



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 09:30 PM BST

PDB ID : 4V7G  
Title : Crystal Structure of Lumazine Synthase from Bacillus Anthracis  
Authors : Morgunova, E.; Illarionov, B.; Saller, S.; Popov, A.; Sambaiah, T.; Bacher, A.;  
Cushman, M.; Fischer, M.; Ladenstein, R.  
Deposited on : 2009-09-16  
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

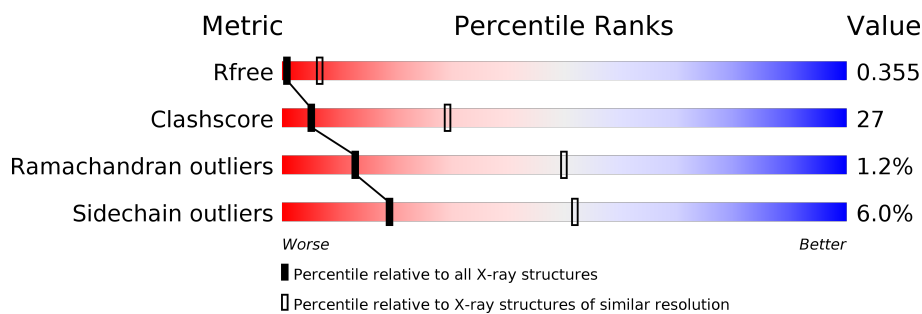
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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




























Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A1	153	56% 40% ..
1	A2	153	58% 38% ..
1	A3	153	55% 37% 7% .
1	A4	153	56% 37% 6% .
1	AA	153	61% 35% ..
1	AB	153	55% 41% ..
1	AC	153	56% 41% ..















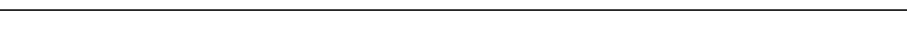




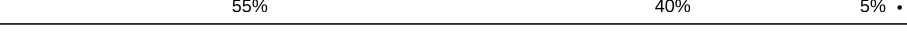





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Mol	Chain	Length	Quality of chain
1	AD	153	 52% 41% 7% .
1	AE	153	 55% 39% 6% .
1	AF	153	 59% 37% . .
1	AG	153	 54% 42% . .
1	AH	153	 58% 38% . .
1	AI	153	 53% 40% 7% .
1	AJ	153	 55% 39% 6% .
1	AK	153	 58% 37% . .
1	AL	153	 57% 39% . .
1	AM	153	 57% 39% . .
1	AN	153	 54% 39% 7% .
1	AO	153	 55% 39% 6% .
1	AP	153	 58% 37% . .
1	AQ	153	 55% 41% . .
1	AR	153	 56% 41% . .
1	AS	153	 54% 39% 7% .
1	AT	153	 57% 37% 6% .
1	AU	153	 58% 38% . .
1	AV	153	 56% 40% . .
1	AW	153	 57% 39% . .
1	AX	153	 55% 39% 6% .
1	AY	153	 56% 37% 6% .
1	AZ	153	 61% 35% . .
1	B1	153	 56% 39% 5% .
1	B2	153	 58% 38% . .


























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Mol	Chain	Length	Quality of chain
1	B3	153	 55% 39% 6% .
1	B4	153	 57% 37% 6% .
1	BA	153	 59% 36% . .
1	BB	153	 54% 41% 5% .
1	BC	153	 55% 41% . .
1	BD	153	 52% 41% 7% .
1	BE	153	 56% 37% 6% .
1	BF	153	 55% 41% . .
1	BG	153	 56% 39% 5% .
1	BH	153	 56% 40% . .
1	BI	153	 55% 38% 7% .
1	BJ	153	 54% 39% 6% .
1	BK	153	 59% 37% . .
1	BL	153	 54% 41% 5% .
1	BM	153	 58% 38% . .
1	BN	153	 54% 39% 7% .
1	BO	153	 56% 37% 6% .
1	BP	153	 60% 35% . .
1	BQ	153	 55% 40% 5% .
1	BR	153	 55% 41% . .
1	BS	153	 54% 39% 7% .
1	BT	153	 56% 37% 6% .
1	BU	153	 55% 41% . .
1	BV	153	 55% 40% 5% .
1	BW	153	 56% 40% . .

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Mol	Chain	Length	Quality of chain
1	BX	153	 55% 38% 7% .
1	BY	153	 55% 39% 6% ..
1	BZ	153	 60% 35% . .
1	C1	153	 56% 39% 5% .
1	C2	153	 55% 41% . .
1	C3	153	 50% 43% 6% .
1	C4	153	 56% 38% 6% .
1	CA	153	 57% 39% . .
1	CB	153	 55% 40% 5% .
1	CC	153	 57% 39% . .
1	CD	153	 52% 41% 7% .
1	CE	153	 57% 37% 6% .
1	CF	153	 55% 41% . .
1	CG	153	 52% 43% 5% .
1	CH	153	 54% 41% . .
1	CI	153	 54% 39% 7% .
1	CJ	153	 56% 38% 6% .
1	CK	153	 59% 37% . .
1	CL	153	 56% 39% 5% .
1	CM	153	 55% 41% . .
1	CN	153	 53% 39% 7% .
1	CO	153	 54% 39% 6% .
1	CP	153	 58% 38% . .
1	CQ	153	 55% 40% 5% .
1	CR	153	 54% 41% . .

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Mol	Chain	Length	Quality of chain
1	CS	153	 54% 39% 7% .
1	CT	153	 53% 41% 6% .
1	CU	153	 56% 39% . .
1	CV	153	 56% 39% 5% .
1	CW	153	 53% 42% . .
1	CX	153	 52% 41% 7% .
1	CY	153	 56% 37% 6% .
1	CZ	153	 59% 37% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A2	1001	-	-	X	-
2	PO4	A4	1001	-	-	X	-
2	PO4	AC	1001	-	-	X	-
2	PO4	AE	1001	-	-	X	-
2	PO4	AH	1001	-	-	X	-
2	PO4	AJ	1001	-	-	X	-
2	PO4	AM	1001	-	-	X	-
2	PO4	AO	1001	-	-	X	-
2	PO4	AR	1001	-	-	X	-
2	PO4	AT	1001	-	-	X	-
2	PO4	AW	201	-	-	X	-
2	PO4	AY	1001	-	-	X	-
2	PO4	B2	1001	-	-	X	-
2	PO4	B4	1001	-	-	X	-
2	PO4	BC	1001	-	-	X	-
2	PO4	BE	1001	-	-	X	-
2	PO4	BH	1001	-	-	X	-
2	PO4	BJ	1001	-	-	X	-
2	PO4	BM	1001	-	-	X	-
2	PO4	BO	1001	-	-	X	-
2	PO4	BR	1001	-	-	X	-
2	PO4	BT	1001	-	-	X	-
2	PO4	BW	1001	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	BY	1001	-	-	X	-
2	PO4	C2	2201	-	-	X	-
2	PO4	C4	4201	-	-	X	-
2	PO4	CC	1001	-	-	X	-
2	PO4	CE	1001	-	-	X	-
2	PO4	CH	2201	-	-	X	-
2	PO4	CJ	4201	-	-	X	-
2	PO4	CM	2201	-	-	X	-
2	PO4	CO	4201	-	-	X	-
2	PO4	CR	2201	-	-	X	-
2	PO4	CT	4201	-	-	X	-
2	PO4	CW	2201	-	-	X	-
2	PO4	CY	4201	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 102534 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 6,7-dimethyl-8-ribityllumazine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	152	Total	C	N	O	S	0	0	0
			1129	723	193	210	3			
1	AB	152	Total	C	N	O	S	0	0	0
			1129	723	193	210	3			
1	AC	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AD	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AE	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AF	152	Total	C	N	O	S	0	0	0
			1129	723	193	210	3			
1	AG	152	Total	C	N	O	S	0	0	0
			1129	723	193	210	3			
1	AH	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AI	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AJ	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AK	152	Total	C	N	O	S	0	0	0
			1129	723	193	210	3			
1	AL	152	Total	C	N	O	S	0	0	0
			1129	723	193	210	3			
1	AM	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AN	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AO	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AP	152	Total	C	N	O	S	0	0	0
			1129	723	193	210	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	152	Total	C	N	O	S	0	0	0
			1129	723	193	210	3			
1	AR	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AS	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AT	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AU	152	Total	C	N	O	S	0	0	0
			1129	723	193	210	3			
1	AV	152	Total	C	N	O	S	0	0	0
			1129	723	193	210	3			
1	AW	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AX	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AY	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	AZ	152	Total	C	N	O	S	0	0	0
			1129	723	193	210	3			
1	A1	152	Total	C	N	O	S	0	0	0
			1129	723	193	210	3			
1	A2	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	A3	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	A4	152	Total	C	N	O	S	0	0	0
			1132	724	193	212	3			
1	BA	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BB	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BC	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BD	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BE	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BF	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BG	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BH	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BI	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BJ	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BK	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BL	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BM	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BN	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BO	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BP	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BQ	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BR	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BS	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BT	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BU	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BV	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BW	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BX	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BY	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	BZ	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	B1	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	B2	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			

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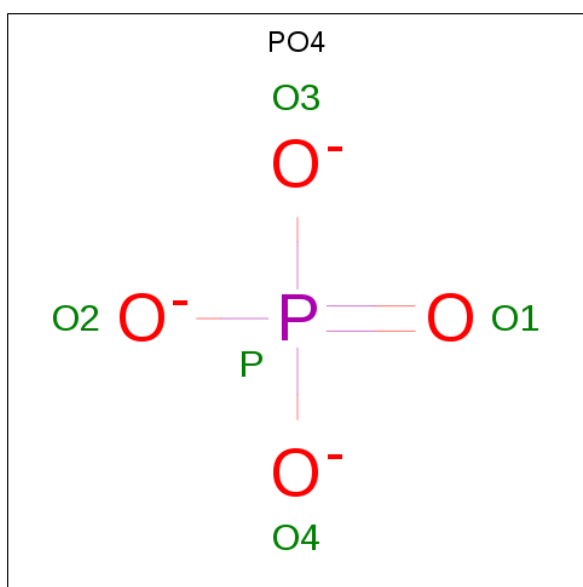
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B3	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	B4	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CA	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CB	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CC	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CD	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CE	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CF	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CG	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CH	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CI	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CJ	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CK	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CL	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CM	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CN	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CO	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CP	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CQ	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CR	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0
1	CS	152	Total 1136	C 726	N 193	O 214	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CT	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	CU	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	CV	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	CW	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	CX	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	CY	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	CZ	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	C1	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	C2	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	C3	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			
1	C4	152	Total	C	N	O	S	0	0	0
			1136	726	193	214	3			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AA	1	Total	O	P	0	0
			5	4	1		
2	AB	1	Total	O	P	0	0
			5	4	1		
2	AC	1	Total	O	P	0	0
			5	4	1		
2	AD	1	Total	O	P	0	0
			5	4	1		
2	AE	1	Total	O	P	0	0
			5	4	1		
2	AF	1	Total	O	P	0	0
			5	4	1		
2	AG	1	Total	O	P	0	0
			5	4	1		
2	AH	1	Total	O	P	0	0
			5	4	1		
2	AI	1	Total	O	P	0	0
			5	4	1		
2	AJ	1	Total	O	P	0	0
			5	4	1		
2	AK	1	Total	O	P	0	0
			5	4	1		
2	AL	1	Total	O	P	0	0
			5	4	1		
2	AM	1	Total	O	P	0	0
			5	4	1		
2	AN	1	Total	O	P	0	0
			5	4	1		
2	AO	1	Total	O	P	0	0
			5	4	1		
2	AP	1	Total	O	P	0	0
			5	4	1		
2	AQ	1	Total	O	P	0	0
			5	4	1		
2	AR	1	Total	O	P	0	0
			5	4	1		
2	AS	1	Total	O	P	0	0
			5	4	1		
2	AT	1	Total	O	P	0	0
			5	4	1		
2	AU	1	Total	O	P	0	0
			5	4	1		
2	AV	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AW	1	Total	O	P	0	0
			5	4	1		
2	AX	1	Total	O	P	0	0
			5	4	1		
2	AY	1	Total	O	P	0	0
			5	4	1		
2	AZ	1	Total	O	P	0	0
			5	4	1		
2	A1	1	Total	O	P	0	0
			5	4	1		
2	A2	1	Total	O	P	0	0
			5	4	1		
2	A3	1	Total	O	P	0	0
			5	4	1		
2	A4	1	Total	O	P	0	0
			5	4	1		
2	BA	1	Total	O	P	0	0
			5	4	1		
2	BB	1	Total	O	P	0	0
			5	4	1		
2	BC	1	Total	O	P	0	0
			5	4	1		
2	BD	1	Total	O	P	0	0
			5	4	1		
2	BE	1	Total	O	P	0	0
			5	4	1		
2	BF	1	Total	O	P	0	0
			5	4	1		
2	BG	1	Total	O	P	0	0
			5	4	1		
2	BH	1	Total	O	P	0	0
			5	4	1		
2	BI	1	Total	O	P	0	0
			5	4	1		
2	BJ	1	Total	O	P	0	0
			5	4	1		
2	BK	1	Total	O	P	0	0
			5	4	1		
2	BL	1	Total	O	P	0	0
			5	4	1		
2	BM	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	BN	1	Total	O	P	0	0
			5	4	1		
2	BO	1	Total	O	P	0	0
			5	4	1		
2	BP	1	Total	O	P	0	0
			5	4	1		
2	BQ	1	Total	O	P	0	0
			5	4	1		
2	BR	1	Total	O	P	0	0
			5	4	1		
2	BS	1	Total	O	P	0	0
			5	4	1		
2	BT	1	Total	O	P	0	0
			5	4	1		
2	BU	1	Total	O	P	0	0
			5	4	1		
2	BV	1	Total	O	P	0	0
			5	4	1		
2	BW	1	Total	O	P	0	0
			5	4	1		
2	BX	1	Total	O	P	0	0
			5	4	1		
2	BY	1	Total	O	P	0	0
			5	4	1		
2	BZ	1	Total	O	P	0	0
			5	4	1		
2	B1	1	Total	O	P	0	0
			5	4	1		
2	B2	1	Total	O	P	0	0
			5	4	1		
2	B3	1	Total	O	P	0	0
			5	4	1		
2	B4	1	Total	O	P	0	0
			5	4	1		
2	CA	1	Total	O	P	0	0
			5	4	1		
2	CB	1	Total	O	P	0	0
			5	4	1		
2	CC	1	Total	O	P	0	0
			5	4	1		
2	CD	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	CE	1	Total	O	P	0	0
			5	4	1		
2	CF	1	Total	O	P	0	0
			5	4	1		
2	CG	1	Total	O	P	0	0
			5	4	1		
2	CH	1	Total	O	P	0	0
			5	4	1		
2	CI	1	Total	O	P	0	0
			5	4	1		
2	CJ	1	Total	O	P	0	0
			5	4	1		
2	CK	1	Total	O	P	0	0
			5	4	1		
2	CL	1	Total	O	P	0	0
			5	4	1		
2	CM	1	Total	O	P	0	0
			5	4	1		
2	CN	1	Total	O	P	0	0
			5	4	1		
2	CO	1	Total	O	P	0	0
			5	4	1		
2	CP	1	Total	O	P	0	0
			5	4	1		
2	CQ	1	Total	O	P	0	0
			5	4	1		
2	CR	1	Total	O	P	0	0
			5	4	1		
2	CS	1	Total	O	P	0	0
			5	4	1		
2	CT	1	Total	O	P	0	0
			5	4	1		
2	CU	1	Total	O	P	0	0
			5	4	1		
2	CV	1	Total	O	P	0	0
			5	4	1		
2	CW	1	Total	O	P	0	0
			5	4	1		
2	CX	1	Total	O	P	0	0
			5	4	1		
2	CY	1	Total	O	P	0	0
			5	4	1		

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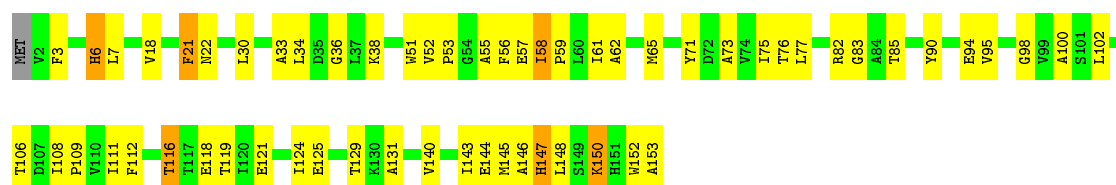
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	CZ	1	Total	O	P	0	0
			5	4	1		
2	C1	1	Total	O	P	0	0
			5	4	1		
2	C2	1	Total	O	P	0	0
			5	4	1		
2	C3	1	Total	O	P	0	0
			5	4	1		
2	C4	1	Total	O	P	0	0
			5	4	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

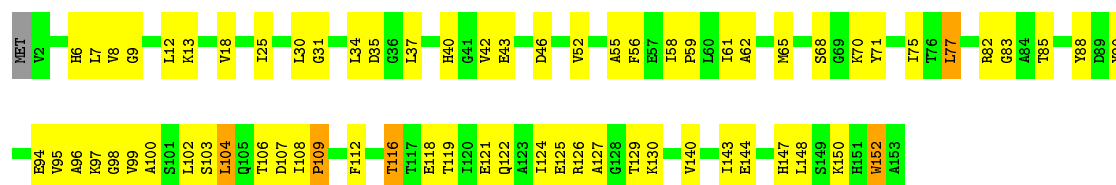
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AA: 



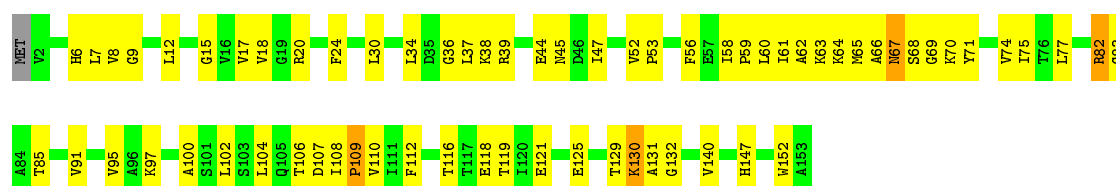
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AB: 



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

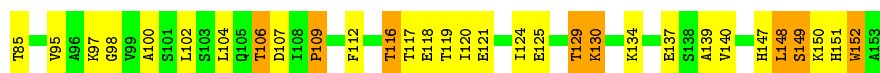
Chain AC: 



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

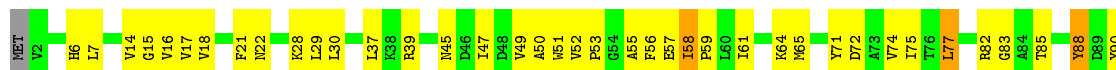
Chain AD: 





- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AE: 55% 39% 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AF: 59% 37%



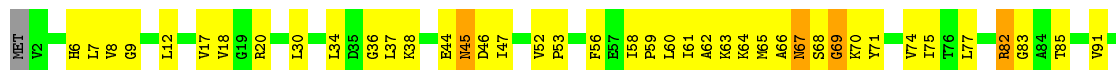
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AG: 54% 42%



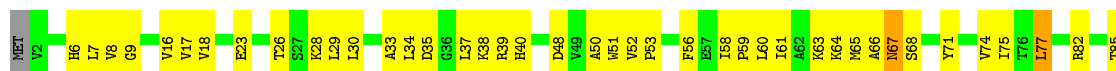
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AH: 58% 38%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

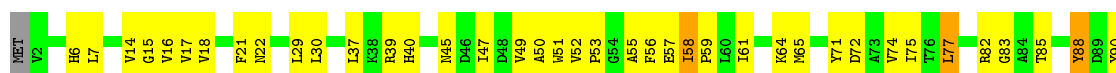
Chain AI: 53% 40% 7%





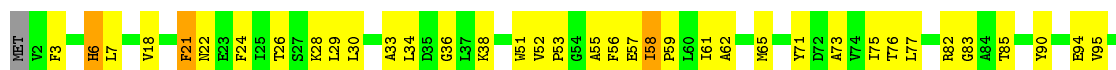
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AJ: 55% 39% 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AK: 58% 37%



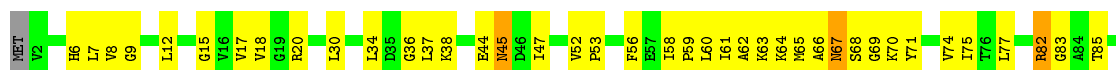
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AL: 57% 39%



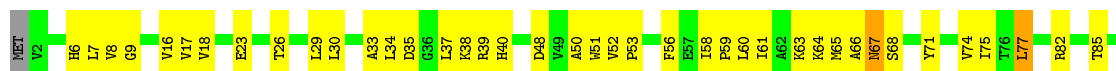
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AM: 57% 39%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

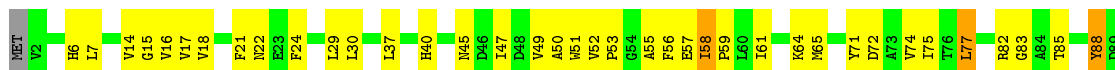
Chain AN: 54% 39% 7%





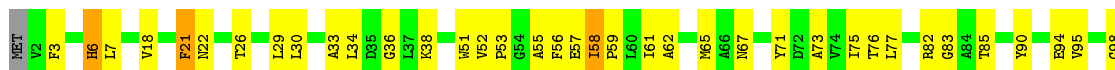
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AO: 55% 39% 6% •



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AP: 58% 37% • •



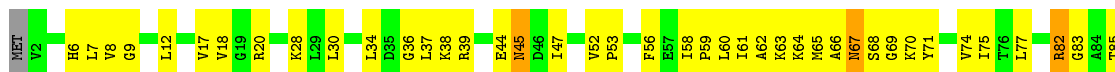
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AQ: 55% 41% • •



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

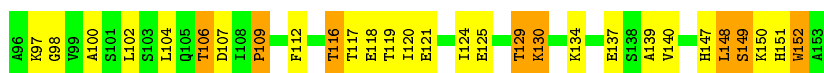
Chain AR: 56% 41% • •



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

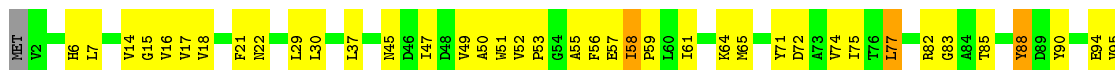
Chain AS: 54% 39% 7% •





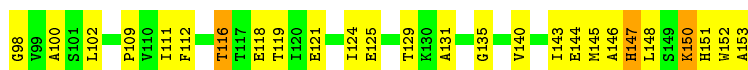
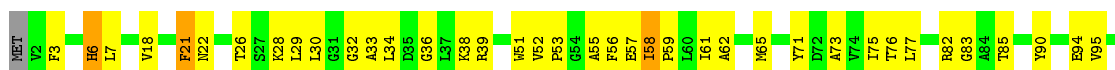
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AT: 57% 37% 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AU: 58% 38% 4%



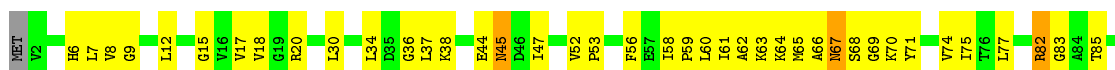
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AV: 56% 40% 4%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AW: 57% 39% 4%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

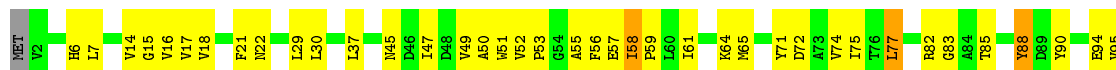
Chain AX: 55% 39% 6%





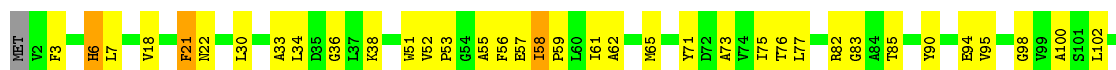
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AY: 56% 37% 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain AZ: 61% 35% 4%



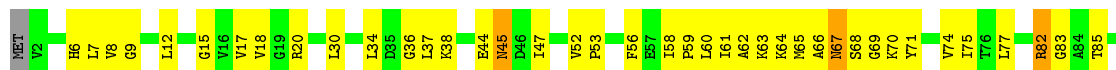
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain A1: 56% 40% 4%



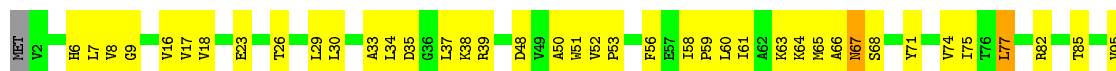
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain A2: 58% 38% 4%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

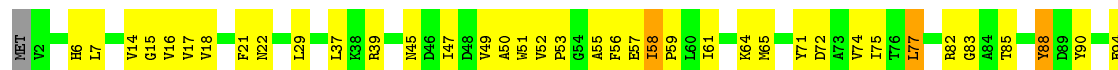
Chain A3: 55% 37% 7%





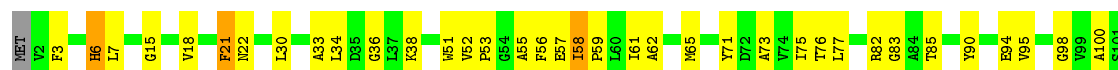
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain A4: 56% 37% 6% •



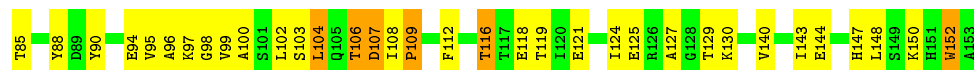
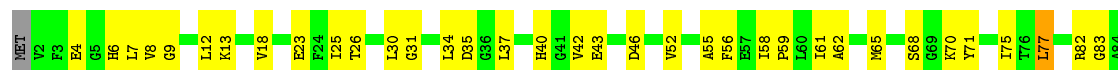
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BA: 59% 36% • •



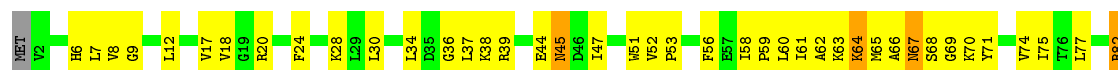
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BB: 54% 41% 5% •



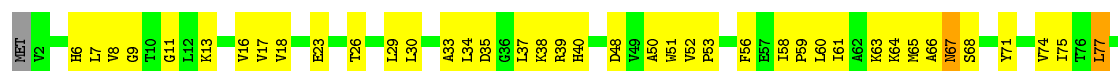
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BC: 55% 41% • •

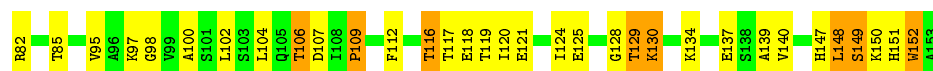


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BD: 52% 41% 7% •

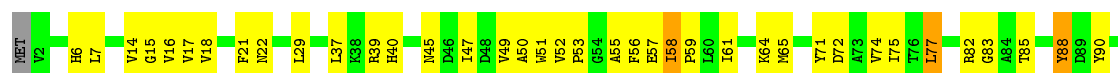






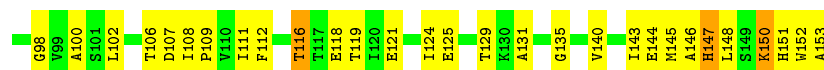
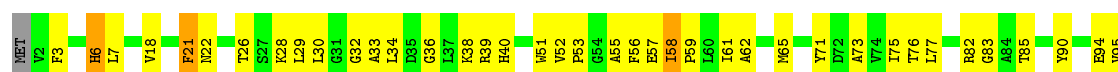
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BE: 56% 37% 6% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BF: 55% 41% . .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BG: 56% 39% 5% .



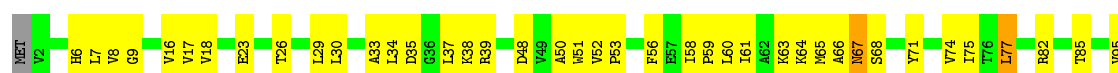
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BH: 56% 40% . .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

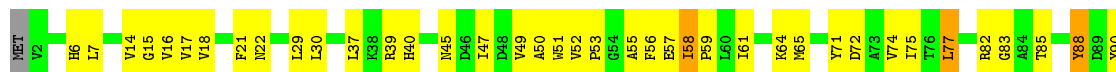
Chain BI: 55% 38% 7% .





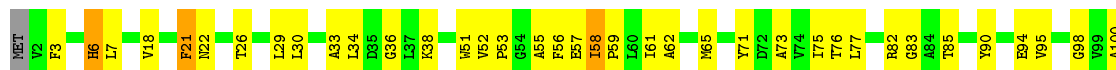
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BJ: 54% 39% 6% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BK: 59% 37% . .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BL: 54% 41% 5% .



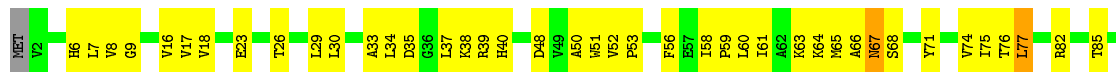
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BM: 58% 38% . .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BN: 54% 39% 7% .





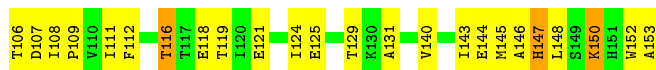
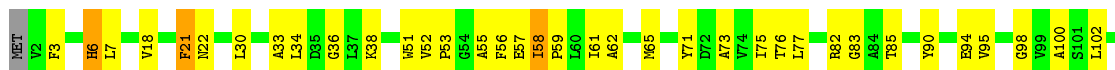
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BO: 56% 37% 6% .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BP: 60% 35% . .



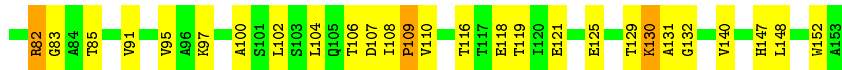
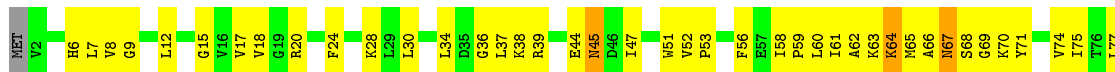
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BQ: 55% 40% 5% .



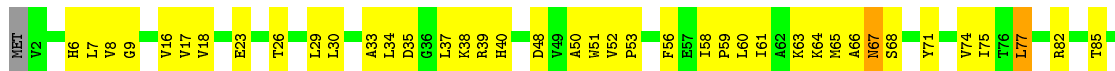
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BR: 55% 41% . .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

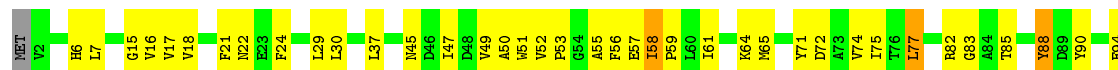
Chain BS: 54% 39% 7% .





- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BT: 56% 37% 6% •



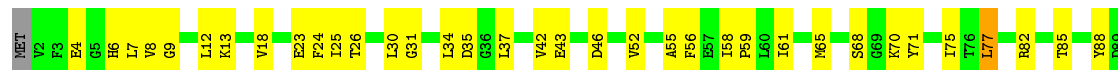
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BU: 55% 41% • •



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BV: 55% 40% 5% •



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BW: 56% 40% • •



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

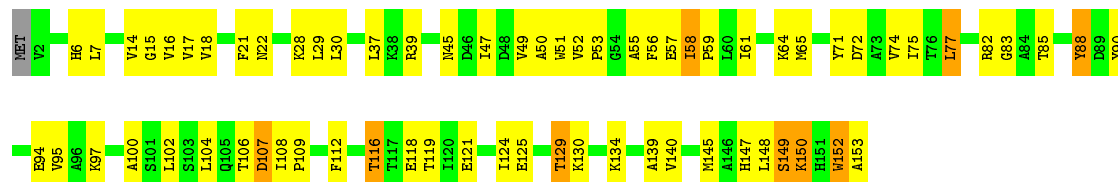
Chain BX: 55% 38% 7% •





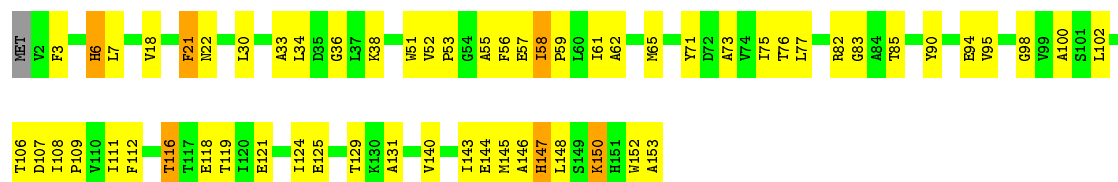
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BY: 55% 39% 6%



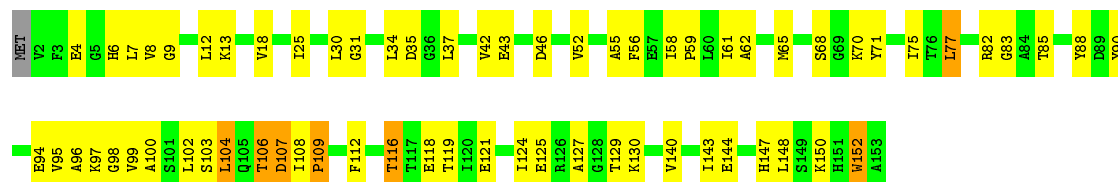
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain BZ: 60% 35% 5%



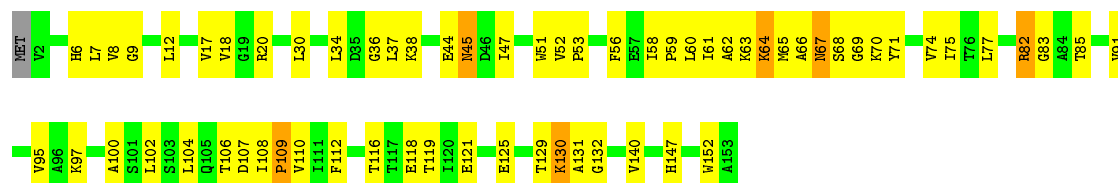
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B1: 56% 39% 5%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B2: 58% 38% 4%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

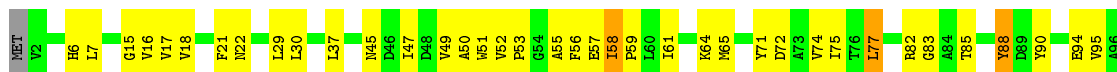
Chain B3: 55% 39% 6%





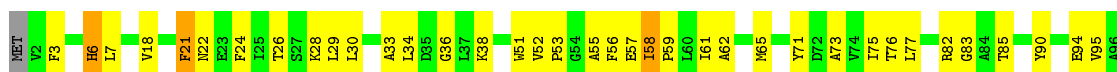
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain B4: 57% 37% 6%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CA: 57% 39% 4%



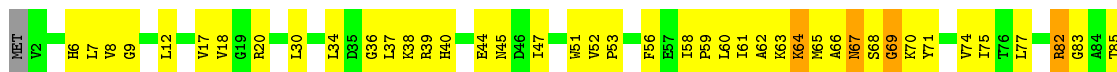
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CB: 55% 40% 5%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

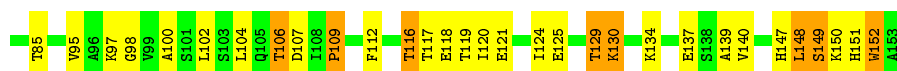
Chain CC: 57% 39% 4%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

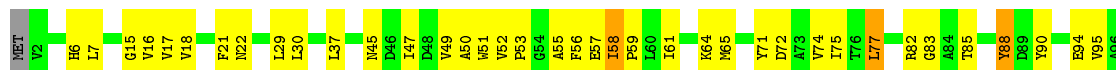
Chain CD: 52% 41% 7%





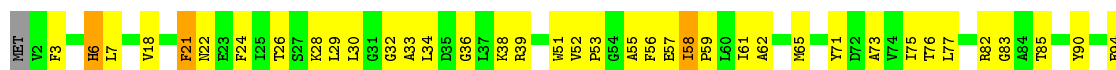
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CE: 57% 37% 6%



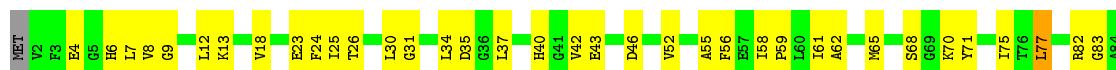
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CF: 55% 41% 4%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CG: 52% 43% 5%



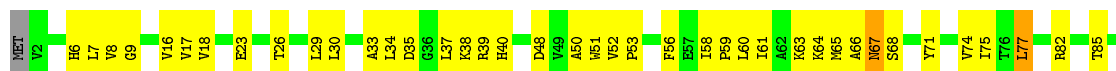
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CH: 54% 41% 5%



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

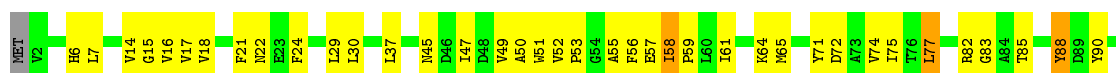
Chain CI: 54% 39% 7%





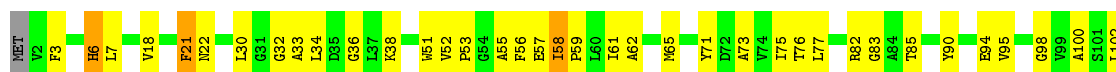
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CJ: 56% 38% 6% .



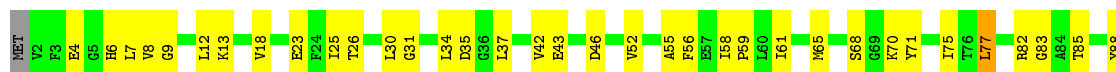
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CK: 59% 37% . .



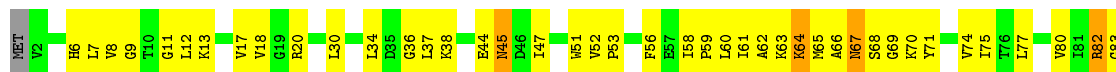
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CL: 56% 39% 5% .



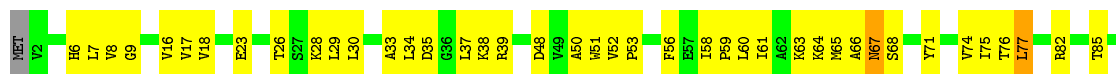
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CM: 55% 41% . .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CN: 53% 39% 7% .

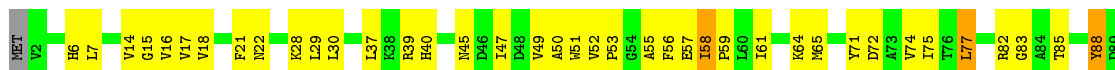






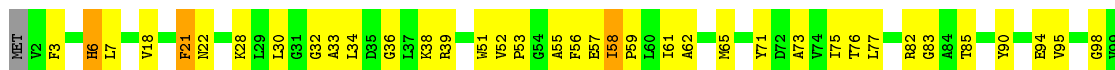
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CO: 54% 39% 6% .



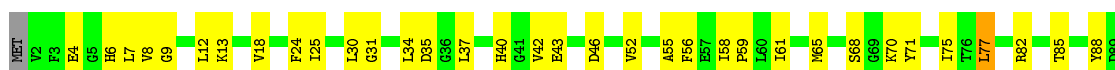
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CP: 58% 38% . .



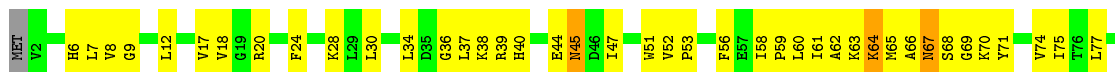
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CQ: 55% 40% 5% .



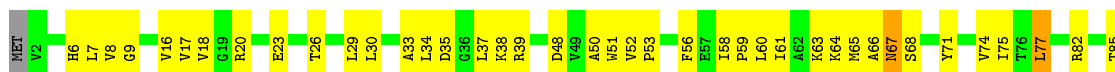
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

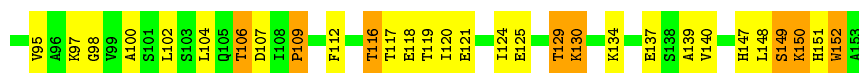
Chain CR: 54% 41% . .



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

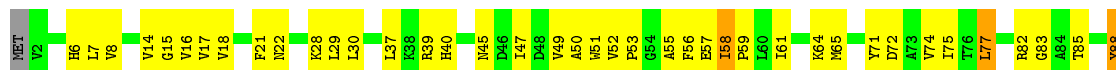
Chain CS: 54% 39% 7% .





- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CT: 53% 41% 6% •



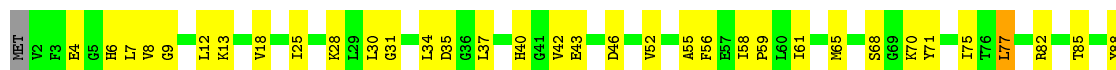
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CU: 56% 39% • •



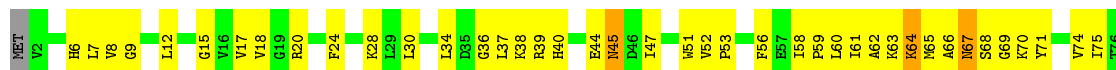
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CV: 56% 39% 5% •



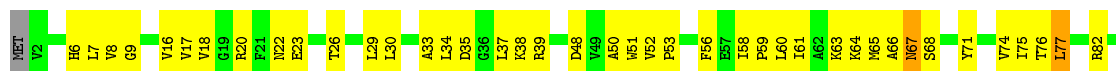
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

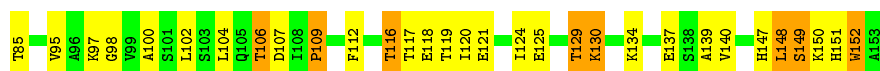
Chain CW: 53% 42% • •



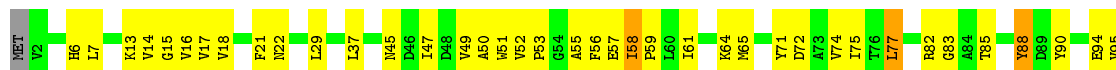
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

Chain CX: 52% 41% 7% •

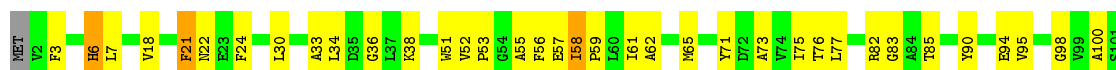




- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



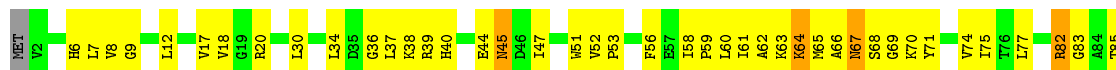
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



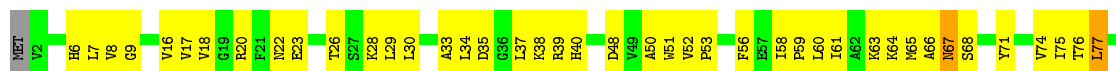
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

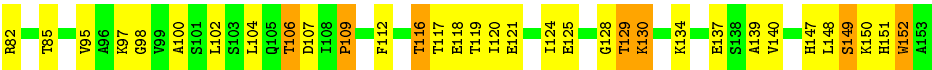


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase





● Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.20 Å   222.24 Å   473.49 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	15.00 – 3.50 39.90 – 3.50	Depositor EDS
% Data completeness (in resolution range)	89.8 (15.00-3.50) 93.0 (39.90-3.50)	Depositor EDS
$R_{merge}$	0.29	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 3.48 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.235   ,   0.286 0.351   ,   0.355	Depositor DCC
$R_{free}$ test set	3896 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.0	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 79.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.73	EDS
Total number of atoms	102534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	A1	0.44	0/1149	0.71	2/1558 (0.1%)
1	A2	0.32	0/1152	0.62	1/1562 (0.1%)
1	A3	0.31	0/1152	0.85	5/1562 (0.3%)
1	A4	0.34	0/1152	0.58	1/1562 (0.1%)
1	AA	0.33	0/1149	0.49	1/1558 (0.1%)
1	AB	0.44	0/1149	0.71	2/1558 (0.1%)
1	AC	0.32	0/1152	0.62	1/1562 (0.1%)
1	AD	0.31	0/1152	0.85	5/1562 (0.3%)
1	AE	0.34	0/1152	0.58	1/1562 (0.1%)
1	AF	0.33	0/1149	0.49	1/1558 (0.1%)
1	AG	0.44	0/1149	0.71	2/1558 (0.1%)
1	AH	0.32	0/1152	0.63	1/1562 (0.1%)
1	AI	0.31	0/1152	0.85	5/1562 (0.3%)
1	AJ	0.34	0/1152	0.58	1/1562 (0.1%)
1	AK	0.33	0/1149	0.49	1/1558 (0.1%)
1	AL	0.44	0/1149	0.71	2/1558 (0.1%)
1	AM	0.32	0/1152	0.63	1/1562 (0.1%)
1	AN	0.31	0/1152	0.85	5/1562 (0.3%)
1	AO	0.34	0/1152	0.58	1/1562 (0.1%)
1	AP	0.33	0/1149	0.49	1/1558 (0.1%)
1	AQ	0.44	0/1149	0.71	2/1558 (0.1%)
1	AR	0.32	0/1152	0.62	1/1562 (0.1%)
1	AS	0.31	0/1152	0.85	5/1562 (0.3%)
1	AT	0.34	0/1152	0.58	1/1562 (0.1%)
1	AU	0.33	0/1149	0.49	1/1558 (0.1%)
1	AV	0.44	0/1149	0.71	2/1558 (0.1%)
1	AW	0.32	0/1152	0.63	1/1562 (0.1%)
1	AX	0.31	0/1152	0.85	5/1562 (0.3%)
1	AY	0.34	0/1152	0.58	1/1562 (0.1%)
1	AZ	0.33	0/1149	0.49	1/1558 (0.1%)
1	B1	0.44	0/1156	0.72	3/1567 (0.2%)
1	B2	0.32	0/1156	0.62	1/1567 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	B3	0.31	0/1156	0.85	5/1567 (0.3%)
1	B4	0.34	0/1156	0.58	1/1567 (0.1%)
1	BA	0.32	0/1156	0.51	2/1567 (0.1%)
1	BB	0.44	0/1156	0.72	3/1567 (0.2%)
1	BC	0.32	0/1156	0.62	1/1567 (0.1%)
1	BD	0.31	0/1156	0.85	5/1567 (0.3%)
1	BE	0.34	0/1156	0.58	1/1567 (0.1%)
1	BF	0.32	0/1156	0.51	2/1567 (0.1%)
1	BG	0.44	0/1156	0.72	3/1567 (0.2%)
1	BH	0.32	0/1156	0.62	1/1567 (0.1%)
1	BI	0.31	0/1156	0.85	5/1567 (0.3%)
1	BJ	0.34	0/1156	0.58	1/1567 (0.1%)
1	BK	0.32	0/1156	0.51	2/1567 (0.1%)
1	BL	0.44	0/1156	0.72	3/1567 (0.2%)
1	BM	0.32	0/1156	0.62	1/1567 (0.1%)
1	BN	0.31	0/1156	0.85	5/1567 (0.3%)
1	BO	0.34	0/1156	0.58	1/1567 (0.1%)
1	BP	0.33	0/1156	0.51	2/1567 (0.1%)
1	BQ	0.44	0/1156	0.72	3/1567 (0.2%)
1	BR	0.32	0/1156	0.62	1/1567 (0.1%)
1	BS	0.31	0/1156	0.85	5/1567 (0.3%)
1	BT	0.34	0/1156	0.58	1/1567 (0.1%)
1	BU	0.33	0/1156	0.51	2/1567 (0.1%)
1	BV	0.44	0/1156	0.72	3/1567 (0.2%)
1	BW	0.32	0/1156	0.62	1/1567 (0.1%)
1	BX	0.31	0/1156	0.85	5/1567 (0.3%)
1	BY	0.34	0/1156	0.58	1/1567 (0.1%)
1	BZ	0.33	0/1156	0.51	2/1567 (0.1%)
1	C1	0.44	0/1156	0.72	3/1567 (0.2%)
1	C2	0.32	0/1156	0.62	1/1567 (0.1%)
1	C3	0.31	0/1156	0.85	5/1567 (0.3%)
1	C4	0.34	0/1156	0.58	1/1567 (0.1%)
1	CA	0.33	0/1156	0.51	2/1567 (0.1%)
1	CB	0.44	0/1156	0.72	3/1567 (0.2%)
1	CC	0.32	0/1156	0.62	1/1567 (0.1%)
1	CD	0.31	0/1156	0.85	5/1567 (0.3%)
1	CE	0.34	0/1156	0.58	1/1567 (0.1%)
1	CF	0.33	0/1156	0.51	2/1567 (0.1%)
1	CG	0.44	0/1156	0.72	3/1567 (0.2%)
1	CH	0.32	0/1156	0.62	1/1567 (0.1%)
1	CI	0.31	0/1156	0.85	5/1567 (0.3%)
1	CJ	0.34	0/1156	0.58	1/1567 (0.1%)
1	CK	0.33	0/1156	0.51	2/1567 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	CL	0.44	0/1156	0.72	3/1567 (0.2%)
1	CM	0.32	0/1156	0.62	1/1567 (0.1%)
1	CN	0.31	0/1156	0.85	5/1567 (0.3%)
1	CO	0.34	0/1156	0.58	1/1567 (0.1%)
1	CP	0.32	0/1156	0.51	2/1567 (0.1%)
1	CQ	0.44	0/1156	0.72	3/1567 (0.2%)
1	CR	0.32	0/1156	0.62	1/1567 (0.1%)
1	CS	0.31	0/1156	0.85	5/1567 (0.3%)
1	CT	0.34	0/1156	0.58	1/1567 (0.1%)
1	CU	0.33	0/1156	0.51	2/1567 (0.1%)
1	CV	0.44	0/1156	0.72	3/1567 (0.2%)
1	CW	0.32	0/1156	0.62	1/1567 (0.1%)
1	CX	0.31	0/1156	0.85	5/1567 (0.3%)
1	CY	0.34	0/1156	0.58	1/1567 (0.1%)
1	CZ	0.33	0/1156	0.51	2/1567 (0.1%)
All	All	0.35	0/103884	0.67	204/140832 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A1	0	1
1	AB	0	1
1	AG	0	1
1	AL	0	1
1	AQ	0	1
1	AV	0	1
1	B1	0	1
1	BB	0	1
1	BG	0	1
1	BL	0	1
1	BQ	0	1
1	BV	0	1
1	C1	0	1
1	CB	0	1
1	CG	0	1
1	CL	0	1
1	CQ	0	1
1	CV	0	1
All	All	0	18



There are no bond length outliers.

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BD	149	SER	CB-CA-C	-14.91	81.78	110.10
1	CD	149	SER	CB-CA-C	-14.90	81.79	110.10
1	C3	149	SER	CB-CA-C	-14.89	81.80	110.10
1	BI	149	SER	CB-CA-C	-14.89	81.81	110.10
1	CX	149	SER	CB-CA-C	-14.89	81.81	110.10

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	99	VAL	Peptide
1	AG	99	VAL	Peptide
1	AL	99	VAL	Peptide
1	AQ	99	VAL	Peptide
1	AV	99	VAL	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	1129	0	1143	68	0
1	A2	1132	0	1145	77	0
1	A3	1132	0	1145	64	0
1	A4	1132	0	1145	75	0
1	AA	1129	0	1143	52	0
1	AB	1129	0	1143	73	0
1	AC	1132	0	1145	81	0
1	AD	1132	0	1145	71	0
1	AE	1132	0	1145	82	0
1	AF	1129	0	1143	57	0
1	AG	1129	0	1143	68	2
1	AH	1132	0	1145	76	3
1	AI	1132	0	1145	70	0
1	AJ	1132	0	1145	81	0
1	AK	1129	0	1143	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AL	1129	0	1143	68	0
1	AM	1132	0	1145	78	0
1	AN	1132	0	1145	64	0
1	AO	1132	0	1145	80	0
1	AP	1129	0	1143	53	0
1	AQ	1129	0	1143	90	0
1	AR	1132	0	1145	85	0
1	AS	1132	0	1145	65	0
1	AT	1132	0	1145	75	0
1	AU	1129	0	1143	58	0
1	AV	1129	0	1143	67	0
1	AW	1132	0	1145	78	0
1	AX	1132	0	1145	62	0
1	AY	1132	0	1145	75	0
1	AZ	1129	0	1143	50	0
1	B1	1136	0	1149	73	0
1	B2	1136	0	1149	78	0
1	B3	1136	0	1149	60	0
1	B4	1136	0	1149	73	0
1	BA	1136	0	1149	49	0
1	BB	1136	0	1149	81	0
1	BC	1136	0	1149	88	0
1	BD	1136	0	1149	75	0
1	BE	1136	0	1149	74	0
1	BF	1136	0	1149	64	0
1	BG	1136	0	1149	76	0
1	BH	1136	0	1149	80	0
1	BI	1136	0	1149	63	0
1	BJ	1136	0	1149	78	1
1	BK	1136	0	1149	51	0
1	BL	1136	0	1149	74	3
1	BM	1136	0	1149	78	0
1	BN	1136	0	1149	65	0
1	BO	1136	0	1149	75	0
1	BP	1136	0	1149	49	0
1	BQ	1136	0	1149	81	0
1	BR	1136	0	1149	90	0
1	BS	1136	0	1149	67	0
1	BT	1136	0	1149	74	0
1	BU	1136	0	1149	77	0
1	BV	1136	0	1149	75	0
1	BW	1136	0	1149	80	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BX	1136	0	1149	63	0
1	BY	1136	0	1149	77	0
1	BZ	1136	0	1149	49	0
1	C1	1136	0	1149	74	0
1	C2	1136	0	1149	91	0
1	C3	1136	0	1149	76	0
1	C4	1136	0	1149	74	1
1	CA	1136	0	1149	55	0
1	CB	1136	0	1149	75	2
1	CC	1136	0	1149	96	2
1	CD	1136	0	1149	75	0
1	CE	1136	0	1149	76	0
1	CF	1136	0	1149	64	0
1	CG	1136	0	1149	84	3
1	CH	1136	0	1149	86	3
1	CI	1136	0	1149	68	0
1	CJ	1136	0	1149	77	0
1	CK	1136	0	1149	52	0
1	CL	1136	0	1149	74	0
1	CM	1136	0	1149	86	3
1	CN	1136	0	1149	68	0
1	CO	1136	0	1149	80	0
1	CP	1136	0	1149	59	0
1	CQ	1136	0	1149	81	0
1	CR	1136	0	1149	96	0
1	CS	1136	0	1149	71	0
1	CT	1136	0	1149	83	0
1	CU	1136	0	1149	61	0
1	CV	1136	0	1149	77	0
1	CW	1136	0	1149	92	0
1	CX	1136	0	1149	69	0
1	CY	1136	0	1149	73	1
1	CZ	1136	0	1149	52	1
2	A1	5	0	0	0	0
2	A2	5	0	0	3	0
2	A3	5	0	0	0	0
2	A4	5	0	0	2	0
2	AA	5	0	0	1	0
2	AB	5	0	0	1	0
2	AC	5	0	0	3	0
2	AD	5	0	0	0	0
2	AE	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AF	5	0	0	1	0
2	AG	5	0	0	1	0
2	AH	5	0	0	3	0
2	AI	5	0	0	0	0
2	AJ	5	0	0	2	0
2	AK	5	0	0	1	0
2	AL	5	0	0	0	0
2	AM	5	0	0	3	0
2	AN	5	0	0	0	0
2	AO	5	0	0	2	0
2	AP	5	0	0	1	0
2	AQ	5	0	0	1	0
2	AR	5	0	0	3	0
2	AS	5	0	0	0	0
2	AT	5	0	0	2	0
2	AU	5	0	0	1	0
2	AV	5	0	0	1	0
2	AW	5	0	0	3	0
2	AX	5	0	0	0	0
2	AY	5	0	0	2	0
2	AZ	5	0	0	1	0
2	B1	5	0	0	1	0
2	B2	5	0	0	3	0
2	B3	5	0	0	0	0
2	B4	5	0	0	2	0
2	BA	5	0	0	1	0
2	BB	5	0	0	1	0
2	BC	5	0	0	3	0
2	BD	5	0	0	0	0
2	BE	5	0	0	2	0
2	BF	5	0	0	1	0
2	BG	5	0	0	1	0
2	BH	5	0	0	3	0
2	BI	5	0	0	0	0
2	BJ	5	0	0	2	0
2	BK	5	0	0	1	0
2	BL	5	0	0	1	0
2	BM	5	0	0	3	0
2	BN	5	0	0	0	0
2	BO	5	0	0	2	0
2	BP	5	0	0	1	0
2	BQ	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BR	5	0	0	3	0
2	BS	5	0	0	0	0
2	BT	5	0	0	2	0
2	BU	5	0	0	1	0
2	BV	5	0	0	0	0
2	BW	5	0	0	3	0
2	BX	5	0	0	0	0
2	BY	5	0	0	2	0
2	BZ	5	0	0	1	0
2	C1	5	0	0	1	0
2	C2	5	0	0	3	0
2	C3	5	0	0	0	0
2	C4	5	0	0	2	0
2	CA	5	0	0	1	0
2	CB	5	0	0	1	0
2	CC	5	0	0	3	0
2	CD	5	0	0	0	0
2	CE	5	0	0	2	0
2	CF	5	0	0	1	0
2	CG	5	0	0	1	0
2	CH	5	0	0	3	0
2	CI	5	0	0	0	0
2	CJ	5	0	0	2	0
2	CK	5	0	0	1	0
2	CL	5	0	0	1	0
2	CM	5	0	0	3	0
2	CN	5	0	0	0	0
2	CO	5	0	0	2	0
2	CP	5	0	0	1	0
2	CQ	5	0	0	0	0
2	CR	5	0	0	3	0
2	CS	5	0	0	0	0
2	CT	5	0	0	2	0
2	CU	5	0	0	1	0
2	CV	5	0	0	0	0
2	CW	5	0	0	3	0
2	CX	5	0	0	0	0
2	CY	5	0	0	2	0
2	CZ	5	0	0	1	0
All	All	102534	0	103266	5521	13

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

The worst 5 of 5521 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CT:53:PRO:CG	1:CT:57:GLU:HG3	1.49	1.43
1:CJ:53:PRO:CG	1:CJ:57:GLU:HG3	1.49	1.42
1:AE:53:PRO:CG	1:AE:57:GLU:HG3	1.49	1.42
1:B4:53:PRO:CG	1:B4:57:GLU:HG3	1.49	1.42
1:C4:53:PRO:CG	1:C4:57:GLU:HG3	1.49	1.42

The worst 5 of 13 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:153:ALA:O	1:AH:46:ASP:OD1[2_565]	1.84	0.36
1:AH:69:GLY:O	1:AH:69:GLY:O[2_565]	1.90	0.30
1:BJ:151:HIS:CE1	1:CY:13:LYS:CE[2_665]	1.91	0.29
1:CB:153:ALA:O	1:CC:69:GLY:CA[2_565]	1.94	0.26
1:CH:39:ARG:NH2	1:CM:20:ARG:NH1[2_665]	1.96	0.24

## 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	A1	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	A2	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	A3	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	A4	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	AA	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	AB	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	AC	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	AD	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AE	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	AF	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	AG	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	AH	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	AI	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	AJ	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	AK	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	AL	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	AM	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	AN	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	AO	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	AP	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	AQ	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	AR	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	AS	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	AT	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	AU	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	AV	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	AW	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	AX	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	AY	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	AZ	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	B1	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	B2	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	B3	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	B4	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	BA	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	BB	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	BC	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	BD	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	BE	150/153 (98%)	133 (89%)	17 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BF	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	BG	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	BH	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	BI	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	BJ	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	BK	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	BL	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	BM	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	BN	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	BO	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	BP	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	BQ	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	BR	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	BS	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	BT	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	BU	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	BV	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	BW	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	BX	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	BY	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	BZ	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	C1	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	C2	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	C3	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	C4	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	CA	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	CB	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	CC	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	CD	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	CE	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	CF	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CG	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	CH	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	CI	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	CJ	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	CK	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	CL	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	CM	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	CN	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	CO	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	CP	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	CQ	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	CR	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	CS	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	CT	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	CU	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
1	CV	150/153 (98%)	132 (88%)	18 (12%)	0	100	100
1	CW	150/153 (98%)	126 (84%)	19 (13%)	5 (3%)	4	28
1	CX	150/153 (98%)	137 (91%)	11 (7%)	2 (1%)	12	48
1	CY	150/153 (98%)	133 (89%)	17 (11%)	0	100	100
1	CZ	150/153 (98%)	129 (86%)	19 (13%)	2 (1%)	12	48
All	All	13500/13770 (98%)	11826 (88%)	1512 (11%)	162 (1%)	13	50

5 of 162 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AC	130	LYS
1	AH	130	LYS
1	AM	130	LYS
1	AR	130	LYS
1	AW	130	LYS

### 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	A1	115/118 (98%)	105 (91%)	10 (9%)	10	38
1	A2	116/118 (98%)	112 (97%)	4 (3%)	37	68
1	A3	116/118 (98%)	108 (93%)	8 (7%)	15	47
1	A4	116/118 (98%)	108 (93%)	8 (7%)	15	47
1	AA	115/118 (98%)	110 (96%)	5 (4%)	29	62
1	AB	115/118 (98%)	105 (91%)	10 (9%)	10	38
1	AC	116/118 (98%)	112 (97%)	4 (3%)	37	68
1	AD	116/118 (98%)	108 (93%)	8 (7%)	15	47
1	AE	116/118 (98%)	108 (93%)	8 (7%)	15	47
1	AF	115/118 (98%)	110 (96%)	5 (4%)	29	62
1	AG	115/118 (98%)	105 (91%)	10 (9%)	10	38
1	AH	116/118 (98%)	112 (97%)	4 (3%)	37	68
1	AI	116/118 (98%)	108 (93%)	8 (7%)	15	47
1	AJ	116/118 (98%)	108 (93%)	8 (7%)	15	47
1	AK	115/118 (98%)	110 (96%)	5 (4%)	29	62
1	AL	115/118 (98%)	105 (91%)	10 (9%)	10	38
1	AM	116/118 (98%)	112 (97%)	4 (3%)	37	68
1	AN	116/118 (98%)	108 (93%)	8 (7%)	15	47
1	AO	116/118 (98%)	108 (93%)	8 (7%)	15	47
1	AP	115/118 (98%)	110 (96%)	5 (4%)	29	62
1	AQ	115/118 (98%)	105 (91%)	10 (9%)	10	38
1	AR	116/118 (98%)	112 (97%)	4 (3%)	37	68
1	AS	116/118 (98%)	108 (93%)	8 (7%)	15	47
1	AT	116/118 (98%)	108 (93%)	8 (7%)	15	47
1	AU	115/118 (98%)	110 (96%)	5 (4%)	29	62
1	AV	115/118 (98%)	105 (91%)	10 (9%)	10	38
1	AW	116/118 (98%)	112 (97%)	4 (3%)	37	68
1	AX	116/118 (98%)	108 (93%)	8 (7%)	15	47
1	AY	116/118 (98%)	108 (93%)	8 (7%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AZ	115/118 (98%)	110 (96%)	5 (4%)	29	62
1	B1	117/118 (99%)	107 (92%)	10 (8%)	10	39
1	B2	117/118 (99%)	113 (97%)	4 (3%)	37	68
1	B3	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	B4	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	BA	117/118 (99%)	112 (96%)	5 (4%)	29	62
1	BB	117/118 (99%)	107 (92%)	10 (8%)	10	39
1	BC	117/118 (99%)	113 (97%)	4 (3%)	37	68
1	BD	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	BE	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	BF	117/118 (99%)	112 (96%)	5 (4%)	29	62
1	BG	117/118 (99%)	107 (92%)	10 (8%)	10	39
1	BH	117/118 (99%)	113 (97%)	4 (3%)	37	68
1	BI	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	BJ	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	BK	117/118 (99%)	112 (96%)	5 (4%)	29	62
1	BL	117/118 (99%)	107 (92%)	10 (8%)	10	39
1	BM	117/118 (99%)	113 (97%)	4 (3%)	37	68
1	BN	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	BO	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	BP	117/118 (99%)	112 (96%)	5 (4%)	29	62
1	BQ	117/118 (99%)	107 (92%)	10 (8%)	10	39
1	BR	117/118 (99%)	113 (97%)	4 (3%)	37	68
1	BS	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	BT	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	BU	117/118 (99%)	112 (96%)	5 (4%)	29	62
1	BV	117/118 (99%)	107 (92%)	10 (8%)	10	39
1	BW	117/118 (99%)	113 (97%)	4 (3%)	37	68
1	BX	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	BY	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	BZ	117/118 (99%)	112 (96%)	5 (4%)	29	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C1	117/118 (99%)	107 (92%)	10 (8%)	10	39
1	C2	117/118 (99%)	113 (97%)	4 (3%)	37	68
1	C3	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	C4	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	CA	117/118 (99%)	112 (96%)	5 (4%)	29	62
1	CB	117/118 (99%)	107 (92%)	10 (8%)	10	39
1	CC	117/118 (99%)	113 (97%)	4 (3%)	37	68
1	CD	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	CE	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	CF	117/118 (99%)	112 (96%)	5 (4%)	29	62
1	CG	117/118 (99%)	107 (92%)	10 (8%)	10	39
1	CH	117/118 (99%)	113 (97%)	4 (3%)	37	68
1	CI	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	CJ	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	CK	117/118 (99%)	112 (96%)	5 (4%)	29	62
1	CL	117/118 (99%)	107 (92%)	10 (8%)	10	39
1	CM	117/118 (99%)	113 (97%)	4 (3%)	37	68
1	CN	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	CO	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	CP	117/118 (99%)	112 (96%)	5 (4%)	29	62
1	CQ	117/118 (99%)	107 (92%)	10 (8%)	10	39
1	CR	117/118 (99%)	113 (97%)	4 (3%)	37	68
1	CS	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	CT	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	CU	117/118 (99%)	112 (96%)	5 (4%)	29	62
1	CV	117/118 (99%)	107 (92%)	10 (8%)	10	39
1	CW	117/118 (99%)	113 (97%)	4 (3%)	37	68
1	CX	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	CY	117/118 (99%)	109 (93%)	8 (7%)	16	48
1	CZ	117/118 (99%)	112 (96%)	5 (4%)	29	62
All	All	10488/10620 (99%)	9858 (94%)	630 (6%)	19	52

5 of 630 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BK	150	LYS
1	BU	116	THR
1	CX	109	PRO
1	BL	116	THR
1	BP	150	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 252 such sidechains are listed below:

Mol	Chain	Res	Type
1	BK	67	ASN
1	BU	45	ASN
1	CW	93	ASN
1	BL	93	ASN
1	BP	67	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

90 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
2	PO4	BV	1001	-	4,4,4	0.90	0	6,6,6	0.35	0
2	PO4	BI	1001	-	4,4,4	0.98	0	6,6,6	0.41	0
2	PO4	CZ	201	-	4,4,4	0.87	0	6,6,6	0.52	0
2	PO4	BQ	1001	-	4,4,4	0.90	0	6,6,6	0.35	0
2	PO4	C2	2201	-	4,4,4	1.00	0	6,6,6	0.53	0
2	PO4	CA	1001	-	4,4,4	0.87	0	6,6,6	0.52	0
2	PO4	AB	1001	-	4,4,4	0.90	0	6,6,6	0.35	0
2	PO4	AN	1001	-	4,4,4	0.96	0	6,6,6	0.41	0
2	PO4	C4	4201	-	4,4,4	0.95	0	6,6,6	0.58	0
2	PO4	BJ	1001	-	4,4,4	0.95	0	6,6,6	0.59	0
2	PO4	CU	201	-	4,4,4	0.87	0	6,6,6	0.51	0
2	PO4	AD	1001	-	4,4,4	0.97	0	6,6,6	0.41	0
2	PO4	BR	1001	-	4,4,4	1.01	0	6,6,6	0.54	0
2	PO4	CP	201	-	4,4,4	0.87	0	6,6,6	0.52	0
2	PO4	CS	3201	-	4,4,4	0.98	0	6,6,6	0.41	0
2	PO4	BM	1001	-	4,4,4	1.00	0	6,6,6	0.53	0
2	PO4	AG	1001	-	4,4,4	0.90	0	6,6,6	0.35	0
2	PO4	BG	1001	-	4,4,4	0.89	0	6,6,6	0.35	0
2	PO4	CG	1201	-	4,4,4	0.90	0	6,6,6	0.35	0
2	PO4	BY	1001	-	4,4,4	0.95	0	6,6,6	0.59	0
2	PO4	CO	4201	-	4,4,4	0.95	0	6,6,6	0.58	0
2	PO4	AZ	1001	-	4,4,4	0.88	0	6,6,6	0.52	0
2	PO4	CB	1001	-	4,4,4	0.90	0	6,6,6	0.36	0
2	PO4	AJ	1001	-	4,4,4	0.96	0	6,6,6	0.58	0
2	PO4	BB	1001	-	4,4,4	0.91	0	6,6,6	0.36	0
2	PO4	BS	1001	-	4,4,4	0.97	0	6,6,6	0.41	0
2	PO4	AC	1001	-	4,4,4	1.00	0	6,6,6	0.53	0
2	PO4	AR	1001	-	4,4,4	1.00	0	6,6,6	0.53	0
2	PO4	AK	1001	-	4,4,4	0.88	0	6,6,6	0.52	0
2	PO4	BC	1001	-	4,4,4	1.00	0	6,6,6	0.53	0
2	PO4	BZ	1001	-	4,4,4	0.87	0	6,6,6	0.52	0
2	PO4	B1	1001	-	4,4,4	0.91	0	6,6,6	0.36	0
2	PO4	A2	1001	-	4,4,4	1.01	0	6,6,6	0.53	0
2	PO4	BT	1001	-	4,4,4	0.96	0	6,6,6	0.58	0
2	PO4	AM	1001	-	4,4,4	1.00	0	6,6,6	0.53	0
2	PO4	AU	1001	-	4,4,4	0.87	0	6,6,6	0.51	0
2	PO4	CE	1001	-	4,4,4	0.96	0	6,6,6	0.59	0
2	PO4	BD	1001	-	4,4,4	0.96	0	6,6,6	0.41	0
2	PO4	BO	1001	-	4,4,4	0.95	0	6,6,6	0.58	0
2	PO4	AT	1001	-	4,4,4	0.96	0	6,6,6	0.58	0
2	PO4	BW	1001	-	4,4,4	1.00	0	6,6,6	0.54	0
2	PO4	B2	1001	-	4,4,4	1.01	0	6,6,6	0.54	0
2	PO4	A3	1001	-	4,4,4	0.97	0	6,6,6	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	C3	3201	-	4,4,4	0.98	0	6,6,6	0.41	0
2	PO4	CT	4201	-	4,4,4	0.96	0	6,6,6	0.59	0
2	PO4	BH	1001	-	4,4,4	1.01	0	6,6,6	0.54	0
2	PO4	CQ	1201	-	4,4,4	0.90	0	6,6,6	0.36	0
2	PO4	BP	1001	-	4,4,4	0.87	0	6,6,6	0.52	0
2	PO4	AH	1001	-	4,4,4	1.00	0	6,6,6	0.54	0
2	PO4	AE	1001	-	4,4,4	0.95	0	6,6,6	0.58	0
2	PO4	BL	1001	-	4,4,4	0.91	0	6,6,6	0.36	0
2	PO4	B3	1001	-	4,4,4	0.97	0	6,6,6	0.41	0
2	PO4	AP	1001	-	4,4,4	0.88	0	6,6,6	0.52	0
2	PO4	C1	1201	-	4,4,4	0.91	0	6,6,6	0.36	0
2	PO4	BE	1001	-	4,4,4	0.95	0	6,6,6	0.58	0
2	PO4	CW	2201	-	4,4,4	1.01	0	6,6,6	0.54	0
2	PO4	AV	1001	-	4,4,4	0.90	0	6,6,6	0.35	0
2	PO4	CK	201	-	4,4,4	0.88	0	6,6,6	0.52	0
2	PO4	B4	1001	-	4,4,4	0.94	0	6,6,6	0.58	0
2	PO4	CL	1201	-	4,4,4	0.91	0	6,6,6	0.36	0
2	PO4	AF	1001	-	4,4,4	0.87	0	6,6,6	0.51	0
2	PO4	BK	1001	-	4,4,4	0.88	0	6,6,6	0.52	0
2	PO4	CI	3201	-	4,4,4	0.97	0	6,6,6	0.41	0
2	PO4	BX	1001	-	4,4,4	0.96	0	6,6,6	0.40	0
2	PO4	CC	1001	-	4,4,4	1.00	0	6,6,6	0.53	0
2	PO4	BU	1001	-	4,4,4	0.87	0	6,6,6	0.52	0
2	PO4	CF	201	-	4,4,4	0.86	0	6,6,6	0.51	0
2	PO4	CR	2201	-	4,4,4	1.00	0	6,6,6	0.54	0
2	PO4	AQ	1001	-	4,4,4	0.90	0	6,6,6	0.36	0
2	PO4	CM	2201	-	4,4,4	1.00	0	6,6,6	0.54	0
2	PO4	AA	1001	-	4,4,4	0.88	0	6,6,6	0.52	0
2	PO4	A1	1001	-	4,4,4	0.90	0	6,6,6	0.36	0
2	PO4	BA	1001	-	4,4,4	0.88	0	6,6,6	0.52	0
2	PO4	AW	201	-	4,4,4	1.01	0	6,6,6	0.54	0
2	PO4	CN	3201	-	4,4,4	0.97	0	6,6,6	0.41	0
2	PO4	CD	1001	-	4,4,4	0.98	0	6,6,6	0.41	0
2	PO4	CJ	4201	-	4,4,4	0.95	0	6,6,6	0.58	0
2	PO4	AS	1001	-	4,4,4	0.97	0	6,6,6	0.41	0
2	PO4	AL	1001	-	4,4,4	0.90	0	6,6,6	0.35	0
2	PO4	CY	4201	-	4,4,4	0.95	0	6,6,6	0.58	0
2	PO4	BF	1001	-	4,4,4	0.88	0	6,6,6	0.52	0
2	PO4	CH	2201	-	4,4,4	1.01	0	6,6,6	0.53	0
2	PO4	CV	1201	-	4,4,4	0.90	0	6,6,6	0.36	0
2	PO4	BN	1001	-	4,4,4	0.97	0	6,6,6	0.41	0
2	PO4	CX	3201	-	4,4,4	0.96	0	6,6,6	0.41	0
2	PO4	AY	1001	-	4,4,4	0.96	0	6,6,6	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PO4	A4	1001	-	4,4,4	0.96	0	6,6,6	0.59	0
2	PO4	AI	1001	-	4,4,4	0.97	0	6,6,6	0.41	0
2	PO4	AO	1001	-	4,4,4	0.95	0	6,6,6	0.58	0
2	PO4	AX	1001	-	4,4,4	0.97	0	6,6,6	0.41	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.

67 monomers are involved in 121 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CZ	201	PO4	1	0
2	BQ	1001	PO4	1	0
2	C2	2201	PO4	3	0
2	CA	1001	PO4	1	0
2	AB	1001	PO4	1	0
2	C4	4201	PO4	2	0
2	BJ	1001	PO4	2	0
2	CU	201	PO4	1	0
2	BR	1001	PO4	3	0
2	CP	201	PO4	1	0
2	BM	1001	PO4	3	0
2	AG	1001	PO4	1	0
2	BG	1001	PO4	1	0
2	CG	1201	PO4	1	0
2	BY	1001	PO4	2	0
2	CO	4201	PO4	2	0
2	AZ	1001	PO4	1	0
2	CB	1001	PO4	1	0
2	AJ	1001	PO4	2	0
2	BB	1001	PO4	1	0
2	AC	1001	PO4	3	0
2	AR	1001	PO4	3	0
2	AK	1001	PO4	1	0
2	BC	1001	PO4	3	0
2	BZ	1001	PO4	1	0
2	B1	1001	PO4	1	0
2	A2	1001	PO4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BT	1001	PO4	2	0
2	AM	1001	PO4	3	0
2	AU	1001	PO4	1	0
2	CE	1001	PO4	2	0
2	BO	1001	PO4	2	0
2	AT	1001	PO4	2	0
2	BW	1001	PO4	3	0
2	B2	1001	PO4	3	0
2	CT	4201	PO4	2	0
2	BH	1001	PO4	3	0
2	BP	1001	PO4	1	0
2	AH	1001	PO4	3	0
2	AE	1001	PO4	2	0
2	BL	1001	PO4	1	0
2	AP	1001	PO4	1	0
2	C1	1201	PO4	1	0
2	BE	1001	PO4	2	0
2	CW	2201	PO4	3	0
2	AV	1001	PO4	1	0
2	CK	201	PO4	1	0
2	B4	1001	PO4	2	0
2	CL	1201	PO4	1	0
2	AF	1001	PO4	1	0
2	BK	1001	PO4	1	0
2	CC	1001	PO4	3	0
2	BU	1001	PO4	1	0
2	CF	201	PO4	1	0
2	CR	2201	PO4	3	0
2	AQ	1001	PO4	1	0
2	CM	2201	PO4	3	0
2	AA	1001	PO4	1	0
2	BA	1001	PO4	1	0
2	AW	201	PO4	3	0
2	CJ	4201	PO4	2	0
2	CY	4201	PO4	2	0
2	BF	1001	PO4	1	0
2	CH	2201	PO4	3	0
2	AY	1001	PO4	2	0
2	A4	1001	PO4	2	0
2	AO	1001	PO4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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