



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:56 AM UTC

PDB ID : 6EKC / pdb_00006ekc
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

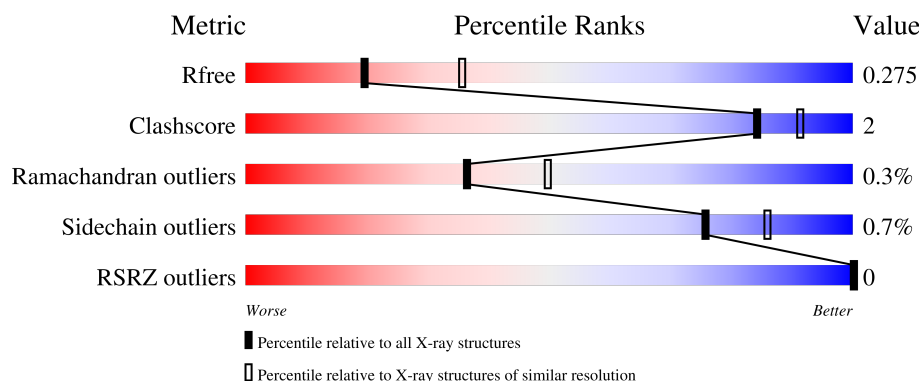
1 Overall quality at a glance

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.



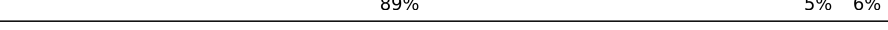
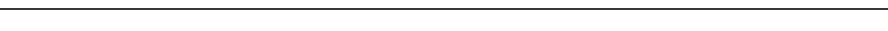
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

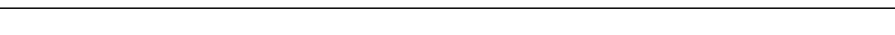
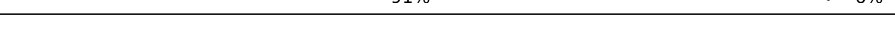
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Mol	Chain	Length	Quality of chain
1	A6	475	 89% 6%
1	A7	475	 87% 7% 6%
1	A8	475	 88% 6% 6%
1	C1	475	 88% 6% 6%
1	C2	475	 89% 5% 6%
1	C3	475	 88% 6% 6%
1	C4	475	 89% 5% 6%
1	C5	475	 90% 6%
1	C6	475	 91% 6%
1	C7	475	 86% 8% 6%
1	C8	475	 88% 6% 6%
1	E1	475	 87% 7% 6%
1	E2	475	 88% 6% 6%
1	E3	475	 89% 5% 6%
1	E4	475	 87% 7% 6%
1	E5	475	 88% 6% 6%
1	E6	475	 91% 6%
1	E7	475	 88% 6% 6%
1	E8	475	 87% 7% 6%
1	G1	475	 88% 6% 6%
1	G2	475	 88% 6% 6%
1	G3	475	 89% 5% 6%
1	G4	475	 89% 5% 6%
1	G5	475	 90% 6%
1	G6	475	 90% 6%

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Mol	Chain	Length	Quality of chain
1	G7	475	 90% 5% 6%
1	G8	475	 88% 5% 6%
1	I1	475	 89% 5% 6%
1	I2	475	 89% 5% 6%
1	I3	475	 88% 7% 6%
1	I4	475	 89% 5% 6%
1	I5	475	 88% 6% 6%
1	I6	475	 88% 6% 6%
1	I7	475	 88% 6% 6%
1	I8	475	 89% 5% 6%
1	K1	475	 87% 7% 6%
1	K2	475	 88% 6% 6%
1	K3	475	 87% 7% 6%
1	K4	475	 86% 8% 6%
1	K5	475	 91% 5% 6%
1	K6	475	 90% 5% 6%
1	K7	475	 89% 5% 6%
1	K8	475	 88% 5% 6%
1	M1	475	 89% 5% 6%
1	M2	475	 89% 5% 6%
1	M3	475	 89% 5% 6%
1	M4	475	 89% 5% 6%
1	M5	475	 89% 5% 6%
1	M6	475	 90% 5% 6%
1	M7	475	 88% 5% 6%

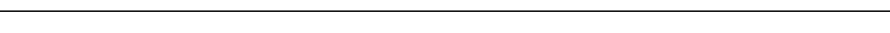
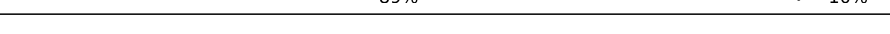
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Mol	Chain	Length	Quality of chain
1	M8	475	 89% 5% 6%
1	O1	475	 89% 5% 6%
1	O2	475	 88% 6% 6%
1	O3	475	 89% 5% 6%
1	O4	475	 87% 7% 6%
1	O5	475	 89% 5% 6%
1	O6	475	 88% 5% 6%
1	O7	475	 88% 7% 6%
1	O8	475	 87% 6% 6%
1	Q1	475	 90% • 6%
1	Q2	475	 89% 5% 6%
1	Q3	475	 90% • 6%
1	Q4	475	 89% 5% 6%
1	Q5	475	 89% 5% 6%
1	Q6	475	 88% 6% 6%
1	Q7	475	 88% 5% 6%
1	Q8	475	 87% 7% 6%
1	S1	475	 89% 5% 6%
1	S2	475	 88% 5% 6%
1	S3	475	 89% 5% 6%
1	S4	475	 88% 6% 6%
1	S5	475	 90% • 6%
1	S6	475	 88% 6% 6%
1	S7	475	 88% 6% 6%
1	S8	475	 89% 5% 6%

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Mol	Chain	Length	Quality of chain
2	B1	81	 88% 10%
2	B2	81	 86% 10%
2	B3	81	 89% 10%
2	B4	81	 86% 10%
2	B5	81	 90% 10%
2	B6	81	 89% 10%
2	B7	81	 90% 10%
2	B8	81	 86% 10%
2	D1	81	 88% 10%
2	D2	81	 88% 10%
2	D3	81	 89% 10%
2	D4	81	 86% 10%
2	D5	81	 90% 10%
2	D6	81	 89% 10%
2	D7	81	 89% 10%
2	D8	81	 86% 10%
2	F1	81	 84% 6% 10%
2	F2	81	 90% 10%
2	F3	81	 88% 10%
2	F4	81	 88% 10%
2	F5	81	 90% 10%
2	F6	81	 88% 10%
2	F7	81	 89% 10%
2	F8	81	 88% 10%
2	H1	81	 88% 10%

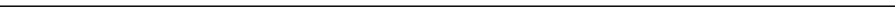
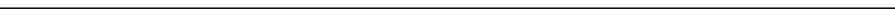
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Mol	Chain	Length	Quality of chain
2	H2	81	 88% • 10%
2	H3	81	 89% • 10%
2	H4	81	 86% • 10%
2	H5	81	 89% • 10%
2	H6	81	 86% • 10%
2	H7	81	 88% • 10%
2	H8	81	 90% 10%
2	J1	81	 88% •• 10%
2	J2	81	 86% •• 10%
2	J3	81	 88% • 10%
2	J4	81	 86% •• 10%
2	J5	81	 90% 10%
2	J6	81	 89% • 10%
2	J7	81	 89% • 10%
2	J8	81	 89% • 10%
2	L1	81	 88% • 10%
2	L2	81	 85% 5% 10%
2	L3	81	 86% • 10%
2	L4	81	 81% 9% 10%
2	L5	81	 90% 10%
2	L6	81	 90% 10%
2	L7	81	 88% • 10%
2	L8	81	 88% • 10%
2	N1	81	 86% • 10%
2	N2	81	 89% • 10%

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Mol	Chain	Length	Quality of chain
2	N3	81	 90% 10%
2	N4	81	 89% 10%
2	N5	81	 89% 10%
2	N6	81	 90% 10%
2	N7	81	 89% 10%
2	N8	81	 88% 10%
2	P1	81	 88% 10%
2	P2	81	 89% 10%
2	P3	81	 86% 10%
2	P4	81	 89% 10%
2	P5	81	 88% 10%
2	P6	81	 89% 10%
2	P7	81	 88% 10%
2	P8	81	 90% 10%
2	R1	81	 88% 10%
2	R2	81	 88% 10%
2	R3	81	 88% 10%
2	R4	81	 88% 10%
2	R5	81	 89% 10%
2	R6	81	 89% 10%
2	R7	81	 89% 10%
2	R8	81	 85% 5% 10%
2	T1	81	 86% 10%
2	T2	81	 88% 10%
2	T3	81	 86% 10%

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Mol	Chain	Length	Quality of chain
2	T4	81	 88% 10%
2	T5	81	 86% 10%
2	T6	81	 86% 10%
2	T7	81	 89% 10%
2	T8	81	 84% 6% 10%

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 biphosphate carboxylase large chain.

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

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

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

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

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

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 520	C 320	N 91	O 100	S 9	0	0	0
2	B2	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	B3	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	B4	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	B5	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	B6	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	B7	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	B8	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	D1	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	D2	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	D3	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	D4	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	D5	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	D6	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	D7	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	D8	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	F1	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	F2	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	F3	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	F4	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	F5	73	Total 520	C 320	N 91	O 100	S 9	0	0	0
2	F6	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	F7	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	F8	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	H1	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	H2	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	H3	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	H4	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	H5	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	H6	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	H7	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	H8	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	J1	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	J2	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	J3	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	J4	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	J5	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	J6	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	J7	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	J8	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	L1	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	L2	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	L3	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			

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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	C	N	O	S	0	0	0
			520	320	91	100	9			
2	R2	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	R3	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	R4	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	R5	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	R6	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	R7	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	R8	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	T1	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	T2	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	T3	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	T4	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	T5	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	T6	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	T7	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			
2	T8	73	Total	C	N	O	S	0	0	0
			520	320	91	100	9			

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 (CCD ID: 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 2	Zn 2	0	0
3	B6	2	Total 2	Zn 2	0	0
3	B7	2	Total 2	Zn 2	0	0
3	B8	2	Total 2	Zn 2	0	0
3	D1	2	Total 2	Zn 2	0	0
3	D2	2	Total 2	Zn 2	0	0
3	D3	2	Total 2	Zn 2	0	0
3	D4	2	Total 2	Zn 2	0	0
3	D5	2	Total 2	Zn 2	0	0
3	D6	2	Total 2	Zn 2	0	0
3	D7	2	Total 2	Zn 2	0	0
3	D8	2	Total 2	Zn 2	0	0
3	F1	2	Total 2	Zn 2	0	0
3	F2	2	Total 2	Zn 2	0	0
3	F3	2	Total 2	Zn 2	0	0
3	F4	2	Total 2	Zn 2	0	0
3	F5	2	Total 2	Zn 2	0	0
3	F6	2	Total 2	Zn 2	0	0
3	F7	2	Total 2	Zn 2	0	0
3	F8	2	Total 2	Zn 2	0	0
3	H1	2	Total 2	Zn 2	0	0

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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A1	6	Total 6	O 6	0	0
4	A2	16	Total 16	O 16	0	0
4	A3	25	Total 25	O 25	0	0
4	A4	29	Total 29	O 29	0	0
4	A5	34	Total 34	O 34	0	0
4	A6	22	Total 22	O 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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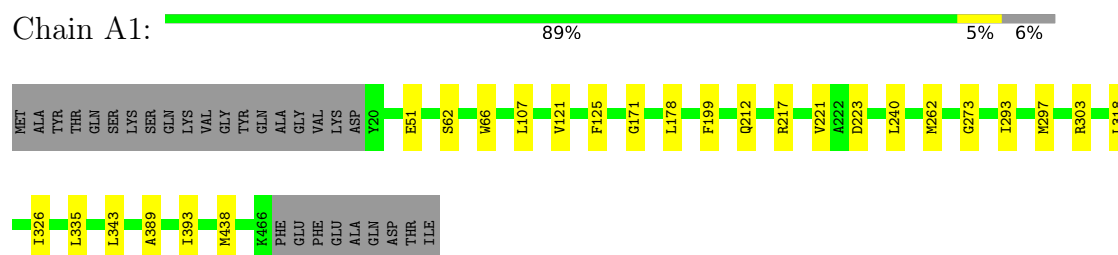
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P8	1	Total	O	0	0
			1	1		
4	T1	1	Total	O	0	0
			1	1		

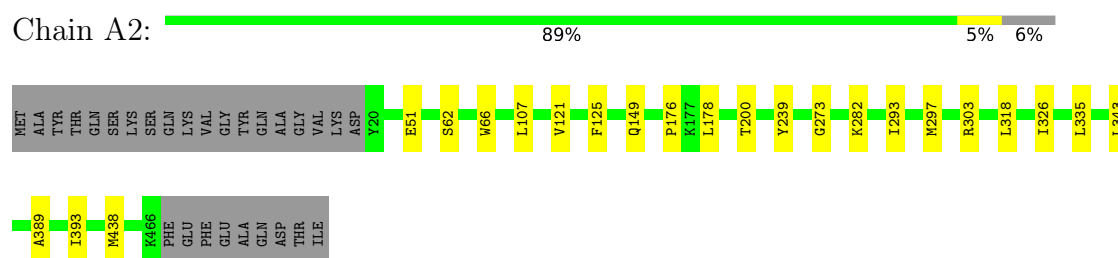
3 Residue-property plots [i](#)

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.

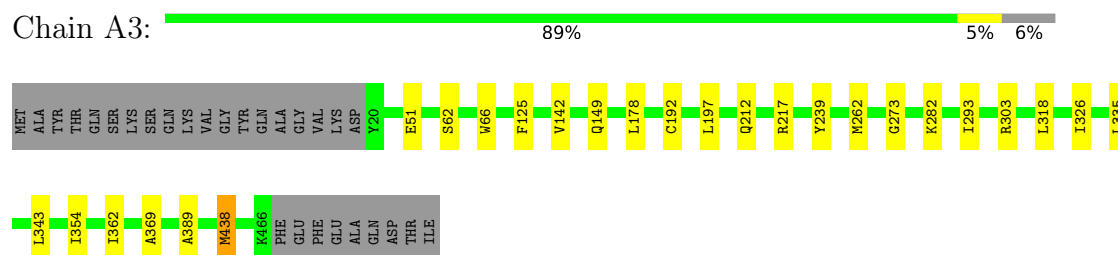
- Molecule 1: Ribulose biphosphate carboxylase large chain



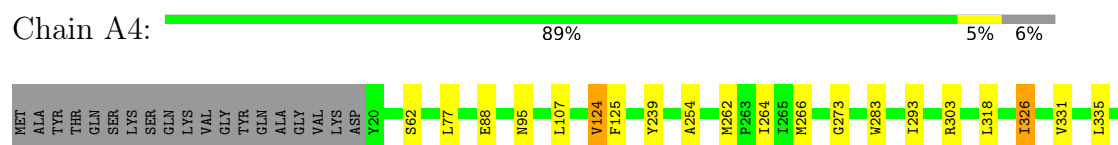
- Molecule 1: Ribulose biphosphate carboxylase large chain

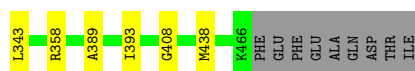


- Molecule 1: Ribulose bisphosphate carboxylase large chain



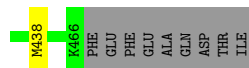
- Molecule 1: Ribulose bisphosphate carboxylase large chain





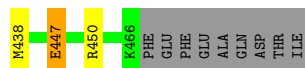
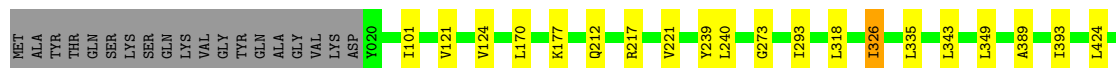
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain A5: 89% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain A6: 89% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain A7: 87% 7% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain A8: 88% 6% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

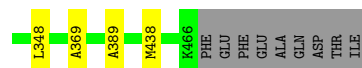
Chain C1: 88% 6% 6%





- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain C2: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain C3: 88% 6% 6%



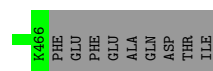
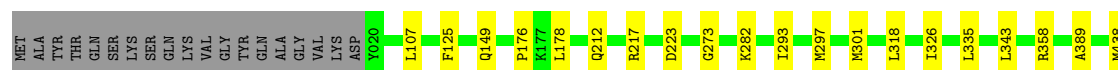
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain C4: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain C5: 90% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

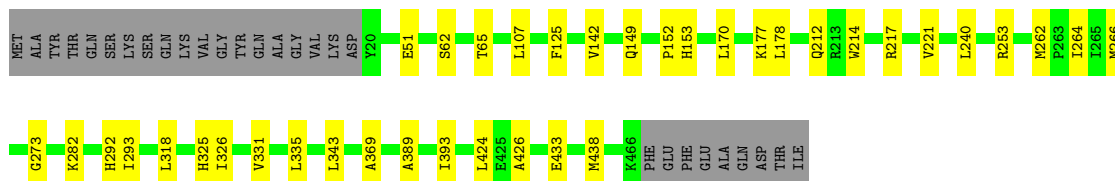
Chain C6: 91% 6%



GLN
ASP
THR
ILE

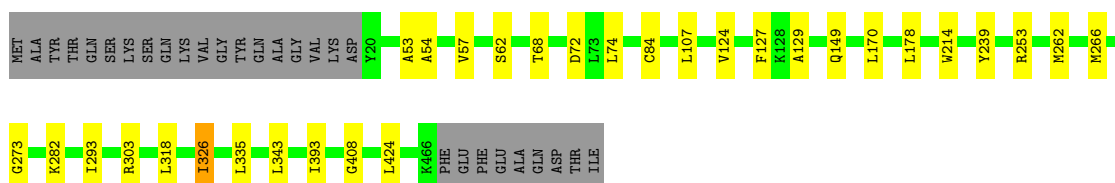
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain C7:  86% 8% 6%



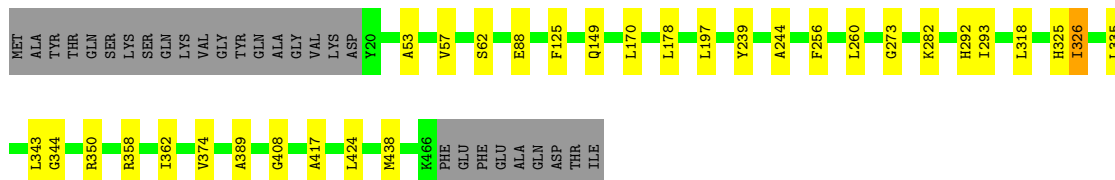
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain C8:  88% 6% 6%



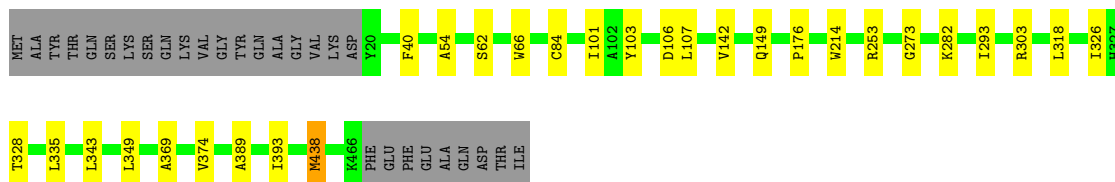
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain E1:  87% 7% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

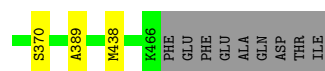
Chain E2:  88% 6% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain E3:  89% 5% 6%





- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain E4: 87% 7% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain E5: 88% 6% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain E6: 91% 6% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain E7: 88% 6% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain E8: 87% 7% 6%





- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain G1: 88% 6% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain G2: 88% 6% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain G3: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain G4: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain G5: 90% 6% 4%



PHE
GLU
ALA
GLN
ASP
THR
ILE

- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain G6:  90% 6%

MET ALA TYR THR GLN SER LYS GLN VAL GLY TYR GLN ALA GLY VAL LYS ASP Y20 V124 Q149 Q212 R217 Y239 I264 I265 M266 G273 K282 H292 I293 R303 L318 I326 L335 L343 V384 A389 G408 M438

K466
PHE
GLU
PHE
GLU
ALA
GLN
ASP
THR
ILE

- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain G7:  90% 6%

MET ALA TYR THR GLN SER LYS GLN VAL GLY TYR GLN ALA GLY VAL LYS ASP Y20 S61 S62 T65 L107 V124 Q149 L178 Q212 R217 Y239 M262 G273 K282 I293 K316 C317 L318 I326 L335 L343 L348

K466
PHE
GLU
PHE
GLU
ALA
GLN
ASP
THR
ILE

- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain G8:  88% 5% 6%

MET ALA TYR THR GLN SER LYS GLN VAL GLY TYR GLN ALA GLY VAL LYS ASP Y20 T23 E52 S62 W66 L107 Q149 L170 T173 I174 K175 L178 Y239 M262 A244 P245 M266 G273 K282 H292 I293 L318 I326 V331

L335 L343 R350 V374 I393 L424 K466
PHE
GLU
PHE
GLU
ALA
GLN
ASP
THR
ILE

- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain I1:  89% 5% 6%

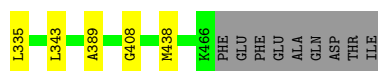
MET ALA TYR THR GLN SER LYS GLN VAL GLY TYR GLN ALA GLY VAL LYS ASP Y20 R41 E51 S62 W66 I87 L90 V142 E158 L178 T200 H238 A244 M266 G273 I293 H294 M297 L318 H325 I326 L335

L343 A369 A369 I393 M438 K466
PHE
GLU
PHE
GLU
ALA
GLN
ASP
THR
ILE

- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain I2:  89% 5% 6%

MET ALA TYR THR GLN SER LYS GLN VAL GLY TYR GLN ALA GLY VAL LYS ASP Y20 W66 L107 F108 E109 M115 V121 Q149 Q212 R213 V214 R217 Y239 R253 F256 L260 M266 G273 K282 H292 I293 L318 I326



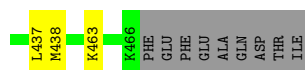
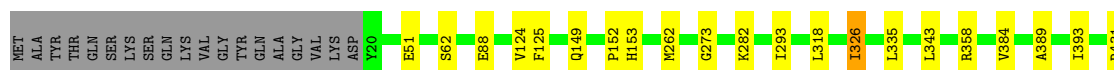
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain I3: 88% 7% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain I4: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain I5: 88% 6% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain I6: 88% 6% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

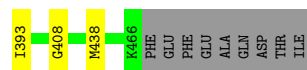
Chain I7: 88% 6% 6%





- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain I8: 89% 5% 6%



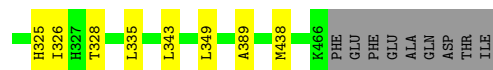
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain K1: 87% 7% 6%



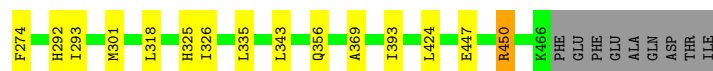
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain K2: 88% 6% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain K3: 87% 7% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

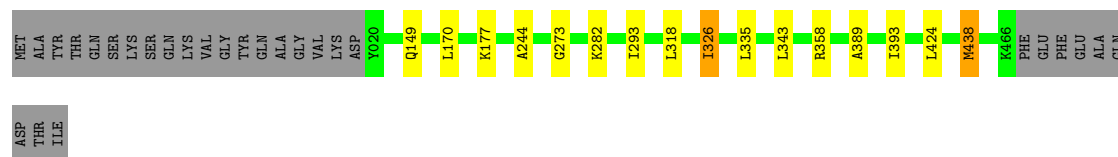
Chain K4: 86% 8% 6%





- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain K5: 91% 6%



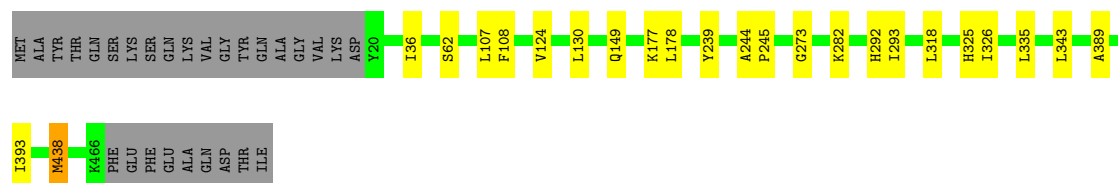
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain K6: 90% 6%



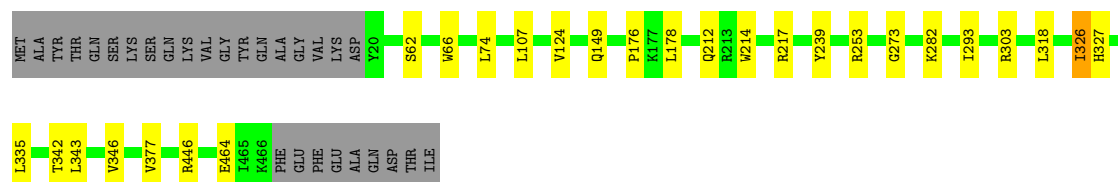
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain K7: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

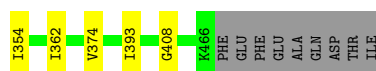
Chain K8: 88% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain M1: 89% 5% 6%





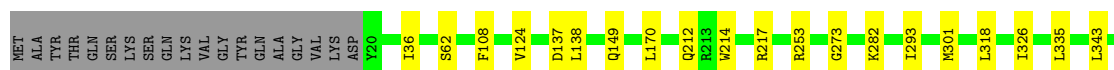
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain M2: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain M3: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain M4: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

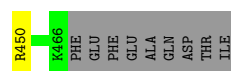
Chain M5: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

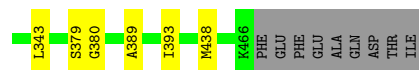
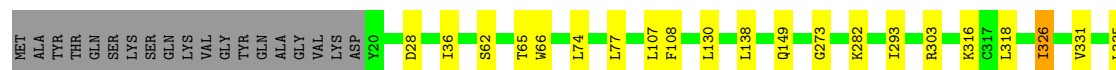
Chain M6: 90% 5% 6%





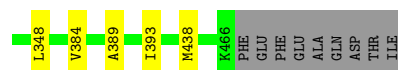
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain M7: 88% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain M8: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain O1: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

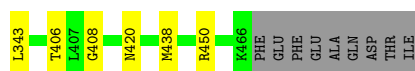
Chain O2: 88% 6% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain O3: 89% 5% 6%





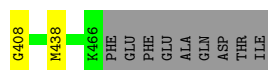
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain O4: 87% 7% 6%



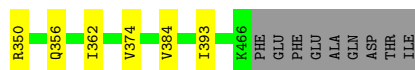
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain O5: 89% 5% 6%



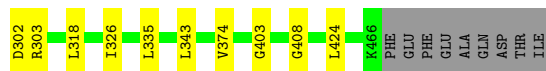
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain O6: 88% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain O7: 88% 7% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

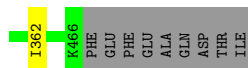
Chain O8: 87% 6% 6%





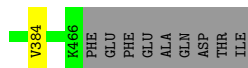
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain Q1: 90% 6%



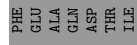
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain Q2: 89% 5% 6%



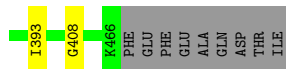
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain Q3: 90% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

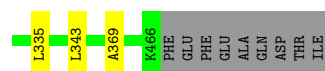
Chain Q4: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain Q5: 89% 5% 6%





- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain Q6: 88% 6% 6%



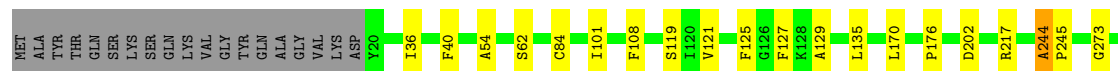
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain Q7: 88% 5% 6%



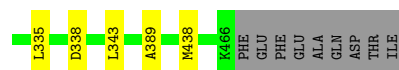
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain Q8: 87% 7% 6%



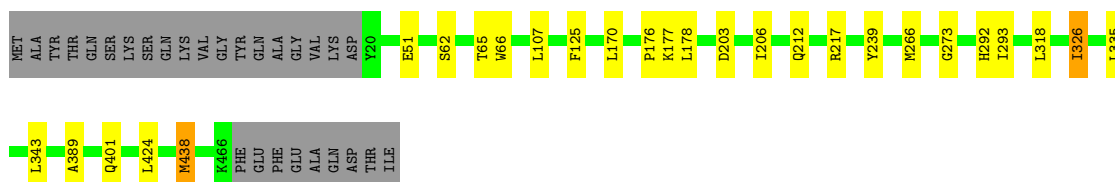
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain S1: 89% 5% 6%



- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain S2: 88% 5% 6%



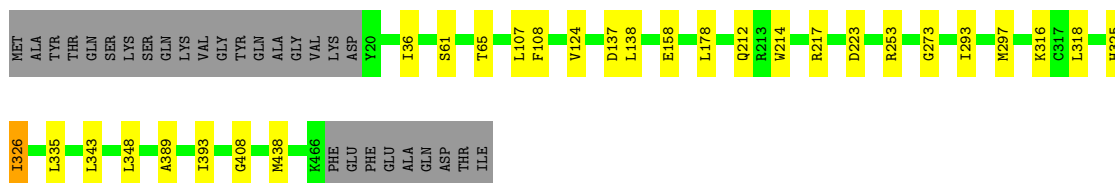
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain S3: 89% 5% 6%



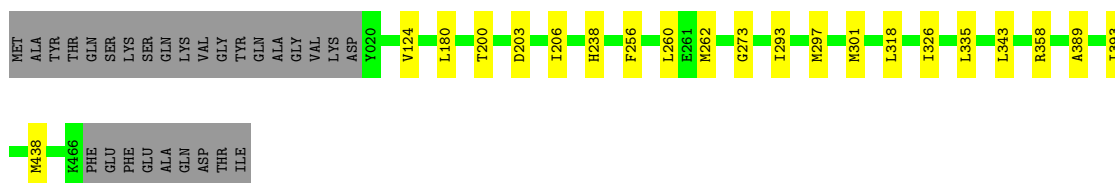
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain S4: 88% 6% 6%



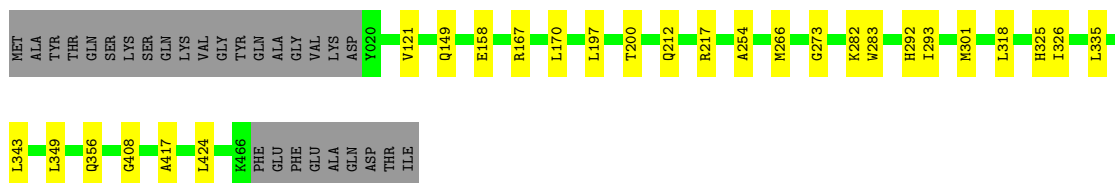
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain S5: 90% 6% 4%



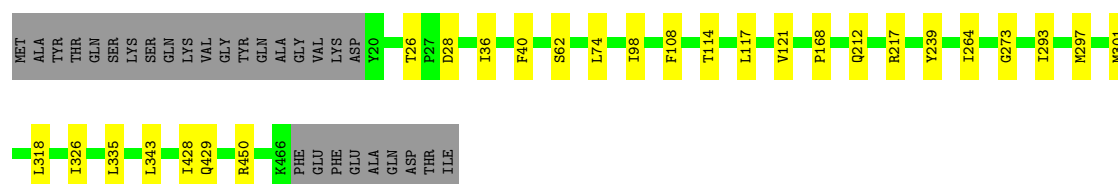
- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain S6: 88% 6% 6%



- Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain S7: 88% 6% 6%



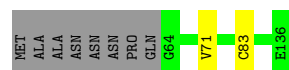
- Molecule 1: Ribulose biphosphate carboxylase large chain

Chain S8: 89% 5% 6%



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

Chain B1: 88% 10%



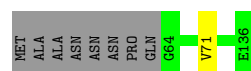
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain B2: 86% 10%



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

Chain B3: 89% 10%



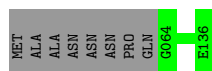
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain B4: 86% 10%



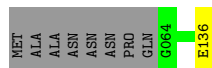
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain B5: 90% 10%



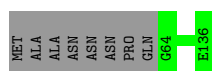
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain B6:  89% 10%



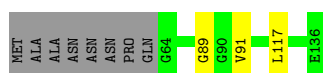
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain B7:  90% 10%



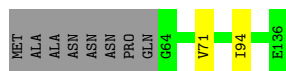
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain B8:  86% 10%



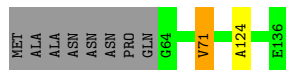
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain D1:  88% 10%



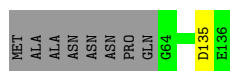
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain D2:  88% 10%



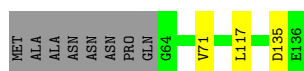
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain D3:  89% 10%

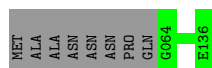


- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

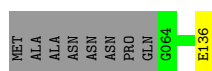
Chain D4:  86% 10%



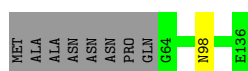
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



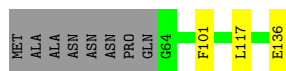
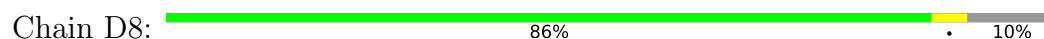
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



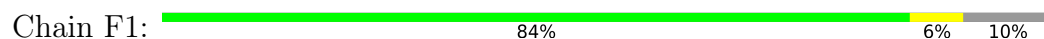
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



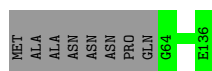
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



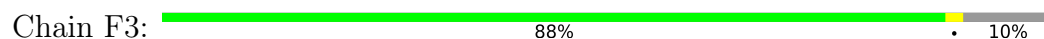
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

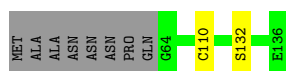


- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

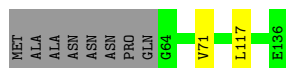
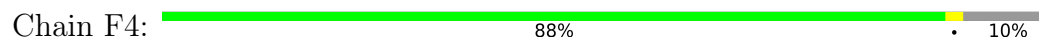


- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

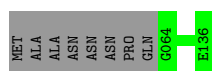




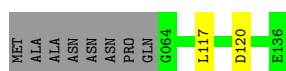
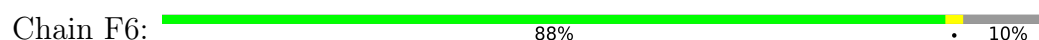
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



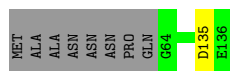
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



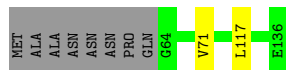
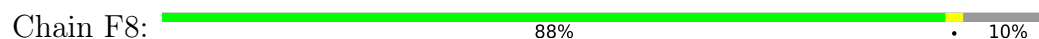
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



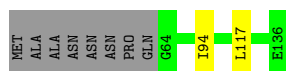
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



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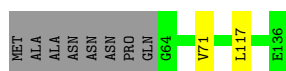


- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

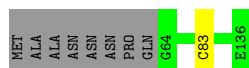


- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

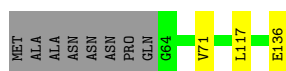
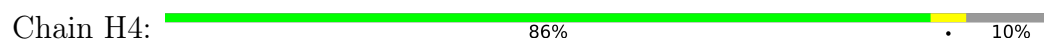




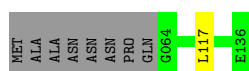
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



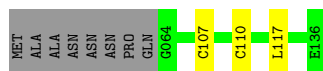
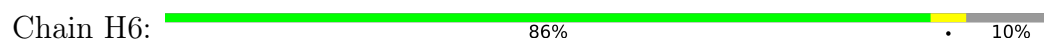
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



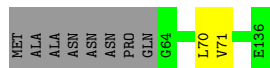
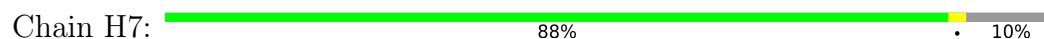
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



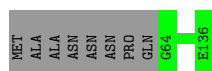
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



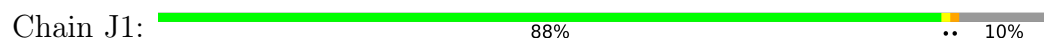
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

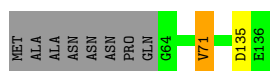


- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



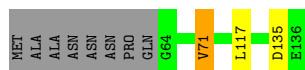
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein





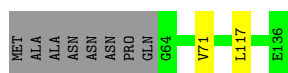
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J2: 86% 10%



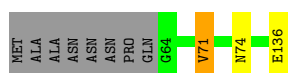
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J3: 88% 10%



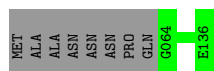
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J4: 86% 10%



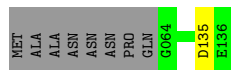
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J5: 90% 10%



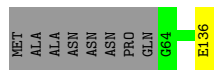
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J6: 89% 10%



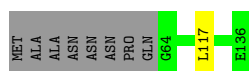
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain J7: 89% 10%



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

Chain J8: 89% 10%



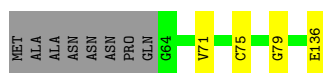
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L1: 88% 10%



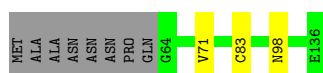
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L2: 85% 5% 10%



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

Chain L3: 86% 10%



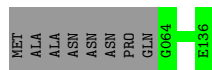
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L4: 81% 9% 10%



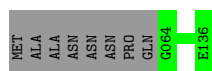
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L5: 90% 10%



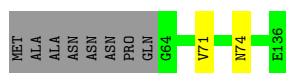
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L6: 90% 10%



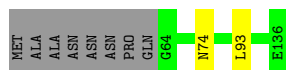
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L7: 88% 10%



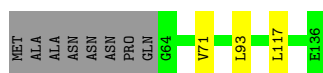
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain L8:  88% 10%



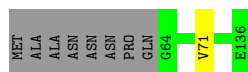
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N1:  86% 10%

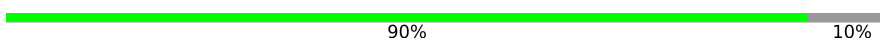


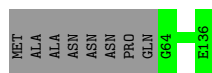
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N2:  89% 10%



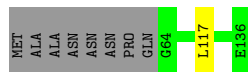
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N3:  90% 10%



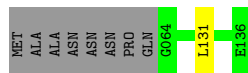
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N4:  89% 10%

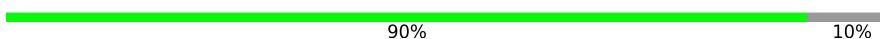


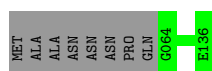
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N5:  89% 10%



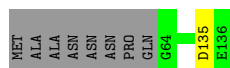
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N6:  90% 10%



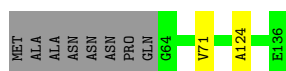
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N7: 89% 10%



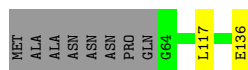
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain N8: 88% 10%



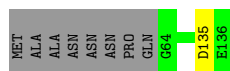
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P1: 88% 10%



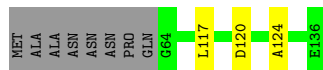
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P2: 89% 10%



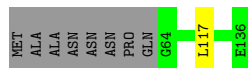
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P3: 86% 10%



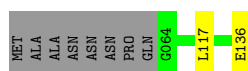
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P4: 89% 10%



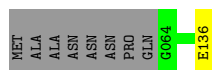
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P5: 88% 10%



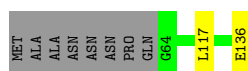
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P6: 89% 10%



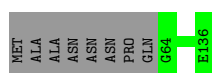
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P7: 88% 10%



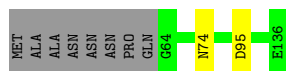
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain P8: 90% 10%



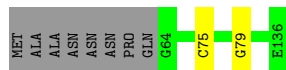
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R1: 88% 10%



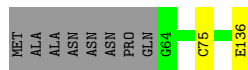
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R2: 88% 10%



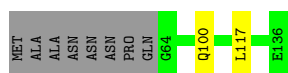
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R3: 88% 10%



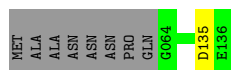
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R4: 88% 10%



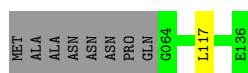
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R5: 89% 10%



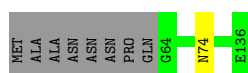
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R6: 89% 10%



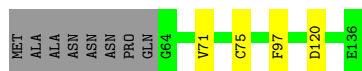
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R7: 89% 10%



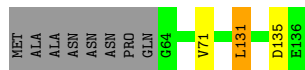
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain R8: 85% 5% 10%



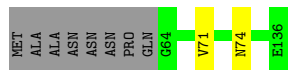
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain T1: 86% 2% 10%



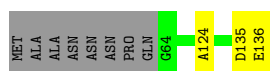
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

Chain T2: 88% 10%

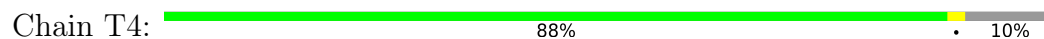


- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein

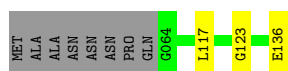
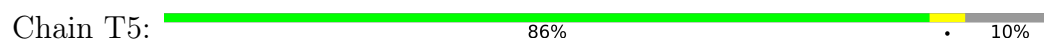
Chain T3: 86% 10%



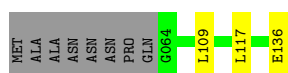
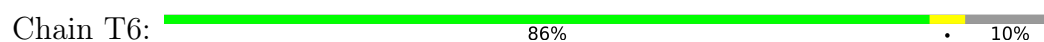
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



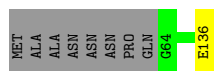
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



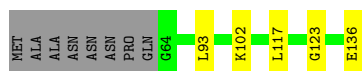
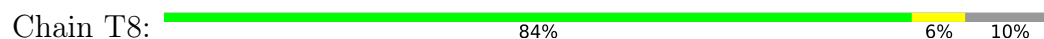
- Molecule 2: DnaJ/Hsp40 cysteine-rich domain superfamily protein



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



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



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 50.01 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.01-2.63) 97.9 (50.01-2.63)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.93%)	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)	0.31 , 18.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.377 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.97	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.54	0/3570	0.82	0/4844
1	A2	0.55	0/3577	0.82	0/4853
1	A3	0.55	0/3577	0.83	0/4853
1	A4	0.55	0/3570	0.83	1/4844 (0.0%)
1	A5	0.55	0/2927	0.85	2/3956 (0.1%)
1	A6	0.55	0/2927	0.86	0/3956
1	A7	0.55	0/3577	0.83	1/4853 (0.0%)
1	A8	0.56	0/3577	0.81	0/4853
1	C1	0.56	0/3577	0.82	1/4853 (0.0%)
1	C2	0.55	0/3577	0.82	0/4853
1	C3	0.56	0/3577	0.82	1/4853 (0.0%)
1	C4	0.56	0/3577	0.81	2/4853 (0.0%)
1	C5	0.56	0/2927	0.84	0/3956
1	C6	0.55	0/2927	0.84	0/3956
1	C7	0.55	0/3577	0.82	1/4853 (0.0%)
1	C8	0.55	0/3577	0.83	1/4853 (0.0%)
1	E1	0.59	0/3577	0.84	1/4853 (0.0%)
1	E2	0.59	0/3577	0.83	0/4853
1	E3	0.59	0/3577	0.83	0/4853
1	E4	0.59	0/3577	0.83	0/4853
1	E5	0.59	0/2927	0.84	0/3956
1	E6	0.58	0/2927	0.86	0/3956
1	E7	0.58	0/3577	0.84	0/4853
1	E8	0.58	0/3577	0.82	1/4853 (0.0%)
1	G1	0.57	0/3577	0.83	1/4853 (0.0%)
1	G2	0.58	0/3577	0.82	0/4853
1	G3	0.58	0/3577	0.84	0/4853
1	G4	0.57	0/3577	0.82	0/4853
1	G5	0.54	0/2927	0.85	1/3956 (0.0%)
1	G6	0.55	0/2927	0.85	2/3956 (0.1%)
1	G7	0.55	0/3577	0.81	0/4853
1	G8	0.55	0/3577	0.82	0/4853

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I1	0.55	0/3577	0.81	1/4853 (0.0%)
1	I2	0.57	0/3577	0.83	0/4853
1	I3	0.55	0/3577	0.82	1/4853 (0.0%)
1	I4	0.56	0/3577	0.82	2/4853 (0.0%)
1	I5	0.52	0/2927	0.83	0/3956
1	I6	0.55	0/2927	0.85	0/3956
1	I7	0.54	0/3577	0.83	0/4853
1	I8	0.57	0/3577	0.83	0/4853
1	K1	0.58	0/3577	0.82	0/4853
1	K2	0.58	0/3577	0.83	0/4853
1	K3	0.57	0/3577	0.83	0/4853
1	K4	0.57	0/3577	0.82	1/4853 (0.0%)
1	K5	0.55	0/2927	0.84	1/3956 (0.0%)
1	K6	0.55	0/2927	0.85	1/3956 (0.0%)
1	K7	0.55	0/3577	0.80	0/4853
1	K8	0.58	0/3577	0.82	0/4853
1	M1	0.55	0/3577	0.81	0/4853
1	M2	0.57	0/3577	0.84	1/4853 (0.0%)
1	M3	0.55	0/3577	0.83	1/4853 (0.0%)
1	M4	0.54	0/3577	0.80	1/4853 (0.0%)
1	M5	0.53	0/2927	0.82	0/3956
1	M6	0.54	0/2927	0.86	0/3956
1	M7	0.54	0/3577	0.82	0/4853
1	M8	0.56	0/3577	0.82	1/4853 (0.0%)
1	O1	0.57	0/3577	0.83	2/4853 (0.0%)
1	O2	0.55	1/3577 (0.0%)	0.83	0/4853
1	O3	0.56	0/3577	0.82	0/4853
1	O4	0.56	0/3577	0.82	0/4853
1	O5	0.58	0/2927	0.84	0/3956
1	O6	0.60	0/2927	0.87	1/3956 (0.0%)
1	O7	0.60	0/3577	0.85	3/4853 (0.1%)
1	O8	0.59	1/3577 (0.0%)	0.84	2/4853 (0.0%)
1	Q1	0.58	0/3577	0.83	1/4853 (0.0%)
1	Q2	0.58	0/3577	0.82	2/4853 (0.0%)
1	Q3	0.56	0/3577	0.81	1/4853 (0.0%)
1	Q4	0.54	0/3577	0.81	1/4853 (0.0%)
1	Q5	0.56	0/2927	0.86	0/3956
1	Q6	0.58	0/2927	0.87	1/3956 (0.0%)
1	Q7	0.62	0/3577	0.84	2/4853 (0.0%)
1	Q8	0.60	0/3577	0.83	1/4853 (0.0%)
1	S1	0.54	0/3577	0.81	0/4853
1	S2	0.55	0/3577	0.82	0/4853
1	S3	0.56	0/3577	0.84	1/4853 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	S4	0.58	0/3577	0.82	0/4853
1	S5	0.58	0/2927	0.84	0/3956
1	S6	0.62	0/2927	0.88	1/3956 (0.0%)
1	S7	0.57	0/3577	0.83	1/4853 (0.0%)
1	S8	0.55	0/3577	0.81	1/4853 (0.0%)
2	B1	0.58	0/528	0.70	0/705
2	B2	0.56	0/528	0.72	0/705
2	B3	0.56	0/528	0.72	0/705
2	B4	0.59	0/528	0.75	0/705
2	B5	0.54	0/280	0.75	0/371
2	B6	0.56	0/280	0.75	0/371
2	B7	0.55	0/528	0.71	0/705
2	B8	0.59	0/528	0.75	1/705 (0.1%)
2	D1	0.56	0/528	0.72	0/705
2	D2	0.51	0/528	0.74	0/705
2	D3	0.55	0/528	0.70	0/705
2	D4	0.59	0/528	0.71	0/705
2	D5	0.58	0/280	0.76	0/371
2	D6	0.56	0/280	0.77	0/371
2	D7	0.57	0/528	0.71	0/705
2	D8	0.59	0/528	0.76	0/705
2	F1	0.59	0/528	0.72	0/705
2	F2	0.59	0/528	0.70	0/705
2	F3	0.63	0/528	0.72	0/705
2	F4	0.62	0/528	0.73	0/705
2	F5	0.59	0/280	0.68	0/371
2	F6	0.55	0/280	0.75	0/371
2	F7	0.58	0/528	0.70	0/705
2	F8	0.59	0/528	0.74	0/705
2	H1	0.60	0/528	0.72	0/705
2	H2	0.62	0/528	0.72	0/705
2	H3	0.59	0/528	0.70	0/705
2	H4	0.60	0/528	0.75	0/705
2	H5	0.55	0/280	0.74	0/371
2	H6	0.53	0/280	0.68	0/371
2	H7	0.57	0/528	0.72	0/705
2	H8	0.59	0/528	0.74	0/705
2	J1	0.55	0/528	0.69	0/705
2	J2	0.58	0/528	0.73	0/705
2	J3	0.59	0/528	0.71	0/705
2	J4	0.57	0/528	0.71	0/705
2	J5	0.55	0/280	0.71	0/371
2	J6	0.52	0/280	0.75	0/371

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	J7	0.57	0/528	0.72	0/705
2	J8	0.58	0/528	0.73	0/705
2	L1	0.60	0/528	0.71	0/705
2	L2	0.60	0/528	0.72	0/705
2	L3	0.59	0/528	0.73	0/705
2	L4	0.61	0/528	0.75	0/705
2	L5	0.48	0/280	0.68	0/371
2	L6	0.52	0/280	0.69	0/371
2	L7	0.60	0/528	0.72	0/705
2	L8	0.61	0/528	0.72	0/705
2	N1	0.59	0/528	0.76	0/705
2	N2	0.61	0/528	0.71	0/705
2	N3	0.55	0/528	0.68	0/705
2	N4	0.61	0/528	0.76	0/705
2	N5	0.51	0/280	0.69	0/371
2	N6	0.52	0/280	0.73	0/371
2	N7	0.58	0/528	0.71	0/705
2	N8	0.56	0/528	0.72	0/705
2	P1	0.57	0/528	0.73	0/705
2	P2	0.58	0/528	0.73	0/705
2	P3	0.58	0/528	0.73	0/705
2	P4	0.60	0/528	0.73	0/705
2	P5	0.64	0/280	0.78	0/371
2	P6	0.65	0/280	0.75	0/371
2	P7	0.59	0/528	0.71	0/705
2	P8	0.57	0/528	0.75	0/705
2	R1	0.62	0/528	0.75	0/705
2	R2	0.60	0/528	0.76	0/705
2	R3	0.59	0/528	0.70	0/705
2	R4	0.60	0/528	0.77	0/705
2	R5	0.59	0/280	0.71	0/371
2	R6	0.59	0/280	0.70	0/371
2	R7	0.62	0/528	0.74	0/705
2	R8	0.65	0/528	0.73	0/705
2	T1	0.56	0/528	0.70	0/705
2	T2	0.54	0/528	0.72	0/705
2	T3	0.62	0/528	0.71	0/705
2	T4	0.60	0/528	0.71	0/705
2	T5	0.60	0/280	0.74	0/371
2	T6	0.59	0/280	0.77	0/371
2	T7	0.58	0/528	0.71	0/705
2	T8	0.62	0/528	0.79	0/705
All	All	0.57	2/310426 (0.0%)	0.82	49/420002 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O8	207	ASN	CA-C	5.44	1.55	1.52
1	O2	207	ASN	CA-C	5.01	1.55	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S3	244	ALA	N-CA-C	6.28	113.66	108.07
1	Q8	244	ALA	N-CA-C	6.18	113.57	108.07
1	A5	244	ALA	N-CA-C	6.05	113.67	108.22
1	G6	384	VAL	N-CA-C	5.94	117.39	110.62
1	S7	264	ILE	N-CA-C	5.93	116.18	108.35
1	Q2	384	VAL	N-CA-C	5.93	117.38	110.62
1	E1	244	ALA	N-CA-C	5.78	113.21	108.07
1	C1	244	ALA	N-CA-C	5.74	113.38	108.22
1	A7	124	VAL	N-CA-C	5.73	119.08	111.17
1	O8	244	ALA	N-CA-C	5.69	113.14	108.07
2	B8	89	GLY	N-CA-C	5.66	119.52	112.73
1	K4	167	ARG	N-CA-C	5.65	113.22	108.13
1	O1	124	VAL	N-CA-C	5.64	118.95	111.17
1	Q4	384	VAL	N-CA-C	5.63	117.04	110.62
1	S6	167	ARG	N-CA-C	5.62	113.19	108.13
1	I4	124	VAL	N-CA-C	5.62	118.93	111.17
1	M2	167	ARG	N-CA-C	5.61	113.27	108.22
1	K5	244	ALA	N-CA-C	5.53	113.19	108.22
1	C7	264	ILE	N-CA-C	5.52	115.12	108.06
1	O8	124	VAL	N-CA-C	5.45	118.69	111.17
1	I4	384	VAL	N-CA-C	5.44	116.82	110.62
1	S8	244	ALA	N-CA-C	5.42	112.89	108.07
1	C3	244	ALA	N-CA-C	5.40	113.08	108.22
1	Q7	124	VAL	N-CA-C	5.38	119.64	111.89
1	A5	384	VAL	N-CA-C	5.37	116.74	110.62
1	I3	384	VAL	N-CA-C	5.30	116.66	110.62
1	M8	384	VAL	N-CA-C	5.29	116.66	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I1	244	ALA	N-CA-C	5.29	114.23	108.14
1	C4	384	VAL	N-CA-C	5.29	116.64	110.62
1	Q1	167	ARG	N-CA-C	5.27	112.88	108.13
1	A4	264	ILE	N-CA-C	5.27	115.31	108.35
1	O1	384	VAL	N-CA-C	5.24	116.59	110.62
1	Q6	167	ARG	N-CA-C	5.22	112.92	108.22
1	O7	124	VAL	N-CA-C	5.22	120.20	109.34
1	E8	124	VAL	N-CA-C	5.21	116.56	110.62
1	C4	264	ILE	N-CA-C	5.18	115.03	107.88
1	O7	244	ALA	N-CA-C	5.16	112.67	108.07
1	G6	264	ILE	N-CA-C	5.14	114.97	107.88
1	Q2	106	ASP	N-CA-C	5.12	117.60	111.71
1	G5	302	ASP	N-CA-C	5.12	119.50	113.16
1	O7	264	ILE	N-CA-C	5.11	115.10	108.35
1	Q3	384	VAL	N-CA-C	5.11	116.44	110.62
1	O6	384	VAL	N-CA-C	5.10	116.43	110.62
1	K6	384	VAL	N-CA-C	5.08	116.41	110.62
1	M4	384	VAL	N-CA-C	5.06	118.16	111.17
1	C8	124	VAL	N-CA-C	5.06	116.39	110.62
1	M3	124	VAL	N-CA-C	5.06	118.15	111.17
1	Q7	264	ILE	N-CA-C	5.02	115.60	108.42
1	G1	269	PHE	N-CA-C	5.02	117.48	111.71

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	21	0
1	A2	3493	0	3418	19	0
1	A3	3493	0	3418	18	0
1	A4	3486	0	3412	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A5	3493	0	2831	19	0
1	A6	3493	0	2831	19	0
1	A7	3493	0	3418	21	0
1	A8	3493	0	3418	23	0
1	C1	3493	0	3418	22	0
1	C2	3493	0	3418	16	0
1	C3	3493	0	3418	16	0
1	C4	3493	0	3418	17	0
1	C5	3493	0	2831	15	0
1	C6	3493	0	2831	15	0
1	C7	3493	0	3418	27	0
1	C8	3493	0	3418	24	0
1	E1	3493	0	3418	20	0
1	E2	3493	0	3418	24	0
1	E3	3493	0	3418	18	0
1	E4	3493	0	3418	23	0
1	E5	3493	0	2831	20	0
1	E6	3493	0	2831	13	0
1	E7	3493	0	3418	23	1
1	E8	3493	0	3418	24	0
1	G1	3493	0	3418	20	0
1	G2	3493	0	3418	19	0
1	G3	3493	0	3418	21	0
1	G4	3493	0	3418	19	0
1	G5	3493	0	2831	17	0
1	G6	3493	0	2831	15	0
1	G7	3493	0	3418	14	0
1	G8	3493	0	3418	20	0
1	I1	3493	0	3418	20	0
1	I2	3493	0	3418	20	0
1	I3	3493	0	3418	22	1
1	I4	3493	0	3418	17	0
1	I5	3493	0	2831	21	0
1	I6	3493	0	2831	22	0
1	I7	3493	0	3418	20	0
1	I8	3493	0	3418	16	0
1	K1	3493	0	3418	22	0
1	K2	3493	0	3418	22	0
1	K3	3493	0	3418	26	1
1	K4	3493	0	3418	26	0
1	K5	3493	0	2831	14	0
1	K6	3493	0	2831	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K7	3493	0	3418	17	0
1	K8	3493	0	3418	18	0
1	M1	3493	0	3418	21	0
1	M2	3493	0	3418	18	0
1	M3	3493	0	3418	18	0
1	M4	3493	0	3418	16	0
1	M5	3493	0	2831	16	0
1	M6	3493	0	2831	18	0
1	M7	3493	0	3418	22	0
1	M8	3493	0	3418	20	0
1	O1	3493	0	3418	16	0
1	O2	3493	0	3418	20	0
1	O3	3493	0	3418	19	0
1	O4	3493	0	3418	25	0
1	O5	3493	0	2831	19	0
1	O6	3493	0	2831	19	0
1	O7	3493	0	3418	21	1
1	O8	3493	0	3418	21	0
1	Q1	3493	0	3418	14	0
1	Q2	3493	0	3418	15	0
1	Q3	3493	0	3418	16	0
1	Q4	3493	0	3418	20	0
1	Q5	3493	0	2831	22	0
1	Q6	3493	0	2831	25	0
1	Q7	3493	0	3418	19	0
1	Q8	3493	0	3418	22	0
1	S1	3493	0	3418	21	0
1	S2	3493	0	3418	20	0
1	S3	3493	0	3418	19	0
1	S4	3493	0	3418	22	0
1	S5	3493	0	2831	18	0
1	S6	3493	0	2831	20	0
1	S7	3493	0	3418	19	0
1	S8	3493	0	3418	17	0
2	B1	520	0	486	3	0
2	B2	520	0	485	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1418	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 (1418) 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
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
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
2:F3:110:CYS:HG	3:F3:302:ZN:ZN	0.61	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:H3:83:CYS:HG	3:H3:302:ZN:ZN	0.98	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H3:83:CYS:SG	3:H3:302:ZN:ZN	1.82	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
1:A3:318:LEU:HD23	1:A3:326:ILE:HD12	1.77	0.66
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:Q3:262:MET:HE2	1:Q3:262:MET:HA	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
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
2:R8:75:CYS:HG	3:R8:301:ZN:ZN	0.45	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
2:R3:75:CYS:SG	3:R3:301:ZN:ZN	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K6:262:MET:HE2	1:K6:262:MET:HA	1.80	0.62
1:Q5:293:ILE:CG2	1:Q5:318:LEU:HD21	2.28	0.62
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:C5:301:MET:HE2	1:C6:301:MET:HE2	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:A8:262:MET:HA	1:A8:262:MET:HE2	1.82	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:O7:262:MET:HE2	1:O7:262:MET:HA	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:S5:262:MET:HE2	1:S5:262:MET:HA	1.84	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:M1:301:MET:HE2	1:M2:301:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M3:301:MET:HE2	1:M4:301:MET:HE2	1.85	0.58
1:G1:293:ILE:CG2	1:G1:318:LEU:HD21	2.33	0.58
1:I7:301:MET:HE2	1:I8:301:MET:HE2	1.86	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:C8:262:MET:HA	1:C8:262:MET:HE2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E7:301:MET:HE2	1:E8:301:MET:HE2	1.87	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
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:A5:389:ALA:CB	1:A5:438:MET:HE1	2.35	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:O3:301:MET:HE2	1:O4:301:MET:HE2	1.88	0.56
1:S1:318:LEU:HD23	1:S1:326:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A4:262:MET:HA	1:A4:262:MET:HE2	1.87	0.55
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:G1:389:ALA:CB	1:G1:438:MET:HE1	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
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:I4:389:ALA:CB	1:I4:438:MET:HE1	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S5:301:MET:HE2	1:S6:301:MET:HE2	1.90	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:O2:262:MET:HE2	1:O2:262:MET:HA	1.89	0.52
1:A8:214:TRP:CE3	1:A8:253:ARG:HG2	2.44	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E3:301:MET:HE2	1:E4:301:MET:HE2	1.92	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:I8:389:ALA:CB	1:I8:438:MET:HE1	2.40	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:S1:262:MET:HE2	1:S1:262:MET:HA	1.91	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
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:K3:262:MET:HA	1:K3:262:MET:HE2	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G6:389:ALA:CB	1:G6:438:MET:HE1	2.41	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:I1:389:ALA:CB	1:I1:438:MET:HE1	2.41	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:E2:389:ALA:CB	1:E2:438:MET:HE1	2.41	0.50
1:E7:335:LEU:HD21	1:E7:393:ILE:HG12	1.93	0.50
1:G4:389:ALA:CB	1:G4:438:MET:HE1	2.41	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:A2:389:ALA:CB	1:A2:438:MET:HE1	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A8:389:ALA:CB	1:A8:438:MET:HE1	2.42	0.50
1:K2:389:ALA:CB	1:K2:438:MET:HE1	2.42	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:Q7:262:MET:HE2	1:Q7:262:MET:HA	1.94	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:S7:301:MET:HE2	1:S8:301:MET:HE2	1.93	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M2:266:MET:HE3	1:M2:294:HIS:HB2	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:M4:389:ALA:CB	1:M4:438:MET:HE1	2.43	0.49
1:O4:34:THR:HG21	1:O5:142:VAL:HG11	1.95	0.49
1:Q7:389:ALA:CB	1:Q7:438:MET:HE1	2.43	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:A3:262:MET:HE2	1:A3:262:MET:HA	1.95	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:S7:26:THR:C	1:S7:28:ASP:H	2.21	0.49
1:E6:389:ALA:HB2	1:E6:438:MET:HE1	1.93	0.48
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:O5:389:ALA:CB	1:O5:438:MET:HE1	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K7:389:ALA:CB	1:K7:438:MET:HE1	2.42	0.48
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:Q6:389:ALA:CB	1:Q6:438:MET:HE1	2.44	0.48
1:S5:389:ALA:CB	1:S5:438:MET:HE1	2.43	0.48
1:I6:266:MET:HE3	1:I6:294:HIS:HB2	1.94	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:M8:389:ALA:CB	1:M8:438:MET:HE1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G1:262:MET:HE2	1:G1:262:MET:HA	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
1:G7:262:MET:HE2	1:G7:262:MET:HA	1.96	0.47
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:Q7:301:MET:HE2	1:Q8:301:MET:HE2	1.96	0.47
1:S4:61:SER:HB3	1:S4:124:VAL:HG11	1.96	0.47
1:S4:389:ALA:HB2	1:S4:438:MET:HE1	1.95	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:E6:389:ALA:CB	1:E6:438:MET:HE1	2.45	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:S3:389:ALA:CB	1:S3:438:MET:HE1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A1:262:MET:HE2	1:A1:262:MET:HA	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:O4:389:ALA:CB	1:O4:438:MET:HE1	2.44	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
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:I7:262:MET:HA	1:I7:262:MET:HE2	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:I7:389:ALA:CB	1:I7:438:MET:HE1	2.44	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:O3:262:MET:HE2	1:O3:262:MET:HA	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C7:262:MET:HE2	1:C7:262:MET:HA	1.97	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:A1:389:ALA:CB	1:A1:438:MET:HE1	2.46	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:O1:262:MET:HA	1:O1:262:MET:HE2	1.98	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:C1:389:ALA:CB	1:C1:438:MET:HE1	2.45	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
1:I6:389:ALA:CB	1:I6:438:MET:HE1	2.46	0.46
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:S2:389:ALA:CB	1:S2:438:MET:HE1	2.46	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:A3:389:ALA:CB	1:A3:438:MET:HE1	2.46	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:Q2:262:MET:HA	1:Q2:262:MET:HE2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E3:389:ALA:CB	1:E3:438:MET:HE1	2.47	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
1:C1:68:THR:O	1:C1:72:ASP:HB2	2.17	0.45
1:G5:262:MET:HE2	1:G5:262:MET:HA	1.98	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:I5:262:MET:HE2	1:I5:262:MET:HA	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M5:200:THR:HG1	1:M5:238:HIS:HD1	1.63	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:C2:389:ALA:CB	1:C2:438:MET:HE1	2.46	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:O2:389:ALA:CB	1:O2:438:MET:HE1	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O2:266:MET:HE3	1:O2:294:HIS:HB2	1.99	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:M6:389:ALA:CB	1:M6:438:MET:HE1	2.46	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:S1:200:THR:OG1	1:S1:238:HIS:ND1	2.44	0.44
1:A5:389:ALA:HB2	1:A5:438:MET:HE1	1.99	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:M7:389:ALA:CB	1:M7:438:MET:HE1	2.47	0.44
1:O2:149:GLN:HE22	1:O2:282:LYS:HA	1.82	0.44
1:O5:266:MET:HE3	1:O5:294:HIS:HB2	1.99	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
1:E5:335:LEU:HD21	1:E5:393:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I5:389:ALA:CB	1:I5:438:MET:HE1	2.48	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:S8:200:THR:OG1	1:S8:238:HIS:ND1	2.49	0.44
1:C3:88:GLU:OE2	1:C3:358:ARG:NH1	2.49	0.44
1:E1:389:ALA:CB	1:E1:438:MET:HE1	2.47	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:S1:200:THR:HG1	1:S1:238:HIS:HD1	1.61	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:C5:389:ALA:CB	1:C5:438:MET:HE1	2.48	0.44
1:K5:389:ALA:CB	1:K5:438:MET:HE1	2.48	0.44
1:K7:335:LEU:HD21	1:K7:393:ILE:HG12	2.00	0.44
1:O5:389:ALA:HB2	1:O5:438:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C4:389:ALA:CB	1:C4:438:MET:HE1	2.48	0.43
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
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:A4:389:ALA:CB	1:A4:438:MET:HE1	2.48	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:I4:262:MET:HE2	1:I4:262:MET:HA	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M8:262:MET:HA	1:M8:262:MET:HE2	2.01	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
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:M7:138:LEU:O	1:M7:316:LYS:NZ	2.45	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:S4:389:ALA:CB	1:S4:438:MET:HE1	2.49	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:E2:389:ALA:HB2	1:E2:438:MET:HE1	2.01	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:O4:389:ALA:HB2	1:O4:438:MET:HE1	2.00	0.43
1:Q2:266:MET:HE3	1:Q2:294:HIS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:K1:301:MET:HE2	1:K2:301:MET:HE2	2.01	0.43
1:K2:266:MET:HE3	1:K2:294:HIS:HB2	2.00	0.43
1:K2:335:LEU:HD22	1:K2:343:LEU:CD1	2.49	0.43
1:K6:389:ALA:CB	1:K6:438:MET:HE1	2.48	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
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:E2:106:ASP:OD2	1:E3:370:SER:OG	2.31	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:C7:389:ALA:CB	1:C7:438:MET:HE1	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:E7:262:MET:HE2	1:E7:262:MET:HA	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O8:138:LEU:O	1:O8:316:LYS:NZ	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C7:389:ALA:HB1	1:C7:438:MET:HE1	2.01	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:A6:389:ALA:CB	1:A6:438:MET:HE1	2.50	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
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:O8:266:MET:HE3	1:O8:294:HIS:HB2	2.02	0.42
1:O8:389:ALA:CB	1:O8:438:MET:HE1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I4:389:ALA:HB2	1:I4:438:MET:HE1	2.02	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:I1:266:MET:HE3	1:I1:294:HIS:HB2	2.02	0.41
1:I5:350:ARG:HG2	1:I5:374:VAL:O	2.21	0.41
1:I6:262:MET:HA	1:I6:262:MET:HE2	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K3:301:MET:HE2	1:K4:301:MET:HE2	2.03	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
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
2:B2:94:ILE:C	2:B2:103:ALA:HB2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K4:389:ALA:CB	1:K4:438:MET:HE1	2.50	0.41
1:K6:335:LEU:HD22	1:K6:343:LEU:CD1	2.50	0.41
1:M5:389:ALA:CB	1:M5:438:MET:HE1	2.51	0.41
1:M6:262:MET:HE2	1:M6:262:MET:HA	2.01	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
1:S7:114:THR:HG23	1:S8:271:THR:C	2.46	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
1:A7:262:MET:HE2	1:A7:262:MET:HA	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I1:200:THR:OG1	1:I1:238:HIS:ND1	2.49	0.41
1:I3:262:MET:HA	1:I3:262:MET:HE2	2.02	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:I1:389:ALA:HB2	1:I1:438:MET:HE1	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:I2:389:ALA:CB	1:I2:438:MET:HE1	2.50	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:M4:266:MET:HE3	1:M4:294:HIS:HB2	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C3:389:ALA:CB	1:C3:438:MET:HE1	2.51	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:G6:389:ALA:HB2	1:G6:438:MET:HE1	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
1:I2:66:TRP:HZ3	2:J1:71:VAL:HG12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A8:158:GLU:CD	1:A8:325:HIS:HE2	2.28	0.40
1:G2:328:THR:HG22	1:G2:349:LEU:CD1	2.52	0.40
1:G3:266:MET:HE3	1:G3:294:HIS:HB2	2.03	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:S1:389:ALA:CB	1:S1:438:MET:HE1	2.52	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%)	43	58
1	A2	445/475 (94%)	430 (97%)	13 (3%)	2 (0%)	30	42
1	A3	445/475 (94%)	429 (96%)	15 (3%)	1 (0%)	43	58
1	A4	445/475 (94%)	429 (96%)	13 (3%)	3 (1%)	18	27
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%)	30	42
1	A8	445/475 (94%)	427 (96%)	17 (4%)	1 (0%)	43	58
1	C1	445/475 (94%)	427 (96%)	16 (4%)	2 (0%)	30	42
1	C2	445/475 (94%)	431 (97%)	12 (3%)	2 (0%)	30	42
1	C3	445/475 (94%)	425 (96%)	19 (4%)	1 (0%)	43	58
1	C4	445/475 (94%)	428 (96%)	14 (3%)	3 (1%)	18	27
1	C5	366/475 (77%)	354 (97%)	11 (3%)	1 (0%)	36	50
1	C6	366/475 (77%)	352 (96%)	14 (4%)	0	100	100
1	C7	445/475 (94%)	429 (96%)	15 (3%)	1 (0%)	43	58
1	C8	445/475 (94%)	429 (96%)	15 (3%)	1 (0%)	43	58
1	E1	445/475 (94%)	423 (95%)	21 (5%)	1 (0%)	43	58
1	E2	445/475 (94%)	426 (96%)	17 (4%)	2 (0%)	30	42
1	E3	445/475 (94%)	424 (95%)	20 (4%)	1 (0%)	43	58
1	E4	445/475 (94%)	420 (94%)	22 (5%)	3 (1%)	18	27
1	E5	366/475 (77%)	353 (96%)	12 (3%)	1 (0%)	36	50
1	E6	366/475 (77%)	351 (96%)	15 (4%)	0	100	100
1	E7	445/475 (94%)	425 (96%)	19 (4%)	1 (0%)	43	58
1	E8	445/475 (94%)	428 (96%)	16 (4%)	1 (0%)	43	58
1	G1	445/475 (94%)	427 (96%)	17 (4%)	1 (0%)	43	58
1	G2	445/475 (94%)	425 (96%)	18 (4%)	2 (0%)	30	42
1	G3	445/475 (94%)	432 (97%)	12 (3%)	1 (0%)	43	58
1	G4	445/475 (94%)	424 (95%)	19 (4%)	2 (0%)	30	42
1	G5	366/475 (77%)	358 (98%)	8 (2%)	0	100	100
1	G6	366/475 (77%)	353 (96%)	12 (3%)	1 (0%)	36	50
1	G7	445/475 (94%)	425 (96%)	19 (4%)	1 (0%)	43	58
1	G8	445/475 (94%)	432 (97%)	12 (3%)	1 (0%)	43	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I1	445/475 (94%)	428 (96%)	16 (4%)	1 (0%)	43	58
1	I2	445/475 (94%)	433 (97%)	12 (3%)	0	100	100
1	I3	445/475 (94%)	426 (96%)	18 (4%)	1 (0%)	43	58
1	I4	445/475 (94%)	429 (96%)	15 (3%)	1 (0%)	43	58
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%)	30	42
1	I8	445/475 (94%)	428 (96%)	16 (4%)	1 (0%)	43	58
1	K1	445/475 (94%)	431 (97%)	11 (2%)	3 (1%)	18	27
1	K2	445/475 (94%)	428 (96%)	15 (3%)	2 (0%)	30	42
1	K3	445/475 (94%)	424 (95%)	19 (4%)	2 (0%)	30	42
1	K4	445/475 (94%)	425 (96%)	18 (4%)	2 (0%)	30	42
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%)	30	42
1	K8	445/475 (94%)	425 (96%)	17 (4%)	3 (1%)	18	27
1	M1	445/475 (94%)	427 (96%)	17 (4%)	1 (0%)	43	58
1	M2	445/475 (94%)	430 (97%)	14 (3%)	1 (0%)	43	58
1	M3	445/475 (94%)	426 (96%)	18 (4%)	1 (0%)	43	58
1	M4	445/475 (94%)	430 (97%)	13 (3%)	2 (0%)	30	42
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%)	30	42
1	M8	445/475 (94%)	427 (96%)	17 (4%)	1 (0%)	43	58
1	O1	445/475 (94%)	425 (96%)	19 (4%)	1 (0%)	43	58
1	O2	445/475 (94%)	422 (95%)	22 (5%)	1 (0%)	43	58
1	O3	445/475 (94%)	431 (97%)	13 (3%)	1 (0%)	43	58
1	O4	445/475 (94%)	428 (96%)	15 (3%)	2 (0%)	30	42
1	O5	366/475 (77%)	351 (96%)	15 (4%)	0	100	100
1	O6	366/475 (77%)	357 (98%)	8 (2%)	1 (0%)	36	50
1	O7	445/475 (94%)	425 (96%)	18 (4%)	2 (0%)	30	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O8	445/475 (94%)	428 (96%)	16 (4%)	1 (0%)	43	58
1	Q1	445/475 (94%)	419 (94%)	25 (6%)	1 (0%)	43	58
1	Q2	445/475 (94%)	423 (95%)	20 (4%)	2 (0%)	30	42
1	Q3	445/475 (94%)	422 (95%)	21 (5%)	2 (0%)	30	42
1	Q4	445/475 (94%)	421 (95%)	23 (5%)	1 (0%)	43	58
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%)	43	58
1	Q8	445/475 (94%)	426 (96%)	17 (4%)	2 (0%)	30	42
1	S1	445/475 (94%)	427 (96%)	17 (4%)	1 (0%)	43	58
1	S2	445/475 (94%)	429 (96%)	14 (3%)	2 (0%)	30	42
1	S3	445/475 (94%)	422 (95%)	20 (4%)	3 (1%)	18	27
1	S4	445/475 (94%)	426 (96%)	19 (4%)	0	100	100
1	S5	366/475 (77%)	347 (95%)	18 (5%)	1 (0%)	36	50
1	S6	366/475 (77%)	351 (96%)	15 (4%)	0	100	100
1	S7	445/475 (94%)	420 (94%)	24 (5%)	1 (0%)	43	58
1	S8	445/475 (94%)	422 (95%)	20 (4%)	3 (1%)	18	27
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%)	9	12
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%)	36	50

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%)	78	87
1	A2	359/385 (93%)	356 (99%)	3 (1%)	73	84
1	A3	359/385 (93%)	356 (99%)	3 (1%)	73	84
1	A4	357/385 (93%)	354 (99%)	3 (1%)	73	84
1	A5	292/385 (76%)	291 (100%)	1 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A6	292/385 (76%)	289 (99%)	3 (1%)	68	80
1	A7	359/385 (93%)	355 (99%)	4 (1%)	65	79
1	A8	359/385 (93%)	358 (100%)	1 (0%)	86	93
1	C1	359/385 (93%)	358 (100%)	1 (0%)	86	93
1	C2	359/385 (93%)	355 (99%)	4 (1%)	65	79
1	C3	359/385 (93%)	354 (99%)	5 (1%)	59	75
1	C4	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	C5	292/385 (76%)	291 (100%)	1 (0%)	86	93
1	C6	292/385 (76%)	289 (99%)	3 (1%)	68	80
1	C7	359/385 (93%)	356 (99%)	3 (1%)	73	84
1	C8	359/385 (93%)	358 (100%)	1 (0%)	86	93
1	E1	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	E2	359/385 (93%)	358 (100%)	1 (0%)	86	93
1	E3	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	E4	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	E5	292/385 (76%)	291 (100%)	1 (0%)	86	93
1	E6	292/385 (76%)	290 (99%)	2 (1%)	76	86
1	E7	359/385 (93%)	356 (99%)	3 (1%)	73	84
1	E8	359/385 (93%)	359 (100%)	0	100	100
1	G1	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	G2	359/385 (93%)	358 (100%)	1 (0%)	86	93
1	G3	359/385 (93%)	358 (100%)	1 (0%)	86	93
1	G4	359/385 (93%)	359 (100%)	0	100	100
1	G5	292/385 (76%)	292 (100%)	0	100	100
1	G6	292/385 (76%)	290 (99%)	2 (1%)	76	86
1	G7	359/385 (93%)	356 (99%)	3 (1%)	73	84
1	G8	359/385 (93%)	356 (99%)	3 (1%)	73	84
1	I1	359/385 (93%)	358 (100%)	1 (0%)	86	93
1	I2	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	I3	359/385 (93%)	358 (100%)	1 (0%)	86	93
1	I4	359/385 (93%)	357 (99%)	2 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I5	292/385 (76%)	288 (99%)	4 (1%)	59	75
1	I6	292/385 (76%)	291 (100%)	1 (0%)	86	93
1	I7	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	I8	359/385 (93%)	355 (99%)	4 (1%)	65	79
1	K1	359/385 (93%)	356 (99%)	3 (1%)	73	84
1	K2	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	K3	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	K4	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	K5	292/385 (76%)	290 (99%)	2 (1%)	76	86
1	K6	292/385 (76%)	288 (99%)	4 (1%)	59	75
1	K7	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	K8	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	M1	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	M2	359/385 (93%)	359 (100%)	0	100	100
1	M3	359/385 (93%)	359 (100%)	0	100	100
1	M4	359/385 (93%)	355 (99%)	4 (1%)	65	79
1	M5	292/385 (76%)	290 (99%)	2 (1%)	76	86
1	M6	292/385 (76%)	289 (99%)	3 (1%)	68	80
1	M7	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	M8	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	O1	359/385 (93%)	354 (99%)	5 (1%)	59	75
1	O2	359/385 (93%)	356 (99%)	3 (1%)	73	84
1	O3	359/385 (93%)	354 (99%)	5 (1%)	59	75
1	O4	359/385 (93%)	358 (100%)	1 (0%)	86	93
1	O5	292/385 (76%)	291 (100%)	1 (0%)	86	93
1	O6	292/385 (76%)	289 (99%)	3 (1%)	68	80
1	O7	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	O8	359/385 (93%)	356 (99%)	3 (1%)	73	84
1	Q1	359/385 (93%)	358 (100%)	1 (0%)	86	93
1	Q2	359/385 (93%)	358 (100%)	1 (0%)	86	93
1	Q3	359/385 (93%)	358 (100%)	1 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q4	359/385 (93%)	358 (100%)	1 (0%)	86	93
1	Q5	292/385 (76%)	292 (100%)	0	100	100
1	Q6	292/385 (76%)	291 (100%)	1 (0%)	86	93
1	Q7	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	Q8	359/385 (93%)	356 (99%)	3 (1%)	73	84
1	S1	359/385 (93%)	355 (99%)	4 (1%)	65	79
1	S2	359/385 (93%)	356 (99%)	3 (1%)	73	84
1	S3	359/385 (93%)	359 (100%)	0	100	100
1	S4	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	S5	292/385 (76%)	292 (100%)	0	100	100
1	S6	292/385 (76%)	290 (99%)	2 (1%)	76	86
1	S7	359/385 (93%)	357 (99%)	2 (1%)	78	87
1	S8	359/385 (93%)	356 (99%)	3 (1%)	73	84
2	B1	54/60 (90%)	54 (100%)	0	100	100
2	B2	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	B3	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	B4	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	B5	27/60 (45%)	27 (100%)	0	100	100
2	B6	27/60 (45%)	26 (96%)	1 (4%)	30	49
2	B7	54/60 (90%)	54 (100%)	0	100	100
2	B8	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	D1	54/60 (90%)	52 (96%)	2 (4%)	30	49
2	D2	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	D3	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	D4	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	D5	27/60 (45%)	27 (100%)	0	100	100
2	D6	27/60 (45%)	26 (96%)	1 (4%)	30	49
2	D7	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	D8	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	F1	54/60 (90%)	53 (98%)	1 (2%)	50	70
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%)	53 (98%)	1 (2%)	50	70
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%)	30	49
2	F7	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	F8	54/60 (90%)	54 (100%)	0	100	100
2	H1	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	H2	54/60 (90%)	54 (100%)	0	100	100
2	H3	54/60 (90%)	54 (100%)	0	100	100
2	H4	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	H5	27/60 (45%)	27 (100%)	0	100	100
2	H6	27/60 (45%)	27 (100%)	0	100	100
2	H7	54/60 (90%)	54 (100%)	0	100	100
2	H8	54/60 (90%)	54 (100%)	0	100	100
2	J1	54/60 (90%)	52 (96%)	2 (4%)	30	49
2	J2	54/60 (90%)	52 (96%)	2 (4%)	30	49
2	J3	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	J4	54/60 (90%)	52 (96%)	2 (4%)	30	49
2	J5	27/60 (45%)	27 (100%)	0	100	100
2	J6	27/60 (45%)	26 (96%)	1 (4%)	30	49
2	J7	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	J8	54/60 (90%)	54 (100%)	0	100	100
2	L1	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	L2	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	L3	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	L4	54/60 (90%)	51 (94%)	3 (6%)	19	31
2	L5	27/60 (45%)	27 (100%)	0	100	100
2	L6	27/60 (45%)	27 (100%)	0	100	100
2	L7	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	L8	54/60 (90%)	52 (96%)	2 (4%)	30	49
2	N1	54/60 (90%)	53 (98%)	1 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N2	54/60 (90%)	54 (100%)	0	100	100
2	N3	54/60 (90%)	54 (100%)	0	100	100
2	N4	54/60 (90%)	54 (100%)	0	100	100
2	N5	27/60 (45%)	26 (96%)	1 (4%)	30	49
2	N6	27/60 (45%)	27 (100%)	0	100	100
2	N7	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	N8	54/60 (90%)	54 (100%)	0	100	100
2	P1	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	P2	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	P3	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	P4	54/60 (90%)	54 (100%)	0	100	100
2	P5	27/60 (45%)	26 (96%)	1 (4%)	30	49
2	P6	27/60 (45%)	26 (96%)	1 (4%)	30	49
2	P7	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	P8	54/60 (90%)	54 (100%)	0	100	100
2	R1	54/60 (90%)	52 (96%)	2 (4%)	30	49
2	R2	54/60 (90%)	54 (100%)	0	100	100
2	R3	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	R4	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	R5	27/60 (45%)	26 (96%)	1 (4%)	30	49
2	R6	27/60 (45%)	27 (100%)	0	100	100
2	R7	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	R8	54/60 (90%)	52 (96%)	2 (4%)	30	49
2	T1	54/60 (90%)	52 (96%)	2 (4%)	30	49
2	T2	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	T3	54/60 (90%)	52 (96%)	2 (4%)	30	49
2	T4	54/60 (90%)	54 (100%)	0	100	100
2	T5	27/60 (45%)	26 (96%)	1 (4%)	30	49
2	T6	27/60 (45%)	26 (96%)	1 (4%)	30	49
2	T7	54/60 (90%)	53 (98%)	1 (2%)	50	70
2	T8	54/60 (90%)	51 (94%)	3 (6%)	19	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	31156/35600 (88%)	30926 (99%)	230 (1%)	76	86

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	51	GLU
1	A1	223	ASP
1	A2	51	GLU
1	A2	200	THR
1	A2	239	TYR
1	A3	51	GLU
1	A3	239	TYR
1	A3	438	MET
1	A4	124	VAL
1	A4	326	ILE
1	A4	331	VAL
1	A5	331	VAL
1	A6	239	TYR
1	A6	326	ILE
1	A6	447	GLU
1	A7	23	THR
1	A7	51	GLU
1	A7	239	TYR
1	A7	326	ILE
1	A8	326	ILE
1	C1	239	TYR
1	C2	51	GLU
1	C2	239	TYR
1	C2	326	ILE
1	C2	338	ASP
1	C3	23	THR
1	C3	51	GLU
1	C3	181	SER
1	C3	200	THR
1	C3	223	ASP
1	C4	326	ILE
1	C4	450	ARG
1	C5	223	ASP
1	C6	239	TYR
1	C6	326	ILE
1	C6	379	SER
1	C7	51	GLU

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Mol	Chain	Res	Type
1	C7	65	THR
1	C7	331	VAL
1	C8	326	ILE
1	E1	239	TYR
1	E1	326	ILE
1	E2	438	MET
1	E3	200	THR
1	E3	239	TYR
1	E4	239	TYR
1	E4	326	ILE
1	E5	223	ASP
1	E6	200	THR
1	E6	239	TYR
1	E7	200	THR
1	E7	239	TYR
1	E7	356	GLN
1	G1	239	TYR
1	G1	438	MET
1	G2	239	TYR
1	G3	200	THR
1	G6	239	TYR
1	G6	326	ILE
1	G7	65	THR
1	G7	239	TYR
1	G7	326	ILE
1	G8	23	THR
1	G8	326	ILE
1	G8	331	VAL
1	I1	51	GLU
1	I2	239	TYR
1	I2	326	ILE
1	I3	223	ASP
1	I4	51	GLU
1	I4	326	ILE
1	I5	223	ASP
1	I5	239	TYR
1	I5	331	VAL
1	I5	450	ARG
1	I6	239	TYR
1	I7	239	TYR
1	I7	326	ILE
1	I8	71	THR

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Mol	Chain	Res	Type
1	I8	223	ASP
1	I8	239	TYR
1	I8	326	ILE
1	K1	119	SER
1	K1	223	ASP
1	K1	239	TYR
1	K2	51	GLU
1	K2	200	THR
1	K3	356	GLN
1	K3	450	ARG
1	K4	239	TYR
1	K4	326	ILE
1	K5	326	ILE
1	K5	438	MET
1	K6	239	TYR
1	K6	326	ILE
1	K6	338	ASP
1	K6	438	MET
1	K7	239	TYR
1	K7	438	MET
1	K8	239	TYR
1	K8	326	ILE
1	M1	23	THR
1	M1	326	ILE
1	M4	200	THR
1	M4	223	ASP
1	M4	326	ILE
1	M4	331	VAL
1	M5	338	ASP
1	M5	438	MET
1	M6	326	ILE
1	M6	438	MET
1	M6	450	ARG
1	M7	326	ILE
1	M7	331	VAL
1	M8	51	GLU
1	M8	326	ILE
1	O1	51	GLU
1	O1	223	ASP
1	O1	239	TYR
1	O1	326	ILE
1	O1	331	VAL

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Mol	Chain	Res	Type
1	O2	177	LYS
1	O2	239	TYR
1	O2	326	ILE
1	O3	200	THR
1	O3	239	TYR
1	O3	326	ILE
1	O3	438	MET
1	O3	450	ARG
1	O4	326	ILE
1	O5	331	VAL
1	O6	239	TYR
1	O6	326	ILE
1	O6	356	GLN
1	O7	51	GLU
1	O7	302	ASP
1	O8	326	ILE
1	O8	331	VAL
1	O8	450	ARG
1	Q1	200	THR
1	Q2	23	THR
1	Q3	181	SER
1	Q4	326	ILE
1	Q6	356	GLN
1	Q7	51	GLU
1	Q7	200	THR
1	Q8	119	SER
1	Q8	326	ILE
1	Q8	356	GLN
1	S1	36	ILE
1	S1	239	TYR
1	S1	326	ILE
1	S1	338	ASP
1	S2	51	GLU
1	S2	326	ILE
1	S2	438	MET
1	S4	223	ASP
1	S4	326	ILE
1	S6	200	THR
1	S6	356	GLN
1	S7	239	TYR
1	S7	450	ARG
1	S8	36	ILE

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Mol	Chain	Res	Type
1	S8	223	ASP
1	S8	326	ILE
2	B2	71	VAL
2	B3	71	VAL
2	B4	136	GLU
2	B6	136	GLU
2	B8	91	VAL
2	D1	71	VAL
2	D1	94	ILE
2	D2	71	VAL
2	D3	135	ASP
2	D4	135	ASP
2	D6	136	GLU
2	D7	98	ASN
2	D8	136	GLU
2	F1	135	ASP
2	F3	132	SER
2	F6	120	ASP
2	F7	135	ASP
2	H1	94	ILE
2	H4	136	GLU
2	J1	71	VAL
2	J1	135	ASP
2	J2	71	VAL
2	J2	135	ASP
2	J3	71	VAL
2	J4	71	VAL
2	J4	136	GLU
2	J6	135	ASP
2	J7	136	GLU
2	L1	91	VAL
2	L2	136	GLU
2	L3	98	ASN
2	L4	71	VAL
2	L4	135	ASP
2	L4	136	GLU
2	L7	74	ASN
2	L8	74	ASN
2	L8	93	LEU
2	N1	93	LEU
2	N5	131	LEU
2	N7	135	ASP

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Mol	Chain	Res	Type
2	P1	136	GLU
2	P2	135	ASP
2	P3	120	ASP
2	P5	136	GLU
2	P6	136	GLU
2	P7	136	GLU
2	R1	74	ASN
2	R1	95	ASP
2	R3	136	GLU
2	R4	100	GLN
2	R5	135	ASP
2	R7	74	ASN
2	R8	97	PHE
2	R8	120	ASP
2	T1	131	LEU
2	T1	135	ASP
2	T2	74	ASN
2	T3	135	ASP
2	T3	136	GLU
2	T5	136	GLU
2	T6	136	GLU
2	T7	136	GLU
2	T8	93	LEU
2	T8	102	LYS
2	T8	136	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (477) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	95	ASN
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	386	HIS
1	A3	115	ASN
1	A3	149	GLN
1	A3	153	HIS

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Mol	Chain	Res	Type
1	A3	207	ASN
1	A3	401	GLN
1	A3	420	ASN
1	A4	115	ASN
1	A4	149	GLN
1	A4	153	HIS
1	A4	207	ASN
1	A4	209	GLN
1	A4	304	GLN
1	A5	383	HIS
1	A5	386	HIS
1	A6	149	GLN
1	A6	153	HIS
1	A6	327	HIS
1	A6	401	GLN
1	A7	277	ASN
1	A7	310	HIS
1	A7	386	HIS
1	A7	401	GLN
1	A7	420	ASN
1	A8	149	GLN
1	A8	163	ASN
1	A8	310	HIS
1	A8	386	HIS
1	C1	115	ASN
1	C1	149	GLN
1	C1	153	HIS
1	C1	207	ASN
1	C1	310	HIS
1	C1	327	HIS
1	C2	96	GLN
1	C2	115	ASN
1	C2	149	GLN
1	C2	153	HIS
1	C2	207	ASN
1	C2	401	GLN
1	C2	413	ASN
1	C2	420	ASN
1	C3	149	GLN
1	C3	153	HIS
1	C3	277	ASN
1	C3	310	HIS

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Mol	Chain	Res	Type
1	C4	96	GLN
1	C4	149	GLN
1	C4	153	HIS
1	C4	241	ASN
1	C4	386	HIS
1	C4	420	ASN
1	C5	149	GLN
1	C5	207	ASN
1	C5	356	GLN
1	C5	386	HIS
1	C5	420	ASN
1	C6	115	ASN
1	C6	149	GLN
1	C6	153	HIS
1	C6	310	HIS
1	C6	386	HIS
1	C6	401	GLN
1	C6	420	ASN
1	C7	115	ASN
1	C7	149	GLN
1	C7	153	HIS
1	C7	163	ASN
1	C7	207	ASN
1	C7	356	GLN
1	C7	401	GLN
1	C7	413	ASN
1	C7	420	ASN
1	C8	95	ASN
1	C8	96	GLN
1	C8	149	GLN
1	C8	207	ASN
1	C8	356	GLN
1	E1	149	GLN
1	E1	304	GLN
1	E1	327	HIS
1	E1	420	ASN
1	E2	115	ASN
1	E2	149	GLN
1	E2	153	HIS
1	E2	307	HIS
1	E2	327	HIS
1	E2	356	GLN

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Mol	Chain	Res	Type
1	E2	386	HIS
1	E3	149	GLN
1	E3	304	GLN
1	E3	310	HIS
1	E3	327	HIS
1	E3	356	GLN
1	E3	401	GLN
1	E3	420	ASN
1	E4	95	ASN
1	E4	327	HIS
1	E4	386	HIS
1	E4	420	ASN
1	E5	149	GLN
1	E5	205	ASN
1	E5	207	ASN
1	E5	241	ASN
1	E5	304	GLN
1	E5	327	HIS
1	E5	386	HIS
1	E5	420	ASN
1	E6	115	ASN
1	E6	149	GLN
1	E6	153	HIS
1	E6	241	ASN
1	E6	277	ASN
1	E6	304	GLN
1	E6	327	HIS
1	E7	96	GLN
1	E7	115	ASN
1	E7	153	HIS
1	E7	163	ASN
1	E7	241	ASN
1	E7	287	ASN
1	E7	310	HIS
1	E7	356	GLN
1	E7	386	HIS
1	E7	420	ASN
1	E8	96	GLN
1	E8	149	GLN
1	E8	153	HIS
1	E8	327	HIS
1	E8	386	HIS

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Mol	Chain	Res	Type
1	G1	149	GLN
1	G1	153	HIS
1	G1	420	ASN
1	G2	115	ASN
1	G2	149	GLN
1	G2	327	HIS
1	G2	356	GLN
1	G2	401	GLN
1	G2	420	ASN
1	G3	207	ASN
1	G3	241	ASN
1	G3	432	ASN
1	G4	96	GLN
1	G4	115	ASN
1	G4	149	GLN
1	G4	153	HIS
1	G4	277	ASN
1	G4	386	HIS
1	G5	115	ASN
1	G5	153	HIS
1	G5	386	HIS
1	G5	420	ASN
1	G6	115	ASN
1	G6	149	GLN
1	G6	153	HIS
1	G6	207	ASN
1	G6	310	HIS
1	G6	356	GLN
1	G6	386	HIS
1	G6	401	GLN
1	G7	149	GLN
1	G7	207	ASN
1	G7	277	ASN
1	G7	304	GLN
1	G7	310	HIS
1	G7	401	GLN
1	G7	413	ASN
1	G7	420	ASN
1	G7	429	GLN
1	G7	432	ASN
1	G8	115	ASN
1	G8	149	GLN

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Mol	Chain	Res	Type
1	G8	153	HIS
1	G8	163	ASN
1	G8	386	HIS
1	I1	95	ASN
1	I1	115	ASN
1	I1	149	GLN
1	I1	153	HIS
1	I1	327	HIS
1	I2	95	ASN
1	I2	115	ASN
1	I2	149	GLN
1	I2	153	HIS
1	I2	310	HIS
1	I2	383	HIS
1	I2	386	HIS
1	I2	401	GLN
1	I3	115	ASN
1	I3	149	GLN
1	I3	153	HIS
1	I3	207	ASN
1	I3	304	GLN
1	I3	420	ASN
1	I4	115	ASN
1	I4	149	GLN
1	I4	153	HIS
1	I4	207	ASN
1	I4	327	HIS
1	I4	356	GLN
1	I4	386	HIS
1	I4	420	ASN
1	I5	115	ASN
1	I5	149	GLN
1	I5	327	HIS
1	I5	356	GLN
1	I5	386	HIS
1	I5	401	GLN
1	I5	420	ASN
1	I6	115	ASN
1	I6	149	GLN
1	I6	153	HIS
1	I6	205	ASN
1	I6	386	HIS

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Mol	Chain	Res	Type
1	I6	401	GLN
1	I6	420	ASN
1	I7	149	GLN
1	I7	153	HIS
1	I7	163	ASN
1	I7	356	GLN
1	I7	420	ASN
1	I8	149	GLN
1	I8	277	ASN
1	I8	327	HIS
1	I8	386	HIS
1	K1	115	ASN
1	K1	149	GLN
1	K1	241	ASN
1	K1	277	ASN
1	K1	401	GLN
1	K1	420	ASN
1	K2	149	GLN
1	K2	205	ASN
1	K2	310	HIS
1	K2	356	GLN
1	K2	386	HIS
1	K2	401	GLN
1	K2	420	ASN
1	K3	45	GLN
1	K3	153	HIS
1	K3	205	ASN
1	K3	327	HIS
1	K3	356	GLN
1	K3	429	GLN
1	K4	96	GLN
1	K4	149	GLN
1	K4	153	HIS
1	K4	156	GLN
1	K4	310	HIS
1	K4	327	HIS
1	K4	356	GLN
1	K4	413	ASN
1	K4	420	ASN
1	K5	115	ASN
1	K5	149	GLN
1	K5	327	HIS

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Mol	Chain	Res	Type
1	K5	420	ASN
1	K6	115	ASN
1	K6	310	HIS
1	K6	356	GLN
1	K6	386	HIS
1	K6	420	ASN
1	K7	149	GLN
1	K7	356	GLN
1	K8	96	GLN
1	K8	149	GLN
1	K8	153	HIS
1	K8	310	HIS
1	K8	386	HIS
1	M1	115	ASN
1	M1	149	GLN
1	M1	153	HIS
1	M1	205	ASN
1	M1	356	GLN
1	M1	386	HIS
1	M1	401	GLN
1	M2	115	ASN
1	M2	149	GLN
1	M2	153	HIS
1	M2	327	HIS
1	M2	383	HIS
1	M2	386	HIS
1	M2	401	GLN
1	M2	420	ASN
1	M3	96	GLN
1	M3	115	ASN
1	M3	149	GLN
1	M3	356	GLN
1	M3	420	ASN
1	M4	96	GLN
1	M4	149	GLN
1	M4	153	HIS
1	M4	156	GLN
1	M4	207	ASN
1	M4	356	GLN
1	M4	386	HIS
1	M5	149	GLN
1	M5	153	HIS

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Mol	Chain	Res	Type
1	M5	310	HIS
1	M5	327	HIS
1	M5	420	ASN
1	M6	115	ASN
1	M6	149	GLN
1	M6	153	HIS
1	M6	163	ASN
1	M6	241	ASN
1	M6	277	ASN
1	M6	386	HIS
1	M6	420	ASN
1	M7	96	GLN
1	M7	149	GLN
1	M7	153	HIS
1	M7	356	GLN
1	M7	386	HIS
1	M8	153	HIS
1	M8	209	GLN
1	M8	327	HIS
1	M8	356	GLN
1	M8	386	HIS
1	M8	420	ASN
1	O1	115	ASN
1	O1	149	GLN
1	O1	153	HIS
1	O1	310	HIS
1	O1	401	GLN
1	O2	115	ASN
1	O2	149	GLN
1	O2	304	GLN
1	O2	401	GLN
1	O3	96	GLN
1	O3	149	GLN
1	O3	153	HIS
1	O3	420	ASN
1	O4	149	GLN
1	O4	153	HIS
1	O4	287	ASN
1	O4	327	HIS
1	O4	420	ASN
1	O5	153	HIS
1	O5	356	GLN

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Mol	Chain	Res	Type
1	O5	401	GLN
1	O6	149	GLN
1	O6	241	ASN
1	O6	420	ASN
1	O7	149	GLN
1	O7	153	HIS
1	O7	310	HIS
1	O7	420	ASN
1	O8	96	GLN
1	O8	115	ASN
1	O8	149	GLN
1	O8	205	ASN
1	O8	241	ASN
1	O8	356	GLN
1	O8	386	HIS
1	O8	420	ASN
1	Q1	149	GLN
1	Q1	277	ASN
1	Q1	327	HIS
1	Q1	356	GLN
1	Q2	96	GLN
1	Q2	149	GLN
1	Q2	153	HIS
1	Q2	207	ASN
1	Q2	226	HIS
1	Q2	310	HIS
1	Q2	327	HIS
1	Q2	386	HIS
1	Q2	401	GLN
1	Q3	96	GLN
1	Q3	115	ASN
1	Q3	153	HIS
1	Q3	327	HIS
1	Q3	356	GLN
1	Q4	310	HIS
1	Q4	327	HIS
1	Q5	149	GLN
1	Q5	205	ASN
1	Q5	386	HIS
1	Q5	401	GLN
1	Q5	420	ASN
1	Q6	241	ASN

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Mol	Chain	Res	Type
1	Q6	277	ASN
1	Q6	401	GLN
1	Q6	413	ASN
1	Q6	420	ASN
1	Q7	209	GLN
1	Q7	241	ASN
1	Q7	267	HIS
1	Q7	327	HIS
1	Q8	149	GLN
1	Q8	153	HIS
1	Q8	156	GLN
1	Q8	205	ASN
1	Q8	209	GLN
1	Q8	277	ASN
1	Q8	356	GLN
1	S1	149	GLN
1	S1	310	HIS
1	S1	420	ASN
1	S2	115	ASN
1	S2	149	GLN
1	S2	153	HIS
1	S2	277	ASN
1	S2	401	GLN
1	S3	96	GLN
1	S3	149	GLN
1	S3	153	HIS
1	S3	304	GLN
1	S3	327	HIS
1	S3	356	GLN
1	S4	153	HIS
1	S4	356	GLN
1	S4	420	ASN
1	S5	149	GLN
1	S5	153	HIS
1	S5	205	ASN
1	S5	241	ASN
1	S5	356	GLN
1	S5	401	GLN
1	S6	115	ASN
1	S6	149	GLN
1	S6	153	HIS
1	S6	207	ASN

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Mol	Chain	Res	Type
1	S6	241	ASN
1	S6	310	HIS
1	S6	327	HIS
1	S6	420	ASN
1	S7	115	ASN
1	S7	304	GLN
1	S7	327	HIS
1	S7	429	GLN
1	S8	149	GLN
1	S8	153	HIS
1	S8	304	GLN
1	S8	307	HIS
1	S8	386	HIS
1	S8	420	ASN
2	B7	96	HIS
2	B7	100	GLN
2	D2	68	ASN
2	D3	100	GLN
2	D5	100	GLN
2	D6	100	GLN
2	F2	98	ASN
2	F4	92	ASN
2	H3	68	ASN
2	H3	100	GLN
2	H7	100	GLN
2	J1	68	ASN
2	J2	100	GLN
2	L2	100	GLN
2	L4	92	ASN
2	L7	100	GLN
2	L8	68	ASN
2	L8	92	ASN
2	N3	74	ASN
2	N7	100	GLN
2	N8	100	GLN
2	P1	100	GLN
2	P3	68	ASN
2	R1	74	ASN
2	R2	68	ASN
2	R2	98	ASN
2	R4	68	ASN
2	R5	100	GLN

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Mol	Chain	Res	Type
2	R7	92	ASN
2	T4	98	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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%)	-1.53	0 100 100	23, 42, 75, 107	0
1	A2	447/475 (94%)	-1.57	0 100 100	24, 39, 66, 119	0
1	A3	447/475 (94%)	-1.60	0 100 100	19, 33, 69, 114	0
1	A4	447/475 (94%)	-1.60	0 100 100	20, 35, 66, 104	0
1	A5	367/475 (77%)	-1.64	0 100 100	20, 32, 53, 104	0
1	A6	367/475 (77%)	-1.61	0 100 100	21, 36, 57, 104	0
1	A7	447/475 (94%)	-1.51	0 100 100	22, 42, 89, 120	0
1	A8	447/475 (94%)	-1.50	0 100 100	22, 44, 87, 132	0
1	C1	447/475 (94%)	-1.61	0 100 100	20, 31, 60, 103	0
1	C2	447/475 (94%)	-1.57	0 100 100	22, 37, 67, 115	0
1	C3	447/475 (94%)	-1.50	0 100 100	23, 41, 84, 125	0
1	C4	447/475 (94%)	-1.47	0 100 100	24, 45, 89, 140	0
1	C5	367/475 (77%)	-1.53	0 100 100	26, 44, 73, 114	0
1	C6	367/475 (77%)	-1.53	0 100 100	27, 42, 63, 109	0
1	C7	447/475 (94%)	-1.53	0 100 100	21, 39, 81, 121	0
1	C8	447/475 (94%)	-1.55	0 100 100	20, 39, 74, 118	0
1	E1	447/475 (94%)	-1.45	0 100 100	32, 54, 94, 123	0
1	E2	447/475 (94%)	-1.45	0 100 100	35, 52, 88, 135	0
1	E3	447/475 (94%)	-1.31	0 100 100	39, 71, 114, 146	0
1	E4	447/475 (94%)	-1.27	0 100 100	40, 79, 119, 161	0
1	E5	367/475 (77%)	-1.27	0 100 100	38, 74, 111, 148	0
1	E6	367/475 (77%)	-1.36	0 100 100	37, 62, 94, 139	0
1	E7	447/475 (94%)	-1.43	0 100 100	32, 53, 97, 130	0
1	E8	447/475 (94%)	-1.39	0 100 100	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%)	-1.50	0 100 100	30, 49, 85, 135	0
1	G2	447/475 (94%)	-1.41	0 100 100	34, 55, 92, 127	0
1	G3	447/475 (94%)	-1.33	0 100 100	34, 61, 106, 138	0
1	G4	447/475 (94%)	-1.37	0 100 100	34, 56, 107, 146	0
1	G5	367/475 (77%)	-1.50	0 100 100	27, 46, 74, 115	0
1	G6	367/475 (77%)	-1.56	0 100 100	24, 39, 63, 116	0
1	G7	447/475 (94%)	-1.52	0 100 100	24, 39, 78, 132	0
1	G8	447/475 (94%)	-1.52	0 100 100	24, 43, 81, 124	0
1	I1	447/475 (94%)	-1.57	0 100 100	19, 36, 70, 112	0
1	I2	447/475 (94%)	-1.54	0 100 100	26, 42, 85, 124	0
1	I3	447/475 (94%)	-1.50	0 100 100	24, 42, 83, 115	0
1	I4	447/475 (94%)	-1.51	0 100 100	25, 44, 82, 133	0
1	I5	367/475 (77%)	-1.59	0 100 100	22, 35, 58, 101	0
1	I6	367/475 (77%)	-1.57	0 100 100	22, 38, 64, 114	0
1	I7	447/475 (94%)	-1.60	0 100 100	21, 35, 75, 112	0
1	I8	447/475 (94%)	-1.54	0 100 100	23, 39, 72, 123	0
1	K1	447/475 (94%)	-1.37	0 100 100	38, 61, 101, 144	0
1	K2	447/475 (94%)	-1.41	0 100 100	38, 58, 95, 135	0
1	K3	447/475 (94%)	-1.42	0 100 100	26, 55, 99, 147	0
1	K4	447/475 (94%)	-1.45	0 100 100	30, 54, 93, 123	0
1	K5	367/475 (77%)	-1.57	0 100 100	25, 36, 58, 101	0
1	K6	367/475 (77%)	-1.55	0 100 100	26, 39, 64, 104	0
1	K7	447/475 (94%)	-1.44	0 100 100	30, 54, 92, 135	0
1	K8	447/475 (94%)	-1.41	0 100 100	31, 58, 105, 138	0
1	M1	447/475 (94%)	-1.49	0 100 100	29, 46, 83, 121	0
1	M2	447/475 (94%)	-1.44	0 100 100	31, 51, 89, 134	0
1	M3	447/475 (94%)	-1.51	0 100 100	23, 44, 84, 125	0
1	M4	447/475 (94%)	-1.48	0 100 100	27, 45, 81, 117	0
1	M5	367/475 (77%)	-1.64	0 100 100	22, 31, 52, 83	0
1	M6	367/475 (77%)	-1.60	0 100 100	21, 35, 60, 98	0
1	M7	447/475 (94%)	-1.53	0 100 100	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%)	-1.50	0 100 100	23, 43, 84, 131	0
1	O1	447/475 (94%)	-1.50	0 100 100	25, 46, 91, 121	0
1	O2	447/475 (94%)	-1.51	0 100 100	22, 42, 79, 122	0
1	O3	447/475 (94%)	-1.56	0 100 100	23, 41, 80, 113	0
1	O4	447/475 (94%)	-1.47	0 100 100	28, 49, 87, 125	0
1	O5	367/475 (77%)	-1.44	0 100 100	33, 53, 80, 122	0
1	O6	367/475 (77%)	-1.29	0 100 100	40, 62, 96, 125	0
1	O7	447/475 (94%)	-1.34	0 100 100	33, 62, 103, 141	0
1	O8	447/475 (94%)	-1.36	0 100 100	33, 59, 100, 139	0
1	Q1	447/475 (94%)	-1.23	0 100 100	43, 79, 119, 147	0
1	Q2	447/475 (94%)	-1.37	0 100 100	35, 56, 99, 142	0
1	Q3	447/475 (94%)	-1.46	0 100 100	33, 52, 90, 132	0
1	Q4	447/475 (94%)	-1.33	0 100 100	33, 66, 107, 138	0
1	Q5	367/475 (77%)	-1.31	0 100 100	37, 66, 98, 137	0
1	Q6	367/475 (77%)	-1.30	0 100 100	43, 67, 101, 138	0
1	Q7	447/475 (94%)	-1.20	0 100 100	49, 79, 124, 147	0
1	Q8	447/475 (94%)	-1.18	0 100 100	47, 82, 127, 182	0
1	S1	447/475 (94%)	-1.54	0 100 100	23, 43, 80, 112	0
1	S2	447/475 (94%)	-1.51	0 100 100	24, 44, 81, 110	0
1	S3	447/475 (94%)	-1.50	0 100 100	28, 49, 88, 121	0
1	S4	447/475 (94%)	-1.43	0 100 100	30, 55, 97, 140	0
1	S5	367/475 (77%)	-1.39	0 100 100	40, 63, 92, 130	0
1	S6	367/475 (77%)	-1.26	0 100 100	44, 72, 103, 141	0
1	S7	447/475 (94%)	-1.31	0 100 100	29, 69, 120, 157	0
1	S8	447/475 (94%)	-1.31	0 100 100	35, 70, 104, 147	0
2	B1	73/81 (90%)	-1.28	0 100 100	45, 73, 102, 112	0
2	B2	73/81 (90%)	-1.47	0 100 100	41, 57, 80, 86	0
2	B3	73/81 (90%)	-1.36	0 100 100	32, 54, 79, 100	0
2	B4	73/81 (90%)	-1.28	0 100 100	45, 62, 99, 134	0
2	B5	37/81 (45%)	-1.52	0 100 100	35, 44, 65, 74	0
2	B6	37/81 (45%)	-1.42	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%)	-1.25	0 100 100	51, 76, 106, 122	0
2	B8	73/81 (90%)	-1.25	0 100 100	52, 71, 102, 139	0
2	D1	73/81 (90%)	-1.50	0 100 100	34, 46, 72, 86	0
2	D2	73/81 (90%)	-1.45	0 100 100	36, 56, 75, 81	0
2	D3	73/81 (90%)	-1.23	0 100 100	52, 72, 99, 112	0
2	D4	73/81 (90%)	-1.30	0 100 100	53, 73, 104, 132	0
2	D5	37/81 (45%)	-1.34	0 100 100	50, 66, 97, 108	0
2	D6	37/81 (45%)	-1.31	0 100 100	46, 58, 76, 82	0
2	D7	73/81 (90%)	-1.34	0 100 100	41, 60, 89, 114	0
2	D8	73/81 (90%)	-1.23	0 100 100	54, 71, 99, 142	0
2	F1	73/81 (90%)	-1.23	0 100 100	55, 76, 101, 117	0
2	F2	73/81 (90%)	-1.21	0 100 100	51, 80, 97, 104	0
2	F3	73/81 (90%)	-0.95	0 100 100	81, 116, 142, 152	0
2	F4	73/81 (90%)	-1.09	0 100 100	73, 99, 130, 154	0
2	F5	37/81 (45%)	-1.00	0 100 100	78, 107, 126, 134	0
2	F6	37/81 (45%)	-1.14	0 100 100	75, 97, 113, 116	0
2	F7	73/81 (90%)	-1.03	0 100 100	66, 86, 111, 137	0
2	F8	73/81 (90%)	-1.13	0 100 100	64, 80, 125, 159	0
2	H1	73/81 (90%)	-1.21	0 100 100	52, 70, 97, 119	0
2	H2	73/81 (90%)	-1.24	0 100 100	58, 80, 101, 107	0
2	H3	73/81 (90%)	-0.85	0 100 100	71, 109, 129, 142	0
2	H4	73/81 (90%)	-1.23	0 100 100	63, 82, 120, 140	0
2	H5	37/81 (45%)	-1.32	0 100 100	54, 67, 103, 108	0
2	H6	37/81 (45%)	-1.26	0 100 100	48, 56, 74, 87	0
2	H7	73/81 (90%)	-1.32	0 100 100	44, 62, 87, 117	0
2	H8	73/81 (90%)	-1.28	0 100 100	45, 64, 97, 127	0
2	J1	73/81 (90%)	-1.40	0 100 100	39, 53, 79, 94	0
2	J2	73/81 (90%)	-1.26	0 100 100	49, 67, 101, 111	0
2	J3	73/81 (90%)	-1.15	0 100 100	46, 74, 104, 132	0
2	J4	73/81 (90%)	-1.35	0 100 100	43, 64, 111, 135	0
2	J5	37/81 (45%)	-1.33	0 100 100	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%)	-1.39	0 100 100	47, 60, 83, 86	0
2	J7	73/81 (90%)	-1.34	0 100 100	36, 59, 91, 103	0
2	J8	73/81 (90%)	-1.36	0 100 100	45, 59, 96, 127	0
2	L1	73/81 (90%)	-1.08	0 100 100	70, 100, 128, 129	0
2	L2	73/81 (90%)	-1.29	0 100 100	57, 74, 94, 105	0
2	L3	73/81 (90%)	-1.13	0 100 100	60, 83, 104, 128	0
2	L4	73/81 (90%)	-1.13	0 100 100	74, 90, 120, 155	0
2	L5	37/81 (45%)	-1.50	0 100 100	42, 52, 68, 77	0
2	L6	37/81 (45%)	-1.41	0 100 100	43, 56, 78, 87	0
2	L7	73/81 (90%)	-1.13	0 100 100	66, 92, 118, 123	0
2	L8	73/81 (90%)	-1.21	0 100 100	66, 82, 110, 140	0
2	N1	73/81 (90%)	-1.25	0 100 100	51, 82, 110, 115	0
2	N2	73/81 (90%)	-1.28	0 100 100	59, 79, 105, 117	0
2	N3	73/81 (90%)	-1.24	0 100 100	48, 71, 101, 114	0
2	N4	73/81 (90%)	-1.14	0 100 100	61, 80, 109, 154	0
2	N5	37/81 (45%)	-1.44	0 100 100	35, 42, 61, 70	0
2	N6	37/81 (45%)	-1.37	0 100 100	39, 56, 88, 98	0
2	N7	73/81 (90%)	-1.27	0 100 100	42, 70, 108, 123	0
2	N8	73/81 (90%)	-1.34	0 100 100	47, 61, 91, 136	0
2	P1	73/81 (90%)	-1.30	0 100 100	46, 72, 100, 103	0
2	P2	73/81 (90%)	-1.37	0 100 100	51, 74, 102, 120	0
2	P3	73/81 (90%)	-1.22	0 100 100	47, 73, 100, 115	0
2	P4	73/81 (90%)	-1.32	0 100 100	49, 63, 101, 128	0
2	P5	37/81 (45%)	-1.18	0 100 100	58, 69, 91, 114	0
2	P6	37/81 (45%)	-1.11	0 100 100	72, 93, 121, 124	0
2	P7	73/81 (90%)	-1.14	0 100 100	65, 95, 135, 142	0
2	P8	73/81 (90%)	-1.09	0 100 100	68, 86, 124, 160	0
2	R1	73/81 (90%)	-0.86	0 100 100	90, 121, 147, 161	0
2	R2	73/81 (90%)	-1.20	0 100 100	55, 76, 129, 145	0
2	R3	73/81 (90%)	-1.21	0 100 100	66, 88, 126, 149	0
2	R4	73/81 (90%)	-1.17	0 100 100	64, 84, 119, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9	
2	R5	37/81 (45%)	-1.03	0	100100	72, 83, 105, 114	0
2	R6	37/81 (45%)	-1.04	0	100100	80, 107, 127, 131	0
2	R7	73/81 (90%)	-0.77	0	100100	95, 143, 165, 173	0
2	R8	73/81 (90%)	-0.99	0	100100	85, 107, 126, 150	0
2	T1	73/81 (90%)	-1.36	0	100100	40, 56, 84, 95	0
2	T2	73/81 (90%)	-1.26	0	100100	51, 80, 107, 114	0
2	T3	73/81 (90%)	-1.15	0	100100	59, 85, 116, 138	0
2	T4	73/81 (90%)	-1.36	0	100100	53, 69, 101, 141	0
2	T5	37/81 (45%)	-1.13	0	100100	76, 96, 122, 123	0
2	T6	37/81 (45%)	-1.15	0	100100	81, 98, 124, 128	0
2	T7	73/81 (90%)	-1.10	0	100100	70, 96, 121, 136	0
2	T8	73/81 (90%)	-1.03	0	100100	77, 110, 147, 180	0
All	All	39280/44480 (88%)	-1.43	0	100100	19, 52, 103, 182	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	0.99	0.02	172,172,172,172	0
3	ZN	R6	302	1/1	0.99	0.02	110,110,110,110	0
3	ZN	R7	302	1/1	0.99	0.03	170,170,170,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	T8	301	1/1	0.99	0.02	114,114,114,114	0
3	ZN	B3	301	1/1	1.00	0.01	44,44,44,44	0
3	ZN	B3	302	1/1	1.00	0.01	49,49,49,49	0
3	ZN	B4	301	1/1	1.00	0.01	55,55,55,55	0
3	ZN	B4	302	1/1	1.00	0.01	59,59,59,59	0
3	ZN	B5	301	1/1	1.00	0.01	45,45,45,45	0
3	ZN	B5	302	1/1	1.00	0.01	48,48,48,48	0
3	ZN	B6	301	1/1	1.00	0.02	44,44,44,44	0
3	ZN	B6	302	1/1	1.00	0.01	56,56,56,56	0
3	ZN	B7	301	1/1	1.00	0.01	67,67,67,67	0
3	ZN	B7	302	1/1	1.00	0.01	65,65,65,65	0
3	ZN	B8	301	1/1	1.00	0.01	57,57,57,57	0
3	ZN	B8	302	1/1	1.00	0.01	57,57,57,57	0
3	ZN	D1	301	1/1	1.00	0.01	41,41,41,41	0
3	ZN	D1	302	1/1	1.00	0.01	40,40,40,40	0
3	ZN	D2	301	1/1	1.00	0.01	42,42,42,42	0
3	ZN	D2	302	1/1	1.00	0.01	58,58,58,58	0
3	ZN	D3	301	1/1	1.00	0.02	62,62,62,62	0
3	ZN	D3	302	1/1	1.00	0.01	67,67,67,67	0
3	ZN	D4	301	1/1	1.00	0.01	55,55,55,55	0
3	ZN	D4	302	1/1	1.00	0.01	69,69,69,69	0
3	ZN	D5	301	1/1	1.00	0.01	65,65,65,65	0
3	ZN	D5	302	1/1	1.00	0.01	73,73,73,73	0
3	ZN	D6	301	1/1	1.00	0.02	62,62,62,62	0
3	ZN	D6	302	1/1	1.00	0.01	55,55,55,55	0
3	ZN	D7	301	1/1	1.00	0.01	42,42,42,42	0
3	ZN	D7	302	1/1	1.00	0.01	60,60,60,60	0
3	ZN	D8	301	1/1	1.00	0.01	62,62,62,62	0
3	ZN	D8	302	1/1	1.00	0.01	69,69,69,69	0
3	ZN	F1	301	1/1	1.00	0.01	56,56,56,56	0
3	ZN	F1	302	1/1	1.00	0.01	62,62,62,62	0
3	ZN	F2	301	1/1	1.00	0.01	62,62,62,62	0
3	ZN	F2	302	1/1	1.00	0.01	74,74,74,74	0
3	ZN	F3	301	1/1	1.00	0.02	99,99,99,99	0
3	ZN	B1	301	1/1	1.00	0.01	56,56,56,56	0
3	ZN	F4	301	1/1	1.00	0.01	92,92,92,92	0
3	ZN	F4	302	1/1	1.00	0.01	79,79,79,79	0
3	ZN	F5	301	1/1	1.00	0.01	99,99,99,99	0
3	ZN	F5	302	1/1	1.00	0.01	93,93,93,93	0
3	ZN	F6	301	1/1	1.00	0.01	88,88,88,88	0
3	ZN	F6	302	1/1	1.00	0.02	107,107,107,107	0
3	ZN	F7	301	1/1	1.00	0.01	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	F7	302	1/1	1.00	0.01	78,78,78,78	0
3	ZN	F8	301	1/1	1.00	0.01	70,70,70,70	0
3	ZN	F8	302	1/1	1.00	0.01	73,73,73,73	0
3	ZN	H1	301	1/1	1.00	0.01	60,60,60,60	0
3	ZN	H1	302	1/1	1.00	0.01	67,67,67,67	0
3	ZN	H2	301	1/1	1.00	0.01	65,65,65,65	0
3	ZN	H2	302	1/1	1.00	0.01	80,80,80,80	0
3	ZN	H3	301	1/1	1.00	0.02	71,71,71,71	0
3	ZN	H3	302	1/1	1.00	0.02	116,116,116,116	0
3	ZN	H4	301	1/1	1.00	0.01	70,70,70,70	0
3	ZN	H4	302	1/1	1.00	0.01	69,69,69,69	0
3	ZN	H5	301	1/1	1.00	0.02	59,59,59,59	0
3	ZN	H5	302	1/1	1.00	0.01	91,91,91,91	0
3	ZN	H6	301	1/1	1.00	0.01	55,55,55,55	0
3	ZN	H6	302	1/1	1.00	0.01	47,47,47,47	0
3	ZN	H7	301	1/1	1.00	0.01	49,49,49,49	0
3	ZN	H7	302	1/1	1.00	0.01	63,63,63,63	0
3	ZN	H8	301	1/1	1.00	0.01	54,54,54,54	0
3	ZN	H8	302	1/1	1.00	0.01	52,52,52,52	0
3	ZN	J1	301	1/1	1.00	0.01	46,46,46,46	0
3	ZN	J1	302	1/1	1.00	0.01	43,43,43,43	0
3	ZN	J2	301	1/1	1.00	0.01	54,54,54,54	0
3	ZN	J2	302	1/1	1.00	0.01	65,65,65,65	0
3	ZN	J3	301	1/1	1.00	0.01	59,59,59,59	0
3	ZN	J3	302	1/1	1.00	0.02	64,64,64,64	0
3	ZN	J4	301	1/1	1.00	0.01	56,56,56,56	0
3	ZN	J4	302	1/1	1.00	0.01	54,54,54,54	0
3	ZN	J5	301	1/1	1.00	0.01	54,54,54,54	0
3	ZN	J5	302	1/1	1.00	0.01	55,55,55,55	0
3	ZN	J6	301	1/1	1.00	0.01	55,55,55,55	0
3	ZN	J6	302	1/1	1.00	0.01	67,67,67,67	0
3	ZN	J7	301	1/1	1.00	0.01	50,50,50,50	0
3	ZN	J7	302	1/1	1.00	0.01	49,49,49,49	0
3	ZN	J8	301	1/1	1.00	0.01	52,52,52,52	0
3	ZN	J8	302	1/1	1.00	0.01	51,51,51,51	0
3	ZN	L1	301	1/1	1.00	0.01	94,94,94,94	0
3	ZN	L1	302	1/1	1.00	0.02	92,92,92,92	0
3	ZN	L2	301	1/1	1.00	0.01	77,77,77,77	0
3	ZN	L2	302	1/1	1.00	0.01	65,65,65,65	0
3	ZN	L3	301	1/1	1.00	0.01	54,54,54,54	0
3	ZN	L3	302	1/1	1.00	0.01	85,85,85,85	0
3	ZN	L4	301	1/1	1.00	0.01	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	L4	302	1/1	1.00	0.01	70,70,70,70	0
3	ZN	L5	301	1/1	1.00	0.01	49,49,49,49	0
3	ZN	L5	302	1/1	1.00	0.01	47,47,47,47	0
3	ZN	L6	301	1/1	1.00	0.01	48,48,48,48	0
3	ZN	L6	302	1/1	1.00	0.01	60,60,60,60	0
3	ZN	L7	301	1/1	1.00	0.02	80,80,80,80	0
3	ZN	L7	302	1/1	1.00	0.01	89,89,89,89	0
3	ZN	L8	301	1/1	1.00	0.01	72,72,72,72	0
3	ZN	L8	302	1/1	1.00	0.01	78,78,78,78	0
3	ZN	N1	301	1/1	1.00	0.01	63,63,63,63	0
3	ZN	N1	302	1/1	1.00	0.01	69,69,69,69	0
3	ZN	N2	301	1/1	1.00	0.01	62,62,62,62	0
3	ZN	N2	302	1/1	1.00	0.01	75,75,75,75	0
3	ZN	N3	301	1/1	1.00	0.01	65,65,65,65	0
3	ZN	N3	302	1/1	1.00	0.01	64,64,64,64	0
3	ZN	N4	301	1/1	1.00	0.01	76,76,76,76	0
3	ZN	N4	302	1/1	1.00	0.01	63,63,63,63	0
3	ZN	N5	301	1/1	1.00	0.01	40,40,40,40	0
3	ZN	N5	302	1/1	1.00	0.01	39,39,39,39	0
3	ZN	N6	301	1/1	1.00	0.01	48,48,48,48	0
3	ZN	N6	302	1/1	1.00	0.01	60,60,60,60	0
3	ZN	N7	301	1/1	1.00	0.01	56,56,56,56	0
3	ZN	N7	302	1/1	1.00	0.01	64,64,64,64	0
3	ZN	N8	301	1/1	1.00	0.01	63,63,63,63	0
3	ZN	N8	302	1/1	1.00	0.01	56,56,56,56	0
3	ZN	P1	301	1/1	1.00	0.01	62,62,62,62	0
3	ZN	P1	302	1/1	1.00	0.01	64,64,64,64	0
3	ZN	P2	301	1/1	1.00	0.01	59,59,59,59	0
3	ZN	P2	302	1/1	1.00	0.01	70,70,70,70	0
3	ZN	P3	301	1/1	1.00	0.01	60,60,60,60	0
3	ZN	P3	302	1/1	1.00	0.01	58,58,58,58	0
3	ZN	P4	301	1/1	1.00	0.01	61,61,61,61	0
3	ZN	P4	302	1/1	1.00	0.01	58,58,58,58	0
3	ZN	P5	301	1/1	1.00	0.01	71,71,71,71	0
3	ZN	P5	302	1/1	1.00	0.01	64,64,64,64	0
3	ZN	P6	301	1/1	1.00	0.01	82,82,82,82	0
3	ZN	P6	302	1/1	1.00	0.02	109,109,109,109	0
3	ZN	P7	301	1/1	1.00	0.01	76,76,76,76	0
3	ZN	P7	302	1/1	1.00	0.02	88,88,88,88	0
3	ZN	P8	301	1/1	1.00	0.01	70,70,70,70	0
3	ZN	P8	302	1/1	1.00	0.01	82,82,82,82	0
3	ZN	R1	301	1/1	1.00	0.01	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	R1	302	1/1	1.00	0.02	131,131,131,131	0
3	ZN	R2	301	1/1	1.00	0.01	70,70,70,70	0
3	ZN	R2	302	1/1	1.00	0.01	70,70,70,70	0
3	ZN	R3	301	1/1	1.00	0.01	78,78,78,78	0
3	ZN	R3	302	1/1	1.00	0.02	92,92,92,92	0
3	ZN	R4	301	1/1	1.00	0.01	73,73,73,73	0
3	ZN	R4	302	1/1	1.00	0.01	74,74,74,74	0
3	ZN	R5	301	1/1	1.00	0.01	73,73,73,73	0
3	ZN	R5	302	1/1	1.00	0.01	78,78,78,78	0
3	ZN	R6	301	1/1	1.00	0.01	101,101,101,101	0
3	ZN	B1	302	1/1	1.00	0.01	68,68,68,68	0
3	ZN	R7	301	1/1	1.00	0.02	118,118,118,118	0
3	ZN	B2	301	1/1	1.00	0.01	52,52,52,52	0
3	ZN	R8	301	1/1	1.00	0.01	97,97,97,97	0
3	ZN	R8	302	1/1	1.00	0.01	97,97,97,97	0
3	ZN	T1	301	1/1	1.00	0.01	46,46,46,46	0
3	ZN	T1	302	1/1	1.00	0.01	55,55,55,55	0
3	ZN	T2	301	1/1	1.00	0.01	57,57,57,57	0
3	ZN	T2	302	1/1	1.00	0.01	66,66,66,66	0
3	ZN	T3	301	1/1	1.00	0.01	72,72,72,72	0
3	ZN	T3	302	1/1	1.00	0.02	92,92,92,92	0
3	ZN	T4	301	1/1	1.00	0.01	64,64,64,64	0
3	ZN	T4	302	1/1	1.00	0.01	61,61,61,61	0
3	ZN	T5	301	1/1	1.00	0.01	88,88,88,88	0
3	ZN	T5	302	1/1	1.00	0.01	94,94,94,94	0
3	ZN	T6	301	1/1	1.00	0.01	89,89,89,89	0
3	ZN	T6	302	1/1	1.00	0.02	117,117,117,117	0
3	ZN	T7	301	1/1	1.00	0.01	84,84,84,84	0
3	ZN	T7	302	1/1	1.00	0.01	103,103,103,103	0
3	ZN	B2	302	1/1	1.00	0.01	46,46,46,46	0
3	ZN	T8	302	1/1	1.00	0.02	118,118,118,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.