Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 09:49 pm GMT

PDB ID	:	6EKC
Title	:	Crystal structure of the BSD2 homolog of Arabidopsis thaliana bound to the octameric assembly of RbcL from Thermosynechococcus elongatus
Authors	:	Aigner, H.; Wilson, R.H.; Bracher, A.; Calisse, L.; Bhat, J.Y.; Hartl, F.U.; Hayer-Hartl, M.
Deposited on	:	2017-09-26
Resolution	:	2.63 Å(reported)

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

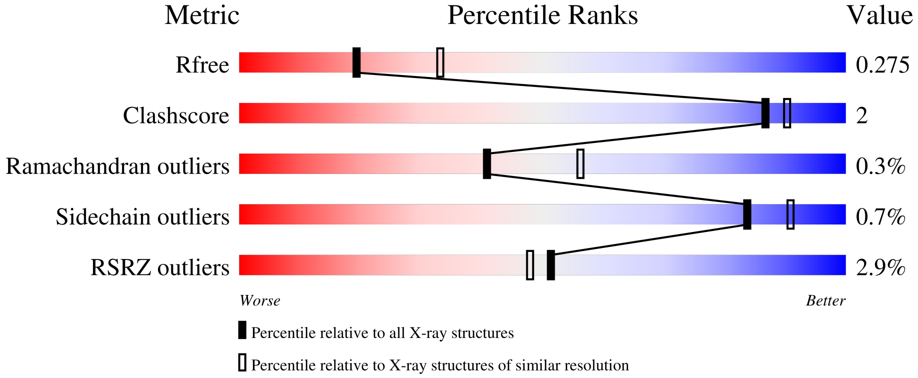
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

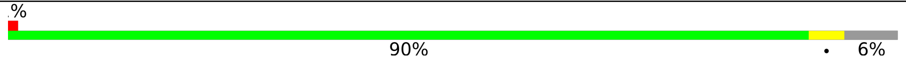
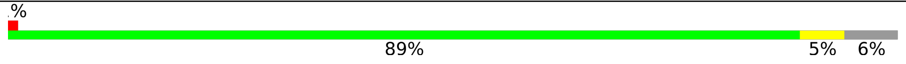
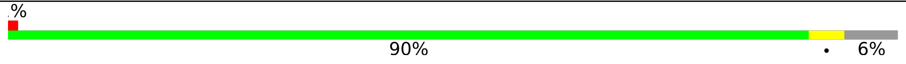
The reported resolution of this entry is 2.63 Å.

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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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

Mol	Chain	Length	Quality of chain
1	A1	475	
1	A2	475	
1	A3	475	
1	A4	475	
1	A5	475	

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Mol	Chain	Length	Quality of chain
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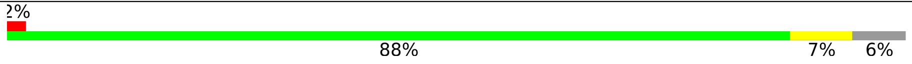
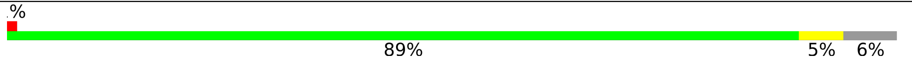
1	A7	475	
1	A8	475	
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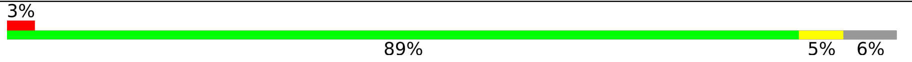
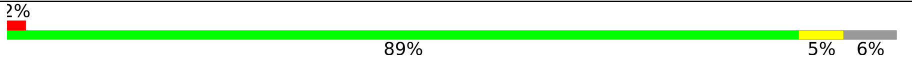
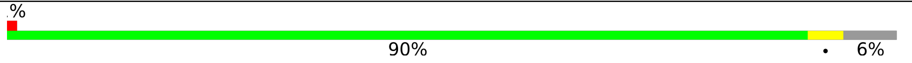
1	C3	475	
1	C4	475	
1	C5	475	
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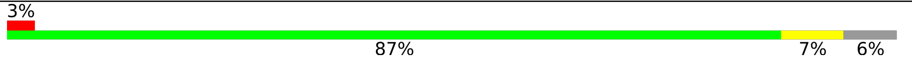
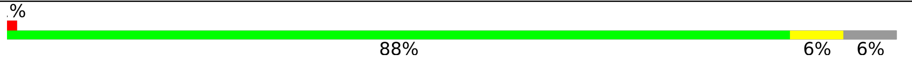
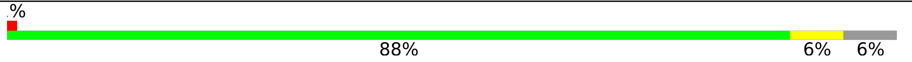
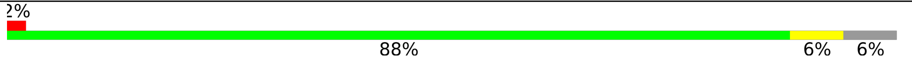
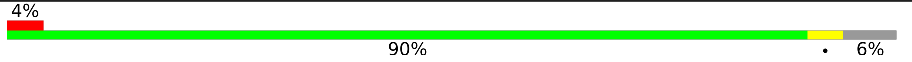
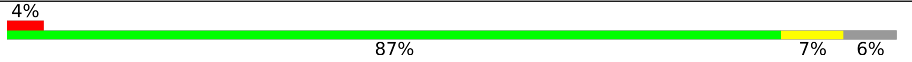
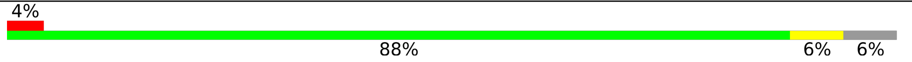
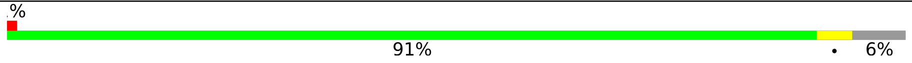
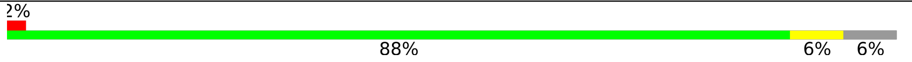
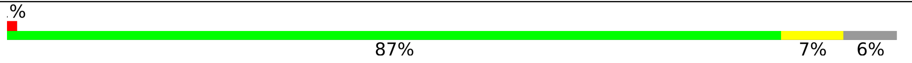
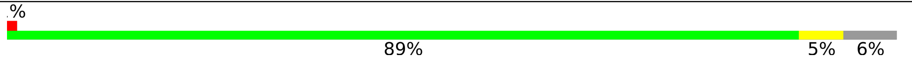
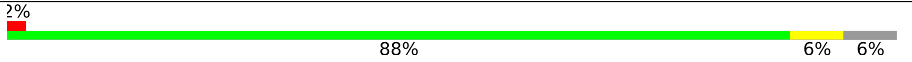
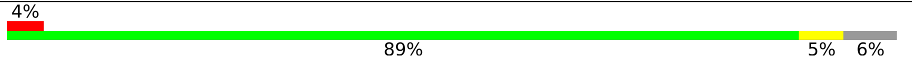
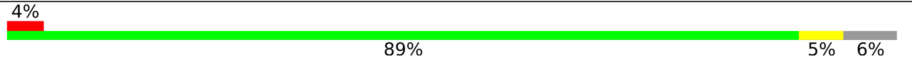
1	C7	475	
1	C8	475	
1	E1	475	
1	E2	475	
1	E3	475	
1	E4	475	
1	E5	475	
1	E6	475	
1	E7	475	
1	E8	475	
1	G1	475	
1	G2	475	
1	G3	475	
1	G4	475	
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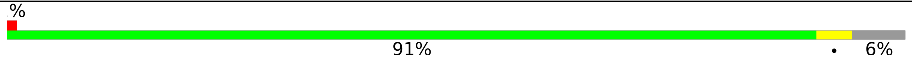
1	G6	475	

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Mol	Chain	Length	Quality of chain
1	G7	475	2% 90% • 6%
1	G8	475	2% 89% 5% 6%
1	I1	475	2% 90% • 6%
1	I2	475	% 89% 5% 6%
1	I3	475	2% 88% 6% 6%
1	I4	475	2% 90% • 6%
1	I5	475	% 89% 5% 6%
1	I6	475	89% 5% 6%
1	I7	475	% 89% 5% 6%
1	I8	475	% 90% • 6%
1	K1	475	2% 87% 7% 6%
1	K2	475	2% 89% 5% 6%
1	K3	475	3% 87% 7% 6%
1	K4	475	% 87% 7% 6%
1	K5	475	91% • 6%
1	K6	475	% 91% • 6%
1	K7	475	3% 89% 5% 6%
1	K8	475	3% 88% 6% 6%
1	M1	475	3% 89% 5% 6%
1	M2	475	2% 89% 5% 6%
1	M3	475	2% 89% 5% 6%
1	M4	475	% 90% • 6%
1	M5	475	90% • 6%
1	M6	475	90% • 6%
1	M7	475	% 89% 5% 6%

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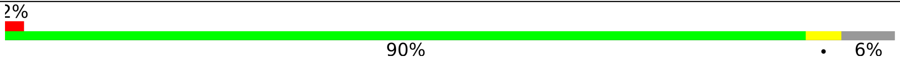
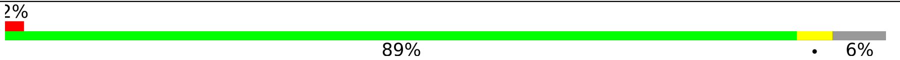
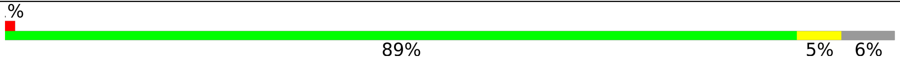
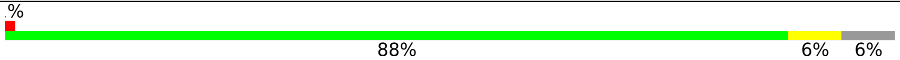
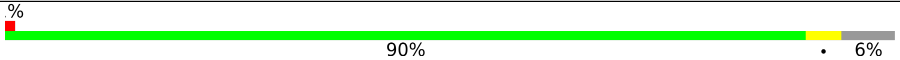
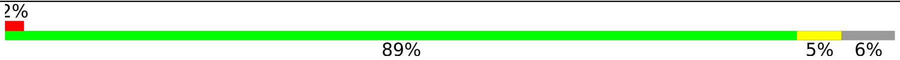
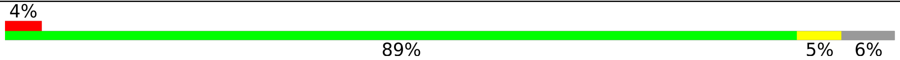
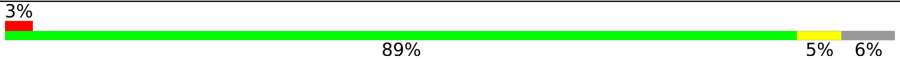
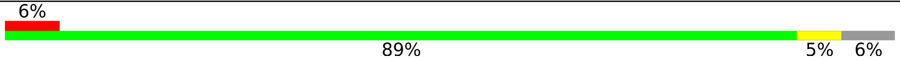
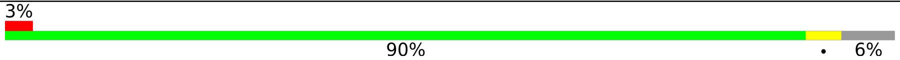
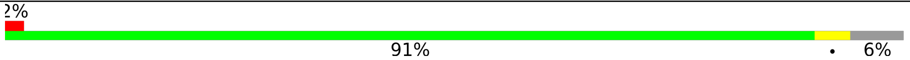
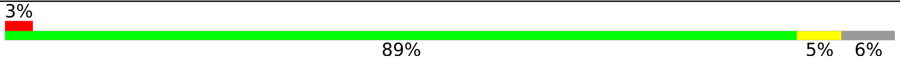
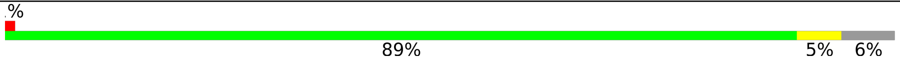
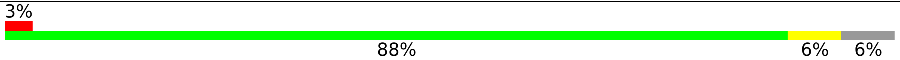
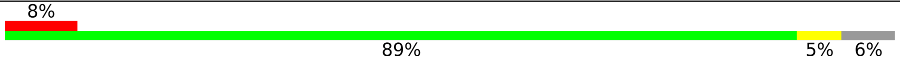
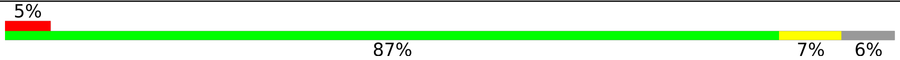
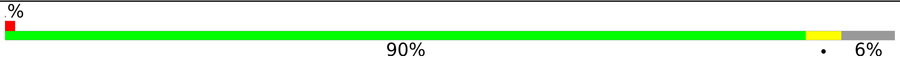
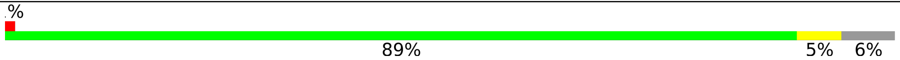
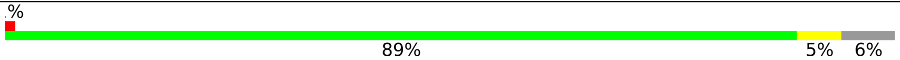
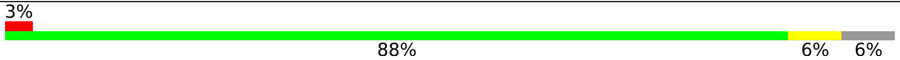
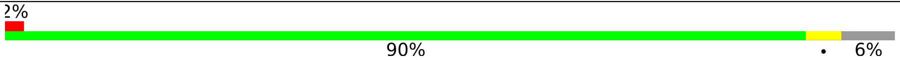
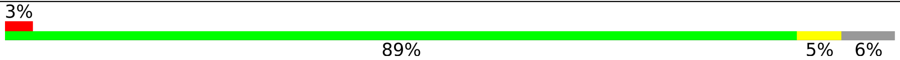
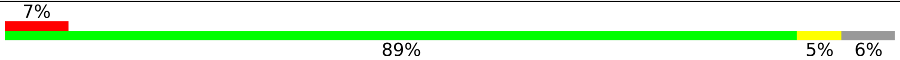
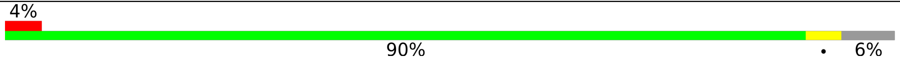
Mol	Chain	Length	Quality of chain
1	M8	475	
1	O1	475	
1	O2	475	
1	O3	475	
1	O4	475	
1	O5	475	
1	O6	475	
1	O7	475	
1	O8	475	
1	Q1	475	
1	Q2	475	
1	Q3	475	
1	Q4	475	
1	Q5	475	
1	Q6	475	
1	Q7	475	
1	Q8	475	
1	S1	475	
1	S2	475	
1	S3	475	
1	S4	475	
1	S5	475	
1	S6	475	
1	S7	475	
1	S8	475	

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Mol	Chain	Length	Quality of chain
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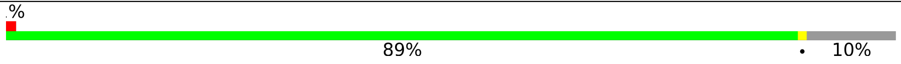
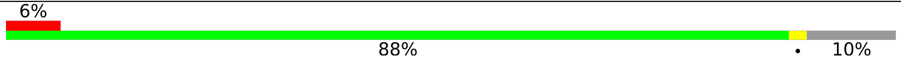
2	B2	81	
2	B3	81	
2	B4	81	
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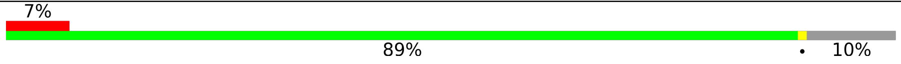
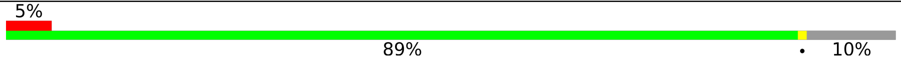
2	B6	81	
2	B7	81	
2	B8	81	
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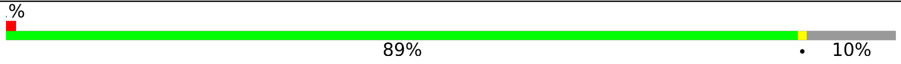
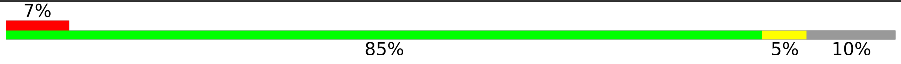
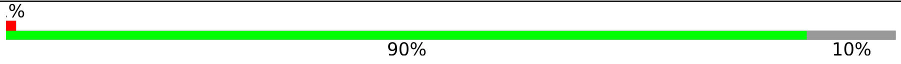
2	D2	81	
2	D3	81	
2	D4	81	
2	D5	81	
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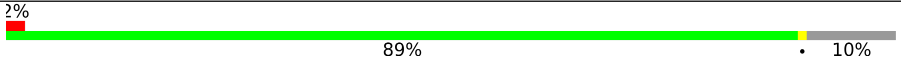
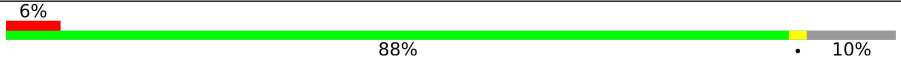
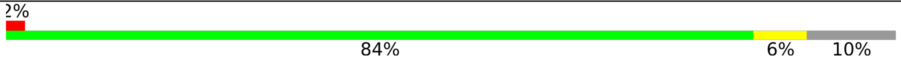
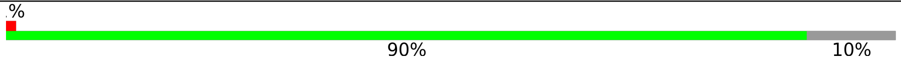
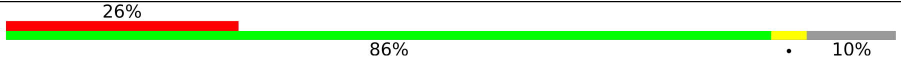
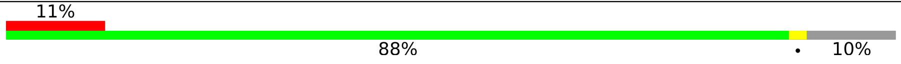
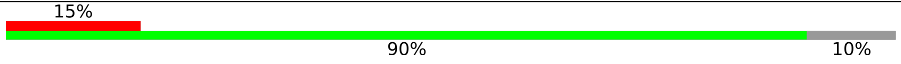
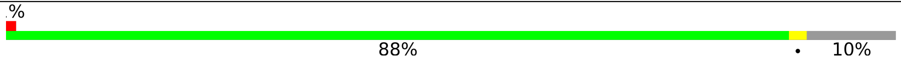
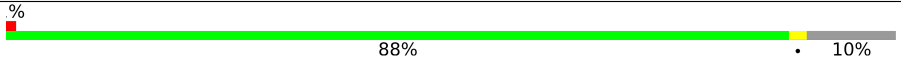
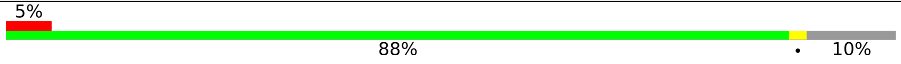
2	D7	81	
2	D8	81	
2	F1	81	
2	F2	81	
2	F3	81	
2	F4	81	
2	F5	81	
2	F6	81	
2	F7	81	
2	F8	81	
2	H1	81	

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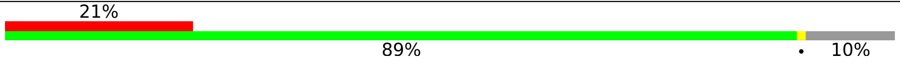
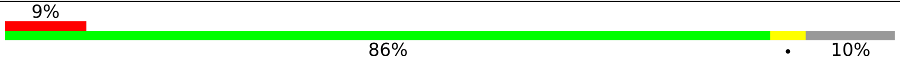
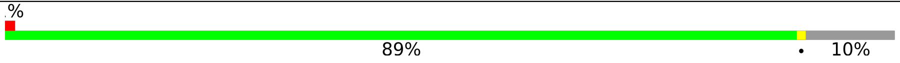
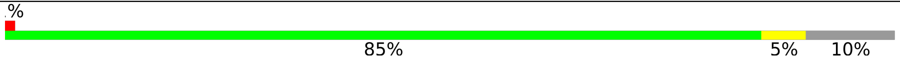
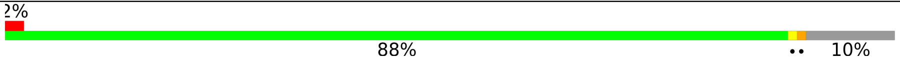
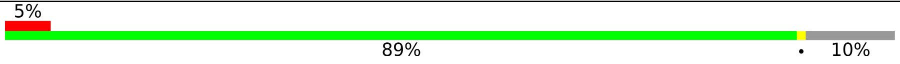
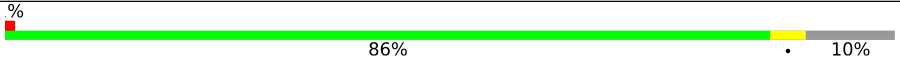
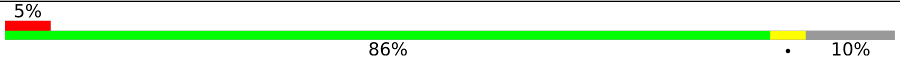
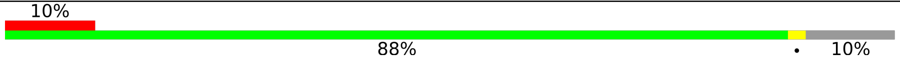
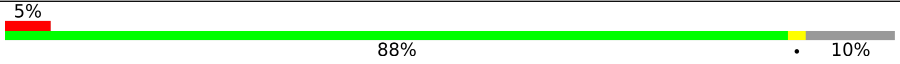
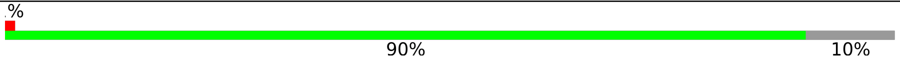
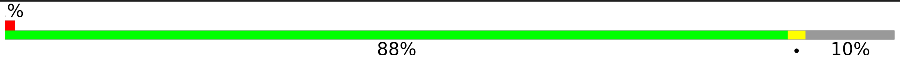
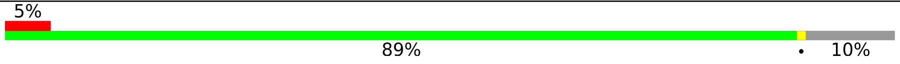
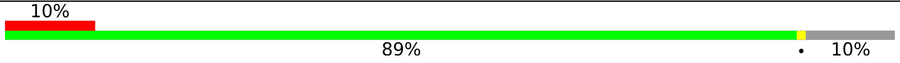
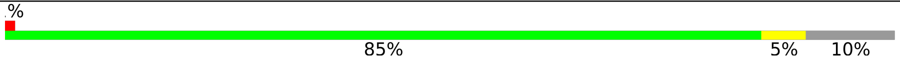
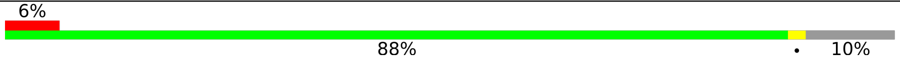
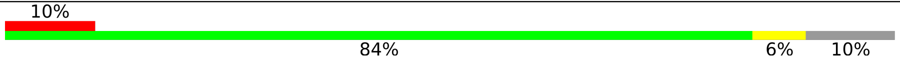
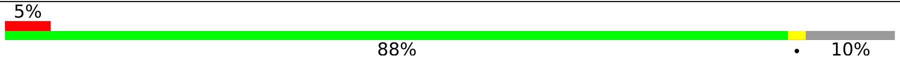
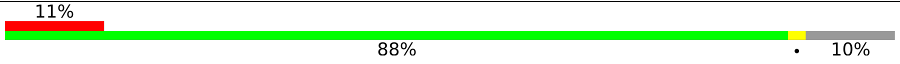
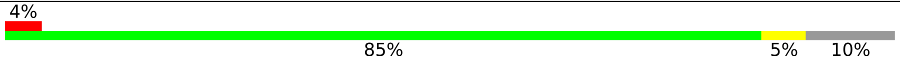
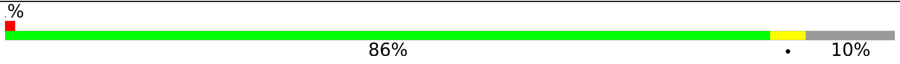
Mol	Chain	Length	Quality of chain
2	H2	81	
2	H3	81	
2	H4	81	
2	H5	81	
2	H6	81	
2	H7	81	
2	H8	81	
2	J1	81	
2	J2	81	
2	J3	81	
2	J4	81	
2	J5	81	
2	J6	81	
2	J7	81	
2	J8	81	
2	L1	81	
2	L2	81	
2	L3	81	
2	L4	81	
2	L5	81	
2	L6	81	
2	L7	81	
2	L8	81	
2	N1	81	
2	N2	81	

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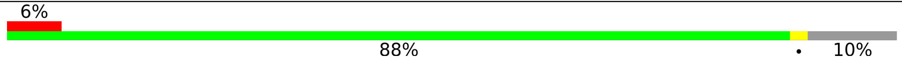
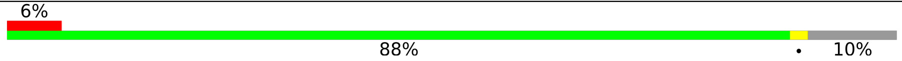
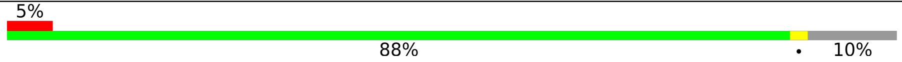
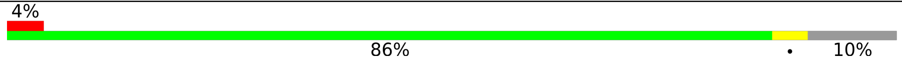
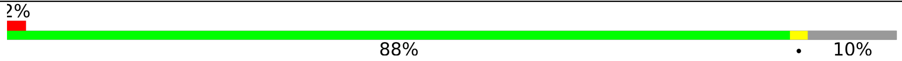
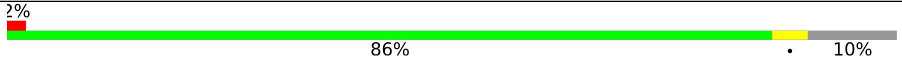
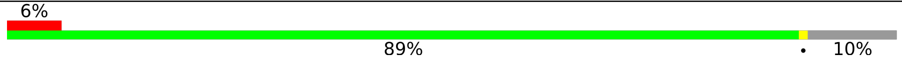
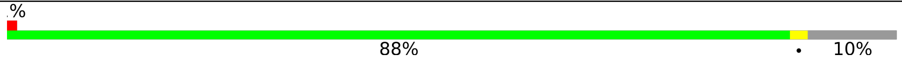
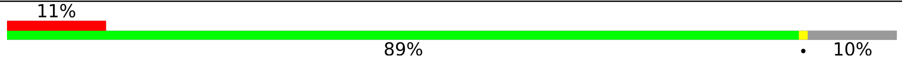
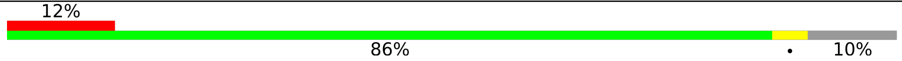
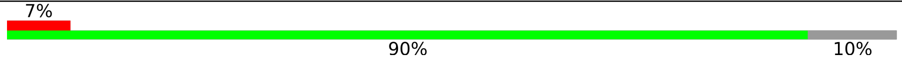
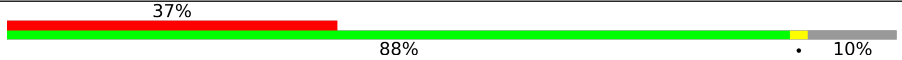
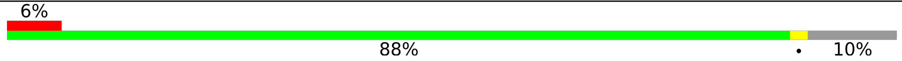
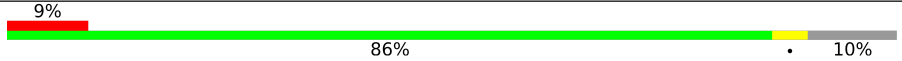
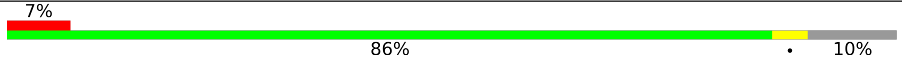
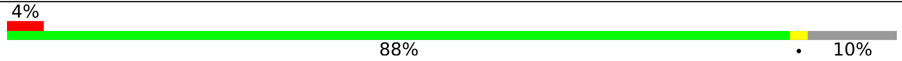
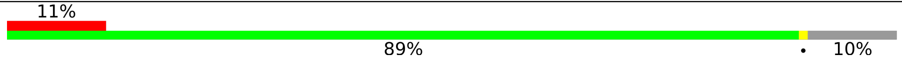
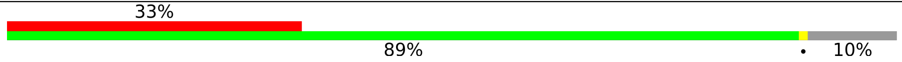
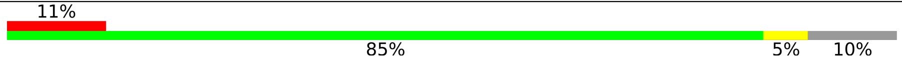
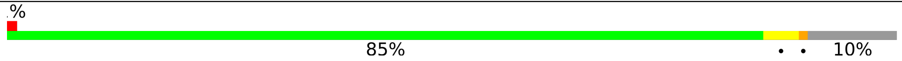
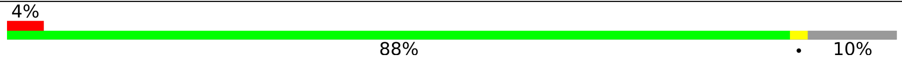
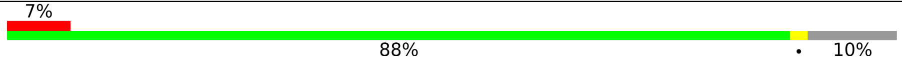
Mol	Chain	Length	Quality of chain
2	N3	81	
2	N4	81	
2	N5	81	
2	N6	81	
2	N7	81	
2	N8	81	
2	P1	81	
2	P2	81	
2	P3	81	
2	P4	81	
2	P5	81	
2	P6	81	
2	P7	81	
2	P8	81	
2	R1	81	
2	R2	81	
2	R3	81	
2	R4	81	
2	R5	81	
2	R6	81	
2	R7	81	
2	R8	81	
2	T1	81	
2	T2	81	
2	T3	81	

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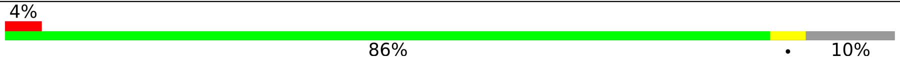
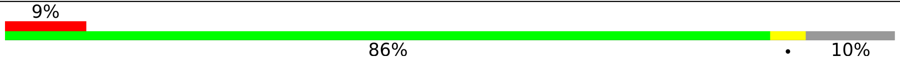
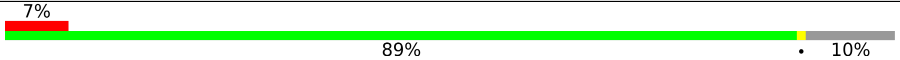
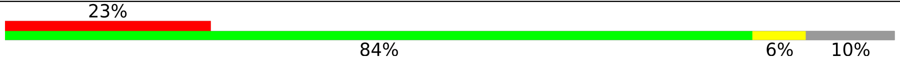
Mol	Chain	Length	Quality of chain
2	T4	81	
2	T5	81	
2	T6	81	
2	T7	81	
2	T8	81	

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
3	ZN	F3	302	-	-	X	-
3	ZN	H3	302	-	-	X	-
3	ZN	H5	302	-	-	X	-
3	ZN	R6	302	-	-	X	-
3	ZN	R8	301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 321799 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 Ribulose bisphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A1	447	3486	2215	612	638	21	0	0	0
1	A2	447	3493	2218	612	642	21	0	0	0
1	A3	447	3493	2218	612	642	21	0	0	0
1	A4	447	3486	2215	612	638	21	0	0	0
1	A5	447	3493	2218	612	642	21	0	0	0
1	A6	447	3493	2218	612	642	21	0	0	0
1	A7	447	3493	2218	612	642	21	0	0	0
1	A8	447	3493	2218	612	642	21	0	0	0
1	C1	447	3493	2218	612	642	21	0	0	0
1	C2	447	3493	2218	612	642	21	0	0	0
1	C3	447	3493	2218	612	642	21	0	0	0
1	C4	447	3493	2218	612	642	21	0	0	0
1	C5	447	3493	2218	612	642	21	0	0	0
1	C6	447	3493	2218	612	642	21	0	0	0
1	C7	447	3493	2218	612	642	21	0	0	0
1	C8	447	3493	2218	612	642	21	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	E1	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	E2	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	E3	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	E4	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	E5	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	E6	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	E7	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	E8	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	G1	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	G2	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	G3	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	G4	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	G5	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	G6	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	G7	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	G8	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	I1	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	I2	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	I3	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	I4	447	Total C N O S 3493 2218 612 642 21	0	0	0
1	I5	447	Total C N O S 3493 2218 612 642 21	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	I6	447	3493	2218	612	642	21	0	0	0
1	I7	447	3493	2218	612	642	21	0	0	0
1	I8	447	3493	2218	612	642	21	0	0	0
1	K1	447	3493	2218	612	642	21	0	0	0
1	K2	447	3493	2218	612	642	21	0	0	0
1	K3	447	3493	2218	612	642	21	0	0	0
1	K4	447	3493	2218	612	642	21	0	0	0
1	K5	447	3493	2218	612	642	21	0	0	0
1	K6	447	3493	2218	612	642	21	0	0	0
1	K7	447	3493	2218	612	642	21	0	0	0
1	K8	447	3493	2218	612	642	21	0	0	0
1	M1	447	3493	2218	612	642	21	0	0	0
1	M2	447	3493	2218	612	642	21	0	0	0
1	M3	447	3493	2218	612	642	21	0	0	0
1	M4	447	3493	2218	612	642	21	0	0	0
1	M5	447	3493	2218	612	642	21	0	0	0
1	M6	447	3493	2218	612	642	21	0	0	0
1	M7	447	3493	2218	612	642	21	0	0	0
1	M8	447	3493	2218	612	642	21	0	0	0
1	O1	447	3493	2218	612	642	21	0	0	0
1	O2	447	3493	2218	612	642	21	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	O3	447	3493	2218	612	642	21	0	0	0
1	O4	447	3493	2218	612	642	21	0	0	0
1	O5	447	3493	2218	612	642	21	0	0	0
1	O6	447	3493	2218	612	642	21	0	0	0
1	O7	447	3493	2218	612	642	21	0	0	0
1	O8	447	3493	2218	612	642	21	0	0	0
1	Q1	447	3493	2218	612	642	21	0	0	0
1	Q2	447	3493	2218	612	642	21	0	0	0
1	Q3	447	3493	2218	612	642	21	0	0	0
1	Q4	447	3493	2218	612	642	21	0	0	0
1	Q5	447	3493	2218	612	642	21	0	0	0
1	Q6	447	3493	2218	612	642	21	0	0	0
1	Q7	447	3493	2218	612	642	21	0	0	0
1	Q8	447	3493	2218	612	642	21	0	0	0
1	S1	447	3493	2218	612	642	21	0	0	0
1	S2	447	3493	2218	612	642	21	0	0	0
1	S3	447	3493	2218	612	642	21	0	0	0
1	S4	447	3493	2218	612	642	21	0	0	0
1	S5	447	3493	2218	612	642	21	0	0	0
1	S6	447	3493	2218	612	642	21	0	0	0
1	S7	447	3493	2218	612	642	21	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	S8	447	3493	2218	612	642	21	0	0	0

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	345	ILE	PHE	engineered mutation	UNP Q8DIS5
A1	415	ALA	PRO	engineered mutation	UNP Q8DIS5
A2	345	ILE	PHE	engineered mutation	UNP Q8DIS5
A2	415	ALA	PRO	engineered mutation	UNP Q8DIS5
A3	345	ILE	PHE	engineered mutation	UNP Q8DIS5
A3	415	ALA	PRO	engineered mutation	UNP Q8DIS5
A4	345	ILE	PHE	engineered mutation	UNP Q8DIS5
A4	415	ALA	PRO	engineered mutation	UNP Q8DIS5
A5	345	ILE	PHE	engineered mutation	UNP Q8DIS5
A5	415	ALA	PRO	engineered mutation	UNP Q8DIS5
A6	345	ILE	PHE	engineered mutation	UNP Q8DIS5
A6	415	ALA	PRO	engineered mutation	UNP Q8DIS5
A7	345	ILE	PHE	engineered mutation	UNP Q8DIS5
A7	415	ALA	PRO	engineered mutation	UNP Q8DIS5
A8	345	ILE	PHE	engineered mutation	UNP Q8DIS5
A8	415	ALA	PRO	engineered mutation	UNP Q8DIS5
C1	345	ILE	PHE	engineered mutation	UNP Q8DIS5
C1	415	ALA	PRO	engineered mutation	UNP Q8DIS5
C2	345	ILE	PHE	engineered mutation	UNP Q8DIS5
C2	415	ALA	PRO	engineered mutation	UNP Q8DIS5
C3	345	ILE	PHE	engineered mutation	UNP Q8DIS5
C3	415	ALA	PRO	engineered mutation	UNP Q8DIS5
C4	345	ILE	PHE	engineered mutation	UNP Q8DIS5
C4	415	ALA	PRO	engineered mutation	UNP Q8DIS5
C5	345	ILE	PHE	engineered mutation	UNP Q8DIS5
C5	415	ALA	PRO	engineered mutation	UNP Q8DIS5
C6	345	ILE	PHE	engineered mutation	UNP Q8DIS5
C6	415	ALA	PRO	engineered mutation	UNP Q8DIS5
C7	345	ILE	PHE	engineered mutation	UNP Q8DIS5
C7	415	ALA	PRO	engineered mutation	UNP Q8DIS5
C8	345	ILE	PHE	engineered mutation	UNP Q8DIS5
C8	415	ALA	PRO	engineered mutation	UNP Q8DIS5
E1	345	ILE	PHE	engineered mutation	UNP Q8DIS5
E1	415	ALA	PRO	engineered mutation	UNP Q8DIS5
E2	345	ILE	PHE	engineered mutation	UNP Q8DIS5
E2	415	ALA	PRO	engineered mutation	UNP Q8DIS5

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Chain	Residue	Modelled	Actual	Comment	Reference
E3	345	ILE	PHE	engineered mutation	UNP Q8DIS5
E3	415	ALA	PRO	engineered mutation	UNP Q8DIS5
E4	345	ILE	PHE	engineered mutation	UNP Q8DIS5
E4	415	ALA	PRO	engineered mutation	UNP Q8DIS5
E5	345	ILE	PHE	engineered mutation	UNP Q8DIS5
E5	415	ALA	PRO	engineered mutation	UNP Q8DIS5
E6	345	ILE	PHE	engineered mutation	UNP Q8DIS5
E6	415	ALA	PRO	engineered mutation	UNP Q8DIS5
E7	345	ILE	PHE	engineered mutation	UNP Q8DIS5
E7	415	ALA	PRO	engineered mutation	UNP Q8DIS5
E8	345	ILE	PHE	engineered mutation	UNP Q8DIS5
E8	415	ALA	PRO	engineered mutation	UNP Q8DIS5
G1	345	ILE	PHE	engineered mutation	UNP Q8DIS5
G1	415	ALA	PRO	engineered mutation	UNP Q8DIS5
G2	345	ILE	PHE	engineered mutation	UNP Q8DIS5
G2	415	ALA	PRO	engineered mutation	UNP Q8DIS5
G3	345	ILE	PHE	engineered mutation	UNP Q8DIS5
G3	415	ALA	PRO	engineered mutation	UNP Q8DIS5
G4	345	ILE	PHE	engineered mutation	UNP Q8DIS5
G4	415	ALA	PRO	engineered mutation	UNP Q8DIS5
G5	345	ILE	PHE	engineered mutation	UNP Q8DIS5
G5	415	ALA	PRO	engineered mutation	UNP Q8DIS5
G6	345	ILE	PHE	engineered mutation	UNP Q8DIS5
G6	415	ALA	PRO	engineered mutation	UNP Q8DIS5
G7	345	ILE	PHE	engineered mutation	UNP Q8DIS5
G7	415	ALA	PRO	engineered mutation	UNP Q8DIS5
G8	345	ILE	PHE	engineered mutation	UNP Q8DIS5
G8	415	ALA	PRO	engineered mutation	UNP Q8DIS5
I1	345	ILE	PHE	engineered mutation	UNP Q8DIS5
I1	415	ALA	PRO	engineered mutation	UNP Q8DIS5
I2	345	ILE	PHE	engineered mutation	UNP Q8DIS5
I2	415	ALA	PRO	engineered mutation	UNP Q8DIS5
I3	345	ILE	PHE	engineered mutation	UNP Q8DIS5
I3	415	ALA	PRO	engineered mutation	UNP Q8DIS5
I4	345	ILE	PHE	engineered mutation	UNP Q8DIS5
I4	415	ALA	PRO	engineered mutation	UNP Q8DIS5
I5	345	ILE	PHE	engineered mutation	UNP Q8DIS5
I5	415	ALA	PRO	engineered mutation	UNP Q8DIS5
I6	345	ILE	PHE	engineered mutation	UNP Q8DIS5
I6	415	ALA	PRO	engineered mutation	UNP Q8DIS5
I7	345	ILE	PHE	engineered mutation	UNP Q8DIS5
I7	415	ALA	PRO	engineered mutation	UNP Q8DIS5

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Chain	Residue	Modelled	Actual	Comment	Reference
I8	345	ILE	PHE	engineered mutation	UNP Q8DIS5
I8	415	ALA	PRO	engineered mutation	UNP Q8DIS5
K1	345	ILE	PHE	engineered mutation	UNP Q8DIS5
K1	415	ALA	PRO	engineered mutation	UNP Q8DIS5
K2	345	ILE	PHE	engineered mutation	UNP Q8DIS5
K2	415	ALA	PRO	engineered mutation	UNP Q8DIS5
K3	345	ILE	PHE	engineered mutation	UNP Q8DIS5
K3	415	ALA	PRO	engineered mutation	UNP Q8DIS5
K4	345	ILE	PHE	engineered mutation	UNP Q8DIS5
K4	415	ALA	PRO	engineered mutation	UNP Q8DIS5
K5	345	ILE	PHE	engineered mutation	UNP Q8DIS5
K5	415	ALA	PRO	engineered mutation	UNP Q8DIS5
K6	345	ILE	PHE	engineered mutation	UNP Q8DIS5
K6	415	ALA	PRO	engineered mutation	UNP Q8DIS5
K7	345	ILE	PHE	engineered mutation	UNP Q8DIS5
K7	415	ALA	PRO	engineered mutation	UNP Q8DIS5
K8	345	ILE	PHE	engineered mutation	UNP Q8DIS5
K8	415	ALA	PRO	engineered mutation	UNP Q8DIS5
M1	345	ILE	PHE	engineered mutation	UNP Q8DIS5
M1	415	ALA	PRO	engineered mutation	UNP Q8DIS5
M2	345	ILE	PHE	engineered mutation	UNP Q8DIS5
M2	415	ALA	PRO	engineered mutation	UNP Q8DIS5
M3	345	ILE	PHE	engineered mutation	UNP Q8DIS5
M3	415	ALA	PRO	engineered mutation	UNP Q8DIS5
M4	345	ILE	PHE	engineered mutation	UNP Q8DIS5
M4	415	ALA	PRO	engineered mutation	UNP Q8DIS5
M5	345	ILE	PHE	engineered mutation	UNP Q8DIS5
M5	415	ALA	PRO	engineered mutation	UNP Q8DIS5
M6	345	ILE	PHE	engineered mutation	UNP Q8DIS5
M6	415	ALA	PRO	engineered mutation	UNP Q8DIS5
M7	345	ILE	PHE	engineered mutation	UNP Q8DIS5
M7	415	ALA	PRO	engineered mutation	UNP Q8DIS5
M8	345	ILE	PHE	engineered mutation	UNP Q8DIS5
M8	415	ALA	PRO	engineered mutation	UNP Q8DIS5
O1	345	ILE	PHE	engineered mutation	UNP Q8DIS5
O1	415	ALA	PRO	engineered mutation	UNP Q8DIS5
O2	345	ILE	PHE	engineered mutation	UNP Q8DIS5
O2	415	ALA	PRO	engineered mutation	UNP Q8DIS5
O3	345	ILE	PHE	engineered mutation	UNP Q8DIS5
O3	415	ALA	PRO	engineered mutation	UNP Q8DIS5
O4	345	ILE	PHE	engineered mutation	UNP Q8DIS5
O4	415	ALA	PRO	engineered mutation	UNP Q8DIS5

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Chain	Residue	Modelled	Actual	Comment	Reference
O5	345	ILE	PHE	engineered mutation	UNP Q8DIS5
O5	415	ALA	PRO	engineered mutation	UNP Q8DIS5
O6	345	ILE	PHE	engineered mutation	UNP Q8DIS5
O6	415	ALA	PRO	engineered mutation	UNP Q8DIS5
O7	345	ILE	PHE	engineered mutation	UNP Q8DIS5
O7	415	ALA	PRO	engineered mutation	UNP Q8DIS5
O8	345	ILE	PHE	engineered mutation	UNP Q8DIS5
O8	415	ALA	PRO	engineered mutation	UNP Q8DIS5
Q1	345	ILE	PHE	engineered mutation	UNP Q8DIS5
Q1	415	ALA	PRO	engineered mutation	UNP Q8DIS5
Q2	345	ILE	PHE	engineered mutation	UNP Q8DIS5
Q2	415	ALA	PRO	engineered mutation	UNP Q8DIS5
Q3	345	ILE	PHE	engineered mutation	UNP Q8DIS5
Q3	415	ALA	PRO	engineered mutation	UNP Q8DIS5
Q4	345	ILE	PHE	engineered mutation	UNP Q8DIS5
Q4	415	ALA	PRO	engineered mutation	UNP Q8DIS5
Q5	345	ILE	PHE	engineered mutation	UNP Q8DIS5
Q5	415	ALA	PRO	engineered mutation	UNP Q8DIS5
Q6	345	ILE	PHE	engineered mutation	UNP Q8DIS5
Q6	415	ALA	PRO	engineered mutation	UNP Q8DIS5
Q7	345	ILE	PHE	engineered mutation	UNP Q8DIS5
Q7	415	ALA	PRO	engineered mutation	UNP Q8DIS5
Q8	345	ILE	PHE	engineered mutation	UNP Q8DIS5
Q8	415	ALA	PRO	engineered mutation	UNP Q8DIS5
S1	345	ILE	PHE	engineered mutation	UNP Q8DIS5
S1	415	ALA	PRO	engineered mutation	UNP Q8DIS5
S2	345	ILE	PHE	engineered mutation	UNP Q8DIS5
S2	415	ALA	PRO	engineered mutation	UNP Q8DIS5
S3	345	ILE	PHE	engineered mutation	UNP Q8DIS5
S3	415	ALA	PRO	engineered mutation	UNP Q8DIS5
S4	345	ILE	PHE	engineered mutation	UNP Q8DIS5
S4	415	ALA	PRO	engineered mutation	UNP Q8DIS5
S5	345	ILE	PHE	engineered mutation	UNP Q8DIS5
S5	415	ALA	PRO	engineered mutation	UNP Q8DIS5
S6	345	ILE	PHE	engineered mutation	UNP Q8DIS5
S6	415	ALA	PRO	engineered mutation	UNP Q8DIS5
S7	345	ILE	PHE	engineered mutation	UNP Q8DIS5
S7	415	ALA	PRO	engineered mutation	UNP Q8DIS5
S8	345	ILE	PHE	engineered mutation	UNP Q8DIS5
S8	415	ALA	PRO	engineered mutation	UNP Q8DIS5

- Molecule 2 is a protein called DnaJ/Hsp40 cysteine-rich domain superfamily protein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B1	73	Total C N O S 520 320 91 100 9	0	0	0
2	B2	73	Total C N O S 520 320 91 100 9	0	0	0
2	B3	73	Total C N O S 520 320 91 100 9	0	0	0
2	B4	73	Total C N O S 520 320 91 100 9	0	0	0
2	B5	73	Total C N O S 520 320 91 100 9	0	0	0
2	B6	73	Total C N O S 520 320 91 100 9	0	0	0
2	B7	73	Total C N O S 520 320 91 100 9	0	0	0
2	B8	73	Total C N O S 520 320 91 100 9	0	0	0
2	D1	73	Total C N O S 520 320 91 100 9	0	0	0
2	D2	73	Total C N O S 520 320 91 100 9	0	0	0
2	D3	73	Total C N O S 520 320 91 100 9	0	0	0
2	D4	73	Total C N O S 520 320 91 100 9	0	0	0
2	D5	73	Total C N O S 520 320 91 100 9	0	0	0
2	D6	73	Total C N O S 520 320 91 100 9	0	0	0
2	D7	73	Total C N O S 520 320 91 100 9	0	0	0
2	D8	73	Total C N O S 520 320 91 100 9	0	0	0
2	F1	73	Total C N O S 520 320 91 100 9	0	0	0
2	F2	73	Total C N O S 520 320 91 100 9	0	0	0
2	F3	73	Total C N O S 520 320 91 100 9	0	0	0
2	F4	73	Total C N O S 520 320 91 100 9	0	0	0
2	F5	73	Total C N O S 520 320 91 100 9	0	0	0
2	F6	73	Total C N O S 520 320 91 100 9	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F7	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	F8	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	H1	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	H2	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	H3	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	H4	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	H5	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	H6	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	H7	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	H8	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	J1	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	J2	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	J3	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	J4	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	J5	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	J6	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	J7	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	J8	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	L1	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	L2	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	L3	73	Total 520	C 320	N 91	O 100	S 9	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L4	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	L5	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	L6	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	L7	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	L8	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	N1	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	N2	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	N3	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	N4	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	N5	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	N6	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	N7	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	N8	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	P1	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	P2	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	P3	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	P4	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	P5	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	P6	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	P7	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	P8	73	Total 520	C 320	N 91	O 100	S 9	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R1	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	R2	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	R3	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	R4	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	R5	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	R6	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	R7	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	R8	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	T1	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	T2	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	T3	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	T4	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	T5	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	T6	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	T7	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	T8	73	Total 520	C 320	N 91	O 100	S 9	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	56	MET	-	initiating methionine	UNP Q9SN73
B2	56	MET	-	initiating methionine	UNP Q9SN73
B3	56	MET	-	initiating methionine	UNP Q9SN73
B4	56	MET	-	initiating methionine	UNP Q9SN73
B5	56	MET	-	initiating methionine	UNP Q9SN73
B6	56	MET	-	initiating methionine	UNP Q9SN73
B7	56	MET	-	initiating methionine	UNP Q9SN73

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Chain	Residue	Modelled	Actual	Comment	Reference
B8	56	MET	-	initiating methionine	UNP Q9SN73
D1	56	MET	-	initiating methionine	UNP Q9SN73
D2	56	MET	-	initiating methionine	UNP Q9SN73
D3	56	MET	-	initiating methionine	UNP Q9SN73
D4	56	MET	-	initiating methionine	UNP Q9SN73
D5	56	MET	-	initiating methionine	UNP Q9SN73
D6	56	MET	-	initiating methionine	UNP Q9SN73
D7	56	MET	-	initiating methionine	UNP Q9SN73
D8	56	MET	-	initiating methionine	UNP Q9SN73
F1	56	MET	-	initiating methionine	UNP Q9SN73
F2	56	MET	-	initiating methionine	UNP Q9SN73
F3	56	MET	-	initiating methionine	UNP Q9SN73
F4	56	MET	-	initiating methionine	UNP Q9SN73
F5	56	MET	-	initiating methionine	UNP Q9SN73
F6	56	MET	-	initiating methionine	UNP Q9SN73
F7	56	MET	-	initiating methionine	UNP Q9SN73
F8	56	MET	-	initiating methionine	UNP Q9SN73
H1	56	MET	-	initiating methionine	UNP Q9SN73
H2	56	MET	-	initiating methionine	UNP Q9SN73
H3	56	MET	-	initiating methionine	UNP Q9SN73
H4	56	MET	-	initiating methionine	UNP Q9SN73
H5	56	MET	-	initiating methionine	UNP Q9SN73
H6	56	MET	-	initiating methionine	UNP Q9SN73
H7	56	MET	-	initiating methionine	UNP Q9SN73
H8	56	MET	-	initiating methionine	UNP Q9SN73
J1	56	MET	-	initiating methionine	UNP Q9SN73
J2	56	MET	-	initiating methionine	UNP Q9SN73
J3	56	MET	-	initiating methionine	UNP Q9SN73
J4	56	MET	-	initiating methionine	UNP Q9SN73
J5	56	MET	-	initiating methionine	UNP Q9SN73
J6	56	MET	-	initiating methionine	UNP Q9SN73
J7	56	MET	-	initiating methionine	UNP Q9SN73
J8	56	MET	-	initiating methionine	UNP Q9SN73
L1	56	MET	-	initiating methionine	UNP Q9SN73
L2	56	MET	-	initiating methionine	UNP Q9SN73
L3	56	MET	-	initiating methionine	UNP Q9SN73
L4	56	MET	-	initiating methionine	UNP Q9SN73
L5	56	MET	-	initiating methionine	UNP Q9SN73
L6	56	MET	-	initiating methionine	UNP Q9SN73
L7	56	MET	-	initiating methionine	UNP Q9SN73
L8	56	MET	-	initiating methionine	UNP Q9SN73
N1	56	MET	-	initiating methionine	UNP Q9SN73

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Chain	Residue	Modelled	Actual	Comment	Reference
N2	56	MET	-	initiating methionine	UNP Q9SN73
N3	56	MET	-	initiating methionine	UNP Q9SN73
N4	56	MET	-	initiating methionine	UNP Q9SN73
N5	56	MET	-	initiating methionine	UNP Q9SN73
N6	56	MET	-	initiating methionine	UNP Q9SN73
N7	56	MET	-	initiating methionine	UNP Q9SN73
N8	56	MET	-	initiating methionine	UNP Q9SN73
P1	56	MET	-	initiating methionine	UNP Q9SN73
P2	56	MET	-	initiating methionine	UNP Q9SN73
P3	56	MET	-	initiating methionine	UNP Q9SN73
P4	56	MET	-	initiating methionine	UNP Q9SN73
P5	56	MET	-	initiating methionine	UNP Q9SN73
P6	56	MET	-	initiating methionine	UNP Q9SN73
P7	56	MET	-	initiating methionine	UNP Q9SN73
P8	56	MET	-	initiating methionine	UNP Q9SN73
R1	56	MET	-	initiating methionine	UNP Q9SN73
R2	56	MET	-	initiating methionine	UNP Q9SN73
R3	56	MET	-	initiating methionine	UNP Q9SN73
R4	56	MET	-	initiating methionine	UNP Q9SN73
R5	56	MET	-	initiating methionine	UNP Q9SN73
R6	56	MET	-	initiating methionine	UNP Q9SN73
R7	56	MET	-	initiating methionine	UNP Q9SN73
R8	56	MET	-	initiating methionine	UNP Q9SN73
T1	56	MET	-	initiating methionine	UNP Q9SN73
T2	56	MET	-	initiating methionine	UNP Q9SN73
T3	56	MET	-	initiating methionine	UNP Q9SN73
T4	56	MET	-	initiating methionine	UNP Q9SN73
T5	56	MET	-	initiating methionine	UNP Q9SN73
T6	56	MET	-	initiating methionine	UNP Q9SN73
T7	56	MET	-	initiating methionine	UNP Q9SN73
T8	56	MET	-	initiating methionine	UNP Q9SN73

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B1	2	Total Zn 2 2	0	0
3	B2	2	Total Zn 2 2	0	0
3	B3	2	Total Zn 2 2	0	0
3	B4	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B5	2	Total Zn 2 2	0	0
3	B6	2	Total Zn 2 2	0	0
3	B7	2	Total Zn 2 2	0	0
3	B8	2	Total Zn 2 2	0	0
3	D1	2	Total Zn 2 2	0	0
3	D2	2	Total Zn 2 2	0	0
3	D3	2	Total Zn 2 2	0	0
3	D4	2	Total Zn 2 2	0	0
3	D5	2	Total Zn 2 2	0	0
3	D6	2	Total Zn 2 2	0	0
3	D7	2	Total Zn 2 2	0	0
3	D8	2	Total Zn 2 2	0	0
3	F1	2	Total Zn 2 2	0	0
3	F2	2	Total Zn 2 2	0	0
3	F3	2	Total Zn 2 2	0	0
3	F4	2	Total Zn 2 2	0	0
3	F5	2	Total Zn 2 2	0	0
3	F6	2	Total Zn 2 2	0	0
3	F7	2	Total Zn 2 2	0	0
3	F8	2	Total Zn 2 2	0	0
3	H1	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H2	2	Total Zn 2 2	0	0
3	H3	2	Total Zn 2 2	0	0
3	H4	2	Total Zn 2 2	0	0
3	H5	2	Total Zn 2 2	0	0
3	H6	2	Total Zn 2 2	0	0
3	H7	2	Total Zn 2 2	0	0
3	H8	2	Total Zn 2 2	0	0
3	J1	2	Total Zn 2 2	0	0
3	J2	2	Total Zn 2 2	0	0
3	J3	2	Total Zn 2 2	0	0
3	J4	2	Total Zn 2 2	0	0
3	J5	2	Total Zn 2 2	0	0
3	J6	2	Total Zn 2 2	0	0
3	J7	2	Total Zn 2 2	0	0
3	J8	2	Total Zn 2 2	0	0
3	L1	2	Total Zn 2 2	0	0
3	L2	2	Total Zn 2 2	0	0
3	L3	2	Total Zn 2 2	0	0
3	L4	2	Total Zn 2 2	0	0
3	L5	2	Total Zn 2 2	0	0
3	L6	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L7	2	Total Zn 2 2	0	0
3	L8	2	Total Zn 2 2	0	0
3	N1	2	Total Zn 2 2	0	0
3	N2	2	Total Zn 2 2	0	0
3	N3	2	Total Zn 2 2	0	0
3	N4	2	Total Zn 2 2	0	0
3	N5	2	Total Zn 2 2	0	0
3	N6	2	Total Zn 2 2	0	0
3	N7	2	Total Zn 2 2	0	0
3	N8	2	Total Zn 2 2	0	0
3	P1	2	Total Zn 2 2	0	0
3	P2	2	Total Zn 2 2	0	0
3	P3	2	Total Zn 2 2	0	0
3	P4	2	Total Zn 2 2	0	0
3	P5	2	Total Zn 2 2	0	0
3	P6	2	Total Zn 2 2	0	0
3	P7	2	Total Zn 2 2	0	0
3	P8	2	Total Zn 2 2	0	0
3	R1	2	Total Zn 2 2	0	0
3	R2	2	Total Zn 2 2	0	0
3	R3	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	R4	2	Total Zn 2 2	0	0
3	R5	2	Total Zn 2 2	0	0
3	R6	2	Total Zn 2 2	0	0
3	R7	2	Total Zn 2 2	0	0
3	R8	2	Total Zn 2 2	0	0
3	T1	2	Total Zn 2 2	0	0
3	T2	2	Total Zn 2 2	0	0
3	T3	2	Total Zn 2 2	0	0
3	T4	2	Total Zn 2 2	0	0
3	T5	2	Total Zn 2 2	0	0
3	T6	2	Total Zn 2 2	0	0
3	T7	2	Total Zn 2 2	0	0
3	T8	2	Total Zn 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A1	6	Total O 6 6	0	0
4	A2	16	Total O 16 16	0	0
4	A3	25	Total O 25 25	0	0
4	A4	29	Total O 29 29	0	0
4	A5	34	Total O 34 34	0	0
4	A6	22	Total O 22 22	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A7	13	Total O 13 13	0	0
4	A8	17	Total O 17 17	0	0
4	C1	19	Total O 19 19	0	0
4	C2	16	Total O 16 16	0	0
4	C3	9	Total O 9 9	0	0
4	C4	12	Total O 12 12	0	0
4	C5	10	Total O 10 10	0	0
4	C6	4	Total O 4 4	0	0
4	C7	11	Total O 11 11	0	0
4	C8	11	Total O 11 11	0	0
4	E1	5	Total O 5 5	0	0
4	E2	5	Total O 5 5	0	0
4	E3	2	Total O 2 2	0	0
4	E6	1	Total O 1 1	0	0
4	E7	1	Total O 1 1	0	0
4	G1	8	Total O 8 8	0	0
4	G2	6	Total O 6 6	0	0
4	G3	3	Total O 3 3	0	0
4	G4	2	Total O 2 2	0	0
4	G5	6	Total O 6 6	0	0
4	G6	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G7	10	Total O 10 10	0	0
4	G8	7	Total O 7 7	0	0
4	I1	19	Total O 19 19	0	0
4	I2	8	Total O 8 8	0	0
4	I3	8	Total O 8 8	0	0
4	I4	4	Total O 4 4	0	0
4	I5	15	Total O 15 15	0	0
4	I6	5	Total O 5 5	0	0
4	I7	14	Total O 14 14	0	0
4	I8	7	Total O 7 7	0	0
4	K1	1	Total O 1 1	0	0
4	K2	2	Total O 2 2	0	0
4	K3	5	Total O 5 5	0	0
4	K4	7	Total O 7 7	0	0
4	K5	8	Total O 8 8	0	0
4	K6	7	Total O 7 7	0	0
4	K7	4	Total O 4 4	0	0
4	K8	5	Total O 5 5	0	0
4	M1	7	Total O 7 7	0	0
4	M2	3	Total O 3 3	0	0
4	M3	11	Total O 11 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M4	7	Total O 7 7	0	0
4	M5	6	Total O 6 6	0	0
4	M6	16	Total O 16 16	0	0
4	M7	9	Total O 9 9	0	0
4	M8	4	Total O 4 4	0	0
4	O1	8	Total O 8 8	0	0
4	O2	5	Total O 5 5	0	0
4	O3	13	Total O 13 13	0	0
4	O4	5	Total O 5 5	0	0
4	O5	3	Total O 3 3	0	0
4	O6	4	Total O 4 4	0	0
4	O7	6	Total O 6 6	0	0
4	O8	3	Total O 3 3	0	0
4	Q1	1	Total O 1 1	0	0
4	Q2	2	Total O 2 2	0	0
4	Q3	5	Total O 5 5	0	0
4	Q5	2	Total O 2 2	0	0
4	Q6	6	Total O 6 6	0	0
4	Q8	1	Total O 1 1	0	0
4	S1	6	Total O 6 6	0	0
4	S2	9	Total O 9 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S3	2	Total O 2 2	0	0
4	S4	5	Total O 5 5	0	0
4	S5	1	Total O 1 1	0	0
4	S7	2	Total O 2 2	0	0
4	B1	2	Total O 2 2	0	0
4	B2	2	Total O 2 2	0	0
4	B8	2	Total O 2 2	0	0
4	D1	2	Total O 2 2	0	0
4	D2	1	Total O 1 1	0	0
4	D4	1	Total O 1 1	0	0
4	D6	1	Total O 1 1	0	0
4	F7	1	Total O 1 1	0	0
4	F8	1	Total O 1 1	0	0
4	J1	2	Total O 2 2	0	0
4	J4	2	Total O 2 2	0	0
4	L5	1	Total O 1 1	0	0
4	L8	1	Total O 1 1	0	0
4	N2	1	Total O 1 1	0	0
4	N5	2	Total O 2 2	0	0
4	N8	1	Total O 1 1	0	0
4	P4	1	Total O 1 1	0	0

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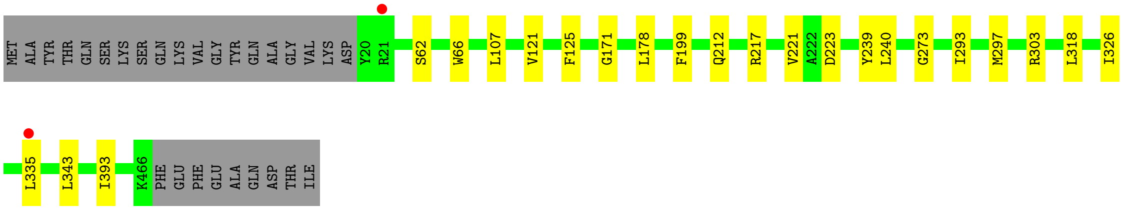
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P8	1	Total O 1 1	0	0
4	T1	1	Total O 1 1	0	0

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

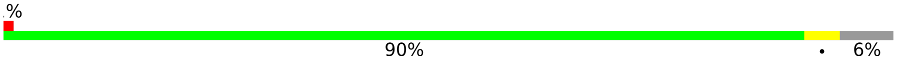
- Molecule 1: Ribulose bisphosphate carboxylase large chain

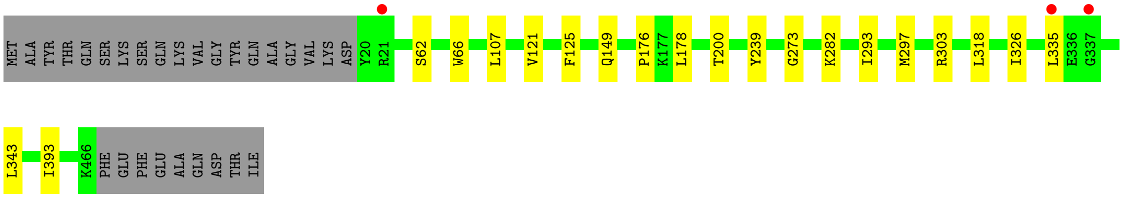
Chain A1:



- Molecule 1: Ribulose bisphosphate carboxylase large chain

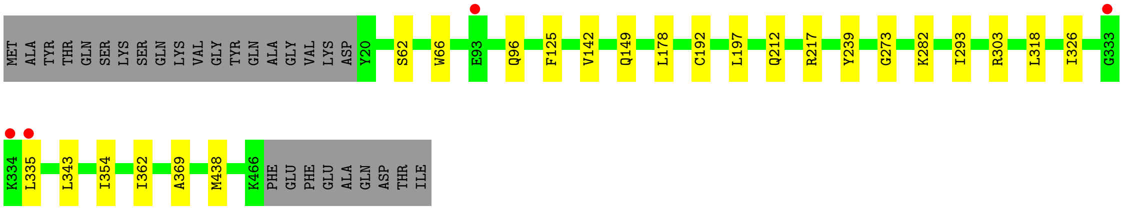
Chain A2:





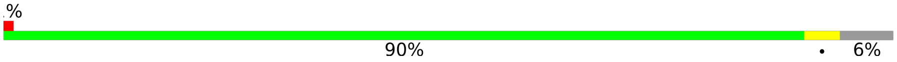
- Molecule 1: Ribulose bisphosphate carboxylase large chain

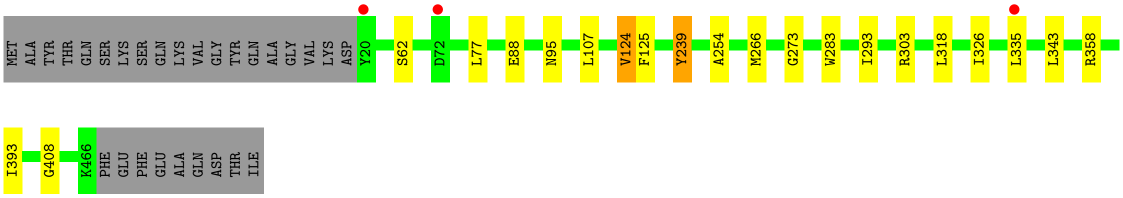
Chain A3:



- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain A4:



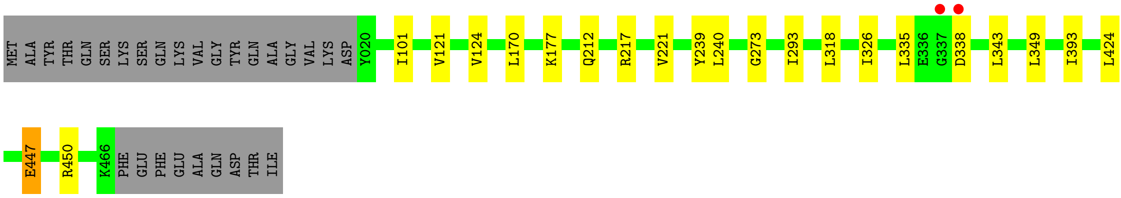


- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain A5:

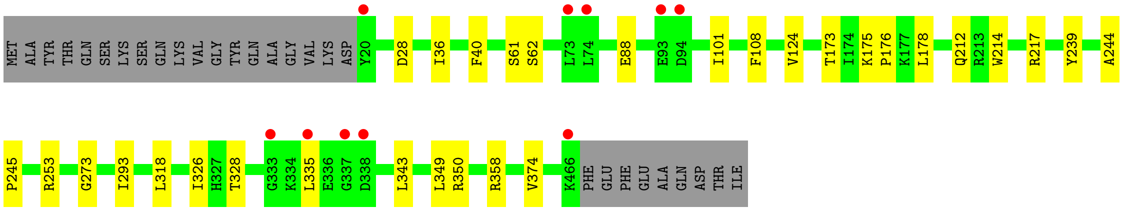
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain A6:



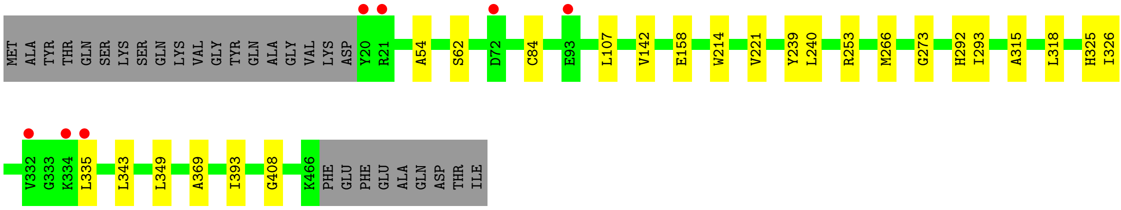
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain A7:

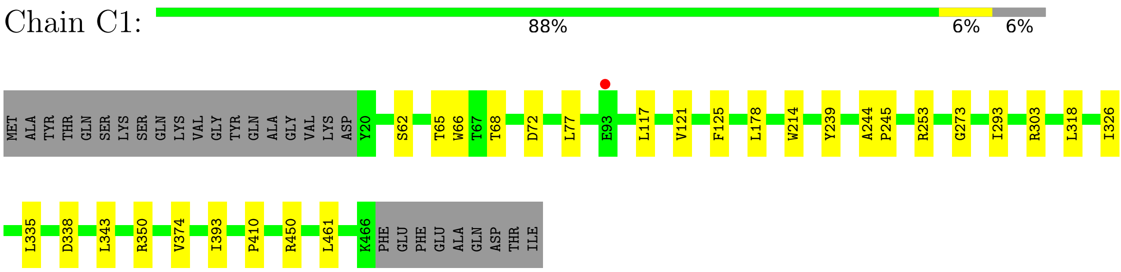


- Molecule 1: Ribulose bisphosphate carboxylase large chain

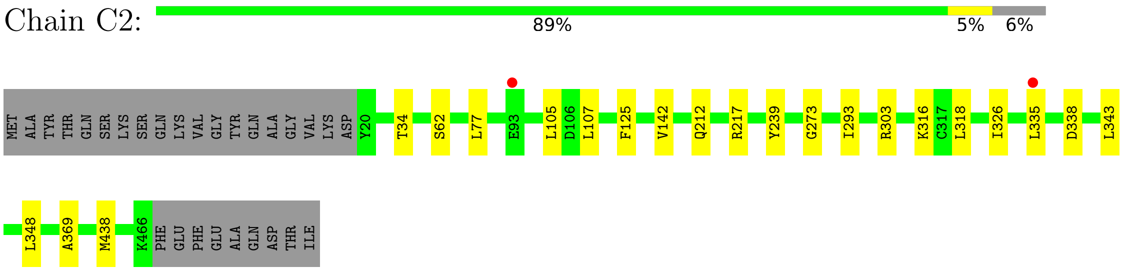
Chain A8:



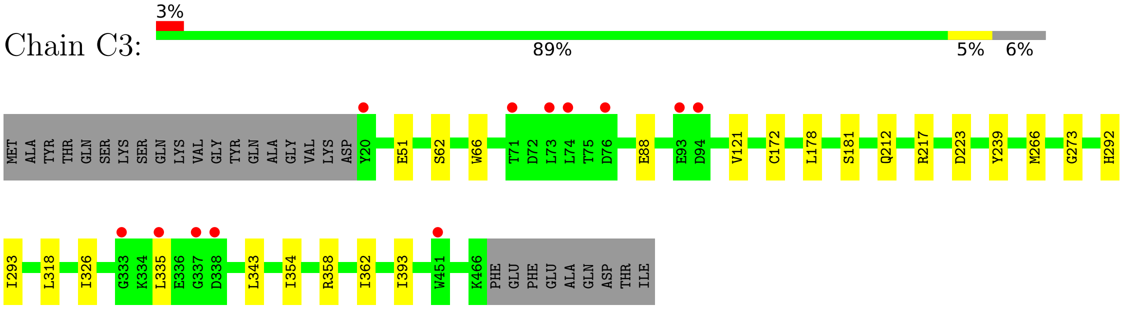
- Molecule 1: Ribulose bisphosphate carboxylase large chain



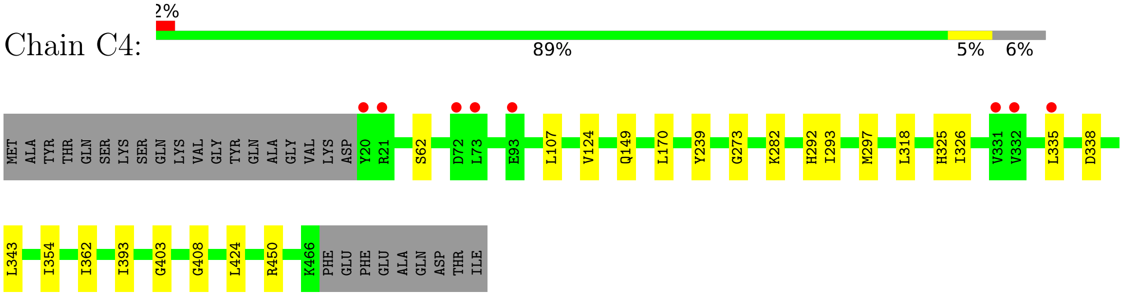
- Molecule 1: Ribulose bisphosphate carboxylase large chain



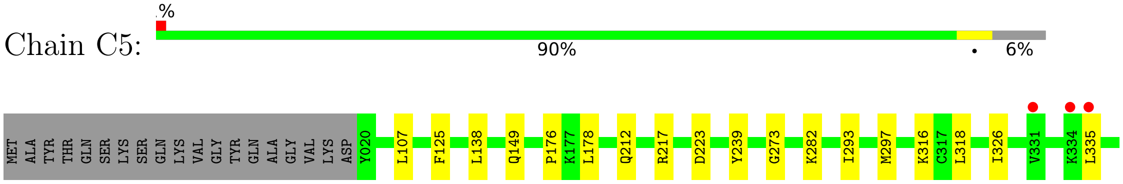
- Molecule 1: Ribulose bisphosphate carboxylase large chain

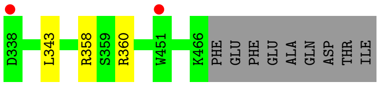


- Molecule 1: Ribulose bisphosphate carboxylase large chain



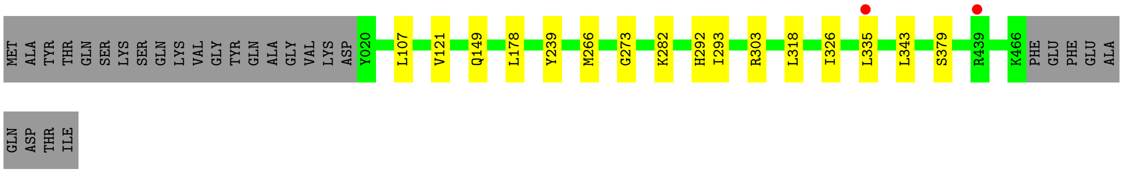
- Molecule 1: Ribulose bisphosphate carboxylase large chain





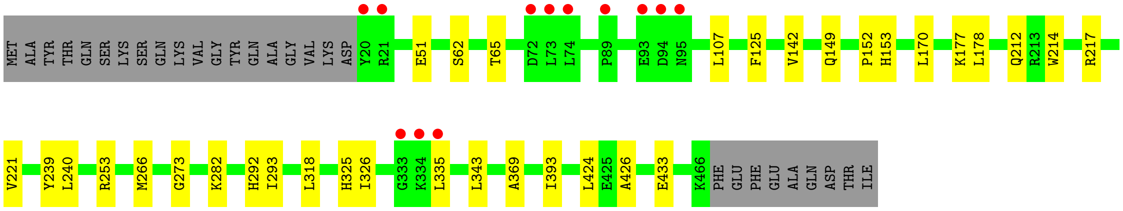
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain C6:



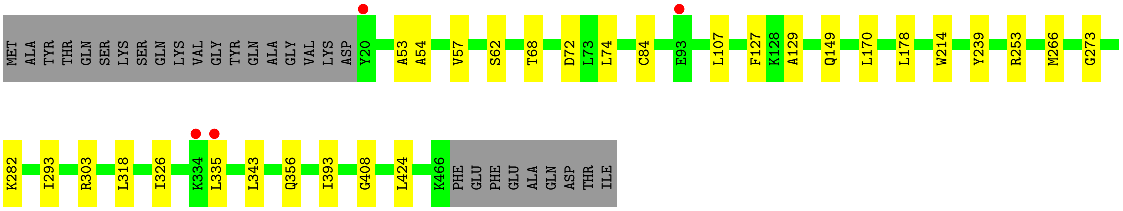
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain C7:



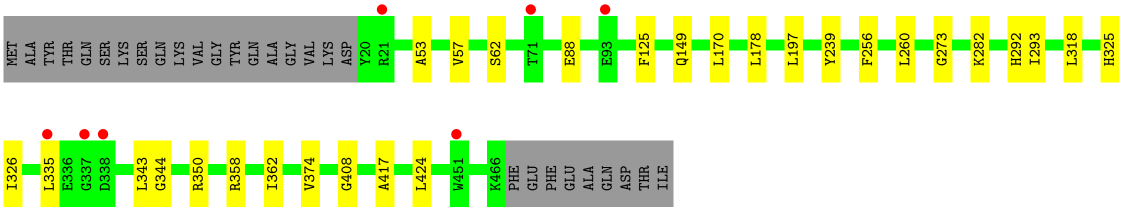
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain C8:



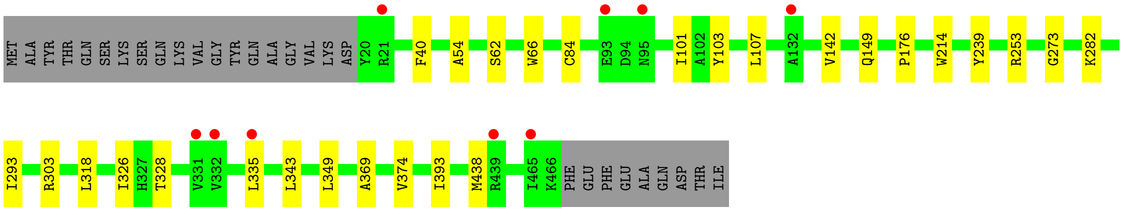
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain E1:



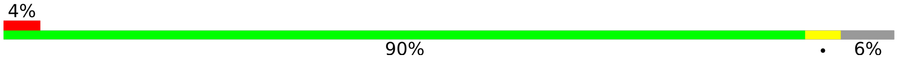
- Molecule 1: Ribulose bisphosphate carboxylase large chain

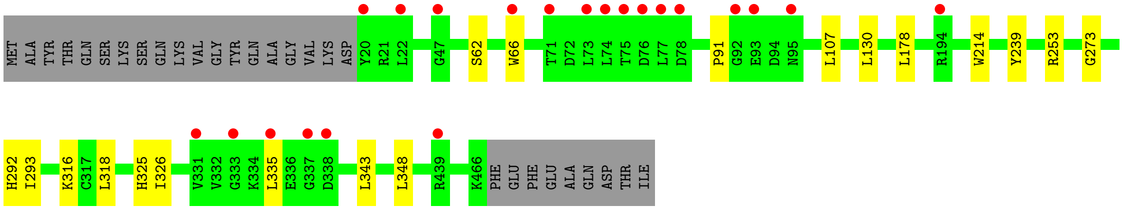
Chain E2:



- Molecule 1: Ribulose bisphosphate carboxylase large chain

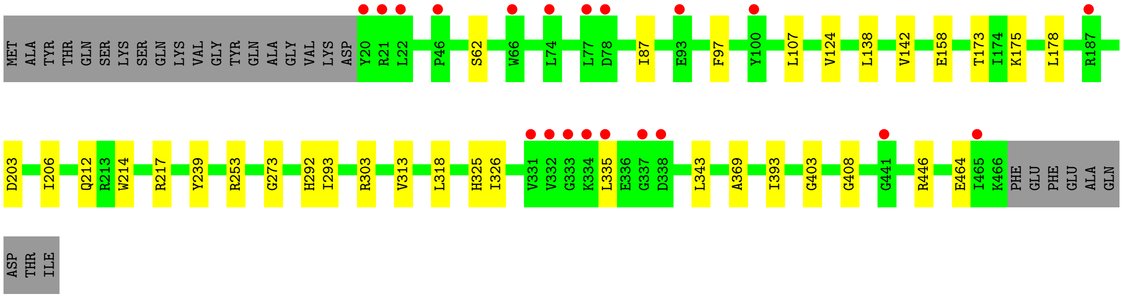
Chain E3:





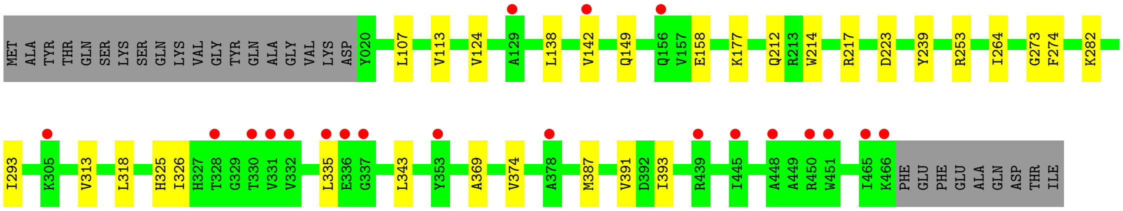
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain E4:



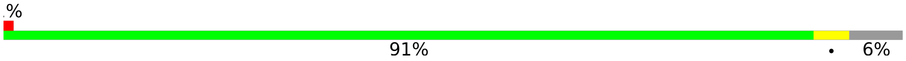
- Molecule 1: Ribulose bisphosphate carboxylase large chain

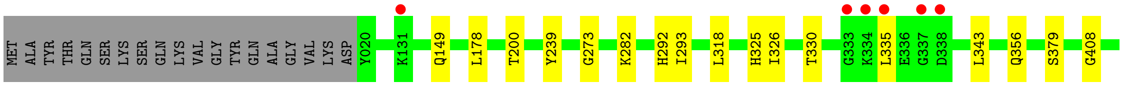
Chain E5:

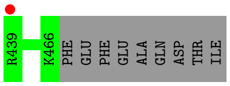


- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain E6:

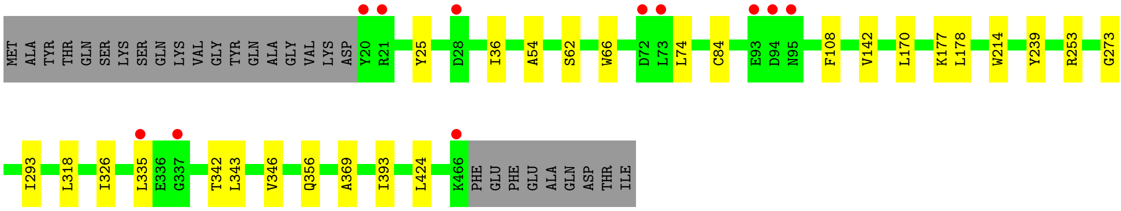






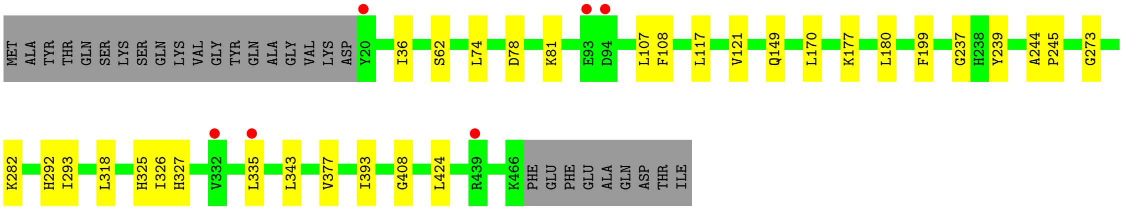
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain E7:



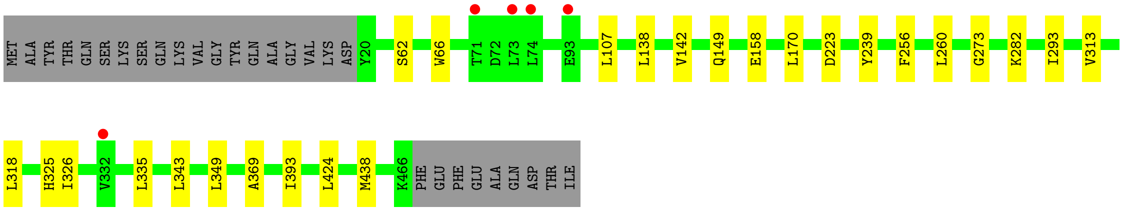
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain E8:



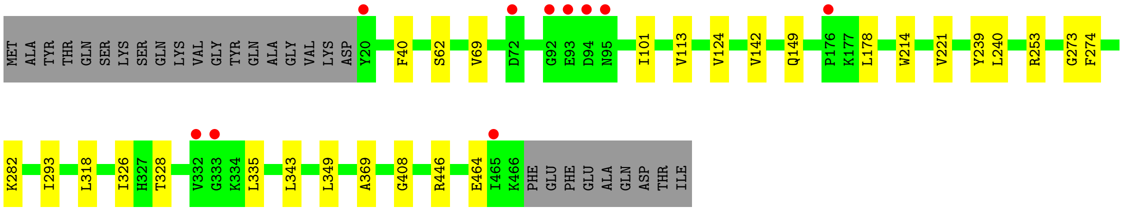
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain G1:



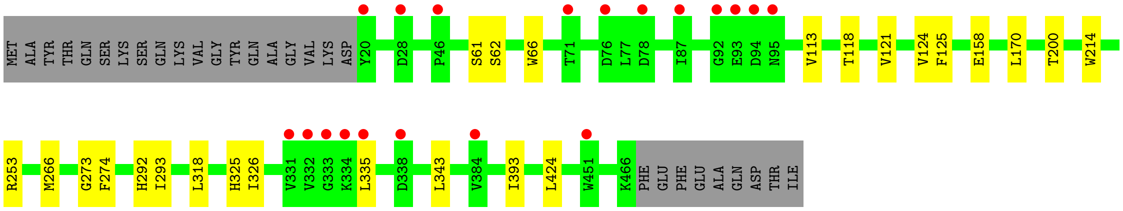
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain G2:



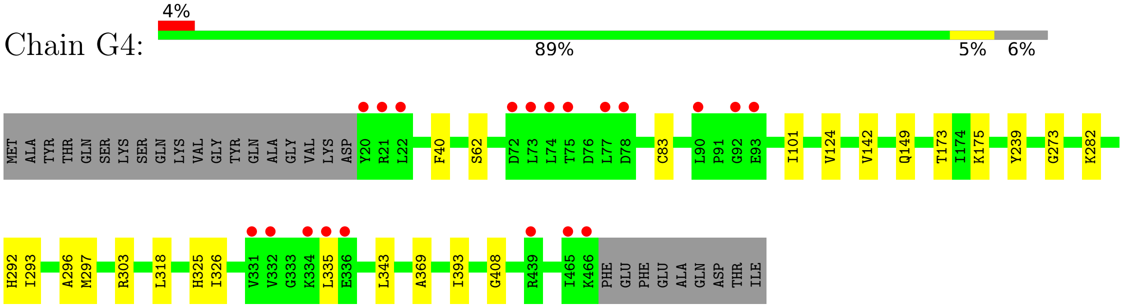
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain G3:



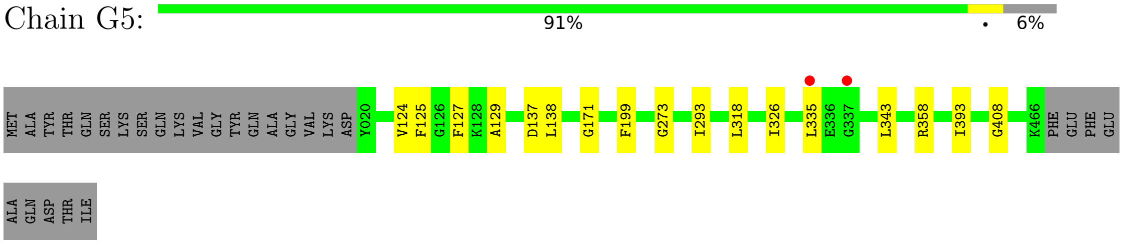
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain G4:



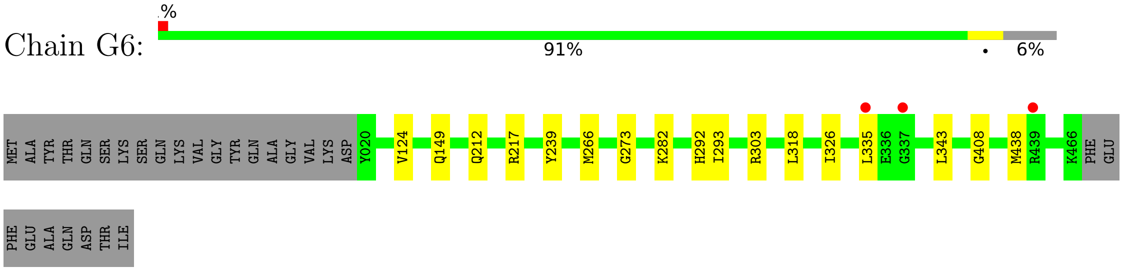
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain G5:



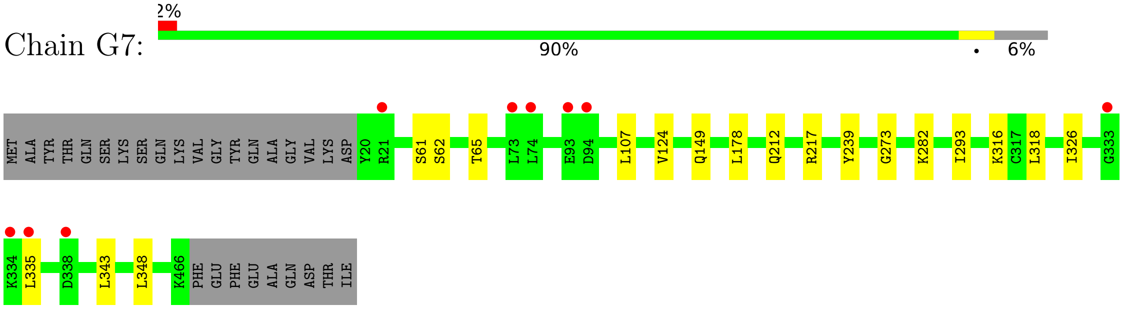
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain G6:



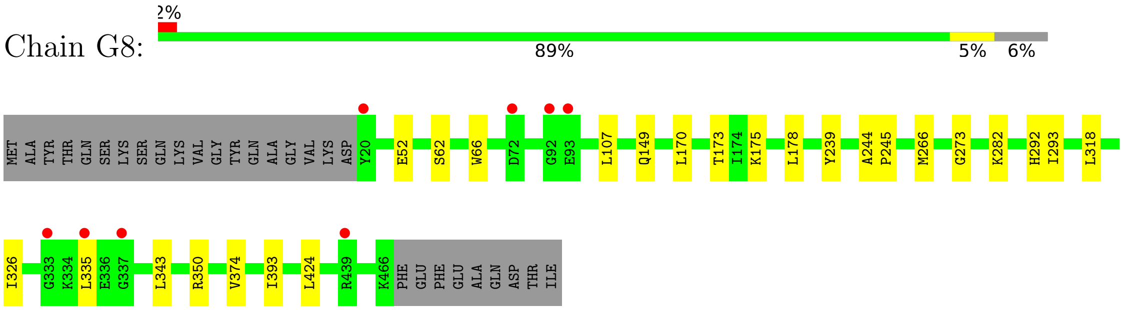
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain G7:



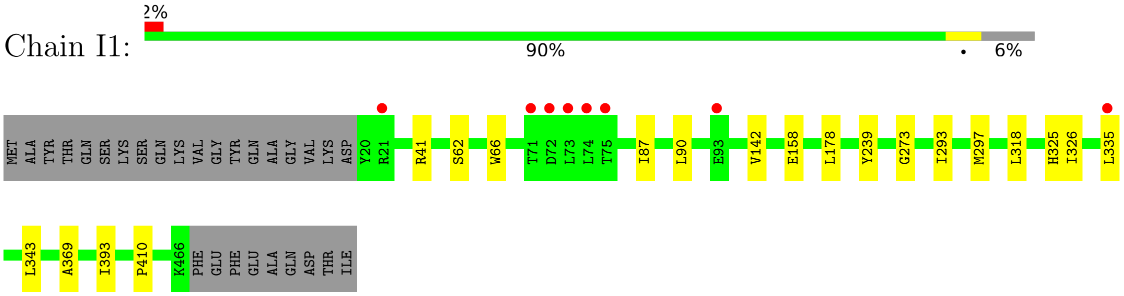
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain G8:



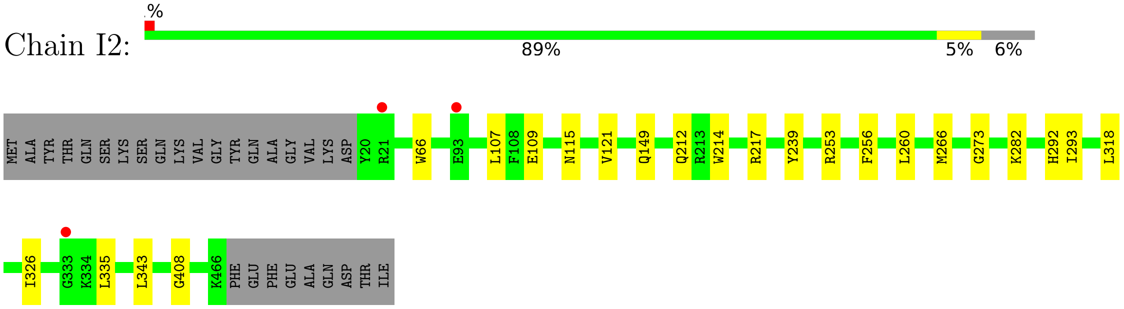
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain I1:



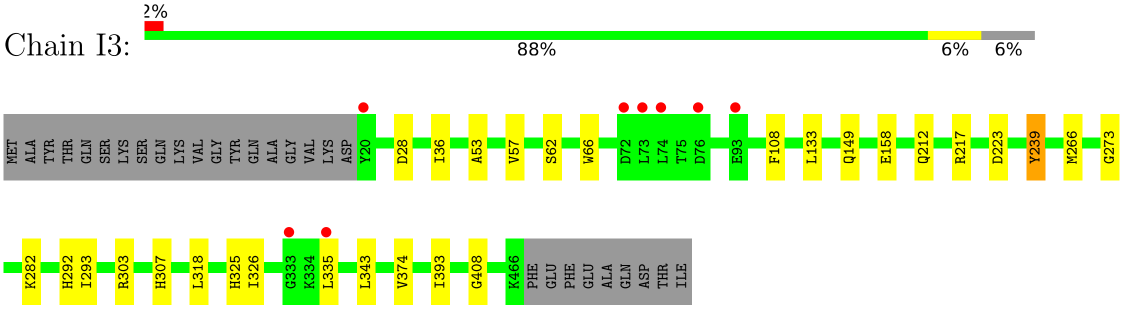
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain I2:



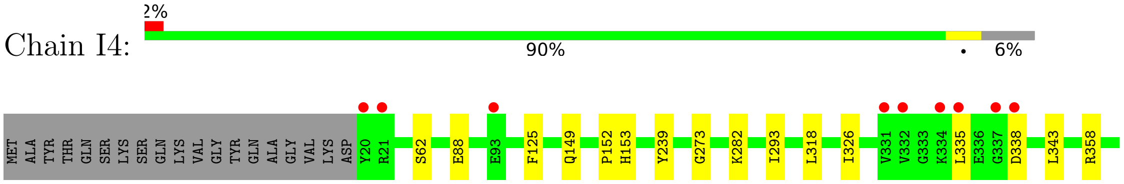
- Molecule 1: Ribulose bisphosphate carboxylase large chain

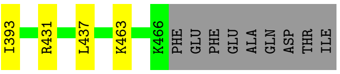
Chain I3:



- Molecule 1: Ribulose bisphosphate carboxylase large chain

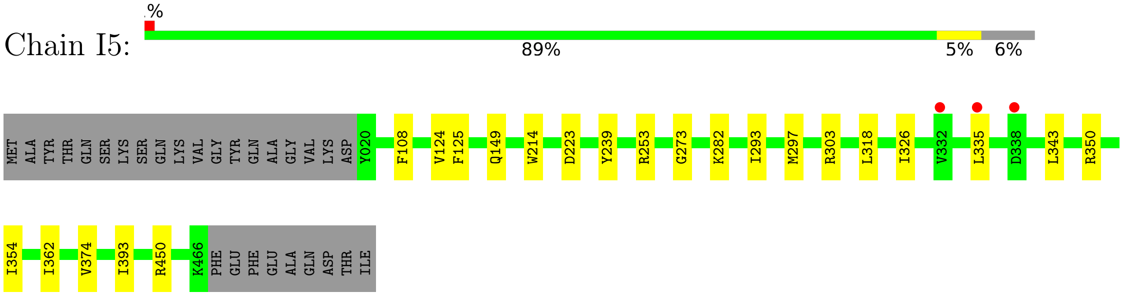
Chain I4:





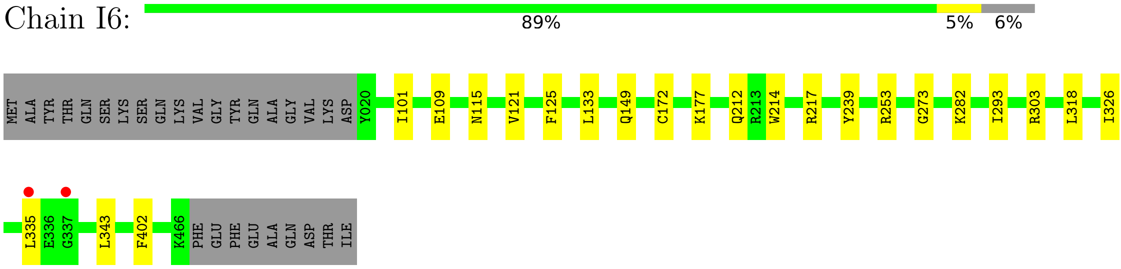
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain I5:



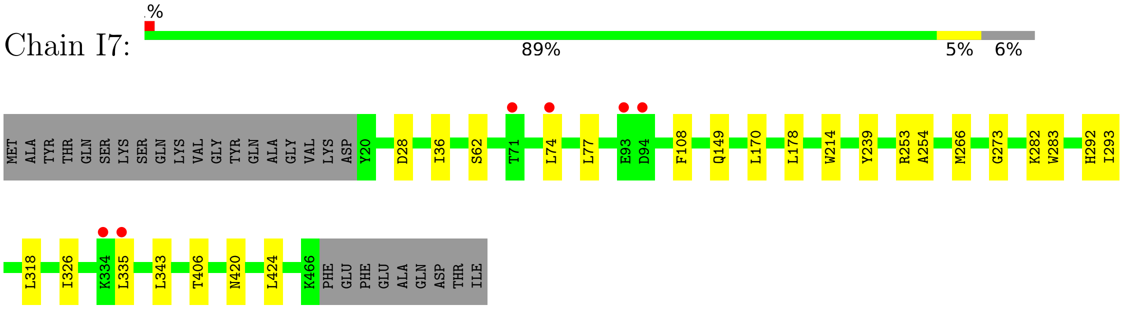
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain I6:



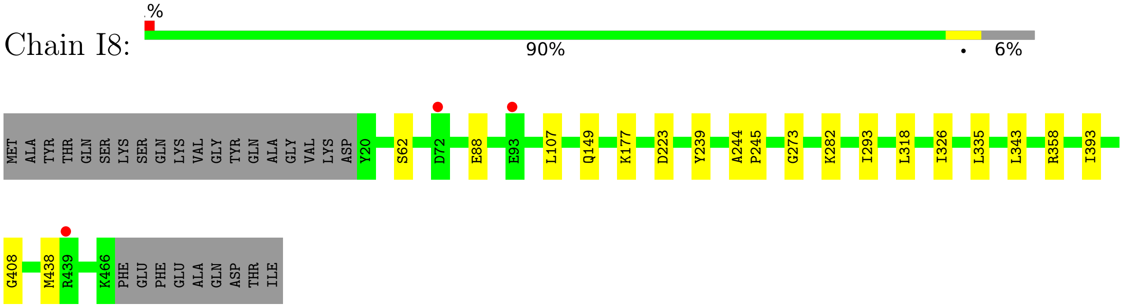
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain I7:



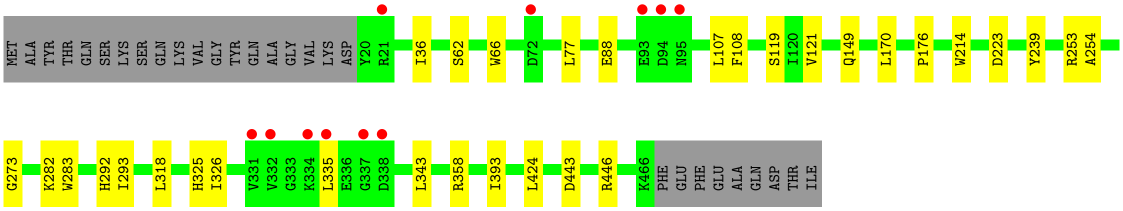
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain I8:



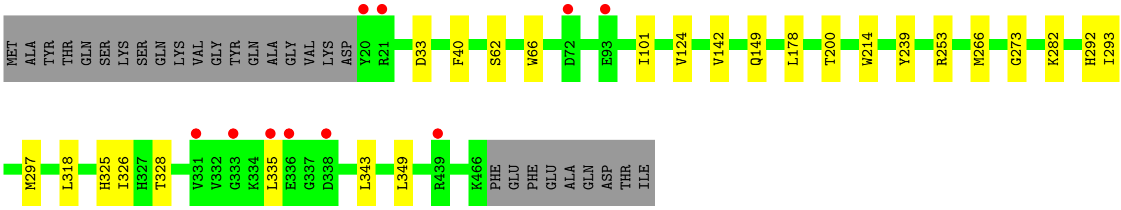
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain K1:



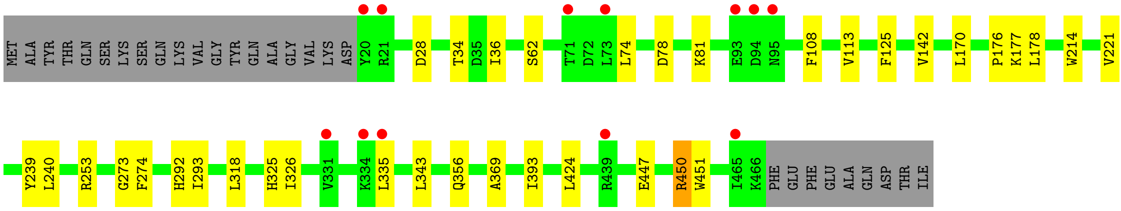
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain K2:



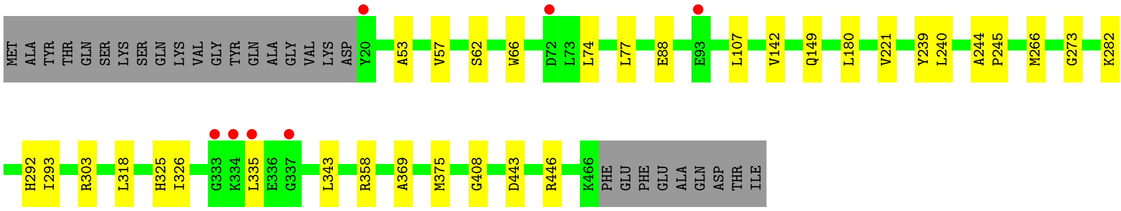
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain K3:



• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain K4:

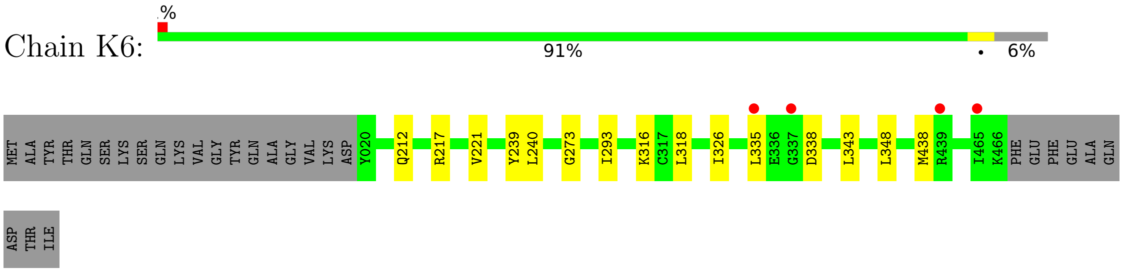


• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain K5:

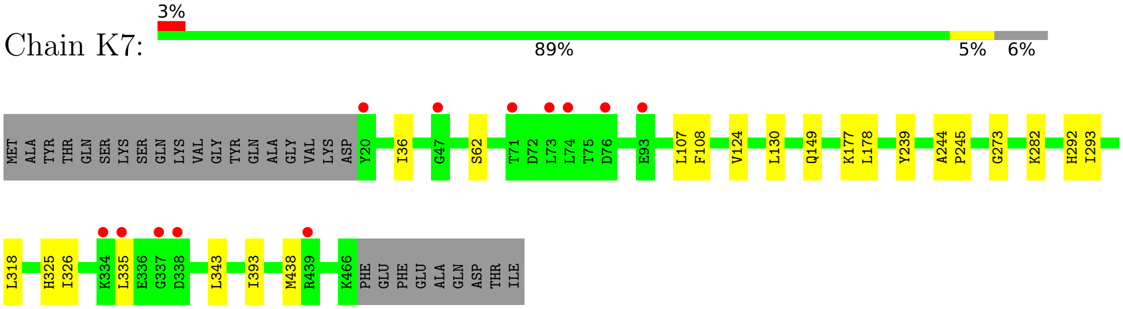
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain K6:



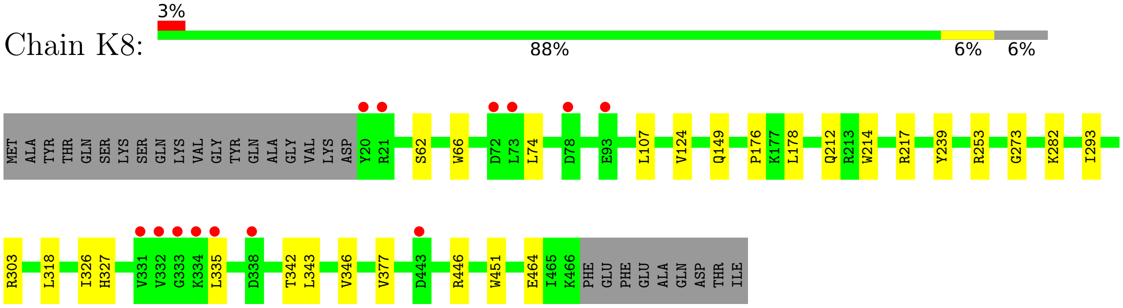
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain K7:



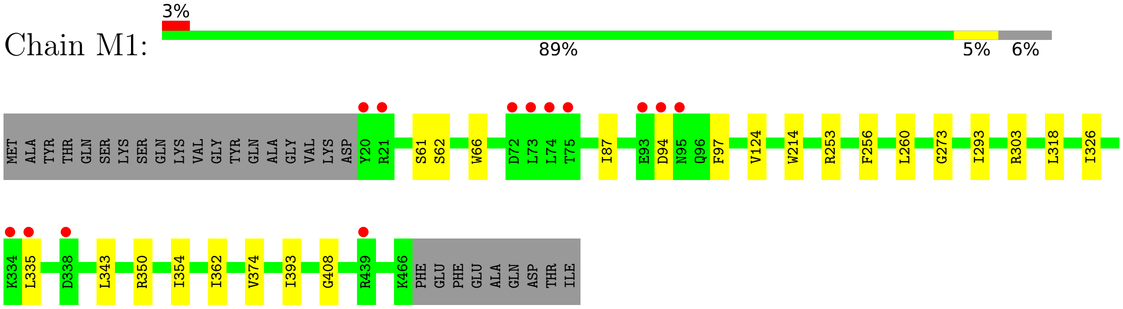
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain K8:



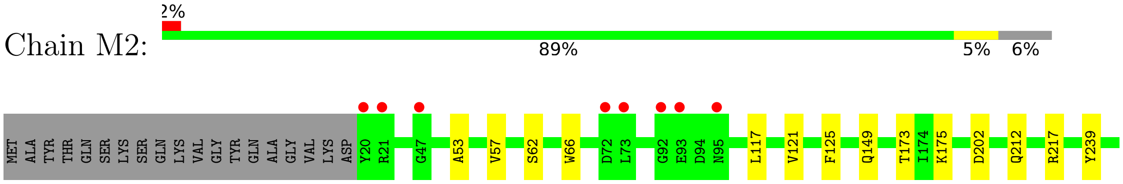
- Molecule 1: Ribulose bisphosphate carboxylase large chain

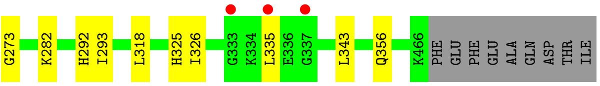
Chain M1:



- Molecule 1: Ribulose bisphosphate carboxylase large chain

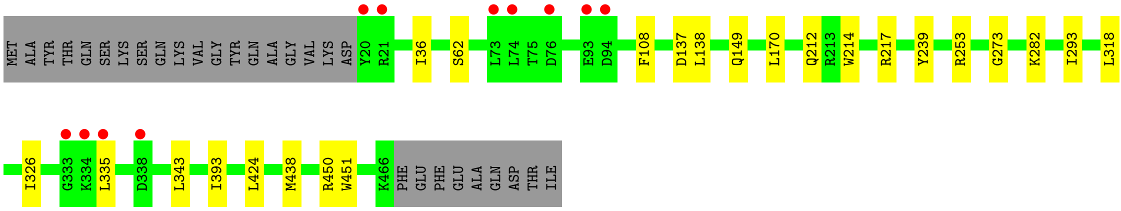
Chain M2:





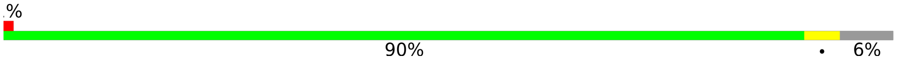
- Molecule 1: Ribulose bisphosphate carboxylase large chain

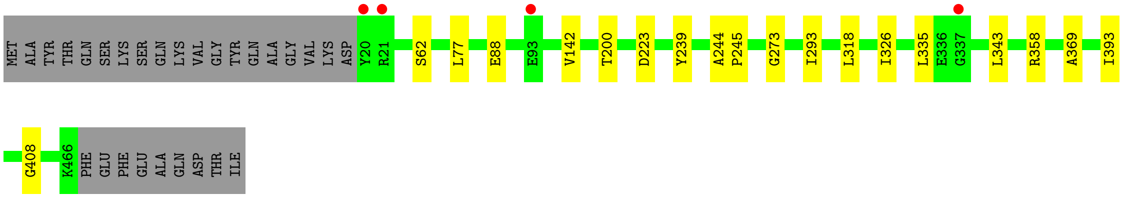
Chain M3:



- Molecule 1: Ribulose bisphosphate carboxylase large chain

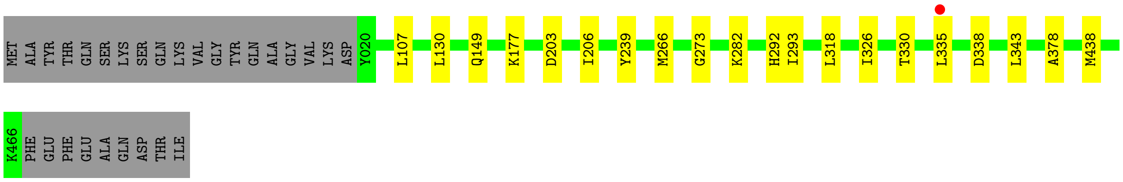
Chain M4:





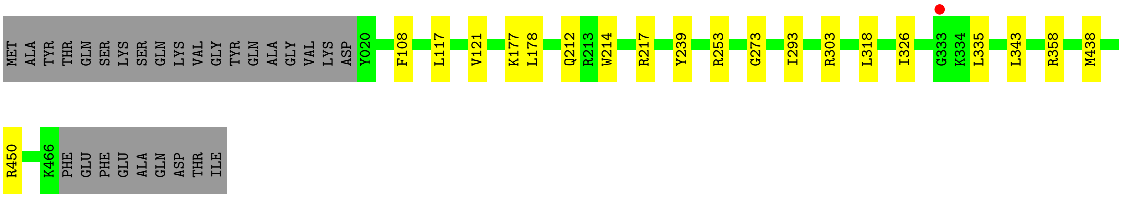
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain M5:



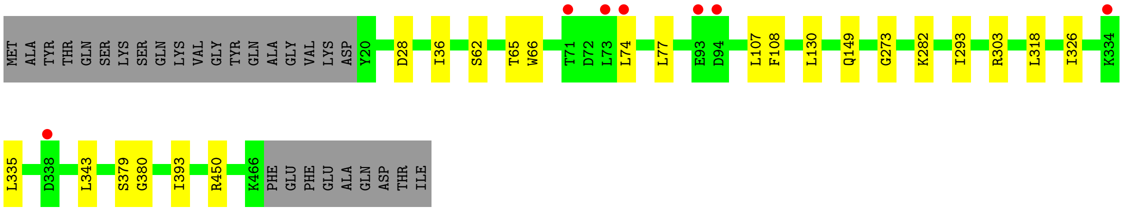
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain M6:



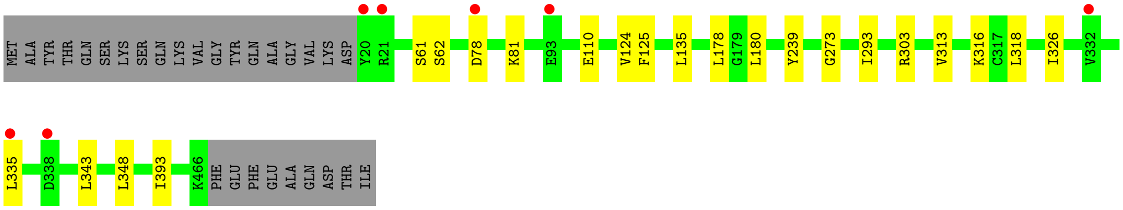
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain M7:



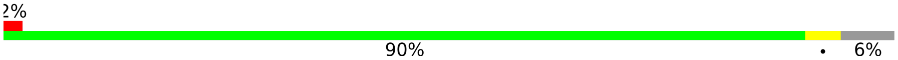
- Molecule 1: Ribulose bisphosphate carboxylase large chain

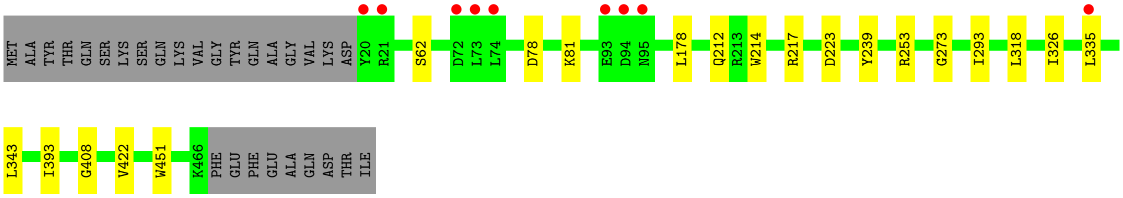
Chain M8:



- Molecule 1: Ribulose bisphosphate carboxylase large chain

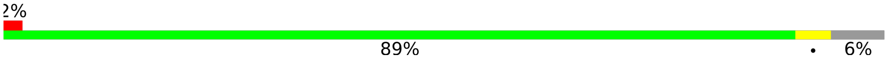
Chain O1:

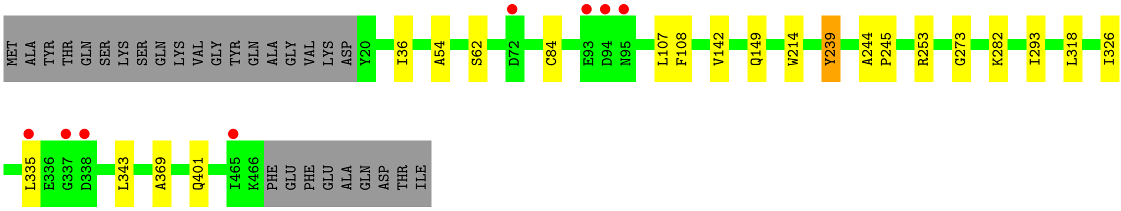




- Molecule 1: Ribulose bisphosphate carboxylase large chain

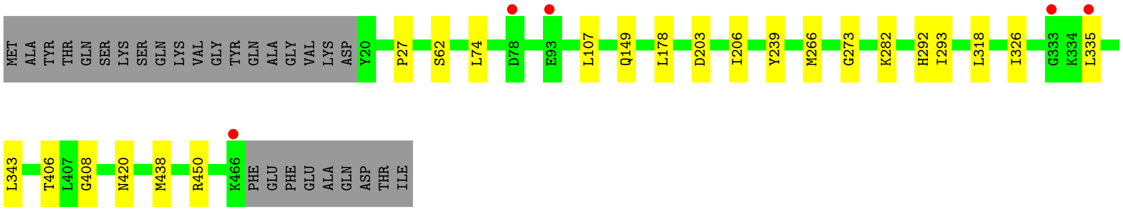
Chain O2:





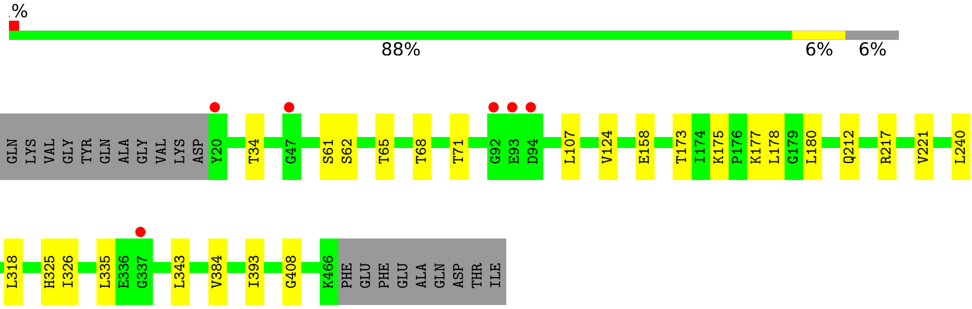
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain O3:



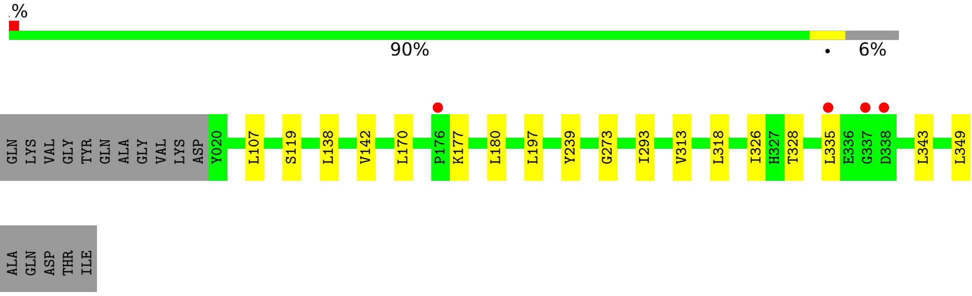
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain O4:



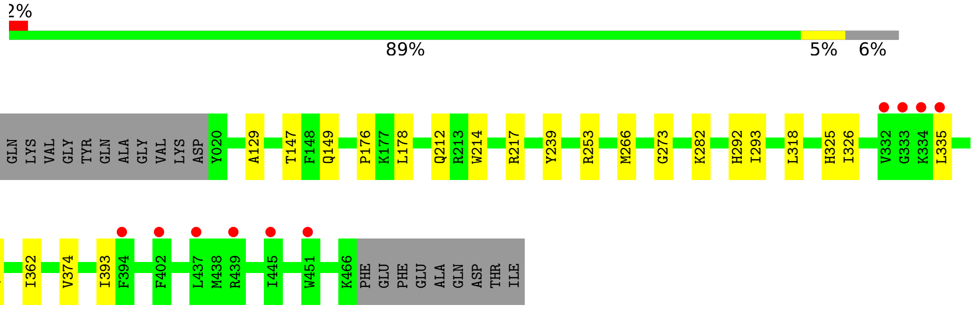
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain O5:



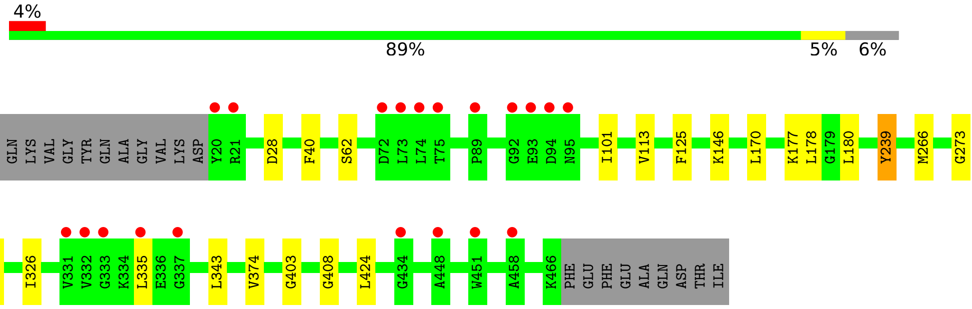
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain O6:



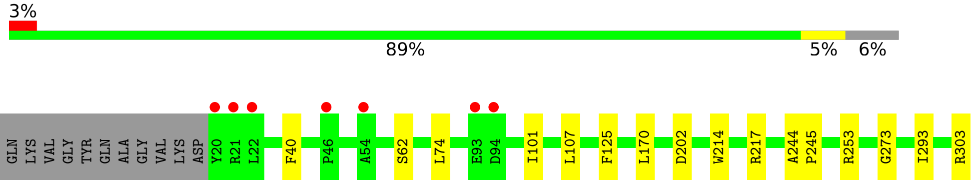
- Molecule 1: Ribulose bisphosphate carboxylase large chain

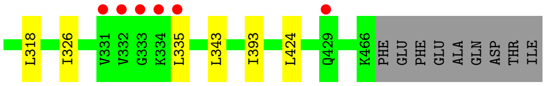
Chain O7:



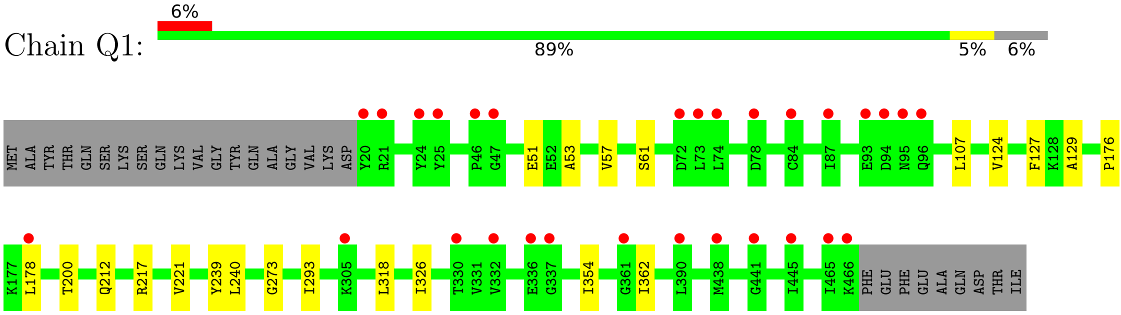
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain O8:

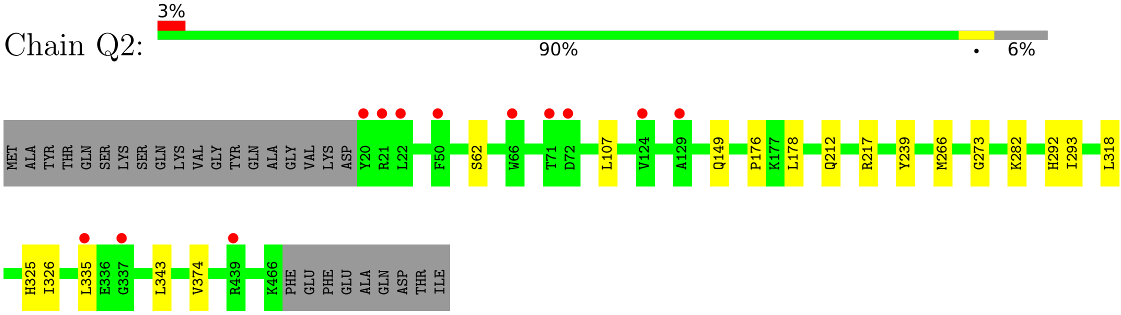




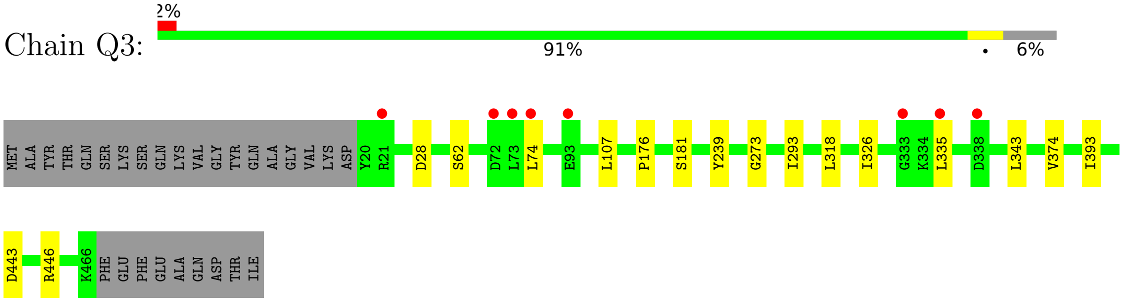
- Molecule 1: Ribulose bisphosphate carboxylase large chain



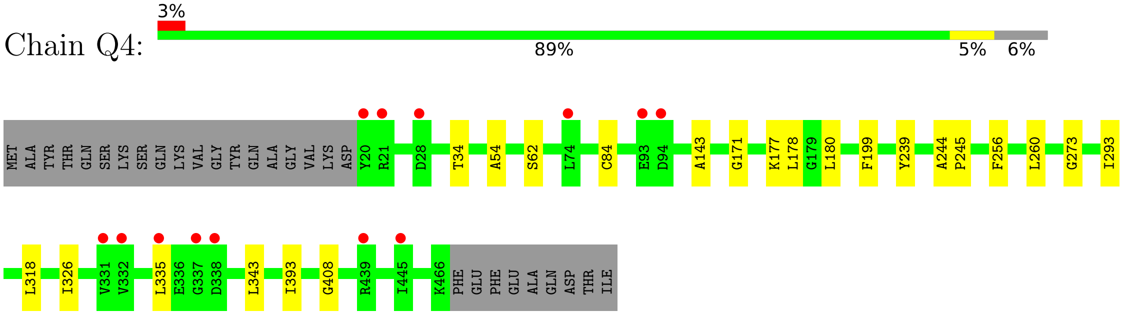
- Molecule 1: Ribulose bisphosphate carboxylase large chain



- Molecule 1: Ribulose bisphosphate carboxylase large chain

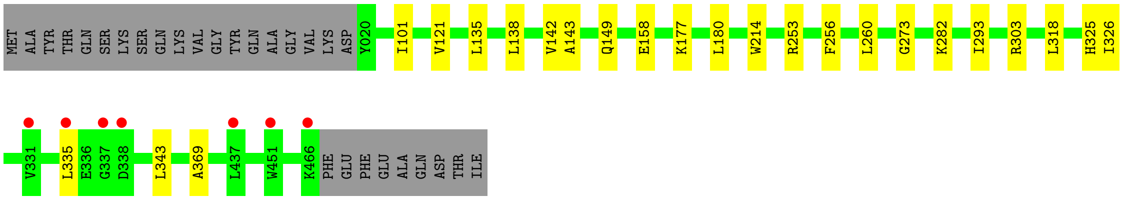


- Molecule 1: Ribulose bisphosphate carboxylase large chain



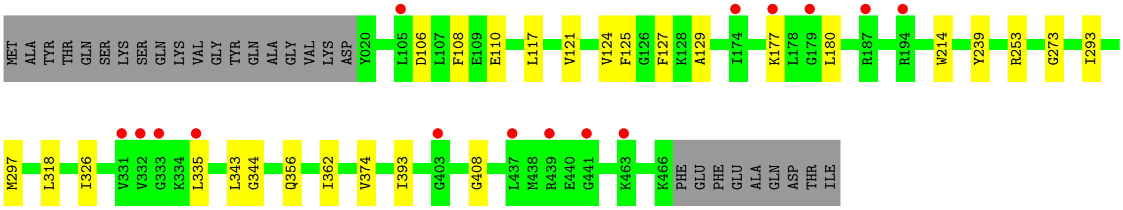
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain Q5:



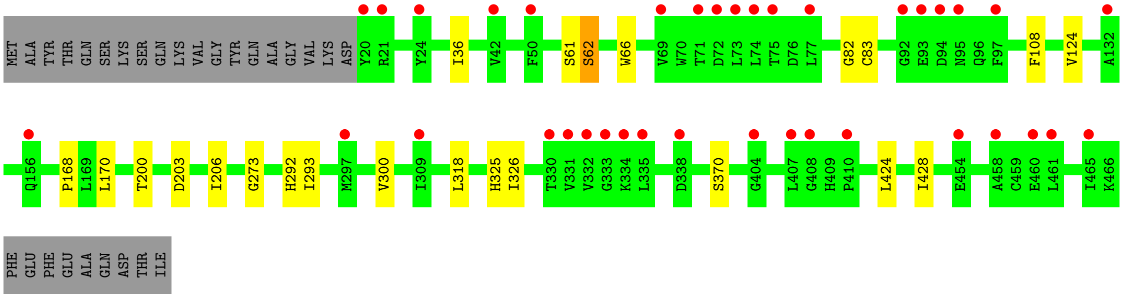
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain Q6:



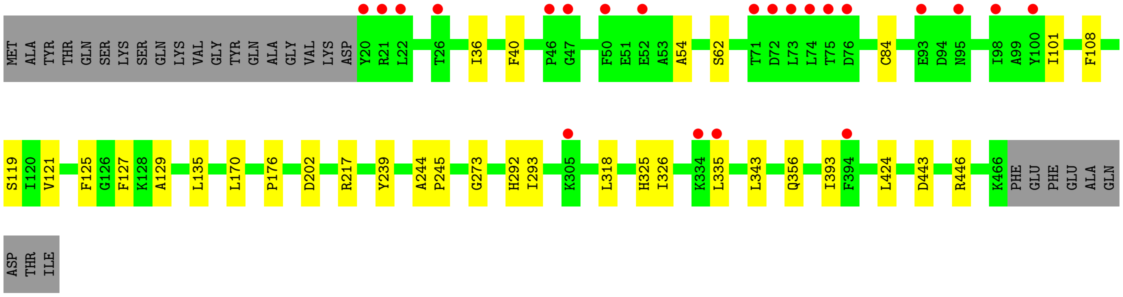
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain Q7:



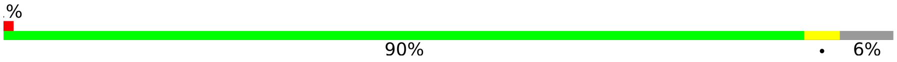
- Molecule 1: Ribulose bisphosphate carboxylase large chain

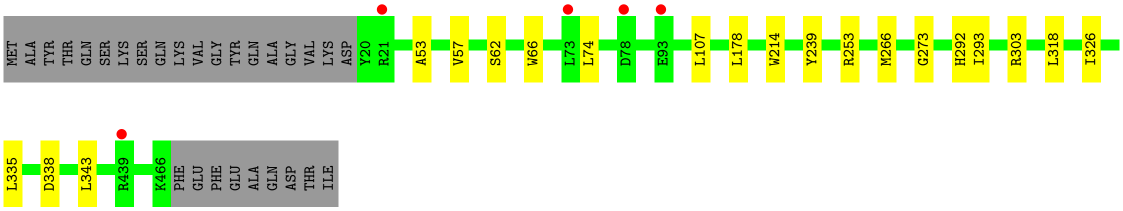
Chain Q8:



- Molecule 1: Ribulose bisphosphate carboxylase large chain

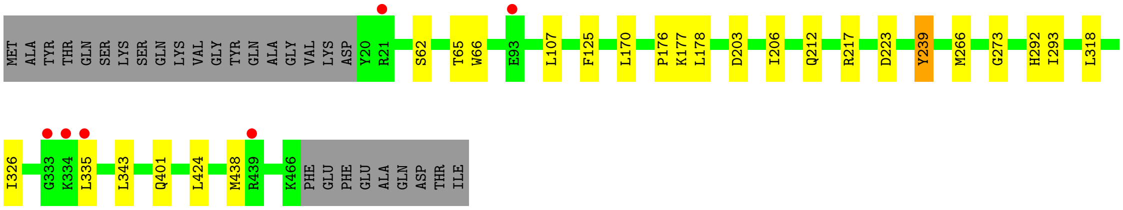
Chain S1:





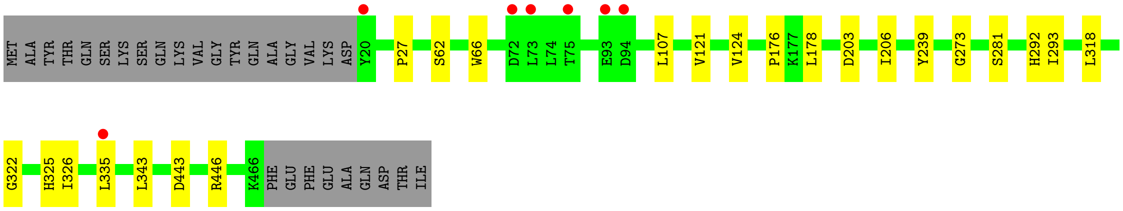
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain S2:



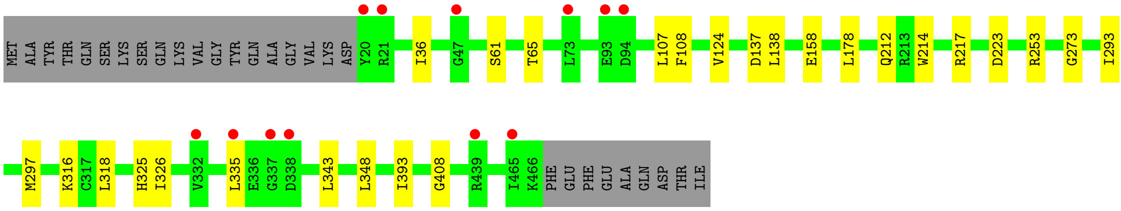
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain S3:



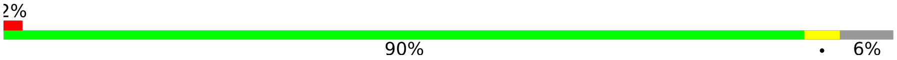
- Molecule 1: Ribulose bisphosphate carboxylase large chain

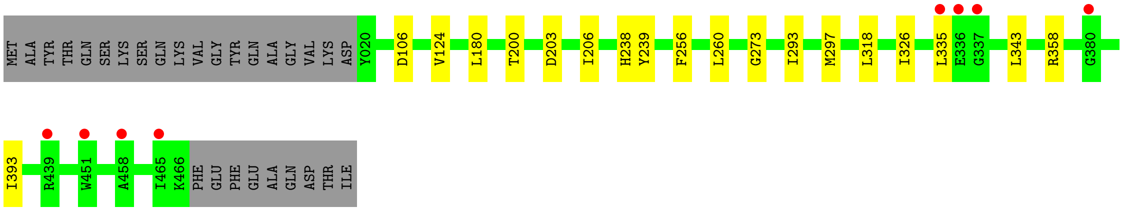
Chain S4:



- Molecule 1: Ribulose bisphosphate carboxylase large chain

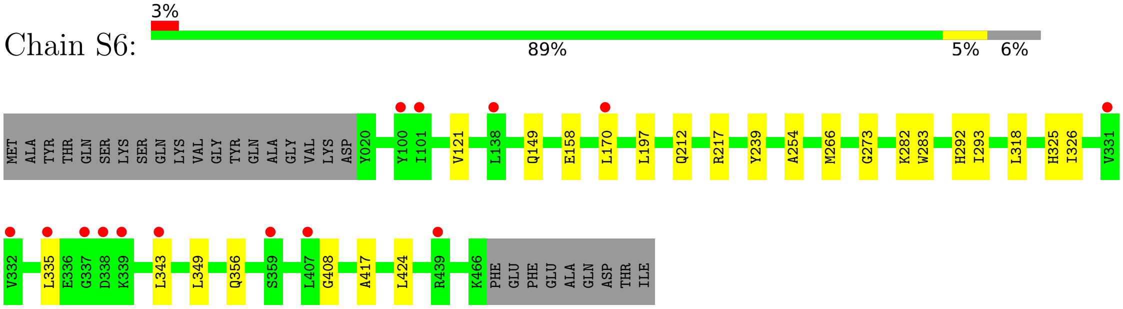
Chain S5:





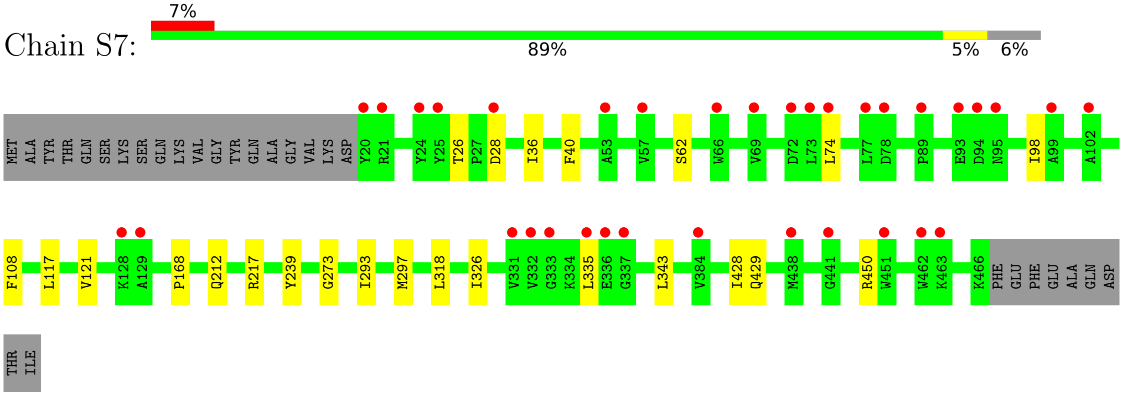
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain S6:



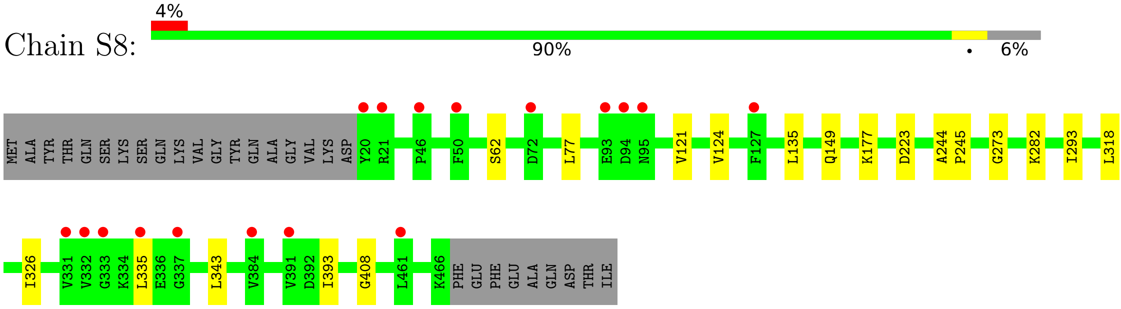
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain S7:



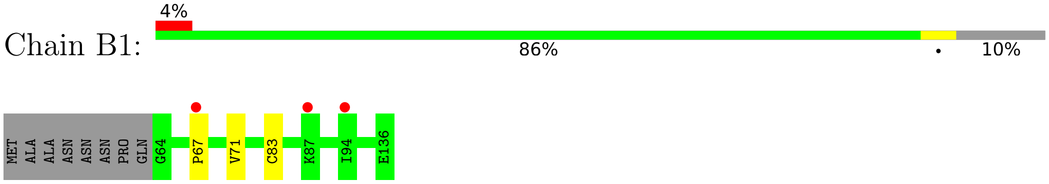
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain S8:



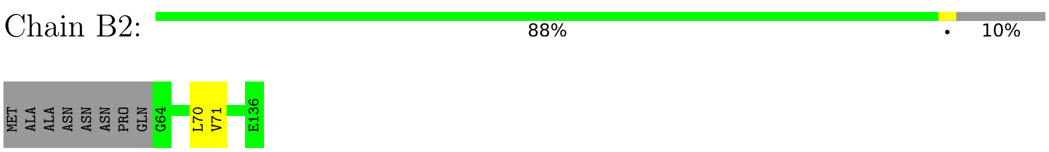
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain B1:



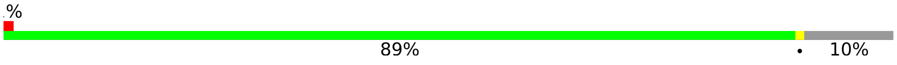
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

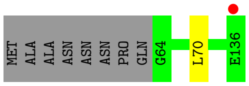
Chain B2:



- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

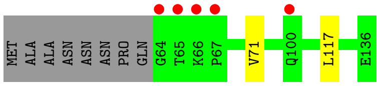
Chain B3:





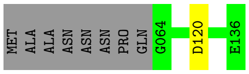
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain B4:



- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain B5:

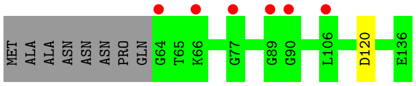


- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain B6:

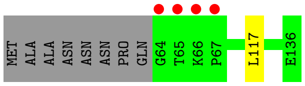
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain B7:



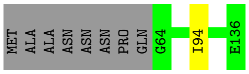
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain B8:



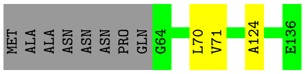
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain D1:



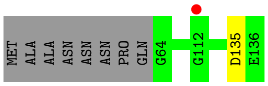
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain D2:



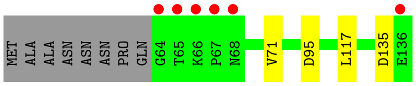
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain D3:



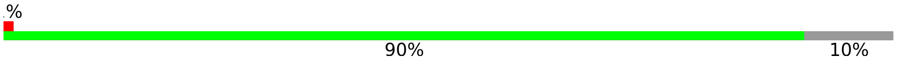
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

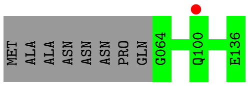
Chain D4:



- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

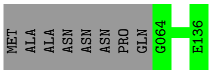
Chain D5:





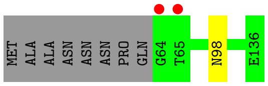
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain D6:



- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain D7:



- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

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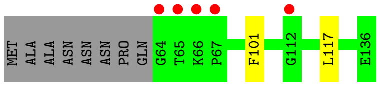
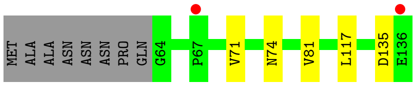


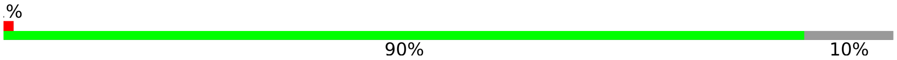
• Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

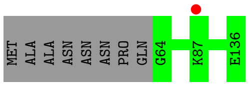
Chain F1:



• Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain F2:





• Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

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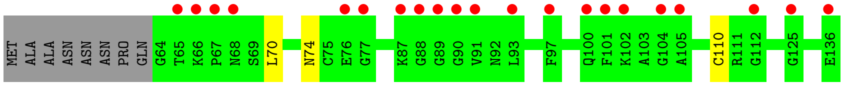

• Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

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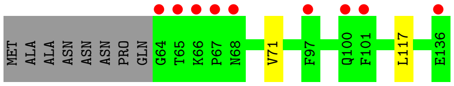

• Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

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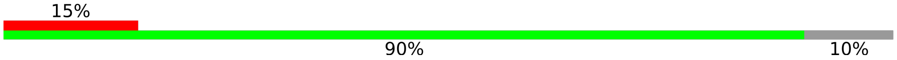

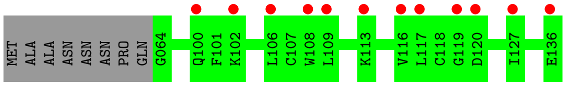

• Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

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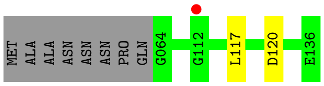
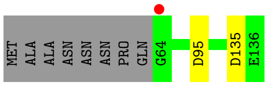


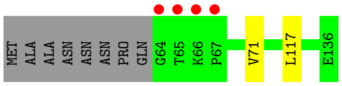
• Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain F7:



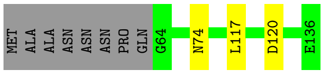
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain F8:



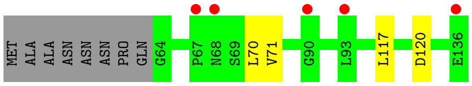
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain H1:



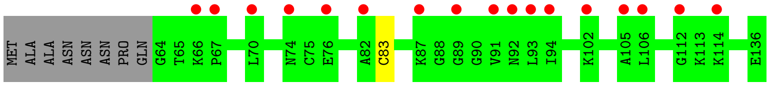
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain H2:



- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain H3:



- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

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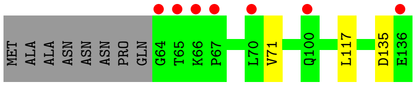
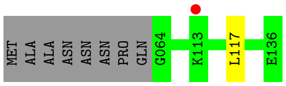


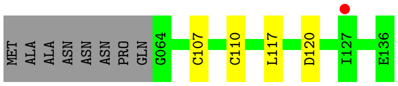
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain H5:



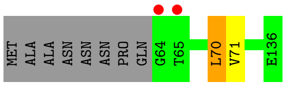
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain H6:



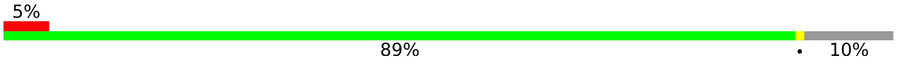
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

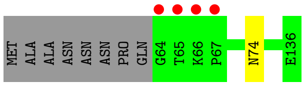
Chain H7:



- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

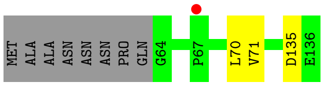
Chain H8:





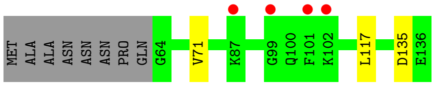
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J1:



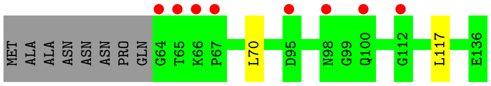
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J2:



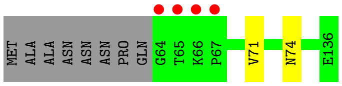
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J3:



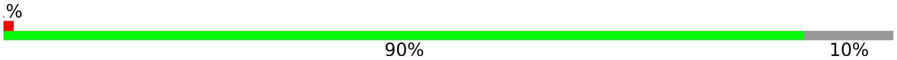
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

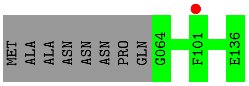
Chain J4:



- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J5:



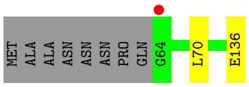


- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J6:

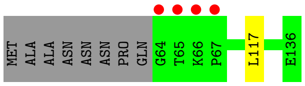
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J7:



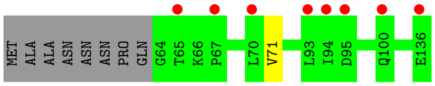
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J8:



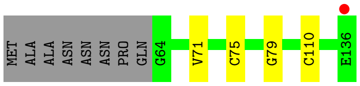
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L1:



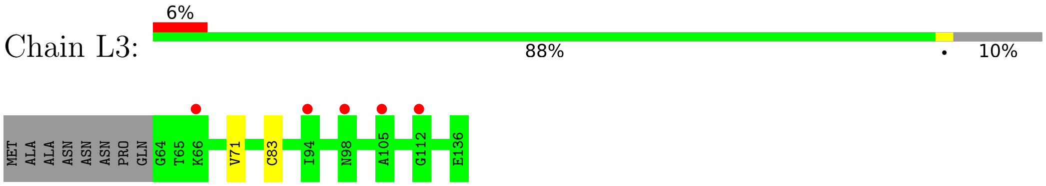
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L2:



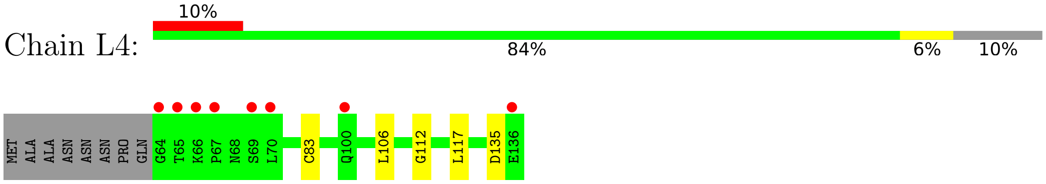
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L3:



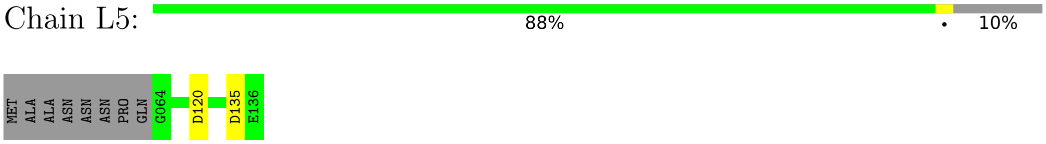
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L4:



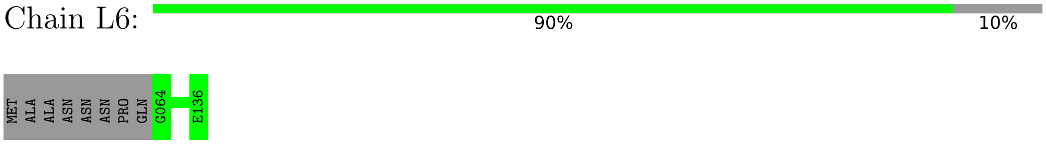
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L5:



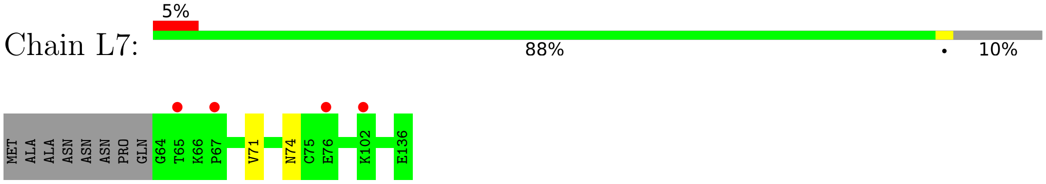
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L6:



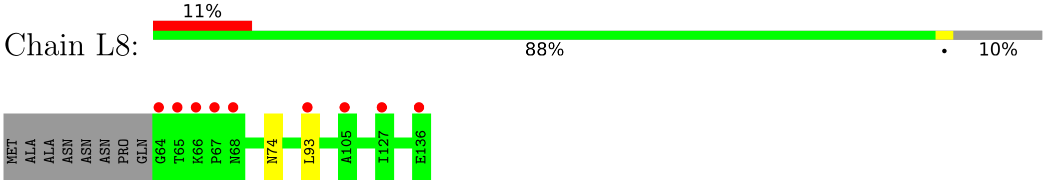
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L7:



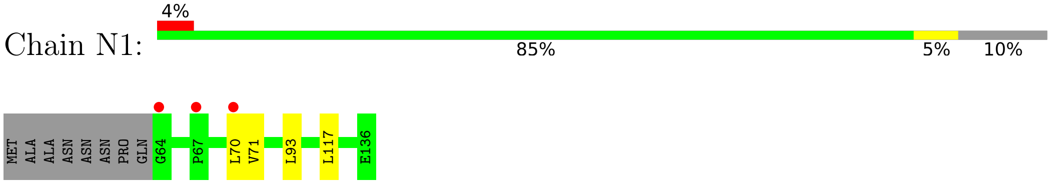
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L8:



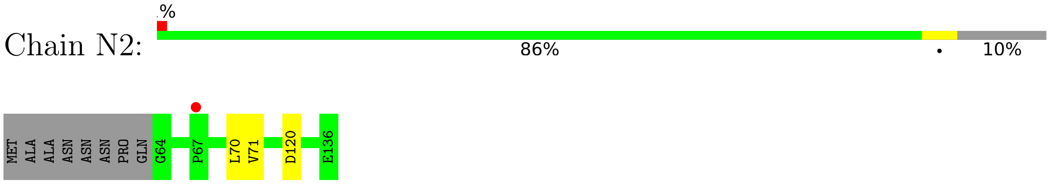
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N1:



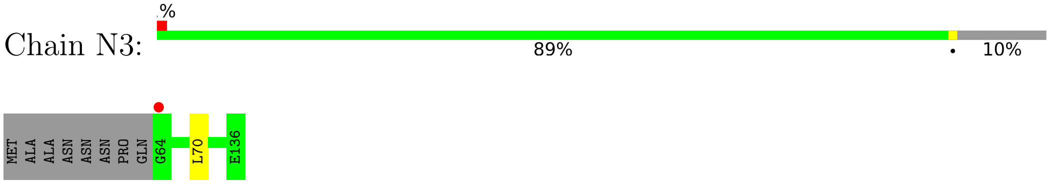
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N2:



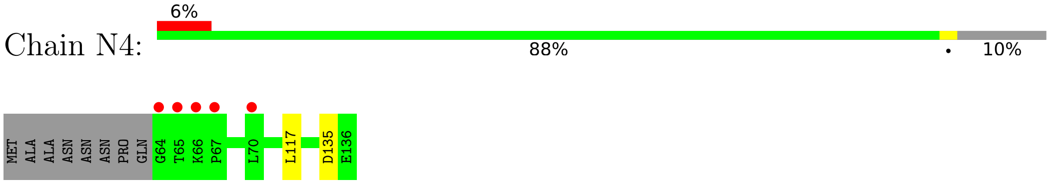
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N3:



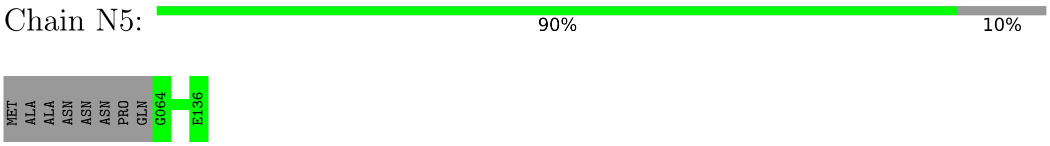
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N4:



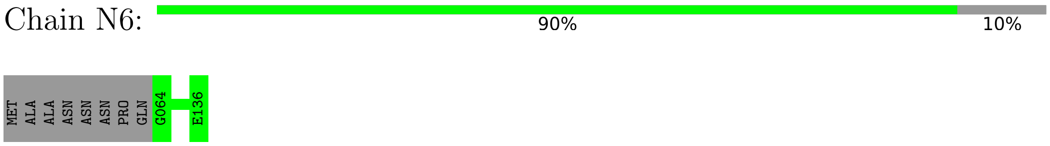
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N5:



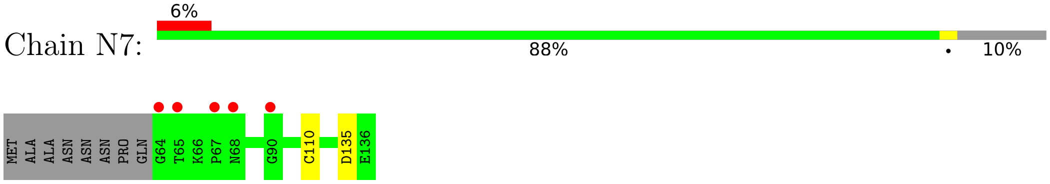
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N6:



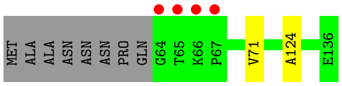
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N7:



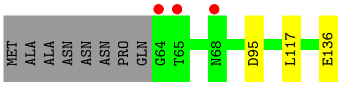
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N8:



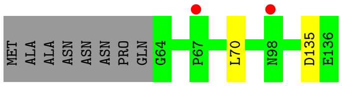
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P1:

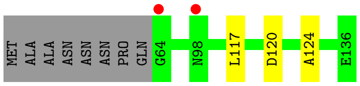
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P2:

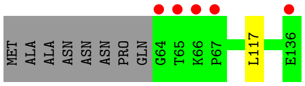
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P3:

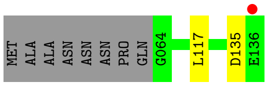
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P4:

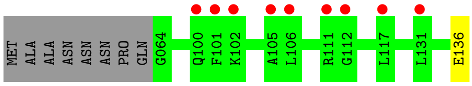
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P5:

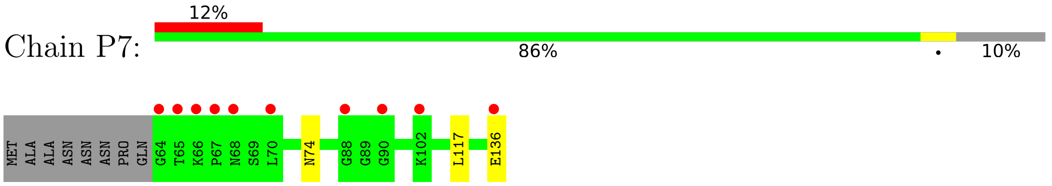
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P6:

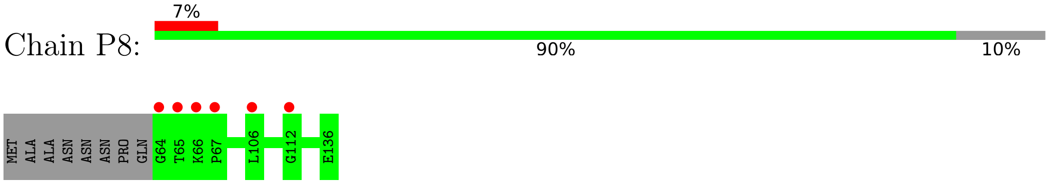
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P7:



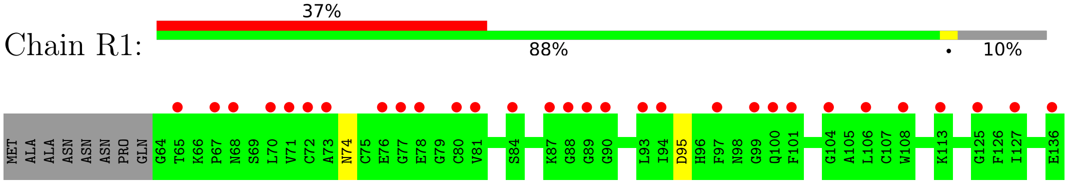
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P8:



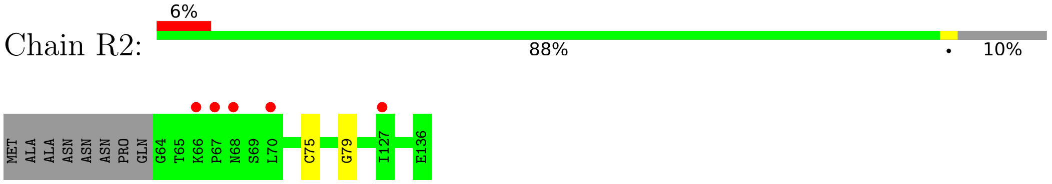
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R1:



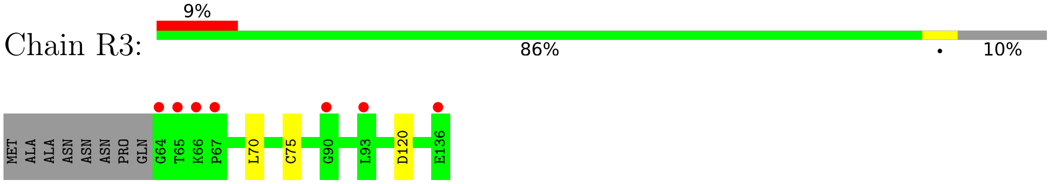
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R2:



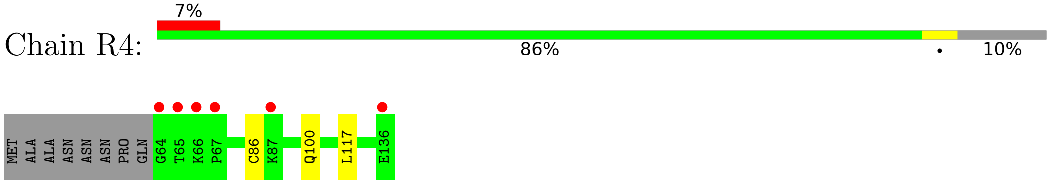
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R3:



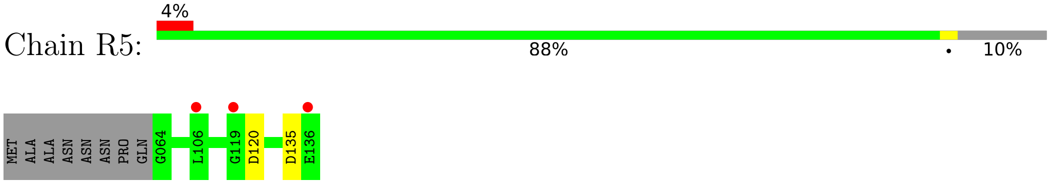
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R4:



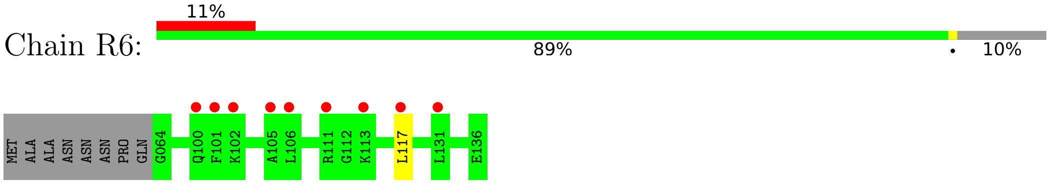
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R5:



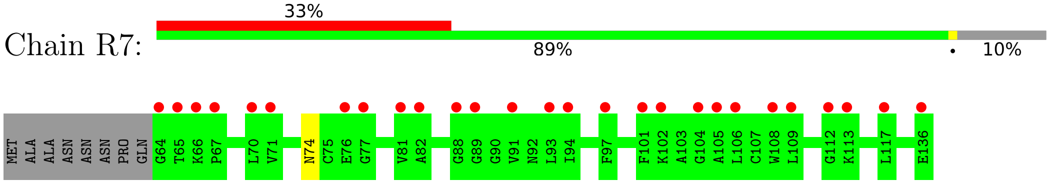
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R6:



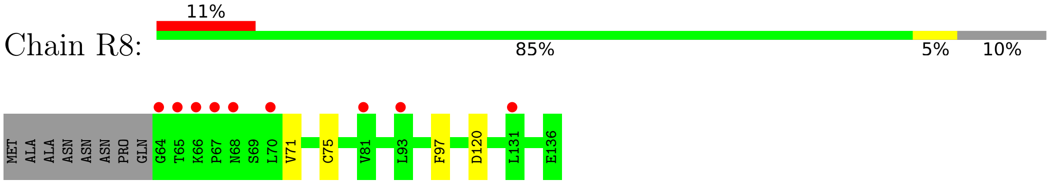
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R7:



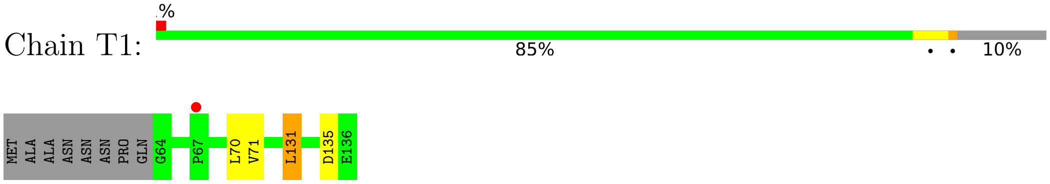
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R8:



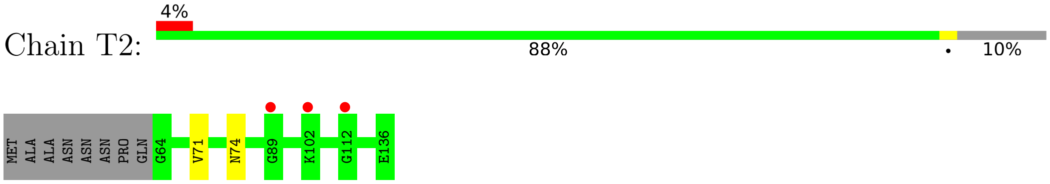
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain T1:



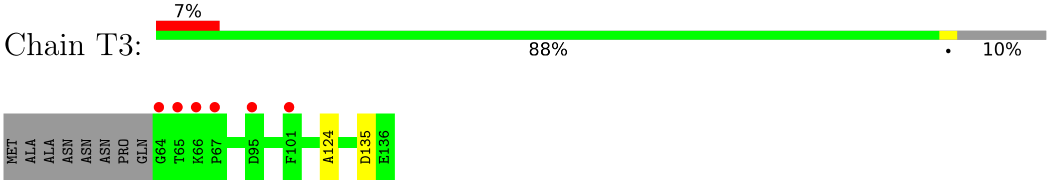
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain T2:



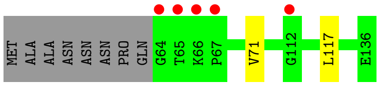
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain T3:



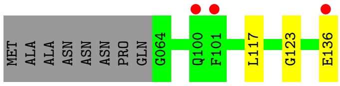
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain T4:



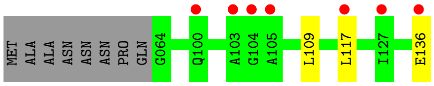
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain T5:



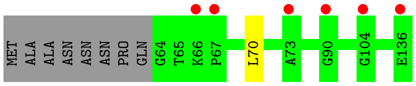
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain T6:



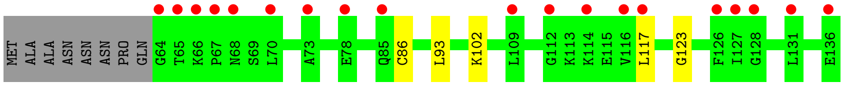
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain T7:



- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain T8:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	217.92Å 218.59Å 310.27Å 69.40° 81.51° 65.50°	Depositor
Resolution (Å)	50.01 – 2.63 49.49 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.01-2.63) 97.9 (49.49-2.63)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.235 , 0.274 0.239 , 0.275	Depositor DCC
R_{free} test set	71428 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 12.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.377 for -h,-k,-k+l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	321799	wwPDB-VP
Average B, all atoms (Å^2)	57.0	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 45.35 % 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 1.3382e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.37	0/3570	0.61	0/4844
1	A2	0.37	0/3577	0.63	0/4853
1	A3	0.37	0/3577	0.63	0/4853
1	A4	0.38	0/3570	0.64	0/4844
1	A5	0.37	0/2927	0.64	0/3956
1	A6	0.37	0/2927	0.64	0/3956
1	A7	0.38	0/3577	0.63	0/4853
1	A8	0.38	0/3577	0.62	0/4853
1	C1	0.38	0/3577	0.64	0/4853
1	C2	0.38	0/3577	0.63	0/4853
1	C3	0.38	0/3577	0.63	0/4853
1	C4	0.38	0/3577	0.62	0/4853
1	C5	0.37	0/2927	0.62	1/3956 (0.0%)
1	C6	0.37	0/2927	0.62	0/3956
1	C7	0.38	0/3577	0.63	0/4853
1	C8	0.38	0/3577	0.63	0/4853
1	E1	0.40	0/3577	0.61	0/4853
1	E2	0.40	0/3577	0.60	0/4853
1	E3	0.40	0/3577	0.59	0/4853
1	E4	0.39	0/3577	0.59	0/4853
1	E5	0.39	0/2927	0.61	0/3956
1	E6	0.39	0/2927	0.61	0/3956
1	E7	0.39	0/3577	0.62	0/4853
1	E8	0.40	0/3577	0.61	0/4853
1	G1	0.39	0/3577	0.61	0/4853
1	G2	0.39	0/3577	0.62	0/4853
1	G3	0.40	0/3577	0.62	0/4853
1	G4	0.39	0/3577	0.61	0/4853
1	G5	0.38	0/2927	0.61	0/3956
1	G6	0.37	0/2927	0.63	0/3956
1	G7	0.37	0/3577	0.62	0/4853
1	G8	0.38	0/3577	0.62	0/4853

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	I1	0.37	0/3577	0.62	0/4853
1	I2	0.39	0/3577	0.62	0/4853
1	I3	0.38	0/3577	0.62	0/4853
1	I4	0.38	0/3577	0.62	0/4853
1	I5	0.36	0/2927	0.64	0/3956
1	I6	0.38	0/2927	0.63	0/3956
1	I7	0.37	0/3577	0.63	0/4853
1	I8	0.39	0/3577	0.63	0/4853
1	K1	0.40	0/3577	0.60	0/4853
1	K2	0.39	0/3577	0.61	0/4853
1	K3	0.40	0/3577	0.61	0/4853
1	K4	0.39	0/3577	0.61	0/4853
1	K5	0.37	0/2927	0.63	1/3956 (0.0%)
1	K6	0.37	0/2927	0.62	0/3956
1	K7	0.38	0/3577	0.60	0/4853
1	K8	0.39	0/3577	0.61	0/4853
1	M1	0.37	0/3577	0.61	0/4853
1	M2	0.38	0/3577	0.63	0/4853
1	M3	0.38	0/3577	0.62	0/4853
1	M4	0.38	0/3577	0.62	0/4853
1	M5	0.36	0/2927	0.62	0/3956
1	M6	0.37	0/2927	0.63	0/3956
1	M7	0.37	0/3577	0.62	0/4853
1	M8	0.38	0/3577	0.62	0/4853
1	O1	0.39	0/3577	0.62	0/4853
1	O2	0.37	0/3577	0.62	0/4853
1	O3	0.38	0/3577	0.63	0/4853
1	O4	0.39	0/3577	0.62	0/4853
1	O5	0.40	0/2927	0.62	0/3956
1	O6	0.41	0/2927	0.62	0/3956
1	O7	0.41	0/3577	0.61	0/4853
1	O8	0.40	0/3577	0.62	0/4853
1	Q1	0.40	0/3577	0.59	0/4853
1	Q2	0.39	0/3577	0.61	0/4853
1	Q3	0.38	0/3577	0.61	0/4853
1	Q4	0.37	0/3577	0.60	0/4853
1	Q5	0.39	0/2927	0.63	0/3956
1	Q6	0.39	0/2927	0.62	0/3956
1	Q7	0.41	0/3577	0.61	0/4853
1	Q8	0.41	0/3577	0.60	0/4853
1	S1	0.37	0/3577	0.62	0/4853
1	S2	0.38	0/3577	0.61	0/4853
1	S3	0.39	0/3577	0.63	0/4853

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	S4	0.40	0/3577	0.60	0/4853
1	S5	0.40	0/2927	0.61	0/3956
1	S6	0.41	0/2927	0.62	0/3956
1	S7	0.39	0/3577	0.61	0/4853
1	S8	0.39	0/3577	0.60	0/4853
2	B1	0.41	0/528	0.51	0/705
2	B2	0.41	0/528	0.54	0/705
2	B3	0.41	0/528	0.55	0/705
2	B4	0.41	0/528	0.56	0/705
2	B5	0.41	0/280	0.58	0/371
2	B6	0.40	0/280	0.56	0/371
2	B7	0.40	0/528	0.51	0/705
2	B8	0.43	0/528	0.54	0/705
2	D1	0.40	0/528	0.57	0/705
2	D2	0.39	0/528	0.54	0/705
2	D3	0.41	0/528	0.52	0/705
2	D4	0.43	0/528	0.51	0/705
2	D5	0.42	0/280	0.55	0/371
2	D6	0.42	0/280	0.53	0/371
2	D7	0.41	0/528	0.54	0/705
2	D8	0.42	0/528	0.55	0/705
2	F1	0.41	0/528	0.53	0/705
2	F2	0.42	0/528	0.53	0/705
2	F3	0.43	0/528	0.51	0/705
2	F4	0.43	0/528	0.51	0/705
2	F5	0.43	0/280	0.49	0/371
2	F6	0.41	0/280	0.49	0/371
2	F7	0.41	0/528	0.52	0/705
2	F8	0.42	0/528	0.55	0/705
2	H1	0.43	0/528	0.56	0/705
2	H2	0.43	0/528	0.54	0/705
2	H3	0.42	0/528	0.52	0/705
2	H4	0.43	0/528	0.53	0/705
2	H5	0.41	0/280	0.52	0/371
2	H6	0.40	0/280	0.52	0/371
2	H7	0.42	0/528	0.54	0/705
2	H8	0.43	0/528	0.53	0/705
2	J1	0.41	0/528	0.55	0/705
2	J2	0.42	0/528	0.52	0/705
2	J3	0.42	0/528	0.55	0/705
2	J4	0.41	0/528	0.54	0/705
2	J5	0.41	0/280	0.55	0/371
2	J6	0.40	0/280	0.53	0/371

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	J7	0.42	0/528	0.56	0/705
2	J8	0.42	0/528	0.54	0/705
2	L1	0.42	0/528	0.51	0/705
2	L2	0.43	0/528	0.54	0/705
2	L3	0.42	0/528	0.52	0/705
2	L4	0.43	0/528	0.54	0/705
2	L5	0.37	0/280	0.54	0/371
2	L6	0.39	0/280	0.54	0/371
2	L7	0.42	0/528	0.50	0/705
2	L8	0.43	0/528	0.52	0/705
2	N1	0.41	0/528	0.57	0/705
2	N2	0.43	0/528	0.53	0/705
2	N3	0.41	0/528	0.52	0/705
2	N4	0.43	0/528	0.54	0/705
2	N5	0.40	0/280	0.58	0/371
2	N6	0.40	0/280	0.54	0/371
2	N7	0.41	0/528	0.54	0/705
2	N8	0.40	0/528	0.51	0/705
2	P1	0.42	0/528	0.52	0/705
2	P2	0.41	0/528	0.51	0/705
2	P3	0.43	0/528	0.54	0/705
2	P4	0.43	0/528	0.52	0/705
2	P5	0.46	0/280	0.56	0/371
2	P6	0.46	0/280	0.56	0/371
2	P7	0.42	0/528	0.53	0/705
2	P8	0.42	0/528	0.54	0/705
2	R1	0.43	0/528	0.52	0/705
2	R2	0.43	0/528	0.56	0/705
2	R3	0.42	0/528	0.51	0/705
2	R4	0.42	0/528	0.54	0/705
2	R5	0.44	0/280	0.52	0/371
2	R6	0.42	0/280	0.52	0/371
2	R7	0.43	0/528	0.52	0/705
2	R8	0.45	0/528	0.56	0/705
2	T1	0.41	0/528	0.54	0/705
2	T2	0.39	0/528	0.53	0/705
2	T3	0.44	0/528	0.53	0/705
2	T4	0.42	0/528	0.53	0/705
2	T5	0.44	0/280	0.52	0/371
2	T6	0.43	0/280	0.53	0/371
2	T7	0.42	0/528	0.53	0/705
2	T8	0.43	0/528	0.54	0/705
All	All	0.39	0/310426	0.61	2/420002 (0.0%)

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	A4	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C5	360	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	K5	360	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A4	95	ASN	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	3486	0	3412	19	0
1	A2	3493	0	3418	18	0
1	A3	3493	0	3418	16	0
1	A4	3486	0	3412	16	0
1	A5	3493	0	2831	17	0
1	A6	3493	0	2831	18	0
1	A7	3493	0	3418	20	0
1	A8	3493	0	3418	20	0
1	C1	3493	0	3418	21	0
1	C2	3493	0	3418	15	0
1	C3	3493	0	3418	15	0
1	C4	3493	0	3418	16	0
1	C5	3493	0	2831	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C6	3493	0	2831	14	0
1	C7	3493	0	3418	24	0
1	C8	3493	0	3418	23	0
1	E1	3493	0	3418	19	0
1	E2	3493	0	3418	21	0
1	E3	3493	0	3418	15	0
1	E4	3493	0	3418	22	0
1	E5	3493	0	2831	20	0
1	E6	3493	0	2831	12	0
1	E7	3493	0	3418	21	1
1	E8	3493	0	3418	23	0
1	G1	3493	0	3418	18	0
1	G2	3493	0	3418	19	0
1	G3	3493	0	3418	20	0
1	G4	3493	0	3418	18	0
1	G5	3493	0	2831	16	0
1	G6	3493	0	2831	13	0
1	G7	3493	0	3418	13	0
1	G8	3493	0	3418	20	0
1	I1	3493	0	3418	16	0
1	I2	3493	0	3418	19	0
1	I3	3493	0	3418	21	1
1	I4	3493	0	3418	14	0
1	I5	3493	0	2831	19	0
1	I6	3493	0	2831	19	0
1	I7	3493	0	3418	17	0
1	I8	3493	0	3418	14	0
1	K1	3493	0	3418	21	0
1	K2	3493	0	3418	19	0
1	K3	3493	0	3418	24	1
1	K4	3493	0	3418	24	0
1	K5	3493	0	2831	13	0
1	K6	3493	0	2831	11	0
1	K7	3493	0	3418	16	0
1	K8	3493	0	3418	18	0
1	M1	3493	0	3418	20	0
1	M2	3493	0	3418	16	0
1	M3	3493	0	3418	17	0
1	M4	3493	0	3418	13	0
1	M5	3493	0	2831	14	0
1	M6	3493	0	2831	16	0
1	M7	3493	0	3418	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M8	3493	0	3418	18	0
1	O1	3493	0	3418	15	0
1	O2	3493	0	3418	17	0
1	O3	3493	0	3418	17	0
1	O4	3493	0	3418	22	0
1	O5	3493	0	2831	16	0
1	O6	3493	0	2831	19	0
1	O7	3493	0	3418	20	1
1	O8	3493	0	3418	18	0
1	Q1	3493	0	3418	14	0
1	Q2	3493	0	3418	13	0
1	Q3	3493	0	3418	15	0
1	Q4	3493	0	3418	20	0
1	Q5	3493	0	2831	22	0
1	Q6	3493	0	2831	24	0
1	Q7	3493	0	3418	16	0
1	Q8	3493	0	3418	21	0
1	S1	3493	0	3418	17	0
1	S2	3493	0	3418	19	0
1	S3	3493	0	3418	18	0
1	S4	3493	0	3418	20	0
1	S5	3493	0	2831	15	0
1	S6	3493	0	2831	19	0
1	S7	3493	0	3418	17	0
1	S8	3493	0	3418	14	0
2	B1	520	0	486	3	0
2	B2	520	0	485	1	0
2	B3	520	0	485	0	0
2	B4	520	0	485	2	0
2	B5	520	0	260	0	0
2	B6	520	0	260	0	0
2	B7	520	0	485	0	0
2	B8	520	0	485	1	0
2	D1	520	0	485	0	0
2	D2	520	0	485	3	0
2	D3	520	0	485	0	0
2	D4	520	0	485	2	0
2	D5	520	0	260	0	0
2	D6	520	0	260	0	0
2	D7	520	0	485	0	0
2	D8	520	0	486	1	0
2	F1	520	0	485	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F2	520	0	486	0	0
2	F3	520	0	488	2	0
2	F4	520	0	486	2	0
2	F5	520	0	261	0	0
2	F6	520	0	261	2	0
2	F7	520	0	487	0	0
2	F8	520	0	487	2	0
2	H1	520	0	485	1	0
2	H2	520	0	485	2	0
2	H3	520	0	490	2	0
2	H4	520	0	487	2	0
2	H5	520	0	260	1	0
2	H6	520	0	260	2	0
2	H7	520	0	485	2	0
2	H8	520	0	485	0	0
2	J1	520	0	485	2	0
2	J2	520	0	486	2	0
2	J3	520	0	486	1	0
2	J4	520	0	485	2	0
2	J5	520	0	260	0	0
2	J6	520	0	260	0	0
2	J7	520	0	485	0	0
2	J8	520	0	485	1	0
2	L1	520	0	486	2	0
2	L2	520	0	486	2	0
2	L3	520	0	487	3	0
2	L4	520	0	489	3	0
2	L5	520	0	260	0	0
2	L6	520	0	260	0	0
2	L7	520	0	485	1	0
2	L8	520	0	485	0	0
2	N1	520	0	486	2	0
2	N2	520	0	486	2	0
2	N3	520	0	485	0	0
2	N4	520	0	485	1	0
2	N5	520	0	260	0	0
2	N6	520	0	260	0	0
2	N7	520	0	485	0	0
2	N8	520	0	485	3	0
2	P1	520	0	485	1	0
2	P2	520	0	485	0	0
2	P3	520	0	485	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P4	520	0	485	1	0
2	P5	520	0	261	1	0
2	P6	520	0	262	0	0
2	P7	520	0	488	1	0
2	P8	520	0	485	0	0
2	R1	520	0	489	0	0
2	R2	520	0	485	1	0
2	R3	520	0	486	1	0
2	R4	520	0	486	1	0
2	R5	520	0	264	0	0
2	R6	520	0	261	2	0
2	R7	520	0	490	0	0
2	R8	520	0	491	3	0
2	T1	520	0	485	2	0
2	T2	520	0	485	2	0
2	T3	520	0	487	1	0
2	T4	520	0	485	3	0
2	T5	520	0	261	1	0
2	T6	520	0	261	4	0
2	T7	520	0	486	0	0
2	T8	520	0	490	2	0
3	B1	2	0	0	1	0
3	B2	2	0	0	0	0
3	B3	2	0	0	0	0
3	B4	2	0	0	0	0
3	B5	2	0	0	0	0
3	B6	2	0	0	0	0
3	B7	2	0	0	0	0
3	B8	2	0	0	0	0
3	D1	2	0	0	0	0
3	D2	2	0	0	0	0
3	D3	2	0	0	0	0
3	D4	2	0	0	0	0
3	D5	2	0	0	0	0
3	D6	2	0	0	0	0
3	D7	2	0	0	0	0
3	D8	2	0	0	0	0
3	F1	2	0	0	0	0
3	F2	2	0	0	0	0
3	F3	2	0	0	2	0
3	F4	2	0	0	0	0
3	F5	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F6	2	0	0	0	0
3	F7	2	0	0	0	0
3	F8	2	0	0	0	0
3	H1	2	0	0	0	0
3	H2	2	0	0	0	0
3	H3	2	0	0	2	0
3	H4	2	0	0	0	0
3	H5	2	0	0	2	0
3	H6	2	0	0	0	0
3	H7	2	0	0	0	0
3	H8	2	0	0	0	0
3	J1	2	0	0	0	0
3	J2	2	0	0	0	0
3	J3	2	0	0	0	0
3	J4	2	0	0	0	0
3	J5	2	0	0	0	0
3	J6	2	0	0	0	0
3	J7	2	0	0	0	0
3	J8	2	0	0	0	0
3	L1	2	0	0	0	0
3	L2	2	0	0	0	0
3	L3	2	0	0	1	0
3	L4	2	0	0	1	0
3	L5	2	0	0	0	0
3	L6	2	0	0	0	0
3	L7	2	0	0	0	0
3	L8	2	0	0	0	0
3	N1	2	0	0	0	0
3	N2	2	0	0	0	0
3	N3	2	0	0	0	0
3	N4	2	0	0	0	0
3	N5	2	0	0	0	0
3	N6	2	0	0	0	0
3	N7	2	0	0	0	0
3	N8	2	0	0	0	0
3	P1	2	0	0	0	0
3	P2	2	0	0	0	0
3	P3	2	0	0	0	0
3	P4	2	0	0	0	0
3	P5	2	0	0	0	0
3	P6	2	0	0	0	0
3	P7	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P8	2	0	0	0	0
3	R1	2	0	0	0	0
3	R2	2	0	0	0	0
3	R3	2	0	0	1	0
3	R4	2	0	0	0	0
3	R5	2	0	0	0	0
3	R6	2	0	0	2	0
3	R7	2	0	0	0	0
3	R8	2	0	0	2	0
3	T1	2	0	0	0	0
3	T2	2	0	0	0	0
3	T3	2	0	0	0	0
3	T4	2	0	0	0	0
3	T5	2	0	0	0	0
3	T6	2	0	0	0	0
3	T7	2	0	0	0	0
3	T8	2	0	0	0	0
4	A1	6	0	0	0	0
4	A2	16	0	0	0	0
4	A3	25	0	0	0	0
4	A4	29	0	0	0	0
4	A5	34	0	0	0	0
4	A6	22	0	0	0	0
4	A7	13	0	0	0	0
4	A8	17	0	0	0	0
4	B1	2	0	0	0	0
4	B2	2	0	0	0	0
4	B8	2	0	0	0	0
4	C1	19	0	0	0	0
4	C2	16	0	0	0	0
4	C3	9	0	0	0	0
4	C4	12	0	0	0	0
4	C5	10	0	0	0	0
4	C6	4	0	0	0	0
4	C7	11	0	0	0	0
4	C8	11	0	0	0	0
4	D1	2	0	0	0	0
4	D2	1	0	0	0	0
4	D4	1	0	0	0	0
4	D6	1	0	0	0	0
4	E1	5	0	0	0	0
4	E2	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E3	2	0	0	0	0
4	E6	1	0	0	0	0
4	E7	1	0	0	0	0
4	F7	1	0	0	0	0
4	F8	1	0	0	0	0
4	G1	8	0	0	0	0
4	G2	6	0	0	0	0
4	G3	3	0	0	0	0
4	G4	2	0	0	0	0
4	G5	6	0	0	0	0
4	G6	6	0	0	0	0
4	G7	10	0	0	0	0
4	G8	7	0	0	0	0
4	I1	19	0	0	0	0
4	I2	8	0	0	0	0
4	I3	8	0	0	0	0
4	I4	4	0	0	0	0
4	I5	15	0	0	0	0
4	I6	5	0	0	0	0
4	I7	14	0	0	0	0
4	I8	7	0	0	0	0
4	J1	2	0	0	0	0
4	J4	2	0	0	0	0
4	K1	1	0	0	0	0
4	K2	2	0	0	0	0
4	K3	5	0	0	0	0
4	K4	7	0	0	0	0
4	K5	8	0	0	0	0
4	K6	7	0	0	0	0
4	K7	4	0	0	0	0
4	K8	5	0	0	0	0
4	L5	1	0	0	0	0
4	L8	1	0	0	0	0
4	M1	7	0	0	0	0
4	M2	3	0	0	0	0
4	M3	11	0	0	0	0
4	M4	7	0	0	0	0
4	M5	6	0	0	0	0
4	M6	16	0	0	0	0
4	M7	9	0	0	0	0
4	M8	4	0	0	0	0
4	N2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N5	2	0	0	0	0
4	N8	1	0	0	0	0
4	O1	8	0	0	0	0
4	O2	5	0	0	0	0
4	O3	13	0	0	0	0
4	O4	5	0	0	0	0
4	O5	3	0	0	0	0
4	O6	4	0	0	0	0
4	O7	6	0	0	0	0
4	O8	3	0	0	0	0
4	P4	1	0	0	0	0
4	P8	1	0	0	0	0
4	Q1	1	0	0	0	0
4	Q2	2	0	0	0	0
4	Q3	5	0	0	0	0
4	Q5	2	0	0	0	0
4	Q6	6	0	0	0	0
4	Q8	1	0	0	0	0
4	S1	6	0	0	0	0
4	S2	9	0	0	0	0
4	S3	2	0	0	0	0
4	S4	5	0	0	0	0
4	S5	1	0	0	0	0
4	S7	2	0	0	0	0
4	T1	1	0	0	0	0
All	All	321799	0	296058	1300	2

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 2.

All (1300) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F3:110:CYS:SG	3:F3:302:ZN:ZN	1.45	1.05
2:R3:75:CYS:HG	3:R3:301:ZN:ZN	0.67	0.97
2:H3:83:CYS:HG	3:H3:302:ZN:ZN	0.77	0.94
1:E3:293:ILE:HG21	1:E3:318:LEU:HD21	1.47	0.93
1:A3:293:ILE:HG21	1:A3:318:LEU:HD21	1.51	0.93
1:S5:293:ILE:HG21	1:S5:318:LEU:HD21	1.51	0.93
1:Q5:293:ILE:HG21	1:Q5:318:LEU:HD21	1.51	0.93
2:L3:83:CYS:HG	3:L3:302:ZN:ZN	0.65	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:293:ILE:HG21	1:C1:318:LEU:HD21	1.53	0.91
1:K3:293:ILE:HG21	1:K3:318:LEU:HD21	1.53	0.91
1:Q6:293:ILE:HG21	1:Q6:318:LEU:HD21	1.51	0.90
1:Q2:293:ILE:HG21	1:Q2:318:LEU:HD21	1.53	0.89
1:I7:293:ILE:HG21	1:I7:318:LEU:HD21	1.54	0.89
2:B1:83:CYS:HG	3:B1:302:ZN:ZN	0.64	0.89
1:Q3:293:ILE:HG21	1:Q3:318:LEU:HD21	1.56	0.89
1:S7:293:ILE:HG21	1:S7:318:LEU:HD21	1.53	0.88
2:F3:110:CYS:HG	3:F3:302:ZN:ZN	0.61	0.88
1:I1:293:ILE:HG21	1:I1:318:LEU:HD21	1.57	0.87
1:O7:293:ILE:HG21	1:O7:318:LEU:HD21	1.57	0.87
1:I4:293:ILE:HG21	1:I4:318:LEU:HD21	1.58	0.86
1:I5:293:ILE:HG21	1:I5:318:LEU:HD21	1.58	0.86
1:K6:293:ILE:HG21	1:K6:318:LEU:HD21	1.57	0.86
1:K1:293:ILE:HG21	1:K1:318:LEU:HD21	1.58	0.85
1:S3:293:ILE:HG21	1:S3:318:LEU:HD21	1.58	0.85
1:K5:293:ILE:HG21	1:K5:318:LEU:HD21	1.59	0.85
1:O1:293:ILE:HG21	1:O1:318:LEU:HD21	1.59	0.85
2:R8:75:CYS:SG	3:R8:301:ZN:ZN	1.64	0.85
1:O3:293:ILE:HG21	1:O3:318:LEU:HD21	1.57	0.84
1:E5:293:ILE:HG21	1:E5:318:LEU:HD21	1.59	0.84
1:M5:293:ILE:HG21	1:M5:318:LEU:HD21	1.60	0.84
1:G1:293:ILE:HG21	1:G1:318:LEU:HD21	1.60	0.84
1:M4:293:ILE:HG21	1:M4:318:LEU:HD21	1.60	0.84
1:S1:293:ILE:HG21	1:S1:318:LEU:HD21	1.58	0.84
1:C5:293:ILE:HG21	1:C5:318:LEU:HD21	1.60	0.83
1:I3:293:ILE:HG21	1:I3:318:LEU:HD21	1.61	0.83
1:K8:293:ILE:HG21	1:K8:318:LEU:HD21	1.59	0.82
1:S8:335:LEU:HD22	1:S8:343:LEU:HD11	1.62	0.82
1:E7:293:ILE:HG21	1:E7:318:LEU:HD21	1.61	0.81
1:G4:293:ILE:HG21	1:G4:318:LEU:HD21	1.63	0.81
1:Q7:293:ILE:HG21	1:Q7:318:LEU:HD21	1.62	0.81
1:I6:293:ILE:HG21	1:I6:318:LEU:HD21	1.61	0.80
1:M2:293:ILE:HG21	1:M2:318:LEU:HD21	1.63	0.80
1:C3:293:ILE:HG21	1:C3:318:LEU:HD21	1.63	0.80
1:M6:293:ILE:HG21	1:M6:318:LEU:HD21	1.62	0.80
1:O5:293:ILE:HG21	1:O5:318:LEU:HD21	1.64	0.80
1:M8:335:LEU:HD22	1:M8:343:LEU:HD11	1.64	0.79
1:E6:293:ILE:HG21	1:E6:318:LEU:HD21	1.63	0.79
1:G5:293:ILE:HG21	1:G5:318:LEU:HD21	1.64	0.79
1:A6:293:ILE:HG21	1:A6:318:LEU:HD21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G6:293:ILE:HG21	1:G6:318:LEU:HD21	1.64	0.79
1:K2:293:ILE:HG21	1:K2:318:LEU:HD21	1.64	0.79
1:M1:293:ILE:HG21	1:M1:318:LEU:HD21	1.63	0.79
1:M8:293:ILE:HG21	1:M8:318:LEU:HD21	1.65	0.79
1:E1:293:ILE:HG21	1:E1:318:LEU:HD21	1.64	0.79
1:C1:318:LEU:HD23	1:C1:326:ILE:HD12	1.65	0.79
1:M3:293:ILE:HG21	1:M3:318:LEU:HD21	1.64	0.79
1:I2:293:ILE:HG21	1:I2:318:LEU:HD21	1.64	0.79
1:Q1:293:ILE:HG21	1:Q1:318:LEU:HD21	1.63	0.79
1:S6:293:ILE:HG21	1:S6:318:LEU:HD21	1.66	0.78
1:O8:335:LEU:HD22	1:O8:343:LEU:HD11	1.65	0.78
1:C6:293:ILE:HG21	1:C6:318:LEU:HD21	1.64	0.77
1:G2:293:ILE:HG21	1:G2:318:LEU:HD21	1.67	0.77
1:K7:335:LEU:HD22	1:K7:343:LEU:HD11	1.66	0.77
1:K3:450:ARG:HB2	1:S7:429:GLN:HE22	1.47	0.77
1:A5:293:ILE:HG21	1:A5:318:LEU:HD21	1.67	0.76
1:S4:335:LEU:HD22	1:S4:343:LEU:HD11	1.67	0.76
1:M7:293:ILE:HG21	1:M7:318:LEU:HD21	1.67	0.76
1:S4:293:ILE:HG21	1:S4:318:LEU:HD21	1.66	0.76
1:I8:293:ILE:HG21	1:I8:318:LEU:HD21	1.66	0.75
1:K4:293:ILE:HG21	1:K4:318:LEU:HD21	1.69	0.75
1:A2:293:ILE:HG21	1:A2:318:LEU:HD21	1.66	0.75
1:A8:293:ILE:HG21	1:A8:318:LEU:HD21	1.69	0.75
1:C7:293:ILE:HG21	1:C7:318:LEU:HD21	1.69	0.75
1:I8:335:LEU:HD22	1:I8:343:LEU:HD11	1.69	0.75
1:K7:293:ILE:HG21	1:K7:318:LEU:HD21	1.69	0.75
1:A1:293:ILE:HG21	1:A1:318:LEU:HD21	1.68	0.74
1:A4:293:ILE:HG21	1:A4:318:LEU:HD21	1.69	0.74
1:I4:318:LEU:HD23	1:I4:326:ILE:HD12	1.70	0.74
1:I2:318:LEU:HD23	1:I2:326:ILE:HD12	1.70	0.74
1:I4:335:LEU:HD22	1:I4:343:LEU:HD11	1.68	0.74
1:O4:335:LEU:HD22	1:O4:343:LEU:HD11	1.68	0.74
1:S2:293:ILE:HG21	1:S2:318:LEU:HD21	1.68	0.74
1:C3:335:LEU:HD22	1:C3:343:LEU:HD11	1.69	0.73
1:E8:293:ILE:HG21	1:E8:318:LEU:HD21	1.69	0.73
1:I8:318:LEU:HD23	1:I8:326:ILE:HD12	1.70	0.73
1:C4:293:ILE:HG21	1:C4:318:LEU:HD21	1.69	0.73
1:E2:293:ILE:HG21	1:E2:318:LEU:HD21	1.69	0.73
1:C7:335:LEU:HD22	1:C7:343:LEU:HD11	1.71	0.73
1:G8:335:LEU:HD22	1:G8:343:LEU:HD11	1.69	0.73
1:O3:318:LEU:HD23	1:O3:326:ILE:HD12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O4:293:ILE:HG21	1:O4:318:LEU:HD21	1.71	0.72
1:E4:335:LEU:HD22	1:E4:343:LEU:HD11	1.71	0.72
1:I7:318:LEU:HD23	1:I7:326:ILE:HD12	1.72	0.72
1:C2:293:ILE:HG21	1:C2:318:LEU:HD21	1.69	0.72
1:A6:335:LEU:HD22	1:A6:343:LEU:HD11	1.72	0.72
1:C8:293:ILE:HG21	1:C8:318:LEU:HD21	1.71	0.71
1:M5:318:LEU:HD23	1:M5:326:ILE:HD12	1.71	0.71
1:M7:318:LEU:HD23	1:M7:326:ILE:HD12	1.72	0.71
1:O6:293:ILE:HG21	1:O6:318:LEU:HD21	1.72	0.71
1:M6:335:LEU:HD22	1:M6:343:LEU:HD11	1.72	0.71
1:O2:335:LEU:HD22	1:O2:343:LEU:HD11	1.73	0.70
1:Q1:273:GLY:HA3	1:Q2:273:GLY:HA3	1.73	0.70
1:A8:335:LEU:HD22	1:A8:343:LEU:HD11	1.73	0.70
1:A7:293:ILE:HG21	1:A7:318:LEU:HD21	1.74	0.70
1:M8:318:LEU:HD23	1:M8:326:ILE:HD12	1.73	0.70
1:K4:335:LEU:HD22	1:K4:343:LEU:HD11	1.74	0.69
1:E2:335:LEU:HD22	1:E2:343:LEU:HD11	1.74	0.69
1:O8:293:ILE:HG21	1:O8:318:LEU:HD21	1.74	0.69
1:G7:335:LEU:HD22	1:G7:343:LEU:HD11	1.73	0.69
1:O6:335:LEU:HD22	1:O6:343:LEU:HD11	1.73	0.69
1:E8:335:LEU:HD22	1:E8:343:LEU:HD11	1.73	0.69
1:K1:335:LEU:HD22	1:K1:343:LEU:HD11	1.75	0.69
1:K8:318:LEU:HD23	1:K8:326:ILE:HD12	1.74	0.69
1:M4:335:LEU:HD22	1:M4:343:LEU:HD11	1.74	0.68
1:S8:293:ILE:HG21	1:S8:318:LEU:HD21	1.75	0.68
1:G3:293:ILE:HG21	1:G3:318:LEU:HD21	1.74	0.68
1:I5:335:LEU:HD22	1:I5:343:LEU:HD11	1.74	0.68
1:K3:335:LEU:HD22	1:K3:343:LEU:HD11	1.74	0.68
1:A4:335:LEU:HD22	1:A4:343:LEU:HD11	1.74	0.68
1:E5:335:LEU:HD22	1:E5:343:LEU:HD11	1.75	0.68
1:C4:335:LEU:HD22	1:C4:343:LEU:HD11	1.77	0.67
1:C8:335:LEU:HD22	1:C8:343:LEU:HD11	1.76	0.67
1:E8:318:LEU:HD23	1:E8:326:ILE:HD12	1.76	0.67
1:I3:335:LEU:HD22	1:I3:343:LEU:HD11	1.76	0.67
1:Q3:335:LEU:HD22	1:Q3:343:LEU:HD11	1.75	0.67
1:S7:318:LEU:HD23	1:S7:326:ILE:HD12	1.76	0.67
1:I3:318:LEU:HD23	1:I3:326:ILE:HD12	1.76	0.67
1:Q4:335:LEU:HD22	1:Q4:343:LEU:HD11	1.77	0.67
1:G8:293:ILE:HG21	1:G8:318:LEU:HD21	1.77	0.66
2:R8:75:CYS:HG	3:R8:301:ZN:ZN	0.45	0.66
1:A3:318:LEU:HD23	1:A3:326:ILE:HD12	1.77	0.66

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:G4:318:LEU:HD23	1:G4:326:ILE:HD12	1.78	0.66
1:E3:318:LEU:HD23	1:E3:326:ILE:HD12	1.77	0.66
1:M4:318:LEU:HD23	1:M4:326:ILE:HD12	1.78	0.66
1:M6:318:LEU:HD23	1:M6:326:ILE:HD12	1.78	0.66
1:C2:318:LEU:HD23	1:C2:326:ILE:HD12	1.76	0.66
1:G6:318:LEU:HD23	1:G6:326:ILE:HD12	1.78	0.66
1:M7:335:LEU:HD22	1:M7:343:LEU:HD11	1.78	0.66
1:C8:318:LEU:HD23	1:C8:326:ILE:HD12	1.77	0.65
1:G2:318:LEU:HD23	1:G2:326:ILE:HD12	1.77	0.65
1:O3:318:LEU:HD23	1:O3:326:ILE:CD1	2.25	0.65
1:G7:293:ILE:HG21	1:G7:318:LEU:HD21	1.78	0.65
1:O5:335:LEU:HD22	1:O5:343:LEU:HD11	1.77	0.65
2:H3:83:CYS:SG	3:H3:302:ZN:ZN	1.82	0.65
1:A5:335:LEU:HD22	1:A5:343:LEU:HD11	1.77	0.65
1:I1:318:LEU:HD23	1:I1:326:ILE:HD12	1.79	0.65
1:A1:335:LEU:HD22	1:A1:343:LEU:HD11	1.79	0.64
1:I7:318:LEU:HD23	1:I7:326:ILE:CD1	2.27	0.64
2:L4:83:CYS:SG	3:L4:302:ZN:ZN	1.87	0.64
1:G5:318:LEU:HD23	1:G5:326:ILE:HD12	1.79	0.64
1:G7:149:GLN:HE22	1:G7:282:LYS:HA	1.63	0.64
1:A5:318:LEU:HD23	1:A5:326:ILE:HD12	1.77	0.64
1:G7:318:LEU:HD23	1:G7:326:ILE:HD12	1.79	0.64
1:E7:318:LEU:HD23	1:E7:326:ILE:HD12	1.78	0.64
1:Q4:293:ILE:HG21	1:Q4:318:LEU:HD21	1.79	0.64
1:A3:318:LEU:HD23	1:A3:326:ILE:CD1	2.28	0.64
1:K3:318:LEU:HD23	1:K3:326:ILE:HD12	1.79	0.63
1:M3:335:LEU:HD22	1:M3:343:LEU:HD11	1.78	0.63
1:A4:318:LEU:HD23	1:A4:326:ILE:HD12	1.79	0.63
1:G3:335:LEU:HD22	1:G3:343:LEU:HD11	1.81	0.63
1:K8:335:LEU:HD22	1:K8:343:LEU:HD11	1.80	0.63
1:O4:318:LEU:HD23	1:O4:326:ILE:HD12	1.80	0.63
1:C3:318:LEU:HD23	1:C3:326:ILE:HD12	1.79	0.63
1:C7:318:LEU:HD23	1:C7:326:ILE:HD12	1.79	0.63
1:K3:293:ILE:CG2	1:K3:318:LEU:HD21	2.28	0.63
1:G6:149:GLN:HE22	1:G6:282:LYS:HA	1.63	0.63
1:I4:318:LEU:HD23	1:I4:326:ILE:CD1	2.29	0.63
1:K3:318:LEU:HD23	1:K3:326:ILE:CD1	2.28	0.63
1:M1:335:LEU:HD22	1:M1:343:LEU:HD11	1.81	0.63
1:A8:318:LEU:HD23	1:A8:326:ILE:HD12	1.79	0.63
1:A1:318:LEU:HD23	1:A1:326:ILE:HD12	1.81	0.62
1:Q5:293:ILE:CG2	1:Q5:318:LEU:HD21	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C2:335:LEU:HD22	1:C2:343:LEU:HD11	1.80	0.62
1:I5:318:LEU:HD23	1:I5:326:ILE:HD12	1.80	0.62
1:K5:318:LEU:HD23	1:K5:326:ILE:HD12	1.81	0.62
1:M7:318:LEU:HD23	1:M7:326:ILE:CD1	2.30	0.62
1:A2:335:LEU:HD22	1:A2:343:LEU:HD11	1.80	0.62
1:E7:318:LEU:HD23	1:E7:326:ILE:CD1	2.29	0.62
1:O2:293:ILE:HG21	1:O2:318:LEU:HD21	1.80	0.62
1:G4:335:LEU:HD22	1:G4:343:LEU:HD11	1.82	0.62
1:Q3:318:LEU:HD23	1:Q3:326:ILE:CD1	2.30	0.62
1:M3:318:LEU:HD23	1:M3:326:ILE:CD1	2.30	0.62
1:C4:149:GLN:HE22	1:C4:282:LYS:HA	1.65	0.62
1:E3:335:LEU:HD22	1:E3:343:LEU:HD11	1.82	0.62
1:A3:293:ILE:CG2	1:A3:318:LEU:HD21	2.29	0.62
1:A2:318:LEU:HD23	1:A2:326:ILE:HD12	1.82	0.62
1:E1:318:LEU:HD23	1:E1:326:ILE:HD12	1.82	0.62
1:I8:408:GLY:HA3	2:J8:117:LEU:HD22	1.82	0.62
1:O1:335:LEU:HD22	1:O1:343:LEU:HD11	1.82	0.61
1:Q6:335:LEU:HD21	1:Q6:393:ILE:HG12	1.82	0.61
1:E6:318:LEU:HD23	1:E6:326:ILE:HD12	1.82	0.61
1:S2:318:LEU:HD23	1:S2:326:ILE:HD12	1.81	0.61
1:O2:318:LEU:HD23	1:O2:326:ILE:HD12	1.82	0.61
1:Q3:318:LEU:HD23	1:Q3:326:ILE:HD12	1.81	0.61
1:E1:149:GLN:HE22	1:E1:282:LYS:HA	1.66	0.61
1:I6:318:LEU:HD23	1:I6:326:ILE:HD12	1.82	0.61
1:A7:88:GLU:OE2	1:A7:358:ARG:NH1	2.33	0.61
1:I6:293:ILE:HG21	1:I6:318:LEU:CD2	2.30	0.61
1:S5:293:ILE:CG2	1:S5:318:LEU:HD21	2.29	0.61
1:I3:318:LEU:HD23	1:I3:326:ILE:CD1	2.30	0.61
1:Q8:293:ILE:HG21	1:Q8:318:LEU:HD21	1.83	0.60
1:S8:335:LEU:HD21	1:S8:393:ILE:HG12	1.82	0.60
1:K5:335:LEU:HD22	1:K5:343:LEU:HD11	1.81	0.60
1:A8:335:LEU:HD21	1:A8:393:ILE:HG12	1.83	0.60
1:M1:318:LEU:HD23	1:M1:326:ILE:HD12	1.83	0.60
1:E4:293:ILE:HG21	1:E4:318:LEU:HD21	1.83	0.60
1:G1:293:ILE:HG21	1:G1:318:LEU:CD2	2.31	0.60
1:E2:318:LEU:HD23	1:E2:326:ILE:HD12	1.82	0.60
1:G4:293:ILE:CG2	1:G4:318:LEU:HD21	2.30	0.60
1:M3:318:LEU:HD23	1:M3:326:ILE:HD12	1.82	0.60
1:M5:293:ILE:HG21	1:M5:318:LEU:CD2	2.31	0.60
1:I8:293:ILE:HG21	1:I8:318:LEU:CD2	2.32	0.60
1:O4:408:GLY:HA3	2:P4:117:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E3:318:LEU:HD23	1:E3:326:ILE:CD1	2.31	0.60
1:I3:335:LEU:HD21	1:I3:393:ILE:HG12	1.83	0.60
1:M8:318:LEU:HD23	1:M8:326:ILE:CD1	2.31	0.60
1:E7:170:LEU:HD21	1:E7:424:LEU:HD22	1.84	0.60
1:I7:335:LEU:HD22	1:I7:343:LEU:HD11	1.83	0.60
1:O1:318:LEU:HD23	1:O1:326:ILE:HD12	1.83	0.59
1:Q3:293:ILE:CG2	1:Q3:318:LEU:HD21	2.31	0.59
1:M4:408:GLY:HA3	2:N4:117:LEU:HD22	1.84	0.59
1:C5:318:LEU:HD23	1:C5:326:ILE:CD1	2.32	0.59
1:G1:335:LEU:HD22	1:G1:343:LEU:HD11	1.84	0.59
1:Q6:335:LEU:HD22	1:Q6:343:LEU:HD11	1.83	0.59
1:C1:318:LEU:HD23	1:C1:326:ILE:CD1	2.32	0.59
1:M2:293:ILE:CG2	1:M2:318:LEU:HD21	2.32	0.59
1:C4:318:LEU:HD23	1:C4:326:ILE:HD12	1.84	0.59
1:K2:293:ILE:CG2	1:K2:318:LEU:HD21	2.32	0.59
1:O8:318:LEU:HD23	1:O8:326:ILE:HD12	1.83	0.59
1:S3:293:ILE:CG2	1:S3:318:LEU:HD21	2.32	0.59
1:C7:149:GLN:HE22	1:C7:282:LYS:HA	1.68	0.59
1:E6:335:LEU:HD22	1:E6:343:LEU:HD11	1.83	0.59
1:G5:335:LEU:HD22	1:G5:343:LEU:HD11	1.85	0.59
1:Q7:318:LEU:HD23	1:Q7:326:ILE:HD12	1.84	0.59
1:S7:318:LEU:HD23	1:S7:326:ILE:CD1	2.32	0.59
1:A8:408:GLY:HA3	2:B8:117:LEU:HD22	1.83	0.59
1:M5:273:GLY:HA3	1:M6:273:GLY:HA3	1.85	0.59
1:A3:335:LEU:HD22	1:A3:343:LEU:HD11	1.85	0.59
1:C7:426:ALA:HB2	1:M3:451:TRP:HH2	1.69	0.58
1:K8:318:LEU:HD23	1:K8:326:ILE:CD1	2.33	0.58
1:G8:318:LEU:HD23	1:G8:326:ILE:HD12	1.84	0.58
1:S3:273:GLY:HA3	1:S4:273:GLY:HA3	1.85	0.58
1:K1:335:LEU:HD21	1:K1:393:ILE:HG12	1.85	0.58
1:M8:335:LEU:HD21	1:M8:393:ILE:HG12	1.84	0.58
1:S1:293:ILE:HG21	1:S1:318:LEU:CD2	2.31	0.58
1:G1:293:ILE:CG2	1:G1:318:LEU:HD21	2.33	0.58
1:O8:335:LEU:HD21	1:O8:393:ILE:HG12	1.86	0.58
1:E3:293:ILE:CG2	1:E3:318:LEU:HD21	2.29	0.58
1:A7:318:LEU:HD23	1:A7:326:ILE:HD12	1.85	0.58
1:C5:318:LEU:HD23	1:C5:326:ILE:HD12	1.85	0.58
1:S6:293:ILE:CG2	1:S6:318:LEU:HD21	2.34	0.58
1:K1:293:ILE:CG2	1:K1:318:LEU:HD21	2.33	0.58
1:M2:149:GLN:HE22	1:M2:282:LYS:HA	1.69	0.58
1:A2:293:ILE:CG2	1:A2:318:LEU:HD21	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:293:ILE:HG21	1:A4:318:LEU:CD2	2.34	0.57
1:M7:273:GLY:HA3	1:M8:273:GLY:HA3	1.85	0.57
1:C1:335:LEU:HD22	1:C1:343:LEU:HD11	1.86	0.57
1:E8:293:ILE:HG21	1:E8:318:LEU:CD2	2.33	0.57
1:I2:318:LEU:HD23	1:I2:326:ILE:CD1	2.33	0.57
1:M2:318:LEU:HD23	1:M2:326:ILE:HD12	1.85	0.57
1:Q2:335:LEU:HD22	1:Q2:343:LEU:HD11	1.86	0.57
1:Q6:318:LEU:HD23	1:Q6:326:ILE:HD12	1.86	0.57
1:K5:293:ILE:CG2	1:K5:318:LEU:HD21	2.33	0.57
1:M6:293:ILE:HG21	1:M6:318:LEU:CD2	2.34	0.57
1:K6:335:LEU:HD22	1:K6:343:LEU:HD11	1.87	0.57
1:O7:318:LEU:HD23	1:O7:326:ILE:CD1	2.34	0.57
1:E2:318:LEU:HD23	1:E2:326:ILE:CD1	2.34	0.57
1:M1:293:ILE:CG2	1:M1:318:LEU:HD21	2.34	0.57
1:O1:293:ILE:CG2	1:O1:318:LEU:HD21	2.33	0.57
1:C6:293:ILE:HG21	1:C6:318:LEU:CD2	2.34	0.57
1:E3:273:GLY:HA3	1:E4:273:GLY:HA3	1.86	0.57
1:O7:293:ILE:CG2	1:O7:318:LEU:HD21	2.32	0.57
1:S5:256:PHE:CE2	1:S5:260:LEU:HD11	2.38	0.57
1:C8:293:ILE:HG21	1:C8:318:LEU:CD2	2.34	0.57
1:G6:335:LEU:HD22	1:G6:343:LEU:HD11	1.87	0.57
1:Q5:293:ILE:HG21	1:Q5:318:LEU:CD2	2.31	0.57
1:C7:273:GLY:HA3	1:C8:273:GLY:HA3	1.86	0.57
1:G7:273:GLY:HA3	1:G8:273:GLY:HA3	1.87	0.57
1:I1:335:LEU:HD22	1:I1:343:LEU:HD11	1.87	0.57
1:K6:318:LEU:HD23	1:K6:326:ILE:HD12	1.87	0.57
1:K7:318:LEU:HD23	1:K7:326:ILE:HD12	1.87	0.57
1:A6:318:LEU:HD23	1:A6:326:ILE:HD12	1.86	0.57
1:I2:293:ILE:HG21	1:I2:318:LEU:CD2	2.35	0.57
1:K2:318:LEU:HD23	1:K2:326:ILE:HD12	1.86	0.56
1:M8:293:ILE:HG21	1:M8:318:LEU:CD2	2.34	0.56
1:S5:293:ILE:HG21	1:S5:318:LEU:CD2	2.31	0.56
1:A6:293:ILE:HG21	1:A6:318:LEU:CD2	2.35	0.56
1:G5:318:LEU:HD23	1:G5:326:ILE:CD1	2.35	0.56
1:M6:293:ILE:CG2	1:M6:318:LEU:HD21	2.35	0.56
1:C6:293:ILE:CG2	1:C6:318:LEU:HD21	2.34	0.56
1:Q6:293:ILE:CG2	1:Q6:318:LEU:HD21	2.29	0.56
1:Q7:318:LEU:HD23	1:Q7:326:ILE:CD1	2.35	0.56
1:I5:318:LEU:HD23	1:I5:326:ILE:CD1	2.34	0.56
1:Q6:318:LEU:HD23	1:Q6:326:ILE:CD1	2.36	0.56
1:E6:149:GLN:HE22	1:E6:282:LYS:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E7:335:LEU:HD22	1:E7:343:LEU:HD11	1.86	0.56
1:G2:318:LEU:HD23	1:G2:326:ILE:CD1	2.34	0.56
1:I4:88:GLU:OE2	1:I4:358:ARG:NH1	2.38	0.56
1:M2:335:LEU:HD22	1:M2:343:LEU:HD11	1.87	0.56
1:Q1:318:LEU:HD23	1:Q1:326:ILE:HD12	1.88	0.56
1:Q5:335:LEU:HD22	1:Q5:343:LEU:HD11	1.88	0.56
1:E5:318:LEU:HD23	1:E5:326:ILE:HD12	1.87	0.56
1:G3:158:GLU:OE2	1:G3:325:HIS:NE2	2.35	0.56
1:K4:149:GLN:HE22	1:K4:282:LYS:HA	1.69	0.56
1:Q8:318:LEU:HD23	1:Q8:326:ILE:HD12	1.86	0.56
1:C3:318:LEU:HD23	1:C3:326:ILE:CD1	2.36	0.56
1:M4:335:LEU:HD21	1:M4:393:ILE:HG12	1.88	0.56
1:Q6:293:ILE:HG21	1:Q6:318:LEU:CD2	2.30	0.56
1:O3:335:LEU:HD22	1:O3:343:LEU:HD11	1.87	0.56
1:S5:318:LEU:HD23	1:S5:326:ILE:HD12	1.87	0.56
1:S7:335:LEU:HD22	1:S7:343:LEU:HD11	1.88	0.56
1:E8:293:ILE:CG2	1:E8:318:LEU:HD21	2.36	0.56
1:G1:149:GLN:HE22	1:G1:282:LYS:HA	1.71	0.56
1:G1:318:LEU:HD23	1:G1:326:ILE:HD12	1.88	0.56
1:G2:149:GLN:HE22	1:G2:282:LYS:HA	1.71	0.56
1:S1:318:LEU:HD23	1:S1:326:ILE:HD12	1.88	0.56
1:C7:318:LEU:HD23	1:C7:326:ILE:CD1	2.36	0.55
1:M4:293:ILE:HG21	1:M4:318:LEU:CD2	2.34	0.55
1:S4:318:LEU:HD23	1:S4:326:ILE:HD12	1.86	0.55
1:S1:293:ILE:CG2	1:S1:318:LEU:HD21	2.33	0.55
1:C6:318:LEU:HD23	1:C6:326:ILE:HD12	1.88	0.55
1:I8:318:LEU:HD23	1:I8:326:ILE:CD1	2.34	0.55
1:G3:335:LEU:HD21	1:G3:393:ILE:HG12	1.89	0.55
1:A5:318:LEU:HD23	1:A5:326:ILE:CD1	2.36	0.55
1:A8:293:ILE:CG2	1:A8:318:LEU:HD21	2.36	0.55
1:G5:273:GLY:HA3	1:G6:273:GLY:HA3	1.88	0.55
1:K3:273:GLY:HA3	1:K4:273:GLY:HA3	1.89	0.55
1:O5:293:ILE:CG2	1:O5:318:LEU:HD21	2.33	0.55
1:I5:293:ILE:CG2	1:I5:318:LEU:HD21	2.34	0.55
1:A6:293:ILE:CG2	1:A6:318:LEU:HD21	2.35	0.55
1:M5:293:ILE:CG2	1:M5:318:LEU:HD21	2.36	0.55
1:Q8:244:ALA:HB1	1:Q8:245:PRO:HD2	1.89	0.55
1:A8:318:LEU:HD23	1:A8:326:ILE:CD1	2.37	0.55
1:C4:293:ILE:HG21	1:C4:318:LEU:CD2	2.36	0.55
1:M7:293:ILE:HG21	1:M7:318:LEU:CD2	2.36	0.55
1:K6:293:ILE:CG2	1:K6:318:LEU:HD21	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C3:273:GLY:HA3	1:C4:273:GLY:HA3	1.89	0.55
1:C3:293:ILE:HG21	1:C3:318:LEU:CD2	2.35	0.55
1:A1:318:LEU:HD23	1:A1:326:ILE:CD1	2.37	0.54
1:A6:170:LEU:HD21	1:A6:424:LEU:HD22	1.87	0.54
1:G1:273:GLY:HA3	1:G2:273:GLY:HA3	1.90	0.54
1:G4:318:LEU:HD23	1:G4:326:ILE:CD1	2.37	0.54
1:I1:293:ILE:HG21	1:I1:318:LEU:CD2	2.34	0.54
1:G1:318:LEU:HD23	1:G1:326:ILE:CD1	2.38	0.54
1:I6:318:LEU:HD23	1:I6:326:ILE:CD1	2.37	0.54
1:O5:293:ILE:HG21	1:O5:318:LEU:CD2	2.37	0.54
1:E2:149:GLN:HE22	1:E2:282:LYS:HA	1.71	0.54
1:I5:273:GLY:HA3	1:I6:273:GLY:HA3	1.90	0.54
1:I5:335:LEU:HD21	1:I5:393:ILE:HG12	1.89	0.54
1:I7:149:GLN:HE22	1:I7:282:LYS:HA	1.73	0.54
1:Q2:293:ILE:CG2	1:Q2:318:LEU:HD21	2.34	0.54
1:S1:335:LEU:HD22	1:S1:343:LEU:HD11	1.88	0.54
1:C7:293:ILE:CG2	1:C7:318:LEU:HD21	2.38	0.54
1:E8:318:LEU:HD23	1:E8:326:ILE:CD1	2.36	0.54
1:G6:318:LEU:HD23	1:G6:326:ILE:CD1	2.37	0.54
1:Q8:335:LEU:HD22	1:Q8:343:LEU:HD11	1.88	0.54
1:I7:293:ILE:CG2	1:I7:318:LEU:HD21	2.32	0.54
1:M7:149:GLN:HE22	1:M7:282:LYS:HA	1.72	0.54
1:Q6:110:GLU:OE1	1:Q6:110:GLU:N	2.41	0.54
1:G3:318:LEU:HD23	1:G3:326:ILE:HD12	1.90	0.54
1:M2:293:ILE:HG21	1:M2:318:LEU:CD2	2.37	0.54
1:C2:293:ILE:HG21	1:C2:318:LEU:CD2	2.37	0.54
1:I3:293:ILE:CG2	1:I3:318:LEU:HD21	2.37	0.54
1:M7:293:ILE:CG2	1:M7:318:LEU:HD21	2.37	0.54
1:I4:335:LEU:HD21	1:I4:393:ILE:HG12	1.89	0.54
1:I6:335:LEU:HD22	1:I6:343:LEU:HD11	1.88	0.54
1:I7:273:GLY:HA3	1:I8:273:GLY:HA3	1.89	0.54
1:K3:450:ARG:HB2	1:S7:429:GLN:NE2	2.19	0.54
1:M4:318:LEU:HD23	1:M4:326:ILE:CD1	2.38	0.54
1:M5:318:LEU:HD23	1:M5:326:ILE:CD1	2.37	0.54
1:Q5:318:LEU:HD23	1:Q5:326:ILE:HD12	1.89	0.54
1:C5:335:LEU:HD22	1:C5:343:LEU:HD11	1.90	0.54
1:C8:149:GLN:HE22	1:C8:282:LYS:HA	1.73	0.54
1:I4:293:ILE:HG21	1:I4:318:LEU:CD2	2.34	0.54
1:S3:318:LEU:HD23	1:S3:326:ILE:CD1	2.38	0.54
1:S6:293:ILE:HG21	1:S6:318:LEU:CD2	2.37	0.53
1:A3:125:PHE:O	1:A4:303:ARG:NH1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G4:293:ILE:HG21	1:G4:318:LEU:CD2	2.36	0.53
1:S2:293:ILE:HG21	1:S2:318:LEU:CD2	2.36	0.53
1:S4:335:LEU:HD21	1:S4:393:ILE:HG12	1.89	0.53
1:S6:212:GLN:OE1	1:S6:217:ARG:HD3	2.08	0.53
1:C6:335:LEU:HD22	1:C6:343:LEU:HD11	1.91	0.53
1:C8:318:LEU:HD23	1:C8:326:ILE:CD1	2.38	0.53
1:M1:335:LEU:HD21	1:M1:393:ILE:HG12	1.91	0.53
1:O6:318:LEU:HD23	1:O6:326:ILE:HD12	1.89	0.53
1:S7:212:GLN:OE1	1:S7:217:ARG:HD3	2.08	0.53
1:I5:293:ILE:HG21	1:I5:318:LEU:CD2	2.35	0.53
1:K7:293:ILE:CG2	1:K7:318:LEU:HD21	2.37	0.53
1:Q4:318:LEU:HD23	1:Q4:326:ILE:HD12	1.91	0.53
1:S4:293:ILE:HG21	1:S4:318:LEU:CD2	2.35	0.53
1:I1:318:LEU:HD23	1:I1:326:ILE:CD1	2.39	0.53
1:K4:293:ILE:CG2	1:K4:318:LEU:HD21	2.38	0.53
1:G7:318:LEU:HD23	1:G7:326:ILE:CD1	2.39	0.53
1:I4:293:ILE:CG2	1:I4:318:LEU:HD21	2.34	0.53
1:K8:293:ILE:HG21	1:K8:318:LEU:CD2	2.34	0.53
1:C1:293:ILE:CG2	1:C1:318:LEU:HD21	2.31	0.53
1:K7:293:ILE:HG21	1:K7:318:LEU:CD2	2.39	0.53
1:S3:318:LEU:HD23	1:S3:326:ILE:HD12	1.91	0.53
2:F1:74:ASN:HD22	2:F1:81:VAL:HG11	1.74	0.53
1:A4:318:LEU:HD23	1:A4:326:ILE:CD1	2.39	0.53
1:O1:273:GLY:HA3	1:O2:273:GLY:HA3	1.91	0.53
1:Q2:318:LEU:HD23	1:Q2:326:ILE:HD12	1.91	0.53
1:A6:318:LEU:HD23	1:A6:326:ILE:CD1	2.39	0.53
1:C8:170:LEU:HD21	1:C8:424:LEU:HD22	1.91	0.53
1:E7:273:GLY:HA3	1:E8:273:GLY:HA3	1.91	0.53
1:G8:293:ILE:HG21	1:G8:318:LEU:CD2	2.38	0.53
1:S4:408:GLY:HA3	2:T4:117:LEU:HD22	1.91	0.53
1:S5:335:LEU:HD22	1:S5:343:LEU:HD11	1.90	0.53
1:S8:318:LEU:HD23	1:S8:326:ILE:HD12	1.90	0.53
1:M3:293:ILE:CG2	1:M3:318:LEU:HD21	2.35	0.53
1:S5:318:LEU:HD23	1:S5:326:ILE:CD1	2.38	0.53
1:C3:293:ILE:CG2	1:C3:318:LEU:HD21	2.35	0.52
1:K5:293:ILE:HG21	1:K5:318:LEU:CD2	2.35	0.52
1:K8:293:ILE:CG2	1:K8:318:LEU:HD21	2.37	0.52
1:Q4:293:ILE:HG21	1:Q4:318:LEU:CD2	2.39	0.52
1:I2:335:LEU:HD22	1:I2:343:LEU:HD11	1.91	0.52
1:I6:293:ILE:CG2	1:I6:318:LEU:HD21	2.35	0.52
1:A8:214:TRP:CE3	1:A8:253:ARG:HG2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A8:293:ILE:HG21	1:A8:318:LEU:CD2	2.37	0.52
1:E5:273:GLY:HA3	1:E6:273:GLY:HA3	1.92	0.52
1:K5:273:GLY:HA3	1:K6:273:GLY:HA3	1.91	0.52
1:O3:293:ILE:CG2	1:O3:318:LEU:HD21	2.35	0.52
1:E1:273:GLY:HA3	1:E2:273:GLY:HA3	1.92	0.52
1:A2:318:LEU:HD23	1:A2:326:ILE:CD1	2.39	0.52
1:K1:293:ILE:HG21	1:K1:318:LEU:CD2	2.35	0.52
1:K2:293:ILE:HG21	1:K2:318:LEU:CD2	2.37	0.52
1:K5:318:LEU:HD23	1:K5:326:ILE:CD1	2.39	0.52
1:A3:293:ILE:HG21	1:A3:318:LEU:CD2	2.33	0.52
1:G5:293:ILE:CG2	1:G5:318:LEU:HD21	2.37	0.52
1:G6:293:ILE:CG2	1:G6:318:LEU:HD21	2.35	0.52
1:K6:293:ILE:HG21	1:K6:318:LEU:CD2	2.34	0.52
1:O7:40:PHE:CD2	1:O7:101:ILE:HD12	2.45	0.52
1:Q1:318:LEU:HD23	1:Q1:326:ILE:CD1	2.40	0.52
1:A4:293:ILE:CG2	1:A4:318:LEU:HD21	2.39	0.52
1:A8:315:ALA:HB1	1:A8:349:LEU:HD21	1.92	0.52
1:C1:273:GLY:HA3	1:C2:273:GLY:HA3	1.92	0.52
1:E6:293:ILE:CG2	1:E6:318:LEU:HD21	2.37	0.52
1:G5:125:PHE:O	1:G6:303:ARG:NH1	2.42	0.52
1:M2:318:LEU:HD23	1:M2:326:ILE:CD1	2.39	0.52
1:C6:318:LEU:HD23	1:C6:326:ILE:CD1	2.40	0.52
1:E5:293:ILE:HG21	1:E5:318:LEU:CD2	2.37	0.52
1:I1:293:ILE:CG2	1:I1:318:LEU:HD21	2.34	0.52
1:K6:318:LEU:HD23	1:K6:326:ILE:CD1	2.39	0.52
1:Q2:318:LEU:HD23	1:Q2:326:ILE:CD1	2.39	0.52
1:C2:318:LEU:HD23	1:C2:326:ILE:CD1	2.39	0.52
1:K3:293:ILE:HG21	1:K3:318:LEU:CD2	2.33	0.52
1:M5:130:LEU:O	1:M6:303:ARG:NH2	2.41	0.52
1:O3:273:GLY:HA3	1:O4:273:GLY:HA3	1.92	0.52
1:Q3:273:GLY:HA3	1:Q4:273:GLY:HA3	1.92	0.52
1:C4:408:GLY:HA3	2:D4:117:LEU:HD22	1.91	0.51
1:E7:293:ILE:HG21	1:E7:318:LEU:CD2	2.38	0.51
1:K6:212:GLN:OE1	1:K6:217:ARG:HD3	2.10	0.51
1:K7:273:GLY:HA3	1:K8:273:GLY:HA3	1.91	0.51
1:C8:293:ILE:CG2	1:C8:318:LEU:HD21	2.41	0.51
1:M5:335:LEU:HD22	1:M5:343:LEU:HD11	1.91	0.51
1:O4:158:GLU:OE2	1:O4:325:HIS:NE2	2.39	0.51
1:C7:178:LEU:HD21	1:C8:107:LEU:CD2	2.40	0.51
1:M1:318:LEU:HD23	1:M1:326:ILE:CD1	2.39	0.51
1:Q4:256:PHE:CE2	1:Q4:260:LEU:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q5:142:VAL:HG13	1:Q5:369:ALA:HB2	1.92	0.51
1:A4:408:GLY:HA3	2:B4:117:LEU:HD22	1.93	0.51
1:A7:293:ILE:HG21	1:A7:318:LEU:CD2	2.41	0.51
1:M3:273:GLY:HA3	1:M4:273:GLY:HA3	1.92	0.51
1:S8:293:ILE:CG2	1:S8:318:LEU:HD21	2.40	0.51
1:A7:273:GLY:HA3	1:A8:273:GLY:HA3	1.92	0.51
1:E6:318:LEU:HD23	1:E6:326:ILE:CD1	2.40	0.51
1:O6:293:ILE:HG21	1:O6:318:LEU:CD2	2.40	0.51
1:S8:408:GLY:HA3	2:T8:117:LEU:HD22	1.92	0.51
1:E4:293:ILE:HG21	1:E4:318:LEU:CD2	2.40	0.51
1:G3:318:LEU:HD23	1:G3:326:ILE:CD1	2.41	0.51
1:K1:318:LEU:HD23	1:K1:326:ILE:CD1	2.40	0.51
1:M6:318:LEU:HD23	1:M6:326:ILE:CD1	2.40	0.51
1:Q7:293:ILE:CG2	1:Q7:318:LEU:HD21	2.38	0.51
1:I6:149:GLN:HE22	1:I6:282:LYS:HA	1.76	0.51
1:M1:66:TRP:HZ3	2:N2:71:VAL:HG12	1.75	0.51
1:O8:170:LEU:HD21	1:O8:424:LEU:HD22	1.91	0.51
1:O8:293:ILE:HG21	1:O8:318:LEU:CD2	2.40	0.51
1:O3:293:ILE:HG21	1:O3:318:LEU:CD2	2.38	0.51
1:O5:318:LEU:HD23	1:O5:326:ILE:HD12	1.92	0.51
1:A7:293:ILE:CG2	1:A7:318:LEU:HD21	2.39	0.51
1:E1:293:ILE:HG21	1:E1:318:LEU:CD2	2.38	0.51
1:E4:335:LEU:HD21	1:E4:393:ILE:HG12	1.93	0.50
1:E5:318:LEU:HD23	1:E5:326:ILE:CD1	2.41	0.50
1:G3:273:GLY:HA3	1:G4:273:GLY:HA3	1.93	0.50
1:K2:318:LEU:HD23	1:K2:326:ILE:CD1	2.41	0.50
1:K8:446:ARG:NH1	1:K8:464:GLU:OE1	2.44	0.50
1:M1:293:ILE:HG21	1:M1:318:LEU:CD2	2.36	0.50
1:Q2:292:HIS:HA	1:Q2:325:HIS:HB2	1.93	0.50
1:S7:273:GLY:HA3	1:S8:273:GLY:HA3	1.92	0.50
1:E7:335:LEU:HD21	1:E7:393:ILE:HG12	1.93	0.50
1:I4:431:ARG:HB2	1:I4:437:LEU:HD11	1.93	0.50
1:C3:178:LEU:HD21	1:C4:107:LEU:CD2	2.41	0.50
1:G7:212:GLN:OE1	1:G7:217:ARG:HD3	2.11	0.50
1:I8:335:LEU:HD21	1:I8:393:ILE:HG12	1.92	0.50
1:K5:149:GLN:HE22	1:K5:282:LYS:HA	1.77	0.50
1:S1:74:LEU:HD21	1:S2:177:LYS:HA	1.94	0.50
1:S2:212:GLN:OE1	1:S2:217:ARG:HD3	2.12	0.50
1:E5:293:ILE:CG2	1:E5:318:LEU:HD21	2.38	0.50
1:O1:178:LEU:HD21	1:O2:107:LEU:CD2	2.42	0.50
1:C5:178:LEU:HD21	1:C6:107:LEU:CD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C5:273:GLY:HA3	1:C6:273:GLY:HA3	1.93	0.50
1:E1:293:ILE:CG2	1:E1:318:LEU:HD21	2.36	0.50
1:E1:318:LEU:HD23	1:E1:326:ILE:CD1	2.41	0.50
1:G7:293:ILE:HG21	1:G7:318:LEU:CD2	2.41	0.50
1:I1:335:LEU:HD22	1:I1:343:LEU:CD1	2.41	0.50
1:I3:273:GLY:HA3	1:I4:273:GLY:HA3	1.94	0.50
1:I3:335:LEU:HD22	1:I3:343:LEU:CD1	2.42	0.50
1:O7:335:LEU:HD22	1:O7:343:LEU:HD11	1.92	0.50
1:S1:66:TRP:HZ3	2:T2:71:VAL:HG12	1.77	0.50
1:S6:335:LEU:HD22	1:S6:343:LEU:HD11	1.92	0.50
1:O7:318:LEU:HD23	1:O7:326:ILE:HD12	1.94	0.50
1:A7:318:LEU:HD23	1:A7:326:ILE:CD1	2.41	0.50
1:I1:66:TRP:HZ3	2:J2:71:VAL:HG12	1.77	0.50
1:K4:408:GLY:HA3	2:L4:117:LEU:HD22	1.93	0.50
1:M4:244:ALA:HB1	1:M4:245:PRO:HD2	1.92	0.50
1:S3:293:ILE:HG21	1:S3:318:LEU:CD2	2.37	0.50
1:C1:335:LEU:HD22	1:C1:343:LEU:CD1	2.42	0.50
1:C3:66:TRP:HZ3	2:D4:71:VAL:HG12	1.77	0.50
1:C5:149:GLN:HE22	1:C5:282:LYS:HA	1.77	0.50
1:G2:408:GLY:HA3	2:H2:117:LEU:HD22	1.94	0.50
1:I3:293:ILE:HG21	1:I3:318:LEU:CD2	2.36	0.50
1:K7:130:LEU:O	1:K8:303:ARG:NH2	2.43	0.50
1:M3:335:LEU:HD21	1:M3:393:ILE:HG12	1.93	0.50
1:S1:273:GLY:HA3	1:S2:273:GLY:HA3	1.92	0.50
1:E4:292:HIS:HA	1:E4:325:HIS:HB2	1.93	0.49
1:G4:335:LEU:HD21	1:G4:393:ILE:HG12	1.94	0.49
1:O6:318:LEU:HD23	1:O6:326:ILE:CD1	2.42	0.49
1:A1:293:ILE:CG2	1:A1:318:LEU:HD21	2.40	0.49
1:E2:328:THR:HG22	1:E2:349:LEU:CD1	2.42	0.49
1:O4:293:ILE:CG2	1:O4:318:LEU:HD21	2.42	0.49
1:Q5:273:GLY:HA3	1:Q6:273:GLY:HA3	1.94	0.49
1:C7:335:LEU:HD21	1:C7:393:ILE:HG12	1.94	0.49
1:O3:408:GLY:HA3	2:P3:117:LEU:HD22	1.94	0.49
1:A5:293:ILE:CG2	1:A5:318:LEU:HD21	2.39	0.49
1:E2:326:ILE:HG22	1:E2:374:VAL:HG12	1.95	0.49
1:G6:293:ILE:HG21	1:G6:318:LEU:CD2	2.40	0.49
1:K8:342:THR:O	1:K8:346:VAL:HG23	2.12	0.49
1:M8:316:LYS:CE	1:M8:348:LEU:HD22	2.42	0.49
1:S4:318:LEU:HD23	1:S4:326:ILE:CD1	2.42	0.49
1:I2:293:ILE:CG2	1:I2:318:LEU:HD21	2.39	0.49
1:I6:212:GLN:OE1	1:I6:217:ARG:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M7:335:LEU:HD21	1:M7:393:ILE:HG12	1.94	0.49
1:S4:316:LYS:HE2	1:S4:348:LEU:HD22	1.94	0.49
1:A1:273:GLY:HA3	1:A2:273:GLY:HA3	1.93	0.49
1:C3:266:MET:HA	1:C3:292:HIS:O	2.13	0.49
1:C7:177:LYS:HA	1:C8:74:LEU:HD21	1.93	0.49
1:G2:293:ILE:CG2	1:G2:318:LEU:HD21	2.40	0.49
1:K1:318:LEU:HD23	1:K1:326:ILE:HD12	1.93	0.49
1:O6:293:ILE:CG2	1:O6:318:LEU:HD21	2.42	0.49
1:O8:318:LEU:HD23	1:O8:326:ILE:CD1	2.42	0.49
1:S2:293:ILE:CG2	1:S2:318:LEU:HD21	2.39	0.49
1:S4:158:GLU:OE2	1:S4:325:HIS:NE2	2.38	0.49
2:L4:106:LEU:HD11	2:L4:112:GLY:HA3	1.94	0.49
1:C4:318:LEU:HD23	1:C4:326:ILE:CD1	2.43	0.49
1:C8:239:TYR:HB3	1:C8:266:MET:HB3	1.94	0.49
1:M5:107:LEU:CD2	1:M6:178:LEU:HD21	2.42	0.49
1:O1:318:LEU:HD23	1:O1:326:ILE:CD1	2.42	0.49
1:O4:335:LEU:HD21	1:O4:393:ILE:HG12	1.94	0.49
1:S2:318:LEU:HD23	1:S2:326:ILE:CD1	2.42	0.49
1:S3:281:SER:OG	1:S3:322:GLY:HA3	2.12	0.49
1:S7:168:PRO:HD2	1:S7:428:ILE:HD11	1.95	0.49
1:A2:293:ILE:HG21	1:A2:318:LEU:CD2	2.40	0.49
1:Q1:354:ILE:HG21	1:Q1:362:ILE:HD13	1.94	0.49
1:K7:149:GLN:HE22	1:K7:282:LYS:HA	1.78	0.49
1:M2:173:THR:HG22	1:M2:175:LYS:HB2	1.95	0.49
1:O4:34:THR:HG21	1:O5:142:VAL:HG11	1.95	0.49
1:S8:149:GLN:HE22	1:S8:282:LYS:HA	1.76	0.49
1:A3:149:GLN:HE22	1:A3:282:LYS:HA	1.78	0.49
1:G3:170:LEU:HD21	1:G3:424:LEU:HD22	1.93	0.49
1:M4:88:GLU:OE2	1:M4:358:ARG:NH1	2.43	0.49
1:K3:178:LEU:HD21	1:K4:107:LEU:CD2	2.44	0.48
2:L2:75:CYS:SG	2:L2:79:GLY:N	2.83	0.48
1:E2:142:VAL:HG13	1:E2:369:ALA:HB2	1.93	0.48
1:E3:292:HIS:HA	1:E3:325:HIS:HB2	1.95	0.48
1:G8:149:GLN:HE22	1:G8:282:LYS:HA	1.78	0.48
1:I6:214:TRP:CD2	1:I6:253:ARG:HG2	2.48	0.48
1:Q3:74:LEU:HD22	1:Q4:180:LEU:HG	1.95	0.48
1:Q4:34:THR:HG21	1:Q5:142:VAL:HG11	1.94	0.48
1:A7:61:SER:HB3	1:A7:124:VAL:HG11	1.96	0.48
1:E4:138:LEU:HD12	1:E4:313:VAL:HG13	1.95	0.48
1:E7:142:VAL:HG13	1:E7:369:ALA:HB2	1.95	0.48
1:E8:117:LEU:O	1:E8:121:VAL:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:66:TRP:CZ3	2:N2:71:VAL:HG12	2.48	0.48
1:C1:293:ILE:HG21	1:C1:318:LEU:CD2	2.32	0.48
1:C4:293:ILE:CG2	1:C4:318:LEU:HD21	2.39	0.48
1:K1:66:TRP:CZ3	2:L2:71:VAL:HG12	2.48	0.48
1:O1:408:GLY:HA3	2:P1:117:LEU:HD22	1.94	0.48
1:Q8:170:LEU:HD21	1:Q8:424:LEU:HD22	1.96	0.48
1:S4:293:ILE:CG2	1:S4:318:LEU:HD21	2.41	0.48
1:A1:335:LEU:HD22	1:A1:343:LEU:CD1	2.43	0.48
1:A5:170:LEU:HD21	1:A5:424:LEU:HD22	1.95	0.48
1:C6:149:GLN:HE22	1:C6:282:LYS:HA	1.79	0.48
1:C7:293:ILE:HG21	1:C7:318:LEU:CD2	2.41	0.48
1:E1:350:ARG:HG2	1:E1:374:VAL:O	2.13	0.48
1:K4:266:MET:HA	1:K4:292:HIS:O	2.14	0.48
1:O4:318:LEU:HD23	1:O4:326:ILE:CD1	2.42	0.48
1:O8:293:ILE:CG2	1:O8:318:LEU:HD21	2.43	0.48
1:A6:221:VAL:HG11	1:A6:240:LEU:HD21	1.94	0.48
1:E7:293:ILE:CG2	1:E7:318:LEU:HD21	2.38	0.48
1:K3:221:VAL:HG11	1:K3:240:LEU:HD21	1.94	0.48
1:M5:149:GLN:HE22	1:M5:282:LYS:HA	1.79	0.48
1:Q3:335:LEU:HD22	1:Q3:343:LEU:CD1	2.43	0.48
1:A7:335:LEU:HD22	1:A7:343:LEU:HD11	1.96	0.48
1:C5:293:ILE:CG2	1:C5:318:LEU:HD21	2.38	0.48
1:K4:318:LEU:HD23	1:K4:326:ILE:HD12	1.96	0.48
1:S2:335:LEU:HD22	1:S2:343:LEU:HD11	1.96	0.48
1:G3:293:ILE:HG21	1:G3:318:LEU:CD2	2.41	0.48
1:K3:177:LYS:HA	1:K4:74:LEU:HD21	1.94	0.48
1:K7:318:LEU:HD23	1:K7:326:ILE:CD1	2.44	0.48
1:M4:293:ILE:CG2	1:M4:318:LEU:HD21	2.37	0.48
1:A8:335:LEU:HD22	1:A8:343:LEU:CD1	2.42	0.48
1:E7:178:LEU:HD21	1:E8:107:LEU:CD2	2.44	0.48
1:I5:297:MET:HG3	1:I6:121:VAL:HG23	1.95	0.48
1:K1:254:ALA:HB1	1:K1:283:TRP:CZ3	2.48	0.48
1:K1:273:GLY:HA3	1:K2:273:GLY:HA3	1.95	0.48
1:K2:335:LEU:HD22	1:K2:343:LEU:HD11	1.96	0.48
1:O4:293:ILE:HG21	1:O4:318:LEU:CD2	2.40	0.48
1:A2:335:LEU:HD21	1:A2:393:ILE:HG12	1.95	0.47
1:A3:273:GLY:HA3	1:A4:273:GLY:HA3	1.95	0.47
1:C2:293:ILE:CG2	1:C2:318:LEU:HD21	2.42	0.47
1:C4:335:LEU:HD21	1:C4:393:ILE:HG12	1.96	0.47
1:A6:335:LEU:HD21	1:A6:393:ILE:HG12	1.96	0.47
1:G4:142:VAL:HG13	1:G4:369:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I1:273:GLY:HA3	1:I2:273:GLY:HA3	1.96	0.47
1:M2:212:GLN:OE1	1:M2:217:ARG:HD3	2.14	0.47
1:O7:408:GLY:HA3	2:P7:117:LEU:HD22	1.94	0.47
1:Q1:178:LEU:HD21	1:Q2:107:LEU:CD2	2.44	0.47
1:S4:61:SER:HB3	1:S4:124:VAL:HG11	1.96	0.47
1:C2:212:GLN:OE1	1:C2:217:ARG:HD3	2.15	0.47
1:C4:292:HIS:HA	1:C4:325:HIS:HB2	1.97	0.47
1:E7:54:ALA:HB1	1:E7:84:CYS:SG	2.54	0.47
1:K1:335:LEU:HD22	1:K1:343:LEU:CD1	2.44	0.47
1:O5:408:GLY:HA3	2:P5:117:LEU:HD22	1.95	0.47
1:Q8:293:ILE:HG21	1:Q8:318:LEU:CD2	2.44	0.47
1:C2:335:LEU:HD22	1:C2:343:LEU:CD1	2.43	0.47
1:E4:318:LEU:HD23	1:E4:326:ILE:HD12	1.96	0.47
1:G5:293:ILE:HG21	1:G5:318:LEU:CD2	2.41	0.47
1:M1:61:SER:HB3	1:M1:124:VAL:HG11	1.96	0.47
1:O1:293:ILE:HG21	1:O1:318:LEU:CD2	2.38	0.47
1:S8:244:ALA:HB1	1:S8:245:PRO:HD2	1.94	0.47
2:T5:117:LEU:HD11	2:T5:123:GLY:HA3	1.96	0.47
1:G1:335:LEU:HD22	1:G1:343:LEU:CD1	2.44	0.47
1:M3:293:ILE:HG21	1:M3:318:LEU:CD2	2.38	0.47
1:O2:214:TRP:CE3	1:O2:253:ARG:HG2	2.50	0.47
1:Q5:318:LEU:HD23	1:Q5:326:ILE:CD1	2.43	0.47
1:C8:335:LEU:HD21	1:C8:393:ILE:HG12	1.96	0.47
1:E3:293:ILE:HG21	1:E3:318:LEU:CD2	2.34	0.47
1:K3:125:PHE:O	1:K4:303:ARG:NH1	2.46	0.47
1:M8:293:ILE:CG2	1:M8:318:LEU:HD21	2.39	0.47
1:O5:273:GLY:HA3	1:O6:273:GLY:HA3	1.96	0.47
1:Q4:244:ALA:HB1	1:Q4:245:PRO:HD2	1.96	0.47
1:A5:273:GLY:HA3	1:A6:273:GLY:HA3	1.97	0.47
1:A5:293:ILE:HG21	1:A5:318:LEU:CD2	2.39	0.47
1:A5:335:LEU:HD22	1:A5:343:LEU:CD1	2.42	0.47
1:E1:170:LEU:HD21	1:E1:424:LEU:HD22	1.96	0.47
1:G2:142:VAL:HG13	1:G2:369:ALA:HB2	1.97	0.47
1:G2:335:LEU:HD22	1:G2:343:LEU:HD11	1.95	0.47
1:M4:335:LEU:HD22	1:M4:343:LEU:CD1	2.43	0.47
1:O7:293:ILE:HG21	1:O7:318:LEU:CD2	2.36	0.47
1:S1:107:LEU:CD2	1:S2:178:LEU:HD21	2.45	0.47
1:A1:303:ARG:NH1	1:A2:125:PHE:O	2.47	0.47
1:E4:142:VAL:HG13	1:E4:369:ALA:HB2	1.96	0.47
1:K2:292:HIS:HA	1:K2:325:HIS:HB2	1.97	0.47
1:Q3:293:ILE:HG21	1:Q3:318:LEU:CD2	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q6:344:GLY:HA2	1:Q6:362:ILE:HD11	1.96	0.47
1:E8:335:LEU:HD21	1:E8:393:ILE:HG12	1.97	0.47
1:G3:61:SER:HB3	1:G3:124:VAL:HG11	1.96	0.47
1:G8:335:LEU:HD21	1:G8:393:ILE:HG12	1.96	0.47
1:A3:212:GLN:OE1	1:A3:217:ARG:HD3	2.15	0.47
1:A5:297:MET:HG3	1:A6:121:VAL:HG23	1.97	0.47
1:G3:121:VAL:HG23	1:G4:297:MET:HG3	1.96	0.47
1:O6:212:GLN:OE1	1:O6:217:ARG:HD3	2.15	0.47
1:O7:303:ARG:NH1	1:O8:125:PHE:O	2.47	0.47
1:Q8:318:LEU:HD23	1:Q8:326:ILE:CD1	2.45	0.47
1:A5:326:ILE:CG2	1:A5:349:LEU:HD13	2.45	0.46
1:G1:256:PHE:CE2	1:G1:260:LEU:HD11	2.50	0.46
1:K1:121:VAL:HG23	1:K2:297:MET:HG3	1.97	0.46
1:O2:318:LEU:HD23	1:O2:326:ILE:CD1	2.44	0.46
1:Q5:135:LEU:HD21	1:Q5:138:LEU:HD21	1.97	0.46
1:S1:318:LEU:HD23	1:S1:326:ILE:CD1	2.44	0.46
1:S1:335:LEU:HD22	1:S1:343:LEU:CD1	2.44	0.46
1:S8:293:ILE:HG21	1:S8:318:LEU:CD2	2.42	0.46
1:G6:212:GLN:OE1	1:G6:217:ARG:HD3	2.15	0.46
1:K2:214:TRP:CE3	1:K2:253:ARG:HG2	2.50	0.46
1:K6:316:LYS:HE2	1:K6:348:LEU:HD22	1.97	0.46
1:M6:212:GLN:OE1	1:M6:217:ARG:HD3	2.16	0.46
1:Q2:212:GLN:OE1	1:Q2:217:ARG:HD3	2.16	0.46
1:A3:66:TRP:CZ3	2:B4:71:VAL:HG12	2.50	0.46
1:O1:214:TRP:CE3	1:O1:253:ARG:HG2	2.50	0.46
1:O7:177:LYS:HA	1:O8:74:LEU:HD21	1.98	0.46
1:G5:335:LEU:HD22	1:G5:343:LEU:CD1	2.46	0.46
1:G5:335:LEU:HD21	1:G5:393:ILE:HG12	1.97	0.46
1:I1:335:LEU:HD21	1:I1:393:ILE:HG12	1.98	0.46
1:S3:335:LEU:HD22	1:S3:343:LEU:HD11	1.97	0.46
1:S6:170:LEU:HD21	1:S6:424:LEU:HD22	1.97	0.46
1:K3:36:ILE:HD12	1:K3:108:PHE:CE2	2.50	0.46
1:O2:142:VAL:HG13	1:O2:369:ALA:CB	2.46	0.46
1:O3:149:GLN:HE22	1:O3:282:LYS:HA	1.80	0.46
1:Q8:443:ASP:OD1	1:Q8:446:ARG:NH2	2.47	0.46
1:S6:197:LEU:HG	1:S6:417:ALA:HB1	1.97	0.46
1:A1:107:LEU:CD2	1:A2:178:LEU:HD21	2.45	0.46
1:A6:335:LEU:HD22	1:A6:343:LEU:CD1	2.44	0.46
1:C4:354:ILE:CG2	1:C4:362:ILE:HD13	2.45	0.46
1:E8:149:GLN:HE22	1:E8:282:LYS:HA	1.79	0.46
1:G1:158:GLU:OE2	1:G1:325:HIS:NE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q2:149:GLN:HE22	1:Q2:282:LYS:HA	1.80	0.46
1:Q7:61:SER:HB3	1:Q7:124:VAL:HG11	1.97	0.46
1:C7:433:GLU:OE1	1:M3:450:ARG:NH1	2.48	0.46
1:G7:316:LYS:CE	1:G7:348:LEU:HD22	2.46	0.46
1:K4:293:ILE:HG21	1:K4:318:LEU:CD2	2.40	0.46
1:I7:178:LEU:HD21	1:I8:107:LEU:CD2	2.46	0.46
1:O7:125:PHE:O	1:O8:303:ARG:NH1	2.48	0.46
1:Q5:158:GLU:OE2	1:Q5:325:HIS:NE2	2.49	0.46
1:Q6:127:PHE:CZ	1:Q6:129:ALA:HB3	2.51	0.46
1:C5:107:LEU:CD2	1:C6:178:LEU:HD21	2.46	0.46
1:E7:36:ILE:HD12	1:E7:108:PHE:CE2	2.51	0.46
1:E7:66:TRP:CZ3	2:F8:71:VAL:HG12	2.51	0.46
1:E7:293:ILE:HG13	1:E7:318:LEU:HD11	1.98	0.46
1:G4:149:GLN:HE22	1:G4:282:LYS:HA	1.80	0.46
1:I5:149:GLN:HE22	1:I5:282:LYS:HA	1.81	0.46
1:K8:212:GLN:OE1	1:K8:217:ARG:HD3	2.16	0.46
1:A1:335:LEU:HD21	1:A1:393:ILE:HG12	1.97	0.46
1:E7:335:LEU:HD22	1:E7:343:LEU:CD1	2.46	0.46
1:G2:221:VAL:HG11	1:G2:240:LEU:HD21	1.98	0.46
1:G3:293:ILE:CG2	1:G3:318:LEU:HD21	2.42	0.46
1:G7:178:LEU:HD21	1:G8:107:LEU:CD2	2.46	0.46
1:I7:170:LEU:HD21	1:I7:424:LEU:HD22	1.98	0.46
1:M3:149:GLN:HE22	1:M3:282:LYS:HA	1.80	0.46
1:O8:244:ALA:HB1	1:O8:245:PRO:HD2	1.97	0.46
1:Q4:335:LEU:HD21	1:Q4:393:ILE:HG12	1.98	0.46
1:S4:212:GLN:OE1	1:S4:217:ARG:HD3	2.17	0.46
1:A2:149:GLN:HE22	1:A2:282:LYS:HA	1.82	0.45
1:G2:40:PHE:CD2	1:G2:101:ILE:HD12	2.51	0.45
1:G4:335:LEU:HD22	1:G4:343:LEU:CD1	2.45	0.45
1:G8:266:MET:HA	1:G8:292:HIS:O	2.16	0.45
1:K1:214:TRP:CE3	1:K1:253:ARG:HG2	2.51	0.45
1:Q5:214:TRP:CE3	1:Q5:253:ARG:HG2	2.51	0.45
1:S3:66:TRP:HZ3	2:T4:71:VAL:HG12	1.81	0.45
1:E3:178:LEU:HD21	1:E4:107:LEU:CD2	2.46	0.45
1:G2:293:ILE:HG21	1:G2:318:LEU:CD2	2.41	0.45
1:G4:408:GLY:HA3	2:H4:117:LEU:HD22	1.97	0.45
1:G7:61:SER:HB3	1:G7:124:VAL:HG11	1.98	0.45
1:G7:107:LEU:CD2	1:G8:178:LEU:HD21	2.46	0.45
1:I6:109:GLU:H	1:I6:115:ASN:HD22	1.64	0.45
1:K2:142:VAL:HG11	1:K3:34:THR:HG21	1.97	0.45
1:Q1:107:LEU:CD2	1:Q2:178:LEU:HD21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:68:THR:O	1:C1:72:ASP:HB2	2.17	0.45
1:M2:53:ALA:O	1:M2:57:VAL:HG23	2.17	0.45
1:Q4:171:GLY:HA2	1:Q4:199:PHE:O	2.16	0.45
1:Q4:335:LEU:HD22	1:Q4:343:LEU:CD1	2.45	0.45
1:A8:292:HIS:HA	1:A8:325:HIS:HB2	1.98	0.45
1:E3:316:LYS:HE2	1:E3:348:LEU:HD22	1.98	0.45
1:G3:335:LEU:HD22	1:G3:343:LEU:CD1	2.46	0.45
1:S6:292:HIS:HA	1:S6:325:HIS:HB2	1.98	0.45
1:S6:408:GLY:HA3	2:T6:117:LEU:HD22	1.97	0.45
1:C1:335:LEU:HD21	1:C1:393:ILE:HG12	1.98	0.45
1:E2:293:ILE:CG2	1:E2:318:LEU:HD21	2.41	0.45
1:G6:266:MET:HA	1:G6:292:HIS:O	2.15	0.45
1:I2:66:TRP:CZ3	2:J1:71:VAL:HG12	2.52	0.45
1:I2:266:MET:HA	1:I2:292:HIS:O	2.16	0.45
1:M2:66:TRP:CZ3	2:N1:71:VAL:HG12	2.51	0.45
1:S6:149:GLN:HE22	1:S6:282:LYS:HA	1.82	0.45
1:O4:173:THR:HG22	1:O4:175:LYS:HB2	1.99	0.45
1:O7:273:GLY:HA3	1:O8:273:GLY:HA3	1.98	0.45
1:Q8:293:ILE:CG2	1:Q8:318:LEU:HD21	2.45	0.45
1:E5:142:VAL:HG13	1:E5:369:ALA:HB2	1.99	0.45
1:E5:239:TYR:CE1	1:E5:264:ILE:HD13	2.52	0.45
1:E8:36:ILE:HD12	1:E8:108:PHE:CE2	2.52	0.45
1:I2:214:TRP:CD2	1:I2:253:ARG:HG2	2.52	0.45
1:M1:87:ILE:HG23	1:M1:97:PHE:CD2	2.52	0.45
1:M7:335:LEU:HD22	1:M7:343:LEU:CD1	2.45	0.45
1:Q1:293:ILE:CG2	1:Q1:318:LEU:HD21	2.39	0.45
1:S7:335:LEU:HD22	1:S7:343:LEU:CD1	2.46	0.45
1:A1:125:PHE:O	1:A2:303:ARG:NH1	2.48	0.45
1:A7:214:TRP:CD2	1:A7:253:ARG:HG2	2.52	0.45
1:C8:408:GLY:HA3	2:D8:117:LEU:HD22	1.99	0.45
1:E7:74:LEU:HD21	1:E8:177:LYS:HA	1.99	0.45
1:I3:408:GLY:HA3	2:J3:117:LEU:HD22	1.99	0.45
1:K4:53:ALA:O	1:K4:57:VAL:HG23	2.17	0.45
1:O5:328:THR:HG22	1:O5:349:LEU:CD1	2.47	0.45
1:Q4:143:ALA:HA	1:Q5:143:ALA:HA	1.98	0.45
1:S4:65:THR:HG22	2:T3:124:ALA:HA	1.99	0.45
1:E1:197:LEU:HG	1:E1:417:ALA:HB1	1.99	0.45
1:G8:293:ILE:CG2	1:G8:318:LEU:HD21	2.47	0.45
1:I8:88:GLU:OE2	1:I8:358:ARG:NH1	2.47	0.45
1:Q8:36:ILE:HD12	1:Q8:108:PHE:CE2	2.52	0.45
1:S8:318:LEU:HD23	1:S8:326:ILE:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H6:107:CYS:HB3	2:H6:110:CYS:SG	2.57	0.45
1:C5:125:PHE:O	1:C6:303:ARG:NH1	2.50	0.45
1:G1:335:LEU:HD21	1:G1:393:ILE:HG12	1.97	0.45
1:I3:158:GLU:OE2	1:I3:325:HIS:NE2	2.42	0.45
1:I7:293:ILE:HG21	1:I7:318:LEU:CD2	2.36	0.45
1:I8:293:ILE:CG2	1:I8:318:LEU:HD21	2.42	0.45
1:M7:28:ASP:OD1	1:O3:27:PRO:HG3	2.17	0.45
1:O6:292:HIS:HA	1:O6:325:HIS:HB2	1.99	0.45
1:S7:117:LEU:O	1:S7:121:VAL:HG22	2.17	0.45
1:I3:149:GLN:HE22	1:I3:282:LYS:HA	1.82	0.44
1:K5:335:LEU:HD21	1:K5:393:ILE:HG12	1.99	0.44
1:O1:78:ASP:HB2	1:O1:81:LYS:HD3	1.99	0.44
1:O1:422:VAL:HG13	1:O1:451:TRP:CZ2	2.51	0.44
1:Q7:293:ILE:HG21	1:Q7:318:LEU:CD2	2.39	0.44
1:S4:137:ASP:OD1	1:S4:138:LEU:N	2.49	0.44
1:S7:36:ILE:HD12	1:S7:108:PHE:CE2	2.53	0.44
1:G3:125:PHE:O	1:G4:303:ARG:NH1	2.50	0.44
1:I2:256:PHE:CE2	1:I2:260:LEU:HD11	2.52	0.44
1:I5:354:ILE:CG2	1:I5:362:ILE:HD13	2.47	0.44
1:I7:254:ALA:HB1	1:I7:283:TRP:CZ3	2.52	0.44
1:K2:149:GLN:HE22	1:K2:282:LYS:HA	1.82	0.44
1:M8:61:SER:HB3	1:M8:124:VAL:HG11	1.99	0.44
1:O5:335:LEU:HD22	1:O5:343:LEU:CD1	2.45	0.44
1:Q1:212:GLN:OE1	1:Q1:217:ARG:HD3	2.17	0.44
1:S1:66:TRP:CZ3	2:T2:71:VAL:HG12	2.52	0.44
1:E1:344:GLY:HA2	1:E1:362:ILE:HD11	1.99	0.44
1:E2:335:LEU:HD21	1:E2:393:ILE:HG12	1.98	0.44
1:G3:113:VAL:HG11	1:G3:274:PHE:CD1	2.52	0.44
1:G4:292:HIS:HA	1:G4:325:HIS:HB2	1.98	0.44
1:I2:109:GLU:H	1:I2:115:ASN:HD22	1.65	0.44
1:I3:133:LEU:O	1:I3:307:HIS:HA	2.18	0.44
1:K5:335:LEU:HD22	1:K5:343:LEU:CD1	2.46	0.44
1:M7:66:TRP:HZ3	2:N8:71:VAL:HG12	1.82	0.44
1:M8:316:LYS:HE2	1:M8:348:LEU:HD22	1.98	0.44
1:Q6:106:ASP:OD2	1:Q7:370:SER:OG	2.33	0.44
1:C7:170:LEU:HD21	1:C7:424:LEU:HD22	1.99	0.44
1:E3:66:TRP:CZ3	2:F4:71:VAL:HG12	2.53	0.44
1:M3:335:LEU:HD22	1:M3:343:LEU:CD1	2.44	0.44
1:O2:149:GLN:HE22	1:O2:282:LYS:HA	1.82	0.44
1:Q3:74:LEU:HD21	1:Q4:177:LYS:HA	1.98	0.44
1:A4:335:LEU:HD21	1:A4:393:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E5:335:LEU:HD21	1:E5:393:ILE:HG12	1.99	0.44
1:E7:74:LEU:HD22	1:E8:180:LEU:HG	1.99	0.44
1:G2:335:LEU:HD22	1:G2:343:LEU:CD1	2.47	0.44
1:K4:221:VAL:HG11	1:K4:240:LEU:HD21	1.99	0.44
1:M3:36:ILE:HD12	1:M3:108:PHE:CE2	2.53	0.44
1:O4:65:THR:HG22	2:P3:124:ALA:HA	1.98	0.44
1:Q6:408:GLY:HA3	2:R6:117:LEU:HD22	2.00	0.44
1:S5:297:MET:HG3	1:S6:121:VAL:HG23	1.99	0.44
1:G2:69:VAL:HG11	2:H1:117:LEU:HD12	1.99	0.44
1:M8:78:ASP:HB2	1:M8:81:LYS:HD3	1.99	0.44
1:Q7:168:PRO:HD2	1:Q7:428:ILE:HD11	1.99	0.44
1:S4:214:TRP:CD2	1:S4:253:ARG:HG2	2.53	0.44
1:A1:121:VAL:HG23	1:A2:297:MET:HG3	2.00	0.44
1:C8:335:LEU:HD22	1:C8:343:LEU:CD1	2.47	0.44
1:K1:107:LEU:CD2	1:K2:178:LEU:HD21	2.48	0.44
1:O2:214:TRP:CD2	1:O2:253:ARG:HG2	2.53	0.44
1:Q2:266:MET:HA	1:Q2:292:HIS:O	2.17	0.44
1:S3:178:LEU:HD21	1:S4:107:LEU:CD2	2.48	0.44
1:S3:203:ASP:HB3	1:S3:206:ILE:HD12	1.98	0.44
1:S6:326:ILE:HG21	1:S6:349:LEU:HD22	1.98	0.44
1:C3:88:GLU:OE2	1:C3:358:ARG:NH1	2.49	0.44
1:G8:244:ALA:HB1	1:G8:245:PRO:HD2	2.00	0.44
1:I4:149:GLN:HE22	1:I4:282:LYS:HA	1.83	0.44
1:O3:178:LEU:HD21	1:O4:107:LEU:CD2	2.48	0.44
1:O4:244:ALA:HB1	1:O4:245:PRO:HD2	2.00	0.44
1:Q1:127:PHE:CZ	1:Q1:129:ALA:HB3	2.53	0.44
1:Q4:408:GLY:HA3	2:R4:117:LEU:HD22	2.00	0.44
1:Q6:326:ILE:HG22	1:Q6:374:VAL:HG12	1.99	0.44
1:S7:74:LEU:HD21	1:S8:177:LYS:HA	2.00	0.44
1:S7:293:ILE:CG2	1:S7:318:LEU:HD21	2.35	0.44
1:C2:316:LYS:HE2	1:C2:348:LEU:HD22	2.00	0.44
1:C5:297:MET:HG3	1:C6:121:VAL:HG23	1.99	0.44
1:K7:335:LEU:HD21	1:K7:393:ILE:HG12	2.00	0.44
1:Q6:335:LEU:HD22	1:Q6:343:LEU:CD1	2.48	0.44
1:S6:254:ALA:HB1	1:S6:283:TRP:CZ3	2.52	0.44
1:E1:335:LEU:HD22	1:E1:343:LEU:HD11	1.99	0.43
1:E4:87:ILE:HG23	1:E4:97:PHE:CD2	2.53	0.43
1:E8:170:LEU:HD21	1:E8:424:LEU:HD22	1.99	0.43
1:I1:41:ARG:NH1	1:I1:90:LEU:HD13	2.33	0.43
1:K1:149:GLN:HE22	1:K1:282:LYS:HA	1.83	0.43
1:K2:266:MET:HA	1:K2:292:HIS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:214:TRP:CE3	1:M1:253:ARG:HG2	2.53	0.43
1:M3:212:GLN:OE1	1:M3:217:ARG:HD3	2.16	0.43
1:Q6:117:LEU:O	1:Q6:121:VAL:HG22	2.18	0.43
1:Q7:66:TRP:CZ3	2:R8:71:VAL:HG12	2.53	0.43
1:Q8:121:VAL:HG11	1:Q8:135:LEU:HD22	2.00	0.43
1:S4:36:ILE:HD12	1:S4:108:PHE:CE2	2.53	0.43
1:A8:221:VAL:HG11	1:A8:240:LEU:HD21	2.00	0.43
1:C7:152:PRO:HB2	1:C7:153:HIS:CD2	2.53	0.43
1:E8:293:ILE:HG13	1:E8:318:LEU:HD11	2.00	0.43
1:M1:335:LEU:HD22	1:M1:343:LEU:CD1	2.45	0.43
1:M8:110:GLU:OE1	1:M8:110:GLU:N	2.49	0.43
1:O2:244:ALA:HB1	1:O2:245:PRO:HD2	1.99	0.43
1:O5:318:LEU:HD23	1:O5:326:ILE:CD1	2.48	0.43
1:O6:147:THR:HG22	1:O7:146:LYS:O	2.18	0.43
1:O6:149:GLN:HE22	1:O6:282:LYS:HA	1.82	0.43
1:S7:26:THR:C	1:S7:28:ASP:H	2.21	0.43
1:K4:66:TRP:CZ3	2:L3:71:VAL:HG12	2.53	0.43
1:Q8:292:HIS:HA	1:Q8:325:HIS:HB2	2.00	0.43
1:S2:335:LEU:HD22	1:S2:343:LEU:CD1	2.48	0.43
1:C4:335:LEU:HD22	1:C4:343:LEU:CD1	2.46	0.43
1:E3:107:LEU:CD2	1:E4:178:LEU:HD21	2.48	0.43
1:E4:173:THR:HG22	1:E4:175:LYS:HB2	1.99	0.43
1:E5:149:GLN:HE22	1:E5:282:LYS:HA	1.82	0.43
1:E6:293:ILE:HG21	1:E6:318:LEU:CD2	2.41	0.43
1:M6:117:LEU:O	1:M6:121:VAL:HG22	2.18	0.43
1:O2:293:ILE:HG21	1:O2:318:LEU:CD2	2.46	0.43
1:O6:335:LEU:HD22	1:O6:343:LEU:CD1	2.46	0.43
1:Q4:34:THR:CG2	1:Q5:142:VAL:HG11	2.48	0.43
1:S2:65:THR:HG22	2:T1:131:LEU:HD22	2.00	0.43
1:S2:66:TRP:CZ3	2:T1:71:VAL:HG12	2.53	0.43
1:A1:178:LEU:HD21	1:A2:107:LEU:CD2	2.48	0.43
1:A3:178:LEU:HD21	1:A4:107:LEU:CD2	2.48	0.43
1:A8:54:ALA:HB1	1:A8:84:CYS:SG	2.58	0.43
1:C2:142:VAL:HG13	1:C2:369:ALA:HB2	2.00	0.43
1:E1:178:LEU:HD21	1:E2:107:LEU:CD2	2.48	0.43
1:S3:66:TRP:CZ3	2:T4:71:VAL:HG12	2.53	0.43
1:S3:335:LEU:HD22	1:S3:343:LEU:CD1	2.49	0.43
1:S5:335:LEU:HD22	1:S5:343:LEU:CD1	2.47	0.43
1:S7:297:MET:HG3	1:S8:121:VAL:HG23	1.99	0.43
1:A1:221:VAL:HG11	1:A1:240:LEU:HD21	2.00	0.43
1:A8:158:GLU:OE2	1:A8:325:HIS:NE2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A8:214:TRP:CD2	1:A8:253:ARG:HG2	2.54	0.43
1:C1:66:TRP:CZ3	2:D2:71:VAL:HG12	2.53	0.43
1:I2:149:GLN:HE22	1:I2:282:LYS:HA	1.83	0.43
1:K4:335:LEU:HD22	1:K4:343:LEU:CD1	2.47	0.43
1:K7:292:HIS:HA	1:K7:325:HIS:HB2	2.01	0.43
1:K8:149:GLN:HE22	1:K8:282:LYS:HA	1.83	0.43
1:M7:130:LEU:O	1:M8:303:ARG:NH2	2.47	0.43
1:A1:293:ILE:HG21	1:A1:318:LEU:CD2	2.43	0.43
1:C3:335:LEU:HD21	1:C3:393:ILE:HG12	2.00	0.43
1:E2:54:ALA:HB1	1:E2:84:CYS:SG	2.59	0.43
1:E2:66:TRP:CZ3	2:F1:71:VAL:HG12	2.54	0.43
1:E4:214:TRP:CD2	1:E4:253:ARG:HG2	2.54	0.43
1:I7:28:ASP:OD1	1:S3:27:PRO:HG3	2.19	0.43
1:K1:254:ALA:HB1	1:K1:283:TRP:CH2	2.54	0.43
1:K4:244:ALA:HB1	1:K4:245:PRO:HD2	2.01	0.43
1:M7:303:ARG:NH1	1:M8:125:PHE:O	2.51	0.43
1:O8:214:TRP:CE3	1:O8:253:ARG:HG2	2.53	0.43
1:Q5:149:GLN:HE22	1:Q5:282:LYS:HA	1.83	0.43
1:Q7:273:GLY:HA3	1:Q8:273:GLY:HA3	2.00	0.43
1:A6:212:GLN:OE1	1:A6:217:ARG:HD3	2.18	0.43
1:C1:303:ARG:NH1	1:C2:125:PHE:O	2.49	0.43
1:E1:256:PHE:CE2	1:E1:260:LEU:HD11	2.54	0.43
1:I1:158:GLU:OE2	1:I1:325:HIS:NE2	2.44	0.43
1:I7:74:LEU:HD21	1:I8:177:LYS:HA	2.00	0.43
1:K4:318:LEU:HD23	1:K4:326:ILE:CD1	2.48	0.43
1:M3:170:LEU:HD21	1:M3:424:LEU:HD22	2.00	0.43
1:O2:36:ILE:HD12	1:O2:108:PHE:CE2	2.54	0.43
1:Q4:293:ILE:CG2	1:Q4:318:LEU:HD21	2.47	0.43
1:A8:239:TYR:HB3	1:A8:266:MET:HB3	2.01	0.43
1:E5:158:GLU:OE2	1:E5:325:HIS:NE2	2.51	0.43
1:E6:330:THR:HG1	1:E6:379:SER:H	1.67	0.43
1:E7:342:THR:O	1:E7:346:VAL:HG23	2.19	0.43
1:I2:408:GLY:HA3	2:J2:117:LEU:HD22	2.01	0.43
1:I3:266:MET:HA	1:I3:292:HIS:O	2.18	0.43
1:K2:335:LEU:HD22	1:K2:343:LEU:CD1	2.49	0.43
1:A2:335:LEU:HD22	1:A2:343:LEU:CD1	2.47	0.43
1:C7:142:VAL:HG13	1:C7:369:ALA:HB2	2.00	0.43
1:E4:212:GLN:OE1	1:E4:217:ARG:HD3	2.18	0.43
1:K3:142:VAL:HG13	1:K3:369:ALA:HB2	2.01	0.43
1:M1:273:GLY:HA3	1:M2:273:GLY:HA3	1.99	0.43
1:O2:54:ALA:HB1	1:O2:84:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O4:68:THR:HA	1:O4:71:THR:HB	2.01	0.43
1:Q8:127:PHE:CZ	1:Q8:129:ALA:HB3	2.54	0.43
1:A5:315:ALA:HB1	1:A5:349:LEU:HD21	2.01	0.42
1:G8:239:TYR:HB3	1:G8:266:MET:HB3	2.01	0.42
1:I6:172:CYS:HA	1:I6:402:PHE:O	2.19	0.42
1:I8:244:ALA:HB1	1:I8:245:PRO:HD2	2.00	0.42
1:K4:88:GLU:OE2	1:K4:358:ARG:NH1	2.51	0.42
1:O1:335:LEU:HD21	1:O1:393:ILE:HG12	2.00	0.42
1:O5:138:LEU:HD12	1:O5:313:VAL:HG13	2.01	0.42
1:O8:202:ASP:OD2	1:O8:217:ARG:NE	2.50	0.42
1:A3:303:ARG:NH1	1:A4:125:PHE:O	2.49	0.42
1:E8:408:GLY:HA3	2:F8:117:LEU:HD22	2.01	0.42
1:K1:292:HIS:HA	1:K1:325:HIS:HB2	2.01	0.42
1:M3:137:ASP:OD1	1:M3:138:LEU:N	2.52	0.42
1:S6:158:GLU:OE2	1:S6:325:HIS:NE2	2.52	0.42
1:A7:212:GLN:OE1	1:A7:217:ARG:HD3	2.19	0.42
1:E7:177:LYS:HA	1:E8:74:LEU:HD21	2.01	0.42
1:G4:173:THR:HG22	1:G4:175:LYS:HB2	2.01	0.42
1:G8:318:LEU:HD23	1:G8:326:ILE:CD1	2.47	0.42
1:I7:36:ILE:HD12	1:I7:108:PHE:CE2	2.54	0.42
1:K4:66:TRP:HZ3	2:L3:71:VAL:HG12	1.83	0.42
1:Q3:443:ASP:OD1	1:Q3:446:ARG:NH2	2.50	0.42
1:Q8:202:ASP:OD2	1:Q8:217:ARG:NE	2.51	0.42
1:A7:335:LEU:HD22	1:A7:343:LEU:CD1	2.49	0.42
1:Q8:293:ILE:HG13	1:Q8:318:LEU:HD11	2.01	0.42
1:C3:212:GLN:OE1	1:C3:217:ARG:HD3	2.19	0.42
1:C6:335:LEU:HD22	1:C6:343:LEU:CD1	2.50	0.42
1:C7:292:HIS:HA	1:C7:325:HIS:HB2	2.01	0.42
1:E5:107:LEU:CD2	1:E6:178:LEU:HD21	2.49	0.42
1:I7:214:TRP:CD2	1:I7:253:ARG:HG2	2.54	0.42
1:K1:443:ASP:OD1	1:K1:446:ARG:NH2	2.51	0.42
1:K2:40:PHE:CD2	1:K2:101:ILE:HD12	2.55	0.42
1:K2:328:THR:HG22	1:K2:349:LEU:CD1	2.49	0.42
1:K3:74:LEU:HD22	1:K4:180:LEU:HG	2.01	0.42
1:O4:61:SER:HB3	1:O4:124:VAL:HG11	1.99	0.42
1:S1:178:LEU:HD21	1:S2:107:LEU:CD2	2.49	0.42
1:S1:266:MET:HA	1:S1:292:HIS:O	2.19	0.42
1:S2:239:TYR:OH	1:S2:401:GLN:NE2	2.52	0.42
1:S5:203:ASP:HB3	1:S5:206:ILE:HD12	2.02	0.42
1:A5:244:ALA:HB1	1:A5:245:PRO:HD2	2.01	0.42
1:G1:107:LEU:CD2	1:G2:178:LEU:HD21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I5:303:ARG:NH1	1:I6:125:PHE:O	2.52	0.42
1:K7:178:LEU:HD21	1:K8:107:LEU:CD2	2.50	0.42
1:M1:354:ILE:CG2	1:M1:362:ILE:HD13	2.50	0.42
1:M6:335:LEU:HD22	1:M6:343:LEU:CD1	2.47	0.42
1:Q1:53:ALA:O	1:Q1:57:VAL:HG23	2.20	0.42
1:Q4:54:ALA:HB1	1:Q4:84:CYS:SG	2.59	0.42
1:Q6:214:TRP:CE3	1:Q6:253:ARG:HG2	2.55	0.42
1:A7:350:ARG:HG2	1:A7:374:VAL:O	2.19	0.42
1:C1:410:PRO:HG3	1:C1:461:LEU:HD11	2.02	0.42
1:C5:212:GLN:OE1	1:C5:217:ARG:HD3	2.20	0.42
1:C7:335:LEU:HD22	1:C7:343:LEU:CD1	2.45	0.42
1:E5:214:TRP:CE3	1:E5:253:ARG:HG2	2.55	0.42
1:E5:326:ILE:HG22	1:E5:374:VAL:HG12	2.00	0.42
1:G2:214:TRP:CD2	1:G2:253:ARG:HG2	2.55	0.42
1:G8:66:TRP:CZ3	2:H7:71:VAL:HG12	2.55	0.42
1:I4:152:PRO:HB2	1:I4:153:HIS:CD2	2.54	0.42
1:I5:125:PHE:O	1:I6:303:ARG:NH1	2.50	0.42
1:K4:325:HIS:HD2	1:K4:375:MET:HB2	1.85	0.42
1:Q5:256:PHE:CE2	1:Q5:260:LEU:HD11	2.55	0.42
1:S3:443:ASP:OD1	1:S3:446:ARG:NH2	2.52	0.42
1:C1:178:LEU:HD21	1:C2:107:LEU:CD2	2.50	0.42
1:E2:214:TRP:CE3	1:E2:253:ARG:HG2	2.54	0.42
1:E3:214:TRP:CE3	1:E3:253:ARG:HG2	2.55	0.42
1:G1:142:VAL:HG13	1:G1:369:ALA:HB2	2.01	0.42
1:I7:406:THR:OG1	1:I7:420:ASN:ND2	2.53	0.42
1:K1:88:GLU:OE2	1:K1:358:ARG:NH1	2.51	0.42
1:M5:266:MET:HA	1:M5:292:HIS:O	2.19	0.42
1:O1:335:LEU:HD22	1:O1:343:LEU:CD1	2.48	0.42
1:O3:74:LEU:HD21	1:O4:177:LYS:HA	2.01	0.42
1:O7:170:LEU:HD21	1:O7:424:LEU:HD22	2.02	0.42
1:S5:200:THR:OG1	1:S5:238:HIS:ND1	2.41	0.42
1:A1:297:MET:HG3	1:A2:121:VAL:HG23	2.02	0.42
1:A3:192:CYS:HB3	1:A3:197:LEU:HD12	2.02	0.42
1:A5:326:ILE:HG21	1:A5:349:LEU:HD13	2.02	0.42
1:A6:326:ILE:CG2	1:A6:349:LEU:HD13	2.49	0.42
1:C7:221:VAL:HG11	1:C7:240:LEU:HD21	2.01	0.42
1:E8:292:HIS:HA	1:E8:325:HIS:HB2	2.00	0.42
1:I2:212:GLN:OE1	1:I2:217:ARG:HD3	2.19	0.42
1:K8:327:HIS:HA	1:K8:377:VAL:HB	2.02	0.42
1:M1:214:TRP:CD2	1:M1:253:ARG:HG2	2.55	0.42
1:M7:65:THR:HG22	2:N8:124:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O2:239:TYR:OH	1:O2:401:GLN:NE2	2.53	0.42
1:O2:293:ILE:CG2	1:O2:318:LEU:HD21	2.49	0.42
1:O4:212:GLN:OE1	1:O4:217:ARG:HD3	2.20	0.42
1:O6:335:LEU:HD21	1:O6:393:ILE:HG12	2.02	0.42
1:O7:326:ILE:HG22	1:O7:374:VAL:HG12	2.02	0.42
1:S3:107:LEU:CD2	1:S4:178:LEU:HD21	2.49	0.42
1:S3:121:VAL:HG23	1:S4:297:MET:HG3	2.02	0.42
1:S5:335:LEU:HD21	1:S5:393:ILE:HG12	2.02	0.42
1:C1:117:LEU:O	1:C1:121:VAL:HG22	2.20	0.42
1:C1:244:ALA:HB1	1:C1:245:PRO:HD2	2.02	0.42
1:E1:408:GLY:HA3	2:F1:117:LEU:HD22	2.02	0.42
1:E2:293:ILE:HG21	1:E2:318:LEU:CD2	2.43	0.42
1:G1:66:TRP:CZ3	2:H2:71:VAL:HG12	2.55	0.42
1:G2:446:ARG:NH1	1:G2:464:GLU:OE1	2.53	0.42
1:I3:36:ILE:HD12	1:I3:108:PHE:CE2	2.54	0.42
1:I3:303:ARG:NH1	1:I4:125:PHE:O	2.53	0.42
1:I3:326:ILE:HG22	1:I3:374:VAL:HG12	2.02	0.42
1:K3:214:TRP:CD2	1:K3:253:ARG:HG2	2.55	0.42
1:K7:36:ILE:HD12	1:K7:108:PHE:CE2	2.55	0.42
1:K7:177:LYS:HA	1:K8:74:LEU:HD21	2.01	0.42
1:M3:214:TRP:CD2	1:M3:253:ARG:HG2	2.55	0.42
1:M5:330:THR:HG23	1:M5:378:ALA:HB1	2.02	0.42
1:O7:335:LEU:HD22	1:O7:343:LEU:CD1	2.50	0.42
1:Q8:40:PHE:CD2	1:Q8:101:ILE:HD12	2.55	0.42
1:I1:297:MET:HG3	1:I2:121:VAL:HG23	2.01	0.41
1:I3:66:TRP:CZ3	2:J4:71:VAL:HG12	2.55	0.41
1:K3:335:LEU:HD21	1:K3:393:ILE:HG12	2.01	0.41
1:O6:266:MET:HA	1:O6:292:HIS:O	2.19	0.41
1:Q3:107:LEU:CD2	1:Q4:178:LEU:HD21	2.49	0.41
1:S5:273:GLY:HA3	1:S6:273:GLY:HA3	2.02	0.41
1:A4:254:ALA:HB1	1:A4:283:TRP:CZ3	2.55	0.41
1:A4:335:LEU:HD22	1:A4:343:LEU:CD1	2.44	0.41
1:A8:142:VAL:HG13	1:A8:369:ALA:HB2	2.02	0.41
1:C1:66:TRP:HZ3	2:D2:71:VAL:HG12	1.85	0.41
1:E6:408:GLY:HA3	2:F6:117:LEU:HD22	2.02	0.41
1:G4:40:PHE:CD2	1:G4:101:ILE:HD12	2.55	0.41
1:I5:350:ARG:HG2	1:I5:374:VAL:O	2.21	0.41
1:I7:266:MET:HA	1:I7:292:HIS:O	2.20	0.41
1:K1:36:ILE:HD12	1:K1:108:PHE:CE2	2.55	0.41
1:K6:221:VAL:HG11	1:K6:240:LEU:HD21	2.02	0.41
1:K7:107:LEU:CD2	1:K8:178:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M1:350:ARG:HG2	1:M1:374:VAL:O	2.20	0.41
1:M7:74:LEU:HD22	1:M8:180:LEU:HG	2.01	0.41
1:Q5:335:LEU:HD22	1:Q5:343:LEU:CD1	2.50	0.41
1:Q7:62:SER:OG	1:Q7:82:GLY:N	2.54	0.41
1:S1:303:ARG:NH1	1:S2:125:PHE:O	2.53	0.41
2:R2:75:CYS:SG	2:R2:79:GLY:N	2.85	0.41
1:C1:125:PHE:O	1:C2:303:ARG:NH1	2.49	0.41
1:E2:335:LEU:HD22	1:E2:343:LEU:CD1	2.45	0.41
1:E7:214:TRP:CD2	1:E7:253:ARG:HG2	2.55	0.41
1:E8:244:ALA:HB1	1:E8:245:PRO:HD2	2.03	0.41
1:G1:138:LEU:HD12	1:G1:313:VAL:HG13	2.02	0.41
1:G3:66:TRP:CZ3	2:H4:71:VAL:HG12	2.55	0.41
1:G3:292:HIS:HA	1:G3:325:HIS:HB2	2.03	0.41
1:G7:293:ILE:CG2	1:G7:318:LEU:HD21	2.47	0.41
1:M1:303:ARG:NH1	1:M2:125:PHE:O	2.51	0.41
1:M5:203:ASP:HB3	1:M5:206:ILE:HD12	2.02	0.41
1:O2:335:LEU:HD22	1:O2:343:LEU:CD1	2.48	0.41
1:A2:66:TRP:CZ3	2:B1:71:VAL:HG12	2.55	0.41
1:A4:88:GLU:OE2	1:A4:358:ARG:NH1	2.52	0.41
1:A7:28:ASP:HB3	1:Q3:28:ASP:HB3	2.03	0.41
1:C1:214:TRP:CE3	1:C1:253:ARG:HG2	2.56	0.41
1:C6:266:MET:HA	1:C6:292:HIS:O	2.19	0.41
1:E4:158:GLU:OE2	1:E4:325:HIS:NE2	2.53	0.41
1:E4:203:ASP:HB3	1:E4:206:ILE:HD12	2.02	0.41
1:G6:335:LEU:HD22	1:G6:343:LEU:CD1	2.51	0.41
1:M6:214:TRP:CD2	1:M6:253:ARG:HG2	2.55	0.41
1:Q2:326:ILE:HG22	1:Q2:374:VAL:CG1	2.50	0.41
1:A5:133:LEU:O	1:A5:307:HIS:HA	2.20	0.41
1:A6:447:GLU:OE1	1:A6:450:ARG:NH1	2.53	0.41
1:A7:40:PHE:CD2	1:A7:101:ILE:HD12	2.56	0.41
1:A7:328:THR:HG22	1:A7:349:LEU:CD1	2.50	0.41
1:C7:266:MET:HA	1:C7:292:HIS:O	2.20	0.41
1:C8:54:ALA:HB1	1:C8:84:CYS:SG	2.60	0.41
1:C8:293:ILE:HG13	1:C8:318:LEU:HD11	2.01	0.41
1:E1:53:ALA:O	1:E1:57:VAL:HG23	2.21	0.41
1:G1:326:ILE:HG21	1:G1:349:LEU:HD13	2.03	0.41
1:I3:53:ALA:O	1:I3:57:VAL:HG23	2.21	0.41
1:O5:107:LEU:CD2	1:O6:178:LEU:HD21	2.51	0.41
1:Q7:300:VAL:HG22	1:Q8:125:PHE:CD2	2.55	0.41
1:C3:121:VAL:HG23	1:C4:297:MET:HG3	2.02	0.41
1:E4:446:ARG:NH1	1:E4:464:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E5:113:VAL:HG11	1:E5:274:PHE:CD1	2.55	0.41
1:I8:149:GLN:HE22	1:I8:282:LYS:HA	1.84	0.41
1:K1:170:LEU:HD21	1:K1:424:LEU:HD22	2.01	0.41
1:K7:244:ALA:HB1	1:K7:245:PRO:HD2	2.03	0.41
1:K8:214:TRP:CD2	1:K8:253:ARG:HG2	2.55	0.41
1:M7:107:LEU:CD2	1:M8:178:LEU:HD21	2.50	0.41
1:Q7:203:ASP:HB3	1:Q7:206:ILE:HD12	2.02	0.41
1:A3:142:VAL:HG13	1:A3:369:ALA:HB2	2.02	0.41
1:C3:354:ILE:CG2	1:C3:362:ILE:HD13	2.51	0.41
1:C7:107:LEU:CD2	1:C8:178:LEU:HD21	2.51	0.41
1:C8:53:ALA:O	1:C8:57:VAL:HG23	2.20	0.41
1:C8:68:THR:O	1:C8:72:ASP:HB2	2.21	0.41
1:C8:214:TRP:CE3	1:C8:253:ARG:HG2	2.55	0.41
1:E2:103:TYR:HB3	1:E2:107:LEU:HD12	2.03	0.41
1:E5:387:MET:O	1:E5:391:VAL:HG23	2.21	0.41
1:E8:327:HIS:HA	1:E8:377:VAL:HB	2.02	0.41
1:G8:52:GLU:HB3	2:H7:70:LEU:HD11	2.03	0.41
1:G8:350:ARG:HG2	1:G8:374:VAL:O	2.20	0.41
1:K3:292:HIS:HA	1:K3:325:HIS:HB2	2.02	0.41
1:K6:335:LEU:HD22	1:K6:343:LEU:CD1	2.50	0.41
1:O3:203:ASP:HB3	1:O3:206:ILE:HD12	2.03	0.41
1:O3:266:MET:HA	1:O3:292:HIS:O	2.20	0.41
1:O6:344:GLY:HA2	1:O6:362:ILE:HD11	2.03	0.41
1:Q3:335:LEU:HD21	1:Q3:393:ILE:HG12	2.03	0.41
1:Q6:214:TRP:CD2	1:Q6:253:ARG:HG2	2.55	0.41
1:S2:170:LEU:HD21	1:S2:424:LEU:HD22	2.02	0.41
1:A7:36:ILE:HD12	1:A7:108:PHE:CE2	2.56	0.41
1:E1:88:GLU:OE2	1:E1:358:ARG:NH1	2.54	0.41
1:E2:142:VAL:HG13	1:E2:369:ALA:CB	2.51	0.41
1:E3:130:LEU:O	1:E4:303:ARG:NH2	2.49	0.41
1:G5:171:GLY:HA2	1:G5:199:PHE:O	2.20	0.41
1:I1:178:LEU:HD21	1:I2:107:LEU:CD2	2.50	0.41
1:I2:214:TRP:CE3	1:I2:253:ARG:HG2	2.56	0.41
1:M2:292:HIS:HA	1:M2:325:HIS:HB2	2.02	0.41
1:M8:135:LEU:HG	1:M8:313:VAL:HG21	2.02	0.41
1:O7:113:VAL:HG11	1:O7:274:PHE:CD1	2.56	0.41
1:Q1:61:SER:HB3	1:Q1:124:VAL:HG11	2.02	0.41
2:T8:117:LEU:HD11	2:T8:123:GLY:HA3	2.03	0.41
1:A1:171:GLY:HA2	1:A1:199:PHE:O	2.20	0.41
1:A1:212:GLN:OE1	1:A1:217:ARG:HD3	2.20	0.41
1:A4:239:TYR:HB3	1:A4:266:MET:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C5:138:LEU:O	1:C5:316:LYS:NZ	2.52	0.41
1:E1:292:HIS:HA	1:E1:325:HIS:HB2	2.03	0.41
1:E2:40:PHE:CD2	1:E2:101:ILE:HD12	2.56	0.41
1:E5:138:LEU:HD12	1:E5:313:VAL:HG13	2.01	0.41
1:E5:212:GLN:OE1	1:E5:217:ARG:HD3	2.21	0.41
1:E8:78:ASP:HB2	1:E8:81:LYS:HD3	2.02	0.41
1:E8:199:PHE:HA	1:E8:237:GLY:O	2.21	0.41
1:G3:118:THR:HG23	1:G4:296:ALA:CB	2.51	0.41
1:G5:127:PHE:CZ	1:G5:129:ALA:HB3	2.55	0.41
1:G8:170:LEU:HD21	1:G8:424:LEU:HD22	2.03	0.41
1:G8:335:LEU:HD22	1:G8:343:LEU:CD1	2.44	0.41
1:I5:214:TRP:CD2	1:I5:253:ARG:HG2	2.55	0.41
1:I5:335:LEU:HD22	1:I5:343:LEU:CD1	2.46	0.41
1:K3:113:VAL:HG11	1:K3:274:PHE:CE1	2.56	0.41
1:K3:170:LEU:HD21	1:K3:424:LEU:HD22	2.02	0.41
1:M1:408:GLY:HA3	2:N1:117:LEU:HD22	2.03	0.41
1:M7:66:TRP:CZ3	2:N8:71:VAL:HG12	2.56	0.41
1:O6:214:TRP:CE3	1:O6:253:ARG:HG2	2.56	0.41
1:Q4:318:LEU:HD23	1:Q4:326:ILE:CD1	2.51	0.41
1:Q5:121:VAL:HG23	1:Q6:297:MET:HG3	2.01	0.41
1:Q5:303:ARG:NH1	1:Q6:125:PHE:O	2.53	0.41
1:A2:66:TRP:HZ3	2:B1:71:VAL:HG12	1.86	0.41
1:C1:350:ARG:HG2	1:C1:374:VAL:O	2.21	0.41
1:C4:170:LEU:HD21	1:C4:424:LEU:HD22	2.02	0.41
1:E1:125:PHE:O	1:E2:303:ARG:NH1	2.52	0.41
1:G1:170:LEU:HD21	1:G1:424:LEU:HD22	2.02	0.41
1:I3:212:GLN:OE1	1:I3:217:ARG:HD3	2.20	0.41
1:I3:239:TYR:HB3	1:I3:266:MET:HB3	2.02	0.41
1:M2:202:ASP:OD2	1:M2:217:ARG:NE	2.53	0.41
1:Q8:335:LEU:HD21	1:Q8:393:ILE:HG12	2.02	0.41
1:S3:292:HIS:HA	1:S3:325:HIS:HB2	2.03	0.41
1:S6:318:LEU:HD23	1:S6:326:ILE:HD12	2.02	0.41
1:E4:408:GLY:HA3	2:F4:117:LEU:HD22	2.03	0.40
1:G3:266:MET:HA	1:G3:292:HIS:O	2.20	0.40
1:G5:137:ASP:OD1	1:G5:138:LEU:N	2.55	0.40
1:G8:173:THR:HG22	1:G8:175:LYS:HB2	2.03	0.40
1:K3:78:ASP:HB2	1:K3:81:LYS:HD3	2.04	0.40
1:K5:170:LEU:HD21	1:K5:424:LEU:HD22	2.03	0.40
1:M7:36:ILE:HD12	1:M7:108:PHE:CE2	2.56	0.40
1:O3:74:LEU:HD22	1:O4:180:LEU:HG	2.03	0.40
1:O4:221:VAL:HG11	1:O4:240:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O6:350:ARG:HG2	1:O6:374:VAL:O	2.21	0.40
1:O7:239:TYR:HB3	1:O7:266:MET:HB3	2.04	0.40
1:O8:40:PHE:CD2	1:O8:101:ILE:HD12	2.56	0.40
1:Q1:221:VAL:HG11	1:Q1:240:LEU:HD21	2.03	0.40
1:Q7:36:ILE:HD12	1:Q7:108:PHE:CE2	2.56	0.40
1:S6:318:LEU:HD23	1:S6:326:ILE:CD1	2.51	0.40
1:A1:66:TRP:CH2	2:B2:71:VAL:HG12	2.56	0.40
1:A5:335:LEU:HD21	1:A5:393:ILE:HG12	2.04	0.40
1:A5:350:ARG:HG2	1:A5:374:VAL:O	2.21	0.40
1:A7:244:ALA:HB1	1:A7:245:PRO:HD2	2.02	0.40
1:C8:127:PHE:CZ	1:C8:129:ALA:HB3	2.56	0.40
1:G2:113:VAL:HG11	1:G2:274:PHE:CD1	2.56	0.40
1:I5:214:TRP:CE3	1:I5:253:ARG:HG2	2.56	0.40
1:K4:142:VAL:HG13	1:K4:369:ALA:HB2	2.03	0.40
1:K8:66:TRP:CZ3	2:L7:71:VAL:HG12	2.56	0.40
1:M7:379:SER:OG	1:M7:380:GLY:N	2.55	0.40
1:O3:107:LEU:CD2	1:O4:178:LEU:HD21	2.51	0.40
1:O7:180:LEU:HG	1:O8:74:LEU:HD22	2.03	0.40
1:S1:214:TRP:CE3	1:S1:253:ARG:HG2	2.56	0.40
1:S6:266:MET:HA	1:S6:292:HIS:O	2.20	0.40
1:S7:40:PHE:O	1:S7:98:ILE:HA	2.21	0.40
1:A3:354:ILE:CG2	1:A3:362:ILE:HD13	2.51	0.40
1:A7:173:THR:HG22	1:A7:175:LYS:HB2	2.04	0.40
1:C7:125:PHE:O	1:C8:303:ARG:NH1	2.54	0.40
1:C7:212:GLN:OE1	1:C7:217:ARG:HD3	2.21	0.40
1:I4:463:LYS:NZ	2:J4:74:ASN:OD1	2.55	0.40
1:K2:66:TRP:CZ3	2:L1:71:VAL:HG12	2.56	0.40
1:M4:142:VAL:HG13	1:M4:369:ALA:HB2	2.02	0.40
1:O1:212:GLN:OE1	1:O1:217:ARG:HD3	2.21	0.40
1:O3:406:THR:OG1	1:O3:420:ASN:ND2	2.55	0.40
1:O7:178:LEU:HD21	1:O8:107:LEU:CD2	2.51	0.40
1:Q8:335:LEU:HD22	1:Q8:343:LEU:CD1	2.51	0.40
1:A7:178:LEU:HD21	1:A8:107:LEU:CD2	2.52	0.40
1:C1:65:THR:HG22	2:D2:124:ALA:HA	2.03	0.40
1:C2:34:THR:HB	1:C2:105:LEU:HD22	2.04	0.40
1:C7:214:TRP:CD2	1:C7:253:ARG:HG2	2.56	0.40
1:E6:292:HIS:HA	1:E6:325:HIS:HB2	2.03	0.40
1:G3:214:TRP:CD2	1:G3:253:ARG:HG2	2.56	0.40
1:G5:408:GLY:HA3	2:H5:117:LEU:HD22	2.03	0.40
1:G6:408:GLY:HA3	2:H6:117:LEU:HD22	2.03	0.40
1:I1:142:VAL:HG13	1:I1:369:ALA:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I2:66:TRP:HZ3	2:J1:71:VAL:HG12	1.86	0.40
1:K2:66:TRP:HZ3	2:L1:71:VAL:HG12	1.85	0.40
1:M1:256:PHE:CE2	1:M1:260:LEU:HD11	2.55	0.40
1:M2:117:LEU:O	1:M2:121:VAL:HG22	2.22	0.40
1:Q3:326:ILE:HG22	1:Q3:374:VAL:CG1	2.51	0.40
1:Q7:170:LEU:HD21	1:Q7:424:LEU:HD22	2.03	0.40
1:Q7:292:HIS:HA	1:Q7:325:HIS:HB2	2.02	0.40
1:S1:53:ALA:O	1:S1:57:VAL:HG23	2.22	0.40
1:S2:266:MET:HA	1:S2:292:HIS:O	2.20	0.40
1:S6:335:LEU:HD22	1:S6:343:LEU:CD1	2.51	0.40
1:G2:328:THR:HG22	1:G2:349:LEU:CD1	2.52	0.40
1:K3:447:GLU:HA	1:K3:450:ARG:HD3	2.04	0.40
1:K4:443:ASP:OD1	1:K4:446:ARG:NH2	2.54	0.40
1:O5:170:LEU:HB3	1:O5:197:LEU:HD22	2.03	0.40
1:Q1:354:ILE:CG2	1:Q1:362:ILE:HD13	2.52	0.40
1:Q8:54:ALA:HB1	1:Q8:84:CYS:SG	2.61	0.40
1:S2:203:ASP:HB3	1:S2:206:ILE:HD12	2.02	0.40
1:S8:121:VAL:CG1	1:S8:135:LEU:HD22	2.52	0.40

All (2) 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:E7:25:TYR:OH	1:I3:28:ASP:OD1[1_554]	1.98	0.22
1:K3:28:ASP:N	1:O7:28:ASP:OD1[1_564]	2.19	0.01

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	445/475 (94%)	429 (96%)	15 (3%)	1 (0%)	47 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A2	445/475 (94%)	430 (97%)	13 (3%)	2 (0%)	34	48
1	A3	445/475 (94%)	429 (96%)	15 (3%)	1 (0%)	47	64
1	A4	445/475 (94%)	429 (96%)	13 (3%)	3 (1%)	22	32
1	A5	366/475 (77%)	356 (97%)	10 (3%)	0	100	100
1	A6	366/475 (77%)	355 (97%)	11 (3%)	0	100	100
1	A7	445/475 (94%)	430 (97%)	13 (3%)	2 (0%)	34	48
1	A8	445/475 (94%)	427 (96%)	17 (4%)	1 (0%)	47	64
1	C1	445/475 (94%)	427 (96%)	16 (4%)	2 (0%)	34	48
1	C2	445/475 (94%)	431 (97%)	12 (3%)	2 (0%)	34	48
1	C3	445/475 (94%)	425 (96%)	19 (4%)	1 (0%)	47	64
1	C4	445/475 (94%)	428 (96%)	14 (3%)	3 (1%)	22	32
1	C5	366/475 (77%)	354 (97%)	11 (3%)	1 (0%)	41	56
1	C6	366/475 (77%)	352 (96%)	14 (4%)	0	100	100
1	C7	445/475 (94%)	429 (96%)	15 (3%)	1 (0%)	47	64
1	C8	445/475 (94%)	429 (96%)	15 (3%)	1 (0%)	47	64
1	E1	445/475 (94%)	423 (95%)	21 (5%)	1 (0%)	47	64
1	E2	445/475 (94%)	426 (96%)	17 (4%)	2 (0%)	34	48
1	E3	445/475 (94%)	424 (95%)	20 (4%)	1 (0%)	47	64
1	E4	445/475 (94%)	420 (94%)	22 (5%)	3 (1%)	22	32
1	E5	366/475 (77%)	353 (96%)	12 (3%)	1 (0%)	41	56
1	E6	366/475 (77%)	351 (96%)	15 (4%)	0	100	100
1	E7	445/475 (94%)	425 (96%)	19 (4%)	1 (0%)	47	64
1	E8	445/475 (94%)	428 (96%)	16 (4%)	1 (0%)	47	64
1	G1	445/475 (94%)	427 (96%)	17 (4%)	1 (0%)	47	64
1	G2	445/475 (94%)	425 (96%)	18 (4%)	2 (0%)	34	48
1	G3	445/475 (94%)	432 (97%)	12 (3%)	1 (0%)	47	64
1	G4	445/475 (94%)	424 (95%)	19 (4%)	2 (0%)	34	48
1	G5	366/475 (77%)	358 (98%)	8 (2%)	0	100	100
1	G6	366/475 (77%)	353 (96%)	12 (3%)	1 (0%)	41	56
1	G7	445/475 (94%)	425 (96%)	19 (4%)	1 (0%)	47	64
1	G8	445/475 (94%)	432 (97%)	12 (3%)	1 (0%)	47	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I1	445/475 (94%)	428 (96%)	16 (4%)	1 (0%)	47	64
1	I2	445/475 (94%)	433 (97%)	12 (3%)	0	100	100
1	I3	445/475 (94%)	426 (96%)	18 (4%)	1 (0%)	47	64
1	I4	445/475 (94%)	429 (96%)	15 (3%)	1 (0%)	47	64
1	I5	366/475 (77%)	357 (98%)	9 (2%)	0	100	100
1	I6	366/475 (77%)	353 (96%)	13 (4%)	0	100	100
1	I7	445/475 (94%)	431 (97%)	12 (3%)	2 (0%)	34	48
1	I8	445/475 (94%)	428 (96%)	16 (4%)	1 (0%)	47	64
1	K1	445/475 (94%)	431 (97%)	11 (2%)	3 (1%)	22	32
1	K2	445/475 (94%)	428 (96%)	15 (3%)	2 (0%)	34	48
1	K3	445/475 (94%)	424 (95%)	19 (4%)	2 (0%)	34	48
1	K4	445/475 (94%)	425 (96%)	18 (4%)	2 (0%)	34	48
1	K5	366/475 (77%)	356 (97%)	10 (3%)	0	100	100
1	K6	366/475 (77%)	353 (96%)	13 (4%)	0	100	100
1	K7	445/475 (94%)	427 (96%)	16 (4%)	2 (0%)	34	48
1	K8	445/475 (94%)	425 (96%)	17 (4%)	3 (1%)	22	32
1	M1	445/475 (94%)	427 (96%)	17 (4%)	1 (0%)	47	64
1	M2	445/475 (94%)	430 (97%)	14 (3%)	1 (0%)	47	64
1	M3	445/475 (94%)	426 (96%)	18 (4%)	1 (0%)	47	64
1	M4	445/475 (94%)	430 (97%)	13 (3%)	2 (0%)	34	48
1	M5	366/475 (77%)	355 (97%)	11 (3%)	0	100	100
1	M6	366/475 (77%)	357 (98%)	9 (2%)	0	100	100
1	M7	445/475 (94%)	425 (96%)	18 (4%)	2 (0%)	34	48
1	M8	445/475 (94%)	427 (96%)	17 (4%)	1 (0%)	47	64
1	O1	445/475 (94%)	425 (96%)	19 (4%)	1 (0%)	47	64
1	O2	445/475 (94%)	422 (95%)	22 (5%)	1 (0%)	47	64
1	O3	445/475 (94%)	431 (97%)	13 (3%)	1 (0%)	47	64
1	O4	445/475 (94%)	428 (96%)	15 (3%)	2 (0%)	34	48
1	O5	366/475 (77%)	351 (96%)	15 (4%)	0	100	100
1	O6	366/475 (77%)	357 (98%)	8 (2%)	1 (0%)	41	56
1	O7	445/475 (94%)	425 (96%)	18 (4%)	2 (0%)	34	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O8	445/475 (94%)	428 (96%)	16 (4%)	1 (0%)	47	64
1	Q1	445/475 (94%)	419 (94%)	25 (6%)	1 (0%)	47	64
1	Q2	445/475 (94%)	423 (95%)	20 (4%)	2 (0%)	34	48
1	Q3	445/475 (94%)	422 (95%)	21 (5%)	2 (0%)	34	48
1	Q4	445/475 (94%)	421 (95%)	23 (5%)	1 (0%)	47	64
1	Q5	366/475 (77%)	351 (96%)	15 (4%)	0	100	100
1	Q6	366/475 (77%)	347 (95%)	19 (5%)	0	100	100
1	Q7	445/475 (94%)	421 (95%)	23 (5%)	1 (0%)	47	64
1	Q8	445/475 (94%)	426 (96%)	17 (4%)	2 (0%)	34	48
1	S1	445/475 (94%)	427 (96%)	17 (4%)	1 (0%)	47	64
1	S2	445/475 (94%)	429 (96%)	14 (3%)	2 (0%)	34	48
1	S3	445/475 (94%)	422 (95%)	20 (4%)	3 (1%)	22	32
1	S4	445/475 (94%)	426 (96%)	19 (4%)	0	100	100
1	S5	366/475 (77%)	347 (95%)	18 (5%)	1 (0%)	41	56
1	S6	366/475 (77%)	351 (96%)	15 (4%)	0	100	100
1	S7	445/475 (94%)	420 (94%)	24 (5%)	1 (0%)	47	64
1	S8	445/475 (94%)	422 (95%)	20 (4%)	3 (1%)	22	32
2	B1	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	B2	71/81 (88%)	66 (93%)	5 (7%)	0	100	100
2	B3	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	B4	71/81 (88%)	66 (93%)	5 (7%)	0	100	100
2	B5	36/81 (44%)	33 (92%)	3 (8%)	0	100	100
2	B6	36/81 (44%)	35 (97%)	1 (3%)	0	100	100
2	B7	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	B8	71/81 (88%)	67 (94%)	4 (6%)	0	100	100
2	D1	71/81 (88%)	70 (99%)	1 (1%)	0	100	100
2	D2	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	D3	71/81 (88%)	70 (99%)	1 (1%)	0	100	100
2	D4	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	D5	36/81 (44%)	34 (94%)	2 (6%)	0	100	100
2	D6	36/81 (44%)	33 (92%)	3 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D7	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	D8	71/81 (88%)	66 (93%)	4 (6%)	1 (1%)	11	15
2	F1	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	F2	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	F3	71/81 (88%)	64 (90%)	7 (10%)	0	100	100
2	F4	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	F5	36/81 (44%)	32 (89%)	4 (11%)	0	100	100
2	F6	36/81 (44%)	34 (94%)	2 (6%)	0	100	100
2	F7	71/81 (88%)	66 (93%)	5 (7%)	0	100	100
2	F8	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	H1	71/81 (88%)	67 (94%)	4 (6%)	0	100	100
2	H2	71/81 (88%)	65 (92%)	6 (8%)	0	100	100
2	H3	71/81 (88%)	70 (99%)	1 (1%)	0	100	100
2	H4	71/81 (88%)	66 (93%)	5 (7%)	0	100	100
2	H5	36/81 (44%)	34 (94%)	2 (6%)	0	100	100
2	H6	36/81 (44%)	34 (94%)	2 (6%)	0	100	100
2	H7	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	H8	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	J1	71/81 (88%)	67 (94%)	4 (6%)	0	100	100
2	J2	71/81 (88%)	70 (99%)	1 (1%)	0	100	100
2	J3	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	J4	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	J5	36/81 (44%)	33 (92%)	3 (8%)	0	100	100
2	J6	36/81 (44%)	34 (94%)	2 (6%)	0	100	100
2	J7	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	J8	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	L1	71/81 (88%)	66 (93%)	5 (7%)	0	100	100
2	L2	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	L3	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	L4	71/81 (88%)	63 (89%)	8 (11%)	0	100	100
2	L5	36/81 (44%)	34 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L6	36/81 (44%)	35 (97%)	1 (3%)	0	100	100
2	L7	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	L8	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	N1	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	N2	71/81 (88%)	67 (94%)	4 (6%)	0	100	100
2	N3	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	N4	71/81 (88%)	67 (94%)	4 (6%)	0	100	100
2	N5	36/81 (44%)	34 (94%)	2 (6%)	0	100	100
2	N6	36/81 (44%)	34 (94%)	2 (6%)	0	100	100
2	N7	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	N8	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	P1	71/81 (88%)	67 (94%)	4 (6%)	0	100	100
2	P2	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	P3	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	P4	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	P5	36/81 (44%)	34 (94%)	2 (6%)	0	100	100
2	P6	36/81 (44%)	35 (97%)	1 (3%)	0	100	100
2	P7	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	P8	71/81 (88%)	67 (94%)	4 (6%)	0	100	100
2	R1	71/81 (88%)	65 (92%)	6 (8%)	0	100	100
2	R2	71/81 (88%)	67 (94%)	4 (6%)	0	100	100
2	R3	71/81 (88%)	67 (94%)	4 (6%)	0	100	100
2	R4	71/81 (88%)	66 (93%)	5 (7%)	0	100	100
2	R5	36/81 (44%)	36 (100%)	0	0	100	100
2	R6	36/81 (44%)	34 (94%)	2 (6%)	0	100	100
2	R7	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	R8	71/81 (88%)	65 (92%)	6 (8%)	0	100	100
2	T1	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
2	T2	71/81 (88%)	69 (97%)	2 (3%)	0	100	100
2	T3	71/81 (88%)	70 (99%)	1 (1%)	0	100	100
2	T4	71/81 (88%)	68 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T5	36/81 (44%)	34 (94%)	2 (6%)	0	100	100
2	T6	36/81 (44%)	33 (92%)	3 (8%)	0	100	100
2	T7	71/81 (88%)	71 (100%)	0	0	100	100
2	T8	71/81 (88%)	63 (89%)	8 (11%)	0	100	100
All	All	39000/44480 (88%)	37399 (96%)	1503 (4%)	98 (0%)	41	56

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A2	62	SER
1	A7	62	SER
1	A8	62	SER
1	C3	62	SER
1	C4	62	SER
1	C7	62	SER
1	C8	62	SER
1	E3	62	SER
1	E7	62	SER
1	E8	62	SER
1	G1	62	SER
1	G4	62	SER
1	G7	62	SER
1	G8	62	SER
1	I4	62	SER
1	K4	62	SER
1	K7	124	VAL
1	K8	62	SER
1	K8	124	VAL
1	M4	62	SER
1	O1	62	SER
1	O2	62	SER
1	O7	62	SER
1	O8	62	SER
1	Q2	62	SER
1	S1	62	SER
1	S3	124	VAL
1	S5	124	VAL
1	S8	62	SER
2	D8	101	PHE
1	A1	62	SER
1	A3	62	SER

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Mol	Chain	Res	Type
1	A4	62	SER
1	C1	62	SER
1	E1	62	SER
1	E2	62	SER
1	E4	62	SER
1	G3	62	SER
1	I1	62	SER
1	I3	62	SER
1	I7	62	SER
1	I8	62	SER
1	K1	62	SER
1	K2	62	SER
1	K3	62	SER
1	K7	62	SER
1	M1	62	SER
1	M2	62	SER
1	M3	62	SER
1	M7	62	SER
1	M8	62	SER
1	O3	62	SER
1	Q3	62	SER
1	S2	62	SER
1	S3	62	SER
1	A4	77	LEU
1	C1	77	LEU
1	C2	62	SER
1	C2	77	LEU
1	G2	62	SER
1	I7	77	LEU
1	K1	77	LEU
1	K4	77	LEU
1	M4	77	LEU
1	O4	62	SER
1	Q4	62	SER
1	Q8	62	SER
1	S8	77	LEU
1	E4	124	VAL
1	G4	124	VAL
1	Q7	62	SER
1	S7	62	SER
1	C4	124	VAL
1	M7	77	LEU

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Mol	Chain	Res	Type
1	K2	124	VAL
1	O4	384	VAL
1	C4	403	GLY
1	E4	403	GLY
1	E5	124	VAL
1	G2	124	VAL
1	G6	124	VAL
1	A4	124	VAL
1	S8	124	VAL
1	O7	403	GLY
1	Q2	176	PRO
1	E2	176	PRO
1	K1	176	PRO
1	Q8	176	PRO
1	S2	176	PRO
1	A2	176	PRO
1	K8	176	PRO
1	Q3	176	PRO
1	A7	176	PRO
1	C5	176	PRO
1	K3	176	PRO
1	S3	176	PRO
1	O6	176	PRO
1	Q1	176	PRO

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	357/385 (93%)	355 (99%)	2 (1%)	86 93
1	A2	359/385 (93%)	357 (99%)	2 (1%)	86 93
1	A3	359/385 (93%)	356 (99%)	3 (1%)	81 89
1	A4	357/385 (93%)	355 (99%)	2 (1%)	86 93
1	A5	292/385 (76%)	291 (100%)	1 (0%)	92 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A6	292/385 (76%)	289 (99%)	3 (1%)	76	86
1	A7	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	A8	359/385 (93%)	359 (100%)	0	100	100
1	C1	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	C2	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	C3	359/385 (93%)	354 (99%)	5 (1%)	67	80
1	C4	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	C5	292/385 (76%)	290 (99%)	2 (1%)	84	91
1	C6	292/385 (76%)	290 (99%)	2 (1%)	84	91
1	C7	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	C8	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	E1	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	E2	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	E3	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	E4	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	E5	292/385 (76%)	291 (100%)	1 (0%)	92	96
1	E6	292/385 (76%)	289 (99%)	3 (1%)	76	86
1	E7	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	E8	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	G1	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	G2	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	G3	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	G4	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	G5	292/385 (76%)	292 (100%)	0	100	100
1	G6	292/385 (76%)	290 (99%)	2 (1%)	84	91
1	G7	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	G8	359/385 (93%)	359 (100%)	0	100	100
1	I1	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	I2	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	I3	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	I4	359/385 (93%)	357 (99%)	2 (1%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I5	292/385 (76%)	289 (99%)	3 (1%)	76	86
1	I6	292/385 (76%)	291 (100%)	1 (0%)	92	96
1	I7	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	I8	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	K1	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	K2	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	K3	359/385 (93%)	355 (99%)	4 (1%)	73	85
1	K4	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	K5	292/385 (76%)	290 (99%)	2 (1%)	84	91
1	K6	292/385 (76%)	289 (99%)	3 (1%)	76	86
1	K7	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	K8	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	M1	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	M2	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	M3	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	M4	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	M5	292/385 (76%)	289 (99%)	3 (1%)	76	86
1	M6	292/385 (76%)	289 (99%)	3 (1%)	76	86
1	M7	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	M8	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	O1	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	O2	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	O3	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	O4	359/385 (93%)	359 (100%)	0	100	100
1	O5	292/385 (76%)	290 (99%)	2 (1%)	84	91
1	O6	292/385 (76%)	290 (99%)	2 (1%)	84	91
1	O7	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	O8	359/385 (93%)	359 (100%)	0	100	100
1	Q1	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	Q2	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	Q3	359/385 (93%)	357 (99%)	2 (1%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q4	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	Q5	292/385 (76%)	292 (100%)	0	100	100
1	Q6	292/385 (76%)	290 (99%)	2 (1%)	84	91
1	Q7	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	Q8	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	S1	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	S2	359/385 (93%)	356 (99%)	3 (1%)	81	89
1	S3	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	S4	359/385 (93%)	358 (100%)	1 (0%)	92	96
1	S5	292/385 (76%)	290 (99%)	2 (1%)	84	91
1	S6	292/385 (76%)	290 (99%)	2 (1%)	84	91
1	S7	359/385 (93%)	357 (99%)	2 (1%)	86	93
1	S8	359/385 (93%)	358 (100%)	1 (0%)	92	96
2	B1	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	B2	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	B3	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	B4	54/60 (90%)	54 (100%)	0	100	100
2	B5	27/60 (45%)	26 (96%)	1 (4%)	34	51
2	B6	27/60 (45%)	26 (96%)	1 (4%)	34	51
2	B7	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	B8	54/60 (90%)	54 (100%)	0	100	100
2	D1	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	D2	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	D3	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	D4	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	D5	27/60 (45%)	27 (100%)	0	100	100
2	D6	27/60 (45%)	27 (100%)	0	100	100
2	D7	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	D8	54/60 (90%)	54 (100%)	0	100	100
2	F1	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	F2	54/60 (90%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F3	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	F4	54/60 (90%)	54 (100%)	0	100	100
2	F5	27/60 (45%)	27 (100%)	0	100	100
2	F6	27/60 (45%)	26 (96%)	1 (4%)	34	51
2	F7	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	F8	54/60 (90%)	54 (100%)	0	100	100
2	H1	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	H2	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	H3	54/60 (90%)	54 (100%)	0	100	100
2	H4	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	H5	27/60 (45%)	27 (100%)	0	100	100
2	H6	27/60 (45%)	26 (96%)	1 (4%)	34	51
2	H7	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	H8	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	J1	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	J2	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	J3	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	J4	54/60 (90%)	54 (100%)	0	100	100
2	J5	27/60 (45%)	27 (100%)	0	100	100
2	J6	27/60 (45%)	26 (96%)	1 (4%)	34	51
2	J7	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	J8	54/60 (90%)	54 (100%)	0	100	100
2	L1	54/60 (90%)	54 (100%)	0	100	100
2	L2	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	L3	54/60 (90%)	54 (100%)	0	100	100
2	L4	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	L5	27/60 (45%)	25 (93%)	2 (7%)	13	21
2	L6	27/60 (45%)	27 (100%)	0	100	100
2	L7	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	L8	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	N1	54/60 (90%)	52 (96%)	2 (4%)	34	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N2	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	N3	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	N4	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	N5	27/60 (45%)	27 (100%)	0	100	100
2	N6	27/60 (45%)	27 (100%)	0	100	100
2	N7	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	N8	54/60 (90%)	54 (100%)	0	100	100
2	P1	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	P2	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	P3	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	P4	54/60 (90%)	54 (100%)	0	100	100
2	P5	27/60 (45%)	26 (96%)	1 (4%)	34	51
2	P6	27/60 (45%)	26 (96%)	1 (4%)	34	51
2	P7	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	P8	54/60 (90%)	54 (100%)	0	100	100
2	R1	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	R2	54/60 (90%)	54 (100%)	0	100	100
2	R3	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	R4	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	R5	27/60 (45%)	25 (93%)	2 (7%)	13	21
2	R6	27/60 (45%)	27 (100%)	0	100	100
2	R7	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	R8	54/60 (90%)	52 (96%)	2 (4%)	34	51
2	T1	54/60 (90%)	51 (94%)	3 (6%)	21	32
2	T2	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	T3	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	T4	54/60 (90%)	54 (100%)	0	100	100
2	T5	27/60 (45%)	26 (96%)	1 (4%)	34	51
2	T6	27/60 (45%)	26 (96%)	1 (4%)	34	51
2	T7	54/60 (90%)	53 (98%)	1 (2%)	57	74
2	T8	54/60 (90%)	51 (94%)	3 (6%)	21	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	31156/35600 (88%)	30927 (99%)	229 (1%)	84	91

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	223	ASP
1	A1	239	TYR
1	A2	200	THR
1	A2	239	TYR
1	A3	96	GLN
1	A3	239	TYR
1	A3	438	MET
1	A4	124	VAL
1	A4	239	TYR
1	A5	239	TYR
1	A6	239	TYR
1	A6	338	ASP
1	A6	447	GLU
1	A7	239	TYR
1	C1	239	TYR
1	C1	338	ASP
1	C1	450	ARG
1	C2	239	TYR
1	C2	338	ASP
1	C2	438	MET
1	C3	51	GLU
1	C3	172	CYS
1	C3	181	SER
1	C3	223	ASP
1	C3	239	TYR
1	C4	239	TYR
1	C4	338	ASP
1	C4	450	ARG
1	C5	223	ASP
1	C5	239	TYR
1	C6	239	TYR
1	C6	379	SER
1	C7	51	GLU
1	C7	65	THR
1	C7	239	TYR
1	C8	356	GLN
1	E1	239	TYR

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Mol	Chain	Res	Type
1	E2	239	TYR
1	E2	438	MET
1	E3	239	TYR
1	E4	239	TYR
1	E5	223	ASP
1	E6	200	THR
1	E6	239	TYR
1	E6	356	GLN
1	E7	239	TYR
1	E7	356	GLN
1	E8	239	TYR
1	G1	223	ASP
1	G1	239	TYR
1	G1	438	MET
1	G2	239	TYR
1	G3	200	THR
1	G4	83	CYS
1	G4	239	TYR
1	G6	239	TYR
1	G6	438	MET
1	G7	65	THR
1	G7	239	TYR
1	I1	239	TYR
1	I1	410	PRO
1	I2	239	TYR
1	I3	223	ASP
1	I3	239	TYR
1	I4	239	TYR
1	I4	338	ASP
1	I5	223	ASP
1	I5	239	TYR
1	I5	450	ARG
1	I6	239	TYR
1	I7	239	TYR
1	I8	223	ASP
1	I8	239	TYR
1	I8	438	MET
1	K1	119	SER
1	K1	223	ASP
1	K1	239	TYR
1	K2	33	ASP
1	K2	200	THR

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Mol	Chain	Res	Type
1	K2	239	TYR
1	K3	239	TYR
1	K3	356	GLN
1	K3	450	ARG
1	K3	451	TRP
1	K4	239	TYR
1	K5	239	TYR
1	K5	438	MET
1	K6	239	TYR
1	K6	338	ASP
1	K6	438	MET
1	K7	239	TYR
1	K7	438	MET
1	K8	239	TYR
1	K8	451	TRP
1	M1	94	ASP
1	M2	239	TYR
1	M2	356	GLN
1	M3	239	TYR
1	M3	438	MET
1	M4	200	THR
1	M4	223	ASP
1	M4	239	TYR
1	M5	239	TYR
1	M5	338	ASP
1	M5	438	MET
1	M6	239	TYR
1	M6	438	MET
1	M6	450	ARG
1	M7	450	ARG
1	M8	239	TYR
1	O1	223	ASP
1	O1	239	TYR
1	O2	239	TYR
1	O3	239	TYR
1	O3	438	MET
1	O3	450	ARG
1	O5	119	SER
1	O5	239	TYR
1	O6	239	TYR
1	O6	356	GLN
1	O7	239	TYR

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Mol	Chain	Res	Type
1	O7	302	ASP
1	Q1	51	GLU
1	Q1	200	THR
1	Q1	239	TYR
1	Q2	239	TYR
1	Q3	181	SER
1	Q3	239	TYR
1	Q4	239	TYR
1	Q6	239	TYR
1	Q6	356	GLN
1	Q7	83	CYS
1	Q7	200	THR
1	Q8	119	SER
1	Q8	239	TYR
1	Q8	356	GLN
1	S1	239	TYR
1	S1	338	ASP
1	S2	223	ASP
1	S2	239	TYR
1	S2	438	MET
1	S3	239	TYR
1	S4	223	ASP
1	S5	106	ASP
1	S5	239	TYR
1	S6	239	TYR
1	S6	356	GLN
1	S7	239	TYR
1	S7	450	ARG
1	S8	223	ASP
2	B1	67	PRO
2	B2	70	LEU
2	B3	70	LEU
2	B5	120	ASP
2	B6	135	ASP
2	B7	120	ASP
2	D1	94	ILE
2	D2	70	LEU
2	D3	135	ASP
2	D4	95	ASP
2	D4	135	ASP
2	D7	98	ASN
2	F1	135	ASP

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Mol	Chain	Res	Type
2	F3	70	LEU
2	F3	74	ASN
2	F6	120	ASP
2	F7	95	ASP
2	F7	135	ASP
2	H1	74	ASN
2	H1	120	ASP
2	H2	70	LEU
2	H2	120	ASP
2	H4	135	ASP
2	H6	120	ASP
2	H7	70	LEU
2	H8	74	ASN
2	J1	70	LEU
2	J1	135	ASP
2	J2	135	ASP
2	J3	70	LEU
2	J6	135	ASP
2	J7	70	LEU
2	J7	136	GLU
2	L2	110	CYS
2	L4	135	ASP
2	L5	120	ASP
2	L5	135	ASP
2	L7	74	ASN
2	L8	74	ASN
2	L8	93	LEU
2	N1	70	LEU
2	N1	93	LEU
2	N2	70	LEU
2	N2	120	ASP
2	N3	70	LEU
2	N4	135	ASP
2	N7	110	CYS
2	N7	135	ASP
2	P1	95	ASP
2	P1	136	GLU
2	P2	70	LEU
2	P2	135	ASP
2	P3	120	ASP
2	P5	135	ASP
2	P6	136	GLU

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Mol	Chain	Res	Type
2	P7	74	ASN
2	P7	136	GLU
2	R1	74	ASN
2	R1	95	ASP
2	R3	70	LEU
2	R3	120	ASP
2	R4	86	CYS
2	R4	100	GLN
2	R5	120	ASP
2	R5	135	ASP
2	R7	74	ASN
2	R8	97	PHE
2	R8	120	ASP
2	T1	70	LEU
2	T1	131	LEU
2	T1	135	ASP
2	T2	74	ASN
2	T3	135	ASP
2	T5	136	GLU
2	T6	136	GLU
2	T7	70	LEU
2	T8	86	CYS
2	T8	93	LEU
2	T8	102	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (313) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	115	ASN
1	A1	149	GLN
1	A1	386	HIS
1	A1	401	GLN
1	A2	115	ASN
1	A2	149	GLN
1	A2	153	HIS
1	A2	207	ASN
1	A2	401	GLN
1	A2	420	ASN
1	A3	149	GLN
1	A3	153	HIS
1	A3	401	GLN
1	A3	420	ASN

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Mol	Chain	Res	Type
1	A4	149	GLN
1	A4	401	GLN
1	A4	420	ASN
1	A5	149	GLN
1	A5	277	ASN
1	A5	420	ASN
1	A6	149	GLN
1	A6	153	HIS
1	A6	401	GLN
1	A6	420	ASN
1	A7	401	GLN
1	A7	420	ASN
1	A8	149	GLN
1	A8	153	HIS
1	C1	115	ASN
1	C1	149	GLN
1	C1	153	HIS
1	C1	277	ASN
1	C1	401	GLN
1	C1	420	ASN
1	C2	149	GLN
1	C2	153	HIS
1	C2	207	ASN
1	C2	401	GLN
1	C2	420	ASN
1	C3	149	GLN
1	C3	277	ASN
1	C3	310	HIS
1	C3	401	GLN
1	C3	420	ASN
1	C4	115	ASN
1	C4	149	GLN
1	C4	153	HIS
1	C4	401	GLN
1	C4	420	ASN
1	C5	115	ASN
1	C5	149	GLN
1	C5	153	HIS
1	C5	401	GLN
1	C5	420	ASN
1	C6	149	GLN
1	C6	386	HIS

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Mol	Chain	Res	Type
1	C6	401	GLN
1	C6	420	ASN
1	C7	149	GLN
1	C7	153	HIS
1	C7	207	ASN
1	C7	401	GLN
1	C7	420	ASN
1	C8	115	ASN
1	C8	149	GLN
1	C8	401	GLN
1	C8	420	ASN
1	E1	149	GLN
1	E1	420	ASN
1	E2	115	ASN
1	E2	149	GLN
1	E2	356	GLN
1	E2	401	GLN
1	E2	420	ASN
1	E3	149	GLN
1	E3	356	GLN
1	E3	401	GLN
1	E3	420	ASN
1	E4	149	GLN
1	E4	401	GLN
1	E4	420	ASN
1	E5	115	ASN
1	E5	149	GLN
1	E5	401	GLN
1	E5	420	ASN
1	E6	149	GLN
1	E6	153	HIS
1	E6	277	ASN
1	E6	401	GLN
1	E6	420	ASN
1	E7	115	ASN
1	E7	153	HIS
1	E7	356	GLN
1	E7	401	GLN
1	E7	420	ASN
1	E8	149	GLN
1	E8	153	HIS
1	E8	401	GLN

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Mol	Chain	Res	Type
1	G1	149	GLN
1	G1	153	HIS
1	G1	401	GLN
1	G1	420	ASN
1	G2	115	ASN
1	G2	149	GLN
1	G2	153	HIS
1	G2	356	GLN
1	G2	401	GLN
1	G2	420	ASN
1	G3	420	ASN
1	G4	149	GLN
1	G4	401	GLN
1	G4	420	ASN
1	G5	149	GLN
1	G5	153	HIS
1	G5	386	HIS
1	G5	401	GLN
1	G5	420	ASN
1	G6	115	ASN
1	G6	149	GLN
1	G6	153	HIS
1	G6	401	GLN
1	G6	420	ASN
1	G7	149	GLN
1	G7	401	GLN
1	G7	420	ASN
1	G8	149	GLN
1	G8	153	HIS
1	G8	420	ASN
1	I1	115	ASN
1	I1	149	GLN
1	I1	153	HIS
1	I1	401	GLN
1	I1	420	ASN
1	I2	115	ASN
1	I2	149	GLN
1	I2	401	GLN
1	I2	420	ASN
1	I3	115	ASN
1	I3	149	GLN
1	I3	153	HIS

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Mol	Chain	Res	Type
1	I3	401	GLN
1	I3	420	ASN
1	I4	149	GLN
1	I4	207	ASN
1	I4	401	GLN
1	I4	420	ASN
1	I5	115	ASN
1	I5	149	GLN
1	I5	401	GLN
1	I5	420	ASN
1	I6	115	ASN
1	I6	149	GLN
1	I6	153	HIS
1	I6	401	GLN
1	I6	420	ASN
1	I7	149	GLN
1	I7	153	HIS
1	I7	420	ASN
1	I8	149	GLN
1	I8	153	HIS
1	I8	277	ASN
1	I8	386	HIS
1	I8	401	GLN
1	I8	420	ASN
1	K1	115	ASN
1	K1	149	GLN
1	K1	401	GLN
1	K1	420	ASN
1	K2	115	ASN
1	K2	149	GLN
1	K2	356	GLN
1	K2	401	GLN
1	K2	420	ASN
1	K3	149	GLN
1	K3	153	HIS
1	K3	401	GLN
1	K4	149	GLN
1	K4	212	GLN
1	K4	277	ASN
1	K4	401	GLN
1	K4	420	ASN
1	K5	115	ASN

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Mol	Chain	Res	Type
1	K5	149	GLN
1	K5	277	ASN
1	K5	401	GLN
1	K5	420	ASN
1	K6	115	ASN
1	K6	401	GLN
1	K6	420	ASN
1	K7	149	GLN
1	K7	401	GLN
1	K8	149	GLN
1	K8	153	HIS
1	K8	401	GLN
1	K8	420	ASN
1	M1	115	ASN
1	M1	149	GLN
1	M1	401	GLN
1	M1	420	ASN
1	M2	115	ASN
1	M2	149	GLN
1	M2	401	GLN
1	M2	420	ASN
1	M3	115	ASN
1	M3	149	GLN
1	M3	420	ASN
1	M4	149	GLN
1	M4	401	GLN
1	M4	420	ASN
1	M5	149	GLN
1	M5	153	HIS
1	M5	401	GLN
1	M5	420	ASN
1	M6	149	GLN
1	M6	153	HIS
1	M6	401	GLN
1	M6	420	ASN
1	M7	149	GLN
1	M7	153	HIS
1	M7	401	GLN
1	M7	420	ASN
1	M8	149	GLN
1	M8	153	HIS
1	M8	401	GLN

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Mol	Chain	Res	Type
1	M8	420	ASN
1	O1	115	ASN
1	O1	149	GLN
1	O1	153	HIS
1	O1	401	GLN
1	O1	420	ASN
1	O2	115	ASN
1	O2	149	GLN
1	O2	401	GLN
1	O2	420	ASN
1	O3	149	GLN
1	O3	153	HIS
1	O3	420	ASN
1	O4	149	GLN
1	O4	153	HIS
1	O4	277	ASN
1	O4	420	ASN
1	O5	356	GLN
1	O5	401	GLN
1	O5	420	ASN
1	O6	149	GLN
1	O6	401	GLN
1	O6	420	ASN
1	O7	115	ASN
1	O7	149	GLN
1	O7	153	HIS
1	O7	420	ASN
1	O8	149	GLN
1	O8	277	ASN
1	O8	420	ASN
1	Q1	115	ASN
1	Q1	149	GLN
1	Q1	277	ASN
1	Q1	401	GLN
1	Q1	420	ASN
1	Q2	149	GLN
1	Q2	153	HIS
1	Q2	207	ASN
1	Q2	401	GLN
1	Q3	115	ASN
1	Q3	149	GLN
1	Q3	401	GLN

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Mol	Chain	Res	Type
1	Q3	420	ASN
1	Q4	149	GLN
1	Q5	149	GLN
1	Q5	401	GLN
1	Q5	420	ASN
1	Q6	401	GLN
1	Q6	420	ASN
1	Q7	356	GLN
1	Q7	420	ASN
1	Q8	149	GLN
1	Q8	153	HIS
1	Q8	356	GLN
1	Q8	420	ASN
1	S1	149	GLN
1	S1	401	GLN
1	S1	420	ASN
1	S2	149	GLN
1	S2	153	HIS
1	S2	401	GLN
1	S2	420	ASN
1	S3	115	ASN
1	S3	149	GLN
1	S3	153	HIS
1	S3	356	GLN
1	S3	401	GLN
1	S3	420	ASN
1	S4	149	GLN
1	S4	153	HIS
1	S4	207	ASN
1	S4	420	ASN
1	S5	149	GLN
1	S5	401	GLN
1	S5	420	ASN
1	S6	149	GLN
1	S6	153	HIS
1	S6	420	ASN
1	S7	115	ASN
1	S7	401	GLN
1	S7	420	ASN
1	S7	429	GLN
1	S8	149	GLN
1	S8	153	HIS

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Mol	Chain	Res	Type
1	S8	304	GLN
1	S8	420	ASN
2	N3	74	ASN
2	P3	96	HIS
2	R1	74	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 ⓘ

Of 160 ligands modelled in this entry, 160 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A1	447/475 (94%)	-0.43	2 (0%)	92	93	23, 42, 75, 107	0
1	A2	447/475 (94%)	-0.46	3 (0%)	87	86	24, 39, 66, 119	0
1	A3	447/475 (94%)	-0.44	4 (0%)	84	83	19, 33, 69, 114	0
1	A4	447/475 (94%)	-0.51	3 (0%)	87	86	20, 35, 66, 104	0
1	A5	367/475 (77%)	-0.52	1 (0%)	94	95	20, 32, 53, 104	0
1	A6	367/475 (77%)	-0.48	2 (0%)	91	90	21, 36, 57, 104	0
1	A7	447/475 (94%)	-0.31	10 (2%)	62	58	22, 42, 89, 120	0
1	A8	447/475 (94%)	-0.33	7 (1%)	72	69	22, 44, 87, 132	0
1	C1	447/475 (94%)	-0.50	1 (0%)	95	96	20, 31, 60, 103	0
1	C2	447/475 (94%)	-0.42	2 (0%)	92	93	22, 37, 67, 115	0
1	C3	447/475 (94%)	-0.35	12 (2%)	54	50	23, 41, 84, 125	0
1	C4	447/475 (94%)	-0.31	8 (1%)	68	66	24, 45, 89, 140	0
1	C5	367/475 (77%)	-0.42	5 (1%)	75	73	26, 44, 73, 114	0
1	C6	367/475 (77%)	-0.43	2 (0%)	91	90	27, 42, 63, 109	0
1	C7	447/475 (94%)	-0.32	12 (2%)	54	50	21, 39, 81, 121	0
1	C8	447/475 (94%)	-0.39	4 (0%)	84	83	20, 39, 74, 118	0
1	E1	447/475 (94%)	-0.15	7 (1%)	72	69	32, 54, 94, 123	0
1	E2	447/475 (94%)	-0.14	9 (2%)	65	61	35, 52, 88, 135	0
1	E3	447/475 (94%)	0.15	21 (4%)	31	27	39, 71, 114, 146	0
1	E4	447/475 (94%)	0.22	20 (4%)	33	30	40, 79, 119, 161	0
1	E5	367/475 (77%)	0.33	20 (5%)	25	22	38, 74, 111, 148	0
1	E6	367/475 (77%)	-0.06	7 (1%)	66	64	37, 62, 94, 139	0
1	E7	447/475 (94%)	-0.05	11 (2%)	57	53	32, 53, 97, 130	0
1	E8	447/475 (94%)	-0.12	6 (1%)	77	75	31, 58, 100, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	G1	447/475 (94%)	-0.22	5 (1%)	80	78	30, 49, 85, 135	0
1	G2	447/475 (94%)	-0.06	10 (2%)	62	58	34, 55, 92, 127	0
1	G3	447/475 (94%)	0.15	19 (4%)	35	31	34, 61, 106, 138	0
1	G4	447/475 (94%)	-0.02	20 (4%)	33	30	34, 56, 107, 146	0
1	G5	367/475 (77%)	-0.36	2 (0%)	91	90	27, 46, 74, 115	0
1	G6	367/475 (77%)	-0.45	3 (0%)	86	85	24, 39, 63, 116	0
1	G7	447/475 (94%)	-0.41	9 (2%)	65	61	24, 39, 78, 132	0
1	G8	447/475 (94%)	-0.32	8 (1%)	68	66	24, 43, 81, 124	0
1	I1	447/475 (94%)	-0.46	8 (1%)	68	66	19, 36, 70, 112	0
1	I2	447/475 (94%)	-0.42	3 (0%)	87	86	26, 42, 85, 124	0
1	I3	447/475 (94%)	-0.38	8 (1%)	68	66	24, 42, 83, 115	0
1	I4	447/475 (94%)	-0.34	9 (2%)	65	61	25, 44, 82, 133	0
1	I5	367/475 (77%)	-0.50	3 (0%)	86	85	22, 35, 58, 101	0
1	I6	367/475 (77%)	-0.43	2 (0%)	91	90	22, 38, 64, 114	0
1	I7	447/475 (94%)	-0.42	6 (1%)	77	75	21, 35, 75, 112	0
1	I8	447/475 (94%)	-0.42	3 (0%)	87	86	23, 39, 72, 123	0
1	K1	447/475 (94%)	-0.03	11 (2%)	57	53	38, 61, 101, 144	0
1	K2	447/475 (94%)	-0.06	10 (2%)	62	58	38, 58, 95, 135	0
1	K3	447/475 (94%)	-0.01	12 (2%)	54	50	26, 55, 99, 147	0
1	K4	447/475 (94%)	-0.14	7 (1%)	72	69	30, 54, 93, 123	0
1	K5	367/475 (77%)	-0.48	0	100	100	25, 36, 58, 101	0
1	K6	367/475 (77%)	-0.49	4 (1%)	80	78	26, 39, 64, 104	0
1	K7	447/475 (94%)	-0.20	12 (2%)	54	50	30, 54, 92, 135	0
1	K8	447/475 (94%)	-0.13	13 (2%)	51	48	31, 58, 105, 138	0
1	M1	447/475 (94%)	-0.31	13 (2%)	51	48	29, 46, 83, 121	0
1	M2	447/475 (94%)	-0.25	11 (2%)	57	53	31, 51, 89, 134	0
1	M3	447/475 (94%)	-0.29	11 (2%)	57	53	23, 44, 84, 125	0
1	M4	447/475 (94%)	-0.34	4 (0%)	84	83	27, 45, 81, 117	0
1	M5	367/475 (77%)	-0.56	1 (0%)	94	95	22, 31, 52, 83	0
1	M6	367/475 (77%)	-0.49	1 (0%)	94	95	21, 35, 60, 98	0
1	M7	447/475 (94%)	-0.42	7 (1%)	72	69	25, 39, 79, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	M8	447/475 (94%)	-0.35	7 (1%)	72	69	23, 43, 84, 131	0
1	O1	447/475 (94%)	-0.33	9 (2%)	65	61	25, 46, 91, 121	0
1	O2	447/475 (94%)	-0.38	8 (1%)	68	66	22, 42, 79, 122	0
1	O3	447/475 (94%)	-0.42	5 (1%)	80	78	23, 41, 80, 113	0
1	O4	447/475 (94%)	-0.30	6 (1%)	77	75	28, 49, 87, 125	0
1	O5	367/475 (77%)	-0.17	4 (1%)	80	78	33, 53, 80, 122	0
1	O6	367/475 (77%)	0.19	11 (2%)	50	46	40, 62, 96, 125	0
1	O7	447/475 (94%)	0.23	20 (4%)	33	30	33, 62, 103, 141	0
1	O8	447/475 (94%)	0.06	13 (2%)	51	48	33, 59, 100, 139	0
1	Q1	447/475 (94%)	0.47	29 (6%)	18	16	43, 79, 119, 147	0
1	Q2	447/475 (94%)	0.06	12 (2%)	54	50	35, 56, 99, 142	0
1	Q3	447/475 (94%)	-0.09	8 (1%)	68	66	33, 52, 90, 132	0
1	Q4	447/475 (94%)	0.17	13 (2%)	51	48	33, 66, 107, 138	0
1	Q5	367/475 (77%)	0.16	7 (1%)	66	64	37, 66, 98, 137	0
1	Q6	367/475 (77%)	0.20	15 (4%)	37	33	43, 67, 101, 138	0
1	Q7	447/475 (94%)	0.47	37 (8%)	11	9	49, 79, 124, 147	0
1	Q8	447/475 (94%)	0.42	22 (4%)	29	25	47, 82, 127, 182	0
1	S1	447/475 (94%)	-0.37	5 (1%)	80	78	23, 43, 80, 112	0
1	S2	447/475 (94%)	-0.39	6 (1%)	77	75	24, 44, 81, 110	0
1	S3	447/475 (94%)	-0.32	7 (1%)	72	69	28, 49, 88, 121	0
1	S4	447/475 (94%)	-0.19	12 (2%)	54	50	30, 55, 97, 140	0
1	S5	367/475 (77%)	-0.10	8 (2%)	62	58	40, 63, 92, 130	0
1	S6	367/475 (77%)	0.21	14 (3%)	40	36	44, 72, 103, 141	0
1	S7	447/475 (94%)	0.35	34 (7%)	13	10	29, 69, 120, 157	0
1	S8	447/475 (94%)	0.17	17 (3%)	40	36	35, 70, 104, 147	0
2	B1	73/81 (90%)	0.03	3 (4%)	37	33	45, 73, 102, 112	0
2	B2	73/81 (90%)	-0.40	0	100	100	41, 57, 80, 86	0
2	B3	73/81 (90%)	-0.22	1 (1%)	75	73	32, 54, 79, 100	0
2	B4	73/81 (90%)	0.10	5 (6%)	17	14	45, 62, 99, 134	0
2	B5	37/81 (45%)	-0.37	0	100	100	35, 44, 65, 74	0
2	B6	37/81 (45%)	-0.34	0	100	100	39, 51, 71, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	B7	73/81 (90%)	0.23	6 (8%) 11 9	51, 76, 106, 122	0
2	B8	73/81 (90%)	0.23	4 (5%) 25 22	52, 71, 102, 139	0
2	D1	73/81 (90%)	-0.39	0 100 100	34, 46, 72, 86	0
2	D2	73/81 (90%)	-0.32	0 100 100	36, 56, 75, 81	0
2	D3	73/81 (90%)	0.26	1 (1%) 75 73	52, 72, 99, 112	0
2	D4	73/81 (90%)	0.24	6 (8%) 11 9	53, 73, 104, 132	0
2	D5	37/81 (45%)	-0.04	1 (2%) 54 50	50, 66, 97, 108	0
2	D6	37/81 (45%)	-0.18	0 100 100	46, 58, 76, 82	0
2	D7	73/81 (90%)	-0.13	2 (2%) 54 50	41, 60, 89, 114	0
2	D8	73/81 (90%)	0.48	5 (6%) 17 14	54, 71, 99, 142	0
2	F1	73/81 (90%)	0.19	2 (2%) 54 50	55, 76, 101, 117	0
2	F2	73/81 (90%)	0.21	1 (1%) 75 73	51, 80, 97, 104	0
2	F3	73/81 (90%)	1.19	21 (28%) 0 0	81, 116, 142, 152	0
2	F4	73/81 (90%)	0.61	9 (12%) 4 2	73, 99, 130, 154	0
2	F5	37/81 (45%)	1.43	12 (32%) 0 0	78, 107, 126, 134	0
2	F6	37/81 (45%)	0.45	1 (2%) 54 50	75, 97, 113, 116	0
2	F7	73/81 (90%)	0.24	1 (1%) 75 73	66, 86, 111, 137	0
2	F8	73/81 (90%)	0.45	4 (5%) 25 22	64, 80, 125, 159	0
2	H1	73/81 (90%)	0.10	0 100 100	52, 70, 97, 119	0
2	H2	73/81 (90%)	0.33	5 (6%) 17 14	58, 80, 101, 107	0
2	H3	73/81 (90%)	1.28	17 (23%) 0 0	71, 109, 129, 142	0
2	H4	73/81 (90%)	0.63	7 (9%) 8 6	63, 82, 120, 140	0
2	H5	37/81 (45%)	0.02	1 (2%) 54 50	54, 67, 103, 108	0
2	H6	37/81 (45%)	-0.05	1 (2%) 54 50	48, 56, 74, 87	0
2	H7	73/81 (90%)	-0.17	2 (2%) 54 50	44, 62, 87, 117	0
2	H8	73/81 (90%)	0.08	4 (5%) 25 22	45, 64, 97, 127	0
2	J1	73/81 (90%)	-0.25	1 (1%) 75 73	39, 53, 79, 94	0
2	J2	73/81 (90%)	0.18	4 (5%) 25 22	49, 67, 101, 111	0
2	J3	73/81 (90%)	0.36	8 (10%) 5 3	46, 74, 104, 132	0
2	J4	73/81 (90%)	0.04	4 (5%) 25 22	43, 64, 111, 135	0
2	J5	37/81 (45%)	-0.08	1 (2%) 54 50	40, 53, 92, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	J6	37/81 (45%)	-0.21	0	100	100	47, 60, 83, 86	0
2	J7	73/81 (90%)	-0.11	1 (1%)	75	73	36, 59, 91, 103	0
2	J8	73/81 (90%)	0.03	4 (5%)	25	22	45, 59, 96, 127	0
2	L1	73/81 (90%)	0.69	8 (10%)	5	3	70, 100, 128, 129	0
2	L2	73/81 (90%)	-0.02	1 (1%)	75	73	57, 74, 94, 105	0
2	L3	73/81 (90%)	0.39	5 (6%)	17	14	60, 83, 104, 128	0
2	L4	73/81 (90%)	0.58	8 (10%)	5	3	74, 90, 120, 155	0
2	L5	37/81 (45%)	-0.26	0	100	100	42, 52, 68, 77	0
2	L6	37/81 (45%)	-0.16	0	100	100	43, 56, 78, 87	0
2	L7	73/81 (90%)	0.50	4 (5%)	25	22	66, 92, 118, 123	0
2	L8	73/81 (90%)	0.54	9 (12%)	4	2	66, 82, 110, 140	0
2	N1	73/81 (90%)	0.31	3 (4%)	37	33	51, 82, 110, 115	0
2	N2	73/81 (90%)	0.09	1 (1%)	75	73	59, 79, 105, 117	0
2	N3	73/81 (90%)	0.08	1 (1%)	75	73	48, 71, 101, 114	0
2	N4	73/81 (90%)	0.46	5 (6%)	17	14	61, 80, 109, 154	0
2	N5	37/81 (45%)	-0.32	0	100	100	35, 42, 61, 70	0
2	N6	37/81 (45%)	-0.15	0	100	100	39, 56, 88, 98	0
2	N7	73/81 (90%)	0.13	5 (6%)	17	14	42, 70, 108, 123	0
2	N8	73/81 (90%)	0.09	4 (5%)	25	22	47, 61, 91, 136	0
2	P1	73/81 (90%)	0.13	3 (4%)	37	33	46, 72, 100, 103	0
2	P2	73/81 (90%)	0.05	2 (2%)	54	50	51, 74, 102, 120	0
2	P3	73/81 (90%)	0.05	2 (2%)	54	50	47, 73, 100, 115	0
2	P4	73/81 (90%)	0.00	5 (6%)	17	14	49, 63, 101, 128	0
2	P5	37/81 (45%)	0.38	1 (2%)	54	50	58, 69, 91, 114	0
2	P6	37/81 (45%)	1.15	9 (24%)	0	0	72, 93, 121, 124	0
2	P7	73/81 (90%)	0.78	10 (13%)	3	1	65, 95, 135, 142	0
2	P8	73/81 (90%)	0.75	6 (8%)	11	9	68, 86, 124, 160	0
2	R1	73/81 (90%)	1.81	30 (41%)	0	0	90, 121, 147, 161	0
2	R2	73/81 (90%)	0.27	5 (6%)	17	14	55, 76, 129, 145	0
2	R3	73/81 (90%)	0.49	7 (9%)	8	6	66, 88, 126, 149	0
2	R4	73/81 (90%)	0.51	6 (8%)	11	9	64, 84, 119, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
2	R5	37/81 (45%)	0.69	3 (8%)	12	9	72, 83, 105, 114	0
2	R6	37/81 (45%)	1.06	9 (24%)	0	0	80, 107, 127, 131	0
2	R7	73/81 (90%)	1.84	27 (36%)	0	0	95, 143, 165, 173	0
2	R8	73/81 (90%)	1.00	9 (12%)	4	2	85, 107, 126, 150	0
2	T1	73/81 (90%)	-0.17	1 (1%)	75	73	40, 56, 84, 95	0
2	T2	73/81 (90%)	0.23	3 (4%)	37	33	51, 80, 107, 114	0
2	T3	73/81 (90%)	0.53	6 (8%)	11	9	59, 85, 116, 138	0
2	T4	73/81 (90%)	0.23	5 (6%)	17	14	53, 69, 101, 141	0
2	T5	37/81 (45%)	0.56	3 (8%)	12	9	76, 96, 122, 123	0
2	T6	37/81 (45%)	0.87	7 (18%)	1	1	81, 98, 124, 128	0
2	T7	73/81 (90%)	0.64	6 (8%)	11	9	70, 96, 121, 136	0
2	T8	73/81 (90%)	1.56	19 (26%)	0	0	77, 110, 147, 180	0
All	All	39280/44480 (88%)	-0.13	1126 (2%)	51	48	19, 52, 103, 182	0

All (1126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T8	65	THR	13.8
1	Q8	20	TYR	11.7
2	T8	66	LYS	11.4
1	S7	335	LEU	11.1
1	E4	20	TYR	11.0
1	G4	20	TYR	11.0
2	F8	64	GLY	10.9
1	K1	94	ASP	10.3
2	D8	65	THR	10.0
1	K3	93	GLU	9.8
2	T4	64	GLY	9.6
2	R8	64	GLY	9.4
1	C4	20	TYR	9.3
1	Q1	47	GLY	8.9
1	K1	335	LEU	8.8
2	J4	67	PRO	8.7
1	G7	93	GLU	8.6
2	R4	64	GLY	8.6
2	T3	64	GLY	8.6
1	Q3	335	LEU	8.6
1	E2	93	GLU	8.5

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Mol	Chain	Res	Type	RSRZ
2	J3	64	GLY	8.5
2	B8	64	GLY	8.4
2	B4	65	THR	8.4
1	E4	335	LEU	8.1
2	L4	66	LYS	8.1
1	E3	337	GLY	8.0
2	N4	64	GLY	8.0
1	Q6	333	GLY	7.9
2	D4	67	PRO	7.9
2	H8	64	GLY	7.9
2	H4	64	GLY	7.7
1	K8	20	TYR	7.7
1	G4	21	ARG	7.7
1	E5	337	GLY	7.5
1	O2	93	GLU	7.4
2	J7	64	GLY	7.4
2	T8	64	GLY	7.3
1	O6	333	GLY	7.3
2	P8	67	PRO	7.3
1	S8	93	GLU	7.2
1	A2	335	LEU	7.2
1	E3	20	TYR	7.2
1	O7	73	LEU	7.2
1	O7	93	GLU	7.1
1	E5	335	LEU	7.0
2	J4	64	GLY	7.0
2	D8	64	GLY	7.0
2	T8	128	GLY	7.0
2	P7	64	GLY	7.0
2	N8	65	THR	6.9
1	I2	93	GLU	6.9
2	H4	65	THR	6.9
1	S4	93	GLU	6.9
2	T4	65	THR	6.9
1	M2	93	GLU	6.8
1	Q7	73	LEU	6.8
2	P4	67	PRO	6.7
1	Q8	21	ARG	6.7
2	T3	67	PRO	6.7
1	Q1	337	GLY	6.7
1	Q8	335	LEU	6.6
2	P6	102	LYS	6.6

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Mol	Chain	Res	Type	RSRZ
2	F7	64	GLY	6.6
1	C8	335	LEU	6.5
1	I4	20	TYR	6.5
1	S6	332	VAL	6.5
2	R8	67	PRO	6.5
1	S7	73	LEU	6.5
2	R7	70	LEU	6.5
1	O8	332	VAL	6.4
1	O7	20	TYR	6.4
2	N4	65	THR	6.4
2	N7	65	THR	6.4
2	J8	67	PRO	6.4
1	M3	93	GLU	6.4
1	E6	337	GLY	6.4
1	E6	335	LEU	6.3
1	C2	93	GLU	6.3
2	F4	65	THR	6.3
1	M8	93	GLU	6.3
1	M2	337	GLY	6.3
2	F8	67	PRO	6.3
1	K2	20	TYR	6.2
1	I4	335	LEU	6.2
2	F4	67	PRO	6.2
1	Q1	94	ASP	6.2
1	K8	93	GLU	6.2
1	E5	331	VAL	6.2
1	Q2	337	GLY	6.2
2	R1	73	ALA	6.1
1	G4	335	LEU	6.1
2	N8	64	GLY	6.1
2	R4	65	THR	6.1
1	I2	333	GLY	6.0
1	C7	93	GLU	6.0
1	K2	93	GLU	6.0
2	J3	65	THR	6.0
1	S7	20	TYR	6.0
2	R7	64	GLY	6.0
1	S5	335	LEU	6.0
2	D4	64	GLY	6.0
2	L4	64	GLY	6.0
2	H4	67	PRO	5.9
2	P5	136	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
1	M8	20	TYR	5.9
1	S6	335	LEU	5.9
1	Q1	93	GLU	5.8
2	R1	67	PRO	5.8
2	L4	65	THR	5.8
1	Q5	451	TRP	5.8
1	Q7	334	LYS	5.8
2	N3	64	GLY	5.8
1	K4	335	LEU	5.8
2	F6	112	GLY	5.7
1	G2	93	GLU	5.7
1	C5	335	LEU	5.7
1	I3	93	GLU	5.7
1	Q7	92	GLY	5.7
1	G3	338	ASP	5.6
1	Q2	21	ARG	5.6
2	L8	67	PRO	5.6
2	T8	67	PRO	5.6
1	E3	333	GLY	5.6
1	E1	93	GLU	5.5
2	R1	97	PHE	5.5
1	I8	93	GLU	5.5
2	B4	67	PRO	5.5
1	A7	335	LEU	5.5
1	E6	333	GLY	5.5
1	G8	337	GLY	5.5
1	S4	20	TYR	5.5
1	O7	337	GLY	5.5
2	R7	136	GLU	5.5
2	P6	105	ALA	5.5
2	L3	112	GLY	5.5
1	O1	93	GLU	5.4
1	Q8	46	PRO	5.4
2	B8	67	PRO	5.4
1	G3	93	GLU	5.4
1	G6	335	LEU	5.4
1	G8	335	LEU	5.4
1	S7	21	ARG	5.3
1	C8	93	GLU	5.3
2	R4	66	LYS	5.3
1	G3	332	VAL	5.3
2	J8	65	THR	5.3

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Mol	Chain	Res	Type	RSRZ
2	L8	64	GLY	5.3
1	E3	92	GLY	5.3
1	O7	95	ASN	5.3
1	C3	93	GLU	5.3
1	M4	93	GLU	5.3
1	E5	465	ILE	5.3
2	F3	66	LYS	5.3
2	D4	65	THR	5.2
2	L8	66	LYS	5.2
1	S8	21	ARG	5.2
1	Q7	74	LEU	5.2
1	G3	331	VAL	5.1
1	O8	93	GLU	5.1
1	Q2	20	TYR	5.1
1	E4	21	ARG	5.1
2	N4	67	PRO	5.1
1	S7	333	GLY	5.1
1	G4	93	GLU	5.0
1	G4	72	ASP	5.0
1	O8	335	LEU	5.0
2	R1	76	GLU	5.0
2	R3	64	GLY	5.0
2	P8	64	GLY	5.0
1	M3	335	LEU	5.0
1	S4	21	ARG	5.0
1	G3	335	LEU	5.0
1	A8	21	ARG	5.0
2	L7	65	THR	5.0
2	R2	67	PRO	4.9
1	G2	333	GLY	4.9
1	M1	93	GLU	4.9
1	Q7	335	LEU	4.9
1	C7	20	TYR	4.9
1	K4	20	TYR	4.9
1	K7	71	THR	4.9
2	R7	93	LEU	4.9
1	M1	335	LEU	4.9
2	R3	65	THR	4.9
1	A5	337	GLY	4.9
1	K3	94	ASP	4.9
1	S4	337	GLY	4.9
1	Q4	335	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A3	333	GLY	4.8
2	L4	67	PRO	4.8
1	G7	334	LYS	4.8
1	O7	333	GLY	4.8
2	T3	65	THR	4.7
2	H3	89	GLY	4.7
1	C3	335	LEU	4.7
1	G3	334	LYS	4.7
2	H8	65	THR	4.7
2	P8	66	LYS	4.7
1	O8	21	ARG	4.7
1	Q7	95	ASN	4.7
1	A7	338	ASP	4.7
1	Q7	333	GLY	4.7
1	I4	93	GLU	4.7
1	Q8	98	ILE	4.7
1	Q2	71	THR	4.6
2	R7	67	PRO	4.6
1	G3	95	ASN	4.6
2	F3	68	ASN	4.6
1	C8	20	TYR	4.6
1	Q7	94	ASP	4.6
2	H4	66	LYS	4.6
2	L8	65	THR	4.6
1	Q7	93	GLU	4.6
1	Q2	335	LEU	4.6
1	C7	21	ARG	4.6
2	N7	67	PRO	4.5
1	M2	335	LEU	4.5
2	R7	82	ALA	4.5
1	E4	338	ASP	4.5
1	M2	95	ASN	4.5
1	K7	74	LEU	4.5
1	A7	93	GLU	4.5
1	E3	76	ASP	4.5
1	O2	335	LEU	4.5
2	R3	67	PRO	4.5
1	K3	465	ILE	4.5
2	R6	106	LEU	4.5
1	O2	337	GLY	4.5
1	C4	21	ARG	4.4
1	Q5	335	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
2	R8	65	THR	4.4
1	G3	333	GLY	4.4
1	I4	338	ASP	4.4
1	C7	335	LEU	4.4
2	J8	66	LYS	4.4
2	P7	67	PRO	4.4
1	G1	73	LEU	4.4
1	I7	93	GLU	4.4
1	G3	451	TRP	4.4
2	R1	68	ASN	4.4
1	Q8	305	LYS	4.4
1	E7	20	TYR	4.4
2	F8	65	THR	4.4
2	N4	66	LYS	4.4
2	R7	89	GLY	4.3
1	G8	20	TYR	4.3
1	Q4	93	GLU	4.3
1	S4	332	VAL	4.3
1	G2	20	TYR	4.3
1	S5	337	GLY	4.3
2	B8	65	THR	4.3
1	M4	21	ARG	4.3
1	S7	93	GLU	4.3
2	R1	81	VAL	4.2
1	E7	95	ASN	4.2
2	J3	67	PRO	4.2
1	O6	332	VAL	4.2
2	P7	90	GLY	4.2
1	Q7	465	ILE	4.2
1	G7	335	LEU	4.2
2	F5	136	GLU	4.2
1	E3	75	THR	4.2
2	L1	65	THR	4.2
2	F5	119	GLY	4.2
2	F5	108	TRP	4.2
1	O5	337	GLY	4.1
1	O7	335	LEU	4.1
2	H3	93	LEU	4.1
1	E7	93	GLU	4.1
1	E1	338	ASP	4.1
2	D8	67	PRO	4.1
1	A8	20	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	Q1	336	GLU	4.1
1	S8	384	VAL	4.1
1	O7	72	ASP	4.1
1	E3	331	VAL	4.1
1	Q7	338	ASP	4.1
1	K6	337	GLY	4.0
2	H4	70	LEU	4.0
2	R7	65	THR	4.0
2	R8	93	LEU	4.0
2	H3	67	PRO	4.0
1	S7	77	LEU	4.0
1	K3	334	LYS	4.0
1	A8	335	LEU	4.0
1	M1	21	ARG	4.0
1	O1	21	ARG	4.0
1	A8	93	GLU	4.0
1	G3	71	THR	4.0
1	I6	335	LEU	4.0
1	I4	337	GLY	3.9
1	Q6	335	LEU	3.9
2	P2	67	PRO	3.9
1	Q7	309	ILE	3.9
2	F4	100	GLN	3.9
1	K3	335	LEU	3.9
1	E5	305	LYS	3.9
1	M7	93	GLU	3.9
2	P6	111	ARG	3.9
1	M1	20	TYR	3.9
1	Q2	66	TRP	3.9
1	K7	47	GLY	3.9
1	E4	332	VAL	3.9
1	S3	73	LEU	3.9
1	S8	335	LEU	3.9
2	L4	100	GLN	3.9
1	S6	439	ARG	3.9
1	K1	338	ASP	3.9
1	G1	71	THR	3.9
1	S5	380	GLY	3.9
2	R1	101	PHE	3.9
1	Q7	332	VAL	3.9
1	E7	335	LEU	3.9
2	F5	113	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
2	R7	91	VAL	3.9
1	O7	75	THR	3.9
2	J4	66	LYS	3.9
1	A2	337	GLY	3.9
1	K2	338	ASP	3.9
1	A3	335	LEU	3.8
2	F4	64	GLY	3.8
1	Q3	93	GLU	3.8
1	Q7	408	GLY	3.8
1	K7	338	ASP	3.8
2	F8	66	LYS	3.8
1	K3	73	LEU	3.8
1	K7	335	LEU	3.8
2	T8	112	GLY	3.8
1	E3	335	LEU	3.8
2	R1	93	LEU	3.8
2	R7	76	GLU	3.8
2	R1	99	GLY	3.8
1	Q7	21	ARG	3.8
1	E4	334	LYS	3.8
2	R8	66	LYS	3.8
1	M4	20	TYR	3.8
1	O4	20	TYR	3.8
1	Q2	439	ARG	3.8
1	K4	93	GLU	3.8
1	K1	331	VAL	3.7
1	Q8	93	GLU	3.7
1	O1	20	TYR	3.7
1	K8	21	ARG	3.7
1	O1	335	LEU	3.7
1	Q7	20	TYR	3.7
1	K8	331	VAL	3.7
2	B4	64	GLY	3.7
2	F3	100	GLN	3.7
2	R1	71	VAL	3.7
2	F3	67	PRO	3.7
1	M1	73	LEU	3.7
1	I4	332	VAL	3.7
1	E2	335	LEU	3.7
1	G1	74	LEU	3.7
1	E4	331	VAL	3.7
2	R7	81	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	E3	71	THR	3.7
2	T2	112	GLY	3.7
2	P4	65	THR	3.7
1	O8	331	VAL	3.6
1	C6	335	LEU	3.6
1	S7	24	TYR	3.6
2	P8	65	THR	3.6
1	C3	74	LEU	3.6
1	K1	95	ASN	3.6
1	Q8	334	LYS	3.6
1	O7	89	PRO	3.6
1	K2	335	LEU	3.6
1	G4	439	ARG	3.6
2	L1	94	ILE	3.6
1	M8	338	ASP	3.6
1	E3	73	LEU	3.6
1	G4	77	LEU	3.6
1	G5	335	LEU	3.6
1	M3	333	GLY	3.6
1	K4	334	LYS	3.5
1	E4	333	GLY	3.5
1	A7	20	TYR	3.5
1	Q5	437	LEU	3.5
1	S7	95	ASN	3.5
1	Q7	97	PHE	3.5
1	O4	93	GLU	3.5
2	F3	88	GLY	3.5
1	O8	20	TYR	3.5
1	S8	20	TYR	3.5
2	R7	117	LEU	3.5
2	R4	136	GLU	3.5
2	N7	64	GLY	3.5
2	P6	112	GLY	3.5
1	G1	93	GLU	3.5
2	T7	136	GLU	3.5
2	J1	67	PRO	3.5
2	P1	68	ASN	3.5
1	O7	74	LEU	3.5
2	L1	93	LEU	3.5
1	S4	439	ARG	3.5
1	O3	93	GLU	3.5
1	E5	332	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	O7	331	VAL	3.5
1	K8	73	LEU	3.5
1	M7	74	LEU	3.5
1	S8	94	ASP	3.5
2	P6	101	PHE	3.5
1	E4	93	GLU	3.5
2	H3	70	LEU	3.5
1	G2	94	ASP	3.5
1	Q4	94	ASP	3.5
2	T8	116	VAL	3.5
2	B7	106	LEU	3.5
2	T4	67	PRO	3.4
1	K6	465	ILE	3.4
1	M1	94	ASP	3.4
1	E8	93	GLU	3.4
1	K8	335	LEU	3.4
2	F3	89	GLY	3.4
1	E6	338	ASP	3.4
1	E3	77	LEU	3.4
1	G2	465	ILE	3.4
1	O7	434	GLY	3.4
1	K8	78	ASP	3.4
2	R1	77	GLY	3.4
1	K2	72	ASP	3.4
1	S5	458	ALA	3.4
1	E5	353	TYR	3.4
1	Q1	332	VAL	3.4
2	H2	93	LEU	3.4
1	Q4	337	GLY	3.4
1	S7	337	GLY	3.4
2	P7	65	THR	3.4
1	E3	93	GLU	3.4
2	T6	103	ALA	3.4
1	O6	335	LEU	3.4
1	Q1	87	ILE	3.4
1	O1	72	ASP	3.4
2	P7	68	ASN	3.4
1	E4	46	PRO	3.4
2	R1	106	LEU	3.4
2	R8	70	LEU	3.4
2	F5	116	VAL	3.4
1	E7	94	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	O7	451	TRP	3.3
1	Q2	129	ALA	3.3
1	G8	93	GLU	3.3
1	S3	93	GLU	3.3
1	Q8	22	LEU	3.3
2	T8	117	LEU	3.3
1	C3	71	THR	3.3
2	T5	101	PHE	3.3
1	A7	333	GLY	3.3
1	E5	451	TRP	3.3
2	H3	82	ALA	3.3
1	C4	332	VAL	3.3
1	G2	332	VAL	3.3
1	I7	71	THR	3.3
1	O8	334	LYS	3.3
2	F4	66	LYS	3.3
2	F3	104	GLY	3.3
1	Q1	46	PRO	3.3
1	Q8	73	LEU	3.3
1	G3	94	ASP	3.3
1	Q1	24	TYR	3.3
1	S5	336	GLU	3.3
2	R1	84	SER	3.3
2	D4	66	LYS	3.3
2	N1	64	GLY	3.3
1	S6	138	LEU	3.3
1	S7	74	LEU	3.3
2	P3	64	GLY	3.3
2	H3	105	ALA	3.3
2	R1	80	CYS	3.3
1	K2	439	ARG	3.3
2	R5	136	GLU	3.3
2	T5	100	GLN	3.3
2	J3	98	ASN	3.2
1	Q4	20	TYR	3.2
2	T7	90	GLY	3.2
1	E6	439	ARG	3.2
2	P6	106	LEU	3.2
2	P7	88	GLY	3.2
2	R7	94	ILE	3.2
1	E3	338	ASP	3.2
2	R4	67	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	M2	21	ARG	3.2
1	E5	378	ALA	3.2
1	S3	335	LEU	3.2
1	O3	335	LEU	3.2
2	H7	64	GLY	3.2
1	O7	94	ASP	3.2
1	A1	335	LEU	3.2
1	C7	95	ASN	3.2
1	K7	337	GLY	3.2
2	L3	66	LYS	3.2
2	R7	77	GLY	3.2
1	S7	72	ASP	3.1
2	H3	87	LYS	3.1
1	K1	21	ARG	3.1
1	O1	74	LEU	3.1
2	B7	89	GLY	3.1
2	P7	70	LEU	3.1
2	R7	104	GLY	3.1
2	L2	136	GLU	3.1
1	C7	94	ASP	3.1
1	Q4	331	VAL	3.1
1	A4	20	TYR	3.1
1	E3	95	ASN	3.1
1	I2	21	ARG	3.1
2	R7	112	GLY	3.1
1	E4	77	LEU	3.1
2	N8	67	PRO	3.1
1	M7	338	ASP	3.1
1	S8	331	VAL	3.1
2	D4	136	GLU	3.1
1	E1	335	LEU	3.1
1	S4	335	LEU	3.1
2	T1	67	PRO	3.1
1	Q6	194	ARG	3.1
1	I5	335	LEU	3.1
1	Q8	71	THR	3.1
1	S1	73	LEU	3.1
2	T8	70	LEU	3.1
1	E8	94	ASP	3.1
1	E2	332	VAL	3.1
1	Q7	461	LEU	3.1
1	A7	94	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	O1	94	ASP	3.1
1	S2	439	ARG	3.1
2	J4	65	THR	3.0
1	E5	142	VAL	3.0
1	C3	76	ASP	3.0
1	E8	335	LEU	3.0
1	I3	72	ASP	3.0
1	K3	21	ARG	3.0
1	K7	76	ASP	3.0
1	Q6	439	ARG	3.0
2	L7	102	LYS	3.0
1	Q1	25	TYR	3.0
1	E5	129	ALA	3.0
1	K7	73	LEU	3.0
1	Q7	404	GLY	3.0
2	R1	90	GLY	3.0
1	A3	334	LYS	3.0
1	O7	21	ARG	3.0
1	Q4	21	ARG	3.0
1	Q8	26	THR	3.0
1	M7	73	LEU	3.0
1	O8	94	ASP	3.0
2	H3	112	GLY	3.0
1	E8	20	TYR	3.0
1	I5	338	ASP	3.0
1	S3	94	ASP	3.0
2	H3	76	GLU	3.0
2	P4	64	GLY	3.0
2	T4	112	GLY	3.0
2	T5	136	GLU	3.0
1	Q4	439	ARG	3.0
2	F4	68	ASN	3.0
1	O7	458	ALA	3.0
1	S7	102	ALA	3.0
2	T6	105	ALA	3.0
2	F5	127	ILE	3.0
2	R1	94	ILE	3.0
1	Q1	466	LYS	3.0
2	R7	66	LYS	3.0
2	T8	126	PHE	3.0
2	F3	125	GLY	3.0
2	R6	105	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	G4	465	ILE	2.9
1	O2	95	ASN	2.9
1	O2	338	ASP	2.9
1	C7	333	GLY	2.9
1	E5	330	THR	2.9
2	R1	70	LEU	2.9
1	G4	331	VAL	2.9
1	S7	94	ASP	2.9
2	F3	97	PHE	2.9
2	L8	93	LEU	2.9
1	Q3	338	ASP	2.9
1	E7	466	LYS	2.9
1	K4	337	GLY	2.9
1	S8	337	GLY	2.9
1	C7	73	LEU	2.9
1	Q1	73	LEU	2.9
1	C4	93	GLU	2.9
2	R7	105	ALA	2.9
1	G4	92	GLY	2.9
2	F4	97	PHE	2.9
2	H4	100	GLN	2.9
1	Q3	73	LEU	2.9
1	O2	72	ASP	2.9
2	F4	136	GLU	2.9
2	H8	66	LYS	2.9
1	G8	72	ASP	2.9
1	Q7	72	ASP	2.9
2	R5	106	LEU	2.9
1	A2	21	ARG	2.9
1	Q3	21	ARG	2.9
1	Q4	338	ASP	2.9
1	Q8	47	GLY	2.8
2	H2	136	GLU	2.8
1	Q1	390	LEU	2.8
1	G4	75	THR	2.8
1	Q8	75	THR	2.8
1	G3	76	ASP	2.8
1	M2	92	GLY	2.8
1	S8	50	PHE	2.8
1	S7	128	LYS	2.8
2	L4	136	GLU	2.8
2	R7	71	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	G7	333	GLY	2.8
1	Q4	74	LEU	2.8
1	O4	94	ASP	2.8
2	R1	113	LYS	2.8
1	Q6	179	GLY	2.8
1	C8	334	LYS	2.8
1	O5	335	LEU	2.8
2	R2	70	LEU	2.8
1	Q1	330	THR	2.8
1	S8	95	ASN	2.8
1	I6	337	GLY	2.8
2	B4	100	GLN	2.8
2	R7	109	LEU	2.8
2	H2	68	ASN	2.8
1	I3	20	TYR	2.8
1	C4	72	ASP	2.8
1	S4	338	ASP	2.8
1	K8	333	GLY	2.8
1	A7	466	LYS	2.8
1	K1	334	LYS	2.8
1	S7	384	VAL	2.8
1	K1	93	GLU	2.8
1	K7	93	GLU	2.8
1	I3	74	LEU	2.8
1	M8	335	LEU	2.8
2	P7	66	LYS	2.8
1	E7	21	ARG	2.8
1	S7	129	ALA	2.7
1	S7	25	TYR	2.7
2	R1	104	GLY	2.7
1	G4	332	VAL	2.7
1	O7	332	VAL	2.7
1	C3	94	ASP	2.7
2	F5	120	ASP	2.7
2	J2	87	LYS	2.7
1	M4	337	GLY	2.7
1	Q3	333	GLY	2.7
2	P2	98	ASN	2.7
2	T8	136	GLU	2.7
2	F3	112	GLY	2.7
1	Q3	74	LEU	2.7
1	S4	73	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	S7	462	TRP	2.7
1	Q1	465	ILE	2.7
1	Q7	330	THR	2.7
1	C3	338	ASP	2.7
1	I1	72	ASP	2.7
1	E7	337	GLY	2.7
1	A7	74	LEU	2.7
2	J2	101	PHE	2.7
2	J2	102	LYS	2.7
2	F3	65	THR	2.7
1	S2	93	GLU	2.7
2	B7	64	GLY	2.7
2	H2	90	GLY	2.7
2	F5	100	GLN	2.7
2	R7	97	PHE	2.7
1	A3	93	GLU	2.7
1	S8	46	PRO	2.7
2	R3	136	GLU	2.7
2	T3	95	ASP	2.7
1	E5	439	ARG	2.7
1	I1	21	ARG	2.7
1	Q6	332	VAL	2.7
1	C3	73	LEU	2.7
1	Q4	445	ILE	2.7
1	S6	338	ASP	2.7
2	R1	136	GLU	2.7
1	S7	53	ALA	2.7
2	N1	67	PRO	2.7
1	Q7	331	VAL	2.7
2	L1	100	GLN	2.7
2	P1	64	GLY	2.7
2	T8	85	GLN	2.7
1	Q2	50	PHE	2.7
2	R6	101	PHE	2.7
1	S1	93	GLU	2.7
1	A8	72	ASP	2.7
1	O3	333	GLY	2.6
1	Q1	21	ARG	2.6
1	G4	78	ASP	2.6
1	M2	20	TYR	2.6
1	G3	92	GLY	2.6
2	T8	68	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	I7	335	LEU	2.6
2	B8	66	LYS	2.6
2	H3	66	LYS	2.6
1	E2	21	ARG	2.6
1	Q7	50	PHE	2.6
2	R7	108	TRP	2.6
1	C3	333	GLY	2.6
1	Q1	84	CYS	2.6
1	Q8	95	ASN	2.6
2	R1	87	LYS	2.6
2	R7	113	LYS	2.6
1	E4	74	LEU	2.6
1	G4	90	LEU	2.6
1	S5	439	ARG	2.6
1	A7	337	GLY	2.6
1	O7	92	GLY	2.6
1	S6	337	GLY	2.6
1	S6	359	SER	2.6
1	Q1	20	TYR	2.6
2	L7	67	PRO	2.6
2	P1	65	THR	2.6
1	K8	332	VAL	2.6
1	M1	439	ARG	2.6
1	M3	21	ARG	2.6
1	O1	73	LEU	2.6
1	Q8	50	PHE	2.6
1	K1	337	GLY	2.6
2	F3	90	GLY	2.6
1	S7	336	GLU	2.6
2	P7	102	LYS	2.6
2	T3	66	LYS	2.6
2	H8	67	PRO	2.6
1	M8	332	VAL	2.6
1	Q1	178	LEU	2.6
1	C5	338	ASP	2.6
1	M6	333	GLY	2.6
2	L8	136	GLU	2.6
1	E4	78	ASP	2.6
1	G4	73	LEU	2.6
1	G7	73	LEU	2.6
1	M3	73	LEU	2.6
1	E4	66	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	K7	20	TYR	2.6
2	B1	87	LYS	2.6
2	P6	100	GLN	2.6
1	C4	335	LEU	2.6
1	E3	78	ASP	2.6
1	O5	338	ASP	2.6
1	Q8	52	GLU	2.6
2	F3	93	LEU	2.6
2	T6	136	GLU	2.6
1	S1	21	ARG	2.6
1	S1	439	ARG	2.6
2	D8	66	LYS	2.5
2	R1	65	THR	2.5
1	K1	72	ASP	2.5
2	F3	76	GLU	2.5
2	L1	95	ASP	2.5
1	M1	75	THR	2.5
2	B1	67	PRO	2.5
1	I1	74	LEU	2.5
1	I3	73	LEU	2.5
1	O4	47	GLY	2.5
2	F5	109	LEU	2.5
1	Q6	187	ARG	2.5
1	I7	334	LYS	2.5
2	R2	66	LYS	2.5
2	R7	101	PHE	2.5
1	M3	94	ASP	2.5
1	E3	439	ARG	2.5
1	G6	439	ARG	2.5
2	P8	112	GLY	2.5
2	T8	114	LYS	2.5
1	O2	465	ILE	2.5
1	O3	78	ASP	2.5
2	H2	67	PRO	2.5
2	N2	67	PRO	2.5
2	T7	73	ALA	2.5
1	A7	73	LEU	2.5
1	G3	28	ASP	2.5
1	K8	72	ASP	2.5
1	K2	333	GLY	2.5
1	O8	54	ALA	2.5
2	F3	105	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	O8	429	GLN	2.5
2	P8	106	LEU	2.5
1	Q6	331	VAL	2.5
1	A8	334	LYS	2.5
1	E6	334	LYS	2.5
2	N4	70	LEU	2.5
1	S7	332	VAL	2.5
1	C7	334	LYS	2.5
1	G7	338	ASP	2.5
1	S1	78	ASP	2.5
1	C3	337	GLY	2.5
1	O5	176	PRO	2.5
1	Q6	174	ILE	2.5
2	T8	73	ALA	2.5
2	F5	102	LYS	2.5
1	K2	331	VAL	2.5
1	Q4	332	VAL	2.5
1	K3	20	TYR	2.5
1	S3	20	TYR	2.5
1	E2	95	ASN	2.5
1	Q8	72	ASP	2.5
1	E7	73	LEU	2.4
1	G7	74	LEU	2.4
1	M5	335	LEU	2.4
1	Q1	445	ILE	2.4
1	Q6	105	LEU	2.4
2	R2	127	ILE	2.4
2	T8	127	ILE	2.4
1	Q2	124	VAL	2.4
2	R8	81	VAL	2.4
1	M3	20	TYR	2.4
1	Q7	297	MET	2.4
1	S7	28	ASP	2.4
2	H3	102	LYS	2.4
1	I1	71	THR	2.4
1	E3	74	LEU	2.4
1	M3	74	LEU	2.4
1	O6	437	LEU	2.4
1	I4	21	ARG	2.4
1	Q7	42	VAL	2.4
1	G2	95	ASN	2.4
2	H5	113	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	R1	88	GLY	2.4
1	C1	93	GLU	2.4
2	F1	136	GLU	2.4
1	M3	338	ASP	2.4
1	Q1	96	GLN	2.4
1	E4	337	GLY	2.4
1	Q8	100	TYR	2.4
2	R1	89	GLY	2.4
1	A4	335	LEU	2.4
1	I3	335	LEU	2.4
1	Q6	437	LEU	2.4
2	B1	94	ILE	2.4
2	P7	136	GLU	2.4
2	T4	66	LYS	2.4
1	E5	156	GLN	2.4
1	S3	72	ASP	2.4
2	H3	92	ASN	2.4
1	G6	337	GLY	2.4
2	J2	99	GLY	2.4
1	C7	89	PRO	2.4
1	S2	334	LYS	2.4
1	Q7	75	THR	2.4
2	F3	136	GLU	2.4
1	Q7	77	LEU	2.4
1	E8	332	VAL	2.4
2	L8	68	ASN	2.4
2	T6	104	GLY	2.4
1	E5	336	GLU	2.4
2	H4	136	GLU	2.4
2	R7	102	LYS	2.4
2	L8	105	ALA	2.4
1	E4	465	ILE	2.4
1	E7	28	ASP	2.4
1	Q1	72	ASP	2.4
2	R1	127	ILE	2.4
1	M1	334	LYS	2.4
1	O6	439	ARG	2.4
1	S7	89	PRO	2.4
2	L1	67	PRO	2.4
2	R1	100	GLN	2.4
2	R6	100	GLN	2.4
1	I3	76	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	Q8	76	ASP	2.4
1	M1	95	ASN	2.4
1	Q1	361	GLY	2.4
2	H3	94	ILE	2.4
2	J3	112	GLY	2.4
1	G1	332	VAL	2.4
1	K3	331	VAL	2.4
1	S2	21	ARG	2.4
2	R6	111	ARG	2.4
2	R6	131	LEU	2.3
2	R7	106	LEU	2.3
1	S7	441	GLY	2.3
2	N8	66	LYS	2.3
2	R3	66	LYS	2.3
2	R7	88	GLY	2.3
1	I8	439	ARG	2.3
1	Q7	69	VAL	2.3
2	T3	101	PHE	2.3
1	S5	451	TRP	2.3
1	E4	100	TYR	2.3
1	G4	334	LYS	2.3
1	G4	74	LEU	2.3
1	O6	338	ASP	2.3
1	G5	337	GLY	2.3
1	O4	92	GLY	2.3
1	S3	75	THR	2.3
2	L7	76	GLU	2.3
1	S4	465	ILE	2.3
2	R6	113	LYS	2.3
1	C3	20	TYR	2.3
1	A1	21	ARG	2.3
1	E1	21	ARG	2.3
1	M1	74	LEU	2.3
1	O8	333	GLY	2.3
1	Q6	403	GLY	2.3
1	Q7	71	THR	2.3
1	I4	334	LYS	2.3
2	B7	66	LYS	2.3
1	K8	443	ASP	2.3
1	M2	333	GLY	2.3
1	Q6	441	GLY	2.3
1	K7	334	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	H6	127	ILE	2.3
1	E8	439	ARG	2.3
1	G7	21	ARG	2.3
2	R1	125	GLY	2.3
1	E4	22	LEU	2.3
1	G4	22	LEU	2.3
1	I1	75	THR	2.3
1	S6	339	LYS	2.3
2	D7	65	THR	2.3
1	K1	332	VAL	2.3
1	G3	78	ASP	2.3
1	E4	441	GLY	2.3
1	K4	333	GLY	2.3
1	Q7	407	LEU	2.3
1	E5	328	THR	2.3
1	C5	331	VAL	2.3
1	E3	194	ARG	2.3
1	I8	72	ASP	2.3
1	E3	47	GLY	2.3
1	S2	333	GLY	2.3
2	R6	102	LYS	2.3
1	E1	451	TRP	2.3
1	E3	22	LEU	2.3
1	M2	73	LEU	2.3
1	Q2	22	LEU	2.3
1	Q8	74	LEU	2.3
1	Q7	458	ALA	2.3
2	L3	105	ALA	2.3
2	P4	136	GLU	2.3
1	C7	72	ASP	2.3
1	E6	131	LYS	2.3
1	K8	334	LYS	2.3
1	M7	334	LYS	2.3
2	F3	101	PHE	2.3
1	S6	331	VAL	2.3
2	T2	89	GLY	2.2
2	T6	100	GLN	2.2
1	K3	95	ASN	2.2
1	Q1	74	LEU	2.2
1	S2	335	LEU	2.2
1	S6	343	LEU	2.2
2	H3	74	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	L1	70	LEU	2.2
2	T7	67	PRO	2.2
2	T8	109	LEU	2.2
1	O6	334	LYS	2.2
1	Q5	466	LYS	2.2
1	A4	72	ASP	2.2
1	G2	72	ASP	2.2
1	Q2	72	ASP	2.2
1	G8	92	GLY	2.2
2	B7	90	GLY	2.2
2	H3	91	VAL	2.2
2	R5	119	GLY	2.2
1	Q7	454	GLU	2.2
1	I1	335	LEU	2.2
1	Q1	305	LYS	2.2
2	F3	87	LYS	2.2
1	E2	439	ARG	2.2
1	M7	94	ASP	2.2
1	Q5	337	GLY	2.2
1	Q7	460	GLU	2.2
1	Q1	95	ASN	2.2
1	Q6	177	LYS	2.2
2	R8	68	ASN	2.2
1	K2	21	ARG	2.2
1	O6	451	TRP	2.2
2	R8	131	LEU	2.2
1	K8	338	ASP	2.2
1	O1	95	ASN	2.2
2	P6	117	LEU	2.2
1	S7	78	ASP	2.2
1	G4	336	GLU	2.2
1	G8	333	GLY	2.2
2	D3	112	GLY	2.2
2	R1	78	GLU	2.2
2	T7	104	GLY	2.2
1	E5	466	LYS	2.2
2	J5	101	PHE	2.2
1	C4	331	VAL	2.2
2	L4	69	SER	2.2
2	F5	106	LEU	2.2
2	L4	70	LEU	2.2
2	R1	72	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E7	72	ASP	2.2
1	I1	93	GLU	2.2
1	K4	72	ASP	2.2
1	Q7	132	ALA	2.2
1	Q7	156	GLN	2.2
2	N7	90	GLY	2.2
1	Q7	24	TYR	2.2
1	S6	100	TYR	2.2
1	I4	331	VAL	2.2
1	G3	46	PRO	2.2
1	I1	73	LEU	2.2
2	R3	93	LEU	2.2
1	Q5	338	ASP	2.2
1	S7	438	MET	2.2
2	B7	77	GLY	2.2
2	L8	127	ILE	2.2
1	C2	335	LEU	2.2
2	F5	117	LEU	2.2
1	I7	94	ASP	2.2
1	Q4	28	ASP	2.2
1	K3	71	THR	2.2
1	K7	439	ARG	2.2
2	L1	136	GLU	2.1
2	T6	127	ILE	2.1
2	F1	67	PRO	2.1
2	P6	131	LEU	2.1
2	T8	131	LEU	2.1
1	M3	76	ASP	2.1
1	C3	451	TRP	2.1
1	K3	439	ARG	2.1
1	S7	99	ALA	2.1
1	G3	20	TYR	2.1
1	S8	332	VAL	2.1
1	I7	74	LEU	2.1
1	Q1	78	ASP	2.1
2	R2	68	ASN	2.1
1	E5	445	ILE	2.1
1	Q5	331	VAL	2.1
1	G7	94	ASP	2.1
1	O8	22	LEU	2.1
1	M8	21	ARG	2.1
1	Q7	410	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	D5	100	GLN	2.1
1	C5	334	LYS	2.1
1	C7	74	LEU	2.1
1	E2	465	ILE	2.1
1	E5	450	ARG	2.1
1	G3	384	VAL	2.1
1	M8	78	ASP	2.1
1	S8	461	LEU	2.1
2	J8	64	GLY	2.1
2	T6	117	LEU	2.1
1	O8	46	PRO	2.1
1	E1	71	THR	2.1
1	O6	402	PHE	2.1
1	M3	334	LYS	2.1
1	O3	466	LYS	2.1
1	E4	187	ARG	2.1
1	G2	92	GLY	2.1
1	M1	338	ASP	2.1
1	O2	94	ASP	2.1
1	K6	335	LEU	2.1
1	S6	101	ILE	2.1
2	R6	117	LEU	2.1
1	K2	336	GLU	2.1
2	B3	136	GLU	2.1
1	G4	466	LYS	2.1
1	A6	337	GLY	2.1
1	M2	72	ASP	2.1
1	A8	332	VAL	2.1
1	S6	170	LEU	2.1
1	S6	407	LEU	2.1
1	O6	445	ILE	2.1
2	F3	91	VAL	2.1
1	S7	463	LYS	2.1
2	P4	66	LYS	2.1
1	M7	71	THR	2.1
2	N7	68	ASN	2.1
1	Q1	441	GLY	2.1
1	S8	333	GLY	2.1
2	F3	77	GLY	2.1
2	R3	90	GLY	2.1
1	C4	73	LEU	2.1
1	S7	57	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	L3	94	ILE	2.1
1	Q6	463	LYS	2.1
2	R4	87	LYS	2.1
1	E2	132	ALA	2.1
1	E3	66	TRP	2.1
1	Q1	438	MET	2.1
1	S7	66	TRP	2.1
2	T8	78	GLU	2.1
1	I3	333	GLY	2.1
1	O6	394	PHE	2.1
1	Q3	72	ASP	2.1
2	J3	95	ASP	2.1
2	F3	102	LYS	2.0
2	H3	114	LYS	2.0
2	N1	70	LEU	2.0
1	E2	331	VAL	2.0
1	I5	332	VAL	2.0
1	S7	331	VAL	2.0
1	S5	465	ILE	2.0
1	E5	448	ALA	2.0
1	K6	439	ARG	2.0
2	D4	68	ASN	2.0
2	P3	98	ASN	2.0
1	E1	337	GLY	2.0
1	M2	47	GLY	2.0
2	H7	65	THR	2.0
1	C5	451	TRP	2.0
1	S8	127	PHE	2.0
2	T2	102	LYS	2.0
1	G2	176	PRO	2.0
1	S8	391	VAL	2.0
1	C6	439	ARG	2.0
1	G3	87	ILE	2.0
1	S8	72	ASP	2.0
2	B4	66	LYS	2.0
2	D8	112	GLY	2.0
2	F2	87	LYS	2.0
1	Q8	394	PHE	2.0
1	S7	451	TRP	2.0
2	J3	100	GLN	2.0
1	G8	439	ARG	2.0
1	A6	338	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	M1	72	ASP	2.0
1	O4	337	GLY	2.0
1	O7	448	ALA	2.0
2	L3	98	ASN	2.0
1	S4	47	GLY	2.0
1	S4	94	ASP	2.0
2	D7	64	GLY	2.0
2	F4	101	PHE	2.0
2	R1	108	TRP	2.0
2	H3	106	LEU	2.0
1	S7	69	VAL	2.0
2	J3	66	LYS	2.0
2	T7	66	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 monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	ZN	F3	302	1/1	0.36	0.14	172,172,172,172	0
3	ZN	R6	302	1/1	0.55	0.14	110,110,110,110	0
3	ZN	T8	302	1/1	0.60	0.14	118,118,118,118	0
3	ZN	R6	301	1/1	0.71	0.16	101,101,101,101	0
3	ZN	H3	302	1/1	0.78	0.14	116,116,116,116	0
3	ZN	R7	301	1/1	0.82	0.11	118,118,118,118	0
3	ZN	P8	302	1/1	0.82	0.17	82,82,82,82	0
3	ZN	T8	301	1/1	0.84	0.10	114,114,114,114	0
3	ZN	R1	301	1/1	0.85	0.11	88,88,88,88	0
3	ZN	R4	301	1/1	0.86	0.15	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	H4	301	1/1	0.87	0.13	70,70,70,70	0
3	ZN	R8	302	1/1	0.87	0.12	97,97,97,97	0
3	ZN	R3	302	1/1	0.88	0.15	92,92,92,92	0
3	ZN	R1	302	1/1	0.88	0.19	131,131,131,131	0
3	ZN	L1	301	1/1	0.89	0.13	94,94,94,94	0
3	ZN	F7	301	1/1	0.89	0.15	79,79,79,79	0
3	ZN	H2	301	1/1	0.90	0.16	65,65,65,65	0
3	ZN	H1	301	1/1	0.90	0.14	60,60,60,60	0
3	ZN	T5	302	1/1	0.90	0.16	94,94,94,94	0
3	ZN	T6	301	1/1	0.90	0.11	89,89,89,89	0
3	ZN	P8	301	1/1	0.90	0.16	70,70,70,70	0
3	ZN	R2	301	1/1	0.90	0.14	70,70,70,70	0
3	ZN	R3	301	1/1	0.91	0.15	78,78,78,78	0
3	ZN	T7	302	1/1	0.91	0.16	103,103,103,103	0
3	ZN	T2	301	1/1	0.91	0.10	57,57,57,57	0
3	ZN	L7	302	1/1	0.91	0.12	89,89,89,89	0
3	ZN	F5	301	1/1	0.92	0.13	99,99,99,99	0
3	ZN	H4	302	1/1	0.92	0.11	69,69,69,69	0
3	ZN	R4	302	1/1	0.92	0.13	74,74,74,74	0
3	ZN	P6	302	1/1	0.92	0.07	109,109,109,109	0
3	ZN	T5	301	1/1	0.92	0.11	88,88,88,88	0
3	ZN	P5	301	1/1	0.93	0.12	71,71,71,71	0
3	ZN	F6	302	1/1	0.93	0.13	107,107,107,107	0
3	ZN	R7	302	1/1	0.93	0.17	170,170,170,170	0
3	ZN	T6	302	1/1	0.93	0.12	117,117,117,117	0
3	ZN	R8	301	1/1	0.93	0.14	97,97,97,97	0
3	ZN	N4	301	1/1	0.93	0.14	76,76,76,76	0
3	ZN	P2	302	1/1	0.93	0.12	70,70,70,70	0
3	ZN	H3	301	1/1	0.94	0.12	71,71,71,71	0
3	ZN	P7	301	1/1	0.94	0.11	76,76,76,76	0
3	ZN	T2	302	1/1	0.94	0.09	66,66,66,66	0
3	ZN	L1	302	1/1	0.94	0.13	92,92,92,92	0
3	ZN	R5	302	1/1	0.94	0.14	78,78,78,78	0
3	ZN	F4	302	1/1	0.94	0.14	79,79,79,79	0
3	ZN	F3	301	1/1	0.94	0.11	99,99,99,99	0
3	ZN	H2	302	1/1	0.94	0.13	80,80,80,80	0
3	ZN	H5	302	1/1	0.94	0.15	91,91,91,91	0
3	ZN	P6	301	1/1	0.94	0.13	82,82,82,82	0
3	ZN	J4	302	1/1	0.95	0.13	54,54,54,54	0
3	ZN	T7	301	1/1	0.95	0.15	84,84,84,84	0
3	ZN	H5	301	1/1	0.95	0.11	59,59,59,59	0
3	ZN	F1	302	1/1	0.95	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	R2	302	1/1	0.95	0.14	70,70,70,70	0
3	ZN	P2	301	1/1	0.96	0.12	59,59,59,59	0
3	ZN	L2	301	1/1	0.96	0.15	77,77,77,77	0
3	ZN	L3	301	1/1	0.96	0.14	54,54,54,54	0
3	ZN	L6	302	1/1	0.96	0.11	60,60,60,60	0
3	ZN	R5	301	1/1	0.96	0.14	73,73,73,73	0
3	ZN	J3	302	1/1	0.96	0.11	64,64,64,64	0
3	ZN	F6	301	1/1	0.96	0.15	88,88,88,88	0
3	ZN	T3	302	1/1	0.96	0.09	92,92,92,92	0
3	ZN	P5	302	1/1	0.97	0.12	64,64,64,64	0
3	ZN	B7	302	1/1	0.97	0.13	65,65,65,65	0
3	ZN	D3	301	1/1	0.97	0.11	62,62,62,62	0
3	ZN	F4	301	1/1	0.97	0.12	92,92,92,92	0
3	ZN	P7	302	1/1	0.97	0.10	88,88,88,88	0
3	ZN	D5	302	1/1	0.97	0.10	73,73,73,73	0
3	ZN	L2	302	1/1	0.97	0.13	65,65,65,65	0
3	ZN	D6	301	1/1	0.97	0.11	62,62,62,62	0
3	ZN	L3	302	1/1	0.97	0.13	85,85,85,85	0
3	ZN	F5	302	1/1	0.97	0.16	93,93,93,93	0
3	ZN	D8	302	1/1	0.97	0.12	69,69,69,69	0
3	ZN	B4	302	1/1	0.97	0.14	59,59,59,59	0
3	ZN	N7	302	1/1	0.97	0.13	64,64,64,64	0
3	ZN	P1	301	1/1	0.97	0.14	62,62,62,62	0
3	ZN	F2	301	1/1	0.97	0.12	62,62,62,62	0
3	ZN	H7	302	1/1	0.97	0.12	63,63,63,63	0
3	ZN	F8	302	1/1	0.97	0.15	73,73,73,73	0
3	ZN	F2	302	1/1	0.98	0.15	74,74,74,74	0
3	ZN	H1	302	1/1	0.98	0.12	67,67,67,67	0
3	ZN	D2	302	1/1	0.98	0.14	58,58,58,58	0
3	ZN	B3	301	1/1	0.98	0.13	44,44,44,44	0
3	ZN	D3	302	1/1	0.98	0.10	67,67,67,67	0
3	ZN	L4	301	1/1	0.98	0.12	77,77,77,77	0
3	ZN	L6	301	1/1	0.98	0.11	48,48,48,48	0
3	ZN	B1	302	1/1	0.98	0.11	68,68,68,68	0
3	ZN	B5	302	1/1	0.98	0.12	48,48,48,48	0
3	ZN	N1	302	1/1	0.98	0.13	69,69,69,69	0
3	ZN	N2	302	1/1	0.98	0.10	75,75,75,75	0
3	ZN	N3	301	1/1	0.98	0.14	65,65,65,65	0
3	ZN	D7	302	1/1	0.98	0.12	60,60,60,60	0
3	ZN	N4	302	1/1	0.98	0.14	63,63,63,63	0
3	ZN	D8	301	1/1	0.98	0.10	62,62,62,62	0
3	ZN	B6	302	1/1	0.98	0.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	ZN	P1	302	1/1	0.98	0.14	64,64,64,64	0
3	ZN	H6	301	1/1	0.98	0.12	55,55,55,55	0
3	ZN	B2	302	1/1	0.98	0.12	46,46,46,46	0
3	ZN	P3	302	1/1	0.98	0.12	58,58,58,58	0
3	ZN	T4	301	1/1	0.98	0.15	64,64,64,64	0
3	ZN	T4	302	1/1	0.98	0.12	61,61,61,61	0
3	ZN	P4	301	1/1	0.98	0.15	61,61,61,61	0
3	ZN	J1	302	1/1	0.98	0.13	43,43,43,43	0
3	ZN	F7	302	1/1	0.98	0.17	78,78,78,78	0
3	ZN	J4	301	1/1	0.98	0.12	56,56,56,56	0
3	ZN	F8	301	1/1	0.98	0.19	70,70,70,70	0
3	ZN	J5	301	1/1	0.98	0.12	54,54,54,54	0
3	ZN	J6	301	1/1	0.98	0.13	55,55,55,55	0
3	ZN	B8	301	1/1	0.98	0.13	57,57,57,57	0
3	ZN	B3	302	1/1	0.99	0.10	49,49,49,49	0
3	ZN	J6	302	1/1	0.99	0.12	67,67,67,67	0
3	ZN	P4	302	1/1	0.99	0.12	58,58,58,58	0
3	ZN	J7	301	1/1	0.99	0.14	50,50,50,50	0
3	ZN	J7	302	1/1	0.99	0.12	49,49,49,49	0
3	ZN	J8	301	1/1	0.99	0.14	52,52,52,52	0
3	ZN	J8	302	1/1	0.99	0.12	51,51,51,51	0
3	ZN	B7	301	1/1	0.99	0.12	67,67,67,67	0
3	ZN	D6	302	1/1	0.99	0.09	55,55,55,55	0
3	ZN	B4	301	1/1	0.99	0.16	55,55,55,55	0
3	ZN	B1	301	1/1	0.99	0.12	56,56,56,56	0
3	ZN	B8	302	1/1	0.99	0.11	57,57,57,57	0
3	ZN	F1	301	1/1	0.99	0.15	56,56,56,56	0
3	ZN	H7	301	1/1	0.99	0.13	49,49,49,49	0
3	ZN	L4	302	1/1	0.99	0.14	70,70,70,70	0
3	ZN	L5	301	1/1	0.99	0.10	49,49,49,49	0
3	ZN	L5	302	1/1	0.99	0.13	47,47,47,47	0
3	ZN	B5	301	1/1	0.99	0.13	45,45,45,45	0
3	ZN	H8	301	1/1	0.99	0.15	54,54,54,54	0
3	ZN	L7	301	1/1	0.99	0.10	80,80,80,80	0
3	ZN	H8	302	1/1	0.99	0.11	52,52,52,52	0
3	ZN	L8	301	1/1	0.99	0.11	72,72,72,72	0
3	ZN	L8	302	1/1	0.99	0.11	78,78,78,78	0
3	ZN	N1	301	1/1	0.99	0.11	63,63,63,63	0
3	ZN	J1	301	1/1	0.99	0.12	46,46,46,46	0
3	ZN	N2	301	1/1	0.99	0.12	62,62,62,62	0
3	ZN	B2	301	1/1	0.99	0.14	52,52,52,52	0
3	ZN	T1	301	1/1	0.99	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	ZN	T1	302	1/1	0.99	0.12	55,55,55,55	0
3	ZN	J2	301	1/1	0.99	0.11	54,54,54,54	0
3	ZN	N3	302	1/1	0.99	0.10	64,64,64,64	0
3	ZN	T3	301	1/1	0.99	0.13	72,72,72,72	0
3	ZN	J2	302	1/1	0.99	0.10	65,65,65,65	0
3	ZN	J3	301	1/1	0.99	0.09	59,59,59,59	0
3	ZN	N6	301	1/1	0.99	0.12	48,48,48,48	0
3	ZN	N7	301	1/1	0.99	0.10	56,56,56,56	0
3	ZN	B6	301	1/1	0.99	0.13	44,44,44,44	0
3	ZN	N8	301	1/1	0.99	0.16	63,63,63,63	0
3	ZN	D4	301	1/1	0.99	0.13	55,55,55,55	0
3	ZN	D4	302	1/1	0.99	0.13	69,69,69,69	0
3	ZN	D5	301	1/1	0.99	0.12	65,65,65,65	0
3	ZN	J5	302	1/1	0.99	0.15	55,55,55,55	0
3	ZN	P3	301	1/1	0.99	0.15	60,60,60,60	0
3	ZN	H6	302	1/1	1.00	0.11	47,47,47,47	0
3	ZN	N6	302	1/1	1.00	0.10	60,60,60,60	0
3	ZN	D2	301	1/1	1.00	0.13	42,42,42,42	0
3	ZN	D7	301	1/1	1.00	0.12	42,42,42,42	0
3	ZN	D1	301	1/1	1.00	0.15	41,41,41,41	0
3	ZN	N8	302	1/1	1.00	0.10	56,56,56,56	0
3	ZN	D1	302	1/1	1.00	0.16	40,40,40,40	0
3	ZN	N5	301	1/1	1.00	0.12	40,40,40,40	0
3	ZN	N5	302	1/1	1.00	0.12	39,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.