



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:01 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

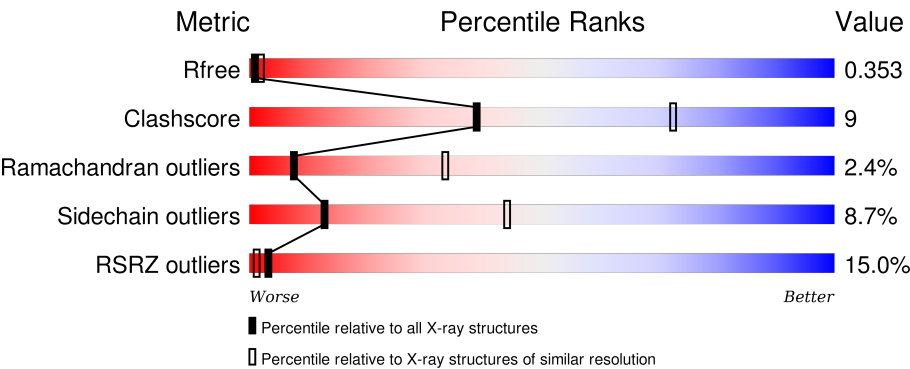


# 1 Overall quality at a glance i

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 <sub>free</sub>	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	119	<div><div></div><div>56%11%..31%</div></div>
1	AI	119	<div><div></div><div>57%10%..31%</div></div>
1	AQ	119	<div><div></div><div>56%11%..31%</div></div>
1	AY	119	<div><div>%</div><div>58%8%..31%</div></div>
1	Ag	119	<div><div></div><div>62%6%•31%</div></div>

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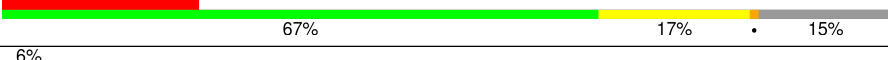

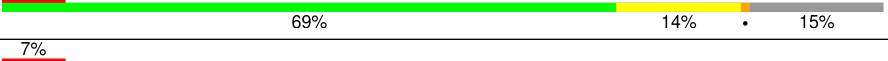

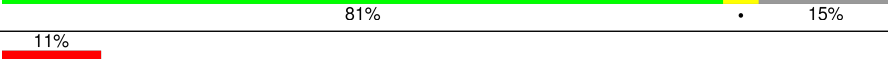
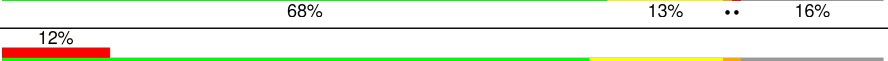
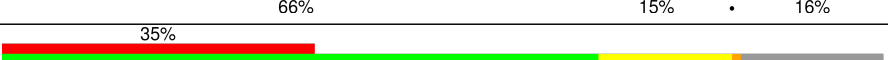
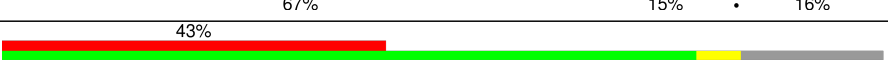
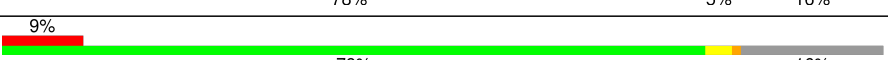
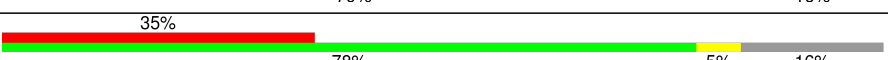
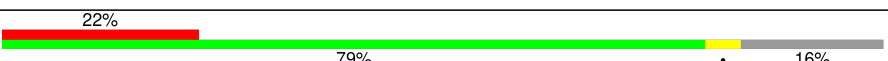
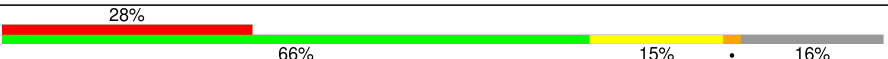
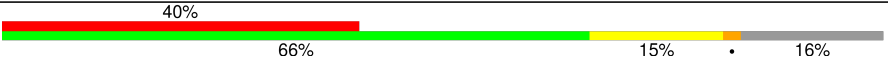



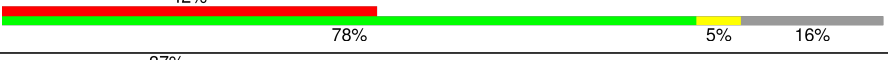
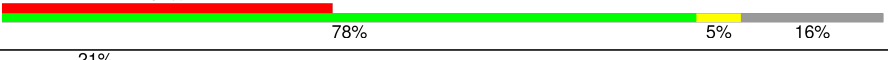
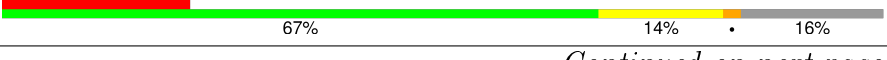

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Mol	Chain	Length	Quality of chain
1	Ao	119	% 64% 31%
1	Aw	119	% 63% 5% 31%
1	BA	119	5% 57% 9% 31%
1	BI	119	12% 57% 9% 31%
1	BQ	119	% 57% 9% 31%
1	BY	119	61% 5% 31%
1	Bg	119	63% 5% 31%
1	Bo	119	62% 6% 31%
1	Bw	119	62% 6% 31%
1	CA	119	58% 9% 31%
1	CI	119	5% 57% 9% 31%
1	CQ	119	57% 9% 31%
1	CY	119	59% 8% 31%
1	Cg	119	62% 6% 31%
1	Co	119	8% 64% 31%
2	AB	118	% 69% 14% 15%
2	AJ	118	67% 17% 15%
2	AR	118	7% 66% 18% 15%
2	AZ	118	8% 69% 15% 15%
2	Ah	118	6% 78% 7% 15%
2	Ap	118	8% 82% 15%
2	Ax	118	3% 81% 15%
2	BB	118	24% 65% 18% 15%
2	BJ	118	32% 65% 17% 15%
2	BR	118	14% 66% 15% 15%

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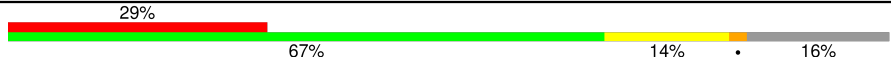
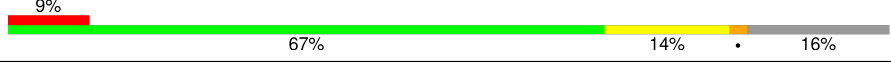
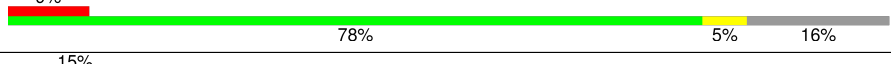


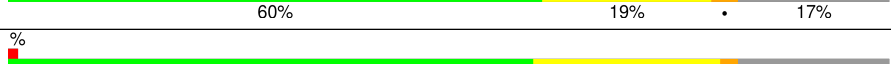
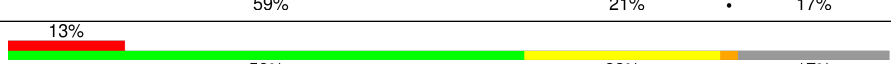
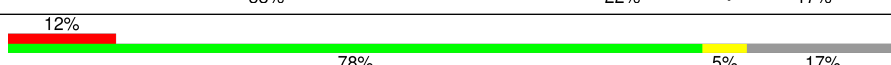
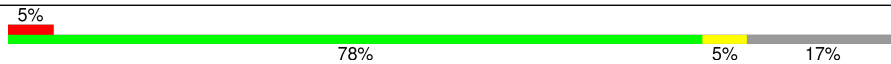


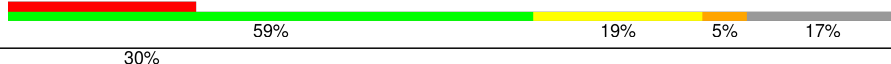
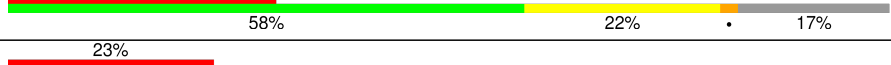

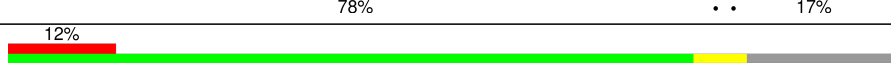










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Mol	Chain	Length	Quality of chain
2	BZ	118	
2	Bh	118	
2	Bp	118	
2	Bx	118	
2	CB	118	
2	CJ	118	
2	CR	118	
2	CZ	118	
2	Ch	118	
2	Cp	118	
3	AC	92	
3	AK	92	
3	AS	92	
3	Aa	92	
3	Ai	92	
3	Aq	92	
3	Ay	92	
3	BC	92	
3	BK	92	
3	BS	92	
3	Ba	92	
3	Bi	92	
3	Bq	92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

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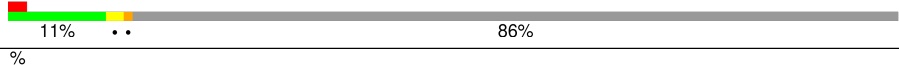
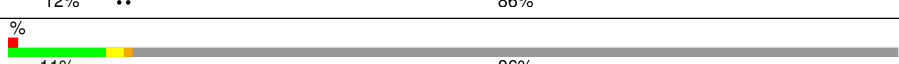
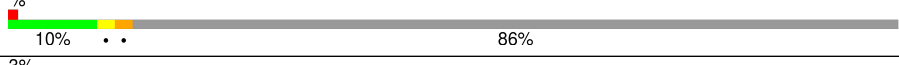



















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Mol	Chain	Length	Quality of chain
3	CK	92	
3	CS	92	
3	Ca	92	
3	Ci	92	
3	Cq	92	
4	AD	86	
4	AL	86	
4	AT	86	
4	Ab	86	
4	Aj	86	
4	Ar	86	
4	Az	86	
4	BD	86	
4	BL	86	
4	BT	86	
4	Bb	86	
4	Bj	86	
4	Br	86	
4	Bz	86	
4	CD	86	
4	CL	86	
4	CT	86	
4	Cb	86	
4	Cj	86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

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Mol	Chain	Length	Quality of chain
5	A1	124	
5	AE	124	
5	AM	124	
5	AU	124	
5	Ac	124	
5	Ak	124	
5	As	124	
5	B1	124	
5	BE	124	
5	BM	124	
5	BU	124	
5	Bc	124	
5	Bk	124	
5	Bs	124	
5	CE	124	
5	CM	124	
5	CU	124	
5	Cc	124	
5	Ck	124	
5	Cs	124	
6	A2	247	
6	AF	247	
6	AN	247	
6	AV	247	
6	Ad	247	

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Mol	Chain	Length	Quality of chain
6	Al	247	
6	At	247	
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	

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Mol	Chain	Length	Quality of chain
7	BW	186	
7	Be	186	
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	

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Mol	Chain	Length	Quality of chain
8	CP	76	<div><div></div><div>29%</div><div>79%</div><div>12%</div><div>8%</div></div>
8	CX	76	<div><div></div><div>12%</div><div>79%</div><div>12%</div><div>8%</div></div>
8	Cf	76	<div><div></div><div>8%</div><div>88%</div><div></div><div>8%</div></div>
8	Cn	76	<div><div></div><div>30%</div><div>88%</div><div></div><div>8%</div></div>
8	Cv	76	<div><div></div><div>70%</div><div>88%</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	C	N	O	S	0	0	0
			638	405	113	115	5			
3	CK	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	CS	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Ca	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Ci	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			
3	Cq	77	Total	C	N	O	S	0	0	0
			638	405	113	115	5			

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

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

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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 133	C 85	N 19	O 29	0	0	0
5	B1	17	Total 133	C 85	N 19	O 29	0	0	0
5	CE	17	Total 133	C 85	N 19	O 29	0	0	0
5	CM	17	Total 133	C 85	N 19	O 29	0	0	0
5	CU	17	Total 133	C 85	N 19	O 29	0	0	0
5	Cc	17	Total 133	C 85	N 19	O 29	0	0	0
5	Ck	17	Total 133	C 85	N 19	O 29	0	0	0
5	Cs	17	Total 133	C 85	N 19	O 29	0	0	0

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			

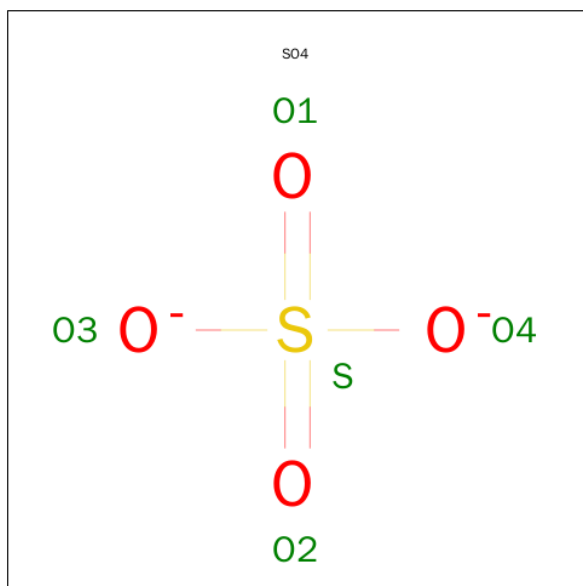
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	Bn	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	Bv	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	B4	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
8	CH	70	Total	C	N	O	S	0	0	0
			544	344	96	98	6			
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: O<sub>4</sub>S).



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		





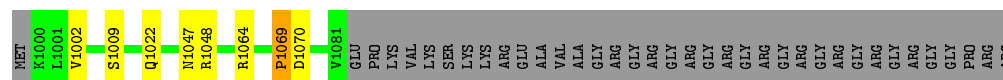
- Molecule 1: Small nuclear ribonucleoprotein Sm D1





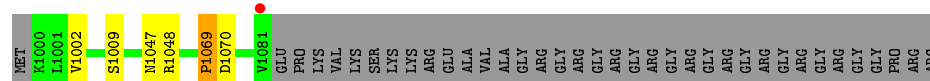
- Molecule 1: Small nuclear ribonucleoprotein Sm D1

Chain Ag: 



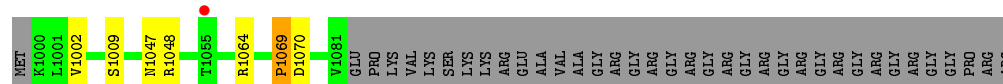
- Molecule 1: Small nuclear ribonucleoprotein Sm D1

Chain Ao: 



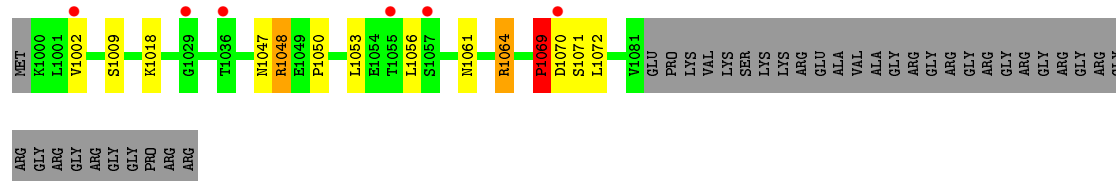
- Molecule 1: Small nuclear ribonucleoprotein Sm D1

Chain Aw: 



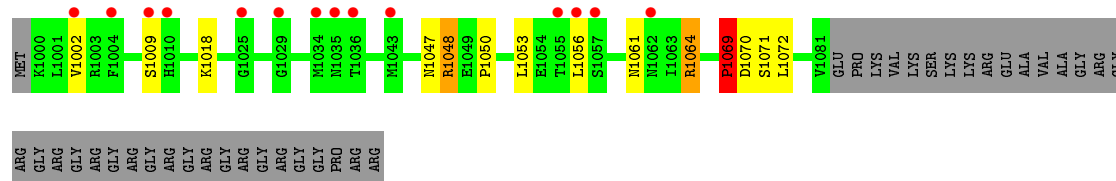
- Molecule 1: Small nuclear ribonucleoprotein Sm D1

Chain BA: 



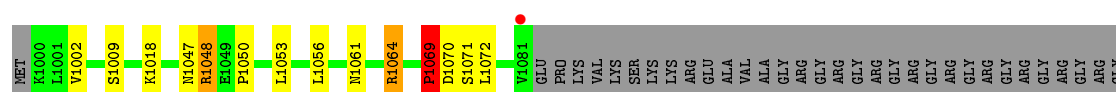
- Molecule 1: Small nuclear ribonucleoprotein Sm D1

Chain BI: 



- Molecule 1: Small nuclear ribonucleoprotein Sm D1

Chain BQ: 









PRO  
ARG  
ARG

- |     |       |       |       |       |       |       |       |       |       |       |       |       |       |       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | K1000 | L1001 | V1002 | S1009 | K1018 | K1042 | N1047 | R1048 | R1064 | P1069 | D1070 | S1071 | L1072 | V1081 | GLU | PRO | LYS | VAL | LYS | SER | LYS | LYS | ARG | GLU | ALA | VAL | ALA | GLY | ARG | GLY | ARG | GLY | GLY | GLY | ARG | GLY | GLY | GLY | PRO | ARG |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- |       |
|-------|
| MET   |
| K1000 |
| L1001 |
| V1002 |
| S1009 |
| N1047 |
| R1048 |
| E1049 |
| R1064 |
| P1069 |
| D1070 |
| V1081 |
| GLU   |
| PRO   |
| LYS   |
| VAL   |
| LYS   |
| SER   |
| LYS   |
| LYS   |
| ARG   |
| GLU   |
| ALA   |
| VAL   |
| ALA   |
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| ARG   |
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| ARG   |
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| ARG   |
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| ARG   |
| GLY   |
| GLY   |
| GLY   |
| GLY   |
| PRO   |
| ARG   |

- [illegible]

GLY  
ARG  
GLY  
GLY  
PRO  
ARG  
ARG

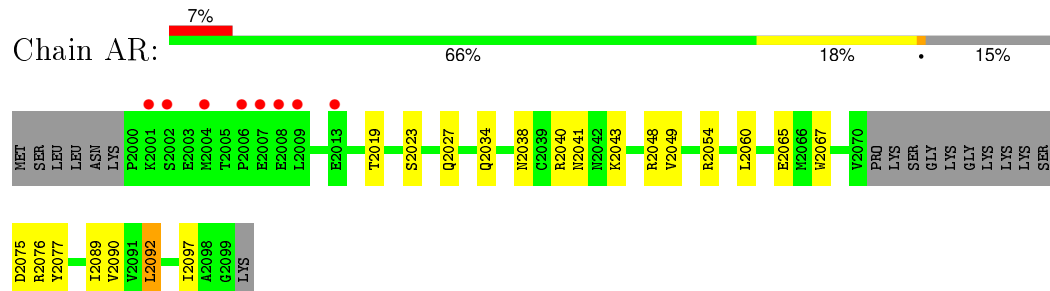
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|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| MET | SER | LEU | LEU | ASN | LYS | P2000 | E2016 | S2023 | Q2027 | Q2034 | N2038 | G2039 | R2040 | N2041 | N2042 | K2043 | R2048 | V2049 | R2054 | L2060 | E2065 | M2066 | W2067 | V2070 | PRO | LYS | LYS | GLY | GLY | LYS | LYS | LYS | LYS | SER | LYS | P2071 | D2075 | R2076 | Y2077 | I2089 | V2090 | L2091 | L2092 | I2097 | A2098 |
|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|

LYS

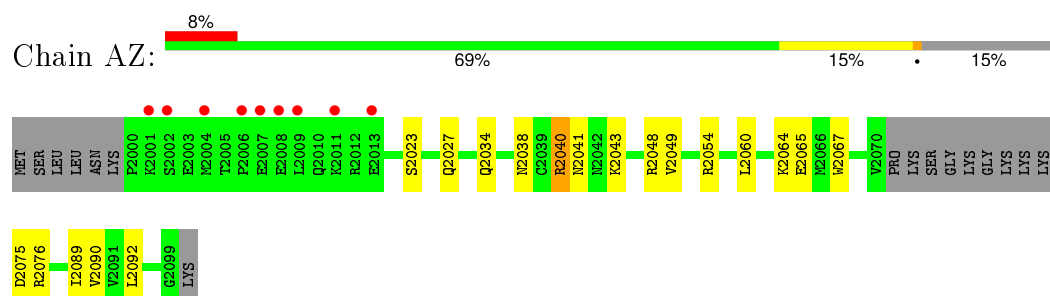
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|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-----|
| NET | SER | LEU | LEU | ASN | LYS | P2000 | R2001 | S2002 | E2016 | S2023 | Q2027 | Q2034 | R2040 | W2041 | W2042 | K2043 | R2048 | V2049 | R2054 | L2060 | E2065 | M2066 | W2067 | V2070 | PRO | LYS | SER | SER | GLY | LYS | GLY | LYS | LYS | LYS | LYS | SER | SER | LYS | P2071 | D2075 | R2076 | Y2077 | L2092 | G2099 | LYS |
|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-----|



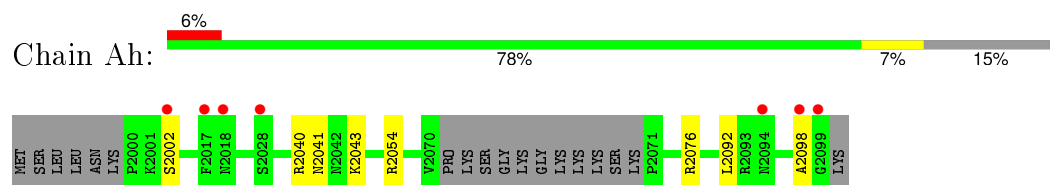
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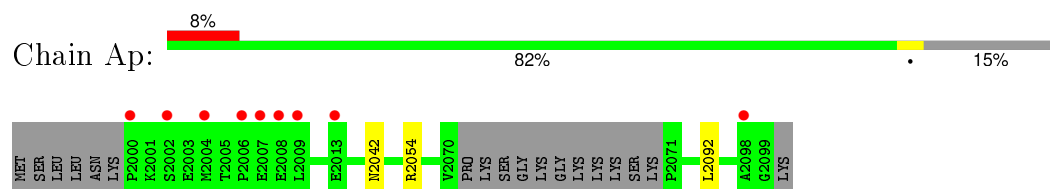
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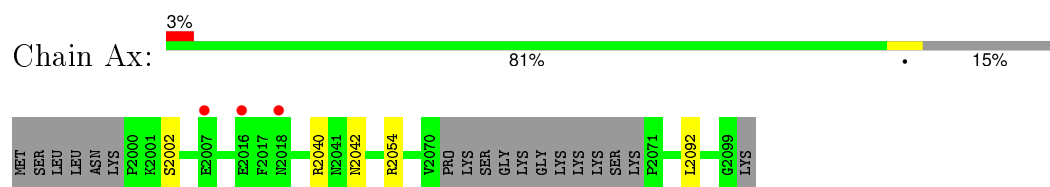
- Molecule 2: Small nuclear ribonucleoprotein Sm D2



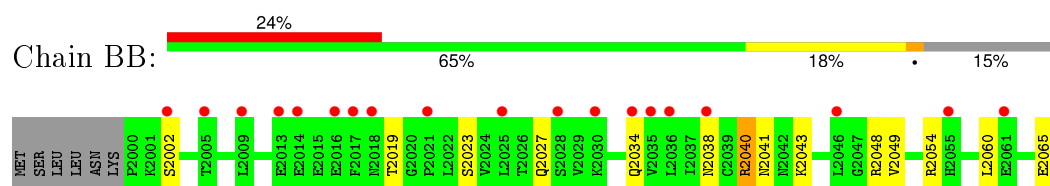
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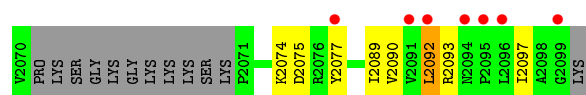
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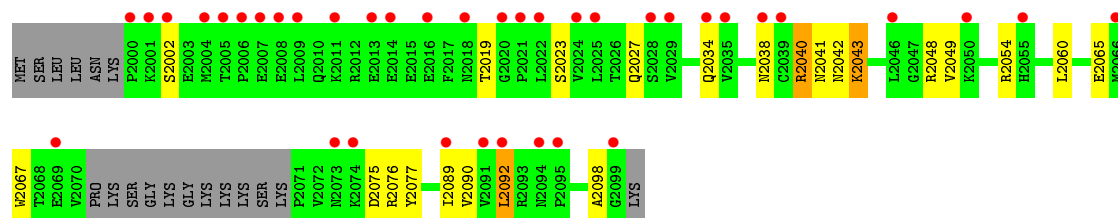
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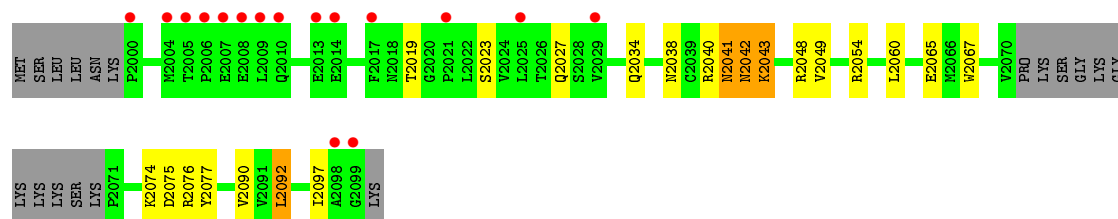




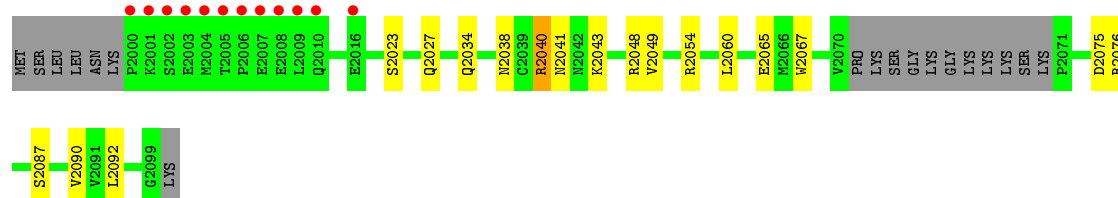
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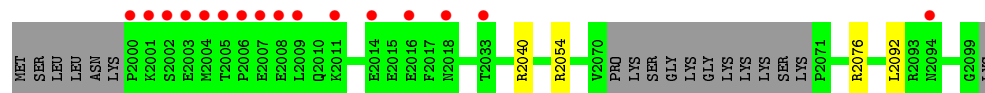
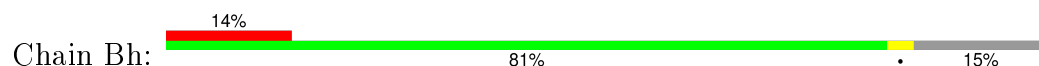
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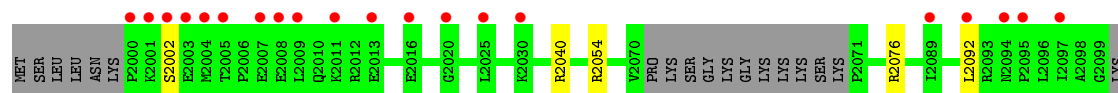
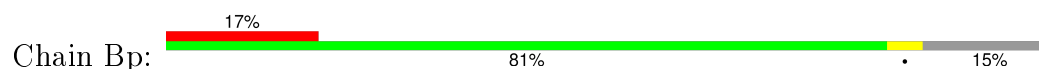
- Molecule 2: Small nuclear ribonucleoprotein Sm D2



- Molecule 2: Small nuclear ribonucleoprotein Sm D2



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

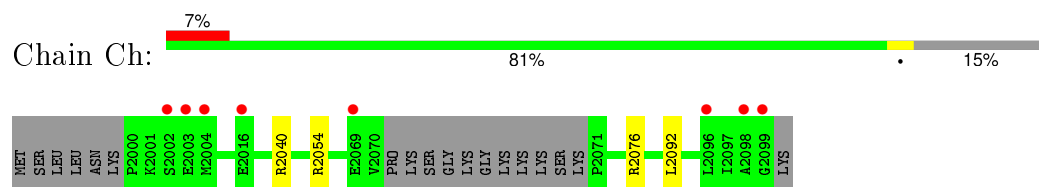




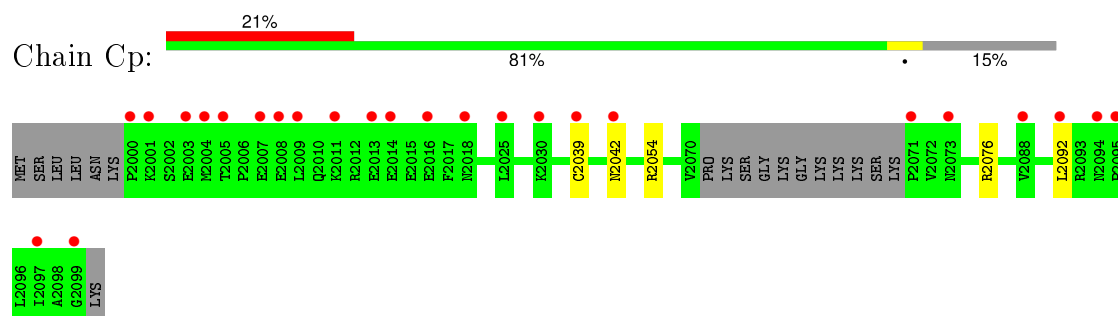
- Chain CZ:
- 
- | Category | Percentage |
|----------|------------|
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| Yellow   | 14%        |
| Red      | 7%         |
| Grey     | 15%        |
- NET  
SER  
LEU  
LEU  
ASN  
LYS  
P2000  
K2001  
S2002  
K2003  
K2004  
E2008  
E2014  
F2017  
S2023  
Q2027  
Q2034  
N2038  
C2039  
R2040  
N2041  
P2042  
K2043  
R2048  
R2054  
E2065  
P2066  
W2067  
V2070  
PRO  
LYS  
SER  
GLY  
LYS  
GLY  
LYS  
LYS  
LYS  
SER  
LYS  
P2071  
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LYS



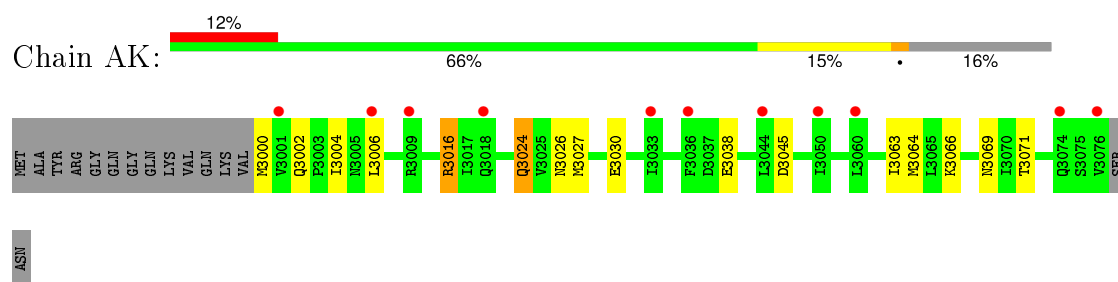
- Molecule 2: Small nuclear ribonucleoprotein Sm D2



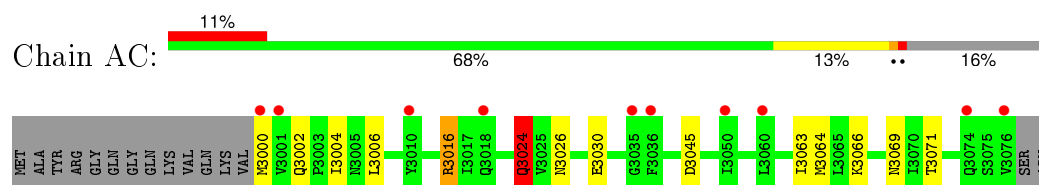
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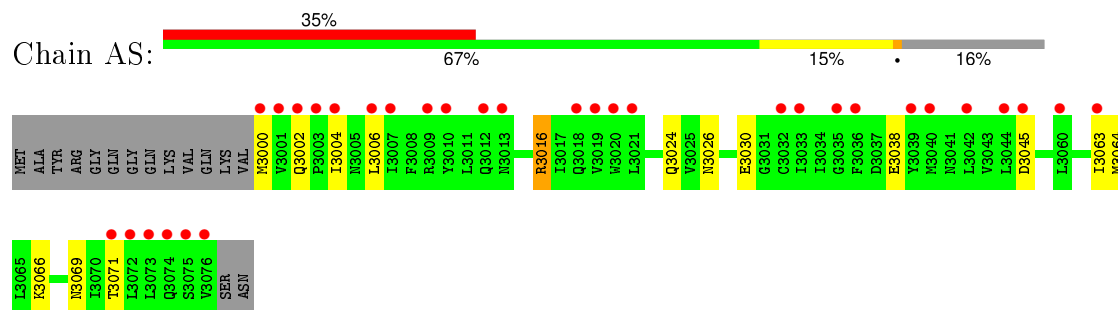
- Molecule 3: Small nuclear ribonucleoprotein E



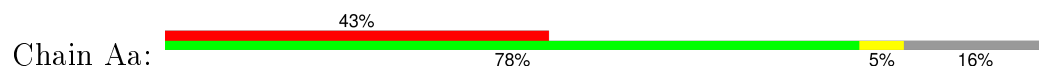
- Molecule 3: Small nuclear ribonucleoprotein E



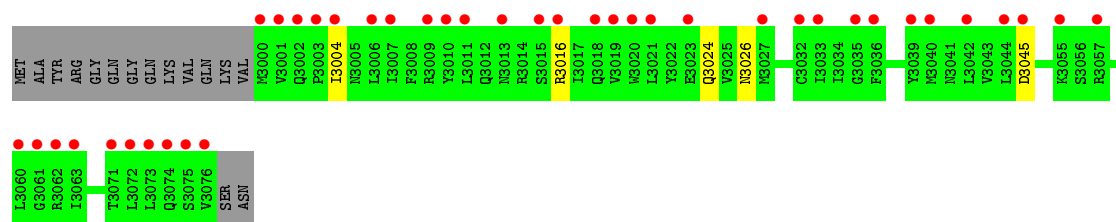
- Molecule 3: Small nuclear ribonucleoprotein E



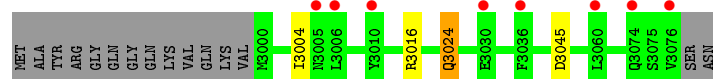
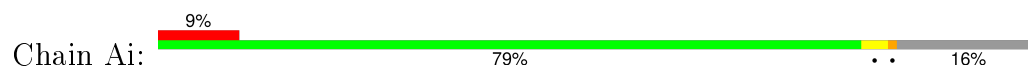
- Molecule 3: Small nuclear ribonucleoprotein E



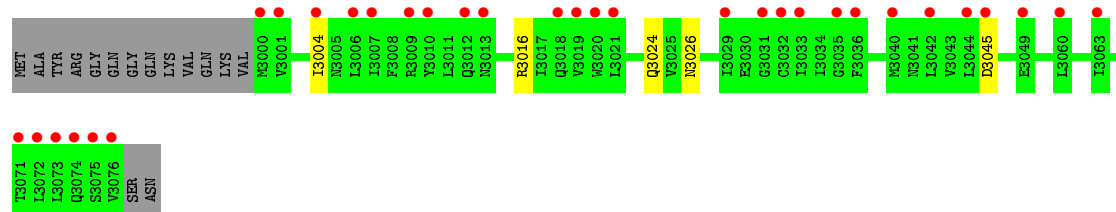
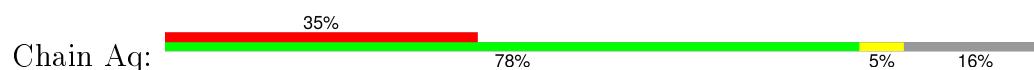




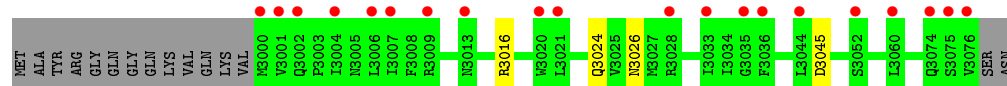
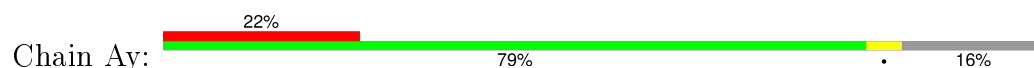
• Molecule 3: Small nuclear ribonucleoprotein E



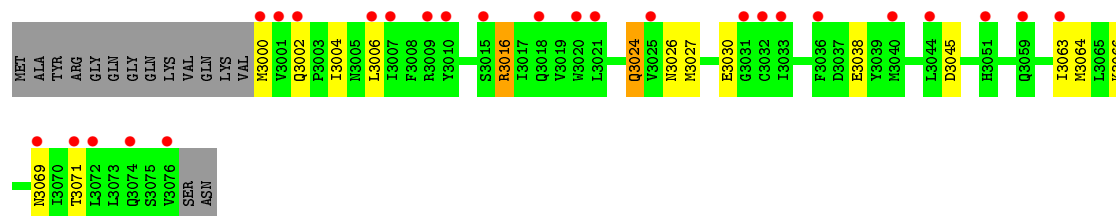
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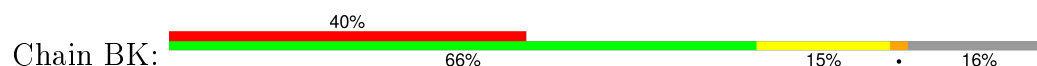
• Molecule 3: Small nuclear ribonucleoprotein E



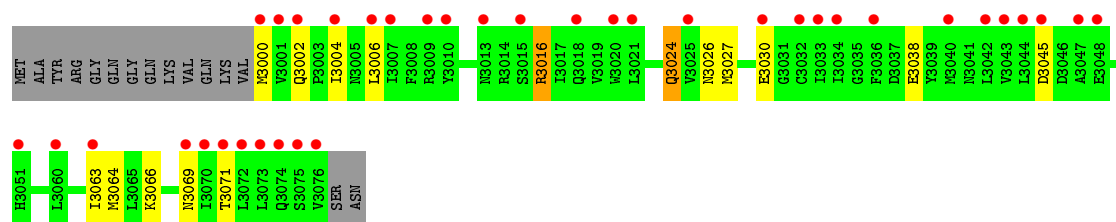
• Molecule 3: Small nuclear ribonucleoprotein E



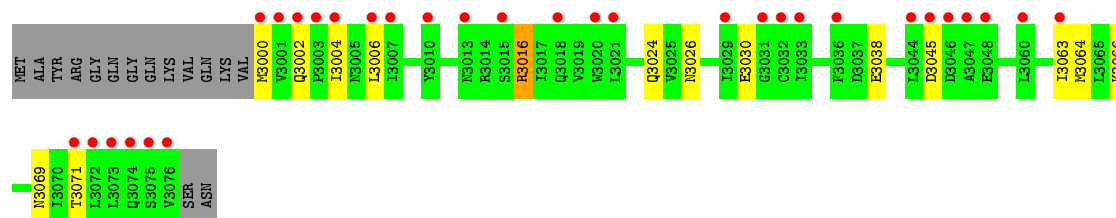
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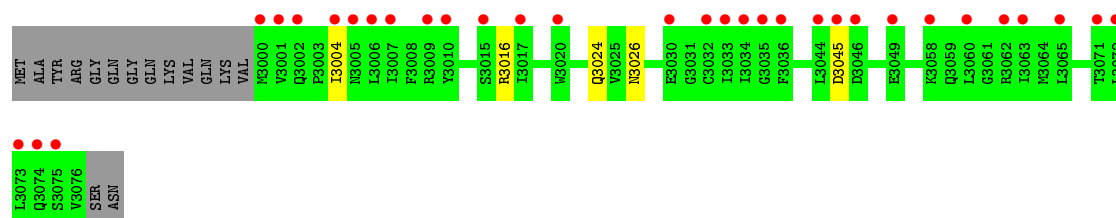
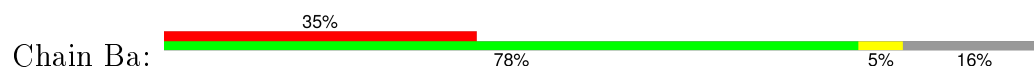




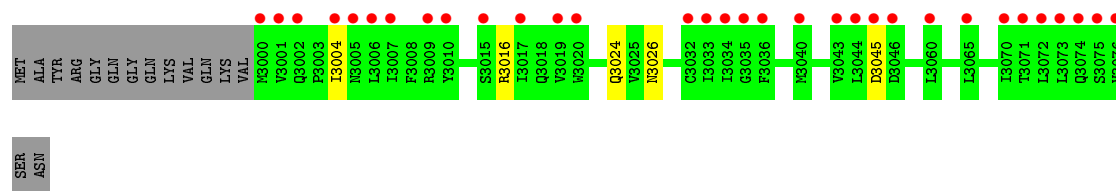
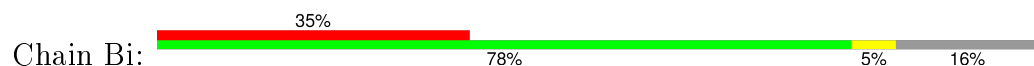
• Molecule 3: Small nuclear ribonucleoprotein E



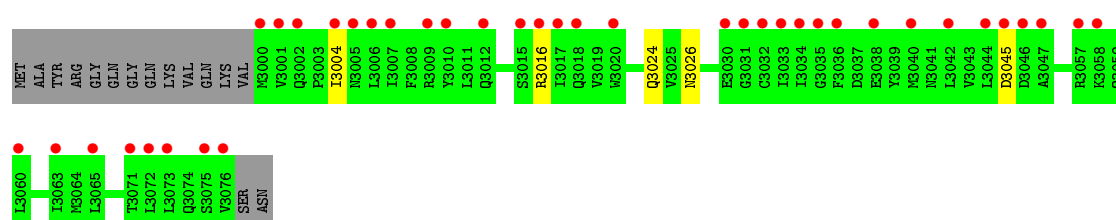
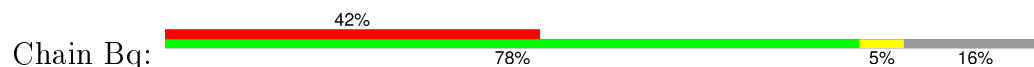
• Molecule 3: Small nuclear ribonucleoprotein E



• Molecule 3: Small nuclear ribonucleoprotein E

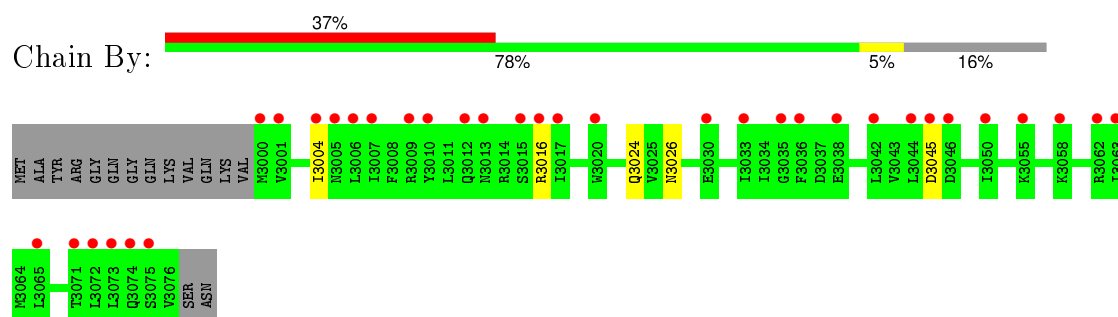


• Molecule 3: Small nuclear ribonucleoprotein E

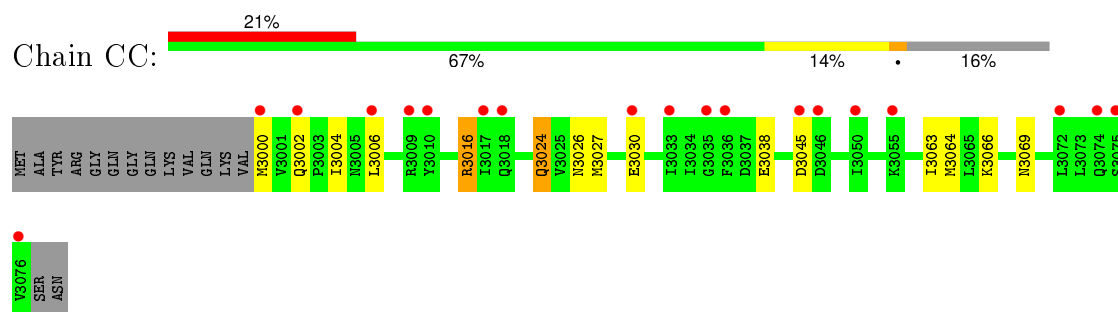




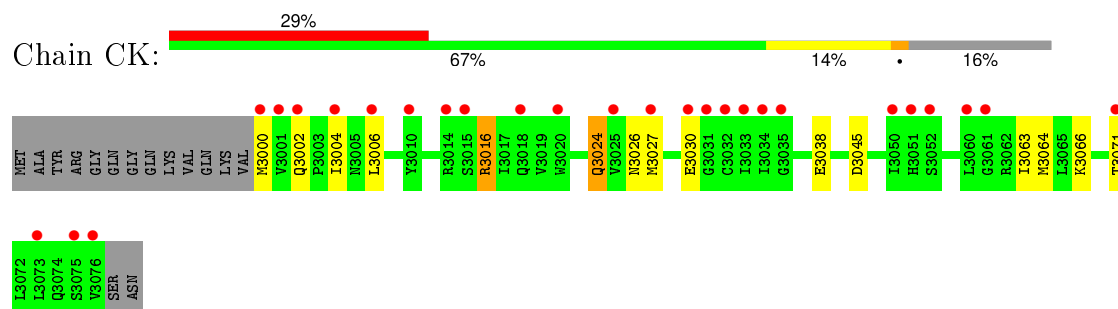
- Molecule 3: Small nuclear ribonucleoprotein E



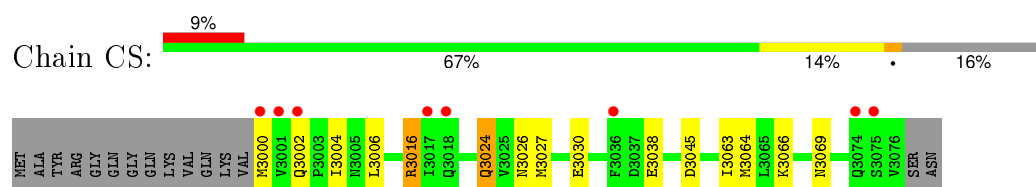
- Molecule 3: Small nuclear ribonucleoprotein E



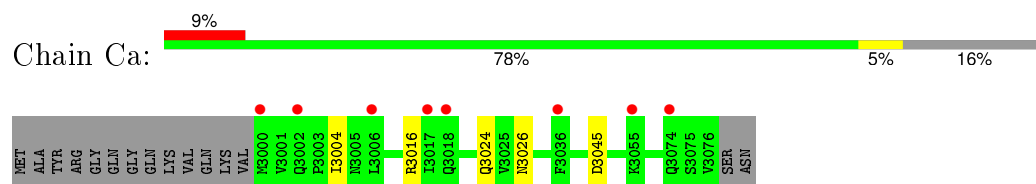
- Molecule 3: Small nuclear ribonucleoprotein E



- Molecule 3: Small nuclear ribonucleoprotein E

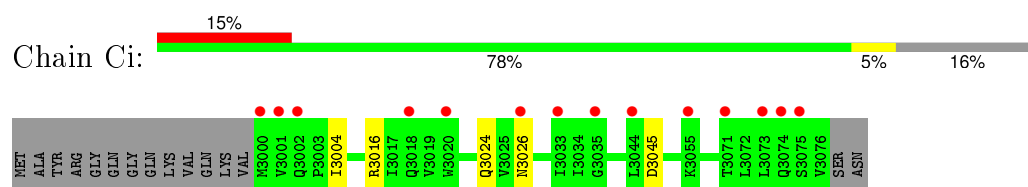


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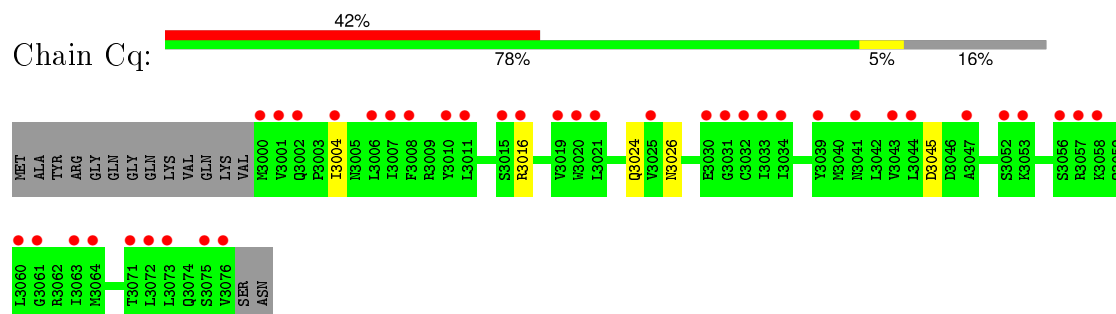


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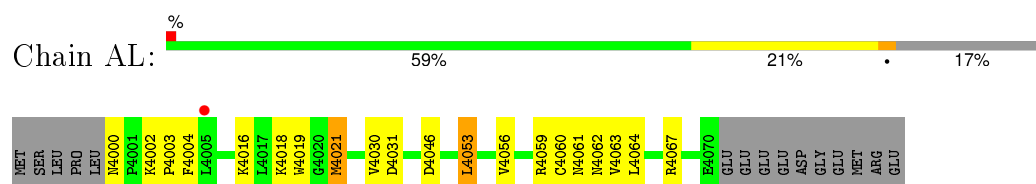




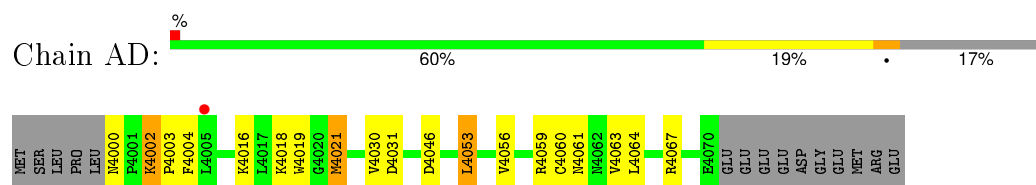
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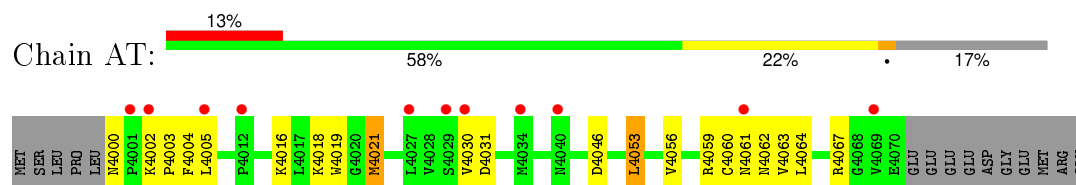
• Molecule 4: Small nuclear ribonucleoprotein F



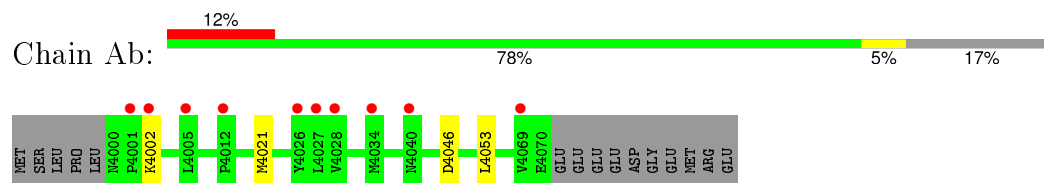
• Molecule 4: Small nuclear ribonucleoprotein F



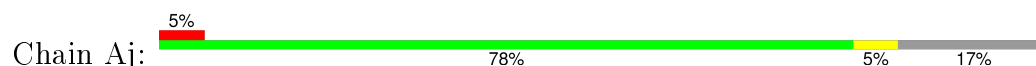
• Molecule 4: Small nuclear ribonucleoprotein F



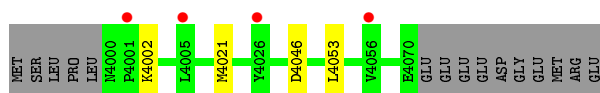
• Molecule 4: Small nuclear ribonucleoprotein F



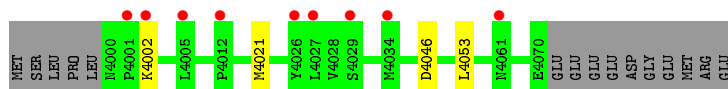
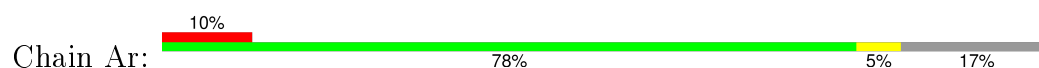
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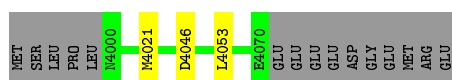
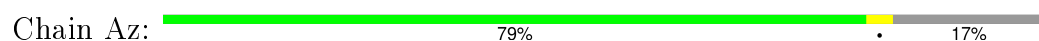




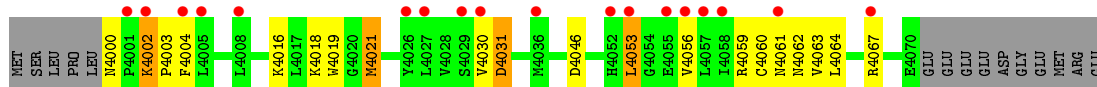
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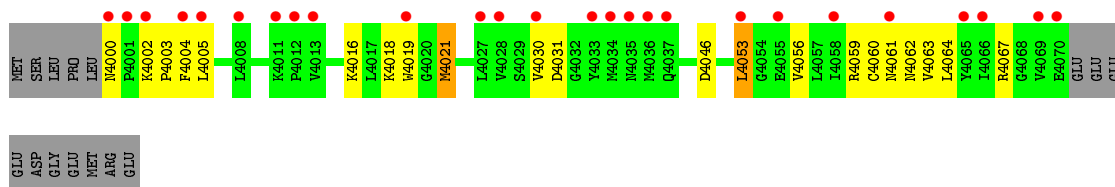
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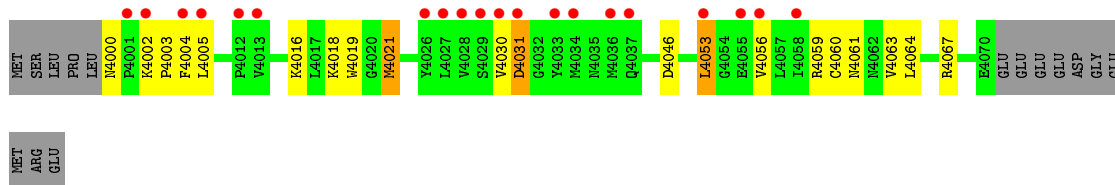
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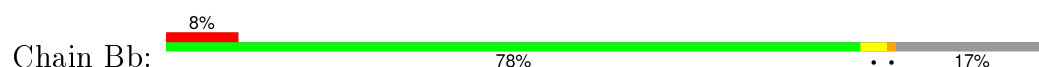
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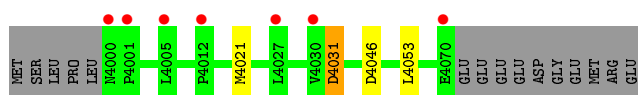
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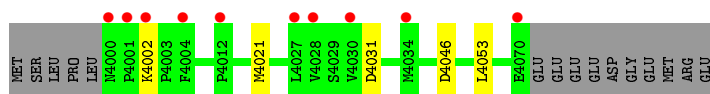
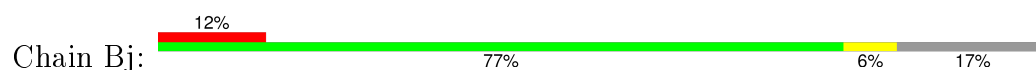
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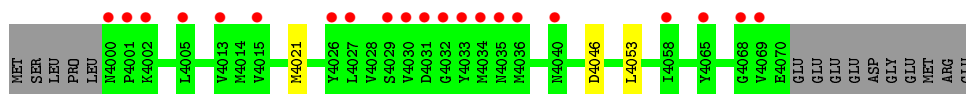
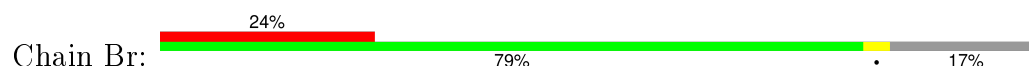




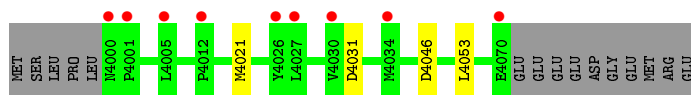
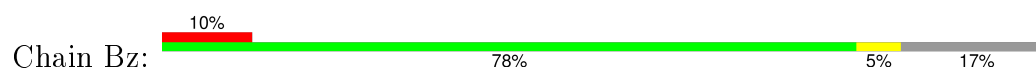
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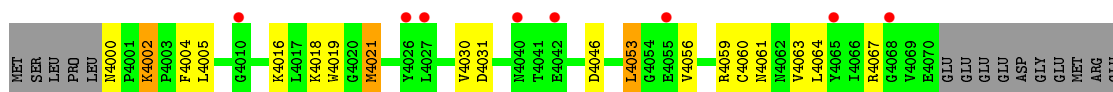
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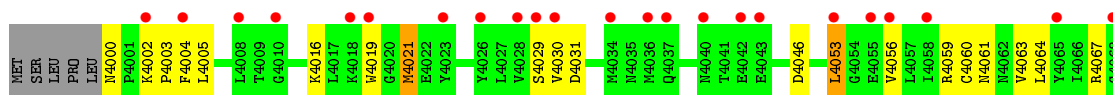
- Molecule 4: Small nuclear ribonucleoprotein F



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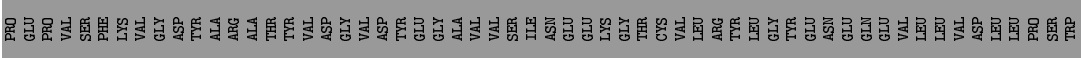
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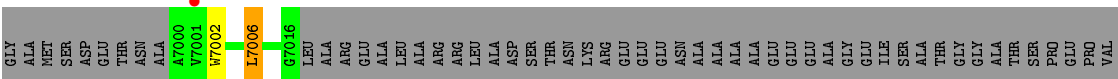




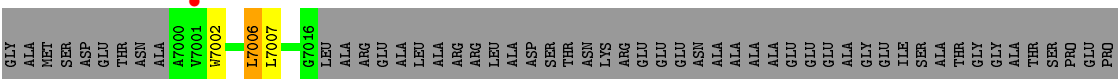
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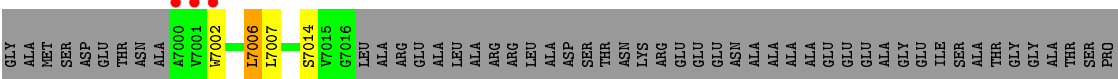
● Molecule 5: LD23602p



● Molecule 5: LD23602p



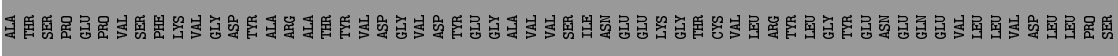
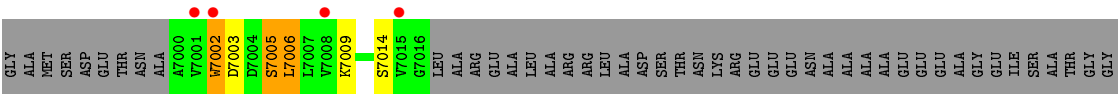
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● Molecule 5: LD23602p

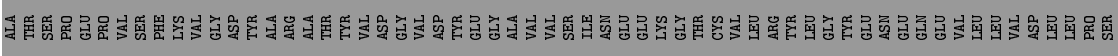
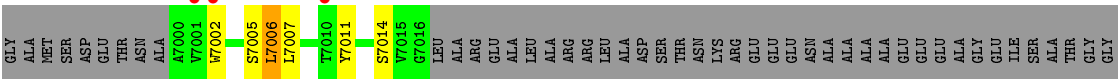






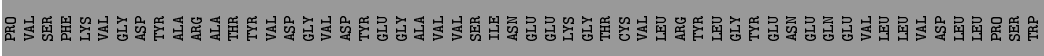
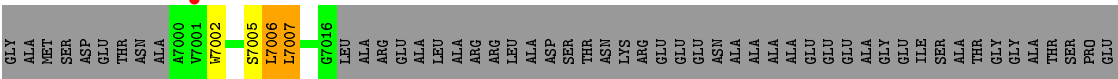
TRP

• Molecule 5: LD23602p



TRP

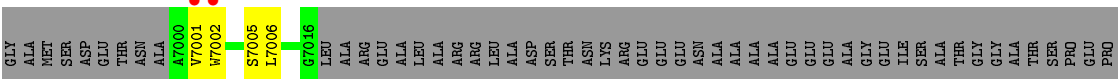
• Molecule 5: LD23602p



• Molecule 5: LD23602p



• Molecule 5: LD23602p





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• Molecule 5: LD23602p



GLY ALA MET SER ASP GLU THR ASN ALA A7000 A7001 W7002 S7005 L7006 T7010 G7016 LEU

GLU PRO SER PHE LYS VAL GLY ASP TYR ARG ALA THR TYR VAL ASP GLY VAL ASP VAL TYR LYS THR CYS VAL LEU ARG GLU TYR LEU ASN GLY ALA ALA ASN GLU GLN GLU VAL LEU VAL LEU VAL ASP LEU PRO SER TRP

• Molecule 5: LD23602p



GLY ALA MET SER ASP GLU THR ASN ALA A7000 A7001 W7002 W7003 L7006 L7007 G7016 LEU

PRO VAL SER PHE LYS VAL GLY ASP TYR ALA ARG ALA THR TYR VAL ASP GLY VAL ASP VAL TYR LYS THR CYS VAL LEU ARG GLU TYR LEU ASN GLY ALA ALA ASN GLU GLN GLU VAL LEU VAL LEU VAL ASP LEU PRO SER TRP

• Molecule 5: LD23602p



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PRO VAL SER PHE LYS VAL GLY ASP TYR ALA ARG ALA THR TYR VAL ASP GLY VAL ASP VAL TYR LYS THR CYS VAL LEU ARG GLU TYR LEU ASN GLY ALA ALA ASN GLU GLN GLU VAL LEU VAL LEU VAL ASP LEU PRO SER TRP

• Molecule 5: LD23602p



GLY ALA MET SER ASP GLU THR ASN ALA A7000 A7001 W7002 L7006 L7007 T7010 T7011 D7012 E7013 V7015 G7016 LEU

ALA THR SER PRO PRO VAL SER PHE LYS VAL GLY ASP TYR ALA ARG ALA THR TYR VAL ASP GLY VAL ASP TYR GLU GLY ALA VAL VAL SER ILE ASN GLU LYS THR CYS VAL LEU ARG TYR LEU ASN GLY ALA ALA ASN GLU GLN GLU TYR GLU VAL LEU VAL LEU VAL ASP LEU PRO SER TRP

TRP

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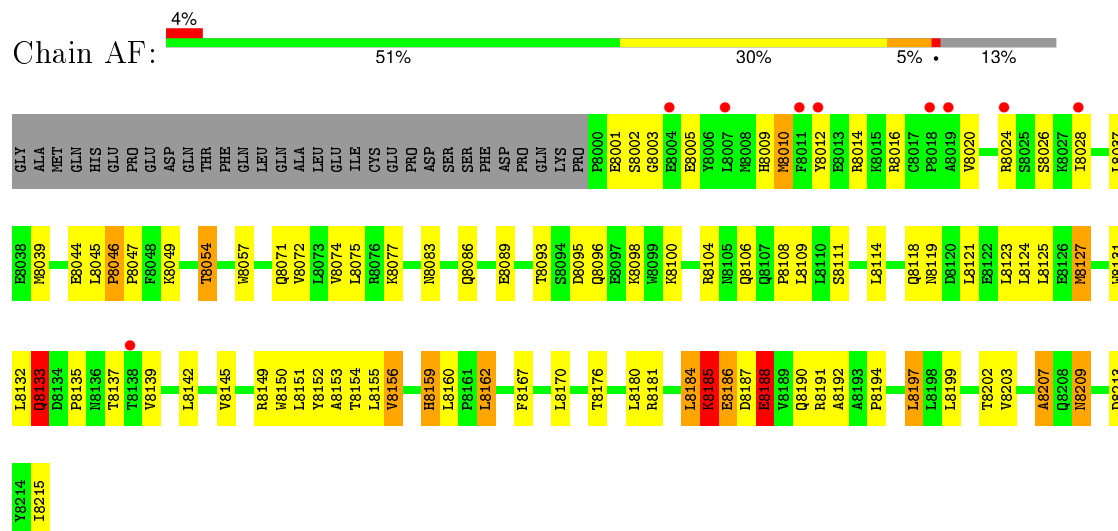




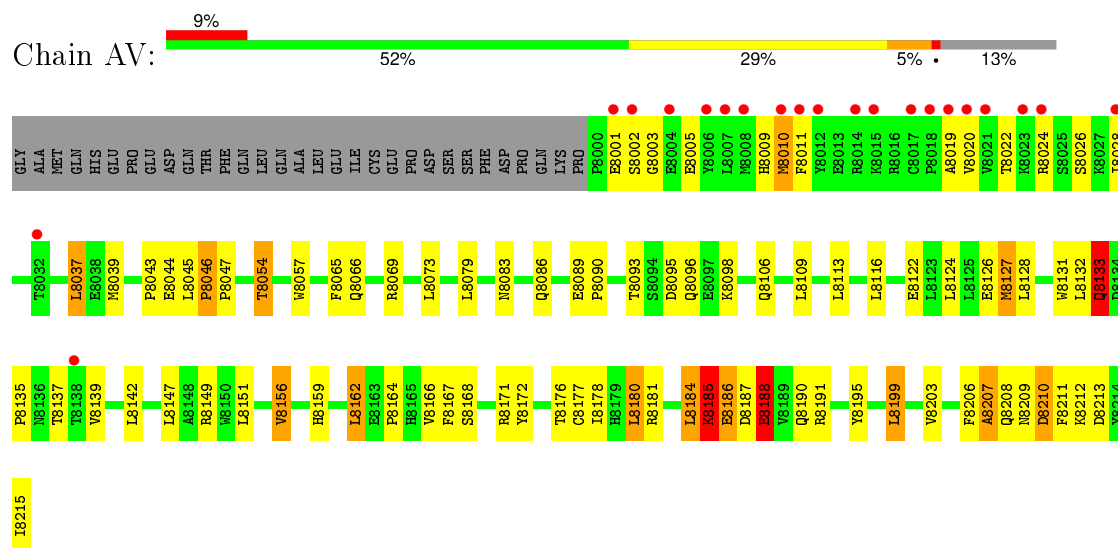




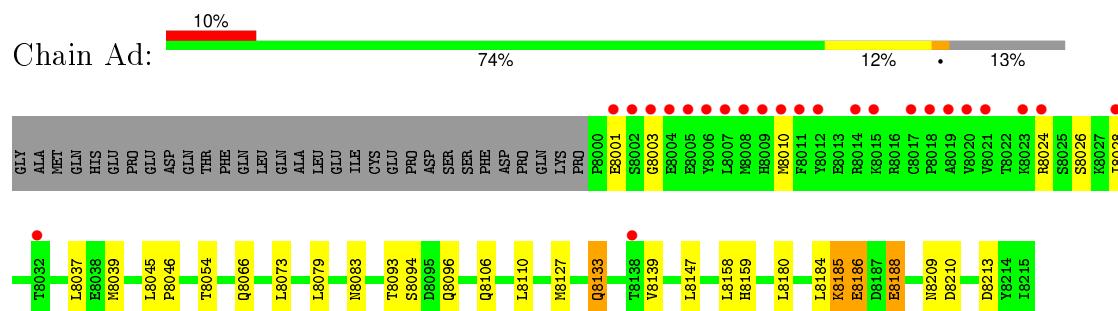
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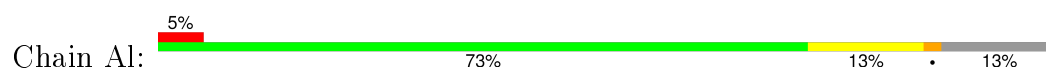
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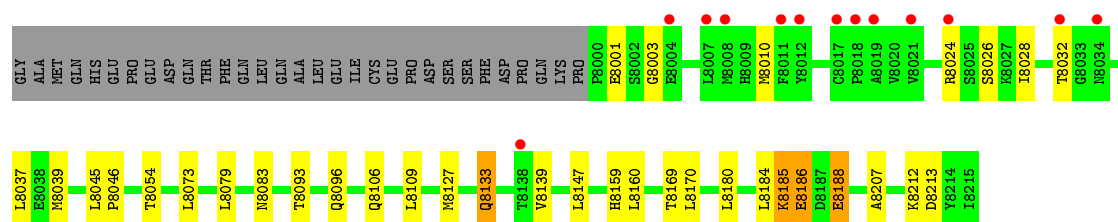
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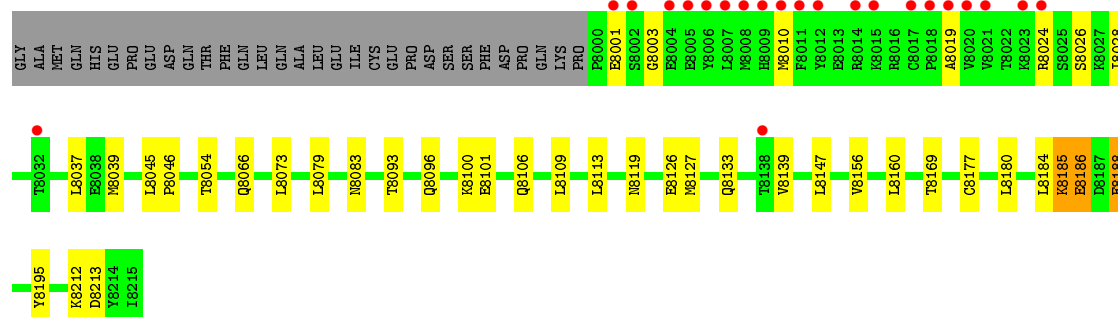
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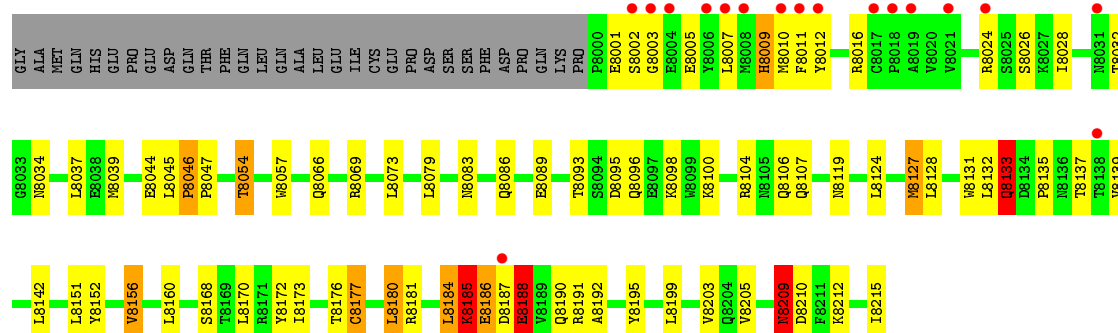




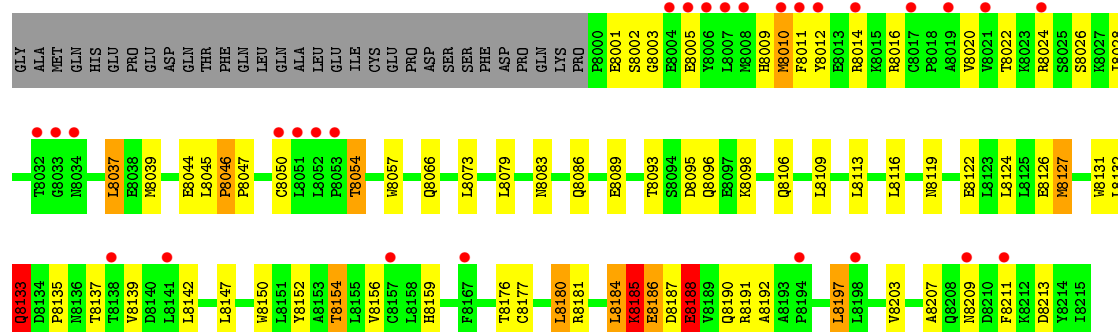
• Molecule 6: CG10419



• Molecule 6: CG10419



• Molecule 6: CG10419





Chain BN:

14% 53% 29% 13%

GLY	ALA	MET	GLN	GLN	GLU	PRO	GLU	ASP	GLN	THR	PHE	GLN	LEU	ALA	LEU	GLU	ILE	CYS	GLU	PRO	ASP	SER	PHE	ASP	PRO	GLN	LYS	PRO	P8000	E8001	S8002	G8003	E8004	E8005	W8006	L8007	L8008	H8008	H8009	H8010	F8011	W8012	E8013	R8014	R8015	R8016	R8017	F8018	A8019	W8020	W8021	T8022	R8023	R8024	S8025	S8026	R8027	T8028
Q8133	D8134	P8135	H8136	T8137	T8138	D8139	L8140	L8141	L8142	W8146	L8147	W8150	L8151	Y8152	A8153	T8154	L8155	L8158	H8159	H8165	F8166	F8167	S8168	T8169	L8170	Y8171	Y8172	R8175	T8176	C8177	I8178	H8179	L8180	R8181	L8184	E8185	D8186	D8187	E8188	W8189	Q8190	R8191	A8192	A8193	F8194	Y8195	H8196	L8197	L8198	L8199	W8203	L8132						

[illegible]

Chain Bd:

Amino Acid	Percentage
GLY	9%
ALA	73%
MET	13%
GLN	13%
HIS	13%
GLU	13%
PRO	13%
LEU	13%
ASP	13%
THR	13%
PHE	13%
GLN	13%
LEU	13%
ALA	13%
GLU	13%
ILE	13%
CYS	13%
GLU	13%
PRO	13%
ASP	13%
SER	13%
PHE	13%
ASP	13%
PRO	13%
GLN	13%
LYS	13%
PRO	13%
P8000	13%
E8001	13%
G8002	13%
G8003	13%
E8004	13%
E8005	13%
Y8006	13%
L8007	13%
M8008	13%
H8009	13%
M8010	13%
F8011	13%
Y8012	13%
E8013	13%
R8014	13%
K8015	13%
R8016	13%
R8024	13%
S8025	13%
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K8027	13%
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T8032	13%
G8033	13%
M8034	13%
L8037	13%

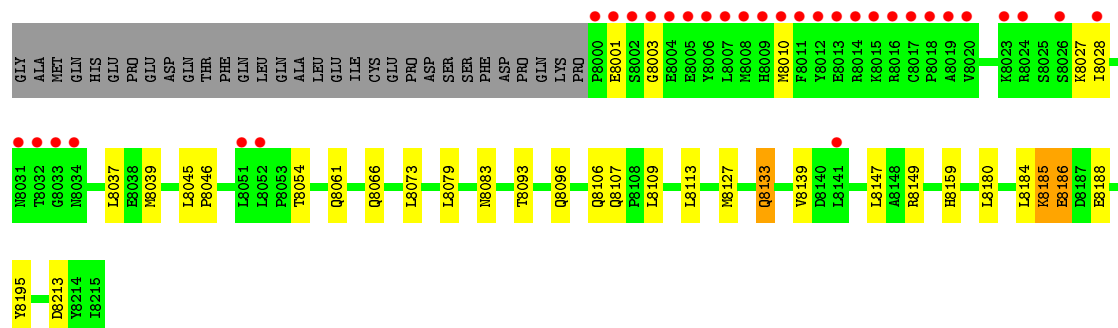
Chain BI:

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ALA  
MET  
GLN  
HIS  
GLU  
PRO  
GLY  
ASP  
GLN  
THR  
PHE  
GLN  
LEU  
GLN  
LEU  
GLU  
ILE  
CYS  
PRO  
ASP  
SER  
PHE  
ASP  
PRO  
GLN  
LVS  
PRO  
P8000  
S8001  
S8002  
G8003  
S8004  
S8005  
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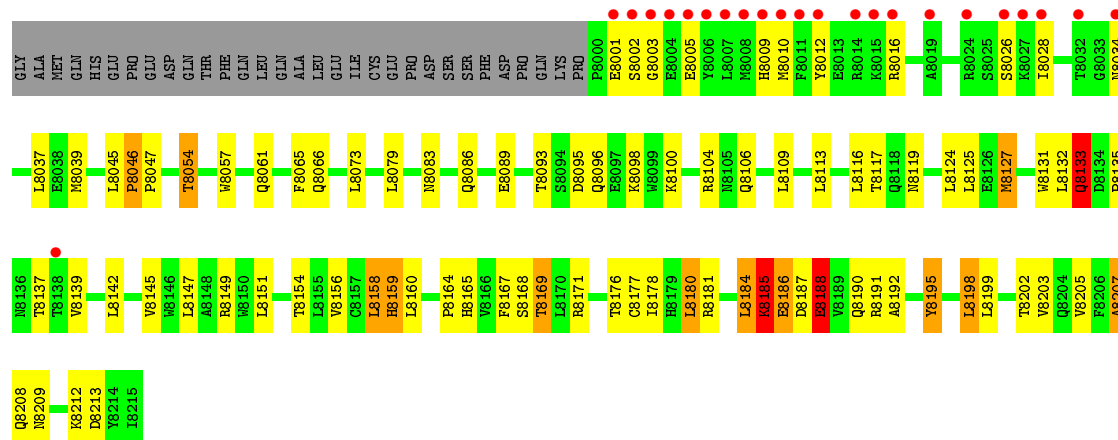




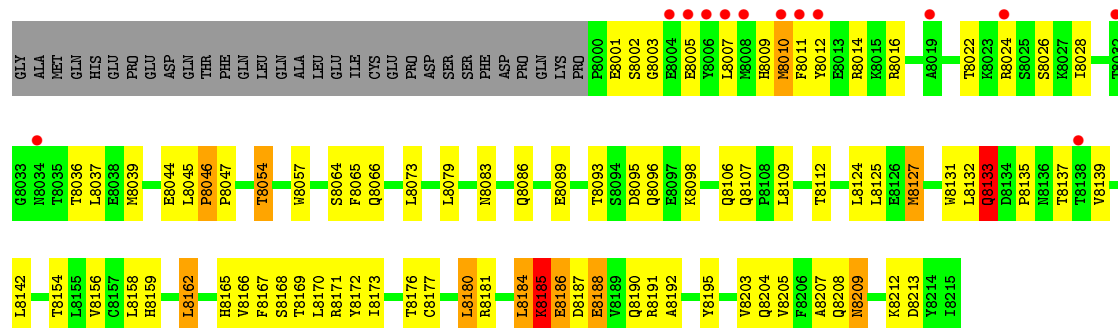
• Molecule 6: CG10419



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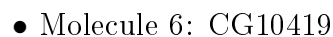
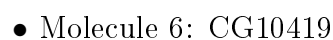
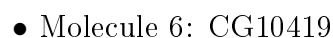


• Molecule 6: CG10419



• Molecule 6: CG10419

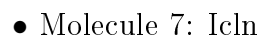
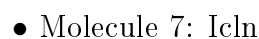




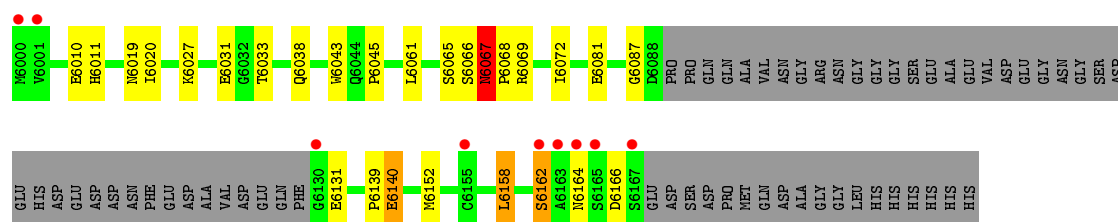




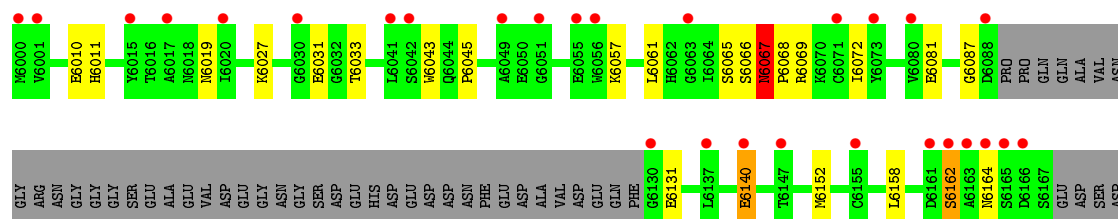




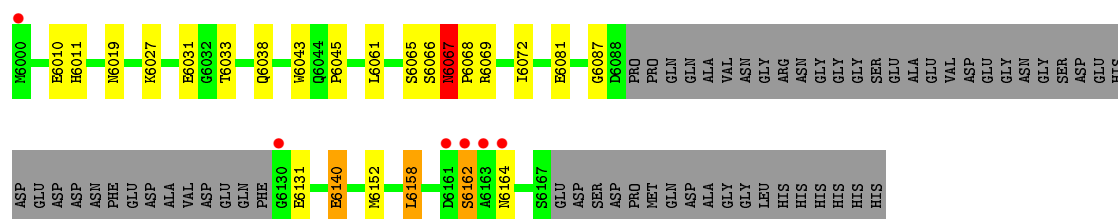




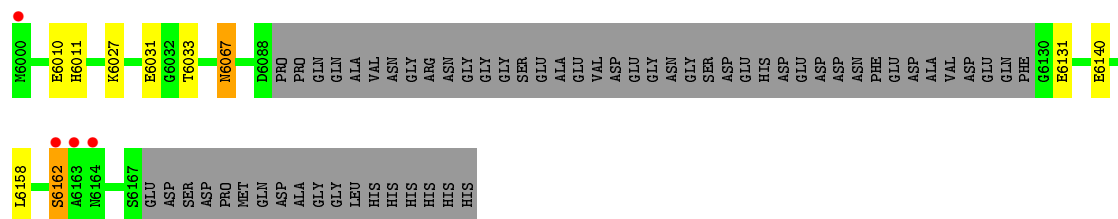
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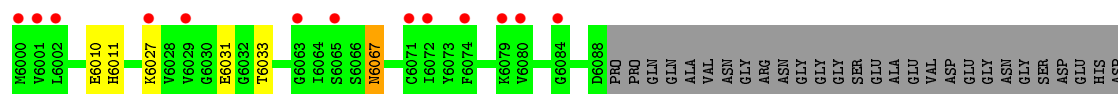
● Molecule 7: Icln



● Molecule 7: Icln



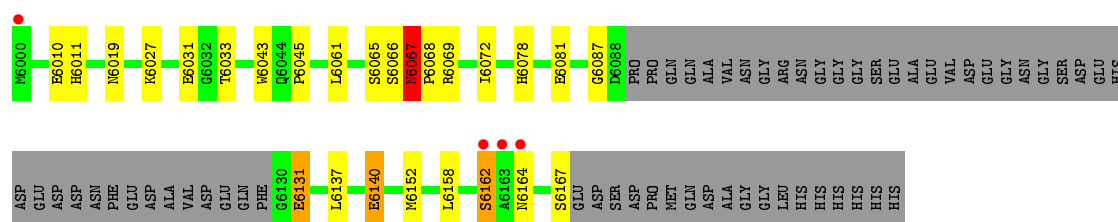
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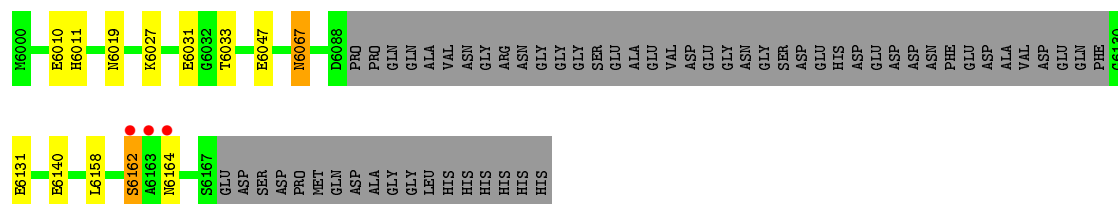




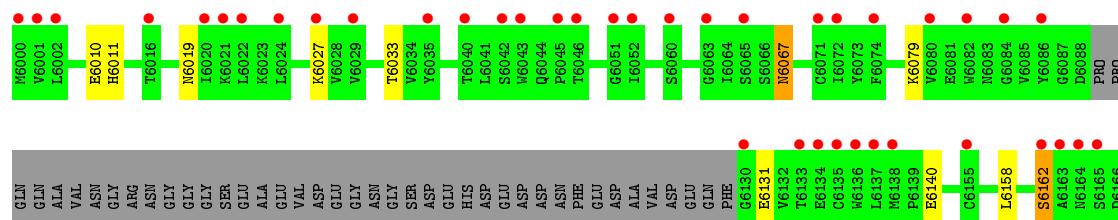




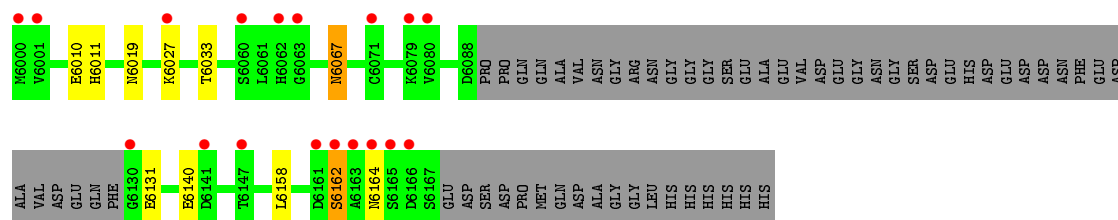
• Molecule 7: Icln



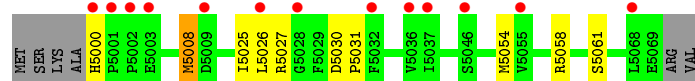
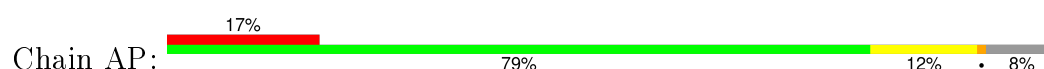
• Molecule 7: Icln



• Molecule 7: Icln

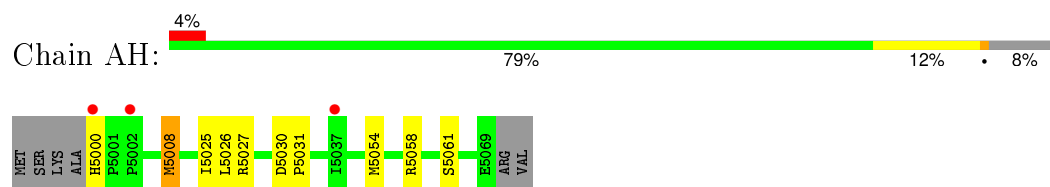


• Molecule 8: Small nuclear ribonucleoprotein G

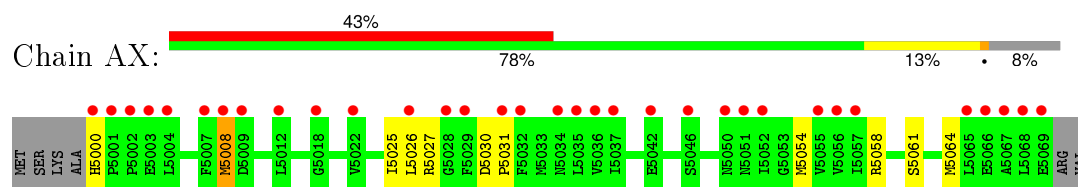




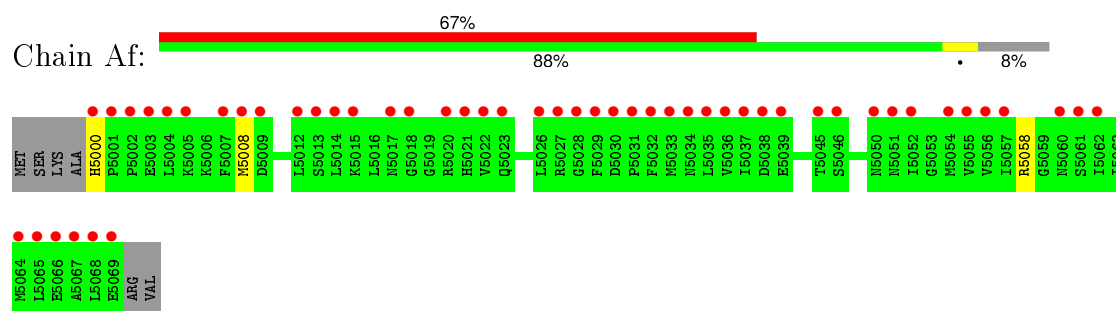
- Molecule 8: Small nuclear ribonucleoprotein G



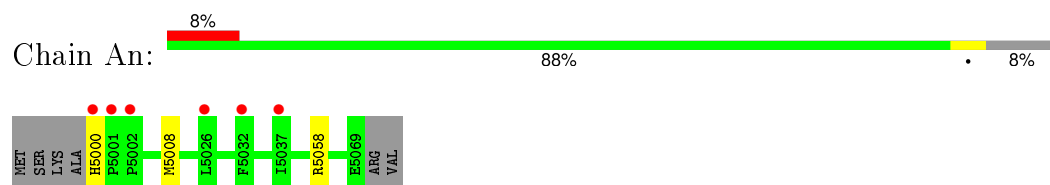
- Molecule 8: Small nuclear ribonucleoprotein G



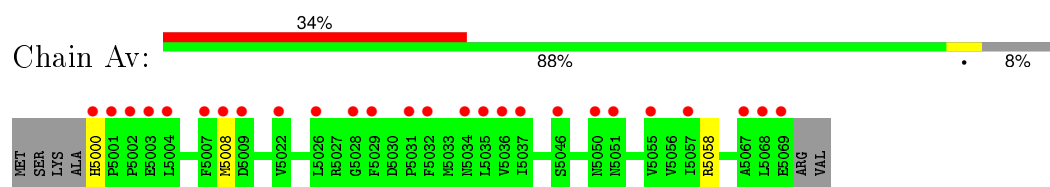
- Molecule 8: Small nuclear ribonucleoprotein G



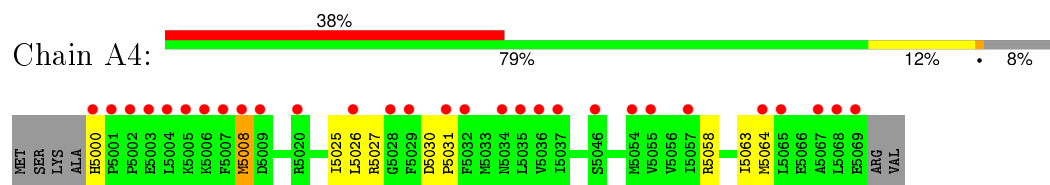
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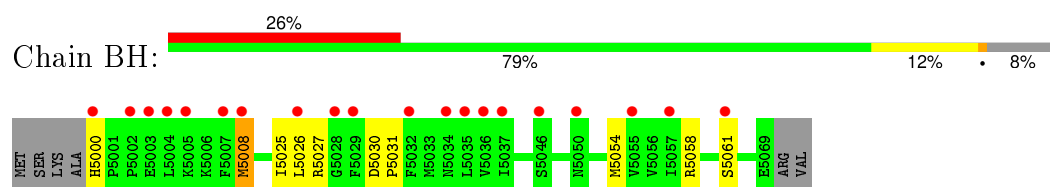


- Molecule 8: Small nuclear ribonucleoprotein G

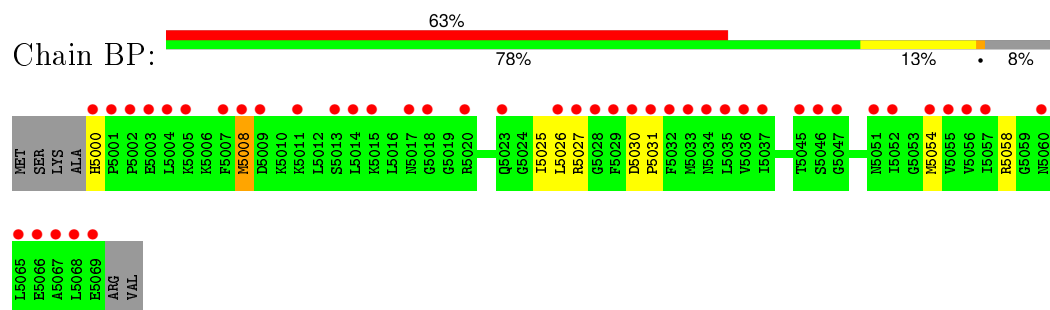


- Molecule 8: Small nuclear ribonucleoprotein G

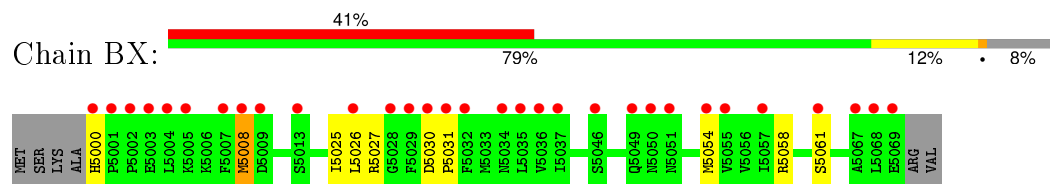




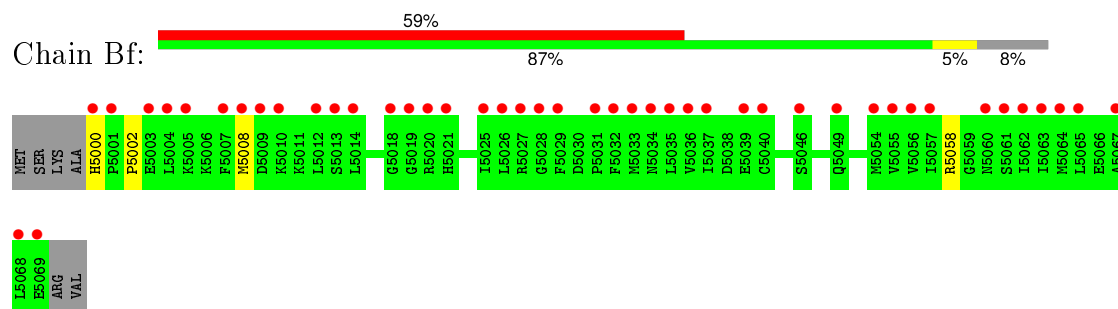
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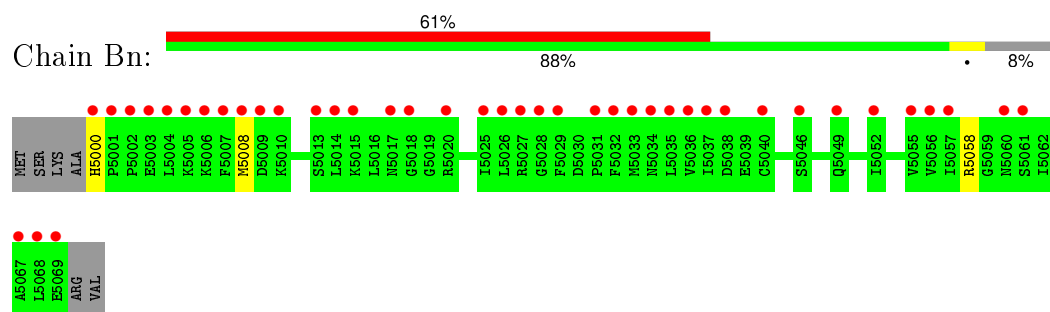
- Molecule 8: Small nuclear ribonucleoprotein G



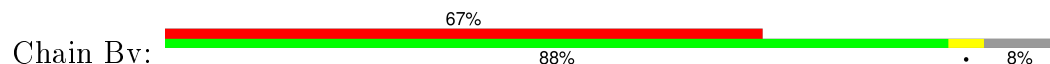
- Molecule 8: Small nuclear ribonucleoprotein G



- Molecule 8: Small nuclear ribonucleoprotein G



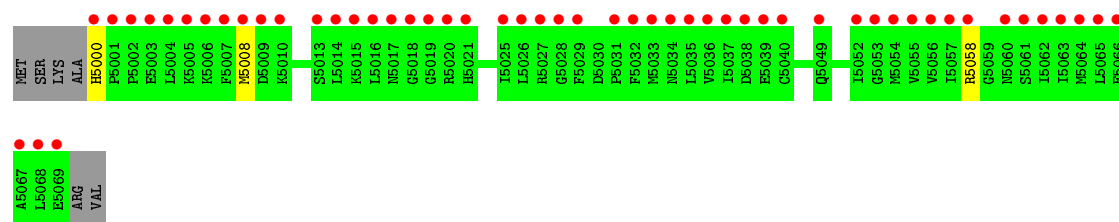
- Molecule 8: Small nuclear ribonucleoprotein G













## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (1.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.1	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 76.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	39 of 281573 reflections (0.014%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	121990	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:CN:8185:LYS:H	6:CN:8187:ASP:HB2	1.46	0.81
6:BV:8185:LYS:H	6:BV:8187:ASP:HB2	1.44	0.81
7:BO:6067:ASN:HB2	7:BO:6068:PRO:CD	2.10	0.81
6:AN:8185:LYS:H	6:AN:8187:ASP:HB2	1.45	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
7:CG:6067:ASN:CB	7:CG:6068:PRO:HD3	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BN:8185:LYS:H	6:BN:8187:ASP:HB2	1.45	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:AW:6067:ASN:CB	7:AW:6068:PRO:HD3	2.12	0.78
7:CO:6067:ASN:CB	7:CO:6068:PRO:HD3	2.14	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
6:B2:8142:LEU:HG	6:B2:8191:ARG:HA	1.71	0.72
4:AT:4060:CYS:O	4:AT:4063:VAL:HG12	1.89	0.72
1:BA:1056:LEU:HD11	7:BG:6061:LEU:HD13	1.71	0.72
2:AZ:2043:LYS:HG2	2:AZ:2067:TRP:HB3	1.72	0.72
4:CT:4060:CYS:O	4:CT:4063:VAL:HG12	1.89	0.72
6:B2:8184:LEU:HD22	6:B2:8192:ALA:HB2	1.71	0.71
6:AV:8203:VAL:HG13	6:AV:8209:ASN:HA	1.72	0.71
1:BQ:1056:LEU:HD11	7:BW:6061:LEU:HD13	1.71	0.71
1:AQ:1050:PRO:HG3	6:AV:8159:HIS:HB2	1.72	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
5:BM:7014:SER:HB3	6:BN:8197:LEU:HD11	1.74	0.69
7:BG:6072:ILE:HD12	7:BG:6152:MET:HE2	1.75	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
6:CN:8184:LEU:HD22	6:CN:8192:ALA:HB2	1.75	0.68
5:CM:7014:SER:HB3	6:CN:8197:LEU:HD11	1.74	0.68
1:CQ:1056:LEU:HD11	7:CW:6061:LEU:HD13	1.76	0.68
2:CB:2043:LYS:HG2	2:CB:2067:TRP:HB3	1.74	0.68
6:AF:8160:LEU:HD12	6:AF:8160:LEU:H	1.58	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:CV:8142:LEU:HG	6:CV:8191:ARG:HA	1.75	0.67
6:B2:8124:LEU:HA	6:B2:8127:MET:HE2	1.76	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
6:AF:8145:VAL:HG22	6:AF:8149:ARG:HD2	1.77	0.67
4:AD:4060:CYS:O	4:AD:4063:VAL:HG12	1.94	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:CO:6068:PRO:HD2	7:CO:6069:ARG:H	1.60	0.67
7:BO:6068:PRO:HD2	7:BO:6069:ARG:H	1.59	0.67
3:BK:3066:LYS:HG3	4:BL:4063:VAL:HG13	1.77	0.66
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
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
3:AC:3016:ARG:NE	3:AC:3030:GLU:HG2	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:A2:8152:TYR:O	6:A2:8156:VAL:HG12	1.95	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:NE	3:BC:3030:GLU:HG2	2.10	0.65
3:BC:3016:ARG:HE	3:BC:3030:GLU:HG2	1.60	0.65
3:CS:3016:ARG:HE	3:CS:3030:GLU:HG2	1.62	0.65
3:BK:3016:ARG:HE	3:BK:3030:GLU:HG2	1.60	0.65
1:AA:1050:PRO:HG3	6:AF:8159:HIS:HB2	1.78	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:3066:LYS:HG3	4:AT:4063:VAL:HG13	1.79	0.64
3:AS:3016:ARG:HE	3:AS:3030:GLU:HG2	1.61	0.64
7:AG:6069:ARG:NH2	7:AG:6140:GLU:O	2.31	0.64
7:A3:6068:PRO:HD2	7:A3:6069:ARG:H	1.60	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
4:AL:4060:CYS:O	4:AL:4063:VAL:HG12	1.97	0.64
1:AA:1064:ARG:HD3	2:AB:2041:ASN:HB3	1.79	0.64
6:BF:8203:VAL:HG13	6:BF:8209:ASN:HA	1.79	0.64
2:AJ:2043:LYS:HG2	2:AJ:2067:TRP:HB3	1.80	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
3:BC:3066:LYS:HG3	4:BD:4063:VAL:HG13	1.79	0.63
8:BX:5030:ASP:HB2	8:BX:5031:PRO:CD	2.29	0.63
8:BP:5030:ASP:HB2	8:BP:5031:PRO:CD	2.29	0.63
6:A2:8199:LEU:O	6:A2:8203:VAL:HG23	1.99	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: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
1:AI:1064:ARG:HD3	2:AJ:2041:ASN:HB3	1.81	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
3:AK:3000:MET:CE	3:AK:3002:GLN:HE22	2.13	0.61
8:AH:5030:ASP:HB2	8:AH:5031:PRO:CD	2.30	0.61
7:BO:6069:ARG:NH2	7:BO:6140:GLU:O	2.33	0.61
3:AC:3000:MET:CE	3:AC:3002:GLN:HE22	2.13	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
7:BO:6067:ASN:CB	7:BO:6068:PRO:CD	2.76	0.61
8:AP:5030:ASP:HB2	8:AP:5031:PRO:CD	2.30	0.61
7:CW:6069:ARG:NH2	7:CW:6140:GLU:O	2.34	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:CG:6069:ARG:NH2	7:CG:6140:GLU:O	2.34	0.61
8:CX:5030:ASP:HB2	8:CX:5031:PRO:CD	2.30	0.61
8:CH:5030:ASP:HB2	8:CH:5031:PRO:CD	2.30	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
6:AV:8128:LEU:HD22	6:AV:8151:LEU:HG	1.82	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
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
7:AG:6018:ASN:HD22	7:AG:6019:ASN:HB2	1.66	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:B2:8203:VAL:O	6:B2:8207:ALA:HA	2.01	0.60
3:BK:3000:MET:CE	3:BK:3002:GLN:HE22	2.15	0.60
6:AN:8146:TRP:O	6:AN:8150:TRP:HD1	1.85	0.60
7:CW:6067:ASN:CB	7:CW:6068:PRO:CD	2.74	0.60
6:CN:8065:PHE:CE2	6:CN:8205:VAL:HG11	2.37	0.60
1:BI:1064:ARG:HD3	2:BJ:2041:ASN:HB3	1.84	0.60
6:AV:8124:LEU:HA	6:AV:8127:MET:HE2	1.84	0.60
6:BV:8124:LEU:HA	6:BV:8127:MET:HE2	1.84	0.60
6:AF:8152:TYR:O	6:AF:8156:VAL:HG12	2.01	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
7:CW:6072:ILE:HD12	7:CW:6152:MET:HE2	1.84	0.60
6:BN:8124:LEU:HA	6:BN:8127:MET:HE2	1.84	0.60
1:BI:1048:ARG:HG3	1:BI:1048:ARG:HH11	1.66	0.59
6:AN:8167:PHE:O	6:AN:8171:ARG:HG3	2.03	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:CG:6068:PRO:CD	7:CG:6069:ARG:H	2.14	0.59
7:B3:6068:PRO:CD	7:B3:6069:ARG:H	2.15	0.59
6:CN:8054:THR:HG23	6:CN:8057:TRP:CB	2.33	0.59
1:CY:1048:ARG:HG3	1:CY:1048:ARG:HH11	1.66	0.58
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
7:CO:6069:ARG:NH2	7:CO:6140:GLU:O	2.36	0.58
6:AV:8177:CYS:HA	6:AV:8180:LEU:HB2	1.85	0.58
7:CW:6068:PRO:CD	7:CW:6069:ARG:H	2.15	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: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
7:AG:6072:ILE:HD12	7:AG:6152:MET:HE2	1.85	0.58
6:AN:8133:GLN:HG3	6:AN:8176:THR:HG21	1.85	0.58
6:AN:8095:ASP:HB3	6:AN:8098:LYS:HB2	1.86	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
8:B4:5008:MET:O	8:B4:5026:LEU:HB3	2.05	0.57
6:AF:8095:ASP:HB3	6:AF:8098:LYS:HB2	1.87	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:BQ:1069:PRO:O	1:BQ:1071:SER:N	2.35	0.57
1:AQ:1069:PRO:O	1:AQ:1071:SER:N	2.36	0.57
6:AV:8203:VAL:O	6:AV:8207:ALA:HA	2.05	0.57
3:AK:3066:LYS:HG3	4:AL:4063:VAL:HG13	1.86	0.57
6:A2:8095:ASP:HB3	6:A2:8098:LYS:HB2	1.87	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
7:BO:6068:PRO:CD	7:BO:6069:ARG:H	2.16	0.57
6:B2:8095:ASP:HB3	6:B2:8098:LYS:HB2	1.87	0.57
7:A3:6072:ILE:HD12	7:A3:6152:MET:HE2	1.86	0.56
1:CQ:1048:ARG:HH11	1:CQ:1048:ARG:HG3	1.70	0.56
6:CF:8133:GLN:HG3	6:CF:8176:THR:HG21	1.87	0.56
2:CR:2040:ARG:HE	4:CT:4019:TRP:HZ2	1.51	0.56
7:BG:6068:PRO:CD	7:BG:6069:ARG:H	2.16	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
1:BQ:1048:ARG:HH11	1:BQ:1048:ARG:HG3	1.70	0.56
1:CA:1069:PRO:O	1:CA:1071:SER:N	2.35	0.56
6:BV:8095:ASP:HB3	6:BV:8098:LYS:HB2	1.87	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:BN:8095:ASP:HB3	6:BN:8098:LYS:HB2	1.88	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
7:BO:6081:GLU:H	8:BP:5064:MET:HE1	1.71	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:CF:8095:ASP:HB3	6:CF:8098:LYS:HB2	1.88	0.56
6:A2:8168:SER:O	6:A2:8172:TYR:HD2	1.89	0.56
6:AV:8095:ASP:HB3	6:AV:8098:LYS:HB2	1.88	0.56
7:BG:6066:SER:HA	7:BG:6069:ARG:O	2.06	0.56
2:AZ:2064:LYS:HE3	2:AZ:2075:ASP:OD2	2.06	0.56
6:CF:8167:PHE:O	6:CF:8171:ARG:HG3	2.06	0.55
6:BN:8155:LEU:HA	6:BN:8158:LEU:HD12	1.87	0.55
6:CV:8203:VAL:HG13	6:CV:8209:ASN:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AG:6066:SER:HA	7:AG:6069:ARG:O	2.06	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
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
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
2:CR:2097:ILE:HG22	6:CV:8037:LEU:HB3	1.88	0.55
8:A4:5008:MET:O	8:A4:5026:LEU:HB3	2.07	0.55
8:CP:5008:MET:O	8:CP:5026:LEU:HB3	2.07	0.55
7:BO:6066:SER:HA	7:BO:6069:ARG:O	2.06	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
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
1:AQ:1064:ARG:HD3	2:AR:2041:ASN:HB3	1.89	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
7:BW:6066:SER:HA	7:BW:6069:ARG:O	2.07	0.54
6:AN:8160:LEU:HD23	6:AN:8161:PRO:HA	1.89	0.54
1:CY:1064:ARG:HD3	2:CZ:2041:ASN:HB3	1.89	0.54
1:BI:1048:ARG:HG3	1:BI:1048:ARG:NH1	2.21	0.54
7:B3:6072:ILE:HD12	7:B3:6152:MET:HE2	1.88	0.54
1:AA:1069:PRO:O	1:AA:1071:SER:N	2.37	0.54
7:CW:6066:SER:HA	7:CW:6069:ARG:O	2.07	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
6:BF:8184:LEU:HD22	6:BF:8192:ALA:HB2	1.88	0.54
6:AV:8209:ASN:C	6:AV:8211:PHE:H	2.11	0.54
6:A2:8199:LEU:HB2	6:A2:8215:ILE:HD13	1.89	0.54
8:B4:5030:ASP:HB2	8:B4:5031:PRO:CD	2.36	0.54
2:BJ:2023:SER:O	2:BJ:2027:GLN:HG3	2.08	0.54
7:CG:6066:SER:HA	7:CG:6069:ARG:O	2.07	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
8:CX:5008:MET:O	8:CX:5026:LEU:HB3	2.08	0.54
6:AN:8054:THR:HG23	6:AN:8057:TRP:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AV:8168:SER:O	6:AV:8172:TYR:HD2	1.91	0.54
2:AJ:2097:ILE:HG22	6:AN:8037:LEU:HB3	1.90	0.54
7:A3:6081:GLU:OE1	7:A3:6088:ASP:HB2	2.07	0.54
8:CH:5008:MET:O	8:CH:5026:LEU:HB3	2.08	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
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
2:BB:2027:GLN:OE1	2:BB:2093:ARG:HD3	2.09	0.53
2:CJ:2040:ARG:HE	4:CL:4019:TRP:HZ2	1.54	0.53
7:BW:6072:ILE:HD12	7:BW:6152:MET:HE2	1.89	0.53
1:BI:1069:PRO:O	1:BI:1071:SER:N	2.37	0.53
2:AB:2040:ARG:C	2:AB:2042:ASN:H	2.11	0.53
7:AW:6066:SER:HA	7:AW:6069:ARG:O	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
8:AX:5008:MET:O	8:AX:5026:LEU:HB3	2.08	0.53
6:B2:8203:VAL:CG1	6:B2:8209:ASN:HA	2.33	0.53
6:AV:8046:PRO:HB2	6:AV:8047:PRO:HD2	1.90	0.53
4:BL:4031:ASP:HA	6:BN:8020:VAL:HG22	1.90	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
6:A2:8133:GLN:HG3	6:A2:8176:THR:HG21	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: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
2:AJ:2077:TYR:CD1	6:AN:8210:ASP:HB3	2.43	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
6:A2:8054:THR:HG23	6:A2:8057:TRP:HB2	1.91	0.53
8:BX:5008:MET:O	8:BX:5026:LEU:HB3	2.08	0.53
6:AV:8054:THR:HG23	6:AV:8057:TRP:HB2	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
6:AV:8171:ARG:NH1	6:AV:8208:GLN:OE1	2.40	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:BV:8203:VAL:HG13	6:BV:8209:ASN:HA	1.90	0.53
2:AJ:2023:SER:O	2:AJ:2027:GLN:HG3	2.09	0.53
6:BV:8153:ALA:O	6:BV:8156:VAL:HG13	2.09	0.53
6:BF:8046:PRO:HB2	6:BF:8047:PRO:HD2	1.91	0.53
3:AK:3000:MET:HE2	3:AK:3002:GLN:HE22	1.73	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
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
7:A3:6047:GLU:HA	6:BF:8054:THR:HB	1.91	0.52
6:CV:8184:LEU:HD22	6:CV:8192:ALA:HB2	1.90	0.52
6:BF:8133:GLN:HG3	6:BF:8176:THR:HG21	1.90	0.52
6:A2:8046:PRO:HB2	6:A2:8047:PRO:HD2	1.91	0.52
2:CJ:2023:SER:O	2:CJ:2027:GLN:HG3	2.08	0.52
2:CB:2065:GLU:O	2:CB:2075:ASP:HA	2.08	0.52
5:AU:7005:SER:O	5:AU:7008:VAL:HG22	2.10	0.52
8:AP:5008:MET:O	8:AP:5026:LEU:HB3	2.09	0.52
2:BB:2065:GLU:O	2:BB:2075:ASP:HA	2.08	0.52
8:AH:5008:MET:O	8:AH:5026:LEU:HB3	2.09	0.52
6:AF:8054:THR:HG23	6:AF:8057:TRP:HB2	1.89	0.52
2:CZ:2034:GLN:HG2	2:CZ:2048:ARG:HG3	1.91	0.52
2:BR:2043:LYS:HG2	2:BR:2067:TRP:CB	2.33	0.52
3:CK:3000:MET:HE2	3:CK:3002:GLN:HE22	1.74	0.52
6:CF:8131:TRP:O	6:CF:8135:PRO:HG3	2.10	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
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
2:BB:2034:GLN:HG2	2:BB:2048:ARG:HG3	1.91	0.52
6:BN:8203:VAL:HG13	6:BN:8209:ASN:HA	1.92	0.52
2:BJ:2065:GLU:O	2:BJ:2075:ASP:HA	2.09	0.52
4:AL:4019:TRP:HB2	4:AL:4021:MET:SD	2.50	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: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:CN:8054:THR:HG23	6:CN:8057:TRP:HB2	1.92	0.52
6:AN:8046:PRO:HB2	6:AN:8047:PRO:HD2	1.92	0.52
6:BV:8054:THR:HG23	6:BV:8057:TRP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CF:8185:LYS:N	6:CF:8187:ASP:HB2	2.21	0.52
6:A2:8044:GLU:HA	6:A2:8044:GLU:OE1	2.10	0.52
6:AF:8135:PRO:C	6:AF:8137:THR:H	2.13	0.52
1:CI:1049:GLU:OE2	6:CN:8117:THR:HB	2.10	0.52
2:AJ:2034:GLN:HG2	2:AJ:2048:ARG:HG3	1.92	0.52
2:AB:2023:SER:O	2:AB:2027:GLN:HG3	2.09	0.52
6:AN:8135:PRO:C	6:AN:8137:THR:H	2.12	0.51
5:AE:7005:SER:O	5:AE:7007:LEU:N	2.43	0.51
7:A3:6048:LEU:HD22	6:BF:8050:CYS:HA	1.92	0.51
6:CN:8199:LEU:HB2	6:CN:8215:ILE:HD13	1.91	0.51
2:BR:2034:GLN:HG2	2:BR:2048:ARG:HG3	1.93	0.51
6:CF:8184:LEU:HD22	6:CF:8192:ALA:HB2	1.91	0.51
6:AV:8135:PRO:C	6:AV:8137:THR:H	2.13	0.51
6:AN:8131:TRP:O	6:AN:8135:PRO:HG3	2.10	0.51
6:AF:8072:VAL:HG13	6:AF:8114:LEU:HD21	1.91	0.51
2:AR:2023:SER:O	2:AR:2027:GLN:HG3	2.10	0.51
6:CN:8046:PRO:HB2	6:CN:8047:PRO:HD2	1.91	0.51
2:CB:2096:LEU:HB3	6:CF:8036:THR:HG22	1.91	0.51
6:CN:8203:VAL:HG13	6:CN:8209:ASN:HA	1.92	0.51
2:CJ:2075:ASP:O	6:CN:8171:ARG:HD3	2.11	0.51
6:A2:8128:LEU:HD22	6:A2:8151:LEU:HG	1.93	0.51
4:CD:4019:TRP:HB2	4:CD:4021:MET:SD	2.51	0.51
4:CT:4019:TRP:HB2	4:CT:4021:MET:SD	2.51	0.51
2:AB:2034:GLN:HG2	2:AB:2048:ARG:HG3	1.92	0.51
4:BD:4019:TRP:HB2	4:BD:4021:MET:SD	2.51	0.51
2:CZ:2043:LYS:HE2	2:CZ:2067:TRP:CD2	2.46	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
1:CA:1048:ARG:HG3	1:CA:1048:ARG:NH1	2.26	0.51
6:BV:8203:VAL:HG22	6:BV:8211:PHE:HB2	1.92	0.51
2:BB:2097:ILE:HG22	6:BF:8037:LEU:HB3	1.93	0.51
6:CF:8054:THR:HG23	6:CF:8057:TRP:HB2	1.93	0.51
2:BZ:2065:GLU:O	2:BZ:2075:ASP:HA	2.11	0.51
7:AO:6043:TRP:CZ3	7:AO:6045:PRO:HG3	2.46	0.51
6:CF:8162:LEU:HD23	6:CF:8166:VAL:HB	1.92	0.51
6:BV:8133:GLN:HG3	6:BV:8176:THR:HG21	1.92	0.51
2:BR:2040:ARG:C	2:BR:2042:ASN:H	2.14	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:AB:2043:LYS:HD3	2:AB:2067:TRP:CE3	2.46	0.51
1:CQ:1053:LEU:CD2	7:CW:6065:SER:HB2	2.41	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:CV:8046:PRO:HB2	6:CV:8047:PRO:HD2	1.91	0.50
7:AG:6043:TRP:CZ3	7:AG:6045:PRO:HG3	2.46	0.50
6:BV:8177:CYS:HA	6:BV:8180:LEU:HB2	1.92	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:BJ:2034:GLN:HG2	2:BJ:2048:ARG:HG3	1.93	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
6:CF:8177:CYS:HA	6:CF:8180:LEU:HB2	1.93	0.50
3:BK:3063:ILE:HG22	4:BL:4067:ARG:HB3	1.93	0.50
6:AN:8184:LEU:HD22	6:AN:8192:ALA:HB2	1.91	0.50
1:BY:1048:ARG:NH1	1:BY:1048:ARG:HG3	2.26	0.50
1:AY:1048:ARG:HG3	1:AY:1048:ARG:HH11	1.76	0.50
6:A2:8135:PRO:C	6:A2:8137:THR:H	2.13	0.50
6:BV:8145:VAL:HG22	6:BV:8149:ARG:HD2	1.94	0.50
3:AS:3063:ILE:HG22	4:AT:4067:ARG:HB3	1.93	0.50
2:AZ:2040:ARG:HA	2:AZ:2089:ILE:HD11	1.93	0.50
3:AS:3000:MET:HE2	3:AS:3002:GLN:HE22	1.75	0.50
3:CC:3063:ILE:HG22	4:CD:4067:ARG:HB3	1.93	0.50
4:AD:4019:TRP:HB2	4:AD:4021:MET:SD	2.50	0.50
6:A2:8177:CYS:HB2	6:A2:8195:TYR:HD1	1.76	0.50
2:CB:2023:SER:O	2:CB:2027:GLN:HG3	2.10	0.50
4:AL:4002:LYS:HB2	4:AL:4003:PRO:HD3	1.93	0.50
6:AV:8177:CYS:HB2	6:AV:8195:TYR:HB3	1.94	0.50
2:BR:2097:ILE:HG22	6:BV:8037:LEU:HB3	1.93	0.50
6:B2:8177:CYS:HA	6:B2:8180:LEU:HB2	1.93	0.50
3:AC:3063:ILE:HG22	4:AD:4067:ARG:HB3	1.94	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
6:CN:8184:LEU:HD23	6:CN:8187:ASP:HB3	1.94	0.50
2:BB:2040:ARG:NH1	7:BG:6166:ASP:O	2.44	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
6:BV:8184:LEU:HD22	6:BV:8192:ALA:HB2	1.92	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
2:BZ:2034:GLN:HG2	2:BZ:2048:ARG:HG3	1.93	0.50
3:BS:3063:ILE:HG22	4:BT:4067:ARG:HB3	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)
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
4:BT:4019:TRP:HB2	4:BT:4021:MET:SD	2.52	0.50
2:BR:2065:GLU:O	2:BR:2075:ASP:HA	2.11	0.50
1:AA:1053:LEU:CD2	7:AG:6065:SER:HB2	2.42	0.49
2:BJ:2043:LYS:HG2	2:BJ:2067:TRP:CB	2.37	0.49
6:B2:8131:TRP:O	6:B2:8135:PRO:HG3	2.11	0.49
2:AJ:2040:ARG:HA	2:AJ:2089:ILE:HD11	1.93	0.49
6:CN:8135:PRO:C	6:CN:8137:THR:H	2.15	0.49
6:AV:8065:PHE:CE1	6:AV:8156:VAL:HG12	2.47	0.49
6:CF:8046:PRO:HB2	6:CF:8047:PRO:HD2	1.92	0.49
2:AJ:2065:GLU:O	2:AJ:2075:ASP:HA	2.12	0.49
7:CG:6081:GLU:HA	7:CG:6087:GLY:HA3	1.94	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: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
7:A3:6043:TRP:CZ3	7:A3:6045:PRO:HG3	2.47	0.49
7:B3:6066:SER:O	7:B3:6067:ASN:O	2.30	0.49
2:AZ:2034:GLN:HG2	2:AZ:2048:ARG:HG3	1.94	0.49
5:BE:7005:SER:HB3	5:BE:7009:LYS:HG3	1.93	0.49
6:CV:8131:TRP:O	6:CV:8135:PRO:HG3	2.13	0.49
1:CI:1048:ARG:NH1	1:CI:1048:ARG:HG3	2.27	0.49
6:BN:8046:PRO:HB2	6:BN:8047:PRO:HD2	1.94	0.49
7:CO:6081:GLU:HA	7:CO:6087:GLY:HA3	1.95	0.49
2:CJ:2092:LEU:HD22	4:CL:4053:LEU:HG	1.95	0.49
6:AN:8181:ARG:HA	6:AN:8184:LEU:HD12	1.95	0.49
6:AV:8131:TRP:O	6:AV:8135:PRO:HG3	2.13	0.49
2:CJ:2040:ARG:C	2:CJ:2042:ASN:H	2.15	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
3:AS:3038:GLU:HB3	6:AV:8011:PHE:HE1	1.78	0.49
7:BW:6066:SER:O	7:BW:6067:ASN:O	2.31	0.49
6:AV:8181:ARG:O	6:AV:8184:LEU:HB2	2.13	0.49
6:CV:8135:PRO:C	6:CV:8137:THR:H	2.16	0.49
6:A2:8132:LEU:O	6:A2:8135:PRO:HD3	2.13	0.49
6:AN:8044:GLU:HA	6:AN:8044:GLU:OE1	2.13	0.49
3:AK:3063:ILE:HG22	4:AL:4067:ARG:HB3	1.94	0.49
1:BQ:1053:LEU:CD2	7:BW:6065:SER:HB2	2.43	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:CQ:1048:ARG:HG3	1:CQ:1048:ARG:NH1	2.27	0.49
2:AB:2065:GLU:O	2:AB:2075:ASP:HA	2.11	0.49
6:AV:8209:ASN:HB3	6:AV:8212:LYS:HE3	1.95	0.49
1:AI:1050:PRO:HG3	6:AN:8159:HIS:HB2	1.93	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
7:AO:6081:GLU:HA	7:AO:6087:GLY:HA3	1.95	0.49
7:AW:6081:GLU:HA	7:AW:6087:GLY:HA3	1.95	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
7:CO:6068:PRO:CD	7:CO:6069:ARG:H	2.17	0.48
1:BA:1048:ARG:HG3	1:BA:1048:ARG:NH1	2.26	0.48
2:BR:2077:TYR:CD1	6:BV:8210:ASP:HB3	2.47	0.48
2:AR:2034:GLN:HG2	2:AR:2048:ARG:HG3	1.95	0.48
6:BN:8054:THR:HG23	6:BN:8057:TRP:HB2	1.94	0.48
6:AF:8188:GLU:CD	6:AF:8190:GLN:HB2	2.33	0.48
2:BJ:2092:LEU:HD22	4:BL:4053:LEU:HG	1.95	0.48
6:AF:8131:TRP:O	6:AF:8135:PRO:HG3	2.13	0.48
6:AF:8108:PRO:HB2	6:AF:8153:ALA:CB	2.43	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
1:BA:1064:ARG:HD3	2:BB:2041:ASN:HB3	1.95	0.48
7:BO:6081:GLU:HA	7:BO:6087:GLY:HA3	1.95	0.48
3:BK:3038:GLU:HB3	6:BN:8011:PHE:HE1	1.78	0.48
4:BD:4000:ASN:ND2	6:BF:8010:MET:HB2	2.27	0.48
6:CV:8132:LEU:O	6:CV:8135:PRO:HD3	2.14	0.48
7:B3:6043:TRP:CZ3	7:B3:6045:PRO:HG3	2.48	0.48
6:BV:8044:GLU:OE1	6:BV:8044:GLU:HA	2.13	0.48
6:BF:8044:GLU:OE1	6:BF:8044:GLU:HA	2.13	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
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
6:CN:8131:TRP:O	6:CN:8135:PRO:HG3	2.14	0.48
7:BO:6043:TRP:CZ3	7:BO:6045:PRO:HG3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BX:5030:ASP:HB2	8:BX:5031:PRO:HD2	1.96	0.48
6:BF:8054:THR:HG23	6:BF:8057:TRP:HB2	1.95	0.48
5:AE:7003:ASP:O	5:AE:7006:LEU:HB2	2.13	0.48
7:BG:6043:TRP:CZ3	7:BG:6045:PRO:HG3	2.49	0.48
6:BF:8113:LEU:HD13	6:BF:8116:LEU:HD12	1.96	0.48
6:AF:8185:LYS:N	6:AF:8187:ASP:HB2	2.21	0.48
6:AF:8044:GLU:OE1	6:AF:8044:GLU:HA	2.13	0.48
6:AV:8133:GLN:HG3	6:AV:8176:THR:HG21	1.96	0.48
1:CA:1053:LEU:CD2	7:CG:6065:SER:HB2	2.44	0.48
6:B2:8184:LEU:HD23	6:B2:8187:ASP:HB3	1.95	0.48
6:B2:8132:LEU:O	6:B2:8135:PRO:HD3	2.14	0.48
6:B2:8054:THR:HG23	6:B2:8057:TRP:HB2	1.95	0.48
4:AL:4016:LYS:HG2	4:AL:4064:LEU:HD23	1.96	0.48
7:CO:6066:SER:O	7:CO:6067:ASN:O	2.32	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
4:CT:4000:ASN:ND2	6:CV:8010:MET:HB2	2.29	0.48
1:CI:1053:LEU:CD2	7:CO:6065:SER:HB2	2.43	0.47
6:CF:8168:SER:HA	6:CF:8171:ARG:HD3	1.96	0.47
2:BR:2092:LEU:HD22	4:BT:4053:LEU:HG	1.96	0.47
6:B2:8181:ARG:O	6:B2:8184:LEU:HB2	2.14	0.47
1:AQ:1048:ARG:NH1	1:AQ:1048:ARG:HG3	2.27	0.47
6:BF:8177:CYS:HA	6:BF:8180:LEU:HB2	1.95	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
2:BB:2043:LYS:HG2	2:BB:2067:TRP:CB	2.39	0.47
4:AT:4016:LYS:HG2	4:AT:4064:LEU:HD23	1.96	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:BN:8177:CYS:HA	6:BN:8180:LEU:HB2	1.95	0.47
6:B2:8135:PRO:C	6:B2:8137:THR:H	2.16	0.47
6:CF:8168:SER:O	6:CF:8172:TYR:HD2	1.96	0.47
6:AN:8201:LEU:HD22	6:AN:8205:VAL:HG21	1.95	0.47
6:BV:8181:ARG:O	6:BV:8184:LEU:HB2	2.15	0.47
4:AD:4016:LYS:HG2	4:AD:4064:LEU:HD23	1.97	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:8135:PRO:C	6:BN:8137:THR:H	2.16	0.47
6:CF:8132:LEU:O	6:CF:8135:PRO:HD3	2.15	0.47
6:BN:8044:GLU:HA	6:BN:8044:GLU:OE1	2.15	0.47
6:CV:8065:PHE:CE2	6:CV:8205:VAL:HG11	2.50	0.47

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:BG:6081:GLU:HA	7:BG:6087:GLY:HA3	1.97	0.46
7:A3:6024:LEU:HD13	7:A3:6080:VAL:HG11	1.97	0.46
2:CZ:2065:GLU:O	2:CZ:2075:ASP:HA	2.14	0.46
6:CF:8184:LEU:HD23	6:CF:8187:ASP:HB3	1.97	0.46
6:BF:8184:LEU:HD23	6:BF:8187:ASP:HB3	1.96	0.46
4:CT:4016:LYS:HG2	4:CT:4064:LEU:HD23	1.96	0.46
3:CC:3064:MET:HB2	4:CD:4004:PHE:CD2	2.50	0.46
7:CO:6043:TRP:CZ3	7:CO:6045:PRO:HG3	2.50	0.46
6:AN:8188:GLU:CD	6:AN:8190:GLN:HB2	2.36	0.46
6:CF:8171:ARG:NH1	6:CF:8208:GLN:OE1	2.49	0.46
6:AF:8002:SER:H	6:AF: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:AN:8002:SER:H	6:AN:8005:GLU:HB2	1.80	0.46
7:CG:6065:SER:OG	7:CG:6066:SER:N	2.48	0.46
6:BF:8152:TYR:HD1	6:BF:8197:LEU:HD21	1.80	0.46
7:BO:6066:SER:O	7:BO:6067:ASN:O	2.34	0.46
6:BN:8195:TYR:HA	6:BN:8198:LEU:HD12	1.97	0.46
2:CB:2040:ARG:HB2	2:CB:2087:SER:O	2.16	0.46
6:CN:8127:MET:HG2	6:CN:8131:TRP:CZ2	2.51	0.46
4:AT:4059:ARG:HD3	4:AT:4061:ASN:OD1	2.16	0.46
7:CG:6043:TRP:CZ3	7:CG:6045:PRO:HG3	2.51	0.46
7:CG:6068:PRO:CD	7:CG:6069:ARG:N	2.79	0.46
6:BN:8203:VAL:HG22	6:BN:8211:PHE:HB2	1.98	0.46
6:AV:8044:GLU:OE1	6:AV:8044:GLU:HA	2.15	0.46
2:CR:2038:ASN:HB2	2:CR:2090:VAL:HG22	1.98	0.46
2:AJ:2092:LEU:HD22	4:AL:4053:LEU:HG	1.97	0.46
6:CV:8184:LEU:HD23	6:CV:8187:ASP:HB3	1.98	0.46
8:AX:5030:ASP:HB2	8:AX:5031:PRO:HD2	1.98	0.46
6:AF:8127:MET:HG2	6:AF:8131:TRP:CZ2	2.51	0.46
6:BF:8002:SER:H	6:BF:8005:GLU:HB2	1.80	0.46
3:CC:3038:GLU:HB3	6:CF:8011:PHE:HE1	1.81	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
7:AW:6068:PRO:CD	7:AW:6069:ARG:N	2.79	0.46
7:CW:6068:PRO:CD	7:CW:6069:ARG:N	2.79	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

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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: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
6:A2:8002:SER:H	6:A2:8005:GLU:HB2	1.81	0.46
2:AB:2092:LEU:HD22	4:AD:4053:LEU:HG	1.98	0.46
6:BV:8184:LEU:HD23	6:BV:8187:ASP:HB3	1.97	0.46
6:AN:8203:VAL:HG22	6:AN:8211:PHE:HB2	1.97	0.46
8:AH:5030:ASP:HB2	8:AH:5031:PRO:HD2	1.97	0.46
3:AS:3064:MET:HB2	4:AT:4004:PHE:CD2	2.51	0.46
2:CZ:2038:ASN:HB2	2:CZ:2090:VAL:HG22	1.98	0.46
6:AV:8002:SER:H	6:AV:8005:GLU:HB2	1.81	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
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:CN:8181:ARG:O	6:CN:8184:LEU:HB2	2.17	0.45
6:AN:8184:LEU:HD23	6:AN:8187:ASP:HB3	1.98	0.45
3:CS:3000:MET:CE	3:CS:3002:GLN:NE2	2.79	0.45
3:AC:3024:GLN:HE21	3:AC:3024:GLN:HB2	1.56	0.45
7:B3:6000:MET:HG3	7:B3:6002:LEU:HD13	1.98	0.45
6:CF:8086:GLN:O	6:CF:8089:GLU:HB2	2.16	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
6:BF:8185:LYS:N	6:BF:8187:ASP:HB2	2.22	0.45
6:AN:8146:TRP:O	6:AN:8150:TRP:CD1	2.67	0.45
6:A2:8007:LEU:HG	6:A2:8011:PHE:CE1	2.52	0.45
3:CS:3006:LEU:HD11	8:CX:5054:MET:HG2	1.98	0.45
4:CL:4016:LYS:HG2	4:CL:4064:LEU:HD23	1.98	0.45
6:B2:8145:VAL:HG22	6:B2:8149:ARG:HD2	1.98	0.45
2:CR:2092:LEU:HD22	4:CT:4053:LEU:HG	1.98	0.45
6:CN:8197:LEU:O	6:CN:8201:LEU:HG	2.16	0.45
3:AK:3000:MET:CE	3:AK:3002:GLN:NE2	2.80	0.45
6:A2:8066:GLN:HE22	6:A2:8205:VAL:HG13	1.82	0.45
4:AL:4059:ARG:HD3	4:AL:4061:ASN:OD1	2.16	0.45
3:CC:3006:LEU:HD11	8:CH:5054:MET:HG2	1.98	0.45
2:CB:2038:ASN:HB2	2:CB:2090:VAL:HG22	1.98	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)
8:CX:5030:ASP:HB2	8:CX:5031:PRO:HD2	1.97	0.45
3:BK:3024:GLN:HE22	3:BK:3027:MET:CE	2.29	0.45
7:CW:6043:TRP:CZ3	7:CW:6045:PRO:HG3	2.51	0.45
4:BT:4059:ARG:HD3	4:BT:4061:ASN:OD1	2.16	0.45
7:AG:6066:SER:O	7:AG:6067:ASN:O	2.35	0.45
6:B2:8209:ASN:HD22	6:B2:8212:LYS:HE3	1.82	0.45
6:A2:8185:LYS:N	6:A2:8187:ASP:HB2	2.22	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
8:CH:5030:ASP:HB2	8:CH:5031:PRO:HD2	1.97	0.45
6:B2:8002:SER:H	6:B2:8005:GLU:HB2	1.81	0.45
6:BV:8002:SER:H	6:BV:8005:GLU:HB2	1.82	0.45
6:AF:8133:GLN:HG3	6:AF:8176:THR:HG21	1.97	0.45
7:CW:6065:SER:OG	7:CW:6066:SER:N	2.49	0.45
6:CN:8185:LYS:N	6:CN:8187:ASP:HB2	2.23	0.45
1:BQ:1050:PRO:HG3	6:BV:8159:HIS:HB2	1.96	0.45
1:CY:1018:LYS:HD3	1:CY:1064:ARG:NH2	2.31	0.45
6:CN:8086:GLN:O	6:CN:8089:GLU:HB2	2.16	0.45
4:BL:4059:ARG:HD3	4:BL:4061:ASN:OD1	2.16	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
6:BN:8172:TYR:HA	6:BN:8175:ARG:HD2	1.98	0.45
6:CF:8065:PHE:CE2	6:CF:8205:VAL:HG11	2.52	0.45
7:AO:6066:SER:O	7:AO:6067:ASN:O	2.35	0.45
6:CN:8195:TYR:HA	6:CN:8198:LEU:HD12	1.99	0.45
6:AN:8174:ALA:HB2	6:AN:8202:THR:HG21	1.97	0.45
3:BK:3069:ASN:OD1	4:BL:4018:LYS:HG2	2.17	0.45
2:CR:2092:LEU:CD2	4:CT:4056:VAL:HG22	2.37	0.45
2:CB:2043:LYS:HE2	2:CB:2067:TRP:CD2	2.51	0.45
6:A2:8069:ARG:HA	6:A2:8156:VAL:HG23	1.99	0.45
6:BN:8132:LEU:O	6:BN:8135:PRO:HD3	2.17	0.45
6:CF:8127:MET:HG2	6:CF:8131:TRP:CZ2	2.52	0.45
6:BN:8002:SER:H	6:BN:8005:GLU:HB2	1.81	0.45
3:CK:3006:LEU:HD11	8:CP:5054:MET:HG2	1.98	0.45
7:BW:6065:SER:OG	7:BW:6066:SER:N	2.50	0.45
6:A2:8184:LEU:HD23	6:A2:8187:ASP:HB3	1.98	0.45
6:A2:8127:MET:HE3	6:A2:8131:TRP:CH2	2.51	0.45
8:B4:5025:ILE:HG21	8:B4:5027:ARG:CZ	2.47	0.45
3:CK:3038:GLU:HB3	6:CN:8011:PHE:HE1	1.82	0.45
4:BT:4000:ASN:ND2	6:BV:8010:MET:HB2	2.31	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
7:AO:6065:SER:OG	7:AO:6066:SER:N	2.50	0.44
7:AG:6065:SER:OG	7:AG:6066:SER:N	2.50	0.44
2:AB:2092:LEU:CD2	4:AD:4056:VAL:HG22	2.36	0.44
7:BO:6072:ILE:HG21	7:BO:6152:MET:CE	2.48	0.44
6:AF:8049:LYS:HG3	7:CG:6084:GLY:HA3	1.98	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:B3:6068:PRO:HD2	7:B3:6069:ARG:N	2.30	0.44
7:A3:6068:PRO:CD	7:A3:6069:ARG:N	2.81	0.44
7:BG:6068:PRO:CD	7:BG:6069:ARG:N	2.80	0.44
3:CS:3000:MET:HE2	3:CS:3002:GLN:NE2	2.32	0.44
3:CC:3000:MET:CE	3:CC:3002:GLN:NE2	2.80	0.44
6:AF:8124:LEU:HA	6:AF:8127:MET:HE2	1.99	0.44
3:BK:3006:LEU:HD11	8:BP:5054:MET:HG2	1.99	0.44
8:CP:5030:ASP:HB2	8:CP:5031:PRO:HD2	1.97	0.44
3:BC:3006:LEU:HD11	8:BH:5054:MET:HG2	2.00	0.44
3:AS:3069:ASN:OD1	4:AT:4018:LYS:HG2	2.18	0.44
6:AF:8155:LEU:HD21	6:AF:8170:LEU:HD13	1.99	0.44
6:B2:8195:TYR:HA	6:B2:8198:LEU:HD12	1.99	0.44
7:A3:6065:SER:OG	7:A3:6066:SER:N	2.50	0.44
6:BV:8132:LEU:O	6:BV:8135:PRO:HD3	2.18	0.44
6:BF:8132:LEU:O	6:BF:8135:PRO:HD3	2.18	0.44
6:A2:8160:LEU:HD12	6:A2:8160:LEU:H	1.82	0.44
6:AV:8122:GLU:O	6:AV:8126:GLU:HG2	2.17	0.44
8:BH:5025:ILE:HG21	8:BH:5027:ARG:CZ	2.48	0.44
1:BY:1064:ARG:NH2	2:BZ:2040:ARG:HB3	2.33	0.44
3:BC:3038:GLU:HB3	6:BF:8011:PHE:HE1	1.83	0.44
2:BB:2038:ASN:HB2	2:BB:2090:VAL:HG22	1.99	0.44
2:CJ:2019:THR:O	6:CN:8022:THR:HG21	2.17	0.44
6:A2:8170:LEU:HA	6:A2:8173:ILE:HD12	2.00	0.44
6:BN:8146:TRP:O	6:BN:8150:TRP:HB2	2.16	0.44
6:BV:8184:LEU:HD21	6:BV:8191:ARG:HB3	2.00	0.44
2:CR:2043:LYS:HG2	2:CR:2067:TRP:CB	2.46	0.44
4:CL:4029:SER:HB2	6:CN:8022:THR:HG22	2.00	0.44
4:BL:4000:ASN:ND2	6:BN:8010:MET:HB2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:CO:6038:GLN:HG2	7:CO:6158:LEU:HD23	2.00	0.44
6:AN:8167:PHE:O	6:AN:8170:LEU:HB3	2.18	0.44
7:BO:6068:PRO:CD	7:BO:6069:ARG:N	2.80	0.44
6:BN:8188:GLU:CD	6:BN:8190:GLN:HB2	2.38	0.44
3:AS:3006:LEU:HD11	8:AX:5054:MET:HG2	2.00	0.44
6:CV:8188:GLU:CD	6:CV:8190:GLN:HB2	2.38	0.44
8:A4:5025:ILE:HG21	8:A4:5027:ARG:CZ	2.48	0.44
8:CX:5025:ILE:HG21	8:CX:5027:ARG:CZ	2.48	0.44
6:AN:8086:GLN:O	6:AN:8089:GLU:HB2	2.17	0.44
6:AF:8086:GLN:O	6:AF:8089:GLU:HB2	2.17	0.44
4:CD:4059:ARG:HD3	4:CD:4061:ASN:OD1	2.18	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
6:AV:8184:LEU:HD21	6:AV:8191:ARG:HB3	2.00	0.44
7:AG:6018:ASN:HD22	7:AG:6018:ASN:C	2.21	0.44
6:AF:8108:PRO:HB3	6:AF:8150:TRP:CD2	2.53	0.44
4:AD:4000:ASN:ND2	6:AF:8010:MET:HB2	2.33	0.44
6:AF:8118:GLN:HA	6:AF:8121:LEU:HD12	1.99	0.44
6:AN:8209:ASN:HB3	6:AN:8212:LYS:HE3	1.99	0.43
3:CK:3000:MET:CE	3:CK:3002:GLN:NE2	2.80	0.43
3:AS:3000:MET:CE	3:AS:3002:GLN:NE2	2.81	0.43
6:CV:8127:MET:HG2	6:CV:8131:TRP:CZ2	2.53	0.43
4:BL:4005:LEU:HD23	4:BL:4030:VAL:HG11	2.00	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:AD:4002:LYS:HG3	6:AF:8014:ARG:CB	2.48	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:8184:LEU:HD21	6:CV:8191:ARG:HB3	1.99	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
3:AK:3071:THR:HG23	8:AP:5061:SER:HB3	2.00	0.43
2:AZ:2049:VAL:HA	2:AZ:2060:LEU:HD23	2.00	0.43
2:AR:2049:VAL:HA	2:AR:2060:LEU:HD23	2.01	0.43
7:CO:6068:PRO:CD	7:CO:6069:ARG:N	2.81	0.43
7:BG:6065:SER:OG	7:BG:6066:SER:N	2.51	0.43
6:AV:8184:LEU:HD23	6:AV:8187:ASP:HB3	1.99	0.43
6:AF:8203:VAL:HG13	6:AF:8209:ASN:HA	2.00	0.43
3:BS:3069:ASN:OD1	4:BT:4018:LYS:HG2	2.19	0.43
8:BP:5025:ILE:HG21	8:BP:5027:ARG:CZ	2.49	0.43
7:CW:6078:HIS:CD2	8:CX:5063:ILE:HG23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CP:5025:ILE:HG21	8:CP:5027:ARG:CZ	2.49	0.43
6:A2:8188:GLU:CD	6:A2:8190:GLN:HB2	2.39	0.43
8:CH:5025:ILE:HG21	8:CH:5027:ARG:CZ	2.49	0.43
7:BG:6066:SER:O	7:BG:6067:ASN:O	2.37	0.43
2:AB:2077:TYR:HE2	6:AF:8209:ASN:HB2	1.71	0.43
4:AT:4030:VAL:HG12	4:AT:4031:ASP:N	2.34	0.43
6:AF:8046:PRO:HB2	6:AF:8047:PRO:CD	2.48	0.43
4:BT:4030:VAL:HG12	4:BT:4031:ASP:N	2.34	0.43
6:B2:8005:GLU:O	6:B2:8009:HIS:ND1	2.52	0.43
4:AL:4031:ASP:HA	6:AN:8020:VAL:HG22	2.01	0.43
3:BC:3069:ASN:OD1	4:BD:4018:LYS:HG2	2.19	0.43
1:AY:1018:LYS:HE2	1:AY:1061:ASN:O	2.18	0.43
4:AD:4059:ARG:HD3	4:AD:4061:ASN:OD1	2.17	0.43
8:AX:5025:ILE:HG21	8:AX:5027:ARG:CZ	2.49	0.43
4:BD:4059:ARG:HD3	4:BD:4061:ASN:OD1	2.17	0.43
6:B2:8086:GLN:O	6:B2:8089:GLU:HB2	2.18	0.43
2:BR:2043:LYS:CG	2:BR:2067:TRP:HB3	2.40	0.43
6:BN:8127:MET:HG2	6:BN:8131:TRP:CZ2	2.53	0.43
6:AN:8127:MET:HG2	6:AN:8131:TRP:CZ2	2.53	0.43
1:CI:1064:ARG:HD3	2:CJ:2041:ASN:HB3	2.00	0.43
7:B3:6000:MET:HG3	7:B3:6002:LEU:CD1	2.48	0.43
6:CF:8044:GLU:HA	6:CF:8044:GLU:OE1	2.18	0.43
8:AP:5025:ILE:HG21	8:AP:5027:ARG:CZ	2.49	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:AC:3006:LEU:HD11	8:AH:5054:MET:HG2	2.00	0.43
6:B2:8127:MET:HG2	6:B2:8131:TRP:CZ2	2.54	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
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
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
6:AV:8127:MET:HG2	6:AV:8131:TRP:CZ2	2.53	0.43
4:BD:4030:VAL:HG12	4:BD:4031:ASP:N	2.34	0.43
8:AP:5008:MET:O	8:AP:5026:LEU:O	2.37	0.43
1:AY:1048:ARG:HG3	1:AY:1048:ARG:NH1	2.32	0.43
6:CF:8188:GLU:OE1	6:CF:8190:GLN:HB2	2.19	0.43
6:AV:8005:GLU:O	6:AV:8009:HIS:ND1	2.52	0.43
2:BR:2019:THR:O	6:BV:8022:THR:HG21	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
1:CI:1069:PRO:HD2	1:CI:1072:LEU:HD22	2.01	0.43
8:AH:5008:MET:O	8:AH:5026:LEU:O	2.37	0.43
6:AF:8188:GLU:OE2	6:AF:8190:GLN:HB2	2.18	0.43
4:CT:4002:LYS:HG3	6:CV:8014:ARG:HB3	2.01	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
7:CO:6065:SER:OG	7:CO:6066:SER:N	2.52	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
6:BF:8152:TYR:CD1	6:BF:8197:LEU:HD21	2.54	0.43
6:A2:8005:GLU:O	6:A2:8009:HIS:ND1	2.52	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
4:AD:4030:VAL:HG12	4:AD:4031:ASP:N	2.33	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
6:B2:8165:HIS:O	6:B2:8169:THR:HG23	2.19	0.43
7:CG:6152:MET:HB2	7:CG:6152:MET:HE3	1.93	0.42
8:A4:5008:MET:O	8:A4:5026:LEU:O	2.37	0.42
2:CJ:2075:ASP:OD1	6:CN:8175:ARG:NH2	2.52	0.42
6:BV:8005:GLU:O	6:BV:8009:HIS:ND1	2.52	0.42
6:CN:8005:GLU:O	6:CN:8009:HIS:ND1	2.52	0.42
6:BF:8122:GLU:O	6:BF:8126:GLU:HG2	2.19	0.42
6:B2:8159:HIS:ND1	6:B2:8159:HIS:N	2.67	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
1:CA:1001:LEU:HD23	1:CA:1001:LEU:HA	1.83	0.42
3:BC:3024:GLN:HE22	3:BC:3027:MET:CE	2.32	0.42
6:CN:8055:PRO:HA	6:CN:8058:ARG:HB2	2.02	0.42
2:CB:2019:THR:O	6:CF:8022:THR:HG21	2.19	0.42
7:AG:6068:PRO:HD2	7:AG:6069:ARG:N	2.29	0.42
2:CR:2043:LYS:HE2	2:CR:2067:TRP:CD2	2.54	0.42
7:CW:6152:MET:HB2	7:CW:6152:MET:HE3	1.90	0.42
1:CQ:1018:LYS:HA	1:CQ:1064:ARG:HD2	2.02	0.42
6:CV:8005:GLU:O	6:CV:8009:HIS:ND1	2.52	0.42
6:CF:8005:GLU:O	6:CF:8009:HIS:ND1	2.52	0.42
4:AL:4030:VAL:HG12	4:AL:4031:ASP:N	2.35	0.42
1:BQ:1018:LYS:HE2	1:BQ:1061:ASN:O	2.19	0.42
6:A2:8086:GLN:O	6:A2:8089:GLU:HB2	2.18	0.42
7:CG:6038:GLN:HG2	7:CG:6158:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CT:4059:ARG:HD3	4:CT:4061:ASN:OD1	2.19	0.42
6:BN:8086:GLN:O	6:BN:8089:GLU:HB2	2.18	0.42
1:BA:1064:ARG:NH2	2:BB:2040:ARG:HB3	2.35	0.42
2:AJ:2040:ARG:C	2:AJ:2042:ASN:H	2.22	0.42
7:AG:6018:ASN:ND2	7:AG:6019:ASN:HB2	2.31	0.42
2:CR:2040:ARG:HB2	2:CR:2087:SER:O	2.20	0.42
4:CL:4005:LEU:HD23	4:CL:4030:VAL:HG11	2.01	0.42
6:BV:8203:VAL:O	6:BV:8207:ALA:HA	2.19	0.42
6:A2:8046:PRO:HB2	6:A2:8047:PRO:CD	2.50	0.42
3:AC:3000:MET:CE	3:AC:3002:GLN:NE2	2.80	0.42
8:BH:5008:MET:O	8:BH:5026:LEU:O	2.38	0.42
6:AN:8046:PRO:HB2	6:AN:8047:PRO:CD	2.50	0.42
6:AF:8188:GLU:OE1	6:AF:8190:GLN:HB2	2.19	0.42
6:BF:8005:GLU:O	6:BF:8009:HIS:ND1	2.52	0.42
4:BD:4002:LYS:HG3	6:BF:8014:ARG:CB	2.50	0.42
3:BC:3000:MET:CE	3:BC:3002:GLN:NE2	2.80	0.42
7:CO:6072:ILE:HB	7:CO:6137:LEU:HB2	2.00	0.42
4:BL:4030:VAL:HG12	4:BL:4031:ASP:N	2.35	0.42
6:B2:8171:ARG:NH1	6:B2:8208:GLN:OE1	2.52	0.42
6:BF:8188:GLU:OE1	6:BF:8190:GLN:HB2	2.19	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
7:AW:6065:SER:OG	7:AW:6066:SER:N	2.52	0.42
4:CL:4030:VAL:HG12	4:CL:4031:ASP:N	2.35	0.42
6:A2:8124:LEU:HD12	6:A2:8127:MET:CE	2.49	0.42
6:AN:8005:GLU:O	6:AN:8009:HIS:ND1	2.53	0.42
6:BV:8043:PRO:HB2	6:BV:8178:ILE:HG21	2.01	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:B2:8113:LEU:HA	6:B2:8116:LEU:HD12	2.00	0.42
4:AT:4005:LEU:HD23	4:AT:4030:VAL:HG11	2.02	0.42
6:AN:8141:LEU:HD12	6:AN:8195:TYR:CD1	2.54	0.42
7:CO:6152:MET:HE3	7:CO:6152:MET:HB2	1.94	0.42
8:AX:5008:MET:O	8:AX:5026:LEU:O	2.38	0.42
6:AV:8046:PRO:HB2	6:AV:8047:PRO:CD	2.50	0.42
4:BT:4005:LEU:HD23	4:BT:4030:VAL:HG11	2.02	0.42
4:AL:4000:ASN:O	4:AL:4003:PRO:HD2	2.20	0.42
6:BN:8012:TYR:O	6:BN:8016:ARG:HG2	2.20	0.42
3:AK:3024:GLN:HE22	3:AK:3027:MET:CE	2.32	0.42
5:B1:7002:TRP:HB2	5:B1:7003:ASP:H	1.60	0.42
7:AW:6081:GLU:HB2	8:AX:5064:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BS:3038:GLU:HB3	6:BV:8011:PHE:CE1	2.55	0.42
6:BN:8005:GLU:O	6:BN:8009:HIS:ND1	2.53	0.42
2:CJ:2043:LYS:HD3	2:CJ:2067:TRP:CD2	2.55	0.42
3:BC:3071:THR:HG23	8:BH:5061:SER:HB3	2.02	0.42
1:AI:1018:LYS:HE2	1:AI:1061:ASN:O	2.20	0.42
6:B2:8012:TYR:O	6:B2:8016:ARG:HG2	2.20	0.42
3:AC:3069:ASN:OD1	4:AD:4018:LYS:HG2	2.19	0.42
3:AC:3071:THR:HG23	8:AH:5061:SER:HB3	2.01	0.42
6:CF:8154:THR:O	6:CF:8158:LEU:HG	2.20	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:BN:8178:ILE:HG13	6:BN:8199:LEU:HD21	2.02	0.41
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
3:CK:3071:THR:HG23	8:CP:5061:SER:HB3	2.01	0.41
6:CF:8012:TYR:O	6:CF:8016:ARG:HG2	2.20	0.41
6:BV:8012:TYR:O	6:BV:8016:ARG:HG2	2.20	0.41
2:CB:2067:TRP:CE2	2:CB:2074:LYS:HB2	2.55	0.41
1:BQ:1069:PRO:HD2	1:BQ:1072:LEU:HD22	2.02	0.41
1:CA:1069:PRO:HD2	1:CA:1072:LEU:HD22	2.02	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:BJ:2049:VAL:HA	2:BJ:2060:LEU:HD23	2.03	0.41
6:A2:8100:LYS:HD3	6:A2:8104:ARG:CZ	2.50	0.41
7:AW:6072:ILE:HB	7:AW:6137:LEU:HB2	2.03	0.41
2:CZ:2040:ARG:HB2	2:CZ:2087:SER:O	2.20	0.41
7:A3:6072:ILE:HB	7:A3:6137:LEU:HB2	2.03	0.41
8:BP:5008:MET:O	8:BP:5026:LEU:O	2.38	0.41
6:BF:8046:PRO:HB2	6:BF:8047:PRO:CD	2.50	0.41
6:B2:8168:SER:HA	6:B2:8171:ARG:HD3	2.01	0.41
6:AN:8196:ASN:HA	6:AN:8215:ILE:HD11	2.02	0.41
2:AZ:2038:ASN:HB2	2:AZ:2090:VAL:HG22	2.01	0.41
2:AR:2038:ASN:HB2	2:AR:2090:VAL:HG22	2.01	0.41
3:CC:3024:GLN:HE22	3:CC:3027:MET:CE	2.33	0.41
6:BN:8209:ASN:C	6:BN:8211:PHE:H	2.24	0.41
3:BK:3000:MET:CE	3:BK:3002:GLN:NE2	2.82	0.41
1:AY:1069:PRO:HD2	1:AY:1072:LEU:HD22	2.02	0.41
6:CN:8172:TYR:CD2	6:CN:8175:ARG:NH1	2.88	0.41
6:B2:8167:PHE:O	6:B2:8171:ARG:HG3	2.20	0.41
6:CN:8046:PRO:HB2	6:CN:8047:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AN:8007:LEU:HG	6:AN:8011:PHE:CE1	2.55	0.41
4:BD:4002:LYS:HG3	6:BF:8014:ARG:HB3	2.01	0.41
2:BJ:2077:TYR:HE2	6:BN:8209:ASN:HB2	1.80	0.41
1:CQ:1001:LEU:HD23	1:CQ:1001:LEU:HA	1.85	0.41
2:AR:2040:ARG:HA	2:AR:2089:ILE:HD11	2.02	0.41
6:CV:8188:GLU:OE1	6:CV:8190:GLN:HB2	2.20	0.41
6:BN:8122:GLU:O	6:BN:8126:GLU:HG2	2.20	0.41
2:AJ:2049:VAL:HA	2:AJ:2060:LEU:HD23	2.03	0.41
6:AN:8203:VAL:O	6:AN:8207:ALA:HA	2.21	0.41
7:CG:6072:ILE:HB	7:CG:6137:LEU:HB2	2.02	0.41
6:AN:8188:GLU:OE2	6:AN:8190:GLN:HB2	2.20	0.41
6:AF:8005:GLU:O	6:AF:8009:HIS:ND1	2.53	0.41
4:AD:4000:ASN:O	4:AD:4003:PRO:HD2	2.20	0.41
7:CW:6078:HIS:HA	7:CW:6131:GLU:O	2.20	0.41
1:CA:1050:PRO:HG3	6:CF:8159:HIS:HB2	2.03	0.41
4:CT:4005:LEU:HD23	4:CT:4030:VAL:HG11	2.02	0.41
2:AB:2049:VAL:HA	2:AB:2060:LEU:HD23	2.03	0.41
2:BR:2049:VAL:HA	2:BR:2060:LEU:HD23	2.03	0.41
6:CV:8012:TYR:O	6:CV:8016:ARG:HG2	2.21	0.41
6:CN:8184:LEU:HD21	6:CN:8191:ARG:HB3	2.02	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
6:CN:8122:GLU:O	6:CN:8126:GLU:HG2	2.21	0.41
8:CH:5063:ILE:HG22	8:CH:5064:MET:HG3	2.03	0.41
6:CV:8168:SER:O	6:CV:8172:TYR:HD2	2.03	0.41
2:BJ:2089:ILE:HA	4:BL:4062:ASN:ND2	2.36	0.41
6:BF:8184:LEU:HD21	6:BF:8191:ARG:HB3	2.03	0.41
1:CY:1069:PRO:HD2	1:CY:1072:LEU:HD22	2.02	0.41
4:BT:4000:ASN:O	4:BT:4003:PRO:HD2	2.21	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
2:AJ:2038:ASN:HB2	2:AJ:2090:VAL:HG22	2.01	0.41
4:CD:4005:LEU:HD23	4:CD:4030:VAL:HG11	2.03	0.41
6:BN:8184:LEU:HD21	6:BN:8191:ARG:HB3	2.03	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
7:CG:6068:PRO:HD2	7:CG:6069:ARG:N	2.29	0.41
6:A2:8209:ASN:HB3	6:A2:8212:LYS:HE3	2.03	0.41
4:CD:4002:LYS:HG3	6:CF:8014:ARG:HB3	2.03	0.41
5:AM:7005:SER:O	5:AM:7007:LEU:N	2.53	0.41
1:AA:1018:LYS:HE2	1:AA:1061:ASN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BM:7011:TYR:HB2	6:BN:8152:TYR:CD2	2.55	0.41
7:AO:6038:GLN:HG2	7:AO:6158:LEU:HD23	2.02	0.41
6:CN:8012:TYR:O	6:CN:8016:ARG:HG2	2.21	0.41
6:BN:8128:LEU:HD23	6:BN:8147:LEU:HD23	2.02	0.41
2:BB:2019:THR:O	6:BF:8022:THR:HG21	2.21	0.41
6:AF:8100:LYS:HD3	6:AF:8104:ARG:CZ	2.51	0.41
2:AJ:2092:LEU:CD2	4:AL:4056:VAL:HG22	2.38	0.41
6:CF:8209:ASN:O	6:CF:8212:LYS:HB2	2.21	0.41
3:AK:3000:MET:HE2	3:AK:3002:GLN:NE2	2.34	0.41
6:AV:8054:THR:HG23	6:AV:8057:TRP:CB	2.51	0.41
6:AF:8054:THR:HG23	6:AF:8057:TRP:CB	2.50	0.41
4:AL:4000:ASN:ND2	6:AN:8010:MET:HB2	2.36	0.41
7:BO:6072:ILE:HG21	7:BO:6152:MET:HE2	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
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:A2:8184:LEU:HD21	6:A2:8191:ARG:HB3	2.03	0.41
6:CN:8069:ARG:O	6:CN:8073:LEU:HD12	2.20	0.41
6:AF:8162:LEU:HB2	6:AF:8167:PHE:CE1	2.56	0.41
2:CJ:2084:ARG:NH2	2:CJ:2086:ASP:OD2	2.54	0.41
8:CP:5008:MET:O	8:CP:5026:LEU:O	2.38	0.41
8:CH:5007:PHE:O	8:CH:5008:MET:O	2.39	0.41
6:CF:8007:LEU:HG	6:CF:8011:PHE:CE1	2.55	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
3:CS:3024:GLN:HE22	3:CS:3027:MET:CE	2.34	0.40
1:BI:1018:LYS:HE2	1:BI:1061:ASN:O	2.21	0.40
6:B2:8178:ILE:HG13	6:B2:8199:LEU:HD21	2.03	0.40
1:BI:1069:PRO:HD2	1:BI:1072:LEU:HD22	2.03	0.40
4:BD:4000:ASN:O	4:BD:4003:PRO:HD2	2.21	0.40
4:CL:4000:ASN:O	4:CL:4003:PRO:HD2	2.21	0.40
2:CJ:2067:TRP:CE2	2:CJ:2074:LYS:HB2	2.56	0.40
7:AG:6038:GLN:HG2	7:AG:6158:LEU:HD23	2.04	0.40
6:AV:8090:PRO:HG3	6:CF:8112:THR:HG23	2.03	0.40
8:B4:5063:ILE:HG22	8:B4:5064:MET:HG3	2.04	0.40
1:CQ:1044:THR:OG1	6:CV:8161:PRO:HD2	2.22	0.40
7:CW:6068:PRO:HD2	7:CW:6069:ARG:N	2.29	0.40
1:CY:1001:LEU:HA	1:CY:1001:LEU:HD23	1.86	0.40
3:AK:3016:ARG:CD	3:AK:3030:GLU:HG2	2.51	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)
3:BS:3000:MET:CE	3:BS:3002:GLN:NE2	2.81	0.40
1:AQ:1069:PRO:HD2	1:AQ:1072:LEU:HD22	2.04	0.40
7:AO:6072:ILE:HB	7:AO:6137:LEU:HB2	2.04	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
6:BN:8188:GLU:OE1	6:BN:8190:GLN:HB2	2.21	0.40
6:AN:8215:ILE:HA	6:AN:8215:ILE:HD12	1.93	0.40
5:AU:7002:TRP:HB2	5:AU:7003:ASP:H	1.66	0.40
7:BW:6038:GLN:HG2	7:BW:6158:LEU:HD23	2.02	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
3:CS:3069:ASN:OD1	4:CT:4018:LYS:HG2	2.20	0.40
1:BY:1069:PRO:HD2	1:BY:1072:LEU:HD22	2.03	0.40
8:CX:5008:MET:O	8:CX:5026:LEU:O	2.38	0.40
2:AR:2089:ILE:HA	4:AT:4062:ASN:ND2	2.36	0.40
6:CF:8188:GLU:OE2	6:CF:8190:GLN:HB2	2.21	0.40
2:AJ:2016:GLU:OE1	6:AN:8020:VAL:HG11	2.21	0.40
7:BG:6020:ILE:CD1	7:BG:6139:PRO:HB3	2.52	0.40
6:AV:8162:LEU:HG	6:AV:8166:VAL:HG11	2.04	0.40
5:CE:7002:TRP:HB2	5:CE:7003:ASP:H	1.68	0.40
3:BK:3071:THR:HG23	8:BP:5061:SER:HB3	2.04	0.40
2:BB:2067:TRP:CE2	2:BB:2074:LYS:HB2	2.56	0.40
2:CB:2043:LYS:HG3	2:CB:2043:LYS:H	1.72	0.40
2:AJ:2089:ILE:HA	4:AL:4062:ASN:ND2	2.37	0.40
6:A2:8012:TYR:O	6:A2:8016:ARG:HG2	2.21	0.40
7:AO:6152:MET:HB2	7:AO:6152:MET:HE3	1.91	0.40
7:B3:6072:ILE:HB	7:B3:6137:LEU:HB2	2.03	0.40
6:BF:8188:GLU:OE2	6:BF:8190:GLN:HB2	2.22	0.40
4:AD:4002:LYS:HG3	6:AF:8014:ARG:HB3	2.02	0.40
2:AR:2067:TRP:CE2	2:AR:2074:LYS:HB2	2.56	0.40
2:BB:2089:ILE:HA	4:BD:4062:ASN:ND2	2.37	0.40
5:BE:7002:TRP:HB2	5:BE:7003:ASP:H	1.67	0.40
2:CR:2077:TYR:CD1	6:CV:8210:ASP:HB3	2.57	0.40
1:AQ:1018:LYS:HE2	1:AQ:1061:ASN:O	2.22	0.40
1:BA:1018:LYS:HE2	1:BA:1061:ASN:O	2.21	0.40
6:BV:8069:ARG:NH2	6:BV:8160:LEU:HD11	2.37	0.40
2:BZ:2049:VAL:HA	2:BZ:2060:LEU:HD23	2.03	0.40
7:CW:6072:ILE:HB	7:CW:6137:LEU:HB2	2.03	0.40
6:AV:8043:PRO:HB2	6:AV:8178:ILE:HG21	2.03	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%)	7	32
1	AI	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	AQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	AY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Ag	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Ao	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	7	32
1	Aw	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	7	32
1	BA	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	BI	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	7	32
1	BQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	BY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Bg	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Bo	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Bw	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	CA	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	CI	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	CQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	CY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Cg	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
1	Co	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	7	32
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%)	5	27

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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%)	19	58
2	BB	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	BJ	96/118 (81%)	90 (94%)	4 (4%)	2 (2%)	9	37
2	BR	96/118 (81%)	90 (94%)	4 (4%)	2 (2%)	9	37
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%)	19	58
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	9
5	AE	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	AM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	AU	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	Ac	15/124 (12%)	9 (60%)	5 (33%)	1 (7%)	1	9
5	Ak	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	9
5	As	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9

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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	9
5	BM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	BU	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	Bc	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	9
5	Bk	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	Bs	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	9
5	CE	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	1	9
5	CM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	CU	15/124 (12%)	10 (67%)	5 (33%)	0	100	100
5	Cc	15/124 (12%)	9 (60%)	5 (33%)	1 (7%)	1	9
5	Ck	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	1	9
5	Cs	15/124 (12%)	10 (67%)	2 (13%)	3 (20%)	0	0
6	A2	214/247 (87%)	187 (87%)	17 (8%)	10 (5%)	3	17
6	AF	214/247 (87%)	182 (85%)	22 (10%)	10 (5%)	3	17
6	AN	214/247 (87%)	174 (81%)	31 (14%)	9 (4%)	3	19
6	AV	214/247 (87%)	182 (85%)	21 (10%)	11 (5%)	2	15
6	Ad	214/247 (87%)	183 (86%)	20 (9%)	11 (5%)	2	15
6	Al	214/247 (87%)	183 (86%)	21 (10%)	10 (5%)	3	17
6	At	214/247 (87%)	182 (85%)	21 (10%)	11 (5%)	2	15
6	B2	214/247 (87%)	179 (84%)	23 (11%)	12 (6%)	2	13
6	BF	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	4	23
6	BN	214/247 (87%)	185 (86%)	22 (10%)	7 (3%)	5	26
6	BV	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	4	23
6	Bd	214/247 (87%)	185 (86%)	19 (9%)	10 (5%)	3	17
6	Bl	214/247 (87%)	186 (87%)	18 (8%)	10 (5%)	3	17
6	Bt	214/247 (87%)	181 (85%)	27 (13%)	6 (3%)	6	30
6	CF	214/247 (87%)	187 (87%)	19 (9%)	8 (4%)	4	23
6	CN	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	4	23
6	CV	214/247 (87%)	182 (85%)	24 (11%)	8 (4%)	4	23
6	Cd	214/247 (87%)	185 (86%)	19 (9%)	10 (5%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Cl	214/247 (87%)	186 (87%)	19 (9%)	9 (4%)	3	19
6	Ct	214/247 (87%)	178 (83%)	26 (12%)	10 (5%)	3	17
7	A3	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	AG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	AO	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	AW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	Ae	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	Am	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	Au	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	B3	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	7	33
7	BG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	BO	123/186 (66%)	115 (94%)	4 (3%)	4 (3%)	5	26
7	BW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	Be	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	7	33
7	Bm	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	7	33
7	Bu	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	CG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	CO	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	CW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	Ce	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
7	Cm	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	7	33
7	Cu	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	5	26
8	A4	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	AH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	AP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	AX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Af	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	An	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Av	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	B4	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	BH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	BP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	BX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Bf	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Bn	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Bv	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	CH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	CP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	CX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Cf	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Cn	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
8	Cv	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	13	46
All	All	14800/20960 (71%)	13553 (92%)	894 (6%)	353 (2%)	7	33

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%)	12	40
1	AI	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	AQ	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	AY	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	Ag	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	Ao	77/101 (76%)	73 (95%)	4 (5%)	29	65
1	Aw	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	BA	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	BI	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	BQ	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	BY	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	Bg	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	Bo	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	Bw	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	CA	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	CI	77/101 (76%)	72 (94%)	5 (6%)	21	57
1	CQ	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	CY	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	Cg	77/101 (76%)	71 (92%)	6 (8%)	16	49
1	Co	77/101 (76%)	73 (95%)	4 (5%)	29	65
2	AB	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	AJ	94/110 (86%)	92 (98%)	2 (2%)	61	86
2	AR	94/110 (86%)	91 (97%)	3 (3%)	46	79
2	AZ	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	Ah	94/110 (86%)	89 (95%)	5 (5%)	28	64
2	Ap	94/110 (86%)	91 (97%)	3 (3%)	46	79
2	Ax	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	BB	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	BJ	94/110 (86%)	88 (94%)	6 (6%)	22	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BR	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	BZ	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	Bh	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	Bp	94/110 (86%)	89 (95%)	5 (5%)	28	64
2	Bx	94/110 (86%)	88 (94%)	6 (6%)	22	57
2	CB	94/110 (86%)	89 (95%)	5 (5%)	28	64
2	CJ	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	CR	94/110 (86%)	91 (97%)	3 (3%)	46	79
2	CZ	94/110 (86%)	88 (94%)	6 (6%)	22	57
2	Ch	94/110 (86%)	90 (96%)	4 (4%)	35	72
2	Cp	94/110 (86%)	89 (95%)	5 (5%)	28	64
3	AC	72/84 (86%)	67 (93%)	5 (7%)	19	55
3	AK	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	AS	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Aa	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Ai	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Aq	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Ay	72/84 (86%)	69 (96%)	3 (4%)	36	73
3	BC	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	BK	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	BS	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Ba	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Bi	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Bq	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	By	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	CC	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	CK	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	CS	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Ca	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Ci	72/84 (86%)	68 (94%)	4 (6%)	26	62
3	Cq	72/84 (86%)	68 (94%)	4 (6%)	26	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	AL	60/74 (81%)	57 (95%)	3 (5%)	30	67
4	AT	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Ab	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Aj	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Ar	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Az	60/74 (81%)	57 (95%)	3 (5%)	30	67
4	BD	60/74 (81%)	55 (92%)	5 (8%)	14	46
4	BL	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	BT	60/74 (81%)	55 (92%)	5 (8%)	14	46
4	Bb	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Bj	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Br	60/74 (81%)	57 (95%)	3 (5%)	30	67
4	Bz	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	CD	60/74 (81%)	55 (92%)	5 (8%)	14	46
4	CL	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	CT	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Cb	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Cj	60/74 (81%)	56 (93%)	4 (7%)	20	56
4	Cr	60/74 (81%)	56 (93%)	4 (7%)	20	56
5	A1	15/97 (16%)	11 (73%)	4 (27%)	0	1
5	AE	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	AM	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	AU	15/97 (16%)	13 (87%)	2 (13%)	5	20
5	Ac	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	Ak	15/97 (16%)	13 (87%)	2 (13%)	5	20
5	As	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	B1	15/97 (16%)	13 (87%)	2 (13%)	5	20
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	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Bc	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	Bk	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	Bs	15/97 (16%)	13 (87%)	2 (13%)	5	20
5	CE	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	CM	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	CU	15/97 (16%)	11 (73%)	4 (27%)	0	1
5	Cc	15/97 (16%)	13 (87%)	2 (13%)	5	20
5	Ck	15/97 (16%)	12 (80%)	3 (20%)	1	7
5	Cs	15/97 (16%)	10 (67%)	5 (33%)	0	0
6	A2	203/231 (88%)	176 (87%)	27 (13%)	5	20
6	AF	203/231 (88%)	170 (84%)	33 (16%)	3	12
6	AN	203/231 (88%)	171 (84%)	32 (16%)	3	13
6	AV	203/231 (88%)	177 (87%)	26 (13%)	5	21
6	Ad	203/231 (88%)	178 (88%)	25 (12%)	6	23
6	Al	203/231 (88%)	176 (87%)	27 (13%)	5	20
6	At	203/231 (88%)	172 (85%)	31 (15%)	3	14
6	B2	203/231 (88%)	169 (83%)	34 (17%)	3	11
6	BF	203/231 (88%)	176 (87%)	27 (13%)	5	20
6	BN	203/231 (88%)	177 (87%)	26 (13%)	5	21
6	BV	203/231 (88%)	178 (88%)	25 (12%)	6	23
6	Bd	203/231 (88%)	176 (87%)	27 (13%)	5	20
6	Bl	203/231 (88%)	175 (86%)	28 (14%)	4	19
6	Bt	203/231 (88%)	174 (86%)	29 (14%)	4	17
6	CF	203/231 (88%)	172 (85%)	31 (15%)	3	14
6	CN	203/231 (88%)	178 (88%)	25 (12%)	6	23
6	CV	203/231 (88%)	175 (86%)	28 (14%)	4	19
6	Cd	203/231 (88%)	174 (86%)	29 (14%)	4	17
6	Cl	203/231 (88%)	172 (85%)	31 (15%)	3	14
6	Ct	203/231 (88%)	174 (86%)	29 (14%)	4	17
7	A3	108/159 (68%)	98 (91%)	10 (9%)	11	39
7	AG	108/159 (68%)	98 (91%)	10 (9%)	11	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AO	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	AW	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	Ae	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	Am	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	Au	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	B3	108/159 (68%)	98 (91%)	10 (9%)	11	39
7	BG	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	BO	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	BW	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	Be	108/159 (68%)	100 (93%)	8 (7%)	17	51
7	Bm	108/159 (68%)	100 (93%)	8 (7%)	17	51
7	Bu	108/159 (68%)	100 (93%)	8 (7%)	17	51
7	CG	108/159 (68%)	98 (91%)	10 (9%)	11	39
7	CO	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	CW	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	Ce	108/159 (68%)	98 (91%)	10 (9%)	11	39
7	Cm	108/159 (68%)	99 (92%)	9 (8%)	14	46
7	Cu	108/159 (68%)	100 (93%)	8 (7%)	17	51
8	A4	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	AH	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	AP	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	AX	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Af	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	An	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Av	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	B4	61/66 (92%)	58 (95%)	3 (5%)	31	68
8	BH	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	BP	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	BX	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Bf	61/66 (92%)	58 (95%)	3 (5%)	31	68
8	Bn	61/66 (92%)	59 (97%)	2 (3%)	45	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Bv	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	CH	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	CP	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	CX	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Cf	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Cn	61/66 (92%)	59 (97%)	2 (3%)	45	79
8	Cv	61/66 (92%)	59 (97%)	2 (3%)	45	79
All	All	13800/18440 (75%)	12594 (91%)	1206 (9%)	13	44

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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	A2	8301	-	4,4,4	0.26	0	6,6,6	0.41	0
9	SO4	Ad	8301	-	4,4,4	0.38	0	6,6,6	0.25	0
9	SO4	At	8301	-	4,4,4	0.56	0	6,6,6	0.38	0
9	SO4	B2	8301	-	4,4,4	0.33	0	6,6,6	0.30	0
9	SO4	BF	8301	-	4,4,4	0.22	0	6,6,6	0.27	0
9	SO4	BV	8301	-	4,4,4	0.40	0	6,6,6	0.34	0
9	SO4	Bd	8301	-	4,4,4	0.27	0	6,6,6	0.42	0
9	SO4	Bt	8301	-	4,4,4	0.42	0	6,6,6	0.27	0
9	SO4	CF	8301	-	4,4,4	0.38	0	6,6,6	0.28	0
9	SO4	Cl	8301	-	4,4,4	0.41	0	6,6,6	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SO4	A2	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	Ad	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	At	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	B2	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	BF	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	BV	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	Bd	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	Bt	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	CF	8301	-	-	0/0/0/0	0/0/0/0
9	SO4	Cl	8301	-	-	0/0/0/0	0/0/0/0

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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	82/119 (68%)	-0.24	0 100 100	16, 44, 80, 155	0
1	AI	82/119 (68%)	-0.40	0 100 100	17, 41, 83, 141	0
1	AQ	82/119 (68%)	-0.28	0 100 100	26, 48, 92, 145	0
1	AY	82/119 (68%)	0.39	1 (1%) 81 64	48, 76, 117, 154	0
1	Ag	82/119 (68%)	-0.29	0 100 100	14, 47, 94, 167	0
1	Ao	82/119 (68%)	-0.32	1 (1%) 81 64	18, 43, 87, 158	0
1	Aw	82/119 (68%)	0.35	1 (1%) 81 64	48, 76, 115, 154	0
1	BA	82/119 (68%)	1.08	6 (7%) 18 6	69, 92, 131, 175	0
1	BI	82/119 (68%)	1.27	14 (17%) 2 1	66, 92, 127, 175	0
1	BQ	82/119 (68%)	0.01	1 (1%) 81 64	34, 60, 107, 179	0
1	BY	82/119 (68%)	-0.17	0 100 100	25, 54, 88, 130	0
1	Bg	82/119 (68%)	0.53	0 100 100	58, 81, 117, 151	0
1	Bo	82/119 (68%)	0.20	0 100 100	41, 68, 117, 164	0
1	Bw	82/119 (68%)	-0.15	0 100 100	24, 53, 90, 142	0
1	CA	82/119 (68%)	0.11	0 100 100	36, 64, 105, 132	0
1	CI	82/119 (68%)	1.11	6 (7%) 18 6	61, 86, 127, 164	0
1	CQ	82/119 (68%)	-0.23	0 100 100	29, 54, 88, 136	0
1	CY	82/119 (68%)	-0.24	0 100 100	17, 47, 88, 130	0
1	Cg	82/119 (68%)	0.55	0 100 100	52, 82, 119, 162	0
1	Co	82/119 (68%)	1.10	10 (12%) 5 2	64, 88, 130, 168	0
2	AB	100/118 (84%)	-0.02	1 (1%) 84 69	19, 63, 168, 181	0
2	AJ	100/118 (84%)	-0.06	0 100 100	20, 63, 167, 179	0
2	AR	100/118 (84%)	0.25	8 (8%) 15 5	29, 69, 190, 201	0
2	AZ	100/118 (84%)	0.43	10 (10%) 9 3	39, 82, 226, 242	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	Ah	100/118 (84%)	0.33	7 (7%) 19 7	44, 82, 207, 217	0
2	Ap	100/118 (84%)	0.30	9 (9%) 12 4	34, 72, 215, 219	0
2	Ax	100/118 (84%)	0.11	3 (3%) 54 29	31, 73, 210, 225	0
2	BB	100/118 (84%)	1.48	28 (28%) 1 0	87, 124, 220, 226	0
2	BJ	100/118 (84%)	1.70	38 (38%) 0 0	77, 113, 245, 255	0
2	BR	100/118 (84%)	0.79	16 (16%) 3 1	45, 94, 235, 237	0
2	BZ	100/118 (84%)	0.45	12 (12%) 6 2	37, 76, 216, 232	0
2	Bh	100/118 (84%)	0.76	16 (16%) 3 1	51, 90, 235, 253	0
2	Bp	100/118 (84%)	1.20	20 (20%) 1 0	56, 111, 242, 250	0
2	Bx	100/118 (84%)	0.47	10 (10%) 9 3	32, 75, 230, 243	0
2	CB	100/118 (84%)	0.71	15 (15%) 3 1	48, 92, 223, 238	0
2	CJ	100/118 (84%)	1.47	26 (26%) 1 0	79, 118, 224, 231	0
2	CR	100/118 (84%)	0.24	7 (7%) 19 7	35, 76, 183, 203	0
2	CZ	100/118 (84%)	0.15	8 (8%) 15 5	28, 72, 184, 205	0
2	Ch	100/118 (84%)	0.64	8 (8%) 15 5	55, 90, 212, 223	0
2	Cp	100/118 (84%)	1.48	25 (25%) 1 0	67, 112, 233, 247	0
3	AC	77/92 (83%)	0.62	10 (12%) 5 2	70, 120, 150, 162	0
3	AK	77/92 (83%)	0.90	11 (14%) 4 2	79, 125, 164, 170	0
3	AS	77/92 (83%)	2.16	32 (41%) 0 0	128, 181, 261, 265	0
3	Aa	77/92 (83%)	2.44	40 (51%) 0 0	134, 199, 268, 274	0
3	Ai	77/92 (83%)	0.80	8 (10%) 8 3	86, 135, 164, 173	0
3	Aq	77/92 (83%)	1.82	32 (41%) 0 0	126, 179, 246, 254	0
3	Ay	77/92 (83%)	1.34	20 (25%) 1 0	87, 140, 220, 227	0
3	BC	77/92 (83%)	1.66	26 (33%) 0 0	128, 157, 177, 185	0
3	BK	77/92 (83%)	2.70	37 (48%) 0 0	177, 242, 280, 286	0
3	BS	77/92 (83%)	2.04	31 (40%) 0 0	148, 203, 244, 256	0
3	Ba	77/92 (83%)	1.95	32 (41%) 0 0	133, 188, 260, 264	0
3	Bi	77/92 (83%)	2.17	32 (41%) 0 0	144, 203, 278, 279	0
3	Bq	77/92 (83%)	2.22	39 (50%) 0 0	200, 257, 282, 293	0
3	By	77/92 (83%)	1.88	34 (44%) 0 0	143, 207, 268, 274	0
3	CC	77/92 (83%)	1.08	19 (24%) 1 0	107, 151, 185, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	CK	77/92 (83%)	1.67	27 (35%) 0 0	131, 181, 212, 222	0
3	CS	77/92 (83%)	0.72	8 (10%) 8 3	81, 121, 161, 172	0
3	Ca	77/92 (83%)	0.67	8 (10%) 8 3	82, 122, 165, 177	0
3	Ci	77/92 (83%)	1.10	14 (18%) 2 1	107, 148, 200, 206	0
3	Cq	77/92 (83%)	2.56	39 (50%) 0 0	172, 241, 284, 286	0
4	AD	71/86 (82%)	0.03	1 (1%) 78 60	46, 93, 120, 142	0
4	AL	71/86 (82%)	0.03	1 (1%) 78 60	50, 89, 113, 143	0
4	AT	71/86 (82%)	0.67	11 (15%) 3 1	64, 115, 159, 182	0
4	Ab	71/86 (82%)	0.81	10 (14%) 4 2	73, 116, 166, 193	0
4	Aj	71/86 (82%)	0.48	4 (5%) 28 11	71, 125, 153, 185	0
4	Ar	71/86 (82%)	0.70	9 (12%) 5 2	66, 122, 172, 191	0
4	Az	71/86 (82%)	0.17	0 100 100	60, 105, 133, 163	0
4	BD	71/86 (82%)	1.41	18 (25%) 1 0	104, 169, 199, 208	0
4	BL	71/86 (82%)	1.68	26 (36%) 0 0	118, 165, 251, 260	0
4	BT	71/86 (82%)	1.12	20 (28%) 1 0	98, 144, 212, 220	0
4	Bb	71/86 (82%)	0.70	7 (9%) 9 3	64, 121, 161, 193	0
4	Bj	71/86 (82%)	0.95	10 (14%) 4 2	80, 130, 174, 203	0
4	Br	71/86 (82%)	1.55	21 (29%) 1 0	118, 183, 264, 271	0
4	Bz	71/86 (82%)	0.76	9 (12%) 5 2	71, 128, 179, 219	0
4	CD	71/86 (82%)	0.65	8 (11%) 7 2	77, 126, 152, 195	0
4	CL	71/86 (82%)	1.67	24 (33%) 0 0	111, 166, 197, 201	0
4	CT	71/86 (82%)	0.04	1 (1%) 78 60	64, 101, 128, 156	0
4	Cb	71/86 (82%)	0.06	2 (2%) 56 32	60, 102, 128, 157	0
4	Cj	71/86 (82%)	0.37	3 (4%) 40 19	79, 117, 152, 178	0
4	Cr	71/86 (82%)	1.63	23 (32%) 1 0	111, 166, 244, 257	0
5	A1	17/124 (13%)	0.70	3 (17%) 2 1	73, 98, 162, 164	0
5	AE	17/124 (13%)	0.28	0 100 100	67, 81, 121, 128	0
5	AM	17/124 (13%)	0.18	1 (5%) 26 11	64, 80, 131, 133	0
5	AU	17/124 (13%)	0.26	1 (5%) 26 11	58, 85, 120, 125	0
5	Ac	17/124 (13%)	0.57	3 (17%) 2 1	52, 86, 141, 144	0
5	Ak	17/124 (13%)	0.44	1 (5%) 26 11	63, 78, 125, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
5	As	17/124 (13%)	0.15	1 (5%) 26 11	59, 76, 128, 128	0
5	B1	17/124 (13%)	0.19	1 (5%) 26 11	56, 69, 129, 130	0
5	BE	17/124 (13%)	1.30	4 (23%) 1 0	115, 129, 153, 167	0
5	BM	17/124 (13%)	1.32	3 (17%) 2 1	96, 109, 152, 152	0
5	BU	17/124 (13%)	0.51	1 (5%) 26 11	83, 94, 129, 132	0
5	Bc	17/124 (13%)	0.34	1 (5%) 26 11	60, 81, 133, 136	0
5	Bk	17/124 (13%)	1.06	2 (11%) 6 2	85, 98, 150, 153	0
5	Bs	17/124 (13%)	0.66	3 (17%) 2 1	81, 95, 149, 151	0
5	CE	17/124 (13%)	0.58	2 (11%) 6 2	77, 93, 139, 142	0
5	CM	17/124 (13%)	1.97	5 (29%) 1 0	111, 124, 163, 163	0
5	CU	17/124 (13%)	0.43	3 (17%) 2 1	54, 78, 134, 134	0
5	Cc	17/124 (13%)	0.28	2 (11%) 6 2	53, 72, 132, 134	0
5	Ck	17/124 (13%)	1.34	3 (17%) 2 1	79, 92, 156, 160	0
5	Cs	17/124 (13%)	1.18	3 (17%) 2 1	101, 114, 151, 152	0
6	A2	216/247 (87%)	0.08	17 (7%) 15 5	24, 73, 196, 212	0
6	AF	216/247 (87%)	-0.00	9 (4%) 40 19	14, 56, 168, 208	0
6	AN	216/247 (87%)	-0.02	10 (4%) 36 17	11, 54, 167, 187	0
6	AV	216/247 (87%)	0.18	21 (9%) 10 3	17, 59, 201, 226	0
6	Ad	216/247 (87%)	0.52	24 (11%) 7 2	27, 75, 214, 236	0
6	Al	216/247 (87%)	0.09	13 (6%) 25 10	16, 62, 189, 235	0
6	At	216/247 (87%)	0.12	22 (10%) 9 3	14, 55, 202, 219	0
6	B2	216/247 (87%)	0.25	23 (10%) 8 3	20, 58, 225, 240	0
6	BF	216/247 (87%)	1.04	28 (12%) 5 2	71, 108, 202, 230	0
6	BN	216/247 (87%)	1.27	35 (16%) 3 1	57, 99, 235, 247	0
6	BV	216/247 (87%)	0.46	23 (10%) 8 3	31, 78, 219, 245	0
6	Bd	216/247 (87%)	0.24	22 (10%) 9 3	24, 61, 215, 236	0
6	Bl	216/247 (87%)	0.57	25 (11%) 6 2	38, 78, 226, 246	0
6	Bt	216/247 (87%)	0.71	32 (14%) 3 1	41, 78, 233, 250	0
6	CF	216/247 (87%)	0.24	13 (6%) 25 10	35, 73, 195, 229	0
6	CN	216/247 (87%)	1.14	35 (16%) 3 1	64, 107, 196, 224	0
6	CV	216/247 (87%)	-0.03	7 (3%) 51 27	23, 61, 175, 202	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
6	Cd	216/247 (87%)	-0.08	9 (4%) 40 19	14, 55, 181, 211	0
6	Cl	216/247 (87%)	0.37	11 (5%) 32 13	32, 76, 204, 225	0
6	Ct	216/247 (87%)	1.28	42 (19%) 1 1	63, 103, 224, 240	0
7	A3	127/186 (68%)	0.99	14 (11%) 7 2	74, 126, 154, 172	0
7	AG	127/186 (68%)	-0.04	2 (1%) 74 55	21, 47, 108, 144	0
7	AO	127/186 (68%)	-0.01	2 (1%) 74 55	19, 58, 119, 143	0
7	AW	127/186 (68%)	0.00	5 (3%) 43 21	29, 60, 122, 152	0
7	Ae	127/186 (68%)	1.61	33 (25%) 1 0	78, 122, 162, 170	0
7	Am	127/186 (68%)	-0.28	5 (3%) 43 21	13, 43, 110, 149	0
7	Au	127/186 (68%)	0.02	6 (4%) 35 16	20, 51, 122, 152	0
7	B3	127/186 (68%)	0.08	4 (3%) 52 28	31, 58, 113, 162	0
7	BG	127/186 (68%)	0.91	9 (7%) 19 7	51, 82, 135, 167	0
7	BO	127/186 (68%)	1.68	28 (22%) 1 0	73, 107, 149, 178	0
7	BW	127/186 (68%)	0.02	6 (4%) 35 16	28, 54, 115, 153	0
7	Be	127/186 (68%)	0.05	4 (3%) 52 28	33, 62, 120, 162	0
7	Bm	127/186 (68%)	1.44	24 (18%) 2 1	62, 110, 152, 178	0
7	Bu	127/186 (68%)	0.14	5 (3%) 43 21	34, 63, 122, 167	0
7	CG	127/186 (68%)	-0.07	4 (3%) 52 28	22, 57, 116, 158	0
7	CO	127/186 (68%)	0.88	12 (9%) 11 4	55, 85, 133, 174	0
7	CW	127/186 (68%)	-0.08	4 (3%) 52 28	23, 59, 126, 158	0
7	Ce	127/186 (68%)	-0.11	3 (2%) 62 39	20, 53, 115, 158	0
7	Cm	127/186 (68%)	1.80	41 (32%) 1 0	67, 125, 157, 179	0
7	Cu	127/186 (68%)	1.32	18 (14%) 4 2	73, 100, 146, 174	0
8	A4	70/76 (92%)	2.36	29 (41%) 0 0	158, 202, 224, 228	0
8	AH	70/76 (92%)	0.32	3 (4%) 39 18	69, 116, 151, 158	0
8	AP	70/76 (92%)	0.98	13 (18%) 2 1	81, 137, 167, 178	0
8	AX	70/76 (92%)	2.54	33 (47%) 0 0	121, 196, 220, 225	0
8	Af	70/76 (92%)	4.55	51 (72%) 0 0	200, 237, 255, 258	0
8	An	70/76 (92%)	0.41	6 (8%) 13 4	67, 110, 152, 158	0
8	Av	70/76 (92%)	1.78	26 (37%) 0 0	109, 176, 200, 214	0
8	B4	70/76 (92%)	3.05	42 (60%) 0 0	176, 224, 253, 261	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
8	BH	70/76 (92%)	1.39	20 (28%)	1	0	102, 140, 170, 178	0
8	BP	70/76 (92%)	4.03	48 (68%)	0	0	180, 237, 261, 266	0
8	BX	70/76 (92%)	2.32	31 (44%)	0	0	114, 173, 192, 201	0
8	Bf	70/76 (92%)	3.09	45 (64%)	0	0	178, 226, 252, 255	0
8	Bn	70/76 (92%)	3.73	46 (65%)	0	0	221, 251, 273, 278	0
8	Bv	70/76 (92%)	3.51	51 (72%)	0	0	185, 237, 271, 277	0
8	CH	70/76 (92%)	0.91	10 (14%)	4	2	106, 144, 166, 172	0
8	CP	70/76 (92%)	1.72	22 (31%)	1	0	135, 167, 187, 206	0
8	CX	70/76 (92%)	0.91	9 (12%)	5	2	103, 135, 162, 171	0
8	Cf	70/76 (92%)	0.64	6 (8%)	13	4	97, 140, 160, 170	0
8	Cn	70/76 (92%)	1.87	23 (32%)	0	0	146, 178, 204, 210	0
8	Cv	70/76 (92%)	4.43	53 (75%)	0	0	231, 267, 287, 290	0
All	All	15200/20960 (72%)	0.77	2274 (14%)	3	1	11, 97, 231, 293	0

All (2274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	Af	5055	VAL	22.6
8	BP	5055	VAL	21.6
7	BO	6164	ASN	21.3
8	Af	5028	GLY	20.6
7	BG	6164	ASN	19.0
7	Cu	6164	ASN	18.6
7	BW	6164	ASN	16.6
7	Bu	6164	ASN	16.0
8	Cv	5065	LEU	15.2
8	Bn	5055	VAL	14.7
8	BP	5028	GLY	14.3
8	A4	5028	GLY	13.9
7	Bm	6164	ASN	13.7
7	Ae	6164	ASN	13.5
8	Bn	5037	ILE	13.2
8	AX	5028	GLY	13.1
8	A4	5055	VAL	12.9
8	Af	5036	VAL	12.3
7	Cm	6164	ASN	12.1
3	BK	3033	ILE	11.8
6	Bd	8011	PHE	11.5

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Mol	Chain	Res	Type	RSRZ
8	Cv	5026	LEU	11.2
3	BK	3076	VAL	11.2
8	BP	5036	VAL	11.1
8	Af	5029	PHE	11.1
6	BN	8006	TYR	11.1
8	Cv	5055	VAL	11.1
7	Cu	6163	ALA	11.1
7	AW	6164	ASN	10.7
8	Af	5035	LEU	10.7
7	CO	6164	ASN	10.6
8	Bn	5064	MET	10.5
7	Be	6164	ASN	10.5
8	Cv	5037	ILE	10.4
8	Bn	5004	LEU	10.3
6	B2	8011	PHE	10.3
8	Cv	5013	SER	10.2
6	BV	8011	PHE	10.1
8	Af	5034	ASN	10.0
7	A3	6164	ASN	10.0
8	BP	5029	PHE	9.9
8	Bn	5065	LEU	9.9
7	Au	6164	ASN	9.9
3	Cq	3000	MET	9.8
8	BP	5026	LEU	9.7
8	Bn	5000	HIS	9.4
8	BX	5028	GLY	9.3
6	BV	8019	ALA	9.3
7	Am	6164	ASN	9.1
8	Cv	5028	GLY	9.0
8	BP	5004	LEU	9.0
3	BK	3044	LEU	8.9
8	Cv	5067	ALA	8.9
8	Bf	5037	ILE	8.9
8	Bv	5028	GLY	8.8
8	A4	5037	ILE	8.8
3	Bi	3000	MET	8.8
8	Cv	5000	HIS	8.7
8	Cv	5064	MET	8.7
7	B3	6164	ASN	8.7
8	A4	5002	PRO	8.7
6	BN	8011	PHE	8.6
8	BP	5001	PRO	8.6

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Mol	Chain	Res	Type	RSRZ
8	Bv	5061	SER	8.6
8	B4	5068	LEU	8.6
8	Bf	5004	LEU	8.6
7	CG	6164	ASN	8.5
8	Bf	5055	VAL	8.4
3	BS	3033	ILE	8.4
8	Cv	5032	PHE	8.4
3	Bq	3000	MET	8.4
3	Aa	3007	ILE	8.3
8	BP	5035	LEU	8.3
7	Bu	6163	ALA	8.3
8	BP	5037	ILE	8.3
8	AX	5055	VAL	8.3
8	Af	5065	LEU	8.2
6	Bl	8011	PHE	8.2
8	B4	5004	LEU	8.2
6	Bt	8002	SER	8.2
8	Bv	5067	ALA	8.2
7	CO	6000	MET	8.1
8	Af	5037	ILE	8.1
3	By	3000	MET	8.1
6	BN	8012	TYR	8.1
3	Ba	3000	MET	8.1
8	Af	5014	LEU	8.0
8	Bv	5026	LEU	8.0
5	Bk	7001	VAL	8.0
8	Cv	5036	VAL	8.0
3	Bq	3036	PHE	8.0
3	BC	3006	LEU	7.9
3	BK	3032	CYS	7.9
7	BO	6163	ALA	7.9
8	B4	5061	SER	7.8
8	Cv	5020	ARG	7.8
6	BN	8010	MET	7.8
8	Bn	5036	VAL	7.7
8	Bv	5036	VAL	7.7
6	BN	8019	ALA	7.7
8	Bn	5026	LEU	7.7
7	AO	6164	ASN	7.7
7	Bm	6163	ALA	7.7
8	A4	5026	LEU	7.6
3	BK	3010	TYR	7.6

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Mol	Chain	Res	Type	RSRZ
6	BN	8002	SER	7.6
8	CP	5001	PRO	7.5
8	Bv	5037	ILE	7.5
3	Aa	3001	VAL	7.5
6	Ad	8017	CYS	7.5
8	Bv	5068	LEU	7.4
8	Bn	5028	GLY	7.4
6	Bl	8012	TYR	7.4
3	Cq	3010	TYR	7.4
8	B4	5037	ILE	7.4
6	Bt	8010	MET	7.4
5	CM	7001	VAL	7.4
3	AS	3036	PHE	7.3
6	Ct	8023	LYS	7.3
8	Cv	5031	PRO	7.3
7	AG	6164	ASN	7.2
8	Av	5028	GLY	7.2
6	Bt	8019	ALA	7.1
6	A2	8004	GLU	7.1
3	Bi	3004	ILE	7.1
3	Aa	3033	ILE	7.1
7	Bm	6000	MET	7.1
3	AS	3033	ILE	7.1
8	Af	5057	ILE	7.0
6	Bt	8011	PHE	7.0
8	Cn	5055	VAL	7.0
8	Af	5000	HIS	7.0
5	BM	7001	VAL	7.0
8	Bf	5000	HIS	7.0
8	AX	5029	PHE	6.9
8	AX	5036	VAL	6.9
8	Bf	5068	LEU	6.9
8	Cv	5057	ILE	6.9
4	Br	4030	VAL	6.9
8	Bv	5004	LEU	6.9
6	BV	8010	MET	6.9
8	Bv	5055	VAL	6.9
6	Cd	8011	PHE	6.8
6	B2	8014	ARG	6.8
6	Ct	8017	CYS	6.8
8	Af	5013	SER	6.8
2	Cp	2009	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
8	BP	5068	LEU	6.8
8	CP	5002	PRO	6.8
3	Cq	3033	ILE	6.8
4	Ar	4005	LEU	6.7
4	Cr	4030	VAL	6.7
8	Bv	5040	CYS	6.7
6	Ct	8014	ARG	6.7
4	BL	4001	PRO	6.7
7	CW	6164	ASN	6.6
8	Bf	5028	GLY	6.6
8	Af	5068	LEU	6.6
8	BX	5001	PRO	6.6
8	B4	5028	GLY	6.6
6	Ad	8011	PHE	6.6
8	Af	5004	LEU	6.6
8	Cv	5054	MET	6.6
6	BF	8012	TYR	6.6
8	A4	5004	LEU	6.6
6	Bt	8034	ASN	6.6
2	BJ	2009	LEU	6.6
8	Av	5001	PRO	6.6
8	Bf	5018	GLY	6.6
8	Af	5069	GLU	6.6
3	AS	3074	GLN	6.5
6	AN	8004	GLU	6.5
3	BK	3045	ASP	6.5
8	BP	5061	SER	6.5
8	Cv	5035	LEU	6.5
8	Af	5002	PRO	6.5
8	BP	5032	PHE	6.5
8	Af	5031	PRO	6.4
6	AV	8017	CYS	6.4
3	BS	3032	CYS	6.4
8	BH	5055	VAL	6.4
8	Af	5032	PHE	6.4
6	Bl	8006	TYR	6.4
6	BF	8004	GLU	6.4
8	Af	5067	ALA	6.4
8	Bn	5029	PHE	6.4
5	Ck	7001	VAL	6.4
8	Bf	5026	LEU	6.4
7	BG	6163	ALA	6.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	Cq	3004	ILE	6.3
6	BN	8017	CYS	6.3
3	Aa	3013	ASN	6.3
8	BP	5003	GLU	6.3
8	CP	5055	VAL	6.3
8	Cv	5056	VAL	6.3
8	Af	5020	ARG	6.3
8	B4	5055	VAL	6.3
4	CL	4053	LEU	6.3
3	BK	3060	LEU	6.3
3	Bq	3030	GLU	6.3
8	Bv	5035	LEU	6.3
4	BT	4001	PRO	6.3
8	B4	5018	GLY	6.3
6	BV	8017	CYS	6.3
8	Bv	5000	HIS	6.2
8	B4	5000	HIS	6.2
8	Bn	5067	ALA	6.2
3	BC	3033	ILE	6.2
7	Ce	6164	ASN	6.2
8	B4	5040	CYS	6.2
8	BX	5029	PHE	6.2
7	Bm	6162	SER	6.2
3	Aq	3036	PHE	6.2
3	Bq	3006	LEU	6.2
3	By	3036	PHE	6.2
7	BO	6000	MET	6.2
6	CF	8011	PHE	6.2
2	BJ	2000	PRO	6.1
6	B2	8007	LEU	6.1
8	BP	5034	ASN	6.1
3	Cq	3057	ARG	6.1
2	Bp	2008	GLU	6.1
8	Bn	5001	PRO	6.1
8	Cv	5004	LEU	6.1
3	AS	3035	GLY	6.1
3	BK	3001	VAL	6.1
8	BP	5065	LEU	6.1
3	Bi	3074	GLN	6.1
8	Cv	5014	LEU	6.1
8	Bf	5003	GLU	6.1
3	AS	3044	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
6	BF	8034	ASN	6.1
3	Aa	3000	MET	6.1
6	At	8007	LEU	6.1
8	Cv	5040	CYS	6.0
6	Ct	8019	ALA	6.0
3	BS	3060	LEU	6.0
8	Cv	5015	LYS	6.0
6	Bt	8014	ARG	6.0
7	Cu	6000	MET	6.0
6	AV	8011	PHE	6.0
6	Ct	8010	MET	6.0
3	Aa	3044	LEU	5.9
3	Aq	3044	LEU	5.9
3	Bq	3033	ILE	5.9
6	At	8011	PHE	5.9
4	Cr	4002	LYS	5.9
7	BO	6161	ASP	5.9
8	AP	5002	PRO	5.9
6	BN	8008	MET	5.9
8	B4	5057	ILE	5.9
8	CP	5000	HIS	5.9
8	BX	5036	VAL	5.9
7	A3	6030	GLY	5.9
8	BP	5000	HIS	5.9
6	Ad	8002	SER	5.9
6	BF	8011	PHE	5.9
8	Cn	5067	ALA	5.8
6	CN	8034	ASN	5.8
8	A4	5068	LEU	5.8
8	AX	5068	LEU	5.8
3	BK	3015	SER	5.8
8	B4	5026	LEU	5.8
6	Ad	8007	LEU	5.7
3	BS	3010	TYR	5.7
8	Bf	5061	SER	5.7
8	Cv	5068	LEU	5.7
2	Bh	2000	PRO	5.7
8	Cv	5063	ILE	5.7
3	BK	3013	ASN	5.7
6	Ct	8018	PRO	5.7
3	BS	3044	LEU	5.7
3	Cq	3007	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
2	Bp	2009	LEU	5.6
7	Cm	6163	ALA	5.6
8	CH	5002	PRO	5.6
8	Av	5031	PRO	5.6
6	CN	8021	VAL	5.6
6	At	8019	ALA	5.6
5	CM	7000	ALA	5.6
8	Cv	5001	PRO	5.6
6	Ct	8011	PHE	5.6
3	Aa	3010	TYR	5.6
3	BS	3076	VAL	5.6
6	Bl	8010	MET	5.6
2	BJ	2025	LEU	5.6
6	Ct	8021	VAL	5.6
8	AP	5055	VAL	5.5
6	Bt	8003	GLY	5.5
8	Af	5026	LEU	5.5
8	BX	5026	LEU	5.5
3	Bi	3075	SER	5.5
8	BX	5055	VAL	5.5
6	At	8010	MET	5.5
8	BP	5009	ASP	5.5
8	BX	5034	ASN	5.5
3	BS	3001	VAL	5.5
3	Aq	3074	GLN	5.5
3	Ba	3074	GLN	5.5
8	Cn	5032	PHE	5.5
2	BB	2095	PRO	5.5
4	Cr	4012	PRO	5.5
7	Ae	6163	ALA	5.5
6	Bd	8004	GLU	5.5
5	BU	7001	VAL	5.5
6	BN	8005	GLU	5.4
6	BV	8006	TYR	5.4
4	Ab	4002	LYS	5.4
7	CO	6165	SER	5.4
3	BK	3072	LEU	5.4
8	Bn	5013	SER	5.4
7	Ae	6001	VAL	5.4
6	BV	8007	LEU	5.4
8	Af	5008	MET	5.4
6	At	8017	CYS	5.4

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Mol	Chain	Res	Type	RSRZ
6	Cl	8012	TYR	5.4
6	B2	8012	TYR	5.4
8	Cn	5001	PRO	5.4
6	BN	8007	LEU	5.4
6	AV	8007	LEU	5.4
6	Ad	8019	ALA	5.4
8	BP	5067	ALA	5.4
2	Cp	2000	PRO	5.4
3	AS	3013	ASN	5.4
7	Cu	6130	GLY	5.4
6	B2	8006	TYR	5.4
6	Bd	8012	TYR	5.3
8	Af	5003	GLU	5.3
6	BF	8138	THR	5.3
6	BF	8051	LEU	5.3
8	AX	5069	GLU	5.3
6	Ad	8006	TYR	5.3
6	BF	8006	TYR	5.3
8	Bf	5057	ILE	5.3
3	CK	3000	MET	5.3
3	Aa	3074	GLN	5.3
3	Aq	3001	VAL	5.3
6	AN	8011	PHE	5.3
8	B4	5012	LEU	5.3
3	AS	3009	ARG	5.3
8	Cv	5027	ARG	5.3
4	Cr	4028	VAL	5.3
5	BE	7001	VAL	5.3
6	Ct	8008	MET	5.3
6	Bl	8004	GLU	5.3
8	Af	5046	SER	5.3
8	BX	5031	PRO	5.3
2	Cp	2094	ASN	5.2
3	Bq	3010	TYR	5.2
8	Af	5056	VAL	5.2
6	Bd	8006	TYR	5.2
3	BK	3000	MET	5.2
8	Bv	5003	GLU	5.2
3	Cq	3060	LEU	5.2
6	Ad	8010	MET	5.2
6	Ct	8012	TYR	5.2
2	BB	2094	ASN	5.2

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Mol	Chain	Res	Type	RSRZ
6	BN	8034	ASN	5.2
8	A4	5035	LEU	5.2
3	Aa	3073	LEU	5.1
8	Bv	5057	ILE	5.1
6	Bt	8006	TYR	5.1
3	By	3006	LEU	5.1
3	Bi	3044	LEU	5.1
3	Bi	3071	THR	5.1
7	Cu	6162	SER	5.1
6	Ct	8006	TYR	5.1
3	BK	3007	ILE	5.1
3	Cq	3032	CYS	5.1
6	A2	8011	PHE	5.1
6	CN	8008	MET	5.1
3	Bi	3073	LEU	5.1
8	AX	5035	LEU	5.1
7	BO	6162	SER	5.1
7	Cm	6027	LYS	5.0
3	Aa	3036	PHE	5.0
3	BS	3007	ILE	5.0
2	CZ	2002	SER	5.0
3	Bq	3017	ILE	5.0
3	Aa	3006	LEU	5.0
6	BF	8007	LEU	5.0
6	Bt	8012	TYR	5.0
2	BJ	2016	GLU	5.0
8	A4	5036	VAL	5.0
5	Bs	7001	VAL	5.0
6	CV	8011	PHE	5.0
6	Ct	8009	HIS	5.0
4	AT	4002	LYS	5.0
3	AS	3007	ILE	5.0
8	BP	5069	GLU	5.0
8	Bf	5040	CYS	5.0
3	Aa	3009	ARG	5.0
8	Bn	5003	GLU	5.0
2	CR	2002	SER	5.0
3	Cq	3076	VAL	5.0
3	Cq	3031	GLY	4.9
6	Ad	8004	GLU	4.9
3	Bi	3015	SER	4.9
6	Ad	8015	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
3	Ay	3074	GLN	4.9
8	Bv	5007	PHE	4.9
6	B2	8010	MET	4.9
3	Bq	3031	GLY	4.9
2	BB	2002	SER	4.9
3	BK	3020	TRP	4.9
7	Cm	6000	MET	4.9
6	BV	8018	PRO	4.9
6	BV	8014	ARG	4.9
6	Bl	8002	SER	4.9
6	BN	8014	ARG	4.9
3	Ba	3004	ILE	4.9
8	BX	5032	PHE	4.9
8	B4	5035	LEU	4.9
8	CP	5026	LEU	4.9
8	A4	5003	GLU	4.9
6	Bd	8007	LEU	4.8
3	Ay	3076	VAL	4.8
3	Ba	3033	ILE	4.8
8	Bf	5007	PHE	4.8
3	Aq	3033	ILE	4.8
3	Bi	3033	ILE	4.8
6	Bt	8007	LEU	4.8
7	BW	6163	ALA	4.8
2	BJ	2094	ASN	4.8
8	Cv	5017	ASN	4.8
8	Bn	5014	LEU	4.8
2	Bx	2008	GLU	4.8
4	BD	4026	TYR	4.8
2	CJ	2000	PRO	4.8
5	Ck	7000	ALA	4.8
3	BS	3000	MET	4.8
8	A4	5057	ILE	4.8
7	Ae	6051	GLY	4.8
8	Cv	5003	GLU	4.8
8	Bn	5057	ILE	4.8
6	AN	8007	LEU	4.8
6	Bl	8008	MET	4.8
8	A4	5000	HIS	4.8
8	BP	5064	MET	4.8
8	CP	5067	ALA	4.8
4	BD	4030	VAL	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	AW	6163	ALA	4.7
3	Aq	3007	ILE	4.7
8	AX	5031	PRO	4.7
8	AX	5034	ASN	4.7
6	Al	8019	ALA	4.7
3	AS	3063	ILE	4.7
7	Be	6163	ALA	4.7
6	Bl	8009	HIS	4.7
8	BX	5003	GLU	4.7
8	Bf	5029	PHE	4.7
6	Bd	8014	ARG	4.7
6	B2	8003	GLY	4.7
6	B2	8002	SER	4.7
4	CL	4030	VAL	4.7
3	Bi	3072	LEU	4.7
8	B4	5007	PHE	4.7
2	Bp	2000	PRO	4.7
8	BX	5009	ASP	4.7
8	CH	5001	PRO	4.7
6	Bt	8008	MET	4.7
3	By	3007	ILE	4.7
6	BF	8019	ALA	4.7
8	Af	5038	ASP	4.7
2	Ch	2099	GLY	4.7
3	Cq	3071	THR	4.6
3	Cq	3061	GLY	4.6
6	BF	8024	ARG	4.6
6	Bt	8009	HIS	4.6
8	Bn	5056	VAL	4.6
8	B4	5036	VAL	4.6
6	Bl	8007	LEU	4.6
3	Aa	3076	VAL	4.6
8	Af	5007	PHE	4.6
2	BB	2016	GLU	4.6
8	CP	5037	ILE	4.6
8	Af	5022	VAL	4.6
3	CC	3006	LEU	4.6
6	AV	8010	MET	4.6
2	BZ	2000	PRO	4.6
6	Ad	8008	MET	4.6
8	Bv	5033	MET	4.6
2	CB	2002	SER	4.6

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Mol	Chain	Res	Type	RSRZ
7	BW	6162	SER	4.6
8	BH	5002	PRO	4.6
6	Ct	8007	LEU	4.6
6	Ct	8002	SER	4.6
8	Cv	5002	PRO	4.6
4	Br	4068	GLY	4.6
2	BZ	2008	GLU	4.6
3	AS	3000	MET	4.6
3	Aa	3020	TRP	4.6
8	Bv	5039	GLU	4.6
8	Bv	5062	ILE	4.6
6	Al	8011	PHE	4.6
6	BN	8032	THR	4.6
8	Af	5001	PRO	4.6
6	BN	8016	ARG	4.5
6	Bd	8002	SER	4.5
8	Bn	5061	SER	4.5
2	BR	2009	LEU	4.5
8	AX	5009	ASP	4.5
6	A2	8008	MET	4.5
3	BK	3036	PHE	4.5
3	Ba	3015	SER	4.5
6	CN	8051	LEU	4.5
7	Ae	6000	MET	4.5
6	Bl	8003	GLY	4.5
3	Ci	3000	MET	4.5
8	BP	5017	ASN	4.5
6	Bt	8024	ARG	4.5
3	Aq	3075	SER	4.5
6	CN	8010	MET	4.5
8	Af	5064	MET	4.5
4	BT	4005	LEU	4.5
8	AX	5002	PRO	4.5
3	BC	3076	VAL	4.5
8	Bn	5032	PHE	4.5
4	Bj	4012	PRO	4.5
8	Bn	5034	ASN	4.5
4	Br	4029	SER	4.5
8	BP	5008	MET	4.5
8	Cf	5001	PRO	4.5
4	BL	4030	VAL	4.5
2	Bx	2016	GLU	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	A3	6130	GLY	4.5
8	BX	5037	ILE	4.5
3	Ay	3006	LEU	4.5
3	BK	3018	GLN	4.5
7	Bm	6130	GLY	4.5
3	CC	3000	MET	4.5
6	BV	8020	VAL	4.4
8	AX	5001	PRO	4.4
8	Bv	5063	ILE	4.4
3	CK	3076	VAL	4.4
3	Aq	3000	MET	4.4
3	Cq	3044	LEU	4.4
8	Av	5029	PHE	4.4
8	Bf	5036	VAL	4.4
6	Al	8012	TYR	4.4
7	A3	6163	ALA	4.4
6	Ct	8020	VAL	4.4
3	CS	3000	MET	4.4
8	A4	5005	LYS	4.4
8	Cn	5004	LEU	4.4
3	AK	3074	GLN	4.4
8	AX	5032	PHE	4.4
4	AT	4005	LEU	4.4
4	BD	4001	PRO	4.4
6	Bl	8005	GLU	4.4
8	Bn	5025	ILE	4.3
8	AP	5028	GLY	4.3
8	CX	5002	PRO	4.3
8	AX	5037	ILE	4.3
3	Bi	3046	ASP	4.3
6	Bd	8010	MET	4.3
8	Bv	5031	PRO	4.3
3	CK	3004	ILE	4.3
6	Ct	8004	GLU	4.3
3	Ba	3072	LEU	4.3
3	Cq	3001	VAL	4.3
2	CJ	2094	ASN	4.3
3	Cq	3002	GLN	4.3
8	Bn	5035	LEU	4.3
8	Bn	5063	ILE	4.3
6	Ct	8003	GLY	4.3
8	B4	5003	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
8	Av	5069	GLU	4.3
3	BK	3063	ILE	4.3
4	BL	4036	MET	4.3
4	Cr	4004	PHE	4.3
3	AS	3073	LEU	4.3
8	Bf	5035	LEU	4.3
7	Be	6000	MET	4.2
8	Bf	5005	LYS	4.2
8	Bf	5067	ALA	4.2
4	CL	4026	TYR	4.2
3	AS	3075	SER	4.2
6	Ct	8000	PRO	4.2
8	AX	5051	ASN	4.2
8	BP	5060	ASN	4.2
8	Cv	5062	ILE	4.2
6	AV	8015	LYS	4.2
8	Af	5018	GLY	4.2
3	Ba	3044	LEU	4.2
8	BH	5026	LEU	4.2
8	Bv	5065	LEU	4.2
8	AX	5057	ILE	4.2
8	Cn	5002	PRO	4.2
4	Cr	4026	TYR	4.2
6	Bd	8003	GLY	4.2
2	Bp	2025	LEU	4.2
6	Ct	8015	LYS	4.2
8	Af	5066	GLU	4.2
8	Bv	5064	MET	4.2
4	BL	4027	LEU	4.2
8	Bf	5012	LEU	4.2
3	Ba	3071	THR	4.2
6	Bt	8033	GLY	4.2
3	CK	3033	ILE	4.2
6	Bd	8028	ILE	4.2
4	BL	4004	PHE	4.2
3	Aa	3072	LEU	4.2
3	BC	3015	SER	4.1
3	Ba	3007	ILE	4.1
7	Au	6163	ALA	4.1
4	Cr	4068	GLY	4.1
8	Cv	5007	PHE	4.1
3	By	3030	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
6	AV	8004	GLU	4.1
2	CJ	2018	ASN	4.1
8	BP	5005	LYS	4.1
8	Bn	5005	LYS	4.1
7	BW	6161	ASP	4.1
8	Bn	5007	PHE	4.1
3	Ay	3009	ARG	4.1
3	BK	3009	ARG	4.1
8	BP	5056	VAL	4.1
2	Ch	2002	SER	4.1
7	A3	6162	SER	4.1
6	BV	8012	TYR	4.1
2	Cp	2007	GLU	4.1
6	AV	8023	LYS	4.1
6	Bt	8000	PRO	4.1
8	CX	5001	PRO	4.1
8	Af	5061	SER	4.1
3	Ba	3036	PHE	4.1
7	CO	6162	SER	4.1
6	Bt	8004	GLU	4.1
8	B4	5031	PRO	4.1
6	CN	8012	TYR	4.1
3	By	3033	ILE	4.1
8	Bn	5066	GLU	4.1
4	Bj	4001	PRO	4.1
6	Bt	8005	GLU	4.1
6	CN	8006	TYR	4.1
8	BH	5032	PHE	4.1
8	Bn	5046	SER	4.1
3	BS	3031	GLY	4.1
6	Bt	8032	THR	4.1
6	Ad	8018	PRO	4.1
8	BP	5062	ILE	4.0
8	Bv	5005	LYS	4.0
8	Bv	5001	PRO	4.0
4	Cr	4040	ASN	4.0
3	BK	3006	LEU	4.0
5	CU	7000	ALA	4.0
3	BK	3071	THR	4.0
6	Bl	8016	ARG	4.0
6	AF	8019	ALA	4.0
6	A2	8003	GLY	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	B3	6163	ALA	4.0
3	Cq	3073	LEU	4.0
7	BO	6130	GLY	4.0
8	CP	5065	LEU	4.0
8	Av	5036	VAL	4.0
2	Bp	2004	MET	4.0
8	BH	5004	LEU	4.0
4	CL	4040	ASN	4.0
6	CF	8034	ASN	4.0
8	Bv	5018	GLY	4.0
6	BF	8008	MET	4.0
8	AX	5004	LEU	4.0
6	Bl	8015	LYS	4.0
8	BX	5000	HIS	4.0
8	Bv	5020	ARG	4.0
8	AX	5007	PHE	4.0
3	BS	3074	GLN	4.0
8	Bn	5008	MET	4.0
8	Cn	5065	LEU	4.0
6	BV	8005	GLU	4.0
8	Bv	5056	VAL	4.0
3	Bi	3045	ASP	4.0
3	CC	3036	PHE	4.0
8	Bn	5068	LEU	4.0
6	Al	8004	GLU	4.0
8	AP	5037	ILE	4.0
8	B4	5062	ILE	4.0
8	Bn	5031	PRO	4.0
6	B2	8004	GLU	4.0
1	Co	1025	GLY	4.0
7	A3	6051	GLY	4.0
3	BS	3015	SER	4.0
8	BP	5046	SER	4.0
6	CV	8138	THR	4.0
3	Bq	3044	LEU	4.0
2	BZ	2004	MET	4.0
6	AF	8004	GLU	4.0
8	Cn	5036	VAL	3.9
6	Cd	8007	LEU	3.9
8	A4	5067	ALA	3.9
8	Cv	5061	SER	3.9
8	Cn	5000	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
8	Cv	5060	ASN	3.9
4	BD	4002	LYS	3.9
6	Bt	8023	LYS	3.9
8	Cv	5033	MET	3.9
8	Af	5009	ASP	3.9
6	B2	8024	ARG	3.9
4	BL	4034	MET	3.9
3	CK	3006	LEU	3.9
8	BX	5035	LEU	3.9
7	Cm	6082	TRP	3.9
2	Bh	2016	GLU	3.9
2	BR	2025	LEU	3.9
3	BS	3072	LEU	3.9
3	By	3017	ILE	3.9
8	Bn	5009	ASP	3.9
7	BG	6130	GLY	3.9
2	Bp	2002	SER	3.9
6	CN	8011	PHE	3.9
8	B4	5067	ALA	3.9
3	Aa	3021	LEU	3.9
3	By	3072	LEU	3.9
3	BS	3075	SER	3.9
6	Bl	8014	ARG	3.9
8	AH	5002	PRO	3.9
7	Be	6162	SER	3.9
2	BJ	2005	THR	3.9
3	Aa	3071	THR	3.9
6	Bd	8015	LYS	3.9
6	B2	8005	GLU	3.9
5	Cs	7001	VAL	3.9
8	BP	5002	PRO	3.9
4	BD	4055	GLU	3.9
6	BN	8004	GLU	3.9
6	AF	8011	PHE	3.8
2	Bx	2004	MET	3.8
6	AV	8019	ALA	3.8
6	Ad	8023	LYS	3.8
8	Bv	5054	MET	3.8
8	Cv	5052	ILE	3.8
8	A4	5029	PHE	3.8
2	Bh	2004	MET	3.8
3	Aa	3004	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
8	B4	5033	MET	3.8
3	AS	3018	GLN	3.8
8	Cv	5029	PHE	3.8
3	By	3065	LEU	3.8
4	Aj	4005	LEU	3.8
4	BD	4005	LEU	3.8
4	BL	4005	LEU	3.8
6	CN	8178	ILE	3.8
8	Bn	5020	ARG	3.8
8	B4	5060	ASN	3.8
8	CX	5000	HIS	3.8
3	Ca	3000	MET	3.8
3	Aq	3060	LEU	3.8
3	Ba	3017	ILE	3.8
6	CV	8012	TYR	3.8
2	Bx	2000	PRO	3.8
8	Av	5009	ASP	3.8
3	AS	3076	VAL	3.8
3	Bi	3076	VAL	3.8
6	BN	8024	ARG	3.8
3	BS	3018	GLN	3.8
3	Ci	3020	TRP	3.8
5	CM	7010	THR	3.8
3	Bq	3060	LEU	3.8
3	Bq	3072	LEU	3.8
7	Cu	6080	VAL	3.8
7	Am	6165	SER	3.8
8	Cn	5064	MET	3.8
3	AK	3036	PHE	3.8
8	CP	5032	PHE	3.8
3	BK	3034	ILE	3.8
8	Cn	5037	ILE	3.8
8	AX	5000	HIS	3.8
8	B4	5069	GLU	3.8
8	Av	5051	ASN	3.8
8	Bf	5034	ASN	3.8
3	Bi	3009	ARG	3.8
3	Cq	3075	SER	3.8
7	Cu	6165	SER	3.8
8	BH	5037	ILE	3.8
4	CL	4002	LYS	3.8
6	At	8006	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
3	BK	3002	GLN	3.8
3	CK	3060	LEU	3.8
2	AZ	2007	GLU	3.8
6	BV	8138	THR	3.8
8	BP	5052	ILE	3.8
8	Av	5034	ASN	3.7
3	Cq	3072	LEU	3.7
4	Br	4001	PRO	3.7
8	Bv	5013	SER	3.7
1	CI	1025	GLY	3.7
3	Aq	3063	ILE	3.7
2	CR	2004	MET	3.7
7	BG	6165	SER	3.7
4	Bj	4070	GLU	3.7
8	B4	5039	GLU	3.7
8	AX	5067	ALA	3.7
3	AK	3076	VAL	3.7
8	Cn	5056	VAL	3.7
7	A3	6000	MET	3.7
7	Bu	6000	MET	3.7
8	BX	5068	LEU	3.7
8	Bf	5013	SER	3.7
8	Bf	5031	PRO	3.7
4	Ab	4069	VAL	3.7
4	Ab	4005	LEU	3.7
8	BX	5002	PRO	3.7
8	Cv	5039	GLU	3.7
8	AX	5003	GLU	3.7
5	Ck	7002	TRP	3.7
3	BS	3063	ILE	3.7
5	A1	7001	VAL	3.7
8	Av	5068	LEU	3.7
4	Bb	4001	PRO	3.7
8	BP	5018	GLY	3.7
6	BN	8009	HIS	3.7
4	BL	4058	ILE	3.7
8	BP	5063	ILE	3.7
4	Br	4032	GLY	3.6
4	Br	4005	LEU	3.6
6	AN	8019	ALA	3.6
7	Bm	6079	LYS	3.6
6	CF	8012	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
7	BG	6000	MET	3.6
8	Av	5037	ILE	3.6
8	Av	5032	PHE	3.6
3	AS	3001	VAL	3.6
8	Av	5055	VAL	3.6
8	BP	5033	MET	3.6
6	Bl	8028	ILE	3.6
8	Bn	5060	ASN	3.6
6	Al	8007	LEU	3.6
7	A3	6050	GLU	3.6
8	BP	5020	ARG	3.6
8	BP	5031	PRO	3.6
6	Bd	8005	GLU	3.6
8	Af	5051	ASN	3.6
3	BS	3045	ASP	3.6
2	BZ	2002	SER	3.6
7	B3	6000	MET	3.6
2	Bx	2002	SER	3.6
3	Bq	3007	ILE	3.6
6	Bd	8008	MET	3.6
3	Ca	3036	PHE	3.6
8	Cv	5066	GLU	3.6
3	BS	3013	ASN	3.6
3	AS	3004	ILE	3.6
8	B4	5063	ILE	3.6
8	CH	5026	LEU	3.6
8	CP	5003	GLU	3.6
8	B4	5005	LYS	3.6
5	CE	7000	ALA	3.6
6	A2	8031	ASN	3.6
8	Bn	5040	CYS	3.6
3	Aq	3035	GLY	3.6
6	AV	8002	SER	3.6
8	Cv	5034	ASN	3.6
8	Bn	5027	ARG	3.6
2	AR	2006	PRO	3.6
8	Av	5000	HIS	3.6
8	CP	5031	PRO	3.6
2	AR	2007	GLU	3.6
2	Cp	2004	MET	3.6
3	AS	3020	TRP	3.6
3	AS	3060	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	Bq	3035	GLY	3.6
7	CG	6000	MET	3.6
8	Bf	5060	ASN	3.6
6	CN	8050	CYS	3.6
8	Cv	5009	ASP	3.6
8	An	5002	PRO	3.6
6	Bt	8020	VAL	3.5
2	Cp	2008	GLU	3.5
3	Cq	3006	LEU	3.5
4	Cr	4039	ALA	3.5
8	Bf	5001	PRO	3.5
4	CL	4029	SER	3.5
6	AV	8006	TYR	3.5
7	Bu	6162	SER	3.5
6	AV	8014	ARG	3.5
2	Bh	2003	GLU	3.5
6	Al	8138	THR	3.5
8	Bv	5032	PHE	3.5
5	Bc	7001	VAL	3.5
7	A3	6046	THR	3.5
8	AX	5026	LEU	3.5
4	Br	4000	ASN	3.5
1	CI	1081	VAL	3.5
3	CK	3002	GLN	3.5
6	Bl	8024	ARG	3.5
8	Bf	5056	VAL	3.5
2	BJ	2013	GLU	3.5
4	Ar	4002	LYS	3.5
6	A2	8017	CYS	3.5
6	Cd	8138	THR	3.5
3	BC	3010	TYR	3.5
8	Cn	5028	GLY	3.5
4	Ab	4028	VAL	3.5
6	Bl	8032	THR	3.5
3	Ay	3004	ILE	3.5
3	Ay	3033	ILE	3.5
3	Bi	3017	ILE	3.5
3	BS	3047	ALA	3.5
3	Bq	3015	SER	3.5
6	BN	8026	SER	3.5
7	BG	6162	SER	3.5
8	Bv	5017	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
8	Cv	5008	MET	3.5
2	Bh	2008	GLU	3.5
3	BC	3020	TRP	3.5
8	CP	5008	MET	3.5
2	Bp	2092	LEU	3.5
2	Bp	2094	ASN	3.5
6	Cl	8011	PHE	3.5
8	Af	5039	GLU	3.5
2	BJ	2021	PRO	3.4
8	B4	5001	PRO	3.4
8	BP	5015	LYS	3.4
6	Cl	8017	CYS	3.4
3	Aq	3073	LEU	3.4
3	CK	3071	THR	3.4
4	BT	4012	PRO	3.4
8	Av	5002	PRO	3.4
8	A4	5009	ASP	3.4
8	CH	5000	HIS	3.4
7	Cm	6136	TRP	3.4
4	BL	4002	LYS	3.4
2	BR	2013	GLU	3.4
4	Bb	4070	GLU	3.4
4	CL	4055	GLU	3.4
8	Af	5052	ILE	3.4
3	AC	3035	GLY	3.4
8	BX	5007	PHE	3.4
2	BJ	2004	MET	3.4
3	Bq	3065	LEU	3.4
7	Cm	6080	VAL	3.4
6	CF	8019	ALA	3.4
6	At	8004	GLU	3.4
3	Aq	3018	GLN	3.4
6	CN	8033	GLY	3.4
8	BP	5013	SER	3.4
6	Ct	8032	THR	3.4
8	Bf	5065	LEU	3.4
3	Ba	3020	TRP	3.4
4	CL	4065	TYR	3.4
8	Cn	5066	GLU	3.4
2	BB	2025	LEU	3.4
3	BC	3044	LEU	3.4
6	CF	8007	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	Cp	2030	LYS	3.4
8	Bf	5025	ILE	3.4
6	Cl	8006	TYR	3.4
8	B4	5056	VAL	3.4
6	B2	8009	HIS	3.4
8	Af	5012	LEU	3.4
2	AZ	2004	MET	3.4
6	BN	8138	THR	3.4
7	Cm	6071	CYS	3.4
2	Bp	2013	GLU	3.4
2	Bp	2016	GLU	3.4
2	CB	2016	GLU	3.4
4	CL	4004	PHE	3.4
6	B2	8016	ARG	3.4
3	AK	3060	LEU	3.4
3	Cq	3052	SER	3.4
2	BZ	2016	GLU	3.4
3	Ba	3009	ARG	3.4
8	Bv	5069	GLU	3.4
8	CX	5032	PHE	3.4
3	Bi	3032	CYS	3.4
5	CE	7001	VAL	3.4
8	Cv	5049	GLN	3.4
2	BR	2000	PRO	3.3
3	AK	3009	ARG	3.3
4	Br	4034	MET	3.3
5	AU	7001	VAL	3.3
8	B4	5041	VAL	3.3
4	BL	4000	ASN	3.3
3	Ay	3007	ILE	3.3
6	Ct	8194	PRO	3.3
3	Ci	3018	GLN	3.3
6	Ct	8013	GLU	3.3
8	Cn	5029	PHE	3.3
8	BX	5004	LEU	3.3
4	Br	4040	ASN	3.3
7	Cm	6001	VAL	3.3
8	Af	5005	LYS	3.3
8	Bf	5008	MET	3.3
2	Cp	2001	LYS	3.3
7	BW	6130	GLY	3.3
3	Ai	3010	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
7	AG	6165	SER	3.3
8	Av	5035	LEU	3.3
5	BM	7002	TRP	3.3
1	BI	1025	GLY	3.3
3	Bq	3071	THR	3.3
8	A4	5032	PHE	3.3
4	Cr	4058	ILE	3.3
8	BH	5036	VAL	3.3
6	CN	8014	ARG	3.3
8	A4	5064	MET	3.3
8	AP	5000	HIS	3.3
7	B3	6162	SER	3.3
3	Ba	3001	VAL	3.3
5	CU	7001	VAL	3.3
8	AX	5008	MET	3.3
8	Af	5060	ASN	3.3
3	BK	3075	SER	3.3
6	Ad	8001	GLU	3.3
8	AX	5018	GLY	3.3
3	BS	3073	LEU	3.3
3	Ci	3073	LEU	3.3
6	Bt	8015	LYS	3.3
7	Bu	6130	GLY	3.3
2	Bx	2009	LEU	3.3
3	Aq	3020	TRP	3.3
3	By	3074	GLN	3.3
8	A4	5034	ASN	3.3
6	Ct	8024	ARG	3.3
2	BB	2092	LEU	3.3
7	BO	6165	SER	3.3
4	Aj	4026	TYR	3.3
4	Cj	4026	TYR	3.3
7	CW	6163	ALA	3.3
6	BN	8020	VAL	3.3
8	Av	5007	PHE	3.3
6	Ct	8051	LEU	3.3
4	Cr	4034	MET	3.3
3	Aa	3018	GLN	3.2
8	AX	5050	ASN	3.2
8	BP	5066	GLU	3.2
3	BK	3073	LEU	3.2
6	BF	8014	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
3	Bq	3038	GLU	3.2
7	CG	6163	ALA	3.2
7	AW	6000	MET	3.2
3	Aa	3063	ILE	3.2
6	At	8009	HIS	3.2
7	Am	6130	GLY	3.2
8	A4	5007	PHE	3.2
8	BH	5000	HIS	3.2
2	BB	2038	ASN	3.2
3	Aq	3013	ASN	3.2
3	Ba	3075	SER	3.2
4	Cr	4056	VAL	3.2
6	B2	8019	ALA	3.2
7	CO	6163	ALA	3.2
6	Ct	8141	LEU	3.2
4	Bz	4001	PRO	3.2
1	Co	1060	GLY	3.2
3	By	3035	GLY	3.2
8	AX	5046	SER	3.2
8	Bv	5027	ARG	3.2
3	Bq	3073	LEU	3.2
2	BJ	2039	CYS	3.2
4	Ar	4001	PRO	3.2
6	Al	8017	CYS	3.2
8	Cn	5008	MET	3.2
2	AR	2008	GLU	3.2
3	CC	3076	VAL	3.2
3	By	3045	ASP	3.2
6	AF	8007	LEU	3.2
7	Bm	6065	SER	3.2
3	Aa	3002	GLN	3.2
3	By	3071	THR	3.2
5	BE	7008	VAL	3.2
2	BB	2028	SER	3.2
2	CJ	2002	SER	3.2
2	BJ	2069	GLU	3.2
6	BV	8004	GLU	3.2
6	B2	8008	MET	3.2
8	A4	5031	PRO	3.2
2	BJ	2020	GLY	3.2
3	Cq	3043	VAL	3.2
4	BT	4028	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
6	A2	8007	LEU	3.2
3	CK	3075	SER	3.2
3	Cq	3016	ARG	3.2
8	Cv	5005	LYS	3.2
7	Au	6162	SER	3.2
6	CN	8018	PRO	3.2
3	AS	3071	THR	3.2
8	Af	5015	LYS	3.2
6	Ct	8005	GLU	3.2
8	Bf	5069	GLU	3.2
8	CH	5003	GLU	3.2
3	BS	3036	PHE	3.2
6	BF	8194	PRO	3.2
8	BH	5028	GLY	3.2
8	Cn	5031	PRO	3.2
3	Aa	3060	LEU	3.2
8	BH	5003	GLU	3.2
3	Cq	3056	SER	3.2
4	Ab	4012	PRO	3.2
6	Ad	8003	GLY	3.2
6	At	8023	LYS	3.2
6	CN	8141	LEU	3.2
8	CP	5020	ARG	3.2
3	Cq	3041	ASN	3.1
6	AV	8001	GLU	3.1
4	Bj	4027	LEU	3.1
2	CJ	2095	PRO	3.1
3	AS	3032	CYS	3.1
3	AS	3042	LEU	3.1
6	BN	8023	LYS	3.1
6	B2	8028	ILE	3.1
8	Bf	5064	MET	3.1
8	B4	5010	LYS	3.1
8	B4	5013	SER	3.1
3	AS	3010	TYR	3.1
3	AC	3074	GLN	3.1
3	By	3004	ILE	3.1
4	CL	4058	ILE	3.1
6	CN	8187	ASP	3.1
7	Cm	6065	SER	3.1
8	A4	5001	PRO	3.1
8	Cv	5069	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
4	Cj	4030	VAL	3.1
4	Cr	4053	LEU	3.1
5	Cc	7001	VAL	3.1
6	At	8020	VAL	3.1
6	Bt	8016	ARG	3.1
6	BF	8032	THR	3.1
6	Cd	8012	TYR	3.1
6	BV	8001	GLU	3.1
3	Aa	3032	CYS	3.1
3	AS	3021	LEU	3.1
4	Bj	4028	VAL	3.1
6	AV	8020	VAL	3.1
8	Bv	5059	GLY	3.1
8	Cn	5035	LEU	3.1
2	BJ	2011	LYS	3.1
2	BZ	2003	GLU	3.1
3	Ay	3075	SER	3.1
8	B4	5029	PHE	3.1
2	AR	2004	MET	3.1
3	Bi	3020	TRP	3.1
3	CK	3010	TYR	3.1
3	Ci	3002	GLN	3.1
8	Bv	5002	PRO	3.1
8	Av	5026	LEU	3.1
8	Bv	5041	VAL	3.1
3	BC	3009	ARG	3.1
6	BV	8009	HIS	3.1
6	At	8018	PRO	3.1
8	Bv	5023	GLN	3.1
8	Cf	5002	PRO	3.1
4	Br	4013	VAL	3.1
7	CW	6162	SER	3.1
3	Bq	3057	ARG	3.1
3	BK	3069	ASN	3.1
2	Cp	2088	VAL	3.1
3	Aq	3076	VAL	3.1
3	Ca	3002	GLN	3.1
7	BO	6166	ASP	3.1
4	BT	4013	VAL	3.1
5	As	7001	VAL	3.1
2	CR	2099	GLY	3.1
4	BL	4055	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
6	CN	8019	ALA	3.1
2	BB	2055	HIS	3.1
4	Cr	4035	ASN	3.1
4	BL	4028	VAL	3.1
3	Bi	3007	ILE	3.1
3	BK	3021	LEU	3.1
7	Cm	6029	VAL	3.1
7	Cu	6141	ASP	3.1
3	Ai	3076	VAL	3.1
3	Bq	3063	ILE	3.1
7	Cu	6161	ASP	3.1
6	CF	8008	MET	3.0
7	Ae	6046	THR	3.0
8	Bf	5039	GLU	3.0
3	Aa	3075	SER	3.0
6	A2	8002	SER	3.0
4	BT	4030	VAL	3.0
2	BJ	2099	GLY	3.0
3	BK	3074	GLN	3.0
3	CC	3050	ILE	3.0
6	Ad	8028	ILE	3.0
3	Ba	3058	LYS	3.0
8	BX	5069	GLU	3.0
8	Cv	5038	ASP	3.0
8	BX	5008	MET	3.0
3	By	3044	LEU	3.0
6	BN	8051	LEU	3.0
4	CL	4019	TRP	3.0
8	Af	5017	ASN	3.0
3	Aa	3057	ARG	3.0
6	Ad	8014	ARG	3.0
8	A4	5008	MET	3.0
3	Bi	3006	LEU	3.0
8	AP	5036	VAL	3.0
2	BJ	2095	PRO	3.0
6	AF	8018	PRO	3.0
2	BR	2098	ALA	3.0
6	Ad	8012	TYR	3.0
8	Bv	5006	LYS	3.0
3	Bq	3002	GLN	3.0
2	Bh	2018	ASN	3.0
8	Bf	5033	MET	3.0

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Mol	Chain	Res	Type	RSRZ
3	By	3010	TYR	3.0
6	A2	8138	THR	3.0
8	Bn	5052	ILE	3.0
8	Cv	5019	GLY	3.0
3	Aq	3009	ARG	3.0
8	Af	5023	GLN	3.0
3	By	3020	TRP	3.0
2	Ch	2004	MET	3.0
8	BX	5054	MET	3.0
7	A3	6001	VAL	3.0
6	Ct	8033	GLY	3.0
4	CL	4037	GLN	3.0
6	Bl	8000	PRO	3.0
8	AX	5056	VAL	3.0
6	Bd	8016	ARG	3.0
2	BB	2069	GLU	3.0
2	Cp	2039	CYS	3.0
2	AB	2002	SER	3.0
5	B1	7001	VAL	3.0
6	BV	8008	MET	3.0
8	BP	5027	ARG	3.0
1	BA	1070	ASP	3.0
4	CT	4026	TYR	3.0
3	BC	3018	GLN	3.0
3	BK	3047	ALA	3.0
6	BV	8021	VAL	3.0
8	Bv	5010	LYS	3.0
4	Bz	4030	VAL	3.0
3	By	3075	SER	3.0
6	Bd	8026	SER	3.0
7	Cm	6084	GLY	3.0
3	Bi	3036	PHE	3.0
3	CC	3002	GLN	3.0
3	BC	3007	ILE	3.0
7	Cm	6072	ILE	3.0
2	BR	2021	PRO	2.9
8	A4	5046	SER	2.9
8	Bf	5009	ASP	2.9
7	Cm	6021	LYS	2.9
7	BW	6000	MET	2.9
8	CP	5036	VAL	2.9
2	Ap	2008	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
3	Bq	3004	ILE	2.9
8	B4	5019	GLY	2.9
4	Cr	4019	TRP	2.9
3	Ba	3032	CYS	2.9
6	CN	8053	PRO	2.9
4	BD	4027	LEU	2.9
6	Ad	8021	VAL	2.9
6	AV	8008	MET	2.9
2	BJ	2055	HIS	2.9
7	Ae	6130	GLY	2.9
8	Bf	5020	ARG	2.9
8	Cf	5000	HIS	2.9
3	Bq	3020	TRP	2.9
3	BC	3036	PHE	2.9
4	BD	4004	PHE	2.9
4	BD	4029	SER	2.9
4	BL	4012	PRO	2.9
2	Ch	2003	GLU	2.9
3	Ci	3074	GLN	2.9
4	BT	4037	GLN	2.9
6	At	8001	GLU	2.9
2	BB	2099	GLY	2.9
6	CN	8024	ARG	2.9
6	Cl	8008	MET	2.9
2	BB	2046	LEU	2.9
4	Bj	4030	VAL	2.9
2	Ch	2096	LEU	2.9
3	BS	3021	LEU	2.9
2	Cp	2011	LYS	2.9
3	Ba	3045	ASP	2.9
8	BH	5008	MET	2.9
2	Cp	2018	ASN	2.9
4	Bb	4000	ASN	2.9
8	Bv	5014	LEU	2.9
2	BB	2035	VAL	2.9
3	Cq	3019	VAL	2.9
7	Cm	6138	MET	2.9
6	Ad	8009	HIS	2.9
8	BH	5050	ASN	2.9
2	BZ	2001	LYS	2.9
2	Cp	2005	THR	2.9
3	Bq	3012	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
6	Bl	8138	THR	2.9
2	Bh	2002	SER	2.9
6	CF	8010	MET	2.9
6	CF	8024	ARG	2.9
2	CJ	2097	ILE	2.9
4	Ab	4034	MET	2.9
6	AN	8138	THR	2.9
8	Af	5033	MET	2.9
3	AS	3072	LEU	2.9
3	Bq	3001	VAL	2.9
4	BD	4056	VAL	2.9
6	Bd	8009	HIS	2.9
8	Bf	5019	GLY	2.9
3	BS	3071	THR	2.9
3	By	3009	ARG	2.9
4	BL	4008	LEU	2.9
7	Cu	6079	LYS	2.9
3	Bi	3043	VAL	2.9
7	Ae	6052	ILE	2.9
2	CB	2017	PHE	2.9
3	Ay	3000	MET	2.9
3	BC	3040	MET	2.9
3	Cq	3064	MET	2.9
4	AT	4027	LEU	2.9
6	Bt	8001	GLU	2.9
6	Al	8024	ARG	2.9
7	Ae	6084	GLY	2.9
8	Bf	5062	ILE	2.8
3	By	3005	ASN	2.8
6	A2	8019	ALA	2.8
2	Ap	2009	LEU	2.8
3	Ay	3060	LEU	2.8
3	CK	3001	VAL	2.8
7	Bm	6080	VAL	2.8
3	CK	3015	SER	2.8
7	BG	6167	SER	2.8
7	Bm	6155	CYS	2.8
8	AP	5046	SER	2.8
8	CP	5009	ASP	2.8
3	BS	3004	ILE	2.8
2	BZ	2009	LEU	2.8
3	AC	3060	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
8	Bf	5032	PHE	2.8
2	BR	2006	PRO	2.8
6	B2	8015	LYS	2.8
7	CO	6079	LYS	2.8
7	Cm	6167	SER	2.8
2	BB	2021	PRO	2.8
3	Bq	3009	ARG	2.8
4	BT	4002	LYS	2.8
6	AV	8024	ARG	2.8
7	Ae	6080	VAL	2.8
3	BC	3063	ILE	2.8
7	Cm	6051	GLY	2.8
4	Bz	4005	LEU	2.8
7	Bm	6161	ASP	2.8
6	At	8005	GLU	2.8
1	BI	1062	ASN	2.8
5	Cs	7002	TRP	2.8
8	Bn	5010	LYS	2.8
6	Al	8018	PRO	2.8
6	Bd	8000	PRO	2.8
6	AV	8028	ILE	2.8
8	Bn	5018	GLY	2.8
6	CF	8138	THR	2.8
6	BF	8209	ASN	2.8
8	CP	5028	GLY	2.8
2	BB	2009	LEU	2.8
3	Bq	3016	ARG	2.8
6	CN	8201	LEU	2.8
8	B4	5008	MET	2.8
8	Bf	5063	ILE	2.8
2	CJ	2016	GLU	2.8
4	Cr	4037	GLN	2.8
2	Cp	2073	ASN	2.8
3	By	3063	ILE	2.8
6	At	8012	TYR	2.8
2	BJ	2014	GLU	2.8
3	Bq	3040	MET	2.8
4	Br	4069	VAL	2.8
1	BI	1009	SER	2.8
2	AR	2002	SER	2.8
2	CB	2097	ILE	2.8
3	Bq	3076	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
4	CL	4056	VAL	2.8
2	Ah	2028	SER	2.8
6	CV	8028	ILE	2.8
3	BS	3003	PRO	2.8
3	Cq	3058	LYS	2.8
4	Cr	4013	VAL	2.8
1	BI	1036	THR	2.8
6	Bt	8017	CYS	2.8
2	BR	2008	GLU	2.8
7	Cm	6165	SER	2.8
6	AN	8018	PRO	2.8
6	BN	8018	PRO	2.8
3	Ci	3001	VAL	2.8
6	Cd	8034	ASN	2.8
7	BO	6001	VAL	2.8
3	CC	3018	GLN	2.8
3	CC	3033	ILE	2.7
4	Cr	4057	LEU	2.7
8	AP	5009	ASP	2.7
8	BH	5035	LEU	2.7
3	CK	3032	CYS	2.7
4	BL	4061	ASN	2.7
2	AZ	2009	LEU	2.7
3	Aq	3004	ILE	2.7
7	Bm	6072	ILE	2.7
8	AH	5000	HIS	2.7
8	An	5000	HIS	2.7
8	BH	5007	PHE	2.7
6	BF	8005	GLU	2.7
6	Bl	8023	LYS	2.7
2	Ap	2098	ALA	2.7
2	Cp	2095	PRO	2.7
4	BT	4029	SER	2.7
4	Bz	4012	PRO	2.7
5	Cc	7000	ALA	2.7
6	BV	8002	SER	2.7
8	Bn	5002	PRO	2.7
8	Bn	5033	MET	2.7
3	Aa	3011	LEU	2.7
3	Cq	3053	LYS	2.7
6	Cl	8028	ILE	2.7
7	Ae	6137	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
8	AP	5003	GLU	2.7
2	CB	2000	PRO	2.7
3	Cq	3047	ALA	2.7
3	Bi	3070	ILE	2.7
3	BC	3001	VAL	2.7
3	By	3001	VAL	2.7
4	Cr	4069	VAL	2.7
3	AS	3012	GLN	2.7
3	Ai	3060	LEU	2.7
6	BN	8033	GLY	2.7
6	CF	8004	GLU	2.7
6	Cd	8024	ARG	2.7
6	BN	8209	ASN	2.7
3	BK	3025	VAL	2.7
8	Av	5067	ALA	2.7
6	Cl	8138	THR	2.7
7	A3	6045	PRO	2.7
2	Cp	2025	LEU	2.7
3	Ay	3044	LEU	2.7
3	Ba	3073	LEU	2.7
4	AD	4005	LEU	2.7
8	BX	5046	SER	2.7
2	Ah	2094	ASN	2.7
3	BC	3025	VAL	2.7
2	CB	2098	ALA	2.7
6	Ad	8024	ARG	2.7
3	Ay	3020	TRP	2.7
3	CK	3031	GLY	2.7
4	BT	4004	PHE	2.7
6	Cl	8010	MET	2.7
7	Cm	6022	LEU	2.7
6	Ad	8020	VAL	2.7
6	At	8014	ARG	2.7
3	AS	3006	LEU	2.7
3	Aq	3006	LEU	2.7
8	BP	5007	PHE	2.7
8	Af	5054	MET	2.7
3	CS	3002	GLN	2.7
6	CF	8032	THR	2.7
8	Bn	5017	ASN	2.7
3	Ba	3006	LEU	2.7
7	Ae	6050	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
4	Bb	4012	PRO	2.7
3	Ay	3002	GLN	2.7
1	Co	1057	SER	2.7
2	BJ	2028	SER	2.7
4	AT	4029	SER	2.7
8	BH	5046	SER	2.7
4	BL	4033	TYR	2.7
2	BB	2096	LEU	2.7
2	BR	2007	GLU	2.7
3	Cq	3008	PHE	2.7
2	Bp	2097	ILE	2.7
2	Ch	2016	GLU	2.7
8	BP	5057	ILE	2.7
2	Bh	2006	PRO	2.7
4	BD	4008	LEU	2.7
6	Bt	8013	GLU	2.7
6	Ct	8037	LEU	2.7
6	AN	8008	MET	2.7
8	BH	5034	ASN	2.7
8	Bf	5049	GLN	2.7
2	Bx	2001	LYS	2.6
3	BS	3048	GLU	2.6
3	Bq	3075	SER	2.6
3	Cq	3030	GLU	2.6
7	AW	6162	SER	2.6
8	BX	5050	ASN	2.6
3	Bi	3002	GLN	2.6
8	Bn	5015	LYS	2.6
8	Cv	5006	LYS	2.6
3	Ba	3035	GLY	2.6
3	Bi	3060	LEU	2.6
3	Bq	3042	LEU	2.6
6	At	8024	ARG	2.6
6	BV	8032	THR	2.6
7	BO	6015	TYR	2.6
3	CK	3061	GLY	2.6
8	Bf	5046	SER	2.6
4	CL	4036	MET	2.6
6	At	8008	MET	2.6
5	Ac	7001	VAL	2.6
6	B2	8034	ASN	2.6
3	Ba	3062	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
3	CK	3014	ARG	2.6
4	Bb	4027	LEU	2.6
8	Cn	5014	LEU	2.6
4	CD	4010	GLY	2.6
3	Ca	3017	ILE	2.6
7	Ae	6042	SER	2.6
1	BQ	1081	VAL	2.6
1	BI	1035	ASN	2.6
3	BC	3002	GLN	2.6
7	Cm	6035	TYR	2.6
6	At	8021	VAL	2.6
7	Bm	6029	VAL	2.6
2	AZ	2071	PRO	2.6
3	Ci	3026	ASN	2.6
4	Ar	4012	PRO	2.6
4	Bj	4000	ASN	2.6
4	Bz	4027	LEU	2.6
2	Bp	2030	LYS	2.6
8	BH	5005	LYS	2.6
1	BA	1036	THR	2.6
6	Ct	8016	ARG	2.6
8	Av	5046	SER	2.6
6	CN	8004	GLU	2.6
7	Cm	6074	PHE	2.6
8	B4	5042	GLU	2.6
8	Cf	5026	LEU	2.6
8	Av	5050	ASN	2.6
3	CC	3046	ASP	2.6
8	An	5037	ILE	2.6
3	Bi	3019	VAL	2.6
4	Bj	4034	MET	2.6
6	CN	8032	THR	2.6
2	AR	2009	LEU	2.6
4	BD	4053	LEU	2.6
8	Cn	5068	LEU	2.6
2	BJ	2006	PRO	2.6
3	BK	3070	ILE	2.6
2	Bh	2007	GLU	2.6
7	Cm	6137	LEU	2.6
8	Av	5003	GLU	2.6
7	Ce	6162	SER	2.6
3	Bq	3047	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
6	Ct	8178	ILE	2.6
7	Ae	6086	TYR	2.6
4	Ab	4040	ASN	2.6
4	Br	4031	ASP	2.6
4	Bz	4000	ASN	2.6
6	Cl	8034	ASN	2.6
7	Bm	6001	VAL	2.6
8	Bv	5009	ASP	2.6
6	BN	8001	GLU	2.6
2	Bp	2005	THR	2.6
3	Aa	3061	GLY	2.6
3	Bi	3034	ILE	2.6
6	B2	8138	THR	2.6
2	Bp	2011	LYS	2.6
3	Bq	3045	ASP	2.6
6	CN	8023	LYS	2.6
8	AX	5066	GLU	2.6
8	BP	5054	MET	2.6
8	Bn	5038	ASP	2.6
2	BJ	2007	GLU	2.6
3	Aq	3021	LEU	2.6
1	CI	1060	GLY	2.6
7	Cm	6135	CYS	2.6
3	Ci	3075	SER	2.6
7	BO	6042	SER	2.6
6	A2	8021	VAL	2.6
3	Ba	3046	ASP	2.6
8	An	5032	PHE	2.6
3	Ba	3063	ILE	2.6
6	AV	8012	TYR	2.6
3	Ay	3001	VAL	2.6
3	CK	3052	SER	2.6
3	Cq	3015	SER	2.6
6	AV	8021	VAL	2.6
7	Au	6165	SER	2.6
7	Cm	6162	SER	2.6
4	Br	4035	ASN	2.5
5	Bk	7002	TRP	2.5
5	Ac	7016	GLY	2.5
7	BO	6051	GLY	2.5
8	Cf	5028	GLY	2.5
2	Bp	2001	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
3	Ba	3034	ILE	2.5
8	Cv	5025	ILE	2.5
2	Cp	2014	GLU	2.5
7	Ae	6155	CYS	2.5
7	CG	6162	SER	2.5
3	Aa	3040	MET	2.5
4	BT	4034	MET	2.5
7	Cm	6155	CYS	2.5
2	BJ	2038	ASN	2.5
2	CZ	2001	LYS	2.5
8	Bv	5060	ASN	2.5
3	AS	3039	TYR	2.5
2	CJ	2069	GLU	2.5
8	BP	5014	LEU	2.5
2	AR	2001	LYS	2.5
2	CB	2001	LYS	2.5
3	CC	3075	SER	2.5
4	Cr	4001	PRO	2.5
7	A3	6165	SER	2.5
8	AP	5001	PRO	2.5
2	Bp	2020	GLY	2.5
4	Ar	4061	ASN	2.5
6	BN	8134	ASP	2.5
2	AZ	2008	GLU	2.5
4	BT	4026	TYR	2.5
4	Cb	4026	TYR	2.5
8	A4	5069	GLU	2.5
3	By	3058	LYS	2.5
8	CH	5010	LYS	2.5
2	BJ	2002	SER	2.5
3	BC	3031	GLY	2.5
5	BM	7010	THR	2.5
2	Bp	2089	ILE	2.5
3	AK	3050	ILE	2.5
5	CM	7002	TRP	2.5
2	BJ	2034	GLN	2.5
4	Cr	4061	ASN	2.5
8	BX	5030	ASP	2.5
7	BO	6049	ALA	2.5
2	AZ	2001	LYS	2.5
2	Bh	2001	LYS	2.5
4	Cr	4036	MET	2.5

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Mol	Chain	Res	Type	RSRZ
6	A2	8010	MET	2.5
6	Bl	8033	GLY	2.5
8	Bv	5043	MET	2.5
5	BE	7002	TRP	2.5
2	BB	2034	GLN	2.5
3	Aq	3010	TYR	2.5
3	BC	3021	LEU	2.5
3	Bq	3005	ASN	2.5
7	Cu	6166	ASP	2.5
3	Bq	3032	CYS	2.5
6	Bd	8024	ARG	2.5
7	Cm	6063	GLY	2.5
6	AN	8032	THR	2.5
2	BJ	2035	VAL	2.5
3	BK	3048	GLU	2.5
3	CC	3030	GLU	2.5
6	BN	8074	VAL	2.5
6	BF	8198	LEU	2.5
7	Ce	6163	ALA	2.5
8	CX	5055	VAL	2.5
3	Ba	3005	ASN	2.5
6	Ct	8034	ASN	2.5
3	Aa	3035	GLY	2.5
3	Aq	3032	CYS	2.5
7	Ae	6045	PRO	2.5
7	CO	6066	SER	2.5
8	BP	5045	THR	2.5
8	B4	5023	GLN	2.5
3	Aq	3031	GLY	2.5
4	BD	4036	MET	2.5
6	BF	8033	GLY	2.5
8	Cv	5053	GLY	2.5
2	BZ	2006	PRO	2.5
6	Bt	8018	PRO	2.5
6	CN	8194	PRO	2.5
3	AK	3018	GLN	2.5
3	BC	3074	GLN	2.5
6	AV	8032	THR	2.5
7	Bm	6002	LEU	2.5
8	B4	5020	ARG	2.5
8	BP	5030	ASP	2.5
4	BL	4035	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
6	CN	8003	GLY	2.5
2	CJ	2070	VAL	2.5
3	CK	3073	LEU	2.5
8	CH	5032	PHE	2.5
1	BI	1057	SER	2.5
3	Ay	3052	SER	2.5
4	Bz	4026	TYR	2.5
6	Ad	8138	THR	2.5
6	B2	8026	SER	2.5
2	CZ	2097	ILE	2.5
3	BC	3069	ASN	2.5
8	B4	5034	ASN	2.5
4	BL	4013	VAL	2.5
4	Bz	4070	GLU	2.5
6	BV	8016	ARG	2.5
3	BS	3002	GLN	2.5
4	BL	4019	TRP	2.5
2	Cp	2099	GLY	2.5
6	At	8002	SER	2.5
7	Cm	6130	GLY	2.5
3	Bq	3034	ILE	2.5
4	Br	4036	MET	2.5
6	Ct	8127	MET	2.5
7	Cm	6020	ILE	2.5
8	A4	5054	MET	2.5
3	By	3038	GLU	2.5
8	Bv	5034	ASN	2.5
8	Cn	5020	ARG	2.5
4	Aj	4001	PRO	2.4
8	BX	5049	GLN	2.4
2	Bh	2005	THR	2.4
3	BC	3071	THR	2.4
2	CB	2003	GLU	2.4
6	BF	8010	MET	2.4
7	Ae	6165	SER	2.4
2	CJ	2088	VAL	2.4
3	Ba	3060	LEU	2.4
3	CC	3055	LYS	2.4
4	AT	4061	ASN	2.4
2	Ch	2098	ALA	2.4
8	BX	5067	ALA	2.4
2	Ap	2013	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	BJ	2008	GLU	2.4
3	CK	3025	VAL	2.4
4	Br	4015	VAL	2.4
6	BF	8050	CYS	2.4
6	Al	8034	ASN	2.4
8	Af	5050	ASN	2.4
8	CP	5034	ASN	2.4
3	Ai	3074	GLN	2.4
6	BV	8024	ARG	2.4
7	CO	6063	GLY	2.4
2	CJ	2011	LYS	2.4
3	BK	3004	ILE	2.4
4	Bz	4034	MET	2.4
7	Cu	6062	HIS	2.4
8	Bv	5008	MET	2.4
3	BS	3046	ASP	2.4
4	Ar	4029	SER	2.4
6	Ct	8187	ASP	2.4
4	AT	4040	ASN	2.4
6	Bd	8034	ASN	2.4
7	AO	6163	ALA	2.4
4	CD	4026	TYR	2.4
6	Cl	8024	ARG	2.4
7	AW	6130	GLY	2.4
6	Cd	8004	GLU	2.4
8	BH	5057	ILE	2.4
1	Co	1043	MET	2.4
3	Ai	3006	LEU	2.4
3	CK	3051	HIS	2.4
6	Ct	8131	TRP	2.4
2	Ah	2002	SER	2.4
6	A2	8187	ASP	2.4
6	Ct	8134	ASP	2.4
3	Ca	3055	LYS	2.4
8	BX	5005	LYS	2.4
2	BZ	2007	GLU	2.4
2	CJ	2007	GLU	2.4
2	CR	2003	GLU	2.4
3	CS	3074	GLN	2.4
6	BF	8053	PRO	2.4
2	Bh	2009	LEU	2.4
3	BK	3042	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	Bi	3065	LEU	2.4
4	BT	4056	VAL	2.4
4	Bb	4030	VAL	2.4
8	BH	5029	PHE	2.4
1	Aw	1055	THR	2.4
4	Bj	4002	LYS	2.4
8	Af	5045	THR	2.4
2	BR	2099	GLY	2.4
4	BL	4066	ILE	2.4
7	Ae	6015	TYR	2.4
3	Ay	3021	LEU	2.4
8	B4	5054	MET	2.4
5	A1	7002	TRP	2.4
7	Bm	6027	LYS	2.4
7	Cm	6016	THR	2.4
2	BR	2010	GLN	2.4
3	CS	3017	ILE	2.4
2	AZ	2006	PRO	2.4
2	Ap	2006	PRO	2.4
3	Bi	3001	VAL	2.4
3	By	3062	ARG	2.4
4	BT	4027	LEU	2.4
6	A2	8024	ARG	2.4
3	Aa	3023	GLU	2.4
6	Ad	8032	THR	2.4
3	AK	3001	VAL	2.4
3	BC	3059	GLN	2.4
3	Ci	3055	LYS	2.4
6	Al	8021	VAL	2.4
8	A4	5065	LEU	2.4
2	BJ	2066	MET	2.4
2	CJ	2038	ASN	2.4
3	Aa	3003	PRO	2.4
3	Cq	3020	TRP	2.4
6	CN	8131	TRP	2.4
5	Bs	7000	ALA	2.4
7	Au	6130	GLY	2.4
3	By	3046	ASP	2.4
3	Cq	3034	ILE	2.4
6	At	8032	THR	2.4
6	CN	8208	GLN	2.4
7	Bm	6167	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	Aq	3040	MET	2.4
3	BC	3051	HIS	2.4
2	BB	2030	LYS	2.4
2	CJ	2014	GLU	2.4
6	BN	8015	LYS	2.4
6	BF	8052	LEU	2.4
6	Ct	8028	ILE	2.4
8	Bf	5010	LYS	2.4
4	BL	4069	VAL	2.4
6	Cd	8021	VAL	2.4
8	AP	5032	PHE	2.4
8	Bf	5014	LEU	2.4
8	Bn	5049	GLN	2.4
2	BB	2005	THR	2.4
6	AV	8018	PRO	2.4
2	Ah	2098	ALA	2.4
3	Ba	3030	GLU	2.4
6	BV	8015	LYS	2.4
7	BO	6055	GLU	2.4
8	Bn	5069	GLU	2.4
2	BR	2017	PHE	2.4
2	CR	2017	PHE	2.4
3	Bi	3010	TYR	2.4
3	By	3073	LEU	2.4
4	CD	4065	TYR	2.4
3	By	3015	SER	2.3
6	Bl	8017	CYS	2.3
7	Ae	6135	CYS	2.3
7	Au	6000	MET	2.3
7	A3	6042	SER	2.3
8	Bv	5046	SER	2.3
4	Ab	4001	PRO	2.3
2	Cp	2013	GLU	2.3
3	CK	3030	GLU	2.3
4	CL	4043	GLU	2.3
8	A4	5020	ARG	2.3
4	CL	4068	GLY	2.3
8	Bv	5019	GLY	2.3
2	BB	2017	PHE	2.3
2	BB	2036	LEU	2.3
2	CJ	2035	VAL	2.3
3	By	3042	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
7	Cm	6052	ILE	2.3
8	CP	5056	VAL	2.3
3	CC	3074	GLN	2.3
6	CN	8134	ASP	2.3
8	Av	5008	MET	2.3
8	Bv	5015	LYS	2.3
2	CB	2008	GLU	2.3
7	BO	6155	CYS	2.3
2	Ax	2018	ASN	2.3
3	AK	3006	LEU	2.3
3	Ay	3013	ASN	2.3
3	AC	3076	VAL	2.3
4	BD	4052	HIS	2.3
8	BP	5023	GLN	2.3
3	BK	3040	MET	2.3
4	Ar	4034	MET	2.3
2	Bx	2003	GLU	2.3
3	Ay	3035	GLY	2.3
3	CK	3035	GLY	2.3
8	CX	5031	PRO	2.3
3	Ba	3065	LEU	2.3
7	A3	6022	LEU	2.3
8	AP	5068	LEU	2.3
4	AT	4069	VAL	2.3
3	Ba	3010	TYR	2.3
4	BL	4065	TYR	2.3
2	Bh	2014	GLU	2.3
2	BJ	2022	LEU	2.3
4	Cr	4029	SER	2.3
6	At	8138	THR	2.3
6	Bd	8032	THR	2.3
7	Ae	6072	ILE	2.3
8	AP	5026	LEU	2.3
8	AX	5012	LEU	2.3
4	Br	4065	TYR	2.3
4	CD	4040	ASN	2.3
2	BB	2066	MET	2.3
2	Cp	2016	GLU	2.3
3	BK	3030	GLU	2.3
3	CK	3027	MET	2.3
2	BJ	2074	LYS	2.3
4	AT	4001	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
7	Cm	6002	LEU	2.3
6	BF	8021	VAL	2.3
7	Cm	6040	THR	2.3
6	Ad	8005	GLU	2.3
7	Bm	6071	CYS	2.3
1	BI	1056	LEU	2.3
6	Bt	8028	ILE	2.3
6	AN	8002	SER	2.3
2	BB	2018	ASN	2.3
3	BS	3020	TRP	2.3
6	CF	8005	GLU	2.3
2	BR	2004	MET	2.3
8	Af	5062	ILE	2.3
4	CD	4055	GLU	2.3
4	BL	4037	GLN	2.3
2	Bh	2094	ASN	2.3
2	CB	2094	ASN	2.3
4	CD	4068	GLY	2.3
2	Cp	2092	LEU	2.3
4	Cb	4005	LEU	2.3
7	BO	6041	LEU	2.3
8	CH	5057	ILE	2.3
2	Ap	2000	PRO	2.3
8	CP	5010	LYS	2.3
3	Aq	3012	GLN	2.3
2	Ah	2017	PHE	2.3
5	Bs	7010	THR	2.3
6	Bd	8138	THR	2.3
7	Cm	6046	THR	2.3
7	Cm	6060	SER	2.3
2	CJ	2025	LEU	2.3
2	CJ	2046	LEU	2.3
3	Ai	3005	ASN	2.3
8	BX	5051	ASN	2.3
3	Bq	3058	LYS	2.3
4	Br	4002	LYS	2.3
6	B2	8027	LYS	2.3
1	CI	1011	GLU	2.3
3	Aq	3045	ASP	2.3
2	BB	2077	TYR	2.3
4	Br	4033	TYR	2.3
3	Bi	3035	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
6	AF	8138	THR	2.3
8	AX	5052	ILE	2.3
4	Cj	4002	LYS	2.3
6	Bd	8027	LYS	2.3
2	CB	2013	GLU	2.3
7	BO	6140	GLU	2.3
1	BI	1004	PHE	2.3
4	Bj	4004	PHE	2.3
3	CS	3075	SER	2.3
6	BN	8131	TRP	2.3
7	Cu	6060	SER	2.3
5	Ac	7000	ALA	2.2
6	AF	8024	ARG	2.2
6	Bl	8019	ALA	2.2
2	Ch	2069	GLU	2.2
8	An	5026	LEU	2.2
4	AT	4034	MET	2.2
4	BT	4036	MET	2.2
7	BO	6020	ILE	2.2
8	Af	5021	HIS	2.2
8	Av	5057	ILE	2.2
8	Cv	5021	HIS	2.2
5	CU	7002	TRP	2.2
2	BB	2013	GLU	2.2
3	Bi	3005	ASN	2.2
2	CB	2099	GLY	2.2
4	BT	4033	TYR	2.2
6	AF	8012	TYR	2.2
7	Cm	6086	TYR	2.2
1	BA	1002	VAL	2.2
4	CL	4028	VAL	2.2
8	BP	5011	LYS	2.2
2	CZ	2017	PHE	2.2
3	CC	3035	GLY	2.2
7	Bm	6084	GLY	2.2
8	Bv	5029	PHE	2.2
3	Aa	3045	ASP	2.2
3	CK	3018	GLN	2.2
6	CN	8028	ILE	2.2
7	BG	6001	VAL	2.2
7	CO	6161	ASP	2.2
8	BX	5057	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
7	BO	6056	TRP	2.2
7	Ae	6053	SER	2.2
3	Aa	3042	LEU	2.2
4	Ar	4027	LEU	2.2
4	CL	4023	TYR	2.2
7	Ae	6014	LEU	2.2
3	CK	3034	ILE	2.2
6	Al	8008	MET	2.2
6	BN	8072	VAL	2.2
6	CN	8020	VAL	2.2
8	Bv	5049	GLN	2.2
2	Ax	2007	GLU	2.2
3	By	3016	ARG	2.2
6	BF	8211	PHE	2.2
6	Bt	8141	LEU	2.2
7	Ae	6007	SER	2.2
3	CC	3010	TYR	2.2
4	Ar	4026	TYR	2.2
3	Bq	3046	ASP	2.2
7	BO	6017	ALA	2.2
8	AX	5042	GLU	2.2
3	Ay	3028	ARG	2.2
3	Ci	3044	LEU	2.2
4	Br	4027	LEU	2.2
6	CN	8007	LEU	2.2
7	BO	6063	GLY	2.2
7	Bm	6063	GLY	2.2
2	BJ	2089	ILE	2.2
2	BR	2005	THR	2.2
3	Ci	3071	THR	2.2
3	Cq	3063	ILE	2.2
5	Ak	7001	VAL	2.2
6	Al	8032	THR	2.2
6	B2	8032	THR	2.2
6	CF	8006	TYR	2.2
7	Cu	6147	THR	2.2
1	BI	1043	MET	2.2
2	BR	2014	GLU	2.2
6	BN	8081	ASN	2.2
7	Cu	6063	GLY	2.2
1	Ao	1081	VAL	2.2
1	BA	1057	SER	2.2

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Mol	Chain	Res	Type	RSRZ
4	BL	4070	GLU	2.2
6	AV	8138	THR	2.2
2	CJ	2048	ARG	2.2
3	AS	3002	GLN	2.2
6	A2	8018	PRO	2.2
3	Ay	3036	PHE	2.2
1	BI	1029	GLY	2.2
6	Bt	8051	LEU	2.2
8	CP	5035	LEU	2.2
4	BL	4011	LYS	2.2
2	AZ	2002	SER	2.2
2	Ap	2002	SER	2.2
2	BB	2014	GLU	2.2
2	Bp	2003	GLU	2.2
8	Af	5027	ARG	2.2
8	Cn	5039	GLU	2.2
8	An	5001	PRO	2.2
2	Bx	2025	LEU	2.2
3	Ai	3036	PHE	2.2
3	Aq	3042	LEU	2.2
3	CC	3045	ASP	2.2
3	Cq	3011	LEU	2.2
6	Ct	8170	LEU	2.2
8	CX	5028	GLY	2.2
8	Cv	5018	GLY	2.2
5	BE	7015	VAL	2.2
6	CN	8203	VAL	2.2
2	CZ	2003	GLU	2.2
7	Cm	6134	GLU	2.2
8	CP	5040	CYS	2.2
7	Am	6000	MET	2.2
1	Co	1055	THR	2.2
2	BZ	2005	THR	2.2
6	BN	8091	PRO	2.2
7	BO	6147	THR	2.2
7	Bm	6144	THR	2.2
3	CC	3072	LEU	2.2
8	Cv	5016	LEU	2.2
1	BA	1029	GLY	2.2
8	Af	5030	ASP	2.2
4	Aj	4056	VAL	2.2
2	CJ	2008	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	AC	3050	ILE	2.2
3	CK	3020	TRP	2.2
2	BJ	2001	LYS	2.2
2	CB	2004	MET	2.2
2	CB	2030	LYS	2.2
1	AY	1055	THR	2.2
3	BS	3006	LEU	2.2
8	BX	5013	SER	2.2
3	By	3013	ASN	2.2
7	Cm	6045	PRO	2.2
3	Aa	3019	VAL	2.2
3	Ai	3030	GLU	2.1
3	BK	3043	VAL	2.2
8	Bv	5038	ASP	2.2
8	Cv	5058	ARG	2.2
3	BS	3029	ILE	2.2
4	CD	4042	GLU	2.1
2	CZ	2004	MET	2.1
8	CX	5004	LEU	2.1
3	AS	3003	PRO	2.1
7	Bm	6147	THR	2.1
2	BJ	2029	VAL	2.1
2	CJ	2003	GLU	2.1
2	Cp	2097	ILE	2.1
4	AT	4030	VAL	2.1
3	AS	3045	ASP	2.1
3	BK	3051	HIS	2.1
6	BV	8034	ASN	2.1
8	AX	5022	VAL	2.1
3	AC	3010	TYR	2.1
3	AK	3044	LEU	2.1
4	Ab	4027	LEU	2.1
4	CD	4027	LEU	2.1
6	CN	8207	ALA	2.1
2	CJ	2028	SER	2.1
3	Aa	3015	SER	2.1
1	Co	1036	THR	2.1
2	AR	2013	GLU	2.1
2	AZ	2013	GLU	2.1
4	BD	4061	ASN	2.1
6	AN	8017	CYS	2.1
7	Ae	6133	THR	2.1

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Mol	Chain	Res	Type	RSRZ
7	CO	6001	VAL	2.1
5	CM	7012	ASP	2.1
6	Bl	8034	ASN	2.1
2	Bx	2017	PHE	2.1
3	Aa	3062	ARG	2.1
3	Ca	3006	LEU	2.1
4	BT	4053	LEU	2.1
3	Ca	3018	GLN	2.1
2	BB	2091	VAL	2.1
2	CZ	2008	GLU	2.1
2	Cp	2003	GLU	2.1
3	CC	3017	ILE	2.1
4	BT	4058	ILE	2.1
7	BO	6080	VAL	2.1
7	Cu	6001	VAL	2.1
8	B4	5025	ILE	2.1
1	CI	1036	THR	2.1
2	Ah	2018	ASN	2.1
2	BJ	2073	ASN	2.1
6	BF	8017	CYS	2.1
6	BF	8157	CYS	2.1
6	Bt	8031	ASN	2.1
6	Ct	8143	HIS	2.1
7	Ae	6083	ASN	2.1
1	Co	1056	LEU	2.1
2	Ap	2004	MET	2.1
3	Aa	3027	MET	2.1
7	Ae	6082	TRP	2.1
8	Av	5004	LEU	2.1
3	Ci	3035	GLY	2.1
2	BJ	2091	VAL	2.1
3	Ba	3049	GLU	2.1
1	BI	1055	THR	2.1
4	Bb	4005	LEU	2.1
7	BO	6088	ASP	2.1
3	Aa	3055	LYS	2.1
7	Ae	6056	TRP	2.1
7	Cu	6027	LYS	2.1
8	CX	5008	MET	2.1
2	BB	2061	GLU	2.1
4	CL	4070	GLU	2.1
6	Ct	8001	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	Aq	3029	ILE	2.1
1	Co	1028	THR	2.1
2	BJ	2046	LEU	2.1
2	BJ	2092	LEU	2.1
3	Aa	3039	TYR	2.1
3	Cq	3039	TYR	2.1
4	Br	4026	TYR	2.1
1	Co	1080	ASP	2.1
4	CL	4034	MET	2.1
7	CO	6027	LYS	2.1
8	B4	5017	ASN	2.1
2	Ah	2099	GLY	2.1
2	CJ	2091	VAL	2.1
3	By	3012	GLN	2.1
2	CR	2097	ILE	2.1
2	Bp	2095	PRO	2.1
3	By	3055	LYS	2.1
4	AT	4012	PRO	2.1
6	Ct	8135	PRO	2.1
4	Ab	4026	TYR	2.1
7	BO	6073	TYR	2.1
2	CJ	2066	MET	2.1
7	Cm	6042	SER	2.1
7	Cm	6133	THR	2.1
2	Ax	2016	GLU	2.1
2	Bp	2007	GLU	2.1
3	Bq	3018	GLN	2.1
3	CS	3001	VAL	2.1
4	BT	4055	GLU	2.1
6	B2	8001	GLU	2.1
8	Av	5022	VAL	2.1
7	BO	6071	CYS	2.1
8	A4	5006	LYS	2.1
3	AC	3036	PHE	2.1
3	Cq	3021	LEU	2.1
4	AL	4005	LEU	2.1
6	Bl	8026	SER	2.1
2	Cp	2042	ASN	2.1
4	BD	4067	ARG	2.1
3	AK	3033	ILE	2.1
3	Ba	3002	GLN	2.1
7	Bm	6133	THR	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	By	3050	ILE	2.1
8	BP	5051	ASN	2.1
3	BC	3072	LEU	2.1
6	BF	8141	LEU	2.1
6	CN	8047	PRO	2.1
3	Aa	3016	ARG	2.1
7	CW	6000	MET	2.1
2	CR	2001	LYS	2.1
3	Cq	3025	VAL	2.1
4	CL	4018	LYS	2.1
7	Bm	6165	SER	2.1
2	BJ	2018	ASN	2.1
6	BN	8125	LEU	2.1
6	Ct	8198	LEU	2.1
3	CC	3009	ARG	2.1
6	A2	8006	TYR	2.1
8	Bf	5027	ARG	2.1
2	Bh	2011	LYS	2.1
3	BC	3032	CYS	2.1
5	Cs	7008	VAL	2.1
6	At	8015	LYS	2.1
8	Cf	5003	GLU	2.1
4	Br	4058	ILE	2.1
1	CI	1012	THR	2.1
6	Bt	8052	LEU	2.1
6	Cl	8136	ASN	2.1
2	CJ	2001	LYS	2.1
7	Ae	6073	TYR	2.1
2	Cp	2071	PRO	2.1
3	AS	3040	MET	2.1
8	Cv	5010	LYS	2.1
3	AC	3018	GLN	2.0
3	Ca	3074	GLN	2.0
7	BG	6155	CYS	2.0
7	Cu	6071	CYS	2.0
1	BA	1055	THR	2.0
7	BO	6137	LEU	2.0
7	Cm	6043	TRP	2.0
2	Ap	2007	GLU	2.0
6	A2	8012	TYR	2.0
1	BI	1002	VAL	2.0
2	CZ	2098	ALA	2.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	BC	3000	MET	2.0
7	CO	6130	GLY	2.0
8	BP	5047	GLY	2.0
5	A1	7000	ALA	2.0
7	Am	6163	ALA	2.0
8	Cn	5022	VAL	2.0
3	CS	3036	PHE	2.0
4	BD	4057	LEU	2.0
8	BH	5061	SER	2.0
8	CH	5020	ARG	2.0
8	CP	5029	PHE	2.0
4	BT	4031	ASP	2.0
2	Bh	2033	THR	2.0
5	AM	7002	TRP	2.0
7	Ae	6043	TRP	2.0
8	Bn	5006	LYS	2.0
4	CL	4010	GLY	2.0
7	BO	6030	GLY	2.0
1	BI	1034	MET	2.0
2	BR	2029	VAL	2.0
3	AC	3000	MET	2.0
3	AC	3001	VAL	2.0
6	CV	8010	MET	2.0
8	CH	5008	MET	2.0
2	CJ	2055	HIS	2.0
3	CK	3050	ILE	2.0
3	Aq	3072	LEU	2.0
6	CN	8211	PHE	2.0
7	Ae	6002	LEU	2.0
7	Bm	6074	PHE	2.0
8	AX	5065	LEU	2.0
8	B4	5006	LYS	2.0
8	B4	5046	SER	2.0
6	CN	8031	ASN	2.0
6	CV	8017	CYS	2.0
7	Ae	6063	GLY	2.0
2	BJ	2024	VAL	2.0
6	AF	8028	ILE	2.0
8	Bf	5054	MET	2.0
1	BI	1010	HIS	2.0
4	CL	4008	LEU	2.0
8	Bf	5021	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
3	Aq	3049	GLU	2.0
4	CL	4042	GLU	2.0
6	CV	8005	GLU	2.0
6	Bt	8026	SER	2.0
3	AS	3019	VAL	2.0
6	Ct	8144	ASP	2.0
2	BJ	2050	LYS	2.0
3	Aq	3071	THR	2.0
3	Bi	3040	MET	2.0
3	Ci	3033	ILE	2.0
4	BD	4058	ILE	2.0
7	Ae	6027	LYS	2.0
2	CB	2092	LEU	2.0
4	BL	4053	LEU	2.0
6	BF	8167	PHE	2.0
6	BN	8194	PRO	2.0
7	Cm	6024	LEU	2.0
2	BZ	2010	GLN	2.0
3	CS	3018	GLN	2.0
2	CJ	2085	GLY	2.0
2	AZ	2011	LYS	2.0
3	Aq	3019	VAL	2.0
7	Ae	6035	TYR	2.0
8	BX	5061	SER	2.0
1	Co	1012	THR	2.0
6	Cd	8028	ILE	2.0
8	AH	5037	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.



The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	SO4	Bt	8301	5/5	0.93	0.20	-0.19	111,113,114,115	0
9	SO4	Cl	8301	5/5	0.76	0.25	-0.27	129,131,132,132	0
9	SO4	Ad	8301	5/5	0.72	0.27	-0.28	137,139,139,140	0
9	SO4	BF	8301	5/5	0.86	0.21	-0.63	129,129,130,131	0
9	SO4	B2	8301	5/5	0.95	0.17	-1.04	97,99,99,103	0
9	SO4	A2	8301	5/5	0.85	0.16	-1.11	150,150,150,151	0
9	SO4	At	8301	5/5	0.89	0.17	-1.29	92,93,96,99	0
9	SO4	BV	8301	5/5	0.90	0.14	-1.42	111,113,114,116	0
9	SO4	CF	8301	5/5	0.94	0.14	-1.47	100,103,104,106	0
9	SO4	Bd	8301	5/5	0.94	0.12	-1.59	108,108,109,112	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.