	THR
6	B2	8180	LEU
6	B2	8184	LEU
6	B2	8186	GLU
6	B2	8188	GLU
6	B2	8195	TYR
6	B2	8198	LEU
6	B2	8202	THR
6	B2	8213	ASP
7	B3	6010	GLU
7	B3	6019	ASN
7	B3	6027	LYS
7	B3	6031	GLU
7	B3	6033	THR
7	B3	6047	GLU
7	B3	6131	GLU
7	B3	6140	GLU
7	B3	6158	LEU
7	B3	6162	SER
8	B4	5000	HIS
8	B4	5002	PRO
8	B4	5058	ARG
1	Bw	1002	VAL
1	Bw	1009	SER
1	Bw	1042	LYS
1	Bw	1047	ASN
1	Bw	1048	ARG
1	Bw	1064	ARG
2	Bx	2014	GLU
2	Bx	2040	ARG

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Mol	Chain	Res	Type
2	Bx	2054	ARG
2	Bx	2066	MET
2	Bx	2076	ARG
2	Bx	2092	LEU
3	By	3004	ILE
3	By	3016	ARG
3	By	3026	ASN
3	By	3045	ASP
4	Bz	4021	MET
4	Bz	4031	ASP
4	Bz	4046	ASP
4	Bz	4053	LEU
1	CA	1002	VAL
1	CA	1009	SER
1	CA	1047	ASN
1	CA	1048	ARG
1	CA	1064	ARG
2	CB	2002	SER
2	CB	2040	ARG
2	CB	2054	ARG
2	CB	2076	ARG
2	CB	2092	LEU
3	CC	3004	ILE
3	CC	3016	ARG
3	CC	3026	ASN
3	CC	3045	ASP
4	CD	4002	LYS
4	CD	4021	MET
4	CD	4031	ASP
4	CD	4046	ASP
4	CD	4053	LEU
5	CE	7002	TRP
5	CE	7006	LEU
5	CE	7007	LEU
6	CF	8001	GLU
6	CF	8010	MET
6	CF	8024	ARG
6	CF	8037	LEU
6	CF	8039	MET
6	CF	8054	THR
6	CF	8064	SER
6	CF	8066	GLN

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Mol	Chain	Res	Type
6	CF	8073	LEU
6	CF	8079	LEU
6	CF	8083	ASN
6	CF	8093	THR
6	CF	8096	GLN
6	CF	8106	GLN
6	CF	8107	GLN
6	CF	8109	LEU
6	CF	8125	LEU
6	CF	8127	MET
6	CF	8133	GLN
6	CF	8139	VAL
6	CF	8156	VAL
6	CF	8162	LEU
6	CF	8165	HIS
6	CF	8169	THR
6	CF	8180	LEU
6	CF	8184	LEU
6	CF	8186	GLU
6	CF	8188	GLU
6	CF	8195	TYR
6	CF	8204	GLN
6	CF	8213	ASP
7	CG	6010	GLU
7	CG	6019	ASN
7	CG	6027	LYS
7	CG	6031	GLU
7	CG	6033	THR
7	CG	6047	GLU
7	CG	6131	GLU
7	CG	6140	GLU
7	CG	6158	LEU
7	CG	6162	SER
8	CH	5000	HIS
8	CH	5058	ARG
1	CI	1002	VAL
1	CI	1009	SER
1	CI	1047	ASN
1	CI	1048	ARG
1	CI	1064	ARG
2	CJ	2002	SER
2	CJ	2054	ARG

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Mol	Chain	Res	Type
2	CJ	2076	ARG
2	CJ	2092	LEU
3	CK	3004	ILE
3	CK	3016	ARG
3	CK	3026	ASN
3	CK	3045	ASP
4	CL	4002	LYS
4	CL	4021	MET
4	CL	4046	ASP
4	CL	4053	LEU
5	CM	7002	TRP
5	CM	7006	LEU
5	CM	7007	LEU
6	CN	8001	GLU
6	CN	8010	MET
6	CN	8024	ARG
6	CN	8037	LEU
6	CN	8039	MET
6	CN	8054	THR
6	CN	8066	GLN
6	CN	8069	ARG
6	CN	8073	LEU
6	CN	8079	LEU
6	CN	8093	THR
6	CN	8096	GLN
6	CN	8106	GLN
6	CN	8107	GLN
6	CN	8125	LEU
6	CN	8127	MET
6	CN	8133	GLN
6	CN	8139	VAL
6	CN	8147	LEU
6	CN	8156	VAL
6	CN	8177	CYS
6	CN	8184	LEU
6	CN	8186	GLU
6	CN	8188	GLU
6	CN	8213	ASP
7	CO	6010	GLU
7	CO	6019	ASN
7	CO	6027	LYS
7	CO	6031	GLU

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Mol	Chain	Res	Type
7	CO	6033	THR
7	CO	6131	GLU
7	CO	6140	GLU
7	CO	6158	LEU
7	CO	6162	SER
8	CP	5000	HIS
8	CP	5058	ARG
1	CQ	1002	VAL
1	CQ	1009	SER
1	CQ	1042	LYS
1	CQ	1047	ASN
1	CQ	1048	ARG
1	CQ	1064	ARG
2	CR	2040	ARG
2	CR	2054	ARG
2	CR	2092	LEU
3	CS	3004	ILE
3	CS	3016	ARG
3	CS	3026	ASN
3	CS	3045	ASP
4	CT	4002	LYS
4	CT	4021	MET
4	CT	4046	ASP
4	CT	4053	LEU
5	CU	7002	TRP
5	CU	7006	LEU
5	CU	7007	LEU
5	CU	7014	SER
6	CV	8001	GLU
6	CV	8010	MET
6	CV	8024	ARG
6	CV	8037	LEU
6	CV	8039	MET
6	CV	8054	THR
6	CV	8066	GLN
6	CV	8073	LEU
6	CV	8079	LEU
6	CV	8083	ASN
6	CV	8093	THR
6	CV	8096	GLN
6	CV	8106	GLN
6	CV	8109	LEU

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Mol	Chain	Res	Type
6	CV	8125	LEU
6	CV	8127	MET
6	CV	8133	GLN
6	CV	8139	VAL
6	CV	8151	LEU
6	CV	8156	VAL
6	CV	8160	LEU
6	CV	8180	LEU
6	CV	8184	LEU
6	CV	8186	GLU
6	CV	8188	GLU
6	CV	8198	LEU
6	CV	8209	ASN
6	CV	8213	ASP
7	CW	6010	GLU
7	CW	6019	ASN
7	CW	6027	LYS
7	CW	6031	GLU
7	CW	6033	THR
7	CW	6131	GLU
7	CW	6140	GLU
7	CW	6158	LEU
7	CW	6162	SER
8	CX	5000	HIS
8	CX	5058	ARG
1	CY	1002	VAL
1	CY	1009	SER
1	CY	1042	LYS
1	CY	1047	ASN
1	CY	1048	ARG
1	CY	1064	ARG
2	CZ	2002	SER
2	CZ	2014	GLU
2	CZ	2040	ARG
2	CZ	2054	ARG
2	CZ	2076	ARG
2	CZ	2092	LEU
3	Ca	3004	ILE
3	Ca	3016	ARG
3	Ca	3026	ASN
3	Ca	3045	ASP
4	Cb	4002	LYS

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Mol	Chain	Res	Type
4	Cb	4021	MET
4	Cb	4046	ASP
4	Cb	4053	LEU
5	Cc	7002	TRP
5	Cc	7006	LEU
6	Cd	8001	GLU
6	Cd	8010	MET
6	Cd	8024	ARG
6	Cd	8037	LEU
6	Cd	8039	MET
6	Cd	8054	THR
6	Cd	8066	GLN
6	Cd	8073	LEU
6	Cd	8079	LEU
6	Cd	8083	ASN
6	Cd	8093	THR
6	Cd	8096	GLN
6	Cd	8100	LYS
6	Cd	8106	GLN
6	Cd	8109	LEU
6	Cd	8125	LEU
6	Cd	8127	MET
6	Cd	8133	GLN
6	Cd	8139	VAL
6	Cd	8142	LEU
6	Cd	8149	ARG
6	Cd	8159	HIS
6	Cd	8168	SER
6	Cd	8180	LEU
6	Cd	8184	LEU
6	Cd	8186	GLU
6	Cd	8188	GLU
6	Cd	8204	GLN
6	Cd	8213	ASP
7	Ce	6010	GLU
7	Ce	6019	ASN
7	Ce	6027	LYS
7	Ce	6031	GLU
7	Ce	6033	THR
7	Ce	6047	GLU
7	Ce	6131	GLU
7	Ce	6140	GLU

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Mol	Chain	Res	Type
7	Ce	6158	LEU
7	Ce	6162	SER
8	Cf	5000	HIS
8	Cf	5058	ARG
1	Cg	1002	VAL
1	Cg	1009	SER
1	Cg	1047	ASN
1	Cg	1048	ARG
1	Cg	1049	GLU
1	Cg	1064	ARG
2	Ch	2040	ARG
2	Ch	2054	ARG
2	Ch	2076	ARG
2	Ch	2092	LEU
3	Ci	3004	ILE
3	Ci	3016	ARG
3	Ci	3026	ASN
3	Ci	3045	ASP
4	Cj	4002	LYS
4	Cj	4021	MET
4	Cj	4046	ASP
4	Cj	4053	LEU
5	Ck	7002	TRP
5	Ck	7007	LEU
5	Ck	7010	THR
6	Cl	8001	GLU
6	Cl	8010	MET
6	Cl	8024	ARG
6	Cl	8037	LEU
6	Cl	8039	MET
6	Cl	8054	THR
6	Cl	8066	GLN
6	Cl	8075	LEU
6	Cl	8079	LEU
6	Cl	8083	ASN
6	Cl	8093	THR
6	Cl	8096	GLN
6	Cl	8106	GLN
6	Cl	8107	GLN
6	Cl	8109	LEU
6	Cl	8110	LEU
6	Cl	8113	LEU

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Mol	Chain	Res	Type
6	Cl	8115	HIS
6	Cl	8127	MET
6	Cl	8133	GLN
6	Cl	8139	VAL
6	Cl	8147	LEU
6	Cl	8154	THR
6	Cl	8156	VAL
6	Cl	8159	HIS
6	Cl	8162	LEU
6	Cl	8180	LEU
6	Cl	8184	LEU
6	Cl	8186	GLU
6	Cl	8188	GLU
6	Cl	8213	ASP
7	Cm	6010	GLU
7	Cm	6019	ASN
7	Cm	6027	LYS
7	Cm	6033	THR
7	Cm	6079	LYS
7	Cm	6131	GLU
7	Cm	6140	GLU
7	Cm	6158	LEU
7	Cm	6162	SER
8	Cn	5000	HIS
8	Cn	5058	ARG
1	Co	1002	VAL
1	Co	1009	SER
1	Co	1047	ASN
1	Co	1048	ARG
2	Cp	2039	CYS
2	Cp	2042	ASN
2	Cp	2054	ARG
2	Cp	2076	ARG
2	Cp	2092	LEU
3	Cq	3004	ILE
3	Cq	3016	ARG
3	Cq	3026	ASN
3	Cq	3045	ASP
4	Cr	4002	LYS
4	Cr	4021	MET
4	Cr	4046	ASP
4	Cr	4053	LEU

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Mol	Chain	Res	Type
5	Cs	7002	TRP
5	Cs	7005	SER
5	Cs	7006	LEU
5	Cs	7007	LEU
5	Cs	7014	SER
6	Ct	8001	GLU
6	Ct	8009	HIS
6	Ct	8010	MET
6	Ct	8024	ARG
6	Ct	8037	LEU
6	Ct	8039	MET
6	Ct	8054	THR
6	Ct	8073	LEU
6	Ct	8079	LEU
6	Ct	8083	ASN
6	Ct	8093	THR
6	Ct	8096	GLN
6	Ct	8106	GLN
6	Ct	8107	GLN
6	Ct	8110	LEU
6	Ct	8113	LEU
6	Ct	8117	THR
6	Ct	8118	GLN
6	Ct	8125	LEU
6	Ct	8127	MET
6	Ct	8139	VAL
6	Ct	8147	LEU
6	Ct	8162	LEU
6	Ct	8180	LEU
6	Ct	8184	LEU
6	Ct	8186	GLU
6	Ct	8188	GLU
6	Ct	8197	LEU
6	Ct	8213	ASP
7	Cu	6010	GLU
7	Cu	6019	ASN
7	Cu	6027	LYS
7	Cu	6033	THR
7	Cu	6131	GLU
7	Cu	6140	GLU
7	Cu	6158	LEU
7	Cu	6162	SER

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Mol	Chain	Res	Type
8	Cv	5000	HIS
8	Cv	5058	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	AI	1047	ASN
2	AJ	2031	ASN
3	AK	3002	GLN
3	AK	3024	GLN
6	AN	8096	GLN
6	AN	8106	GLN
1	AA	1047	ASN
2	AB	2031	ASN
3	AC	3002	GLN
3	AC	3024	GLN
6	AF	8081	ASN
6	AF	8096	GLN
6	AF	8106	GLN
7	AG	6018	ASN
1	AQ	1047	ASN
2	AR	2031	ASN
3	AS	3002	GLN
3	AS	3024	GLN
6	AV	8066	GLN
6	AV	8096	GLN
1	AY	1022	GLN
1	AY	1047	ASN
2	AZ	2031	ASN
3	Aa	3002	GLN
3	Aa	3024	GLN
6	Ad	8096	GLN
6	Ad	8190	GLN
7	Ae	6018	ASN
1	Ag	1047	ASN
2	Ah	2031	ASN
3	Ai	3002	GLN
3	Ai	3024	GLN
6	Al	8066	GLN
6	Al	8081	ASN
6	Al	8096	GLN
6	Al	8119	ASN

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Mol	Chain	Res	Type
1	Ao	1022	GLN
1	Ao	1047	ASN
2	Ap	2031	ASN
3	Aq	3002	GLN
3	Aq	3024	GLN
6	At	8165	HIS
6	At	8209	ASN
7	Au	6018	ASN
6	A2	8096	GLN
1	Aw	1047	ASN
2	Ax	2031	ASN
3	Ay	3002	GLN
3	Ay	3024	GLN
4	Az	4052	HIS
1	BA	1047	ASN
2	BB	2031	ASN
3	BC	3002	GLN
3	BC	3024	GLN
6	BF	8096	GLN
6	BF	8209	ASN
1	BI	1010	HIS
1	BI	1047	ASN
2	BJ	2031	ASN
3	BK	3002	GLN
3	BK	3024	GLN
6	BN	8096	GLN
6	BN	8106	GLN
6	BN	8209	ASN
1	BQ	1047	ASN
2	BR	2031	ASN
3	BS	3002	GLN
3	BS	3024	GLN
6	BV	8096	GLN
6	BV	8209	ASN
1	BY	1047	ASN
2	BZ	2031	ASN
3	Ba	3002	GLN
3	Ba	3024	GLN
6	Bd	8096	GLN
7	Be	6018	ASN
1	Bg	1022	GLN
1	Bg	1047	ASN

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Mol	Chain	Res	Type
2	Bh	2031	ASN
3	Bi	3002	GLN
3	Bi	3024	GLN
6	Bl	8096	GLN
6	Bl	8165	HIS
7	Bm	6018	ASN
1	Bo	1047	ASN
2	Bp	2031	ASN
3	Bq	3002	GLN
3	Bq	3024	GLN
6	Bt	8034	ASN
6	Bt	8096	GLN
6	Bt	8209	ASN
6	B2	8096	GLN
7	B3	6018	ASN
2	Bx	2031	ASN
3	By	3002	GLN
3	By	3024	GLN
1	CA	1047	ASN
2	CB	2031	ASN
3	CC	3002	GLN
3	CC	3024	GLN
6	CF	8096	GLN
6	CF	8159	HIS
7	CG	6018	ASN
1	CI	1047	ASN
2	CJ	2031	ASN
3	CK	3002	GLN
3	CK	3024	GLN
6	CN	8066	GLN
6	CN	8096	GLN
6	CN	8209	ASN
1	CQ	1047	ASN
2	CR	2031	ASN
3	CS	3002	GLN
3	CS	3024	GLN
6	CV	8081	ASN
6	CV	8096	GLN
6	CV	8106	GLN
6	CV	8209	ASN
7	CW	6018	ASN
2	CZ	2031	ASN

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Mol	Chain	Res	Type
3	Ca	3002	GLN
3	Ca	3024	GLN
6	Cd	8096	GLN
6	Cd	8106	GLN
6	Cd	8209	ASN
1	Cg	1047	ASN
2	Ch	2031	ASN
3	Ci	3002	GLN
3	Ci	3024	GLN
6	Cl	8096	GLN
7	Cm	6018	ASN
1	Co	1010	HIS
1	Co	1022	GLN
1	Co	1047	ASN
2	Cp	2031	ASN
2	Cp	2042	ASN
3	Cq	3002	GLN
3	Cq	3024	GLN
4	Cr	4052	HIS
6	Ct	8096	GLN
6	Ct	8106	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	SO4	Ad	8301	-	4,4,4	0.30	0	6,6,6	0.34	0
9	SO4	B2	8301	-	4,4,4	0.27	0	6,6,6	0.32	0
9	SO4	BV	8301	-	4,4,4	0.21	0	6,6,6	0.41	0
9	SO4	CF	8301	-	4,4,4	0.30	0	6,6,6	0.38	0
9	SO4	Bt	8301	-	4,4,4	0.15	0	6,6,6	0.34	0
9	SO4	A2	8301	-	4,4,4	0.14	0	6,6,6	0.39	0
9	SO4	At	8301	-	4,4,4	0.37	0	6,6,6	0.56	0
9	SO4	Cl	8301	-	4,4,4	0.33	0	6,6,6	0.25	0
9	SO4	BF	8301	-	4,4,4	0.09	0	6,6,6	0.28	0
9	SO4	Bd	8301	-	4,4,4	0.25	0	6,6,6	0.37	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.