



# Full wwPDB X-ray Structure Validation Report

Jun 16, 2014 – 06:44 PM BST

PDB ID : 4V98  
Title : The 8S snRNP Assembly Intermediate  
Authors : Grimm, C.; Pelz, J.P.; Schindelin, H.; Diederichs, K.; Kuper, J.; Kisker, C.  
Deposited on : 2012-05-15  
Resolution : 3.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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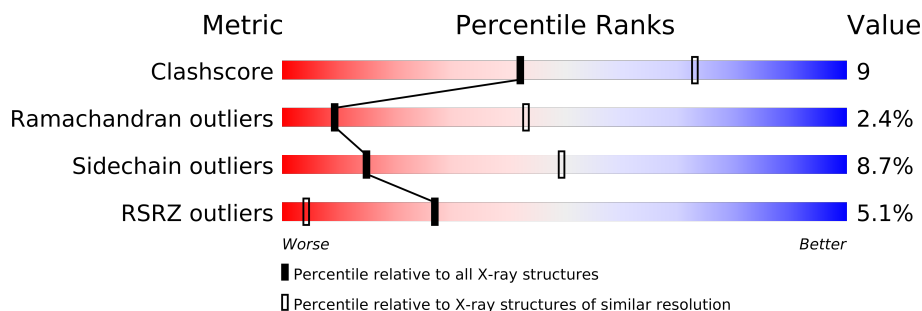
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397

# 1 Overall quality at a glance

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))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	119	
1	AI	119	
1	AQ	119	
1	AY	119	
1	Ag	119	
1	Ao	119	
1	Aw	119	
1	BA	119	
1	BI	119	
1	BQ	119	
1	BY	119	
1	Bg	119	
1	Bo	119	
1	Bw	119	
1	CA	119	
1	CI	119	

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Mol	Chain	Length	Quality of chain
1	CQ	119	
1	CY	119	
1	Cg	119	
1	Co	119	
2	AB	118	
2	AJ	118	
2	AR	118	
2	AZ	118	
2	Ah	118	
2	Ap	118	
2	Ax	118	
2	BB	118	
2	BJ	118	
2	BR	118	
2	BZ	118	
2	Bh	118	
2	Bp	118	
2	Bx	118	
2	CB	118	
2	CJ	118	
2	CR	118	
2	CZ	118	
2	Ch	118	
2	Cp	118	
3	AC	92	
3	AK	92	
3	AS	92	
3	Aa	92	
3	Ai	92	
3	Aq	92	
3	Ay	92	
3	BC	92	
3	BK	92	
3	BS	92	
3	Ba	92	
3	Bi	92	
3	Bq	92	
3	By	92	
3	CC	92	
3	CK	92	
3	CS	92	
3	Ca	92	

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










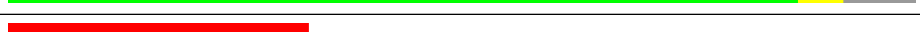

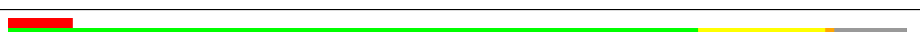


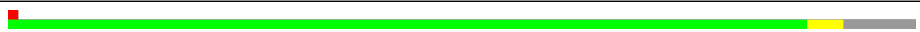



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Mol	Chain	Length	Quality of chain
6	A2	247	
6	AF	247	
6	AN	247	
6	AV	247	
6	Ad	247	
6	Al	247	
6	At	247	
6	B2	247	
6	BF	247	
6	BN	247	
6	BV	247	
6	Bd	247	
6	Bl	247	
6	Bt	247	
6	CF	247	
6	CN	247	
6	CV	247	
6	Cd	247	
6	Cl	247	
6	Ct	247	
7	A3	186	
7	AG	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	
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	

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Mol	Chain	Length	Quality of chain
8	AP	76	
8	AX	76	
8	Af	76	
8	An	76	
8	Av	76	
8	B4	76	
8	BH	76	
8	BP	76	
8	BX	76	
8	Bf	76	
8	Bn	76	
8	Bv	76	
8	CH	76	
8	CP	76	
8	CX	76	
8	Cf	76	
8	Cn	76	
8	Cv	76	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 121990 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 5 is a protein called LD23602p.

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Bs	17	Total 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 Q9V VX0
AN	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
AF	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
AF	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
AV	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
AV	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
Ad	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
Ad	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
Al	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
Al	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
At	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
At	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
A2	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
A2	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
BF	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
BF	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
BN	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
BN	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
BV	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0
BV	7970	ALA	-	EXPRESSION TAG	UNP Q9V VX0
Bd	7969	GLY	-	EXPRESSION TAG	UNP Q9V VX0

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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: SO<sub>4</sub>) (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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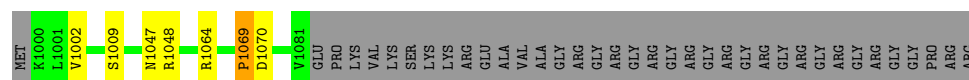
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A2	1	Total	O	S	0	0
			5	4	1		
9	BF	1	Total	O	S	0	0
			5	4	1		
9	BV	1	Total	O	S	0	0
			5	4	1		
9	Bd	1	Total	O	S	0	0
			5	4	1		
9	Bt	1	Total	O	S	0	0
			5	4	1		
9	B2	1	Total	O	S	0	0
			5	4	1		
9	CF	1	Total	O	S	0	0
			5	4	1		
9	Cl	1	Total	O	S	0	0
			5	4	1		

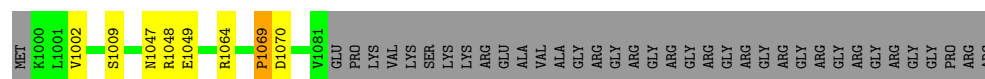




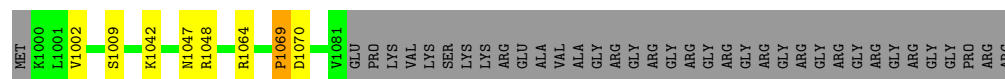
- Chain Bg:



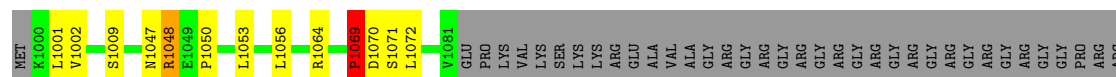
- Chain Bo: 



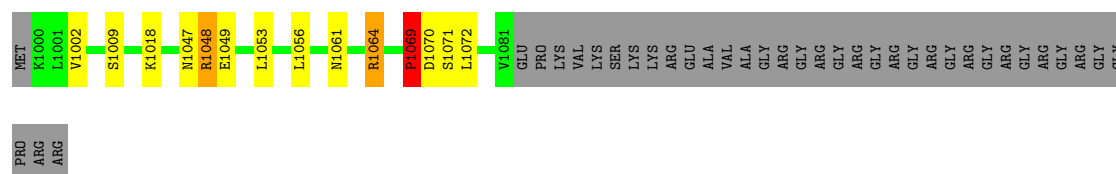
- Chain Bw: 



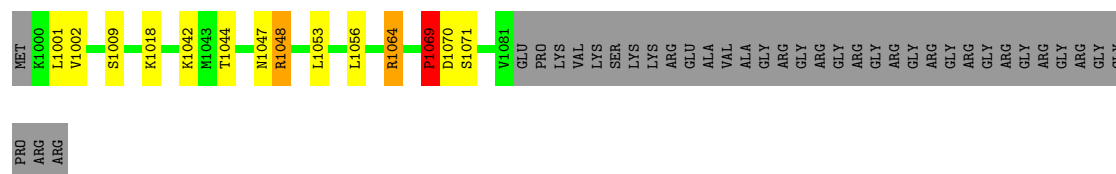
- Chain CA: 



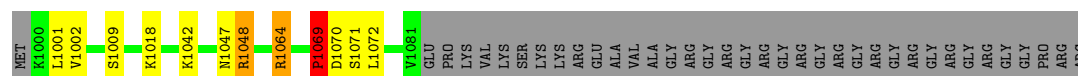
- Chain CI: 



- Chain CQ: 



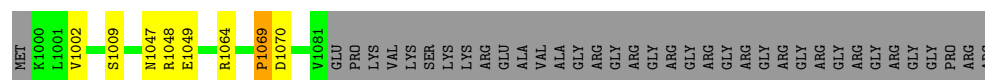
- Chain CY: 





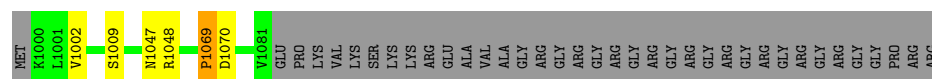
- Molecule 1: Small nuclear ribonucleoprotein Sm D1

Chain Cg: 



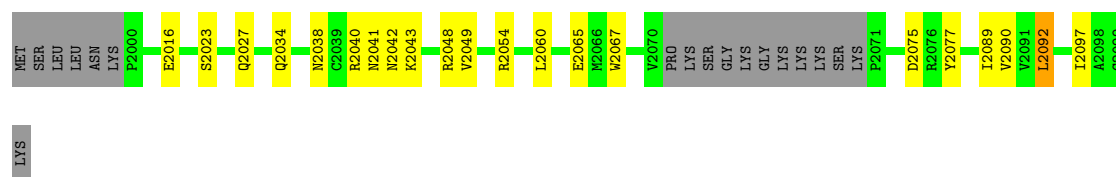
- Molecule 1: Small nuclear ribonucleoprotein Sm D1

Chain Co: 



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain AJ: 



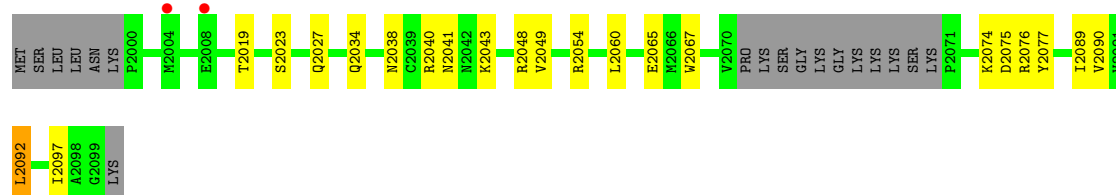
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain AB: 



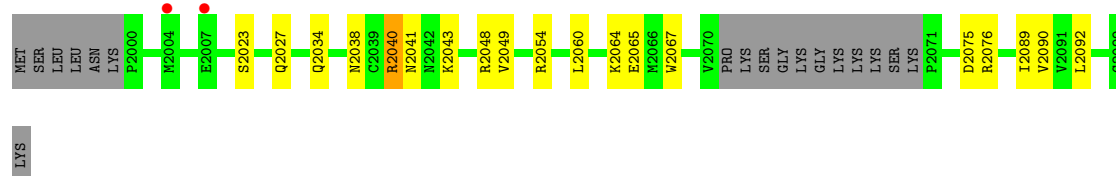
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain AR: 



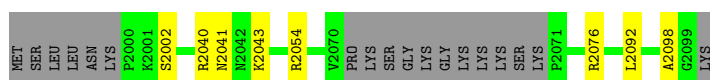
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain AZ: 



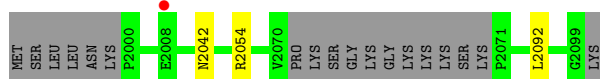
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Ah: 



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Ap:



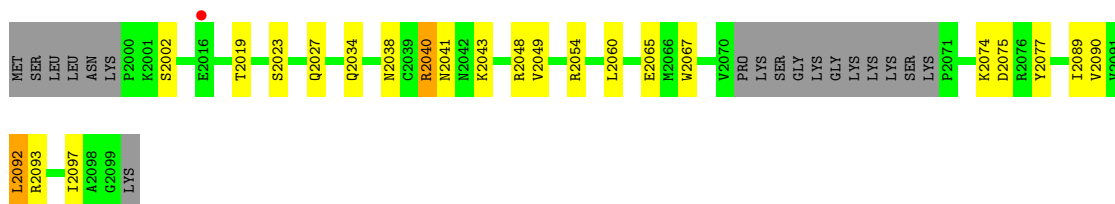
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Ax:



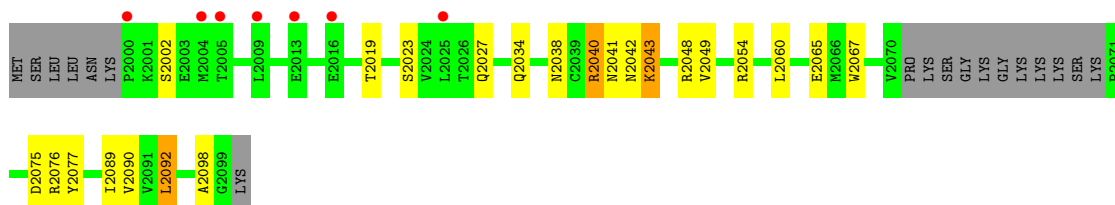
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain BB:



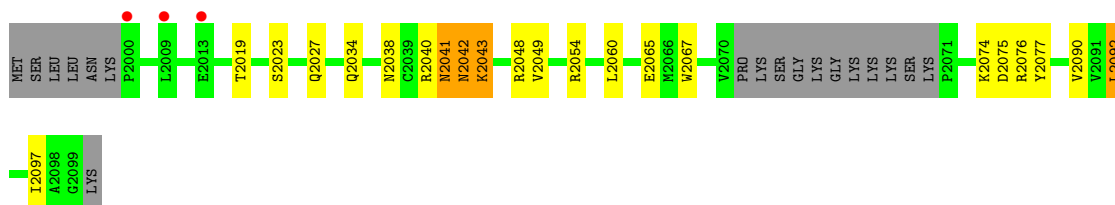
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain BJ:



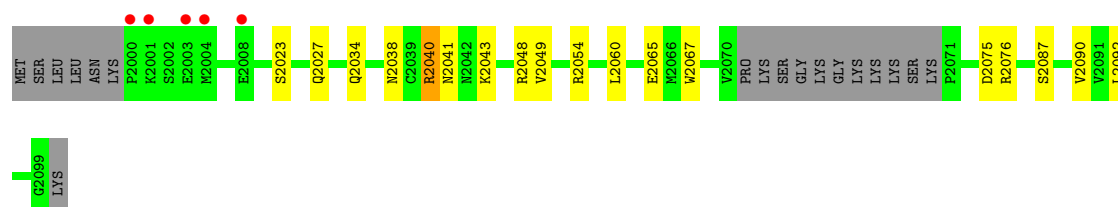
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain BR:



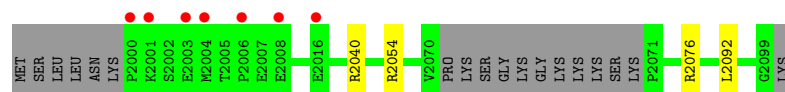
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain BZ:



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Bh:



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Bp:



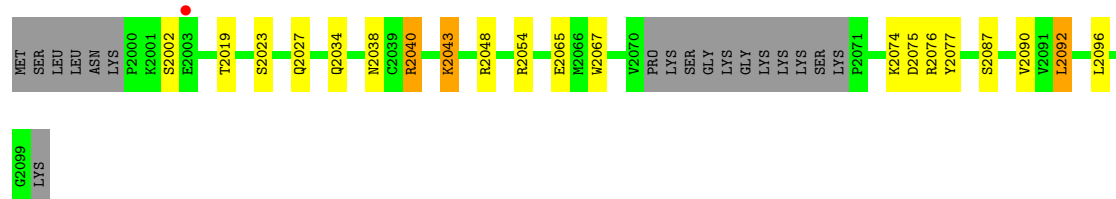
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Bx:



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain CB:



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain CJ:



- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain CR:



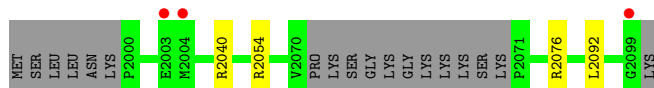
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain CZ: 



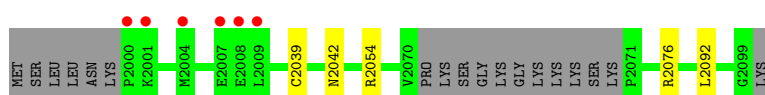
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Ch: 



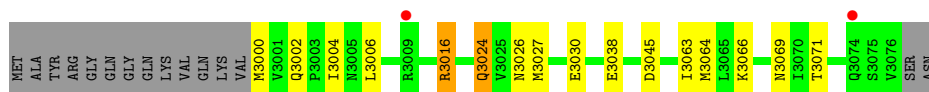
- Molecule 2: Small nuclear ribonucleoprotein Sm D2

Chain Cp: 



- Molecule 3: Small nuclear ribonucleoprotein E

Chain AK: 



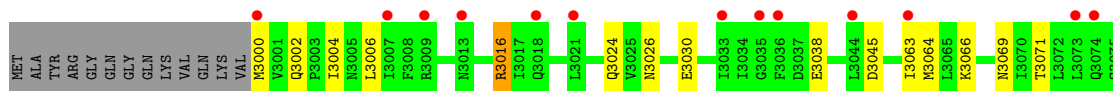
- Molecule 3: Small nuclear ribonucleoprotein E

Chain AC: 



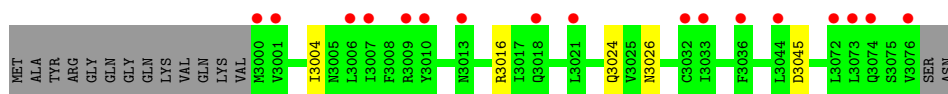
- Molecule 3: Small nuclear ribonucleoprotein E

Chain AS: 



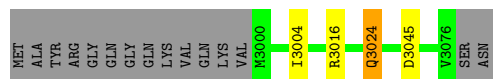
- Molecule 3: Small nuclear ribonucleoprotein E

Chain Aa: 



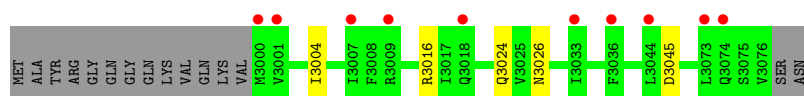
- Molecule 3: Small nuclear ribonucleoprotein E

Chain Ai:



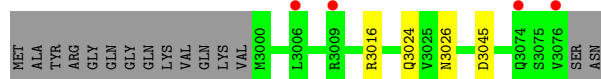
- Molecule 3: Small nuclear ribonucleoprotein E

Chain Aq:



- Molecule 3: Small nuclear ribonucleoprotein E

Chain Ay:



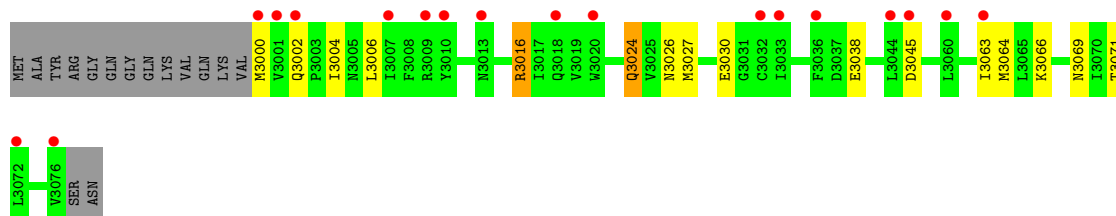
- Molecule 3: Small nuclear ribonucleoprotein E

Chain BC:



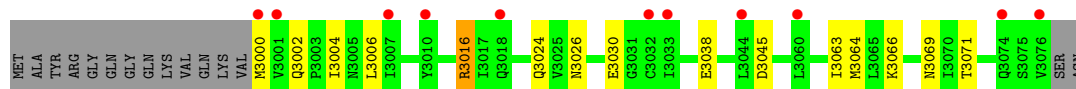
- Molecule 3: Small nuclear ribonucleoprotein E

Chain BK:



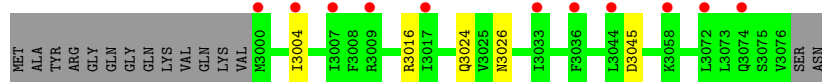
- Molecule 3: Small nuclear ribonucleoprotein E

Chain BS:



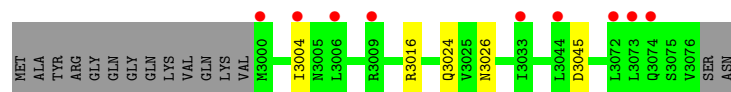
- Molecule 3: Small nuclear ribonucleoprotein E

Chain Ba:



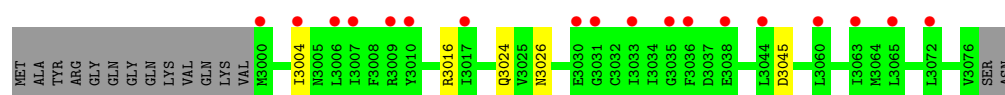
- Molecule 3: Small nuclear ribonucleoprotein E

Chain Bi:



- Molecule 3: Small nuclear ribonucleoprotein E

Chain Bq:



- Molecule 3: Small nuclear ribonucleoprotein E

Chain By:



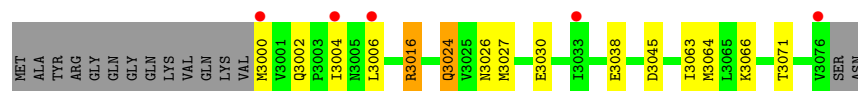
- Molecule 3: Small nuclear ribonucleoprotein E

Chain CC:



- Molecule 3: Small nuclear ribonucleoprotein E

Chain CK:



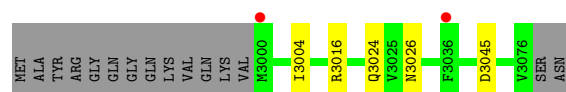
- Molecule 3: Small nuclear ribonucleoprotein E

Chain CS:



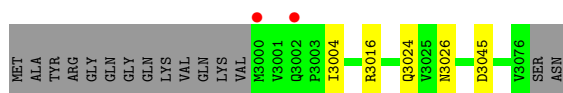
- Molecule 3: Small nuclear ribonucleoprotein E

Chain Ca:



- Molecule 3: Small nuclear ribonucleoprotein E

Chain Ci:



- Molecule 3: Small nuclear ribonucleoprotein E

Chain Cq:



- Molecule 4: Small nuclear ribonucleoprotein F

Chain AL:



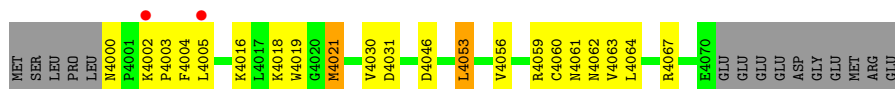
- Molecule 4: Small nuclear ribonucleoprotein F

Chain AD:



- Molecule 4: Small nuclear ribonucleoprotein F

Chain AT: 



- Molecule 4: Small nuclear ribonucleoprotein F

Chain Ab: 



- Molecule 4: Small nuclear ribonucleoprotein F

Chain Aj: 



- Molecule 4: Small nuclear ribonucleoprotein F

Chain Ar: 



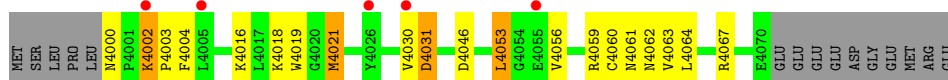
- Molecule 4: Small nuclear ribonucleoprotein F

Chain Az: 



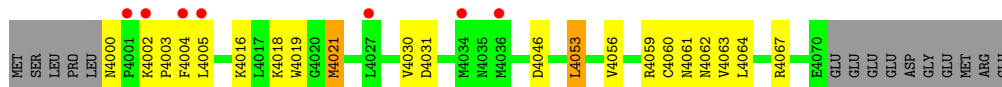
- Molecule 4: Small nuclear ribonucleoprotein F

Chain BD: 



- Molecule 4: Small nuclear ribonucleoprotein F

Chain BL: 



- Molecule 4: Small nuclear ribonucleoprotein F

Chain BT: 



- Molecule 4: Small nuclear ribonucleoprotein F

Chain Bb: 



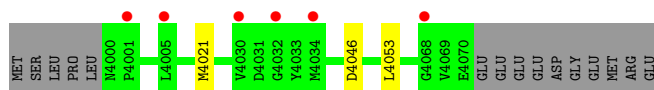
- Molecule 4: Small nuclear ribonucleoprotein F

Chain Bj: 



- Molecule 4: Small nuclear ribonucleoprotein F

Chain Br: 



- Molecule 4: Small nuclear ribonucleoprotein F

Chain Bz: 





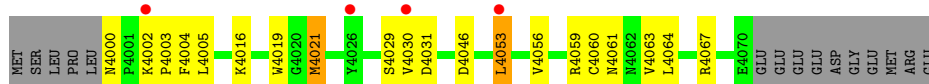
- Molecule 4: Small nuclear ribonucleoprotein F

Chain CD:



- Molecule 4: Small nuclear ribonucleoprotein F

Chain CL:



- Molecule 4: Small nuclear ribonucleoprotein F

Chain CT:



- Molecule 4: Small nuclear ribonucleoprotein F

Chain Cb:



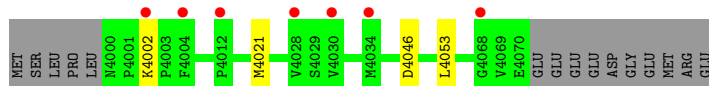
- Molecule 4: Small nuclear ribonucleoprotein F

Chain Cj:



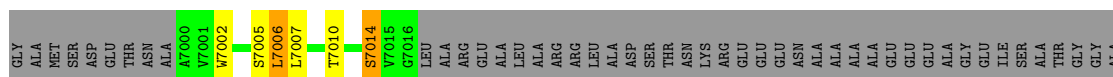
- Molecule 4: Small nuclear ribonucleoprotein F

Chain Cr:



- Molecule 5: LD23602p

Chain AM:



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


- Molecule 5: LD23602p

Chain AE: 

GLY ALA MET SER ASP GLU THR ASN ALA A7000 V7001 W7002 D7003 D7004 S7005 L7006 L7007 G7016 LEU ALA ARG GLU ARG ALA LEU ALA VAL VAL ASP SER THR ASN LYS ARG GLU ARG GLU TYR ASN GLY ALA ALA ASN GLU GLN GLU VAL ALA GLY ILE SER THR GLY ALA THR ASP LEU PRO SER TRP

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

- Molecule 5: LD23602p

Chain AU: 

GLY ALA MET SER ASP GLU THR ASN ALA A7000 V7001 W7002 D7003 D7004 S7005 L7006 L7007 G7016 LEU ALA ARG GLU ARG ALA LEU ALA VAL VAL ASP SER THR ASN LYS ARG GLU ARG GLU TYR ASN GLY ALA ALA ASN GLU GLN GLU VAL ALA GLY ILE SER THR GLY ALA THR ASP LEU PRO SER TRP

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

- Molecule 5: LD23602p

Chain Ac: 

GLY ALA MET SER ASP GLU THR ASN ALA A7000 V7001 W7002 L7006 L7007 G7016 LEU ALA ARG GLU ARG ALA LEU ALA VAL VAL ASP SER THR ASN LYS ARG GLU ARG GLU TYR ASN GLY ALA ALA ASN GLU GLN GLU VAL ALA GLY ILE SER THR GLY ALA THR ASP LEU PRO SER TRP

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

- Molecule 5: LD23602p

Chain Ak: 

GLY ALA MET SER ASP GLU THR ASN ALA A7000 V7001 W7002 L7006 L7007 G7016 LEU ALA ARG GLU ARG ALA LEU ALA VAL VAL ASP SER THR ASN LYS ARG GLU ARG GLU TYR ASN GLY ALA ALA ASN GLU GLN GLU VAL ALA GLY ILE SER THR GLY ALA THR ASP LEU PRO SER TRP

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

- Molecule 5: LD23602p

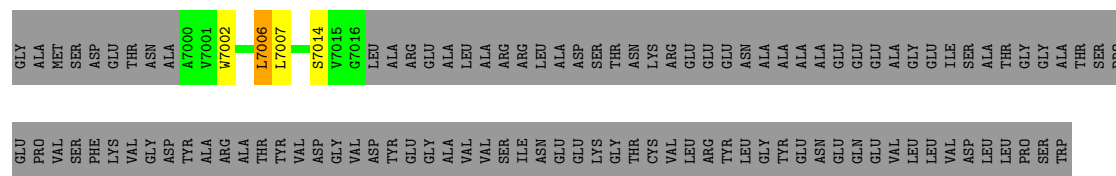
Chain As: 

GLY ALA MET SER ASP GLU THR ASN ALA A7000 V7001 W7002 L7006 L7007 G7016 LEU ALA ARG GLU ARG ALA LEU ALA VAL VAL ASP SER THR ASN LYS ARG GLU ARG GLU TYR ASN GLY ALA ALA ASN GLU GLN GLU VAL ALA GLY ILE SER THR GLY ALA THR ASP LEU PRO SER TRP

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

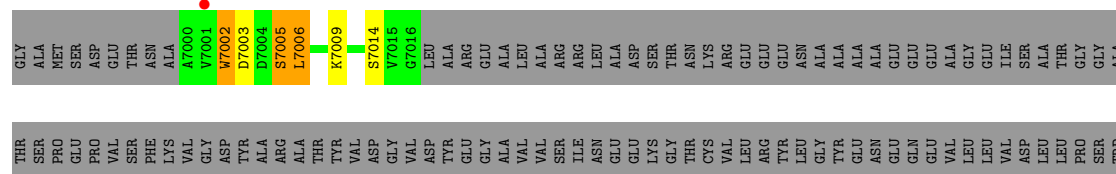
- Molecule 5: LD23602p

Chain A1:



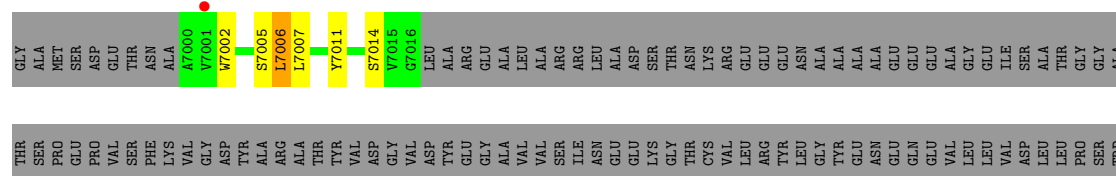
• Molecule 5: LD23602p

Chain BE:



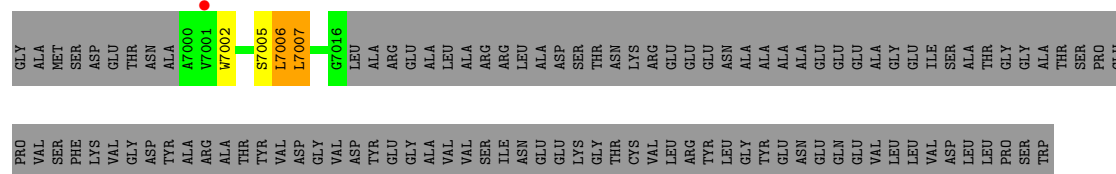
• Molecule 5: LD23602p

Chain BM:



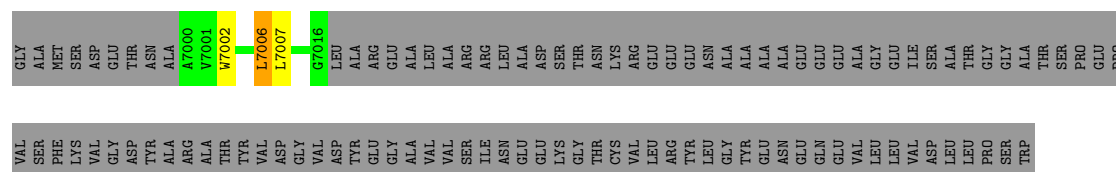
• Molecule 5: LD23602p

Chain BU:



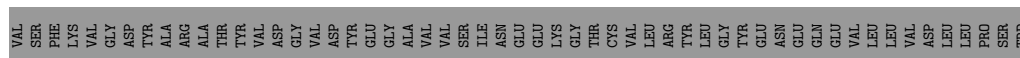
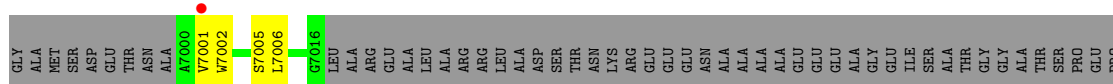
• Molecule 5: LD23602p

Chain Bc:



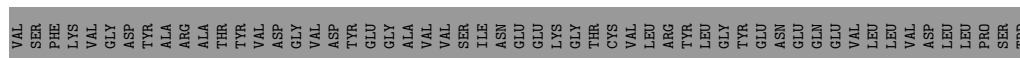
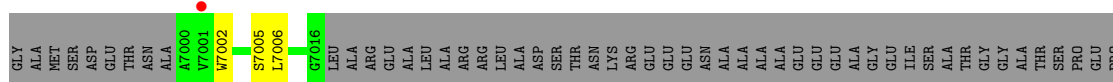
• Molecule 5: LD23602p

Chain Bk:



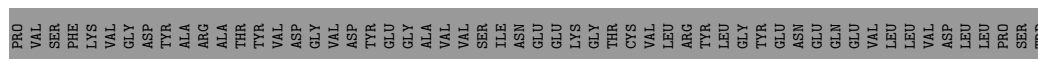
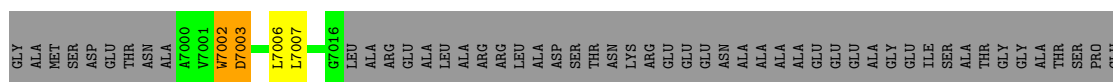
• Molecule 5: LD23602p

Chain Bs:



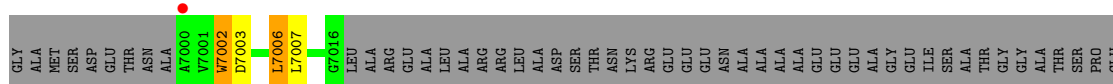
• Molecule 5: LD23602p

Chain B1:



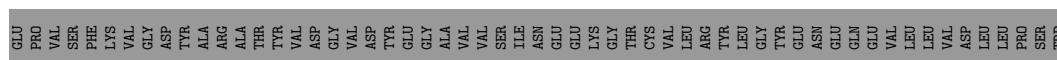
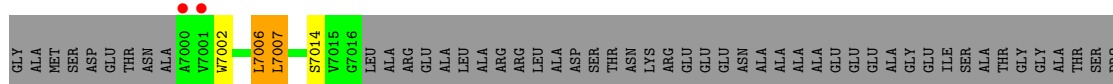
• Molecule 5: LD23602p

Chain CE:



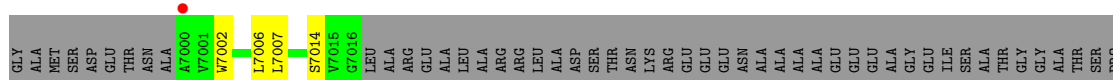
• Molecule 5: LD23602p

Chain CM:

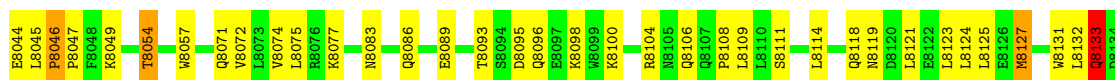


• Molecule 5: LD23602p

Chain CU:

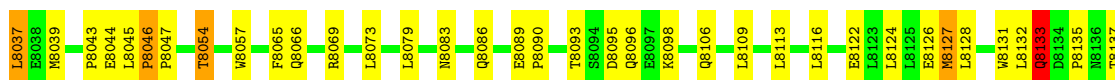
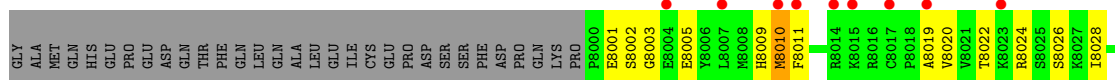






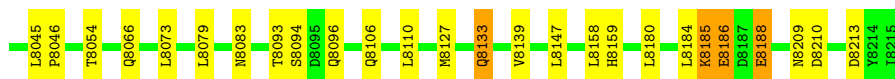
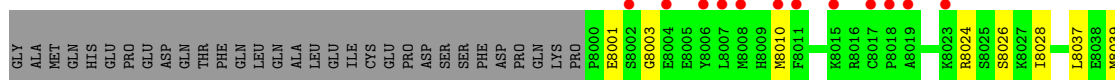
• Molecule 6: CG10419

Chain AV:



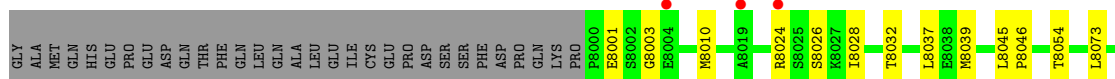
• Molecule 6: CG10419

Chain Ad:



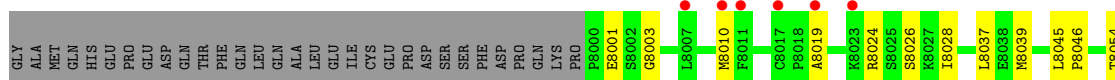
• Molecule 6: CG10419

Chain Al:



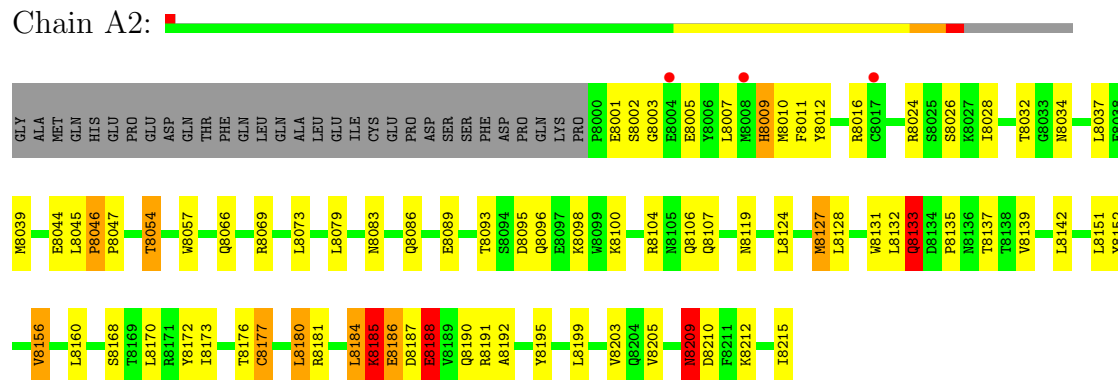
• Molecule 6: CG10419

Chain At:



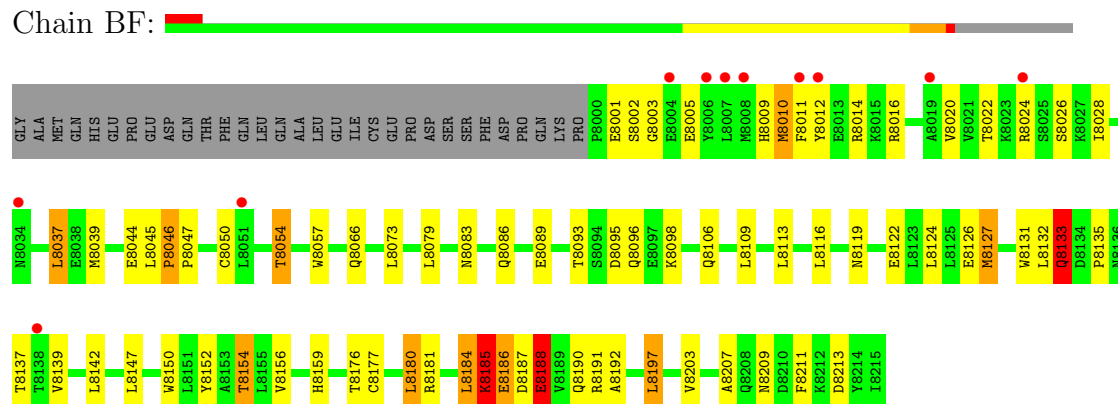
• Molecule 6: CG10419

## Chain A2:



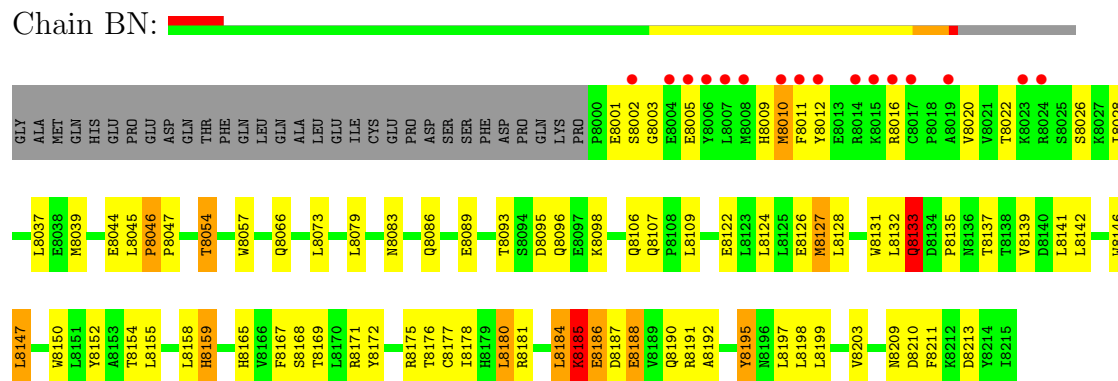
## • Molecule 6: CG10419

## Chain BF:



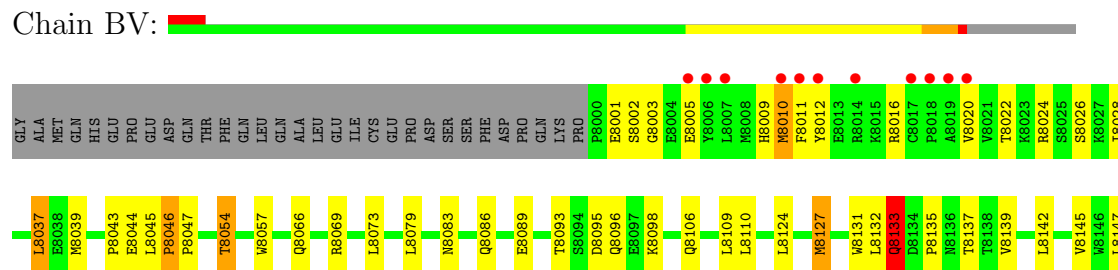
## • Molecule 6: CG10419

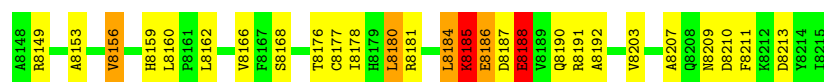
## Chain BN:



## • Molecule 6: CG10419

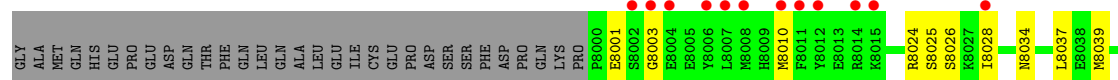
## Chain BV:





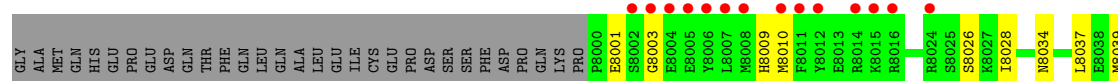
• Molecule 6: CG10419

Chain Bd:



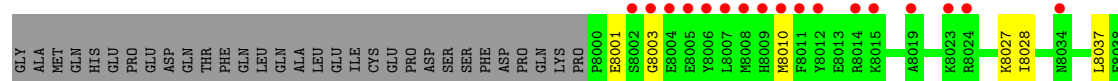
• Molecule 6: CG10419

Chain Bl:



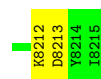
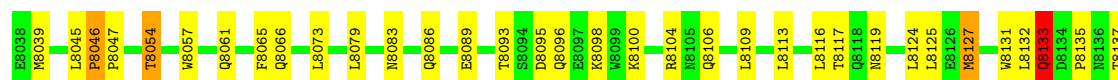
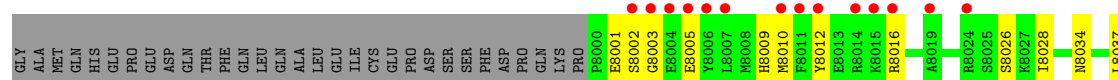
• Molecule 6: CG10419

Chain Bt:



• Molecule 6: CG10419

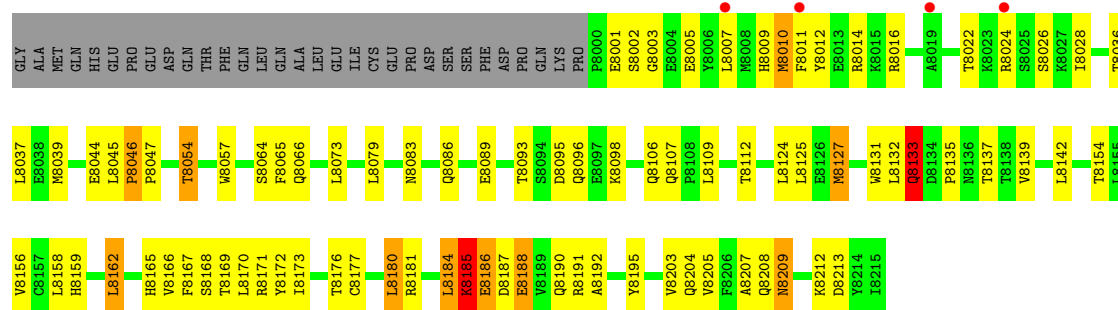
Chain B2:



• Molecule 6: CG10419

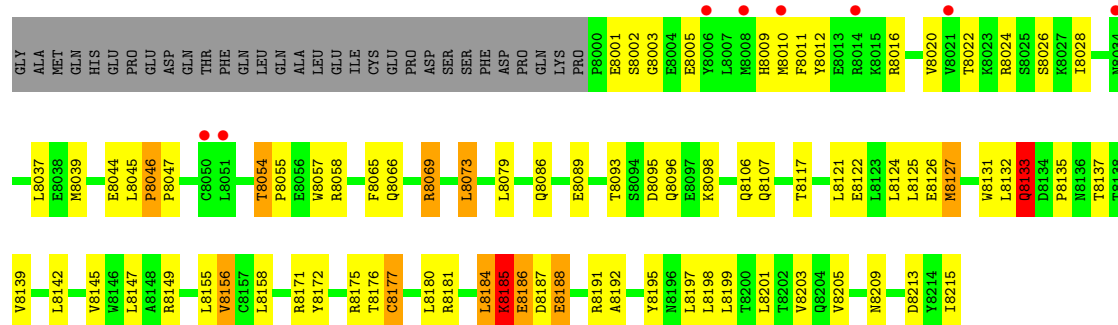


Chain CF:



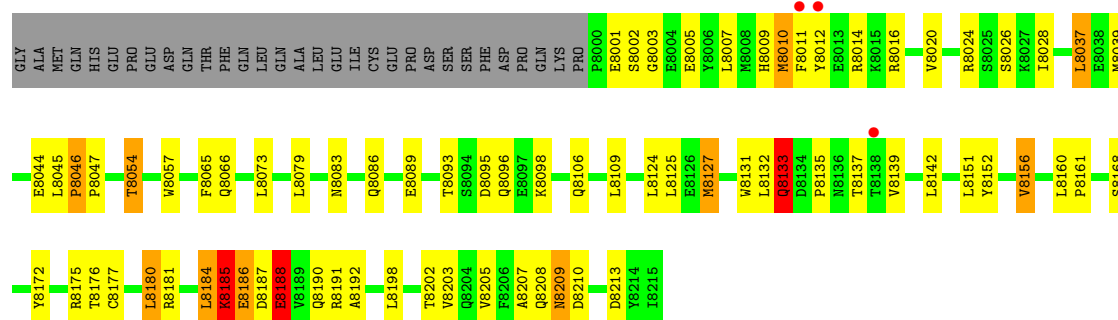
- Molecule 6: CG10419

Chain CN:



- Molecule 6: CG10419

Chain CV:



- Molecule 6: CG10419

Chain Cd:



- Molecule 6: CG10419

[illegible]

- Chain Ct: 

GLY	ALA	MET	GLN	HIS	GLU	PRO	GLU	ASP	THR	PHE	GLN	LEU	GLN	ALA	LEU	GLU	ILE	CYS	GLU	PRO	ASP	SER	SER	PHE	GLN	PRO	LYS	PRO	PRO000	ER001	S8002	G8003	E8004	E8005	Y8006	L8007	M8008	H8009	M8010	F8011	Y8012	E8013	R8014	K8015	R8016	C8017	R8018	A8019	V8020	T8021	T8022	K8023	R8024	S8025	S8026	K8027	T8028
	T8036	L8037	E8038	M8039		L8045	R8046	T8054		L8073		L8079		N8083		T8093		Q8096	Q8106	Q8107		L8110		L8113	T8117	Q8118		L8125	E8126	M8127		Q8133		V8139		L8147		L8162		L8180	L8184	K8185	E8186	L8187	E8188	L8197		Q8204		D8213	Y8214	I8215					

- Chain AO: 

[illegible]

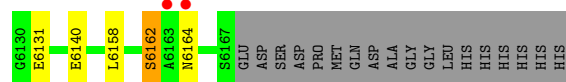
- Chain AG: 

[illegible]

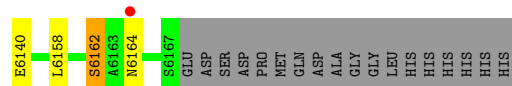
- Chain AW: 

ASP	ASP	ASN	PHE	GLU	ASP	ALA	VAL	ASP	GLU	GLN	PHE	G6130	E6131	L6137	E6140	M6152	L6158	S6162	A6163	N6164	S6167	GLU	ASP	SER	ASP	PRO	MET	GLN	GLN	ASP	ALA	ALA	GLY	GLY	LEU	HIS	HIS	HIS	HIS	HIS				
#6000	E6010	H6011	M6019	K6027	E6031	S6032	T6033	M6043	M6044	P6045	L6061	S6065	S6066	N6067	P6068	R6069	T6072	E6081	S6087	P6098	PRO	PRO	GLN	GLN	ALA	VAL	ASN	GLY	ARG	ASN	GLY	GLY	SER	GLU	ALA	GLU	VAL	ASP	GLU	GLY	ASN	HIS	ASP	GLU

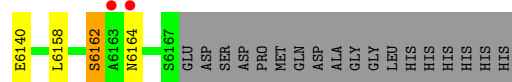
- Chain Ae: 



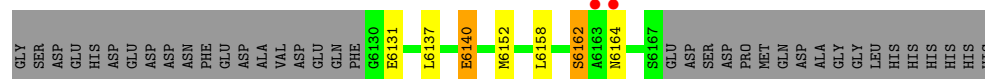
- Molecule 7: Icln



- Molecule 7: Icln



- Molecule 7: Icln

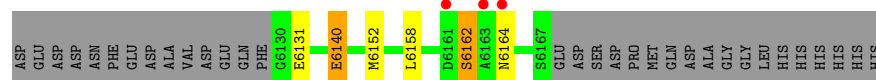


- Molecule 7: Icln



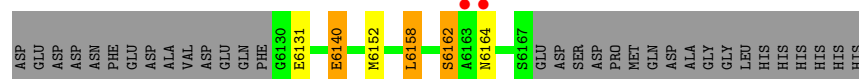
- Molecule 7: Icln





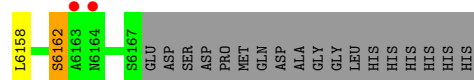
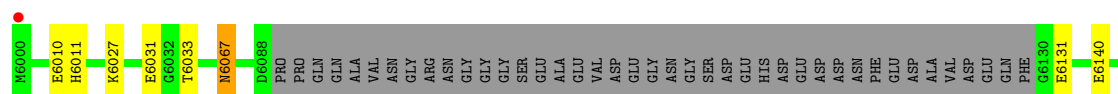
• Molecule 7: Icln

Chain BW:



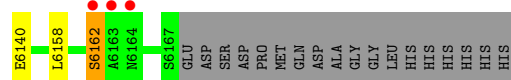
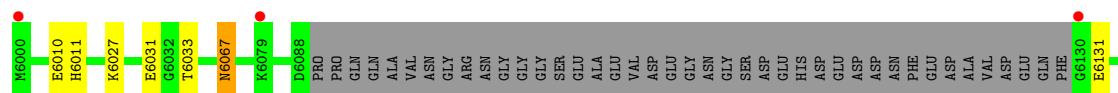
• Molecule 7: Icln

Chain Be:



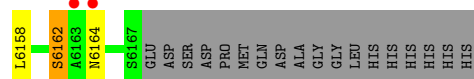
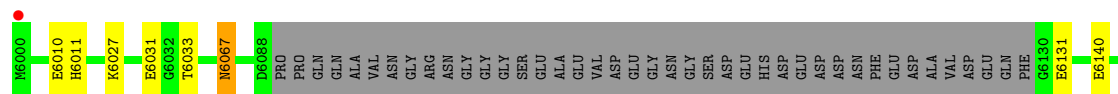
• Molecule 7: Icln

Chain Bm:



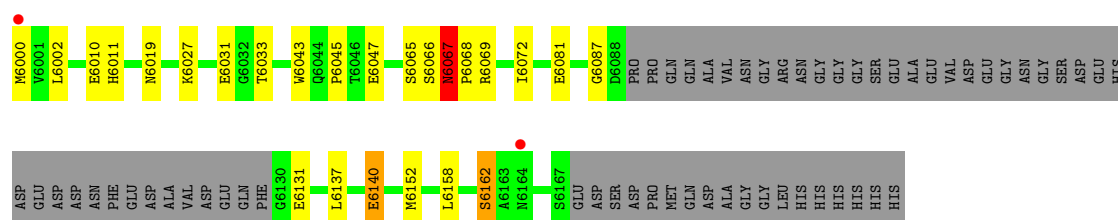
• Molecule 7: Icln

Chain Bu:



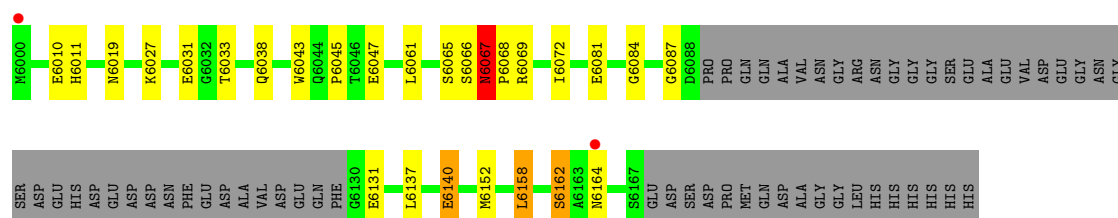
• Molecule 7: Icln

Chain B3:



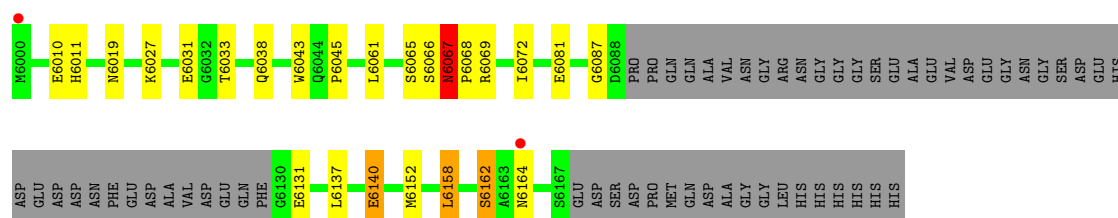
• Molecule 7: Icln

Chain CG:



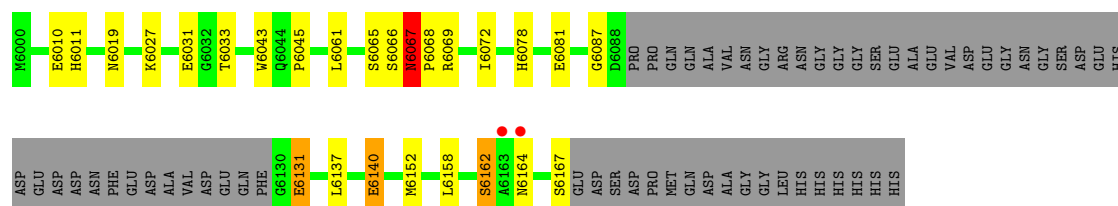
• Molecule 7: Icln

Chain CO:



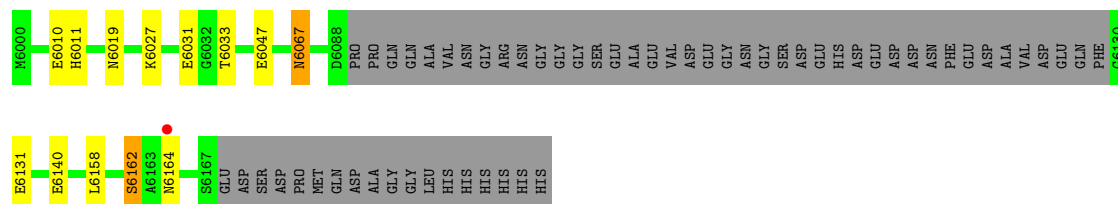
• Molecule 7: Icln

Chain CW:



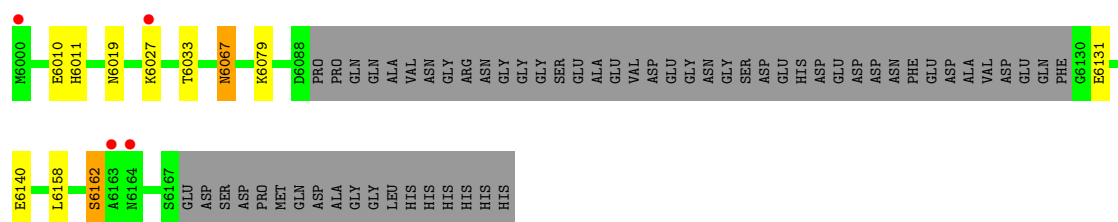
• Molecule 7: Icln

Chain Ce:



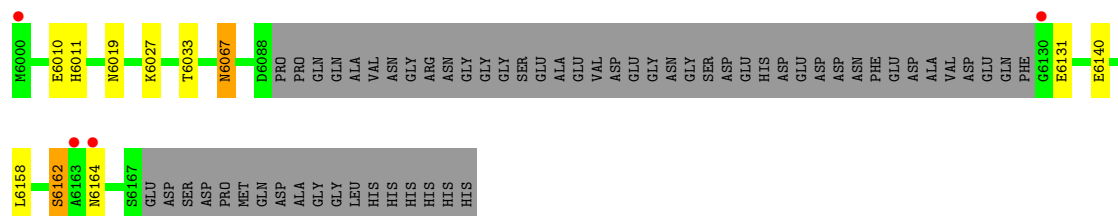
• Molecule 7: Icln

Chain Cm:



• Molecule 7: Icln

Chain Cu:



• Molecule 8: Small nuclear ribonucleoprotein G

Chain AP:



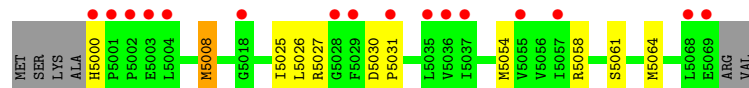
• Molecule 8: Small nuclear ribonucleoprotein G

Chain AH:



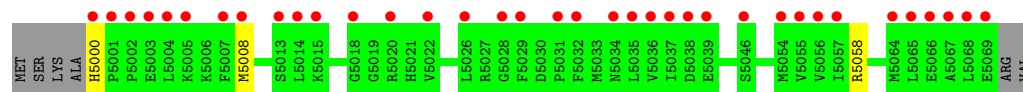
• Molecule 8: Small nuclear ribonucleoprotein G

Chain AX:



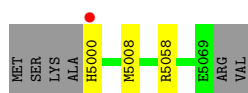
• Molecule 8: Small nuclear ribonucleoprotein G

Chain Af:



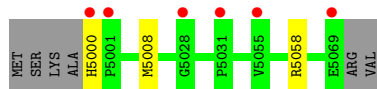
• Molecule 8: Small nuclear ribonucleoprotein G

Chain An:



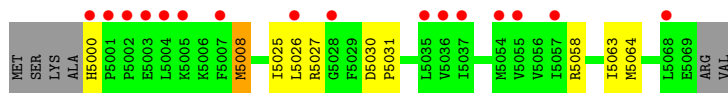
- Molecule 8: Small nuclear ribonucleoprotein G

Chain Av:



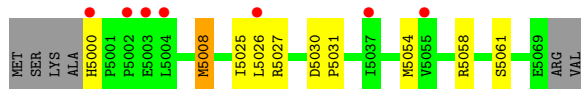
- Molecule 8: Small nuclear ribonucleoprotein G

Chain A4:



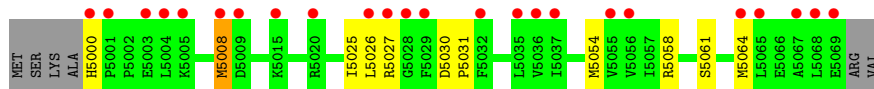
- Molecule 8: Small nuclear ribonucleoprotein G

Chain BH:



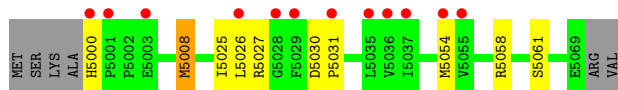
- Molecule 8: Small nuclear ribonucleoprotein G

Chain BP:



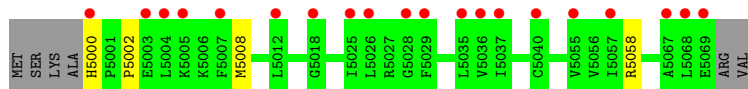
- Molecule 8: Small nuclear ribonucleoprotein G

Chain BX:



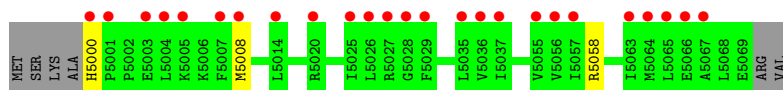
- Molecule 8: Small nuclear ribonucleoprotein G

Chain Bf:



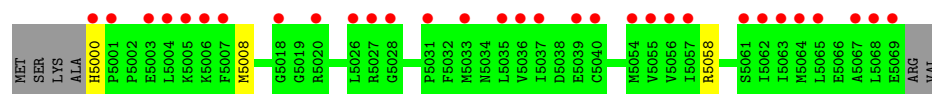
- Molecule 8: Small nuclear ribonucleoprotein G

Chain Bn:



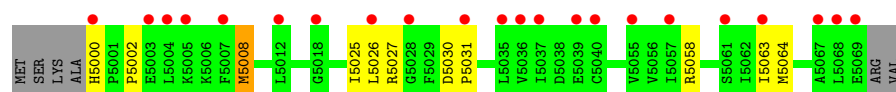
- Molecule 8: Small nuclear ribonucleoprotein G

Chain Bv:



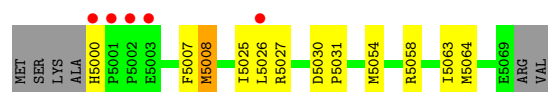
- Molecule 8: Small nuclear ribonucleoprotein G

Chain B4:



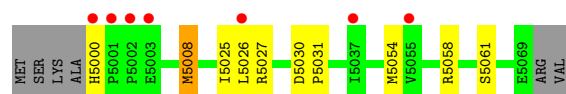
- Molecule 8: Small nuclear ribonucleoprotein G

Chain CH:



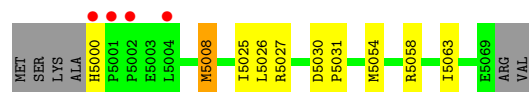
- Molecule 8: Small nuclear ribonucleoprotein G

Chain CP:



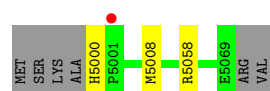
- Molecule 8: Small nuclear ribonucleoprotein G

Chain CX:



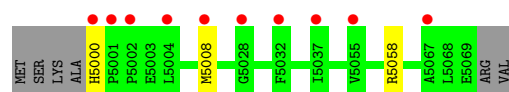
- Molecule 8: Small nuclear ribonucleoprotein G

Chain Cf:



- Molecule 8: Small nuclear ribonucleoprotein G

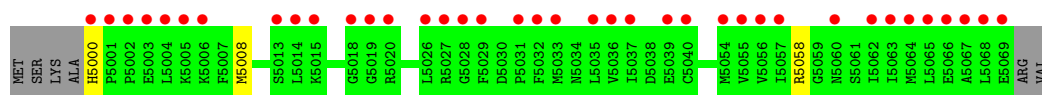
Chain Cn:



- Molecule 8: Small nuclear ribonucleoprotein G

Chain Cv:





## 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 0.367 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	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 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	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.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CY	648	0	690	8	0
1	Cg	648	0	690	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Cq	638	0	657	0	0
4	AD	556	0	561	16	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AF	1787	0	1779	51	0
6	AN	1787	0	1779	57	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AX	544	0	563	8	0
8	Af	544	0	563	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (1154) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
6:BN:8185:LYS:H	6:BN:8187:ASP:HB2	1.45	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	9	42
1	AI	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	AQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	AY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	Ag	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	Ao	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	9	42
1	Aw	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	9	42
1	BA	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	BI	80/119 (67%)	77 (96%)	1 (1%)	2 (2%)	9	42
1	BQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	BY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Bg	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	Bo	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	Bw	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	CA	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	CI	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	CQ	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	CY	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	Cg	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
1	Co	80/119 (67%)	76 (95%)	2 (2%)	2 (2%)	9	42
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%)	7	36
2	Ap	96/118 (81%)	91 (95%)	5 (5%)	0	100	100
2	Ax	96/118 (81%)	92 (96%)	3 (3%)	1 (1%)	22	68
2	BB	96/118 (81%)	90 (94%)	6 (6%)	0	100	100
2	BJ	96/118 (81%)	90 (94%)	4 (4%)	2 (2%)	11	48
2	BR	96/118 (81%)	90 (94%)	4 (4%)	2 (2%)	11	48
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%)	22	68
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	2	14
5	AE	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	AM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	AU	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	Ac	15/124 (12%)	9 (60%)	5 (33%)	1 (7%)	2	14
5	Ak	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	2	14
5	As	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	B1	15/124 (12%)	10 (67%)	3 (20%)	2 (13%)	0	2
5	BE	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	BM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	BU	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	Bc	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	2	14
5	Bk	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	Bs	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	2	14
5	CE	15/124 (12%)	10 (67%)	4 (27%)	1 (7%)	2	14
5	CM	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	CU	15/124 (12%)	10 (67%)	5 (33%)	0	100	100
5	Cc	15/124 (12%)	9 (60%)	5 (33%)	1 (7%)	2	14
5	Ck	15/124 (12%)	11 (73%)	3 (20%)	1 (7%)	2	14
5	Cs	15/124 (12%)	10 (67%)	2 (13%)	3 (20%)	0	0
6	A2	214/247 (87%)	187 (87%)	17 (8%)	10 (5%)	4	23
6	AF	214/247 (87%)	182 (85%)	22 (10%)	10 (5%)	4	23
6	AN	214/247 (87%)	174 (81%)	31 (14%)	9 (4%)	4	27
6	AV	214/247 (87%)	182 (85%)	21 (10%)	11 (5%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Ad	214/247 (87%)	183 (86%)	20 (9%)	11 (5%)	3	22
6	Al	214/247 (87%)	183 (86%)	21 (10%)	10 (5%)	4	23
6	At	214/247 (87%)	182 (85%)	21 (10%)	11 (5%)	3	22
6	B2	214/247 (87%)	179 (84%)	23 (11%)	12 (6%)	3	19
6	BF	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	5	31
6	BN	214/247 (87%)	185 (86%)	22 (10%)	7 (3%)	6	33
6	BV	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	5	31
6	Bd	214/247 (87%)	185 (86%)	19 (9%)	10 (5%)	4	23
6	Bl	214/247 (87%)	186 (87%)	18 (8%)	10 (5%)	4	23
6	Bt	214/247 (87%)	181 (85%)	27 (13%)	6 (3%)	8	39
6	CF	214/247 (87%)	187 (87%)	19 (9%)	8 (4%)	5	31
6	CN	214/247 (87%)	186 (87%)	20 (9%)	8 (4%)	5	31
6	CV	214/247 (87%)	182 (85%)	24 (11%)	8 (4%)	5	31
6	Cd	214/247 (87%)	185 (86%)	19 (9%)	10 (5%)	4	23
6	Cl	214/247 (87%)	186 (87%)	19 (9%)	9 (4%)	4	27
6	Ct	214/247 (87%)	178 (83%)	26 (12%)	10 (5%)	4	23
7	A3	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	AG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	AO	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	AW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	Ae	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	Am	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	Au	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	B3	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	9	43
7	BG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	BO	123/186 (66%)	115 (94%)	4 (3%)	4 (3%)	6	33
7	BW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	Be	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	9	43
7	Bm	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	9	43
7	Bu	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	CG	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	CO	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	CW	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	Ce	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
7	Cm	123/186 (66%)	114 (93%)	6 (5%)	3 (2%)	9	43
7	Cu	123/186 (66%)	114 (93%)	5 (4%)	4 (3%)	6	33
8	A4	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	AH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	AP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	AX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	Af	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	An	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	Av	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	B4	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	BH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	BP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	BX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	Bf	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	Bn	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	Bv	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	CH	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	CP	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	CX	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	Cf	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	Cn	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
8	Cv	68/76 (90%)	64 (94%)	3 (4%)	1 (2%)	15	57
All	All	14800/20960 (71%)	13553 (92%)	894 (6%)	353 (2%)	9	43

All (353) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AM	7006	LEU
6	AN	8028	ILE
6	AN	8185	LYS

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	14	45
1	AI	77/101 (76%)	72 (94%)	5 (6%)	24	65
1	AQ	77/101 (76%)	72 (94%)	5 (6%)	24	65
1	AY	77/101 (76%)	71 (92%)	6 (8%)	18	57
1	Ag	77/101 (76%)	71 (92%)	6 (8%)	18	57
1	Ao	77/101 (76%)	73 (95%)	4 (5%)	32	73
1	Aw	77/101 (76%)	72 (94%)	5 (6%)	24	65
1	BA	77/101 (76%)	72 (94%)	5 (6%)	24	65
1	BI	77/101 (76%)	72 (94%)	5 (6%)	24	65
1	BQ	77/101 (76%)	72 (94%)	5 (6%)	24	65
1	BY	77/101 (76%)	72 (94%)	5 (6%)	24	65
1	Bg	77/101 (76%)	72 (94%)	5 (6%)	24	65
1	Bo	77/101 (76%)	71 (92%)	6 (8%)	18	57
1	Bw	77/101 (76%)	71 (92%)	6 (8%)	18	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CA	77/101 (76%)	72 (94%)	5 (6%)	24	65
1	CI	77/101 (76%)	72 (94%)	5 (6%)	24	65
1	CQ	77/101 (76%)	71 (92%)	6 (8%)	18	57
1	CY	77/101 (76%)	71 (92%)	6 (8%)	18	57
1	Cg	77/101 (76%)	71 (92%)	6 (8%)	18	57
1	Co	77/101 (76%)	73 (95%)	4 (5%)	32	73
2	AB	94/110 (86%)	90 (96%)	4 (4%)	40	80
2	AJ	94/110 (86%)	92 (98%)	2 (2%)	66	92
2	AR	94/110 (86%)	91 (97%)	3 (3%)	51	87
2	AZ	94/110 (86%)	90 (96%)	4 (4%)	40	80
2	Ah	94/110 (86%)	89 (95%)	5 (5%)	32	72
2	Ap	94/110 (86%)	91 (97%)	3 (3%)	51	87
2	Ax	94/110 (86%)	90 (96%)	4 (4%)	40	80
2	BB	94/110 (86%)	90 (96%)	4 (4%)	40	80
2	BJ	94/110 (86%)	88 (94%)	6 (6%)	25	65
2	BR	94/110 (86%)	90 (96%)	4 (4%)	40	80
2	BZ	94/110 (86%)	90 (96%)	4 (4%)	40	80
2	Bh	94/110 (86%)	90 (96%)	4 (4%)	40	80
2	Bp	94/110 (86%)	89 (95%)	5 (5%)	32	72
2	Bx	94/110 (86%)	88 (94%)	6 (6%)	25	65
2	CB	94/110 (86%)	89 (95%)	5 (5%)	32	72
2	CJ	94/110 (86%)	90 (96%)	4 (4%)	40	80
2	CR	94/110 (86%)	91 (97%)	3 (3%)	51	87
2	CZ	94/110 (86%)	88 (94%)	6 (6%)	25	65
2	Ch	94/110 (86%)	90 (96%)	4 (4%)	40	80
2	Cp	94/110 (86%)	89 (95%)	5 (5%)	32	72
3	AC	72/84 (86%)	67 (93%)	5 (7%)	22	62
3	AK	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	AS	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	Aa	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	Ai	72/84 (86%)	68 (94%)	4 (6%)	30	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Aq	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	Ay	72/84 (86%)	69 (96%)	3 (4%)	40	81
3	BC	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	BK	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	BS	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	Ba	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	Bi	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	Bq	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	By	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	CC	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	CK	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	CS	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	Ca	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	Ci	72/84 (86%)	68 (94%)	4 (6%)	30	70
3	Cq	72/84 (86%)	68 (94%)	4 (6%)	30	70
4	AD	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	AL	60/74 (81%)	57 (95%)	3 (5%)	34	75
4	AT	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	Ab	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	Aj	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	Ar	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	Az	60/74 (81%)	57 (95%)	3 (5%)	34	75
4	BD	60/74 (81%)	55 (92%)	5 (8%)	16	53
4	BL	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	BT	60/74 (81%)	55 (92%)	5 (8%)	16	53
4	Bb	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	Bj	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	Br	60/74 (81%)	57 (95%)	3 (5%)	34	75
4	Bz	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	CD	60/74 (81%)	55 (92%)	5 (8%)	16	53
4	CL	60/74 (81%)	56 (93%)	4 (7%)	23	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CT	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	Cb	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	Cj	60/74 (81%)	56 (93%)	4 (7%)	23	63
4	Cr	60/74 (81%)	56 (93%)	4 (7%)	23	63
5	A1	15/97 (16%)	11 (73%)	4 (27%)	1	2
5	AE	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	AM	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	AU	15/97 (16%)	13 (87%)	2 (13%)	6	22
5	Ac	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	Ak	15/97 (16%)	13 (87%)	2 (13%)	6	22
5	As	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	B1	15/97 (16%)	13 (87%)	2 (13%)	6	22
5	BE	15/97 (16%)	11 (73%)	4 (27%)	1	2
5	BM	15/97 (16%)	11 (73%)	4 (27%)	1	2
5	BU	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	Bc	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	Bk	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	Bs	15/97 (16%)	13 (87%)	2 (13%)	6	22
5	CE	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	CM	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	CU	15/97 (16%)	11 (73%)	4 (27%)	1	2
5	Cc	15/97 (16%)	13 (87%)	2 (13%)	6	22
5	Ck	15/97 (16%)	12 (80%)	3 (20%)	2	8
5	Cs	15/97 (16%)	10 (67%)	5 (33%)	0	0
6	A2	203/231 (88%)	176 (87%)	27 (13%)	6	22
6	AF	203/231 (88%)	170 (84%)	33 (16%)	3	12
6	AN	203/231 (88%)	171 (84%)	32 (16%)	4	14
6	AV	203/231 (88%)	177 (87%)	26 (13%)	6	24
6	Ad	203/231 (88%)	178 (88%)	25 (12%)	7	26
6	Al	203/231 (88%)	176 (87%)	27 (13%)	6	22
6	At	203/231 (88%)	172 (85%)	31 (15%)	4	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	B2	203/231 (88%)	169 (83%)	34 (17%)	3	11
6	BF	203/231 (88%)	176 (87%)	27 (13%)	6	22
6	BN	203/231 (88%)	177 (87%)	26 (13%)	6	24
6	BV	203/231 (88%)	178 (88%)	25 (12%)	7	26
6	Bd	203/231 (88%)	176 (87%)	27 (13%)	6	22
6	Bl	203/231 (88%)	175 (86%)	28 (14%)	5	21
6	Bt	203/231 (88%)	174 (86%)	29 (14%)	5	19
6	CF	203/231 (88%)	172 (85%)	31 (15%)	4	15
6	CN	203/231 (88%)	178 (88%)	25 (12%)	7	26
6	CV	203/231 (88%)	175 (86%)	28 (14%)	5	21
6	Cd	203/231 (88%)	174 (86%)	29 (14%)	5	19
6	Cl	203/231 (88%)	172 (85%)	31 (15%)	4	15
6	Ct	203/231 (88%)	174 (86%)	29 (14%)	5	19
7	A3	108/159 (68%)	98 (91%)	10 (9%)	13	44
7	AG	108/159 (68%)	98 (91%)	10 (9%)	13	44
7	AO	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	AW	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	Ae	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	Am	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	Au	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	B3	108/159 (68%)	98 (91%)	10 (9%)	13	44
7	BG	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	BO	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	BW	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	Be	108/159 (68%)	100 (93%)	8 (7%)	20	59
7	Bm	108/159 (68%)	100 (93%)	8 (7%)	20	59
7	Bu	108/159 (68%)	100 (93%)	8 (7%)	20	59
7	CG	108/159 (68%)	98 (91%)	10 (9%)	13	44
7	CO	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	CW	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	Ce	108/159 (68%)	98 (91%)	10 (9%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	Cm	108/159 (68%)	99 (92%)	9 (8%)	16	53
7	Cu	108/159 (68%)	100 (93%)	8 (7%)	20	59
8	A4	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	AH	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	AP	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	AX	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	Af	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	An	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	Av	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	B4	61/66 (92%)	58 (95%)	3 (5%)	35	76
8	BH	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	BP	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	BX	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	Bf	61/66 (92%)	58 (95%)	3 (5%)	35	76
8	Bn	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	Bv	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	CH	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	CP	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	CX	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	Cf	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	Cn	61/66 (92%)	59 (97%)	2 (3%)	50	86
8	Cv	61/66 (92%)	59 (97%)	2 (3%)	50	86
All	All	13800/18440 (75%)	12594 (91%)	1206 (9%)	15	49

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
6	B1	8073	LEU
6	B1	8079	LEU
6	B1	8083	ASN
6	B1	8093	THR
6	B1	8096	GLN
6	B1	8106	GLN
6	B1	8110	LEU
6	B1	8127	MET
6	B1	8133	GLN
6	B1	8139	VAL
6	B1	8147	LEU
6	B1	8154	THR
6	B1	8162	LEU
6	B1	8169	THR
6	B1	8173	ILE
6	B1	8180	LEU
6	B1	8184	LEU
6	B1	8186	GLU
6	B1	8188	GLU
6	B1	8195	TYR
6	B1	8213	ASP
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	0.39	0
9	SO4	Ad	8301	-	4,4,4	0.38	0	6,6,6	0.25	0
9	SO4	At	8301	-	4,4,4	0.55	0	6,6,6	0.37	0
9	SO4	B2	8301	-	4,4,4	0.33	0	6,6,6	0.30	0
9	SO4	BF	8301	-	4,4,4	0.21	0	6,6,6	0.25	0
9	SO4	BV	8301	-	4,4,4	0.39	0	6,6,6	0.33	0
9	SO4	Bd	8301	-	4,4,4	0.27	0	6,6,6	0.41	0
9	SO4	Bt	8301	-	4,4,4	0.41	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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.27	0 100 100	16, 44, 80, 155	0
1	AI	82/119 (68%)	-0.33	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%)	0.07	0 100 100	48, 76, 117, 154	0
1	Ag	82/119 (68%)	-0.25	0 100 100	14, 47, 94, 167	0
1	Ao	82/119 (68%)	-0.28	0 100 100	18, 43, 87, 158	0
1	Aw	82/119 (68%)	0.06	0 100 100	48, 76, 115, 154	0
1	BA	82/119 (68%)	0.40	0 100 100	69, 92, 131, 175	0
1	BI	82/119 (68%)	0.46	0 100 100	66, 92, 127, 175	0
1	BQ	82/119 (68%)	-0.10	0 100 100	34, 60, 107, 179	0
1	BY	82/119 (68%)	-0.20	0 100 100	25, 54, 88, 130	0
1	Bg	82/119 (68%)	0.14	0 100 100	58, 81, 117, 151	0
1	Bo	82/119 (68%)	-0.02	0 100 100	41, 68, 117, 164	0
1	Bw	82/119 (68%)	-0.19	0 100 100	24, 53, 90, 142	0
1	CA	82/119 (68%)	-0.06	0 100 100	36, 64, 105, 132	0
1	CI	82/119 (68%)	0.39	0 100 100	61, 86, 127, 164	0
1	CQ	82/119 (68%)	-0.26	0 100 100	29, 54, 88, 136	0
1	CY	82/119 (68%)	-0.25	0 100 100	17, 47, 88, 130	0
1	Cg	82/119 (68%)	0.16	0 100 100	52, 82, 119, 162	0
1	Co	82/119 (68%)	0.37	0 100 100	64, 88, 130, 168	0
2	AB	100/118 (84%)	-0.13	0 100 100	19, 63, 168, 181	0
2	AJ	100/118 (84%)	-0.16	0 100 100	20, 63, 167, 179	0
2	AR	100/118 (84%)	0.05	2 (2%) 62 12	29, 69, 190, 201	0
2	AZ	100/118 (84%)	0.13	2 (2%) 62 12	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%)	0.03	0 100 100	44, 82, 207, 217	0
2	Ap	100/118 (84%)	0.07	1 (1%) 79 23	34, 72, 215, 219	0
2	Ax	100/118 (84%)	-0.07	0 100 100	31, 73, 210, 225	0
2	BB	100/118 (84%)	0.57	1 (1%) 79 23	87, 124, 220, 226	0
2	BJ	100/118 (84%)	0.67	7 (7%) 16 3	77, 113, 245, 255	0
2	BR	100/118 (84%)	0.30	3 (3%) 48 7	45, 94, 235, 237	0
2	BZ	100/118 (84%)	0.17	5 (5%) 28 4	37, 76, 216, 232	0
2	Bh	100/118 (84%)	0.31	7 (7%) 16 3	51, 90, 235, 253	0
2	Bp	100/118 (84%)	0.49	8 (8%) 12 2	56, 111, 242, 250	0
2	Bx	100/118 (84%)	0.18	6 (6%) 21 3	32, 75, 230, 243	0
2	CB	100/118 (84%)	0.24	1 (1%) 79 23	48, 92, 223, 238	0
2	CJ	100/118 (84%)	0.53	1 (1%) 79 23	79, 118, 224, 231	0
2	CR	100/118 (84%)	0.03	1 (1%) 79 23	35, 76, 183, 203	0
2	CZ	100/118 (84%)	-0.03	0 100 100	28, 72, 184, 205	0
2	Ch	100/118 (84%)	0.21	3 (3%) 48 7	55, 90, 212, 223	0
2	Cp	100/118 (84%)	0.56	6 (6%) 21 3	67, 112, 233, 247	0
3	AC	77/92 (83%)	0.26	0 100 100	70, 120, 150, 162	0
3	AK	77/92 (83%)	0.42	2 (2%) 53 8	79, 125, 164, 170	0
3	AS	77/92 (83%)	1.16	13 (16%) 2 0	128, 181, 261, 265	0
3	Aa	77/92 (83%)	1.33	17 (22%) 1 0	134, 199, 268, 274	0
3	Ai	77/92 (83%)	0.40	0 100 100	86, 135, 164, 173	0
3	Aq	77/92 (83%)	0.95	10 (12%) 4 1	126, 179, 246, 254	0
3	Ay	77/92 (83%)	0.63	4 (5%) 26 4	87, 140, 220, 227	0
3	BC	77/92 (83%)	0.78	3 (3%) 37 5	128, 157, 177, 185	0
3	BK	77/92 (83%)	1.39	18 (23%) 1 0	177, 242, 280, 286	0
3	BS	77/92 (83%)	1.03	11 (14%) 3 1	148, 203, 244, 256	0
3	Ba	77/92 (83%)	1.06	11 (14%) 3 1	133, 188, 260, 264	0
3	Bi	77/92 (83%)	1.09	9 (11%) 5 1	144, 203, 278, 279	0
3	Bq	77/92 (83%)	1.27	18 (23%) 1 0	200, 257, 282, 293	0
3	By	77/92 (83%)	1.04	11 (14%) 3 1	143, 207, 268, 274	0
3	CC	77/92 (83%)	0.55	3 (3%) 37 5	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%)	0.83	5 (6%) 18 3	131, 181, 212, 222	0
3	CS	77/92 (83%)	0.35	1 (1%) 74 19	81, 121, 161, 172	0
3	Ca	77/92 (83%)	0.36	2 (2%) 53 8	82, 122, 165, 177	0
3	Ci	77/92 (83%)	0.54	2 (2%) 53 8	107, 148, 200, 206	0
3	Cq	77/92 (83%)	1.38	16 (20%) 1 0	172, 241, 284, 286	0
4	AD	71/86 (82%)	-0.04	0 100 100	46, 93, 120, 142	0
4	AL	71/86 (82%)	-0.05	0 100 100	50, 89, 113, 143	0
4	AT	71/86 (82%)	0.30	2 (2%) 50 8	64, 115, 159, 182	0
4	Ab	71/86 (82%)	0.36	2 (2%) 50 8	73, 116, 166, 193	0
4	Aj	71/86 (82%)	0.20	1 (1%) 72 17	71, 125, 153, 185	0
4	Ar	71/86 (82%)	0.33	2 (2%) 50 8	66, 122, 172, 191	0
4	Az	71/86 (82%)	0.00	0 100 100	60, 105, 133, 163	0
4	BD	71/86 (82%)	0.68	5 (7%) 16 3	104, 169, 199, 208	0
4	BL	71/86 (82%)	0.77	7 (9%) 8 2	118, 165, 251, 260	0
4	BT	71/86 (82%)	0.51	3 (4%) 35 5	98, 144, 212, 220	0
4	Bb	71/86 (82%)	0.33	1 (1%) 72 17	64, 121, 161, 193	0
4	Bj	71/86 (82%)	0.40	1 (1%) 72 17	80, 130, 174, 203	0
4	Br	71/86 (82%)	0.78	6 (8%) 11 2	118, 183, 264, 271	0
4	Bz	71/86 (82%)	0.36	0 100 100	71, 128, 179, 219	0
4	CD	71/86 (82%)	0.21	0 100 100	77, 126, 152, 195	0
4	CL	71/86 (82%)	0.74	4 (5%) 24 3	111, 166, 197, 201	0
4	CT	71/86 (82%)	-0.06	0 100 100	64, 101, 128, 156	0
4	Cb	71/86 (82%)	-0.06	0 100 100	60, 102, 128, 157	0
4	Cj	71/86 (82%)	0.12	0 100 100	79, 117, 152, 178	0
4	Cr	71/86 (82%)	0.79	7 (9%) 8 2	111, 166, 244, 257	0
5	A1	17/124 (13%)	0.25	0 100 100	73, 98, 162, 164	0
5	AE	17/124 (13%)	0.06	0 100 100	67, 81, 121, 128	0
5	AM	17/124 (13%)	-0.01	0 100 100	64, 80, 131, 133	0
5	AU	17/124 (13%)	0.07	0 100 100	58, 85, 120, 125	0
5	Ac	17/124 (13%)	0.21	0 100 100	52, 86, 141, 144	0
5	Ak	17/124 (13%)	0.14	0 100 100	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%)	0.04	0 <span>100</span> <span>100</span>	59, 76, 128, 128	0
5	B1	17/124 (13%)	0.11	0 <span>100</span> <span>100</span>	56, 69, 129, 130	0
5	BE	17/124 (13%)	0.63	1 (5%) <span>22</span> <span>3</span>	115, 129, 153, 167	0
5	BM	17/124 (13%)	0.56	1 (5%) <span>22</span> <span>3</span>	96, 109, 152, 152	0
5	BU	17/124 (13%)	0.23	1 (5%) <span>22</span> <span>3</span>	83, 94, 129, 132	0
5	Bc	17/124 (13%)	0.21	0 <span>100</span> <span>100</span>	60, 81, 133, 136	0
5	Bk	17/124 (13%)	0.54	1 (5%) <span>22</span> <span>3</span>	85, 98, 150, 153	0
5	Bs	17/124 (13%)	0.33	1 (5%) <span>22</span> <span>3</span>	81, 95, 149, 151	0
5	CE	17/124 (13%)	0.26	1 (5%) <span>22</span> <span>3</span>	77, 93, 139, 142	0
5	CM	17/124 (13%)	0.86	2 (11%) <span>5</span> <span>1</span>	111, 124, 163, 163	0
5	CU	17/124 (13%)	0.24	1 (5%) <span>22</span> <span>3</span>	54, 78, 134, 134	0
5	Cc	17/124 (13%)	0.13	0 <span>100</span> <span>100</span>	53, 72, 132, 134	0
5	Ck	17/124 (13%)	0.65	2 (11%) <span>5</span> <span>1</span>	79, 92, 156, 160	0
5	Cs	17/124 (13%)	0.50	0 <span>100</span> <span>100</span>	101, 114, 151, 152	0
6	A2	216/247 (87%)	-0.09	3 (1%) <span>72</span> <span>17</span>	24, 73, 196, 212	0
6	AF	216/247 (87%)	-0.13	2 (0%) <span>81</span> <span>25</span>	14, 56, 168, 208	0
6	AN	216/247 (87%)	-0.14	2 (0%) <span>81</span> <span>25</span>	11, 54, 167, 187	0
6	AV	216/247 (87%)	-0.01	9 (4%) <span>35</span> <span>5</span>	17, 59, 201, 226	0
6	Ad	216/247 (87%)	0.17	12 (5%) <span>24</span> <span>3</span>	27, 75, 214, 236	0
6	Al	216/247 (87%)	-0.06	3 (1%) <span>72</span> <span>17</span>	16, 62, 189, 235	0
6	At	216/247 (87%)	-0.06	6 (2%) <span>50</span> <span>8</span>	14, 55, 202, 219	0
6	B2	216/247 (87%)	0.04	14 (6%) <span>18</span> <span>3</span>	20, 58, 225, 240	0
6	BF	216/247 (87%)	0.40	11 (5%) <span>27</span> <span>4</span>	71, 108, 202, 230	0
6	BN	216/247 (87%)	0.49	16 (7%) <span>14</span> <span>2</span>	57, 99, 235, 247	0
6	BV	216/247 (87%)	0.13	11 (5%) <span>27</span> <span>4</span>	31, 78, 219, 245	0
6	Bd	216/247 (87%)	0.03	12 (5%) <span>24</span> <span>3</span>	24, 61, 215, 236	0
6	Bl	216/247 (87%)	0.19	14 (6%) <span>18</span> <span>3</span>	38, 78, 226, 246	0
6	Bt	216/247 (87%)	0.27	17 (7%) <span>13</span> <span>2</span>	41, 78, 233, 250	0
6	CF	216/247 (87%)	0.01	4 (1%) <span>64</span> <span>13</span>	35, 73, 195, 229	0
6	CN	216/247 (87%)	0.44	8 (3%) <span>39</span> <span>6</span>	64, 107, 196, 224	0
6	CV	216/247 (87%)	-0.13	3 (1%) <span>72</span> <span>17</span>	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%)	-0.15	3 (1%) 72 17	14, 55, 181, 211	0
6	Cl	216/247 (87%)	0.07	2 (0%) 81 25	32, 76, 204, 225	0
6	Ct	216/247 (87%)	0.52	17 (7%) 13 2	63, 103, 224, 240	0
7	A3	127/186 (68%)	0.31	4 (3%) 47 7	74, 126, 154, 172	0
7	AG	127/186 (68%)	-0.15	1 (0%) 83 28	21, 47, 108, 144	0
7	AO	127/186 (68%)	-0.14	1 (0%) 83 28	19, 58, 119, 143	0
7	AW	127/186 (68%)	-0.10	2 (1%) 68 15	29, 60, 122, 152	0
7	Ae	127/186 (68%)	0.71	5 (3%) 37 5	78, 122, 162, 170	0
7	Am	127/186 (68%)	-0.28	1 (0%) 83 28	13, 43, 110, 149	0
7	Au	127/186 (68%)	-0.10	2 (1%) 68 15	20, 51, 122, 152	0
7	B3	127/186 (68%)	-0.07	2 (1%) 68 15	31, 58, 113, 162	0
7	BG	127/186 (68%)	0.26	3 (2%) 56 9	51, 82, 135, 167	0
7	BO	127/186 (68%)	0.63	4 (3%) 47 7	73, 107, 149, 178	0
7	BW	127/186 (68%)	-0.14	2 (1%) 68 15	28, 54, 115, 153	0
7	Be	127/186 (68%)	-0.06	3 (2%) 56 9	33, 62, 120, 162	0
7	Bm	127/186 (68%)	0.58	6 (4%) 30 4	62, 110, 152, 178	0
7	Bu	127/186 (68%)	-0.05	3 (2%) 56 9	34, 63, 122, 167	0
7	CG	127/186 (68%)	-0.15	2 (1%) 68 15	22, 57, 116, 158	0
7	CO	127/186 (68%)	0.27	2 (1%) 68 15	55, 85, 133, 174	0
7	CW	127/186 (68%)	-0.14	2 (1%) 68 15	23, 59, 126, 158	0
7	Ce	127/186 (68%)	-0.17	1 (0%) 83 28	20, 53, 115, 158	0
7	Cm	127/186 (68%)	0.75	4 (3%) 47 7	67, 125, 157, 179	0
7	Cu	127/186 (68%)	0.50	4 (3%) 47 7	73, 100, 146, 174	0
8	A4	70/76 (92%)	1.31	16 (22%) 1 0	158, 202, 224, 228	0
8	AH	70/76 (92%)	0.11	2 (2%) 49 7	69, 116, 151, 158	0
8	AP	70/76 (92%)	0.49	5 (7%) 16 3	81, 137, 167, 178	0
8	AX	70/76 (92%)	1.32	16 (22%) 1 0	121, 196, 220, 225	0
8	Af	70/76 (92%)	2.44	36 (51%) 0 0	200, 237, 255, 258	0
8	An	70/76 (92%)	0.16	1 (1%) 72 17	67, 110, 152, 158	0
8	Av	70/76 (92%)	0.87	6 (8%) 11 2	109, 176, 200, 214	0
8	B4	70/76 (92%)	1.79	22 (31%) 1 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%)	0.61	7 (10%) 8 2	102, 140, 170, 178	0
8	BP	70/76 (92%)	2.03	24 (34%) 1 0	180, 237, 261, 266	0
8	BX	70/76 (92%)	1.07	12 (17%) 2 0	114, 173, 192, 201	0
8	Bf	70/76 (92%)	1.74	20 (28%) 1 0	178, 226, 252, 255	0
8	Bn	70/76 (92%)	1.93	25 (35%) 1 0	221, 251, 273, 278	0
8	Bv	70/76 (92%)	2.10	31 (44%) 1 0	185, 237, 271, 277	0
8	CH	70/76 (92%)	0.51	5 (7%) 16 3	106, 144, 166, 172	0
8	CP	70/76 (92%)	0.88	7 (10%) 8 2	135, 167, 187, 206	0
8	CX	70/76 (92%)	0.48	4 (5%) 23 3	103, 135, 162, 171	0
8	Cf	70/76 (92%)	0.39	1 (1%) 72 17	97, 140, 160, 170	0
8	Cn	70/76 (92%)	0.95	10 (14%) 3 1	146, 178, 204, 210	0
8	Cv	70/76 (92%)	2.52	38 (54%) 0 0	231, 267, 287, 290	0
All	All	15200/20960 (72%)	0.31	773 (5%) 27 4	11, 97, 231, 293	0

All (773) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	BP	5055	VAL	11.8
8	Af	5055	VAL	11.5
8	Af	5028	GLY	9.7
8	Cv	5065	LEU	7.9
8	Bn	5037	ILE	7.7
7	Cu	6164	ASN	7.7
7	BO	6164	ASN	7.3
8	A4	5028	GLY	7.1
8	AX	5028	GLY	7.0
8	Bn	5055	VAL	6.9
3	BK	3033	ILE	6.9
8	A4	5055	VAL	6.9
6	Bd	8011	PHE	6.7
8	Cv	5026	LEU	6.6
7	BG	6164	ASN	6.6
3	Cq	3000	MET	6.6
8	Af	5035	LEU	6.4
7	Ae	6164	ASN	6.4
8	BP	5028	GLY	6.4
7	Bu	6164	ASN	6.0
8	Cv	5037	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
7	Bm	6164	ASN	6.0
8	Bf	5037	ILE	6.0
8	Cv	5055	VAL	6.0
7	BW	6164	ASN	5.9
8	Bn	5064	MET	5.9
8	Cv	5000	HIS	5.8
8	B4	5004	LEU	5.8
8	Cv	5064	MET	5.8
8	Bf	5004	LEU	5.8
8	Bn	5004	LEU	5.7
8	Af	5014	LEU	5.6
8	BP	5026	LEU	5.6
7	Cm	6164	ASN	5.6
3	Bi	3000	MET	5.6
8	BP	5036	VAL	5.5
8	Cv	5020	ARG	5.5
8	A4	5002	PRO	5.5
8	B4	5037	ILE	5.5
6	B2	8011	PHE	5.5
8	Af	5036	VAL	5.4
8	Bv	5037	ILE	5.4
8	Af	5020	ARG	5.4
8	B4	5068	LEU	5.4
7	Cu	6163	ALA	5.4
3	By	3000	MET	5.3
6	BN	8006	TYR	5.3
8	Bn	5000	HIS	5.2
3	BS	3033	ILE	5.2
8	Af	5029	PHE	5.2
8	Cv	5028	GLY	5.1
8	Bv	5026	LEU	5.1
8	Af	5065	LEU	5.1
6	BN	8012	TYR	5.1
3	BK	3044	LEU	5.0
7	AW	6164	ASN	5.0
8	Bv	5004	LEU	5.0
3	Ba	3000	MET	5.0
6	BN	8011	PHE	4.9
7	CO	6000	MET	4.9
8	Bv	5036	VAL	4.9
6	Ct	8023	LYS	4.9
6	BV	8011	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
3	Bq	3000	MET	4.9
6	Bl	8011	PHE	4.8
8	Bn	5065	LEU	4.8
3	BK	3076	VAL	4.8
7	Au	6164	ASN	4.8
8	AX	5055	VAL	4.7
8	Bv	5028	GLY	4.7
8	A4	5026	LEU	4.7
8	Bf	5003	GLU	4.7
7	Be	6164	ASN	4.6
8	Cv	5067	ALA	4.6
8	Bf	5055	VAL	4.6
8	Bn	5026	LEU	4.6
6	B2	8014	ARG	4.6
4	Ar	4005	LEU	4.6
3	Aa	3033	ILE	4.6
6	BV	8019	ALA	4.6
6	Ct	8014	ARG	4.6
4	Cr	4002	LYS	4.6
8	A4	5037	ILE	4.5
6	BN	8010	MET	4.5
8	BP	5035	LEU	4.5
6	Bt	8010	MET	4.5
8	BP	5029	PHE	4.5
3	Bi	3004	ILE	4.5
3	Cq	3033	ILE	4.5
6	Bd	8004	GLU	4.5
8	BP	5001	PRO	4.5
3	BK	3010	TYR	4.4
7	A3	6164	ASN	4.4
8	BP	5004	LEU	4.4
6	Ad	8017	CYS	4.4
8	Bf	5000	HIS	4.4
8	Bf	5018	GLY	4.4
6	AV	8017	CYS	4.4
8	Bv	5040	CYS	4.4
7	Bu	6163	ALA	4.4
8	Bv	5035	LEU	4.3
8	Af	5000	HIS	4.3
6	A2	8004	GLU	4.3
6	Bl	8012	TYR	4.3
8	Bv	5067	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
8	Af	5069	GLU	4.3
8	Cv	5057	ILE	4.3
6	Bt	8019	ALA	4.3
8	Bv	5055	VAL	4.2
3	Aa	3007	ILE	4.2
8	Cv	5015	LYS	4.2
8	Bf	5026	LEU	4.2
8	BP	5037	ILE	4.2
7	CO	6164	ASN	4.2
8	Cv	5036	VAL	4.2
8	Cv	5054	MET	4.2
8	B4	5055	VAL	4.1
3	Bq	3036	PHE	4.1
3	Bq	3006	LEU	4.1
3	Aa	3001	VAL	4.1
6	Ct	8017	CYS	4.1
8	BX	5028	GLY	4.1
8	B4	5018	GLY	4.1
8	Af	5037	ILE	4.1
8	BP	5003	GLU	4.1
8	Bv	5068	LEU	4.1
5	Bk	7001	VAL	4.1
6	Bl	8004	GLU	4.1
8	A4	5004	LEU	4.0
8	B4	5057	ILE	4.0
8	Bv	5003	GLU	4.0
8	B4	5000	HIS	4.0
7	Bm	6000	MET	4.0
3	Bq	3030	GLU	4.0
8	Bn	5036	VAL	4.0
8	B4	5040	CYS	4.0
6	BN	8019	ALA	4.0
6	Bt	8014	ARG	4.0
8	A4	5000	HIS	4.0
3	Aa	3009	ARG	4.0
6	BV	8010	MET	4.0
6	B2	8007	LEU	4.0
3	AS	3009	ARG	3.9
8	Bv	5000	HIS	3.9
7	Cu	6000	MET	3.9
3	BK	3032	CYS	3.9
3	AS	3033	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
3	Cq	3010	TYR	3.9
6	Ad	8019	ALA	3.9
7	Bm	6163	ALA	3.9
6	BV	8017	CYS	3.9
3	Aa	3000	MET	3.9
8	CP	5001	PRO	3.9
3	Cq	3004	ILE	3.9
6	BF	8024	ARG	3.9
2	Bp	2008	GLU	3.8
8	Cv	5013	SER	3.8
8	Cv	5035	LEU	3.8
2	BJ	2000	PRO	3.8
6	AN	8004	GLU	3.8
3	BC	3006	LEU	3.8
8	Af	5004	LEU	3.8
8	Av	5001	PRO	3.8
4	Cr	4030	VAL	3.8
8	Bf	5068	LEU	3.8
8	Af	5002	PRO	3.7
8	Af	5003	GLU	3.7
7	AG	6164	ASN	3.7
8	Cv	5031	PRO	3.7
8	CP	5002	PRO	3.7
3	Cq	3057	ARG	3.7
7	BO	6163	ALA	3.7
8	CP	5000	HIS	3.7
8	A4	5003	GLU	3.7
8	Af	5057	ILE	3.7
6	Ct	8019	ALA	3.7
8	CP	5055	VAL	3.7
6	BN	8002	SER	3.7
3	BK	3000	MET	3.7
6	BF	8004	GLU	3.6
8	Cv	5003	GLU	3.6
8	BP	5065	LEU	3.6
8	Cv	5004	LEU	3.6
8	Cn	5055	VAL	3.6
7	AO	6164	ASN	3.6
8	Af	5067	ALA	3.6
6	Bl	8006	TYR	3.6
3	AS	3074	GLN	3.6
8	Bn	5028	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
8	Af	5034	ASN	3.6
8	B4	5026	LEU	3.6
2	Cp	2009	LEU	3.6
4	CL	4053	LEU	3.6
4	Ab	4002	LYS	3.6
7	BO	6000	MET	3.6
6	At	8017	CYS	3.5
8	BP	5000	HIS	3.5
6	BN	8017	CYS	3.5
8	B4	5035	LEU	3.5
3	By	3036	PHE	3.5
8	BP	5068	LEU	3.5
6	Bt	8011	PHE	3.5
4	AT	4002	LYS	3.5
2	BJ	2009	LEU	3.5
8	Cv	5032	PHE	3.5
5	BM	7001	VAL	3.5
4	BL	4001	PRO	3.5
8	Bn	5001	PRO	3.5
3	Bi	3074	GLN	3.5
3	CC	3006	LEU	3.5
8	A4	5035	LEU	3.5
6	Cd	8011	PHE	3.4
8	AP	5002	PRO	3.4
3	Bq	3010	TYR	3.4
6	BN	8008	MET	3.4
6	Ct	8010	MET	3.4
3	AS	3036	PHE	3.4
8	Cv	5027	ARG	3.4
3	BS	3032	CYS	3.4
8	Cv	5040	CYS	3.4
3	AS	3044	LEU	3.4
8	Bf	5028	GLY	3.4
7	Cm	6000	MET	3.4
7	CG	6164	ASN	3.4
3	Aq	3044	LEU	3.4
8	Bn	5003	GLU	3.4
7	Am	6164	ASN	3.4
7	B3	6164	ASN	3.4
3	Ba	3004	ILE	3.4
3	CK	3000	MET	3.4
7	Ae	6163	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
8	Af	5068	LEU	3.4
7	CW	6164	ASN	3.4
8	B4	5012	LEU	3.3
2	Bh	2000	PRO	3.3
8	Av	5028	GLY	3.3
8	B4	5028	GLY	3.3
3	Ba	3074	GLN	3.3
8	Bv	5018	GLY	3.3
6	Bl	8007	LEU	3.3
8	BP	5069	GLU	3.3
8	AX	5036	VAL	3.3
8	Af	5031	PRO	3.3
6	Bd	8014	ARG	3.3
3	Aa	3044	LEU	3.3
6	Bl	8010	MET	3.3
8	Cv	5014	LEU	3.3
8	Bf	5057	ILE	3.3
8	Bv	5057	ILE	3.3
8	BH	5055	VAL	3.3
8	Bf	5035	LEU	3.3
6	Bt	8007	LEU	3.3
3	Cq	3032	CYS	3.3
3	BS	3044	LEU	3.3
3	Aq	3074	GLN	3.3
8	Bv	5064	MET	3.2
4	Br	4030	VAL	3.2
6	BN	8005	GLU	3.2
8	Cn	5001	PRO	3.2
6	BN	8014	ARG	3.2
3	BS	3060	LEU	3.2
3	Ay	3009	ARG	3.2
3	Aa	3010	TYR	3.2
3	BK	3060	LEU	3.2
8	A4	5005	LYS	3.2
7	Be	6000	MET	3.2
8	BX	5003	GLU	3.2
8	Cv	5039	GLU	3.2
8	Bn	5005	LYS	3.2
8	Cv	5063	ILE	3.2
8	BX	5055	VAL	3.2
3	By	3006	LEU	3.2
3	Bq	3033	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
6	B2	8010	MET	3.2
8	Bf	5005	LYS	3.1
8	Cv	5001	PRO	3.1
6	At	8010	MET	3.1
6	Ct	8004	GLU	3.1
8	CP	5026	LEU	3.1
6	BV	8014	ARG	3.1
6	Bd	8012	TYR	3.1
8	BX	5001	PRO	3.1
3	CK	3006	LEU	3.1
8	Bv	5039	GLU	3.1
6	BF	8012	TYR	3.1
6	Bt	8004	GLU	3.1
7	Ae	6000	MET	3.1
8	Cn	5004	LEU	3.1
6	Ad	8006	TYR	3.1
6	Ad	8015	LYS	3.1
3	Ci	3000	MET	3.1
8	Cv	5019	GLY	3.1
6	B2	8012	TYR	3.1
6	Bd	8007	LEU	3.1
8	CH	5002	PRO	3.1
6	At	8019	ALA	3.1
2	BJ	2016	GLU	3.1
3	BK	3001	VAL	3.1
6	Ad	8007	LEU	3.1
8	AX	5035	LEU	3.1
2	Bp	2009	LEU	3.1
3	Aq	3036	PHE	3.1
8	CP	5003	GLU	3.1
8	Bn	5029	PHE	3.1
8	Af	5026	LEU	3.0
4	BT	4001	PRO	3.0
8	Af	5001	PRO	3.0
2	Cp	2000	PRO	3.0
7	AW	6163	ALA	3.0
6	Cl	8012	TYR	3.0
3	Aa	3073	LEU	3.0
6	Ad	8023	LYS	3.0
3	BK	3009	ARG	3.0
6	Ad	8010	MET	3.0
6	Ad	8004	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
3	BS	3010	TYR	3.0
6	Bt	8024	ARG	3.0
8	AX	5069	GLU	3.0
8	Bv	5005	LYS	3.0
8	B4	5003	GLU	3.0
3	Cq	3007	ILE	3.0
4	AT	4005	LEU	3.0
3	BS	3000	MET	3.0
3	Cq	3044	LEU	3.0
6	BN	8016	ARG	3.0
6	Bt	8003	GLY	3.0
5	Ck	7001	VAL	3.0
8	BP	5067	ALA	3.0
8	AX	5029	PHE	3.0
3	BC	3033	ILE	3.0
6	Ad	8011	PHE	3.0
3	Aa	3006	LEU	2.9
3	Ay	3006	LEU	2.9
7	Cm	6163	ALA	2.9
6	B2	8004	GLU	2.9
3	Aa	3074	GLN	2.9
3	Ay	3074	GLN	2.9
3	AS	3073	LEU	2.9
8	AX	5068	LEU	2.9
8	BX	5026	LEU	2.9
6	Ct	8018	PRO	2.9
3	Bi	3009	ARG	2.9
6	AV	8023	LYS	2.9
6	Bl	8014	ARG	2.9
8	Cv	5056	VAL	2.9
8	A4	5057	ILE	2.9
8	Af	5032	PHE	2.9
8	Bn	5035	LEU	2.9
6	Ct	8011	PHE	2.9
6	Bl	8003	GLY	2.9
6	Bt	8008	MET	2.9
6	CF	8011	PHE	2.9
6	Bl	8016	ARG	2.9
8	B4	5069	GLU	2.9
2	Bp	2000	PRO	2.9
4	BL	4036	MET	2.9
3	Aq	3033	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
6	Bl	8015	LYS	2.9
7	Ae	6001	VAL	2.9
6	B2	8006	TYR	2.9
7	Ce	6164	ASN	2.9
4	BT	4005	LEU	2.8
8	Cv	5068	LEU	2.8
8	Av	5031	PRO	2.8
8	Bf	5040	CYS	2.8
3	CC	3000	MET	2.8
4	BL	4005	LEU	2.8
6	Ct	8007	LEU	2.8
3	BK	3072	LEU	2.8
2	CR	2004	MET	2.8
8	AX	5002	PRO	2.8
2	Bx	2004	MET	2.8
3	AS	3000	MET	2.8
8	Av	5069	GLU	2.8
3	Bi	3073	LEU	2.8
6	Ct	8008	MET	2.8
2	Bx	2016	GLU	2.8
2	Bp	2004	MET	2.8
8	Bf	5007	PHE	2.8
7	B3	6000	MET	2.8
6	Ct	8006	TYR	2.8
4	BL	4002	LYS	2.8
8	Af	5013	SER	2.8
5	BU	7001	VAL	2.8
8	Af	5008	MET	2.8
6	BN	8024	ARG	2.8
8	AP	5000	HIS	2.8
8	Bv	5007	PHE	2.7
3	CS	3000	MET	2.7
6	Bd	8006	TYR	2.7
2	Bh	2004	MET	2.7
4	BD	4002	LYS	2.7
6	BN	8007	LEU	2.7
8	BH	5002	PRO	2.7
6	At	8007	LEU	2.7
8	Af	5018	GLY	2.7
6	Bt	8002	SER	2.7
3	Cq	3076	VAL	2.7
6	Bd	8015	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
8	Bv	5033	MET	2.7
7	A3	6030	GLY	2.7
8	Bn	5067	ALA	2.7
3	AS	3018	GLN	2.7
3	AS	3035	GLY	2.7
8	Bv	5061	SER	2.7
6	Ad	8018	PRO	2.7
6	Cd	8007	LEU	2.7
8	Cn	5067	ALA	2.7
3	AS	3007	ILE	2.7
3	BK	3045	ASP	2.7
7	Cm	6027	LYS	2.7
8	Bn	5057	ILE	2.7
2	BZ	2004	MET	2.7
8	Af	5064	MET	2.7
6	AV	8007	LEU	2.7
8	Af	5066	GLU	2.7
8	Cv	5069	GLU	2.7
3	Ca	3000	MET	2.7
3	BK	3018	GLN	2.7
8	Cv	5002	PRO	2.7
8	B4	5007	PHE	2.7
3	Bi	3044	LEU	2.7
3	By	3007	ILE	2.7
6	BN	8004	GLU	2.7
8	AX	5003	GLU	2.7
6	Bl	8024	ARG	2.7
3	Bq	3044	LEU	2.7
8	AP	5055	VAL	2.7
8	BP	5064	MET	2.7
8	BX	5036	VAL	2.7
8	B4	5005	LYS	2.7
8	CP	5037	ILE	2.7
3	Aa	3036	PHE	2.6
8	AX	5001	PRO	2.6
6	B2	8024	ARG	2.6
2	BJ	2025	LEU	2.6
3	BK	3013	ASN	2.6
6	BF	8051	LEU	2.6
6	AV	8015	LYS	2.6
7	Au	6163	ALA	2.6
6	Ct	8009	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	BZ	2008	GLU	2.6
2	Bh	2003	GLU	2.6
4	BD	4026	TYR	2.6
8	Cn	5037	ILE	2.6
4	Cr	4012	PRO	2.6
6	Ct	8021	VAL	2.6
8	Cn	5000	HIS	2.6
8	Cv	5062	ILE	2.6
5	CM	7001	VAL	2.6
2	Bx	2008	GLU	2.6
8	Bv	5069	GLU	2.6
3	Aq	3000	MET	2.6
6	BV	8006	TYR	2.6
8	B4	5036	VAL	2.6
3	Bq	3007	ILE	2.6
6	Bt	8006	TYR	2.6
6	Bt	8012	TYR	2.6
8	Bv	5054	MET	2.6
8	Bf	5029	PHE	2.6
8	BP	5032	PHE	2.6
8	A4	5068	LEU	2.6
8	BP	5020	ARG	2.6
8	Bv	5020	ARG	2.6
6	BF	8011	PHE	2.6
6	Bt	8005	GLU	2.6
6	AV	8010	MET	2.6
6	Bl	8008	MET	2.6
3	Ba	3033	ILE	2.6
6	BV	8018	PRO	2.6
2	BB	2016	GLU	2.6
8	Bv	5063	ILE	2.6
5	Ck	7000	ALA	2.6
2	BR	2009	LEU	2.6
3	Aa	3021	LEU	2.6
6	Al	8024	ARG	2.6
6	Bl	8002	SER	2.6
2	BZ	2003	GLU	2.6
3	Bq	3038	GLU	2.6
7	CG	6000	MET	2.5
8	Bv	5006	LYS	2.5
8	CX	5000	HIS	2.5
4	Br	4034	MET	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
7	Bu	6000	MET	2.5
8	CH	5026	LEU	2.5
8	A4	5036	VAL	2.5
3	Aq	3018	GLN	2.5
3	Ba	3036	PHE	2.5
2	AZ	2004	MET	2.5
4	Ab	4005	LEU	2.5
7	Be	6163	ALA	2.5
2	Cp	2007	GLU	2.5
3	AK	3074	GLN	2.5
6	AV	8011	PHE	2.5
2	BZ	2000	PRO	2.5
6	Bt	8034	ASN	2.5
8	Af	5056	VAL	2.5
3	Ba	3007	ILE	2.5
3	Cq	3060	LEU	2.5
8	Bf	5036	VAL	2.5
4	BD	4005	LEU	2.5
3	AS	3063	ILE	2.5
2	Cp	2004	MET	2.5
8	BX	5029	PHE	2.5
5	CM	7000	ALA	2.5
6	Bt	8009	HIS	2.5
3	BS	3018	GLN	2.5
4	Br	4005	LEU	2.5
6	CN	8034	ASN	2.5
8	AX	5004	LEU	2.5
8	Af	5005	LYS	2.5
6	B2	8003	GLY	2.5
8	BX	5031	PRO	2.5
8	Bf	5069	GLU	2.5
3	BK	3007	ILE	2.5
6	CN	8008	MET	2.5
4	Bj	4001	PRO	2.5
4	CL	4002	LYS	2.5
6	Ct	8012	TYR	2.5
7	BG	6163	ALA	2.5
3	By	3030	GLU	2.5
6	AV	8019	ALA	2.5
8	CH	5003	GLU	2.4
3	Aq	3001	VAL	2.4
6	BF	8034	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
6	Ct	8003	GLY	2.4
3	Bi	3033	ILE	2.4
8	BX	5000	HIS	2.4
3	Bi	3072	LEU	2.4
3	CK	3076	VAL	2.4
6	Bl	8005	GLU	2.4
2	Bp	2001	LYS	2.4
8	Cn	5032	PHE	2.4
6	BV	8012	TYR	2.4
8	CX	5002	PRO	2.4
8	Af	5039	GLU	2.4
8	Bn	5066	GLU	2.4
8	AX	5000	HIS	2.4
6	At	8011	PHE	2.4
6	CV	8011	PHE	2.4
6	Bd	8010	MET	2.4
3	Cq	3006	LEU	2.4
8	Af	5054	MET	2.4
7	BO	6161	ASP	2.4
6	BV	8005	GLU	2.4
6	Ct	8015	LYS	2.4
6	BV	8007	LEU	2.4
6	CF	8007	LEU	2.4
2	Cp	2001	LYS	2.4
6	Al	8019	ALA	2.4
2	AZ	2007	GLU	2.4
3	Ay	3076	VAL	2.4
3	BK	3063	ILE	2.4
2	CJ	2000	PRO	2.4
3	AK	3009	ARG	2.4
3	Bq	3031	GLY	2.4
3	Aq	3007	ILE	2.4
3	Bq	3017	ILE	2.4
3	By	3004	ILE	2.4
3	BS	3076	VAL	2.4
5	BE	7001	VAL	2.4
2	Bx	2001	LYS	2.4
8	BP	5015	LYS	2.4
2	BJ	2005	THR	2.4
8	Bv	5031	PRO	2.4
8	Af	5038	ASP	2.4
8	BP	5009	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
3	Ba	3009	ARG	2.4
3	Ba	3058	LYS	2.4
6	Bd	8003	GLY	2.4
4	Aj	4005	LEU	2.4
3	Cq	3031	GLY	2.4
8	AP	5028	GLY	2.3
4	BD	4030	VAL	2.3
8	AH	5000	HIS	2.3
8	Av	5000	HIS	2.3
3	BS	3001	VAL	2.3
4	Ar	4002	LYS	2.3
8	Av	5055	VAL	2.3
6	BF	8019	ALA	2.3
3	Aq	3009	ARG	2.3
3	Aa	3032	CYS	2.3
8	Bv	5065	LEU	2.3
8	Bv	5001	PRO	2.3
6	CN	8010	MET	2.3
8	Cv	5033	MET	2.3
8	Cf	5001	PRO	2.3
6	CF	8024	ARG	2.3
3	Aa	3072	LEU	2.3
3	BS	3074	GLN	2.3
3	Ba	3044	LEU	2.3
3	CC	3036	PHE	2.3
3	CK	3033	ILE	2.3
3	Cq	3002	GLN	2.3
4	Br	4001	PRO	2.3
2	AR	2008	GLU	2.3
2	BZ	2001	LYS	2.3
3	BK	3036	PHE	2.3
6	Bt	8023	LYS	2.3
8	Cv	5005	LYS	2.3
3	Bq	3009	ARG	2.3
8	BH	5026	LEU	2.3
3	BK	3002	GLN	2.3
3	CK	3004	ILE	2.3
8	Bf	5012	LEU	2.3
8	Cn	5008	MET	2.3
8	AH	5002	PRO	2.3
8	CH	5000	HIS	2.3
7	BG	6000	MET	2.3

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Mol	Chain	Res	Type	RSRZ
2	Bp	2025	LEU	2.3
6	Ad	8002	SER	2.3
3	Bq	3004	ILE	2.3
8	Bv	5062	ILE	2.3
8	BP	5056	VAL	2.3
8	CH	5001	PRO	2.3
8	Bn	5014	LEU	2.3
3	Cq	3001	VAL	2.3
6	CN	8021	VAL	2.3
8	BH	5003	GLU	2.3
2	BJ	2004	MET	2.2
8	B4	5031	PRO	2.2
2	Bh	2001	LYS	2.2
8	AX	5037	ILE	2.2
3	Ba	3072	LEU	2.2
6	BF	8007	LEU	2.2
8	A4	5054	MET	2.2
3	Bq	3063	ILE	2.2
2	CB	2003	GLU	2.2
7	A3	6000	MET	2.2
3	Ba	3017	ILE	2.2
3	Bq	3072	LEU	2.2
4	CL	4026	TYR	2.2
3	BS	3007	ILE	2.2
4	BL	4034	MET	2.2
8	AX	5031	PRO	2.2
8	Bn	5063	ILE	2.2
6	AV	8004	GLU	2.2
2	AR	2004	MET	2.2
8	BX	5054	MET	2.2
8	Bv	5056	VAL	2.2
2	Bp	2016	GLU	2.2
8	Af	5015	LYS	2.2
6	CN	8006	TYR	2.2
8	AX	5057	ILE	2.2
8	B4	5061	SER	2.2
6	AN	8007	LEU	2.2
6	B2	8016	ARG	2.2
3	By	3017	ILE	2.2
3	Aa	3013	ASN	2.2
3	Aa	3076	VAL	2.2
2	Bh	2008	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	By	3038	GLU	2.2
4	BT	4002	LYS	2.2
8	BP	5005	LYS	2.2
6	AF	8004	GLU	2.2
3	Bq	3065	LEU	2.2
5	Bs	7001	VAL	2.2
8	Bn	5020	ARG	2.2
2	BR	2000	PRO	2.2
4	Bb	4001	PRO	2.2
8	B4	5039	GLU	2.2
3	Aq	3073	LEU	2.2
3	By	3065	LEU	2.2
2	Ap	2008	GLU	2.2
2	BR	2013	GLU	2.2
6	AV	8014	ARG	2.2
6	BN	8023	LYS	2.2
8	Cv	5018	GLY	2.2
4	Cr	4034	MET	2.2
8	A4	5001	PRO	2.2
6	B2	8005	GLU	2.2
7	BW	6163	ALA	2.2
4	Br	4068	GLY	2.2
6	At	8023	LYS	2.2
8	Bn	5056	VAL	2.2
6	Cl	8024	ARG	2.2
2	Bh	2016	GLU	2.1
8	Af	5007	PHE	2.1
6	Ad	8008	MET	2.1
8	Bn	5027	ARG	2.1
8	Af	5022	VAL	2.1
8	AP	5003	GLU	2.1
8	Bf	5025	ILE	2.1
6	Al	8004	GLU	2.1
3	Ci	3002	GLN	2.1
6	CN	8014	ARG	2.1
6	CN	8050	CYS	2.1
6	BF	8138	THR	2.1
8	BX	5037	ILE	2.1
8	Bn	5025	ILE	2.1
8	Cv	5066	GLU	2.1
7	Ae	6051	GLY	2.1
8	BP	5008	MET	2.1

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Mol	Chain	Res	Type	RSRZ
8	Bf	5067	ALA	2.1
8	CX	5001	PRO	2.1
8	B4	5063	ILE	2.1
8	Bn	5008	MET	2.1
3	Bq	3060	LEU	2.1
4	BL	4027	LEU	2.1
6	CN	8051	LEU	2.1
6	BF	8006	TYR	2.1
8	Cn	5002	PRO	2.1
7	Cu	6130	GLY	2.1
3	Aa	3018	GLN	2.1
3	Ca	3036	PHE	2.1
8	A4	5007	PHE	2.1
2	Ch	2004	MET	2.1
6	B2	8002	SER	2.1
8	B4	5067	ALA	2.1
8	BH	5000	HIS	2.1
7	CW	6163	ALA	2.1
4	Cr	4004	PHE	2.1
6	Bd	8008	MET	2.1
3	BC	3009	ARG	2.1
5	CE	7000	ALA	2.1
7	A3	6163	ALA	2.1
8	BP	5027	ARG	2.1
8	BH	5037	ILE	2.1
6	BN	8015	LYS	2.1
6	B2	8019	ALA	2.1
3	Bq	3035	GLY	2.1
8	Cn	5028	GLY	2.1
8	Cv	5006	LYS	2.1
8	Bn	5007	PHE	2.1
3	By	3033	ILE	2.1
4	Br	4032	GLY	2.1
6	CV	8012	TYR	2.1
7	Bm	6130	GLY	2.1
4	Cr	4028	VAL	2.1
2	Bh	2006	PRO	2.1
2	Cp	2008	GLU	2.1
8	Cv	5060	ASN	2.1
2	Bp	2013	GLU	2.1
3	By	3072	LEU	2.1
4	BL	4004	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
6	CV	8138	THR	2.1
8	AX	5018	GLY	2.1
8	An	5000	HIS	2.1
5	CU	7000	ALA	2.1
6	Bd	8028	ILE	2.1
8	CX	5004	LEU	2.1
4	CL	4030	VAL	2.0
2	BJ	2013	GLU	2.0
8	BX	5035	LEU	2.0
6	A2	8008	MET	2.0
2	Bx	2003	GLU	2.0
3	AS	3013	ASN	2.0
3	AS	3021	LEU	2.0
3	Cq	3030	GLU	2.0
6	A2	8017	CYS	2.0
6	Bd	8002	SER	2.0
8	Bv	5027	ARG	2.0
2	Ch	2099	GLY	2.0
6	AF	8019	ALA	2.0
6	CF	8019	ALA	2.0
8	BH	5004	LEU	2.0
7	Bm	6079	LYS	2.0
6	Cd	8024	ARG	2.0
2	Ch	2003	GLU	2.0
4	BD	4055	GLU	2.0
8	Cv	5029	PHE	2.0
7	Bm	6162	SER	2.0
6	BV	8020	VAL	2.0
2	Bx	2000	PRO	2.0
6	B2	8015	LYS	2.0
6	Ct	8020	VAL	2.0
8	Af	5046	SER	2.0
3	BK	3020	TRP	2.0
3	Bi	3006	LEU	2.0
3	Cq	3072	LEU	2.0
4	Cr	4068	GLY	2.0
6	BF	8008	MET	2.0
6	Bt	8015	LYS	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	SO4	Ad	8301	5/5	0.22	-0.53	137,139,139,140	0
9	SO4	Bt	8301	5/5	0.17	-0.55	111,113,114,115	0
9	SO4	Cl	8301	5/5	0.16	-0.93	129,131,132,132	0
9	SO4	BF	8301	5/5	0.17	-0.96	129,129,130,131	0
9	SO4	B2	8301	5/5	0.15	-1.03	97,99,99,103	0
9	SO4	BV	8301	5/5	0.14	-1.13	111,113,114,116	0
9	SO4	A2	8301	5/5	0.13	-1.37	150,150,150,151	0
9	SO4	At	8301	5/5	0.15	-1.39	92,93,96,99	0
9	SO4	Bd	8301	5/5	0.11	-1.55	108,108,109,112	0
9	SO4	CF	8301	5/5	0.12	-1.61	100,103,104,106	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.