



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:32 PM UTC

PDB ID : 4HW9 / pdb_00004hw9
Title : Crystal Structure of Helicobacter pylori MscS (Closed State)
Authors : Lai, J.Y.; Poon, Y.S.; Kaiser, J.; Rees, D.C.
Deposited on : 2012-11-07
Resolution : 4.14 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

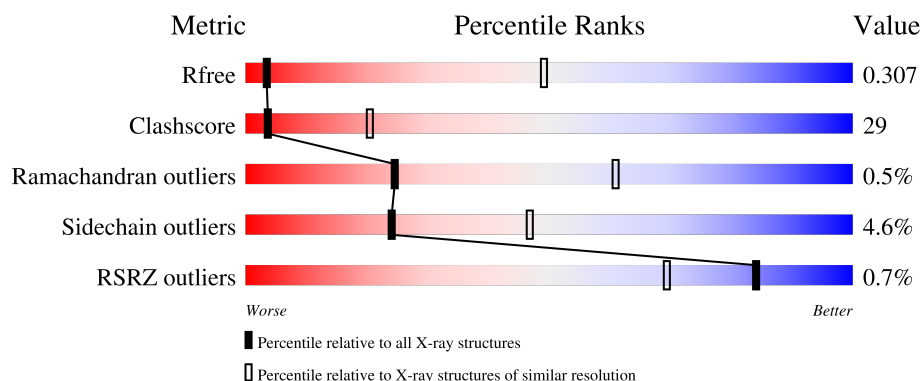
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.14 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	1004 (4.46-3.82)
Clashscore	190562	1004 (4.44-3.84)
Ramachandran outliers	187476	1224 (4.48-3.80)
Sidechain outliers	187428	1211 (4.48-3.80)
RSRZ outliers	180081	1001 (4.46-3.82)

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	A	309	
1	B	309	
1	C	309	
1	D	309	
1	E	309	

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Mol	Chain	Length	Quality of chain
1	F	309	36%37%8%•18%
1	G	309	% 34%34%13%•18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13797 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 Mechanosensitive channel MscS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0
1	B	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0
1	C	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0
1	D	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0
1	E	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0
1	F	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0
1	G	253	Total 1971	C 1284	N 327	O 354	S 6	0	0	0

There are 266 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP E8QGV2
A	-22	GLY	-	expression tag	UNP E8QGV2
A	-21	SER	-	expression tag	UNP E8QGV2
A	-20	SER	-	expression tag	UNP E8QGV2
A	-19	HIS	-	expression tag	UNP E8QGV2
A	-18	HIS	-	expression tag	UNP E8QGV2
A	-17	HIS	-	expression tag	UNP E8QGV2
A	-16	HIS	-	expression tag	UNP E8QGV2
A	-15	HIS	-	expression tag	UNP E8QGV2
A	-14	HIS	-	expression tag	UNP E8QGV2
A	-13	SER	-	expression tag	UNP E8QGV2
A	-12	SER	-	expression tag	UNP E8QGV2
A	-11	GLY	-	expression tag	UNP E8QGV2
A	-10	LEU	-	expression tag	UNP E8QGV2
A	-9	VAL	-	expression tag	UNP E8QGV2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	PRO	-	expression tag	UNP E8QGV2
A	-7	ARG	-	expression tag	UNP E8QGV2
A	-6	GLY	-	expression tag	UNP E8QGV2
A	-5	SER	-	expression tag	UNP E8QGV2
A	-4	HIS	-	expression tag	UNP E8QGV2
A	-3	THR	-	expression tag	UNP E8QGV2
A	-2	LEU	-	expression tag	UNP E8QGV2
A	-1	ILE	-	expression tag	UNP E8QGV2
A	0	ASN	-	expression tag	UNP E8QGV2
A	200	THR	ALA	conflict	UNP E8QGV2
A	202	GLU	ASP	conflict	UNP E8QGV2
A	273	PRO	SER	conflict	UNP E8QGV2
A	275	LEU	-	expression tag	UNP E8QGV2
A	276	ILE	-	expression tag	UNP E8QGV2
A	277	ASN	-	expression tag	UNP E8QGV2
A	278	ASP	-	expression tag	UNP E8QGV2
A	279	TYR	-	expression tag	UNP E8QGV2
A	280	LYS	-	expression tag	UNP E8QGV2
A	281	ASP	-	expression tag	UNP E8QGV2
A	282	ASP	-	expression tag	UNP E8QGV2
A	283	ASP	-	expression tag	UNP E8QGV2
A	284	ASP	-	expression tag	UNP E8QGV2
A	285	LYS	-	expression tag	UNP E8QGV2
B	-23	MET	-	expression tag	UNP E8QGV2
B	-22	GLY	-	expression tag	UNP E8QGV2
B	-21	SER	-	expression tag	UNP E8QGV2
B	-20	SER	-	expression tag	UNP E8QGV2
B	-19	HIS	-	expression tag	UNP E8QGV2
B	-18	HIS	-	expression tag	UNP E8QGV2
B	-17	HIS	-	expression tag	UNP E8QGV2
B	-16	HIS	-	expression tag	UNP E8QGV2
B	-15	HIS	-	expression tag	UNP E8QGV2
B	-14	HIS	-	expression tag	UNP E8QGV2
B	-13	SER	-	expression tag	UNP E8QGV2
B	-12	SER	-	expression tag	UNP E8QGV2
B	-11	GLY	-	expression tag	UNP E8QGV2
B	-10	LEU	-	expression tag	UNP E8QGV2
B	-9	VAL	-	expression tag	UNP E8QGV2
B	-8	PRO	-	expression tag	UNP E8QGV2
B	-7	ARG	-	expression tag	UNP E8QGV2
B	-6	GLY	-	expression tag	UNP E8QGV2
B	-5	SER	-	expression tag	UNP E8QGV2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP E8QGV2
B	-3	THR	-	expression tag	UNP E8QGV2
B	-2	LEU	-	expression tag	UNP E8QGV2
B	-1	ILE	-	expression tag	UNP E8QGV2
B	0	ASN	-	expression tag	UNP E8QGV2
B	200	THR	ALA	conflict	UNP E8QGV2
B	202	GLU	ASP	conflict	UNP E8QGV2
B	273	PRO	SER	conflict	UNP E8QGV2
B	275	LEU	-	expression tag	UNP E8QGV2
B	276	ILE	-	expression tag	UNP E8QGV2
B	277	ASN	-	expression tag	UNP E8QGV2
B	278	ASP	-	expression tag	UNP E8QGV2
B	279	TYR	-	expression tag	UNP E8QGV2
B	280	LYS	-	expression tag	UNP E8QGV2
B	281	ASP	-	expression tag	UNP E8QGV2
B	282	ASP	-	expression tag	UNP E8QGV2
B	283	ASP	-	expression tag	UNP E8QGV2
B	284	ASP	-	expression tag	UNP E8QGV2
B	285	LYS	-	expression tag	UNP E8QGV2
C	-23	MET	-	expression tag	UNP E8QGV2
C	-22	GLY	-	expression tag	UNP E8QGV2
C	-21	SER	-	expression tag	UNP E8QGV2
C	-20	SER	-	expression tag	UNP E8QGV2
C	-19	HIS	-	expression tag	UNP E8QGV2
C	-18	HIS	-	expression tag	UNP E8QGV2
C	-17	HIS	-	expression tag	UNP E8QGV2
C	-16	HIS	-	expression tag	UNP E8QGV2
C	-15	HIS	-	expression tag	UNP E8QGV2
C	-14	HIS	-	expression tag	UNP E8QGV2
C	-13	SER	-	expression tag	UNP E8QGV2
C	-12	SER	-	expression tag	UNP E8QGV2
C	-11	GLY	-	expression tag	UNP E8QGV2
C	-10	LEU	-	expression tag	UNP E8QGV2
C	-9	VAL	-	expression tag	UNP E8QGV2
C	-8	PRO	-	expression tag	UNP E8QGV2
C	-7	ARG	-	expression tag	UNP E8QGV2
C	-6	GLY	-	expression tag	UNP E8QGV2
C	-5	SER	-	expression tag	UNP E8QGV2
C	-4	HIS	-	expression tag	UNP E8QGV2
C	-3	THR	-	expression tag	UNP E8QGV2
C	-2	LEU	-	expression tag	UNP E8QGV2
C	-1	ILE	-	expression tag	UNP E8QGV2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ASN	-	expression tag	UNP E8QGV2
C	200	THR	ALA	conflict	UNP E8QGV2
C	202	GLU	ASP	conflict	UNP E8QGV2
C	273	PRO	SER	conflict	UNP E8QGV2
C	275	LEU	-	expression tag	UNP E8QGV2
C	276	ILE	-	expression tag	UNP E8QGV2
C	277	ASN	-	expression tag	UNP E8QGV2
C	278	ASP	-	expression tag	UNP E8QGV2
C	279	TYR	-	expression tag	UNP E8QGV2
C	280	LYS	-	expression tag	UNP E8QGV2
C	281	ASP	-	expression tag	UNP E8QGV2
C	282	ASP	-	expression tag	UNP E8QGV2
C	283	ASP	-	expression tag	UNP E8QGV2
C	284	ASP	-	expression tag	UNP E8QGV2
C	285	LYS	-	expression tag	UNP E8QGV2
D	-23	MET	-	expression tag	UNP E8QGV2
D	-22	GLY	-	expression tag	UNP E8QGV2
D	-21	SER	-	expression tag	UNP E8QGV2
D	-20	SER	-	expression tag	UNP E8QGV2
D	-19	HIS	-	expression tag	UNP E8QGV2
D	-18	HIS	-	expression tag	UNP E8QGV2
D	-17	HIS	-	expression tag	UNP E8QGV2
D	-16	HIS	-	expression tag	UNP E8QGV2
D	-15	HIS	-	expression tag	UNP E8QGV2
D	-14	HIS	-	expression tag	UNP E8QGV2
D	-13	SER	-	expression tag	UNP E8QGV2
D	-12	SER	-	expression tag	UNP E8QGV2
D	-11	GLY	-	expression tag	UNP E8QGV2
D	-10	LEU	-	expression tag	UNP E8QGV2
D	-9	VAL	-	expression tag	UNP E8QGV2
D	-8	PRO	-	expression tag	UNP E8QGV2
D	-7	ARG	-	expression tag	UNP E8QGV2
D	-6	GLY	-	expression tag	UNP E8QGV2
D	-5	SER	-	expression tag	UNP E8QGV2
D	-4	HIS	-	expression tag	UNP E8QGV2
D	-3	THR	-	expression tag	UNP E8QGV2
D	-2	LEU	-	expression tag	UNP E8QGV2
D	-1	ILE	-	expression tag	UNP E8QGV2
D	0	ASN	-	expression tag	UNP E8QGV2
D	200	THR	ALA	conflict	UNP E8QGV2
D	202	GLU	ASP	conflict	UNP E8QGV2
D	273	PRO	SER	conflict	UNP E8QGV2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	275	LEU	-	expression tag	UNP E8QGV2
D	276	ILE	-	expression tag	UNP E8QGV2
D	277	ASN	-	expression tag	UNP E8QGV2
D	278	ASP	-	expression tag	UNP E8QGV2
D	279	TYR	-	expression tag	UNP E8QGV2
D	280	LYS	-	expression tag	UNP E8QGV2
D	281	ASP	-	expression tag	UNP E8QGV2
D	282	ASP	-	expression tag	UNP E8QGV2
D	283	ASP	-	expression tag	UNP E8QGV2
D	284	ASP	-	expression tag	UNP E8QGV2
D	285	LYS	-	expression tag	UNP E8QGV2
E	-23	MET	-	expression tag	UNP E8QGV2
E	-22	GLY	-	expression tag	UNP E8QGV2
E	-21	SER	-	expression tag	UNP E8QGV2
E	-20	SER	-	expression tag	UNP E8QGV2
E	-19	HIS	-	expression tag	UNP E8QGV2
E	-18	HIS	-	expression tag	UNP E8QGV2
E	-17	HIS	-	expression tag	UNP E8QGV2
E	-16	HIS	-	expression tag	UNP E8QGV2
E	-15	HIS	-	expression tag	UNP E8QGV2
E	-14	HIS	-	expression tag	UNP E8QGV2
E	-13	SER	-	expression tag	UNP E8QGV2
E	-12	SER	-	expression tag	UNP E8QGV2
E	-11	GLY	-	expression tag	UNP E8QGV2
E	-10	LEU	-	expression tag	UNP E8QGV2
E	-9	VAL	-	expression tag	UNP E8QGV2
E	-8	PRO	-	expression tag	UNP E8QGV2
E	-7	ARG	-	expression tag	UNP E8QGV2
E	-6	GLY	-	expression tag	UNP E8QGV2
E	-5	SER	-	expression tag	UNP E8QGV2
E	-4	HIS	-	expression tag	UNP E8QGV2
E	-3	THR	-	expression tag	UNP E8QGV2
E	-2	LEU	-	expression tag	UNP E8QGV2
E	-1	ILE	-	expression tag	UNP E8QGV2
E	0	ASN	-	expression tag	UNP E8QGV2
E	200	THR	ALA	conflict	UNP E8QGV2
E	202	GLU	ASP	conflict	UNP E8QGV2
E	273	PRO	SER	conflict	UNP E8QGV2
E	275	LEU	-	expression tag	UNP E8QGV2
E	276	ILE	-	expression tag	UNP E8QGV2
E	277	ASN	-	expression tag	UNP E8QGV2
E	278	ASP	-	expression tag	UNP E8QGV2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	279	TYR	-	expression tag	UNP E8QGV2
E	280	LYS	-	expression tag	UNP E8QGV2
E	281	ASP	-	expression tag	UNP E8QGV2
E	282	ASP	-	expression tag	UNP E8QGV2
E	283	ASP	-	expression tag	UNP E8QGV2
E	284	ASP	-	expression tag	UNP E8QGV2
E	285	LYS	-	expression tag	UNP E8QGV2
F	-23	MET	-	expression tag	UNP E8QGV2
F	-22	GLY	-	expression tag	UNP E8QGV2
F	-21	SER	-	expression tag	UNP E8QGV2
F	-20	SER	-	expression tag	UNP E8QGV2
F	-19	HIS	-	expression tag	UNP E8QGV2
F	-18	HIS	-	expression tag	UNP E8QGV2
F	-17	HIS	-	expression tag	UNP E8QGV2
F	-16	HIS	-	expression tag	UNP E8QGV2
F	-15	HIS	-	expression tag	UNP E8QGV2
F	-14	HIS	-	expression tag	UNP E8QGV2
F	-13	SER	-	expression tag	UNP E8QGV2
F	-12	SER	-	expression tag	UNP E8QGV2
F	-11	GLY	-	expression tag	UNP E8QGV2
F	-10	LEU	-	expression tag	UNP E8QGV2
F	-9	VAL	-	expression tag	UNP E8QGV2
F	-8	PRO	-	expression tag	UNP E8QGV2
F	-7	ARG	-	expression tag	UNP E8QGV2
F	-6	GLY	-	expression tag	UNP E8QGV2
F	-5	SER	-	expression tag	UNP E8QGV2
F	-4	HIS	-	expression tag	UNP E8QGV2
F	-3	THR	-	expression tag	UNP E8QGV2
F	-2	LEU	-	expression tag	UNP E8QGV2
F	-1	ILE	-	expression tag	UNP E8QGV2
F	0	ASN	-	expression tag	UNP E8QGV2
F	200	THR	ALA	conflict	UNP E8QGV2
F	202	GLU	ASP	conflict	UNP E8QGV2
F	273	PRO	SER	conflict	UNP E8QGV2
F	275	LEU	-	expression tag	UNP E8QGV2
F	276	ILE	-	expression tag	UNP E8QGV2
F	277	ASN	-	expression tag	UNP E8QGV2
F	278	ASP	-	expression tag	UNP E8QGV2
F	279	TYR	-	expression tag	UNP E8QGV2
F	280	LYS	-	expression tag	UNP E8QGV2
F	281	ASP	-	expression tag	UNP E8QGV2
F	282	ASP	-	expression tag	UNP E8QGV2

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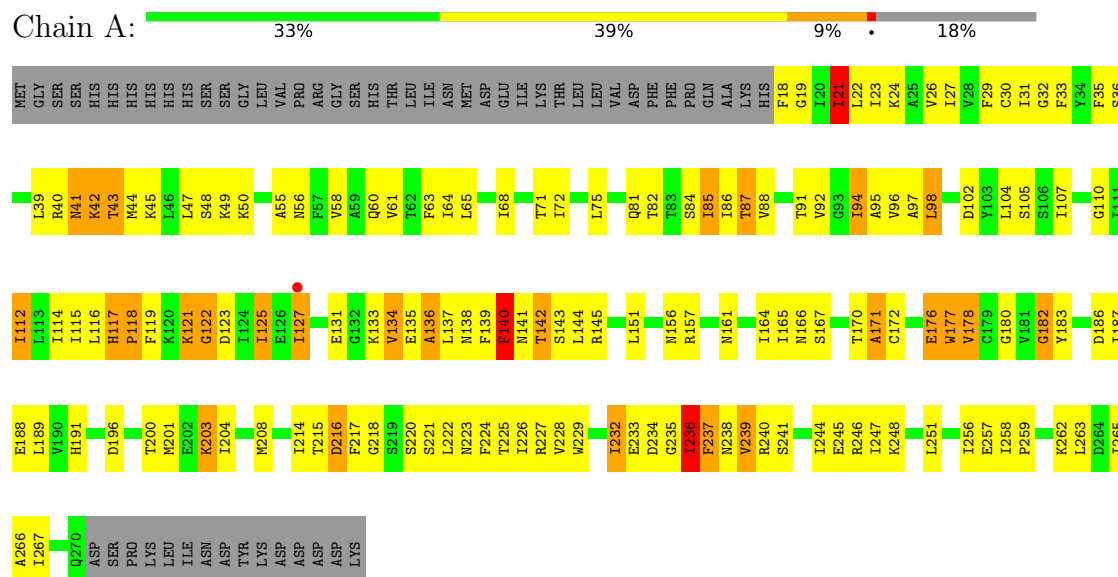
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Chain	Residue	Modelled	Actual	Comment	Reference
F	283	ASP	-	expression tag	UNP E8QGV2
F	284	ASP	-	expression tag	UNP E8QGV2
F	285	LYS	-	expression tag	UNP E8QGV2
G	-23	MET	-	expression tag	UNP E8QGV2
G	-22	GLY	-	expression tag	UNP E8QGV2
G	-21	SER	-	expression tag	UNP E8QGV2
G	-20	SER	-	expression tag	UNP E8QGV2
G	-19	HIS	-	expression tag	UNP E8QGV2
G	-18	HIS	-	expression tag	UNP E8QGV2
G	-17	HIS	-	expression tag	UNP E8QGV2
G	-16	HIS	-	expression tag	UNP E8QGV2
G	-15	HIS	-	expression tag	UNP E8QGV2
G	-14	HIS	-	expression tag	UNP E8QGV2
G	-13	SER	-	expression tag	UNP E8QGV2
G	-12	SER	-	expression tag	UNP E8QGV2
G	-11	GLY	-	expression tag	UNP E8QGV2
G	-10	LEU	-	expression tag	UNP E8QGV2
G	-9	VAL	-	expression tag	UNP E8QGV2
G	-8	PRO	-	expression tag	UNP E8QGV2
G	-7	ARG	-	expression tag	UNP E8QGV2
G	-6	GLY	-	expression tag	UNP E8QGV2
G	-5	SER	-	expression tag	UNP E8QGV2
G	-4	HIS	-	expression tag	UNP E8QGV2
G	-3	THR	-	expression tag	UNP E8QGV2
G	-2	LEU	-	expression tag	UNP E8QGV2
G	-1	ILE	-	expression tag	UNP E8QGV2
G	0	ASN	-	expression tag	UNP E8QGV2
G	200	THR	ALA	conflict	UNP E8QGV2
G	202	GLU	ASP	conflict	UNP E8QGV2
G	273	PRO	SER	conflict	UNP E8QGV2
G	275	LEU	-	expression tag	UNP E8QGV2
G	276	ILE	-	expression tag	UNP E8QGV2
G	277	ASN	-	expression tag	UNP E8QGV2
G	278	ASP	-	expression tag	UNP E8QGV2
G	279	TYR	-	expression tag	UNP E8QGV2
G	280	LYS	-	expression tag	UNP E8QGV2
G	281	ASP	-	expression tag	UNP E8QGV2
G	282	ASP	-	expression tag	UNP E8QGV2
G	283	ASP	-	expression tag	UNP E8QGV2
G	284	ASP	-	expression tag	UNP E8QGV2
G	285	LYS	-	expression tag	UNP E8QGV2

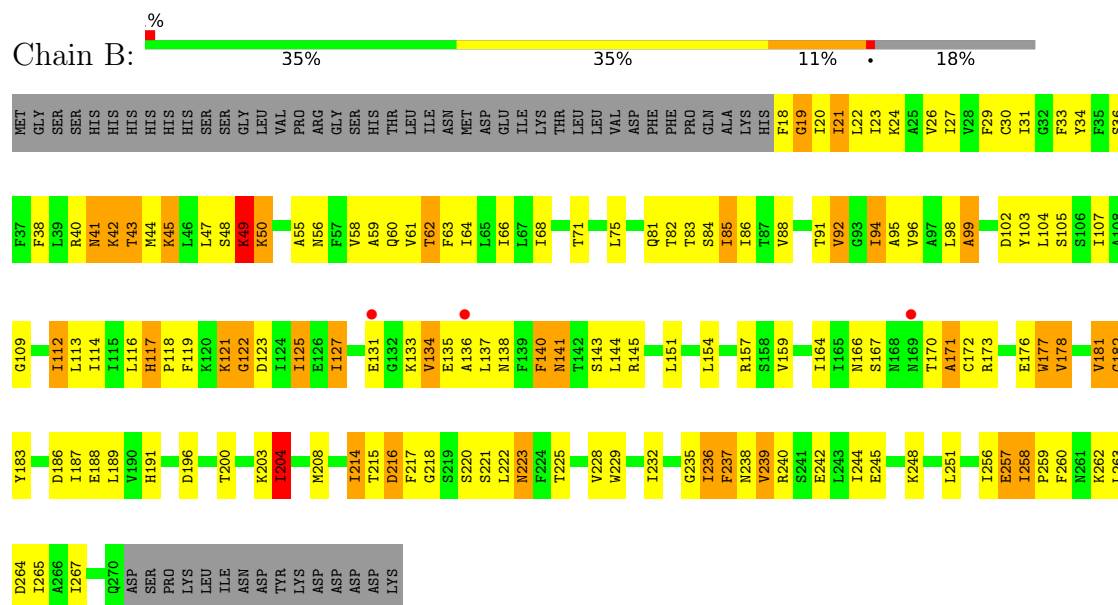
3 Residue-property plots

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

• Molecule 1: Mechanosensitive channel MscS

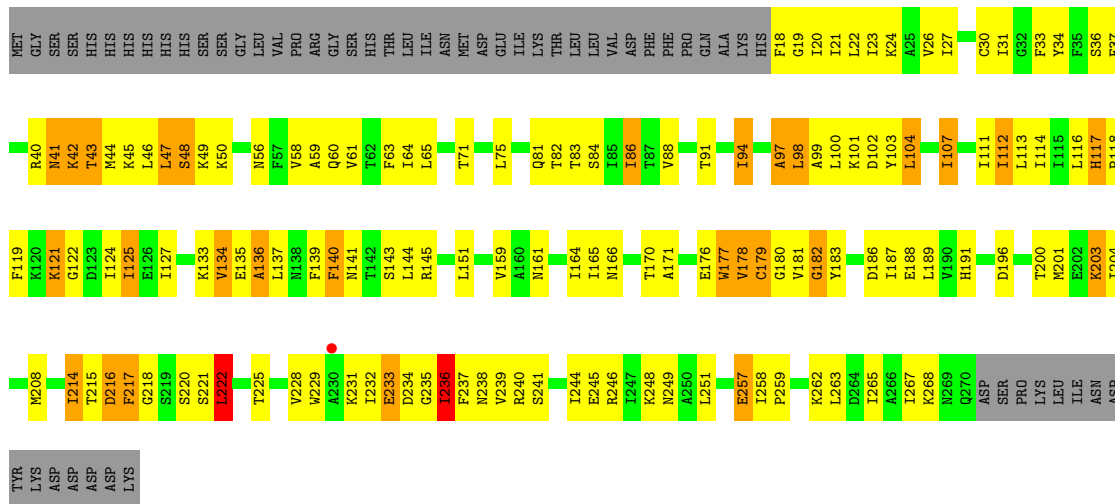


• Molecule 1: Mechanosensitive channel MscS

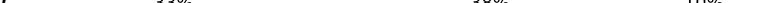


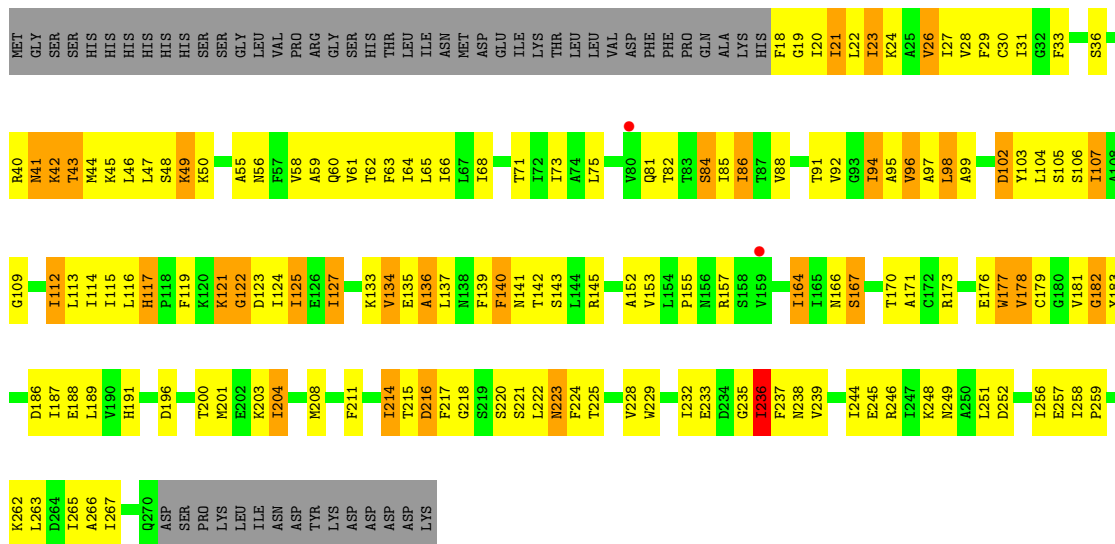
- Molecule 1: Mechanosensitive channel MscS

Chain C: 37% 36% 9% 1% 18%

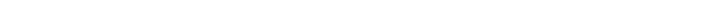


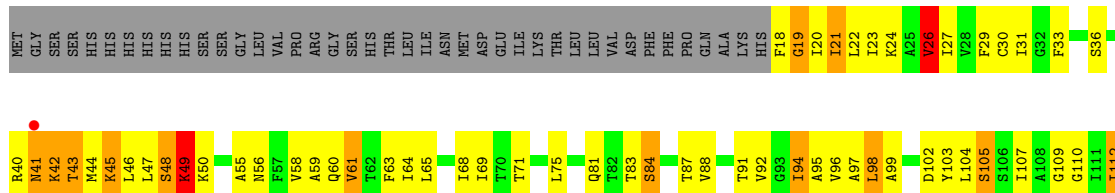
- Molecule 1: Mechanosensitive channel MscS

Chain D: 



- Molecule 1: Mechanosensitive channel MscS

Chain E:  36% 32% 13% 1% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.92Å 143.10Å 178.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.56 – 4.14 44.56 – 4.14	Depositor EDS
% Data completeness (in resolution range)	88.2 (44.56-4.14) 98.5 (44.56-4.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.244 , 0.304 0.255 , 0.307	Depositor DCC
R_{free} test set	1150 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	183.3	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 193.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13797	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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 ⓘ

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	A	1.25	5/2001 (0.2%)	1.80	54/2707 (2.0%)
1	B	1.28	9/2001 (0.4%)	1.73	45/2707 (1.7%)
1	C	1.34	12/2001 (0.6%)	1.78	52/2707 (1.9%)
1	D	1.31	9/2001 (0.4%)	1.78	54/2707 (2.0%)
1	E	1.31	12/2001 (0.6%)	1.82	61/2707 (2.3%)
1	F	1.28	10/2001 (0.5%)	1.81	44/2707 (1.6%)
1	G	1.30	8/2001 (0.4%)	1.85	59/2707 (2.2%)
All	All	1.30	65/14007 (0.5%)	1.80	369/18949 (1.9%)

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	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	1
All	All	0	7

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	236	ILE	CA-CB	11.11	1.69	1.54
1	G	236	ILE	CA-CB	10.94	1.69	1.54
1	F	236	ILE	CA-CB	10.51	1.68	1.54
1	F	141	ASN	CA-C	-9.41	1.41	1.52
1	C	141	ASN	CA-C	-8.96	1.42	1.52
1	E	236	ILE	C-O	8.75	1.34	1.24
1	D	236	ILE	CA-CB	8.40	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	159	VAL	CA-CB	-7.78	1.45	1.54
1	C	86	ILE	CG1-CD1	-7.74	1.21	1.51
1	A	107	ILE	CA-CB	-7.61	1.45	1.54
1	C	94	ILE	CA-CB	-7.34	1.45	1.54
1	B	214	ILE	CA-C	-7.32	1.44	1.52
1	B	50	LYS	CA-C	7.22	1.62	1.52
1	F	236	ILE	C-O	6.83	1.32	1.24
1	A	236	ILE	CA-CB	6.70	1.63	1.54
1	C	107	ILE	CA-CB	-6.67	1.47	1.54
1	G	86	ILE	CG1-CD1	-6.60	1.25	1.51
1	C	139	PHE	CA-C	6.54	1.60	1.52
1	E	46	LEU	CA-C	6.54	1.61	1.52
1	D	73	ILE	CA-CB	-6.48	1.46	1.54
1	G	85	ILE	CA-CB	-6.47	1.46	1.54
1	F	86	ILE	CG1-CD1	-6.43	1.26	1.51
1	C	125	ILE	CA-CB	-6.38	1.46	1.54
1	F	141	ASN	C-O	-6.38	1.15	1.23
1	F	181	VAL	CA-CB	-6.33	1.45	1.54
1	G	107	ILE	CA-CB	-6.33	1.47	1.54
1	E	125	ILE	CA-CB	-6.20	1.46	1.54
1	D	94	ILE	CA-CB	-6.14	1.46	1.54
1	E	181	VAL	CA-CB	-6.13	1.45	1.54
1	B	99	ALA	CA-CB	-5.94	1.43	1.53
1	G	141	ASN	CA-C	-5.90	1.45	1.52
1	C	97	ALA	CA-C	-5.84	1.44	1.52
1	D	26	VAL	CA-CB	-5.83	1.47	1.54
1	B	258	ILE	CA-CB	-5.83	1.47	1.54
1	E	84	SER	CA-C	5.82	1.60	1.52
1	E	177	TRP	CA-C	-5.78	1.45	1.52
1	A	203	LYS	CG-CD	-5.76	1.35	1.52
1	D	141	ASN	CA-C	-5.75	1.45	1.52
1	E	236	ILE	CA-CB	5.71	1.62	1.54
1	E	214	ILE	CA-C	-5.64	1.46	1.53
1	A	125	ILE	CA-CB	-5.61	1.47	1.54
1	B	159	VAL	CA-CB	-5.60	1.47	1.54
1	G	26	VAL	CA-CB	-5.52	1.47	1.54
1	E	107	ILE	CA-CB	-5.50	1.48	1.54
1	D	86	ILE	CG1-CD1	-5.43	1.30	1.51
1	E	141	ASN	CA-C	-5.41	1.45	1.52
1	B	141	ASN	CA-C	-5.40	1.46	1.52
1	C	48	SER	CB-OG	-5.37	1.31	1.42
1	G	21	ILE	CA-CB	-5.33	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	228	VAL	N-CA	5.30	1.52	1.46
1	D	125	ILE	CA-CB	-5.29	1.47	1.54
1	E	26	VAL	CA-CB	-5.29	1.48	1.54
1	C	104	LEU	CA-C	5.23	1.59	1.52
1	F	73	ILE	CA-CB	-5.19	1.48	1.54
1	F	94	ILE	CA-CB	-5.18	1.47	1.54
1	B	85	ILE	CA-CB	-5.17	1.47	1.54
1	D	153	VAL	CA-CB	-5.17	1.47	1.54
1	G	96	VAL	CA-CB	-5.16	1.47	1.54
1	D	164	ILE	CA-C	-5.16	1.48	1.53
1	F	210	THR	CA-C	5.14	1.58	1.52
1	A	85	ILE	CA-CB	-5.12	1.47	1.54
1	E	41	ASN	CA-C	5.07	1.60	1.52
1	C	179	CYS	CB-SG	5.06	1.98	1.81
1	C	159	VAL	CA-CB	-5.05	1.48	1.54
1	B	125	ILE	CA-CB	-5.03	1.48	1.54

All (369) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	235	GLY	N-CA-C	19.40	135.97	112.49
1	F	19	GLY	N-CA-C	17.82	134.11	112.73
1	G	19	GLY	N-CA-C	17.27	133.45	112.73
1	D	50	LYS	N-CA-C	-15.25	94.33	113.55
1	B	182	GLY	N-CA-C	-13.98	95.00	111.36
1	E	235	GLY	N-CA-C	13.73	129.10	112.49
1	C	50	LYS	N-CA-C	-13.34	90.74	111.02
1	A	50	LYS	N-CA-C	-12.28	97.96	113.43
1	G	50	LYS	N-CA-C	-12.16	97.92	113.12
1	F	236	ILE	CG1-CB-CG2	-10.87	78.09	110.70
1	A	21	ILE	CG1-CB-CG2	-10.78	78.36	110.70
1	F	50	LYS	N-CA-C	-10.53	98.93	112.93
1	A	239	VAL	N-CA-C	10.11	120.97	110.36
1	F	236	ILE	N-CA-C	-9.68	89.22	109.34
1	G	49	LYS	CA-CB-CG	9.55	133.21	114.10
1	G	86	ILE	CG1-CB-CG2	-9.15	83.25	110.70
1	D	236	ILE	CA-C-N	9.00	133.99	120.31
1	D	236	ILE	C-N-CA	9.00	133.99	120.31
1	D	98	LEU	N-CA-C	8.86	121.01	111.36
1	E	47	LEU	N-CA-C	8.76	124.10	113.41
1	A	182	GLY	N-CA-C	-8.72	92.50	113.18
1	F	177	TRP	N-CA-C	8.63	122.90	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	177	TRP	N-CA-C	8.62	122.51	109.41
1	D	182	GLY	N-CA-C	-8.62	92.76	113.18
1	E	236	ILE	CA-C-N	8.57	136.36	122.65
1	E	236	ILE	C-N-CA	8.57	136.36	122.65
1	C	177	TRP	N-CA-C	8.53	122.75	109.52
1	G	236	ILE	CA-C-N	8.53	136.06	121.14
1	G	236	ILE	C-N-CA	8.53	136.06	121.14
1	C	49	LYS	CA-CB-CG	8.51	131.11	114.10
1	G	182	GLY	N-CA-C	-8.45	93.15	113.18
1	E	50	LYS	N-CA-C	-8.44	101.31	111.69
1	C	117	HIS	N-CA-C	8.35	119.84	109.57
1	B	19	GLY	N-CA-C	8.32	132.89	113.18
1	G	237	PHE	N-CA-C	8.31	123.20	112.89
1	B	214	ILE	CB-CA-C	-8.24	101.44	111.08
1	F	236	ILE	CA-C-N	8.22	135.53	121.14
1	F	236	ILE	C-N-CA	8.22	135.53	121.14
1	E	19	GLY	N-CA-C	8.22	132.65	113.18
1	B	216	ASP	N-CA-C	8.20	121.87	108.99
1	E	49	LYS	CA-CB-CG	8.20	130.49	114.10
1	D	19	GLY	N-CA-C	8.14	132.47	113.18
1	E	182	GLY	N-CA-C	-8.14	93.89	113.18
1	G	177	TRP	N-CA-C	8.13	121.52	109.24
1	D	176	GLU	N-CA-C	8.09	121.69	108.99
1	G	118	PRO	CA-C-O	8.08	126.05	118.29
1	B	117	HIS	N-CA-C	8.07	119.49	109.57
1	A	139	PHE	CA-C-N	7.96	134.22	120.68
1	A	139	PHE	C-N-CA	7.96	134.22	120.68
1	E	117	HIS	N-CA-C	7.91	119.30	109.57
1	A	19	GLY	N-CA-C	7.86	131.80	113.18
1	C	48	SER	CA-CB-OG	7.83	126.75	111.10
1	G	125	ILE	N-CA-C	7.81	118.34	108.82
1	B	177	TRP	N-CA-C	7.79	121.60	109.52
1	D	139	PHE	N-CA-C	-7.79	102.73	111.14
1	C	19	GLY	N-CA-C	7.78	131.62	113.18
1	B	49	LYS	CA-CB-CG	7.77	129.63	114.10
1	E	118	PRO	CA-C-O	7.77	125.75	118.29
1	D	47	LEU	N-CA-C	7.75	123.65	114.04
1	D	50	LYS	N-CA-CB	7.74	121.63	110.40
1	C	98	LEU	N-CA-C	7.74	121.21	111.69
1	G	171	ALA	N-CA-C	7.73	120.60	111.71
1	E	94	ILE	N-CA-C	7.73	118.52	110.72
1	E	177	TRP	N-CA-C	7.69	120.60	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	LEU	N-CA-C	7.68	123.56	114.04
1	D	117	HIS	N-CA-C	7.66	120.51	109.48
1	A	125	ILE	N-CA-C	7.64	118.14	108.82
1	E	231	LYS	CA-C-N	7.58	130.85	120.46
1	E	231	LYS	C-N-CA	7.58	130.85	120.46
1	D	94	ILE	N-CA-C	7.58	118.37	110.72
1	F	49	LYS	CA-CB-CG	7.54	129.18	114.10
1	E	237	PHE	N-CA-CB	-7.52	99.58	110.56
1	A	122	GLY	N-CA-C	-7.51	105.54	114.48
1	C	182	GLY	N-CA-C	-7.50	95.41	113.18
1	A	117	HIS	N-CA-C	7.46	118.74	109.57
1	D	214	ILE	CB-CA-C	-7.43	103.25	111.35
1	F	98	LEU	N-CA-C	7.42	119.44	111.36
1	F	182	GLY	N-CA-C	-7.41	95.61	113.18
1	C	86	ILE	CA-CB-CG1	-7.41	97.80	110.40
1	E	98	LEU	N-CA-C	7.37	120.36	111.82
1	A	98	LEU	N-CA-C	7.36	120.35	111.82
1	B	20	ILE	N-CA-C	7.34	118.06	110.36
1	F	86	ILE	CA-CB-CG1	-7.34	97.93	110.40
1	B	125	ILE	N-CA-C	7.29	117.72	108.82
1	F	176	GLU	N-CA-C	7.29	120.43	108.99
1	D	177	TRP	N-CA-CB	7.27	122.99	111.43
1	E	177	TRP	N-CA-CB	7.23	123.34	111.62
1	G	47	LEU	N-CA-C	7.17	122.94	114.04
1	B	105	SER	N-CA-C	-7.15	104.59	113.38
1	E	45	LYS	N-CA-C	7.15	120.46	111.24
1	A	94	ILE	N-CA-C	7.13	117.93	110.72
1	B	42	LYS	N-CA-C	-7.11	103.78	113.30
1	G	98	LEU	N-CA-C	7.06	120.37	111.69
1	A	157	ARG	CA-C-N	7.04	129.72	120.28
1	A	157	ARG	C-N-CA	7.04	129.72	120.28
1	C	48	SER	CB-CA-C	-7.00	98.30	112.99
1	G	176	GLU	N-CA-C	6.99	119.69	109.07
1	E	233	GLU	CA-CB-CG	6.98	128.06	114.10
1	G	127	ILE	N-CA-C	6.98	117.47	108.12
1	C	47	LEU	N-CA-C	6.98	122.69	114.04
1	D	49	LYS	N-CA-C	6.97	121.17	112.24
1	D	125	ILE	N-CA-C	6.96	117.31	108.82
1	C	176	GLU	N-CA-C	6.94	119.89	108.99
1	B	176	GLU	N-CA-C	6.94	119.88	108.99
1	E	177	TRP	CB-CG-CD2	-6.92	117.12	126.80
1	E	214	ILE	CB-CA-C	-6.92	103.81	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ASN	N-CA-C	6.89	121.29	113.02
1	D	115	ILE	N-CA-C	6.89	117.03	110.42
1	G	177	TRP	N-CA-CB	6.87	123.64	111.69
1	A	140	PHE	N-CA-C	6.85	120.86	112.23
1	F	102	ASP	N-CA-CB	-6.85	99.67	110.22
1	C	177	TRP	CA-CB-CG	6.84	126.59	113.60
1	G	117	HIS	N-CA-C	6.83	119.41	109.71
1	F	236	ILE	N-CA-CB	6.82	122.48	111.23
1	A	121	LYS	N-CA-C	6.81	120.10	109.96
1	E	231	LYS	N-CA-C	6.75	120.25	109.24
1	B	177	TRP	N-CA-CB	6.75	123.30	111.55
1	E	177	TRP	CA-CB-CG	6.74	126.41	113.60
1	D	122	GLY	N-CA-C	-6.74	106.46	114.48
1	A	105	SER	N-CA-C	-6.73	105.06	113.28
1	G	236	ILE	N-CA-C	-6.73	95.34	109.34
1	F	177	TRP	N-CA-CB	6.71	123.22	111.55
1	E	237	PHE	N-CA-C	6.70	121.16	112.92
1	C	233	GLU	N-CA-CB	6.68	119.94	110.12
1	C	125	ILE	N-CA-C	6.65	116.64	108.53
1	C	216	ASP	N-CA-C	6.63	119.40	108.99
1	A	127	ILE	N-CA-C	6.60	116.96	108.12
1	F	125	ILE	N-CA-C	6.56	116.82	108.82
1	G	214	ILE	CB-CA-C	-6.55	104.22	111.35
1	C	177	TRP	N-CA-CB	6.53	122.91	111.55
1	G	122	GLY	N-CA-C	-6.53	106.71	114.48
1	C	222	LEU	CA-CB-CG	6.52	139.13	116.30
1	C	233	GLU	CB-CA-C	-6.45	100.09	110.79
1	C	102	ASP	N-CA-C	6.44	119.11	111.71
1	A	118	PRO	N-CA-C	-6.42	105.60	114.98
1	E	121	LYS	N-CA-C	6.42	119.52	109.96
1	A	217	PHE	N-CA-C	-6.42	100.54	110.10
1	E	102	ASP	N-CA-CB	-6.41	100.35	110.22
1	E	118	PRO	N-CA-C	-6.39	106.50	114.68
1	D	223	ASN	N-CA-C	6.39	118.93	108.52
1	C	94	ILE	N-CA-C	6.37	117.15	110.72
1	B	102	ASP	N-CA-CB	-6.36	100.43	110.22
1	D	43	THR	N-CA-C	-6.35	101.85	111.56
1	C	20	ILE	N-CA-C	6.34	117.02	110.36
1	C	49	LYS	CA-C-N	6.33	129.97	122.44
1	C	49	LYS	C-N-CA	6.33	129.97	122.44
1	B	167	SER	N-CA-C	-6.32	105.70	113.41
1	C	102	ASP	N-CA-CB	-6.30	100.52	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	SER	N-CA-C	-6.29	105.92	113.97
1	D	42	LYS	N-CA-C	-6.28	104.19	113.61
1	F	237	PHE	N-CA-CB	-6.28	100.17	110.40
1	B	50	LYS	N-CA-C	-6.21	104.05	111.69
1	C	140	PHE	CB-CA-C	-6.20	98.66	109.07
1	E	222	LEU	CA-CB-CG	6.20	137.99	116.30
1	E	171	ALA	N-CA-C	6.19	120.09	112.54
1	B	94	ILE	N-CA-C	6.18	116.97	110.72
1	A	216	ASP	N-CA-C	6.18	118.52	108.76
1	D	216	ASP	N-CA-C	6.17	118.68	108.99
1	G	167	SER	N-CA-C	-6.17	105.88	113.41
1	F	117	HIS	N-CA-C	6.17	117.16	109.57
1	D	177	TRP	CB-CA-C	-6.17	98.08	110.30
1	A	112	ILE	CB-CG1-CD1	6.17	126.75	113.80
1	G	139	PHE	N-CA-C	-6.14	104.13	111.69
1	B	41	ASN	N-CA-C	6.14	120.48	112.92
1	G	216	ASP	N-CA-C	6.14	118.62	108.99
1	B	102	ASP	N-CA-C	6.13	118.75	111.71
1	B	122	GLY	N-CA-C	-6.12	107.19	114.48
1	A	203	LYS	CB-CG-CD	6.12	125.36	111.30
1	E	41	ASN	N-CA-C	6.11	120.44	112.92
1	E	167	SER	N-CA-C	-6.11	105.95	113.41
1	C	42	LYS	N-CA-C	-6.11	105.12	113.30
1	F	86	ILE	CB-CG1-CD1	6.11	126.62	113.80
1	D	127	ILE	N-CA-C	6.10	116.30	108.12
1	G	104	LEU	CB-CG-CD2	-6.09	92.42	110.70
1	D	107	ILE	N-CA-C	6.09	116.21	110.30
1	F	122	GLY	N-CA-C	-6.08	107.25	114.48
1	F	102	ASP	N-CA-C	6.08	118.70	111.71
1	B	83	THR	N-CA-C	-6.07	104.78	111.82
1	E	42	LYS	N-CA-C	-6.06	104.52	113.61
1	B	47	LEU	N-CA-C	6.05	121.54	114.04
1	E	176	GLU	N-CA-C	6.04	118.25	109.07
1	C	233	GLU	CA-CB-CG	6.03	126.17	114.10
1	A	136	ALA	N-CA-C	6.03	119.06	108.75
1	A	238	ASN	N-CA-C	6.02	118.37	111.02
1	C	236	ILE	CA-C-N	6.01	130.86	120.58
1	C	236	ILE	C-N-CA	6.01	130.86	120.58
1	G	102	ASP	N-CA-CB	-6.00	100.98	110.22
1	B	223	ASN	N-CA-C	5.99	118.58	107.99
1	F	94	ILE	N-CA-C	5.96	116.73	110.72
1	B	181	VAL	CB-CA-C	-5.95	103.61	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	20	ILE	N-CA-C	5.95	116.60	110.36
1	G	42	LYS	N-CA-C	-5.94	105.34	113.30
1	E	216	ASP	N-CA-C	5.93	118.30	108.99
1	A	176	GLU	N-CA-C	5.90	118.05	109.07
1	D	217	PHE	N-CA-C	-5.90	101.31	110.10
1	A	203	LYS	CD-CE-NZ	-5.89	93.06	111.90
1	G	157	ARG	CA-C-N	5.89	128.65	120.29
1	G	157	ARG	C-N-CA	5.89	128.65	120.29
1	B	121	LYS	N-CA-C	5.88	118.87	110.10
1	D	28	VAL	N-CA-C	5.88	116.06	110.42
1	A	102	ASP	N-CA-CB	-5.87	101.19	110.28
1	C	83	THR	N-CA-C	-5.85	105.04	111.82
1	B	239	VAL	N-CA-C	5.84	116.49	110.36
1	A	171	ALA	N-CA-C	5.84	119.66	112.54
1	D	155	PRO	CA-C-O	-5.84	114.69	121.34
1	E	240	ARG	N-CA-C	-5.84	104.34	112.45
1	F	121	LYS	N-CA-C	5.83	118.65	109.96
1	G	257	GLU	CA-C-N	-5.80	116.99	123.02
1	G	257	GLU	C-N-CA	-5.80	116.99	123.02
1	B	118	PRO	CA-C-O	5.80	123.85	118.29
1	D	121	LYS	N-CA-C	5.79	118.59	109.96
1	C	257	GLU	CA-C-N	-5.79	117.00	123.02
1	C	257	GLU	C-N-CA	-5.79	117.00	123.02
1	B	257	GLU	CA-C-N	-5.79	117.00	123.02
1	B	257	GLU	C-N-CA	-5.79	117.00	123.02
1	B	21	ILE	CA-C-N	5.78	129.93	120.63
1	B	21	ILE	C-N-CA	5.78	129.93	120.63
1	E	177	TRP	CB-CA-C	-5.78	97.79	110.67
1	F	41	ASN	N-CA-C	5.78	120.02	112.92
1	G	20	ILE	N-CA-C	5.77	116.42	110.36
1	F	43	THR	N-CA-C	-5.75	102.75	111.56
1	A	42	LYS	N-CA-C	-5.75	104.99	113.61
1	A	236	ILE	CA-C-N	5.75	127.91	120.44
1	A	236	ILE	C-N-CA	5.75	127.91	120.44
1	E	43	THR	N-CA-C	-5.75	102.77	111.56
1	E	164	ILE	CB-CA-C	-5.74	105.72	111.80
1	F	125	ILE	CB-CA-C	-5.74	103.31	111.34
1	G	43	THR	N-CA-C	-5.73	102.79	111.56
1	B	62	THR	N-CA-C	-5.73	105.12	111.71
1	E	136	ALA	N-CA-C	5.73	118.54	108.75
1	D	20	ILE	N-CA-C	5.72	116.37	110.36
1	B	177	TRP	CA-CB-CG	5.71	124.46	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	257	GLU	CA-C-N	-5.71	117.08	123.02
1	E	257	GLU	C-N-CA	-5.71	117.08	123.02
1	C	236	ILE	CA-CB-CG2	5.71	120.21	110.50
1	D	177	TRP	CA-CB-CG	5.70	124.44	113.60
1	C	233	GLU	CB-CG-CD	5.70	122.29	112.60
1	B	98	LEU	N-CA-C	5.70	119.41	112.23
1	G	223	ASN	N-CA-C	5.68	117.78	108.52
1	G	170	THR	N-CA-C	5.68	117.66	108.41
1	G	94	ILE	N-CA-C	5.67	116.45	110.72
1	E	233	GLU	N-CA-C	5.66	117.13	111.07
1	F	42	LYS	N-CA-C	-5.66	105.71	113.30
1	C	214	ILE	CB-CA-C	-5.61	103.81	111.33
1	A	102	ASP	N-CA-C	5.61	118.33	111.82
1	E	21	ILE	CA-C-N	5.61	129.66	120.63
1	E	21	ILE	C-N-CA	5.61	129.66	120.63
1	B	260	PHE	N-CA-C	-5.60	103.14	110.53
1	D	41	ASN	N-CA-C	5.59	119.80	112.92
1	E	181	VAL	CB-CA-C	-5.59	103.53	111.19
1	C	101	LYS	CA-C-N	5.59	128.33	120.28
1	C	101	LYS	C-N-CA	5.59	128.33	120.28
1	F	257	GLU	CA-C-N	-5.59	117.21	123.02
1	F	257	GLU	C-N-CA	-5.59	117.21	123.02
1	A	237	PHE	N-CA-C	5.56	117.02	111.07
1	D	167	SER	N-CA-C	-5.56	106.63	113.41
1	B	45	LYS	N-CA-C	5.55	118.18	111.40
1	A	125	ILE	CB-CA-C	-5.55	103.57	111.34
1	C	121	LYS	N-CA-C	5.54	118.36	110.10
1	A	50	LYS	N-CA-CB	5.52	119.89	110.51
1	A	49	LYS	N-CA-C	5.51	119.30	112.24
1	G	115	ILE	N-CA-C	5.50	115.70	110.53
1	E	61	VAL	N-CA-C	5.49	116.12	110.36
1	A	115	ILE	N-CA-C	5.45	115.65	110.53
1	F	177	TRP	CA-CB-CG	5.45	123.95	113.60
1	A	43	THR	N-CA-C	-5.43	103.25	111.56
1	C	43	THR	N-CA-C	-5.43	103.25	111.56
1	F	113	LEU	CB-CG-CD2	-5.43	94.42	110.70
1	A	21	ILE	CB-CG1-CD1	5.42	125.18	113.80
1	B	127	ILE	N-CA-C	5.42	115.38	108.12
1	E	177	TRP	CB-CG-CD1	5.40	135.01	126.90
1	F	260	PHE	N-CA-C	-5.40	103.40	110.53
1	D	252	ASP	N-CA-C	-5.40	105.56	111.82
1	F	165	ILE	N-CA-C	5.38	115.05	106.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	ARG	CA-C-N	5.37	127.92	120.29
1	B	157	ARG	C-N-CA	5.37	127.92	120.29
1	B	204	ILE	N-CA-C	5.37	115.29	107.88
1	G	177	TRP	CA-CB-CG	5.37	123.80	113.60
1	G	83	THR	N-CA-C	-5.35	105.61	111.82
1	B	171	ALA	N-CA-C	5.35	119.07	112.54
1	B	118	PRO	N-CA-C	-5.35	107.84	114.68
1	G	164	ILE	N-CA-C	5.34	114.96	107.37
1	D	125	ILE	CB-CA-C	-5.34	103.86	111.34
1	G	201	MET	CA-C-N	5.34	127.70	120.44
1	G	201	MET	C-N-CA	5.34	127.70	120.44
1	D	177	TRP	CB-CG-CD2	-5.33	119.34	126.80
1	A	177	TRP	CB-CA-C	-5.33	98.78	110.67
1	C	107	ILE	N-CA-C	5.33	115.47	110.30
1	D	233	GLU	CB-CG-CD	5.32	121.64	112.60
1	F	61	VAL	N-CA-C	5.30	115.93	110.36
1	G	121	LYS	N-CA-C	5.30	117.86	109.96
1	E	157	ARG	CA-C-N	5.30	127.81	120.29
1	E	157	ARG	C-N-CA	5.30	127.81	120.29
1	G	111	ILE	N-CA-C	5.30	115.92	110.36
1	F	167	SER	N-CA-C	-5.29	106.96	113.41
1	G	177	TRP	CB-CG-CD2	-5.28	119.41	126.80
1	F	47	LEU	CB-CA-C	-5.27	102.36	109.16
1	D	136	ALA	N-CA-C	5.26	117.75	108.75
1	D	105	SER	N-CA-C	-5.26	106.91	113.38
1	E	122	GLY	N-CA-C	-5.26	108.22	114.48
1	E	237	PHE	CA-CB-CG	5.25	119.05	113.80
1	E	105	SER	N-CA-C	-5.24	106.88	113.28
1	C	104	LEU	CB-CG-CD2	-5.24	94.99	110.70
1	F	105	SER	N-CA-C	-5.23	106.95	113.38
1	D	23	ILE	CA-C-N	5.22	128.01	120.38
1	D	23	ILE	C-N-CA	5.22	128.01	120.38
1	A	87	THR	OG1-CB-CG2	5.22	119.74	109.30
1	B	141	ASN	N-CA-CB	5.22	118.88	111.05
1	G	142	THR	CA-C-N	-5.22	114.27	122.73
1	G	142	THR	C-N-CA	-5.22	114.27	122.73
1	C	41	ASN	N-CA-C	5.22	119.34	112.92
1	E	142	THR	CA-C-N	-5.21	114.30	122.73
1	E	142	THR	C-N-CA	-5.21	114.30	122.73
1	F	142	THR	CA-C-N	-5.21	115.13	122.94
1	F	142	THR	C-N-CA	-5.21	115.13	122.94
1	A	233	GLU	CB-CG-CD	5.20	121.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	SER	N-CA-C	5.19	117.36	111.02
1	C	238	ASN	N-CA-C	5.19	117.35	111.02
1	G	210	THR	N-CA-C	5.19	116.98	108.52
1	F	140	PHE	N-CA-C	5.18	119.87	113.50
1	G	181	VAL	N-CA-C	5.17	116.31	108.96
1	A	232	ILE	CA-C-N	5.17	128.58	120.82
1	A	232	ILE	C-N-CA	5.17	128.58	120.82
1	A	21	ILE	N-CA-C	5.17	115.89	110.62
1	D	142	THR	CA-C-N	-5.17	114.36	122.73
1	D	142	THR	C-N-CA	-5.17	114.36	122.73
1	F	72	ILE	N-CA-C	5.16	115.78	110.36
1	A	165	ILE	N-CA-C	5.16	114.72	106.88
1	A	140	PHE	CB-CA-C	-5.15	99.86	110.38
1	F	177	TRP	CB-CA-C	-5.15	99.23	109.79
1	C	136	ALA	N-CA-C	5.14	117.54	108.75
1	B	43	THR	N-CA-C	-5.14	103.70	111.56
1	C	111	ILE	N-CA-C	5.14	115.76	110.36
1	C	203	LYS	N-CA-CB	-5.14	104.26	110.53
1	C	171	ALA	N-CA-C	5.12	118.79	112.54
1	G	23	ILE	CA-C-N	5.12	127.85	120.38
1	G	23	ILE	C-N-CA	5.12	127.85	120.38
1	C	177	TRP	CB-CA-C	-5.11	99.32	109.79
1	D	181	VAL	CA-C-O	-5.10	116.31	121.67
1	D	96	VAL	CB-CA-C	-5.10	105.36	112.04
1	G	165	ILE	N-CA-C	5.09	114.62	106.88
1	F	114	ILE	N-CA-C	-5.09	105.75	110.53
1	D	157	ARG	CA-C-N	5.09	127.52	120.29
1	D	157	ARG	C-N-CA	5.09	127.52	120.29
1	A	107	ILE	N-CA-C	5.09	115.23	110.30
1	C	177	TRP	CB-CG-CD2	-5.09	119.68	126.80
1	D	21	ILE	CA-C-N	5.09	128.82	120.63
1	D	21	ILE	C-N-CA	5.09	128.82	120.63
1	E	232	ILE	CA-C-N	5.08	127.05	120.44
1	E	232	ILE	C-N-CA	5.08	127.05	120.44
1	C	217	PHE	N-CA-C	-5.08	102.53	110.10
1	D	238	ASN	N-CA-C	5.08	116.50	111.07
1	G	52	GLU	CA-CB-CG	5.07	124.25	114.10
1	E	49	LYS	N-CA-CB	5.07	119.06	110.49
1	G	260	PHE	N-CA-C	-5.07	103.35	110.50
1	B	125	ILE	CB-CA-C	-5.07	104.25	111.34
1	G	172	CYS	N-CA-C	5.07	117.66	109.40
1	D	140	PHE	CB-CA-C	-5.06	100.56	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	ASP	N-CA-C	5.04	119.14	112.89
1	G	232	ILE	CA-C-N	5.04	127.03	120.28
1	G	232	ILE	C-N-CA	5.04	127.03	120.28
1	A	142	THR	CA-C-N	-5.04	114.57	122.73
1	A	142	THR	C-N-CA	-5.04	114.57	122.73
1	E	164	ILE	N-CA-C	5.03	114.52	107.37
1	G	86	ILE	CB-CG1-CD1	5.03	124.36	113.80
1	E	236	ILE	N-CA-C	-5.01	98.91	109.34
1	C	233	GLU	CG-CD-OE2	5.01	129.93	118.40
1	E	246	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	G	102	ASP	N-CA-C	5.00	117.46	111.71

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	49	LYS	Mainchain
1	C	236	ILE	Mainchain
1	D	102	ASP	Mainchain
1	E	237	PHE	Mainchain
1	F	234	ASP	Mainchain
1	F	236	ILE	Mainchain
1	G	234	ASP	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1971	0	2079	137	0
1	B	1971	0	2079	135	0
1	C	1971	0	2079	140	0
1	D	1971	0	2079	144	0
1	E	1971	0	2079	136	0
1	F	1971	0	2079	138	0
1	G	1971	0	2079	137	0
All	All	13797	0	14553	824	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (824) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ILE:HG23	1:C:237:PHE:H	1.30	0.95
1:D:236:ILE:HG23	1:D:237:PHE:H	1.33	0.91
1:F:220:SER:HB2	1:F:262:LYS:H	1.32	0.91
1:F:91:THR:HA	1:F:94:ILE:HD12	1.52	0.91
1:B:91:THR:HA	1:B:94:ILE:HD12	1.52	0.90
1:F:186:ASP:HB3	1:F:189:LEU:HG	1.54	0.89
1:G:186:ASP:HB3	1:G:189:LEU:HG	1.55	0.88
1:F:236:ILE:HG22	1:F:237:PHE:H	1.36	0.88
1:G:220:SER:HB2	1:G:262:LYS:H	1.38	0.87
1:E:186:ASP:HB3	1:E:189:LEU:HG	1.58	0.86
1:B:220:SER:HB2	1:B:262:LYS:H	1.41	0.86
1:D:220:SER:HB2	1:D:262:LYS:H	1.41	0.86
1:C:91:THR:HA	1:C:94:ILE:HD12	1.59	0.85
1:C:220:SER:HB2	1:C:262:LYS:H	1.39	0.85
1:G:91:THR:HA	1:G:94:ILE:HD12	1.59	0.85
1:E:220:SER:HB2	1:E:262:LYS:H	1.41	0.84
1:A:91:THR:HA	1:A:94:ILE:HD12	1.57	0.84
1:G:236:ILE:HG23	1:G:237:PHE:H	1.39	0.84
1:D:214:ILE:HG21	1:E:248:LYS:HE3	1.57	0.84
1:F:236:ILE:HG22	1:F:237:PHE:HB3	1.58	0.83
1:A:220:SER:HB2	1:A:262:LYS:H	1.44	0.82
1:A:186:ASP:HB3	1:A:189:LEU:HG	1.60	0.81
1:F:135:GLU:OE2	1:F:145:ARG:HB2	1.81	0.81
1:D:186:ASP:HB3	1:D:189:LEU:HG	1.61	0.81
1:A:237:PHE:CE2	1:G:211:PHE:HB3	2.18	0.79
1:E:44:MET:HA	1:E:48:SER:HB3	1.65	0.78
1:B:186:ASP:HB3	1:B:189:LEU:HG	1.65	0.78
1:A:215:THR:HG22	1:A:216:ASP:OD2	1.84	0.78
1:D:182:GLY:N	1:D:257:GLU:O	2.17	0.78
1:C:186:ASP:HB3	1:C:189:LEU:HG	1.66	0.77
1:C:236:ILE:CG2	1:C:237:PHE:H	1.95	0.77
1:D:30:CYS:HA	1:D:33:PHE:HB3	1.66	0.77
1:B:214:ILE:HG21	1:C:248:LYS:HE3	1.66	0.77
1:E:30:CYS:HA	1:E:33:PHE:HB3	1.65	0.77
1:A:248:LYS:HE3	1:G:214:ILE:HG21	1.66	0.77
1:C:214:ILE:HG21	1:D:248:LYS:HE3	1.67	0.77
1:B:18:PHE:HE2	1:B:22:LEU:HD13	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLY:HA2	1:A:133:LYS:HE3	1.67	0.76
1:E:117:HIS:HB2	1:E:119:PHE:O	1.86	0.76
1:C:122:GLY:HA2	1:C:133:LYS:HE3	1.68	0.76
1:G:214:ILE:HG23	1:G:222:LEU:HD21	1.68	0.76
1:F:182:GLY:N	1:F:257:GLU:O	2.18	0.75
1:F:18:PHE:HE2	1:F:22:LEU:HD13	1.51	0.75
1:E:235:GLY:HA2	1:E:239:VAL:HG23	1.69	0.75
1:E:182:GLY:N	1:E:257:GLU:O	2.20	0.75
1:G:21:ILE:HG13	1:G:22:LEU:H	1.51	0.75
1:D:215:THR:HG22	1:D:216:ASP:OD2	1.87	0.75
1:A:237:PHE:CD2	1:G:211:PHE:HB3	2.22	0.75
1:C:182:GLY:N	1:C:257:GLU:O	2.18	0.74
1:G:30:CYS:HA	1:G:33:PHE:HB3	1.69	0.74
1:A:82:THR:OG1	1:B:81:GLN:NE2	2.20	0.74
1:G:215:THR:HG22	1:G:216:ASP:OD2	1.87	0.74
1:B:60:GLN:HG3	1:B:64:ILE:HD11	1.69	0.74
1:D:21:ILE:HG13	1:D:22:LEU:H	1.52	0.74
1:E:91:THR:HA	1:E:94:ILE:HD12	1.67	0.74
1:B:30:CYS:HA	1:B:33:PHE:HB3	1.70	0.74
1:A:30:CYS:HA	1:A:33:PHE:HB3	1.70	0.74
1:C:127:ILE:HD11	1:C:164:ILE:HG23	1.70	0.74
1:B:182:GLY:N	1:B:257:GLU:O	2.20	0.73
1:D:122:GLY:HA2	1:D:133:LYS:HE3	1.70	0.73
1:C:21:ILE:HG13	1:C:22:LEU:H	1.52	0.73
1:F:21:ILE:HG13	1:F:22:LEU:H	1.53	0.73
1:F:214:ILE:HG21	1:G:248:LYS:HE3	1.70	0.72
1:D:60:GLN:HG3	1:D:64:ILE:HD11	1.72	0.72
1:D:91:THR:HA	1:D:94:ILE:HD12	1.72	0.72
1:E:18:PHE:HE2	1:E:22:LEU:HD13	1.52	0.72
1:C:18:PHE:HE2	1:C:22:LEU:HD13	1.53	0.72
1:B:21:ILE:HG13	1:B:22:LEU:H	1.55	0.72
1:D:187:ILE:HG23	1:D:214:ILE:HD11	1.73	0.71
1:G:122:GLY:HA2	1:G:133:LYS:HE3	1.72	0.71
1:B:24:LYS:HA	1:B:27:ILE:HD12	1.72	0.71
1:G:237:PHE:HE1	1:G:240:ARG:HH11	1.38	0.71
1:A:135:GLU:OE2	1:A:145:ARG:HB2	1.90	0.71
1:A:60:GLN:HG3	1:A:64:ILE:HD11	1.72	0.70
1:C:30:CYS:HA	1:C:33:PHE:HB3	1.73	0.70
1:F:44:MET:O	1:F:48:SER:OG	2.04	0.70
1:G:236:ILE:CG2	1:G:237:PHE:H	2.03	0.70
1:A:182:GLY:N	1:A:257:GLU:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLU:OE2	1:C:145:ARG:HB2	1.91	0.70
1:E:60:GLN:HG3	1:E:64:ILE:HD11	1.72	0.70
1:B:122:GLY:HA2	1:B:133:LYS:HE3	1.74	0.70
1:G:182:GLY:N	1:G:257:GLU:O	2.24	0.69
1:F:215:THR:HG22	1:F:216:ASP:OD2	1.92	0.69
1:F:30:CYS:HA	1:F:33:PHE:HB3	1.75	0.69
1:F:60:GLN:HG3	1:F:64:ILE:HD11	1.75	0.69
1:A:214:ILE:HG21	1:B:248:LYS:HE3	1.73	0.68
1:B:127:ILE:HD11	1:B:164:ILE:HG23	1.76	0.67
1:A:127:ILE:HD11	1:A:164:ILE:HG23	1.77	0.67
1:D:41:ASN:HA	1:D:44:MET:HB2	1.76	0.67
1:F:236:ILE:CG2	1:F:237:PHE:H	2.01	0.67
1:F:187:ILE:HG23	1:F:214:ILE:HD11	1.75	0.67
1:E:215:THR:HG22	1:E:216:ASP:OD2	1.95	0.67
1:E:122:GLY:HA2	1:E:133:LYS:HE3	1.75	0.67
1:G:44:MET:O	1:G:48:SER:OG	2.09	0.67
1:G:177:TRP:HE3	1:G:178:VAL:H	1.44	0.66
1:F:177:TRP:HE3	1:F:178:VAL:H	1.43	0.66
1:C:60:GLN:HG3	1:C:64:ILE:HD11	1.78	0.66
1:C:27:ILE:O	1:C:31:ILE:HG13	1.95	0.66
1:C:187:ILE:HG23	1:C:214:ILE:HD11	1.78	0.66
1:C:215:THR:HG22	1:C:216:ASP:OD2	1.94	0.66
1:D:116:LEU:HD13	1:E:140:PHE:CE2	2.31	0.65
1:G:92:VAL:O	1:G:96:VAL:HG23	1.96	0.65
1:A:187:ILE:HG23	1:A:214:ILE:HD11	1.78	0.65
1:A:24:LYS:HA	1:A:27:ILE:HD12	1.78	0.65
1:G:187:ILE:HG23	1:G:214:ILE:HD11	1.79	0.65
1:A:18:PHE:HE2	1:A:22:LEU:HD13	1.61	0.65
1:D:235:GLY:HA2	1:D:239:VAL:HG23	1.78	0.65
1:E:21:ILE:HG13	1:E:22:LEU:H	1.60	0.65
1:D:177:TRP:HE3	1:D:178:VAL:H	1.42	0.65
1:G:43:THR:CG2	1:G:58:VAL:HG12	2.27	0.65
1:G:125:ILE:HG22	1:G:166:ASN:HA	1.79	0.65
1:G:237:PHE:CE1	1:G:240:ARG:NH1	2.65	0.65
1:B:215:THR:HG22	1:B:216:ASP:OD2	1.96	0.64
1:F:116:LEU:HD13	1:G:140:PHE:CE2	2.32	0.64
1:F:122:GLY:HA2	1:F:133:LYS:HE3	1.78	0.64
1:A:81:GLN:NE2	1:G:82:THR:OG1	2.26	0.64
1:B:221:SER:HB3	1:B:259:PRO:HG2	1.80	0.64
1:C:112:ILE:HG13	1:D:140:PHE:HE2	1.62	0.64
1:G:18:PHE:HE2	1:G:22:LEU:HD13	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:GLY:HA3	1:G:221:SER:O	1.97	0.64
1:F:122:GLY:H	1:F:134:VAL:HG13	1.63	0.64
1:G:60:GLN:O	1:G:64:ILE:HG13	1.98	0.64
1:E:263:LEU:HD11	1:F:263:LEU:HD23	1.80	0.64
1:F:116:LEU:HD23	1:F:116:LEU:O	1.97	0.63
1:C:177:TRP:O	1:C:225:THR:HA	1.98	0.63
1:E:24:LYS:HA	1:E:27:ILE:HD12	1.81	0.63
1:B:235:GLY:HA2	1:B:239:VAL:HG23	1.81	0.63
1:B:263:LEU:HD11	1:C:263:LEU:HB3	1.81	0.63
1:C:114:ILE:HG13	1:C:137:LEU:HD21	1.80	0.63
1:D:18:PHE:HE2	1:D:22:LEU:HD13	1.63	0.63
1:B:177:TRP:O	1:B:225:THR:HA	1.99	0.62
1:E:214:ILE:HG21	1:F:248:LYS:HE3	1.81	0.62
1:G:60:GLN:HG3	1:G:64:ILE:HD11	1.81	0.62
1:F:263:LEU:HD11	1:G:263:LEU:HD23	1.80	0.62
1:B:265:ILE:HD13	1:C:265:ILE:HD12	1.80	0.62
1:E:48:SER:O	1:E:49:LYS:HG2	1.99	0.62
1:E:23:ILE:O	1:E:27:ILE:HG13	1.99	0.62
1:E:187:ILE:HG23	1:E:214:ILE:HD11	1.81	0.62
1:C:235:GLY:HA2	1:C:239:VAL:HG23	1.81	0.62
1:A:140:PHE:CD1	1:A:140:PHE:N	2.67	0.62
1:E:60:GLN:O	1:E:64:ILE:HG13	2.00	0.62
1:E:135:GLU:OE2	1:E:145:ARG:HB2	1.98	0.62
1:G:122:GLY:H	1:G:134:VAL:HG13	1.64	0.62
1:D:122:GLY:H	1:D:134:VAL:HG13	1.65	0.61
1:E:69:ILE:HD13	1:F:85:ILE:HG13	1.80	0.61
1:E:177:TRP:HE3	1:E:178:VAL:H	1.46	0.61
1:C:82:THR:OG1	1:D:81:GLN:NE2	2.30	0.61
1:C:121:LYS:HG2	1:C:122:GLY:N	2.14	0.61
1:A:125:ILE:HG22	1:A:166:ASN:HA	1.81	0.61
1:B:60:GLN:O	1:B:64:ILE:HG13	2.00	0.61
1:D:82:THR:OG1	1:E:81:GLN:NE2	2.27	0.61
1:D:218:GLY:HA3	1:D:221:SER:O	1.99	0.61
1:C:125:ILE:HG22	1:C:166:ASN:HA	1.81	0.61
1:A:140:PHE:HE2	1:G:112:ILE:HG13	1.64	0.61
1:A:84:SER:HA	1:G:86:ILE:HD11	1.82	0.61
1:C:24:LYS:HA	1:C:27:ILE:HD12	1.83	0.61
1:C:117:HIS:HB2	1:C:119:PHE:O	2.00	0.61
1:F:71:THR:O	1:F:75:LEU:HG	2.00	0.61
1:D:117:HIS:HB2	1:D:119:PHE:O	2.01	0.61
1:D:221:SER:HB3	1:D:259:PRO:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLN:O	1:A:64:ILE:HG13	2.00	0.61
1:D:114:ILE:HG13	1:D:137:LEU:HD21	1.83	0.61
1:A:116:LEU:HD13	1:B:140:PHE:CE2	2.35	0.61
1:E:170:THR:OG1	1:F:151:LEU:HD21	2.01	0.61
1:G:21:ILE:HG13	1:G:22:LEU:N	2.16	0.60
1:A:263:LEU:HD23	1:G:263:LEU:HD11	1.83	0.60
1:B:218:GLY:HA3	1:B:221:SER:O	2.01	0.60
1:F:117:HIS:HB2	1:F:119:PHE:O	2.02	0.60
1:G:196:ASP:O	1:G:200:THR:HG23	2.02	0.60
1:G:221:SER:HB3	1:G:259:PRO:HG2	1.83	0.60
1:A:117:HIS:HB2	1:A:119:PHE:O	2.02	0.60
1:B:135:GLU:OE2	1:B:145:ARG:HB2	2.01	0.60
1:B:177:TRP:HE3	1:B:178:VAL:H	1.50	0.60
1:F:170:THR:O	1:F:232:ILE:HD11	2.01	0.60
1:G:24:LYS:HA	1:G:27:ILE:HD12	1.83	0.60
1:A:114:ILE:HG13	1:A:137:LEU:HD21	1.82	0.60
1:B:170:THR:O	1:B:232:ILE:HD11	2.02	0.60
1:D:263:LEU:HD11	1:E:263:LEU:HB3	1.84	0.60
1:G:27:ILE:O	1:G:31:ILE:HG13	2.01	0.60
1:F:235:GLY:HA2	1:F:239:VAL:HG23	1.83	0.59
1:B:104:LEU:HG	1:C:99:ALA:HB2	1.82	0.59
1:F:218:GLY:HA3	1:F:221:SER:O	2.02	0.59
1:D:211:PHE:CE1	1:E:236:ILE:HD12	2.37	0.59
1:E:27:ILE:O	1:E:31:ILE:HG13	2.02	0.59
1:C:177:TRP:HE3	1:C:178:VAL:H	1.50	0.59
1:C:97:ALA:HA	1:D:95:ALA:HB2	1.85	0.59
1:D:43:THR:CG2	1:D:58:VAL:HG12	2.33	0.59
1:D:177:TRP:CG	1:D:179:CYS:HG	2.20	0.59
1:C:177:TRP:CG	1:C:179:CYS:HG	2.20	0.59
1:E:170:THR:O	1:E:232:ILE:HD11	2.02	0.59
1:G:181:VAL:HG23	1:G:182:GLY:O	2.02	0.59
1:A:41:ASN:HA	1:A:44:MET:HB2	1.83	0.59
1:B:187:ILE:HG23	1:B:214:ILE:HD11	1.85	0.58
1:D:177:TRP:O	1:D:225:THR:HA	2.02	0.58
1:F:44:MET:HA	1:F:48:SER:HB3	1.85	0.58
1:F:265:ILE:HD13	1:G:265:ILE:CD1	2.33	0.58
1:B:41:ASN:HA	1:B:44:MET:HB2	1.85	0.58
1:E:41:ASN:HA	1:E:44:MET:HB2	1.84	0.58
1:F:21:ILE:HG13	1:F:22:LEU:N	2.17	0.58
1:F:177:TRP:O	1:F:225:THR:HA	2.02	0.58
1:B:214:ILE:HG23	1:B:222:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:ASN:HD21	1:G:103:TYR:HE2	1.51	0.58
1:A:218:GLY:HA3	1:A:221:SER:O	2.04	0.58
1:C:21:ILE:HG13	1:C:22:LEU:N	2.18	0.58
1:G:236:ILE:HG23	1:G:237:PHE:N	2.16	0.58
1:D:60:GLN:O	1:D:64:ILE:HG13	2.03	0.57
1:G:56:ASN:O	1:G:60:GLN:HB2	2.04	0.57
1:A:86:ILE:HD12	1:B:84:SER:HA	1.87	0.57
1:A:177:TRP:HE3	1:A:178:VAL:H	1.50	0.57
1:F:43:THR:CG2	1:F:58:VAL:HG12	2.35	0.57
1:G:177:TRP:O	1:G:225:THR:HA	2.04	0.57
1:C:56:ASN:O	1:C:60:GLN:HB2	2.04	0.57
1:C:116:LEU:HD13	1:D:140:PHE:CE2	2.39	0.57
1:D:170:THR:O	1:D:232:ILE:HD11	2.04	0.57
1:B:48:SER:HB2	1:B:55:ALA:HB1	1.87	0.57
1:A:227:ARG:HH22	1:B:236:ILE:CD1	2.18	0.57
1:D:36:SER:HB3	1:D:63:PHE:CE1	2.39	0.57
1:D:125:ILE:HG22	1:D:166:ASN:HA	1.87	0.57
1:F:24:LYS:HA	1:F:27:ILE:HD12	1.86	0.57
1:F:183:TYR:OH	1:G:258:ILE:HG21	2.05	0.57
1:G:127:ILE:HD11	1:G:164:ILE:HG23	1.87	0.57
1:A:136:ALA:HB3	1:A:143:SER:HB3	1.87	0.57
1:B:117:HIS:HB2	1:B:119:PHE:O	2.05	0.57
1:B:236:ILE:O	1:B:238:ASN:N	2.31	0.57
1:D:21:ILE:HG13	1:D:22:LEU:N	2.19	0.57
1:B:122:GLY:H	1:B:134:VAL:HG13	1.70	0.56
1:C:60:GLN:O	1:C:64:ILE:HG13	2.05	0.56
1:E:268:LYS:O	1:F:266:ALA:HA	2.05	0.56
1:A:121:LYS:HG2	1:A:122:GLY:N	2.20	0.56
1:E:56:ASN:O	1:E:60:GLN:HB2	2.05	0.56
1:E:114:ILE:HG13	1:E:137:LEU:HD21	1.87	0.56
1:G:121:LYS:HG2	1:G:122:GLY:N	2.20	0.56
1:D:125:ILE:HD12	1:D:127:ILE:HG12	1.88	0.56
1:F:220:SER:CB	1:F:262:LYS:H	2.14	0.56
1:B:263:LEU:HD11	1:C:263:LEU:HD23	1.87	0.56
1:C:127:ILE:CD1	1:C:164:ILE:HA	2.36	0.56
1:C:41:ASN:HA	1:C:44:MET:HB2	1.88	0.56
1:A:43:THR:CG2	1:A:58:VAL:HG12	2.36	0.56
1:E:183:TYR:OH	1:F:258:ILE:HG21	2.06	0.56
1:F:60:GLN:O	1:F:64:ILE:HG13	2.06	0.56
1:D:88:VAL:HA	1:D:91:THR:HG22	1.88	0.56
1:B:41:ASN:O	1:B:45:LYS:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ILE:HD13	1:C:265:ILE:CD1	2.36	0.55
1:D:177:TRP:CZ2	1:D:244:ILE:HD12	2.41	0.55
1:F:136:ALA:HB3	1:F:143:SER:HB3	1.89	0.55
1:G:43:THR:HG23	1:G:58:VAL:HG12	1.88	0.55
1:A:71:THR:O	1:A:75:LEU:HG	2.07	0.55
1:C:43:THR:CG2	1:C:58:VAL:HG12	2.37	0.55
1:C:88:VAL:HA	1:C:91:THR:HG22	1.87	0.55
1:A:214:ILE:HG21	1:B:248:LYS:CE	2.36	0.55
1:G:72:ILE:HD13	1:G:86:ILE:HD12	1.89	0.55
1:G:117:HIS:HB2	1:G:119:PHE:O	2.07	0.55
1:A:88:VAL:HA	1:A:91:THR:HG22	1.88	0.55
1:A:258:ILE:HG21	1:G:183:TYR:OH	2.05	0.55
1:B:21:ILE:HG13	1:B:22:LEU:N	2.22	0.55
1:B:121:LYS:HG2	1:B:122:GLY:N	2.22	0.55
1:D:112:ILE:HG13	1:E:140:PHE:HE2	1.72	0.55
1:G:41:ASN:HA	1:G:44:MET:HB2	1.87	0.55
1:A:177:TRP:CZ2	1:A:244:ILE:HD12	2.40	0.55
1:B:116:LEU:HD13	1:C:140:PHE:CE2	2.41	0.55
1:E:221:SER:HB3	1:E:259:PRO:HG2	1.89	0.55
1:B:23:ILE:O	1:B:27:ILE:HG13	2.07	0.55
1:D:23:ILE:O	1:D:27:ILE:HG13	2.07	0.55
1:A:221:SER:HB3	1:A:259:PRO:HG2	1.88	0.54
1:E:177:TRP:O	1:E:225:THR:HA	2.06	0.54
1:A:44:MET:O	1:A:48:SER:OG	2.16	0.54
1:A:245:GLU:HG2	1:G:214:ILE:HG13	1.89	0.54
1:B:114:ILE:HG13	1:B:137:LEU:HD21	1.88	0.54
1:D:263:LEU:HD11	1:E:263:LEU:HD23	1.88	0.54
1:E:218:GLY:HA3	1:E:221:SER:O	2.06	0.54
1:B:44:MET:O	1:B:48:SER:OG	2.14	0.54
1:D:214:ILE:HG21	1:E:248:LYS:CE	2.34	0.54
1:G:117:HIS:ND1	1:G:117:HIS:O	2.40	0.54
1:A:215:THR:OG1	1:A:225:THR:OG1	2.23	0.54
1:B:235:GLY:O	1:B:236:ILE:C	2.50	0.54
1:C:214:ILE:HG23	1:C:222:LEU:HD11	1.88	0.54
1:A:27:ILE:O	1:A:31:ILE:HG13	2.07	0.54
1:A:122:GLY:H	1:A:134:VAL:HG13	1.71	0.54
1:E:136:ALA:HB3	1:E:143:SER:HB3	1.89	0.54
1:C:268:LYS:O	1:D:266:ALA:HA	2.07	0.54
1:D:27:ILE:O	1:D:31:ILE:HG13	2.07	0.54
1:D:116:LEU:O	1:D:116:LEU:HD23	2.07	0.54
1:D:117:HIS:O	1:D:117:HIS:ND1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ASN:HA	1:F:44:MET:HB2	1.90	0.54
1:F:121:LYS:HG2	1:F:122:GLY:N	2.22	0.54
1:A:127:ILE:CD1	1:A:164:ILE:HA	2.38	0.54
1:A:263:LEU:HD11	1:B:263:LEU:HB3	1.90	0.54
1:B:56:ASN:O	1:B:60:GLN:HB2	2.08	0.54
1:D:42:LYS:HA	1:D:45:LYS:HB3	1.90	0.54
1:F:18:PHE:CE2	1:F:22:LEU:HD13	2.39	0.54
1:E:109:GLY:HA2	1:F:103:TYR:CE1	2.42	0.53
1:B:183:TYR:OH	1:C:258:ILE:HG21	2.07	0.53
1:D:135:GLU:OE2	1:D:145:ARG:HB2	2.09	0.53
1:E:41:ASN:O	1:E:45:LYS:HB2	2.08	0.53
1:G:41:ASN:O	1:G:45:LYS:HB2	2.07	0.53
1:B:112:ILE:HG13	1:C:140:PHE:HE2	1.72	0.53
1:C:218:GLY:HA3	1:C:221:SER:O	2.08	0.53
1:C:263:LEU:HD11	1:D:263:LEU:HD23	1.90	0.53
1:E:122:GLY:H	1:E:134:VAL:HG13	1.71	0.53
1:C:23:ILE:O	1:C:27:ILE:HG13	2.08	0.53
1:C:40:ARG:HB2	1:C:63:PHE:HD1	1.74	0.53
1:C:116:LEU:HD23	1:C:116:LEU:O	2.07	0.53
1:F:265:ILE:HD13	1:G:265:ILE:HD12	1.89	0.53
1:A:86:ILE:CD1	1:B:84:SER:HA	2.38	0.53
1:D:56:ASN:O	1:D:60:GLN:HB2	2.09	0.53
1:F:215:THR:OG1	1:F:225:THR:OG1	2.23	0.53
1:F:140:PHE:CD1	1:F:140:PHE:N	2.75	0.53
1:D:85:ILE:HD12	1:D:85:ILE:H	1.73	0.53
1:A:188:GLU:HA	1:A:191:HIS:CB	2.39	0.53
1:D:236:ILE:HG23	1:D:237:PHE:N	2.13	0.53
1:A:196:ASP:O	1:A:200:THR:HG23	2.08	0.53
1:D:43:THR:HG23	1:D:58:VAL:HG12	1.91	0.53
1:E:138:ASN:HD22	1:E:141:ASN:HB2	1.74	0.53
1:A:214:ILE:HG23	1:A:222:LEU:HD21	1.91	0.53
1:C:221:SER:HB3	1:C:259:PRO:HG2	1.91	0.53
1:E:88:VAL:HA	1:E:91:THR:HG22	1.90	0.53
1:G:127:ILE:CD1	1:G:164:ILE:HA	2.39	0.53
1:G:170:THR:O	1:G:232:ILE:HD11	2.08	0.53
1:C:112:ILE:HG13	1:D:140:PHE:CE2	2.44	0.52
1:F:196:ASP:O	1:F:200:THR:HG23	2.10	0.52
1:B:71:THR:O	1:B:75:LEU:HG	2.08	0.52
1:B:82:THR:OG1	1:C:81:GLN:NE2	2.32	0.52
1:D:44:MET:O	1:D:48:SER:OG	2.14	0.52
1:F:56:ASN:O	1:F:60:GLN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:SER:HB3	1:A:63:PHE:CE1	2.44	0.52
1:A:140:PHE:CE2	1:G:116:LEU:HD13	2.44	0.52
1:B:140:PHE:N	1:B:140:PHE:CD1	2.76	0.52
1:B:127:ILE:CD1	1:B:164:ILE:HA	2.39	0.52
1:E:127:ILE:HD11	1:E:164:ILE:HG23	1.92	0.52
1:C:122:GLY:H	1:C:134:VAL:HG13	1.74	0.52
1:F:23:ILE:O	1:F:27:ILE:HG13	2.09	0.52
1:F:214:ILE:HG12	1:F:224:PHE:CZ	2.45	0.52
1:B:264:ASP:HB2	1:C:262:LYS:HG3	1.92	0.52
1:D:86:ILE:CD1	1:E:84:SER:HA	2.40	0.52
1:D:123:ASP:O	1:D:134:VAL:HG12	2.10	0.52
1:E:109:GLY:HA2	1:F:103:TYR:CZ	2.45	0.52
1:G:135:GLU:OE2	1:G:145:ARG:HB2	2.09	0.52
1:G:178:VAL:HG12	1:G:223:ASN:HB3	1.92	0.52
1:C:183:TYR:OH	1:D:258:ILE:HG21	2.10	0.52
1:G:177:TRP:CZ2	1:G:244:ILE:HD12	2.44	0.52
1:A:39:LEU:O	1:A:43:THR:OG1	2.26	0.52
1:A:266:ALA:HA	1:G:268:LYS:O	2.09	0.52
1:B:181:VAL:HG23	1:B:222:LEU:HB3	1.92	0.52
1:D:24:LYS:HA	1:D:27:ILE:HD12	1.91	0.52
1:E:71:THR:O	1:E:75:LEU:HG	2.10	0.52
1:F:235:GLY:C	1:F:236:ILE:O	2.45	0.52
1:C:265:ILE:HD13	1:D:265:ILE:CD1	2.40	0.52
1:D:41:ASN:O	1:D:45:LYS:HB2	2.09	0.52
1:D:136:ALA:HB3	1:D:143:SER:HB3	1.92	0.52
1:D:203:LYS:O	1:D:204:ILE:HG13	2.10	0.52
1:A:177:TRP:O	1:A:225:THR:HA	2.10	0.51
1:B:181:VAL:CG2	1:B:222:LEU:HB3	2.40	0.51
1:F:18:PHE:CD2	1:F:22:LEU:HD22	2.44	0.51
1:F:214:ILE:HG23	1:F:222:LEU:HD21	1.90	0.51
1:G:88:VAL:HA	1:G:91:THR:HG22	1.92	0.51
1:C:241:SER:O	1:C:244:ILE:HG22	2.10	0.51
1:E:43:THR:CG2	1:E:58:VAL:HG12	2.39	0.51
1:E:121:LYS:HG2	1:E:122:GLY:N	2.24	0.51
1:A:208:MET:HB2	1:A:229:TRP:HB2	1.92	0.51
1:C:144:LEU:O	1:C:151:LEU:HA	2.10	0.51
1:C:177:TRP:CZ2	1:C:244:ILE:HD12	2.45	0.51
1:A:187:ILE:O	1:A:191:HIS:HB2	2.11	0.51
1:C:18:PHE:CE2	1:C:22:LEU:HD13	2.41	0.51
1:A:42:LYS:HE2	1:A:45:LYS:NZ	2.26	0.51
1:D:188:GLU:HA	1:D:191:HIS:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PHE:CE1	1:B:125:ILE:HD13	2.45	0.51
1:E:104:LEU:HG	1:F:99:ALA:HB2	1.92	0.51
1:F:123:ASP:O	1:F:134:VAL:HG12	2.11	0.51
1:G:119:PHE:CE1	1:G:125:ILE:HD13	2.46	0.51
1:C:43:THR:HG23	1:C:58:VAL:HG12	1.93	0.51
1:C:44:MET:HA	1:C:48:SER:OG	2.11	0.51
1:F:125:ILE:HG22	1:F:166:ASN:HA	1.93	0.51
1:A:18:PHE:CD2	1:A:22:LEU:HD22	2.46	0.50
1:B:125:ILE:HG22	1:B:166:ASN:HA	1.92	0.50
1:E:125:ILE:HG22	1:E:166:ASN:HA	1.93	0.50
1:F:136:ALA:HB3	1:F:143:SER:CB	2.41	0.50
1:B:116:LEU:HD23	1:B:116:LEU:O	2.11	0.50
1:F:263:LEU:HD11	1:G:263:LEU:HB3	1.93	0.50
1:A:235:GLY:O	1:A:236:ILE:C	2.55	0.50
1:E:21:ILE:HG13	1:E:22:LEU:N	2.26	0.50
1:G:23:ILE:O	1:G:27:ILE:HG13	2.11	0.50
1:B:251:LEU:HD22	1:B:256:ILE:HG21	1.93	0.50
1:G:241:SER:O	1:G:244:ILE:HG22	2.12	0.50
1:A:92:VAL:O	1:A:96:VAL:HG23	2.12	0.50
1:F:43:THR:HG23	1:F:58:VAL:HG12	1.93	0.50
1:C:217:PHE:CE2	1:D:258:ILE:HG12	2.46	0.50
1:C:41:ASN:O	1:C:45:LYS:HB2	2.12	0.50
1:C:196:ASP:O	1:C:200:THR:HG23	2.12	0.50
1:D:196:ASP:O	1:D:200:THR:HG23	2.12	0.50
1:F:235:GLY:O	1:F:238:ASN:HB2	2.12	0.50
1:A:41:ASN:O	1:A:45:LYS:HB2	2.11	0.50
1:C:170:THR:O	1:C:232:ILE:HD11	2.11	0.50
1:E:136:ALA:HB3	1:E:143:SER:CB	2.41	0.50
1:E:177:TRP:CZ2	1:E:244:ILE:HD12	2.46	0.50
1:F:48:SER:O	1:F:49:LYS:HG2	2.12	0.50
1:G:42:LYS:HZ2	1:G:46:LEU:HD11	1.76	0.50
1:G:64:ILE:O	1:G:68:ILE:HG13	2.11	0.50
1:C:236:ILE:CG2	1:C:237:PHE:N	2.71	0.50
1:C:263:LEU:HD11	1:D:263:LEU:HB3	1.93	0.50
1:F:187:ILE:O	1:F:191:HIS:HB2	2.12	0.50
1:F:251:LEU:HD22	1:F:256:ILE:HG21	1.94	0.50
1:G:71:THR:O	1:G:75:LEU:HG	2.12	0.50
1:A:56:ASN:O	1:A:60:GLN:HB2	2.11	0.49
1:F:27:ILE:O	1:F:31:ILE:HG13	2.12	0.49
1:B:18:PHE:CE2	1:B:22:LEU:HD13	2.39	0.49
1:D:121:LYS:HG2	1:D:122:GLY:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:PHE:CE2	1:E:22:LEU:HD13	2.40	0.49
1:E:118:PRO:HG2	1:F:141:ASN:ND2	2.26	0.49
1:G:36:SER:HB3	1:G:63:PHE:CE1	2.47	0.49
1:C:208:MET:HB2	1:C:229:TRP:HB2	1.94	0.49
1:D:183:TYR:OH	1:E:258:ILE:HG21	2.12	0.49
1:E:18:PHE:CD2	1:E:22:LEU:HD22	2.47	0.49
1:G:237:PHE:HE1	1:G:240:ARG:NH1	2.04	0.49
1:A:42:LYS:HA	1:A:45:LYS:HB3	1.93	0.49
1:E:42:LYS:HG2	1:E:45:LYS:HE3	1.93	0.49
1:F:41:ASN:O	1:F:45:LYS:HB2	2.12	0.49
1:G:39:LEU:O	1:G:43:THR:OG1	2.23	0.49
1:A:40:ARG:HB2	1:A:63:PHE:HD1	1.76	0.49
1:B:259:PRO:HB3	1:B:262:LYS:NZ	2.27	0.49
1:A:183:TYR:OH	1:B:258:ILE:HG21	2.13	0.49
1:B:208:MET:HB2	1:B:229:TRP:HB2	1.94	0.49
1:D:109:GLY:HA2	1:E:103:TYR:CZ	2.48	0.49
1:E:127:ILE:CD1	1:E:164:ILE:HA	2.43	0.49
1:F:178:VAL:HG12	1:F:223:ASN:HB3	1.94	0.49
1:C:18:PHE:CE1	1:C:21:ILE:HD11	2.48	0.49
1:B:36:SER:HB3	1:B:63:PHE:CE1	2.48	0.49
1:B:40:ARG:HB2	1:B:63:PHE:HD1	1.76	0.49
1:E:203:LYS:NZ	1:E:234:ASP:OD2	2.44	0.49
1:A:188:GLU:HA	1:A:191:HIS:HB2	1.95	0.49
1:B:44:MET:HA	1:B:48:SER:HB3	1.94	0.49
1:F:127:ILE:HD12	1:F:127:ILE:HG23	1.56	0.49
1:C:119:PHE:CE1	1:C:125:ILE:HD13	2.48	0.48
1:D:124:ILE:HG22	1:D:133:LYS:HB2	1.95	0.48
1:E:125:ILE:HD12	1:E:127:ILE:HG12	1.95	0.48
1:G:136:ALA:HB3	1:G:143:SER:HB3	1.94	0.48
1:F:18:PHE:CE2	1:F:22:LEU:HD22	2.47	0.48
1:F:268:LYS:O	1:G:266:ALA:HA	2.13	0.48
1:B:44:MET:HG2	1:B:59:ALA:HB2	1.95	0.48
1:B:48:SER:HB2	1:B:55:ALA:CB	2.44	0.48
1:B:220:SER:CB	1:B:262:LYS:H	2.20	0.48
1:C:44:MET:HE3	1:C:48:SER:OG	2.12	0.48
1:E:188:GLU:HA	1:E:191:HIS:CB	2.43	0.48
1:E:178:VAL:HG12	1:E:223:ASN:HB3	1.94	0.48
1:A:180:GLY:HA2	1:A:222:LEU:O	2.12	0.48
1:B:85:ILE:HD12	1:B:85:ILE:H	1.79	0.48
1:D:98:LEU:HA	1:D:98:LEU:HD23	1.49	0.48
1:D:214:ILE:HG23	1:D:222:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:HIS:ND1	1:B:117:HIS:O	2.47	0.48
1:G:114:ILE:HG13	1:G:137:LEU:HD21	1.95	0.48
1:D:187:ILE:O	1:D:191:HIS:HB2	2.14	0.48
1:G:98:LEU:HA	1:G:98:LEU:HD23	1.54	0.48
1:G:235:GLY:HA2	1:G:239:VAL:HG23	1.95	0.48
1:B:42:LYS:HA	1:B:45:LYS:HB3	1.96	0.48
1:D:127:ILE:CD1	1:D:164:ILE:HA	2.43	0.48
1:C:42:LYS:HA	1:C:45:LYS:HB3	1.96	0.48
1:B:178:VAL:HG12	1:B:223:ASN:HB3	1.95	0.47
1:D:208:MET:HB2	1:D:229:TRP:HB2	1.96	0.47
1:A:136:ALA:HB3	1:A:143:SER:CB	2.44	0.47
1:C:177:TRP:CD1	1:C:179:CYS:HG	2.31	0.47
1:C:203:LYS:NZ	1:C:234:ASP:OD2	2.46	0.47
1:E:112:ILE:HG13	1:F:140:PHE:HE2	1.78	0.47
1:E:235:GLY:O	1:E:236:ILE:C	2.56	0.47
1:B:48:SER:O	1:B:49:LYS:HG2	2.13	0.47
1:G:215:THR:CB	1:G:225:THR:HG1	2.27	0.47
1:A:123:ASP:O	1:A:134:VAL:HG12	2.15	0.47
1:D:71:THR:O	1:D:75:LEU:HG	2.15	0.47
1:D:109:GLY:HA2	1:E:103:TYR:CE1	2.48	0.47
1:E:42:LYS:HA	1:E:45:LYS:HB3	1.96	0.47
1:G:203:LYS:O	1:G:204:ILE:HG13	2.14	0.47
1:B:107:ILE:HG12	1:B:140:PHE:CD1	2.49	0.47
1:F:42:LYS:HG2	1:F:45:LYS:HE3	1.96	0.47
1:G:127:ILE:HD13	1:G:164:ILE:HA	1.95	0.47
1:A:140:PHE:CD2	1:G:116:LEU:HD13	2.50	0.47
1:A:176:GLU:HA	1:A:226:ILE:O	2.15	0.47
1:B:88:VAL:HA	1:B:91:THR:HG22	1.97	0.47
1:C:231:LYS:HE2	1:C:233:GLU:HG2	1.96	0.47
1:D:85:ILE:O	1:D:86:ILE:C	2.56	0.47
1:D:136:ALA:HB3	1:D:143:SER:CB	2.45	0.47
1:D:220:SER:CB	1:D:262:LYS:H	2.20	0.47
1:E:18:PHE:CE1	1:E:21:ILE:HD11	2.50	0.47
1:E:48:SER:HB2	1:E:55:ALA:HB1	1.96	0.47
1:E:171:ALA:HA	1:E:232:ILE:HD12	1.97	0.47
1:F:221:SER:HB3	1:F:259:PRO:HG2	1.96	0.47
1:C:215:THR:OG1	1:C:225:THR:OG1	2.24	0.47
1:D:265:ILE:HD13	1:E:265:ILE:CD1	2.45	0.47
1:F:188:GLU:HA	1:F:191:HIS:CB	2.45	0.47
1:F:208:MET:HB2	1:F:229:TRP:HB2	1.96	0.47
1:G:186:ASP:HB3	1:G:189:LEU:CG	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:ILE:O	1:G:191:HIS:HB2	2.15	0.47
1:B:235:GLY:O	1:B:237:PHE:N	2.48	0.47
1:C:36:SER:HB3	1:C:63:PHE:CE1	2.50	0.47
1:E:116:LEU:HD13	1:F:140:PHE:CE2	2.50	0.47
1:E:161:ASN:OD1	1:F:157:ARG:HD3	2.15	0.47
1:E:196:ASP:O	1:E:200:THR:HG23	2.14	0.47
1:E:220:SER:CB	1:E:262:LYS:H	2.20	0.47
1:F:39:LEU:O	1:F:43:THR:OG1	2.32	0.47
1:F:214:ILE:HG13	1:G:245:GLU:HG2	1.97	0.47
1:D:112:ILE:HG13	1:E:140:PHE:CE2	2.50	0.47
1:E:42:LYS:HE2	1:E:45:LYS:NZ	2.30	0.47
1:B:215:THR:HG23	1:C:240:ARG:HH12	1.80	0.46
1:B:203:LYS:O	1:B:204:ILE:HG13	2.15	0.46
1:C:170:THR:HG21	1:D:145:ARG:CZ	2.45	0.46
1:F:42:LYS:HA	1:F:45:LYS:HB3	1.97	0.46
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.46	0.46
1:A:172:CYS:SG	1:A:208:MET:HE3	2.55	0.46
1:A:241:SER:O	1:A:244:ILE:HG22	2.15	0.46
1:E:92:VAL:O	1:E:96:VAL:HG23	2.16	0.46
1:G:116:LEU:HD23	1:G:116:LEU:O	2.15	0.46
1:G:124:ILE:HG22	1:G:133:LYS:HB2	1.97	0.46
1:A:170:THR:O	1:A:232:ILE:HD11	2.14	0.46
1:B:19:GLY:O	1:B:22:LEU:HB3	2.15	0.46
1:C:71:THR:O	1:C:75:LEU:HG	2.15	0.46
1:D:127:ILE:HD11	1:D:164:ILE:HG23	1.98	0.46
1:E:187:ILE:O	1:E:191:HIS:HB2	2.16	0.46
1:F:116:LEU:HD13	1:G:140:PHE:CD2	2.51	0.46
1:G:42:LYS:NZ	1:G:46:LEU:HD11	2.30	0.46
1:G:201:MET:HE1	1:G:246:ARG:HB2	1.96	0.46
1:B:136:ALA:HB3	1:B:143:SER:HB3	1.97	0.46
1:D:97:ALA:HA	1:E:95:ALA:HB2	1.97	0.46
1:F:98:LEU:HD23	1:F:98:LEU:HA	1.51	0.46
1:G:42:LYS:HA	1:G:45:LYS:HB3	1.97	0.46
1:A:23:ILE:O	1:A:27:ILE:HG13	2.16	0.46
1:A:251:LEU:HD23	1:A:251:LEU:HA	1.71	0.46
1:A:263:LEU:HB3	1:G:263:LEU:HD11	1.96	0.46
1:C:161:ASN:HD21	1:D:103:TYR:HE2	1.64	0.46
1:D:18:PHE:CE1	1:D:21:ILE:HD11	2.51	0.46
1:D:48:SER:HB2	1:D:55:ALA:HB1	1.97	0.46
1:D:65:LEU:HA	1:D:65:LEU:HD12	1.70	0.46
1:E:65:LEU:HD12	1:E:65:LEU:HA	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LYS:HE2	1:B:45:LYS:NZ	2.31	0.46
1:D:236:ILE:CG2	1:D:237:PHE:H	2.05	0.46
1:F:18:PHE:CE1	1:F:21:ILE:HD11	2.50	0.46
1:A:84:SER:CA	1:G:86:ILE:HD11	2.46	0.46
1:E:251:LEU:HD23	1:E:251:LEU:HA	1.60	0.46
1:A:201:MET:HE1	1:A:246:ARG:HB2	1.97	0.46
1:B:86:ILE:CD1	1:C:84:SER:HA	2.46	0.46
1:B:172:CYS:SG	1:B:208:MET:HE3	2.56	0.46
1:C:165:ILE:HA	1:D:152:ALA:HA	1.97	0.46
1:C:214:ILE:HG13	1:D:245:GLU:HG2	1.98	0.46
1:C:251:LEU:HD23	1:C:251:LEU:HA	1.75	0.46
1:E:44:MET:HG2	1:E:59:ALA:HB2	1.97	0.46
1:A:265:ILE:CD1	1:G:265:ILE:HD13	2.46	0.46
1:B:18:PHE:CD2	1:B:22:LEU:HD22	2.51	0.46
1:C:44:MET:O	1:C:48:SER:OG	2.29	0.45
1:D:40:ARG:HB2	1:D:63:PHE:HD1	1.81	0.45
1:C:117:HIS:O	1:C:117:HIS:ND1	2.48	0.45
1:F:88:VAL:HA	1:F:91:THR:HG22	1.98	0.45
1:A:18:PHE:CE2	1:A:22:LEU:HD22	2.50	0.45
1:D:265:ILE:HD13	1:E:265:ILE:HD12	1.98	0.45
1:G:251:LEU:HD22	1:G:256:ILE:HG21	1.99	0.45
1:B:251:LEU:HA	1:B:251:LEU:HD23	1.75	0.45
1:C:18:PHE:CD2	1:C:22:LEU:HD22	2.51	0.45
1:F:177:TRP:HE1	1:F:244:ILE:HD12	1.81	0.45
1:F:259:PRO:HB3	1:F:262:LYS:NZ	2.31	0.45
1:B:123:ASP:O	1:B:134:VAL:HG12	2.17	0.45
1:D:29:PHE:O	1:D:33:PHE:HB2	2.17	0.45
1:D:42:LYS:HA	1:D:45:LYS:CB	2.46	0.45
1:D:214:ILE:HG12	1:D:224:PHE:CZ	2.52	0.45
1:C:136:ALA:HB3	1:C:143:SER:HB3	1.99	0.45
1:D:92:VAL:O	1:D:96:VAL:HG23	2.16	0.45
1:E:127:ILE:HD13	1:E:164:ILE:HA	1.99	0.45
1:E:214:ILE:HG13	1:F:245:GLU:HG2	1.99	0.45
1:G:108:ALA:HA	1:G:111:ILE:HB	1.98	0.45
1:C:201:MET:HE1	1:C:246:ARG:HB2	1.97	0.45
1:D:177:TRP:HZ2	1:D:244:ILE:HD12	1.81	0.45
1:F:173:ARG:HE	1:F:173:ARG:HB3	1.57	0.45
1:G:236:ILE:CG2	1:G:237:PHE:N	2.77	0.45
1:B:127:ILE:HD13	1:B:164:ILE:HA	1.97	0.45
1:D:188:GLU:HA	1:D:191:HIS:HB3	1.98	0.45
1:F:180:GLY:HA2	1:F:222:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ALA:HB2	1:G:97:ALA:HA	1.99	0.45
1:A:116:LEU:HD23	1:A:116:LEU:O	2.17	0.45
1:B:196:ASP:O	1:B:200:THR:HG23	2.16	0.45
1:D:201:MET:HE1	1:D:246:ARG:HB2	1.98	0.45
1:E:29:PHE:O	1:E:33:PHE:HB2	2.17	0.45
1:G:48:SER:O	1:G:49:LYS:HG2	2.17	0.45
1:B:214:ILE:HG13	1:C:245:GLU:HG2	1.99	0.45
1:A:21:ILE:H	1:A:21:ILE:HG13	1.65	0.44
1:A:214:ILE:HG12	1:A:224:PHE:CZ	2.52	0.44
1:B:92:VAL:O	1:B:96:VAL:HG23	2.16	0.44
1:C:113:LEU:HD23	1:C:113:LEU:HA	1.52	0.44
1:C:127:ILE:HD13	1:C:164:ILE:HA	1.97	0.44
1:E:214:ILE:HG12	1:E:224:PHE:CZ	2.51	0.44
1:F:29:PHE:O	1:F:33:PHE:CB	2.65	0.44
1:C:42:LYS:NZ	1:C:46:LEU:HD11	2.32	0.44
1:G:172:CYS:SG	1:G:208:MET:HE3	2.57	0.44
1:A:64:ILE:O	1:A:68:ILE:HG13	2.18	0.44
1:A:87:THR:O	1:A:91:THR:HG22	2.18	0.44
1:A:127:ILE:HD13	1:A:164:ILE:HA	1.98	0.44
1:A:140:PHE:HE2	1:G:112:ILE:CG1	2.30	0.44
1:B:188:GLU:HA	1:B:191:HIS:CB	2.47	0.44
1:E:43:THR:HG23	1:E:58:VAL:HG12	1.99	0.44
1:E:188:GLU:HA	1:E:191:HIS:HB2	1.98	0.44
1:D:29:PHE:O	1:D:33:PHE:CB	2.65	0.44
1:D:259:PRO:HB3	1:D:262:LYS:NZ	2.32	0.44
1:E:40:ARG:HB2	1:E:63:PHE:HD1	1.82	0.44
1:F:117:HIS:O	1:F:117:HIS:ND1	2.51	0.44
1:F:172:CYS:SG	1:F:208:MET:HE3	2.58	0.44
1:F:265:ILE:HD13	1:G:265:ILE:HD11	1.99	0.44
1:A:65:LEU:HA	1:A:65:LEU:HD12	1.74	0.44
1:B:217:PHE:CE2	1:C:258:ILE:HG12	2.53	0.44
1:C:42:LYS:HZ2	1:C:46:LEU:HD11	1.83	0.44
1:A:251:LEU:HD22	1:A:256:ILE:HG21	1.99	0.44
1:C:42:LYS:HG2	1:C:45:LYS:HE3	1.98	0.44
1:E:235:GLY:HA2	1:E:239:VAL:CG2	2.45	0.44
1:G:123:ASP:O	1:G:134:VAL:HG12	2.17	0.44
1:A:48:SER:HB2	1:A:55:ALA:HB1	2.00	0.44
1:C:98:LEU:HA	1:C:98:LEU:HD23	1.55	0.44
1:C:116:LEU:HD13	1:D:140:PHE:CD2	2.52	0.44
1:D:107:ILE:HG12	1:D:140:PHE:CD1	2.53	0.44
1:A:43:THR:HG23	1:A:58:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:THR:O	1:D:66:ILE:HG13	2.17	0.44
1:E:112:ILE:HG13	1:F:140:PHE:CE2	2.52	0.44
1:F:138:ASN:HD22	1:F:141:ASN:HB2	1.82	0.44
1:A:171:ALA:O	1:A:232:ILE:HG13	2.17	0.43
1:D:251:LEU:HD23	1:D:251:LEU:HA	1.73	0.43
1:E:36:SER:HB3	1:E:63:PHE:CE1	2.52	0.43
1:E:116:LEU:HD11	1:F:139:PHE:HD2	1.83	0.43
1:F:127:ILE:HD13	1:F:127:ILE:HA	1.70	0.43
1:G:18:PHE:CE1	1:G:21:ILE:HD11	2.53	0.43
1:G:210:THR:HG22	1:G:228:VAL:HG13	1.99	0.43
1:A:114:ILE:CG1	1:A:137:LEU:HD21	2.46	0.43
1:A:138:ASN:HB2	1:A:141:ASN:C	2.42	0.43
1:B:187:ILE:HG13	1:C:249:ASN:OD1	2.18	0.43
1:C:114:ILE:CG1	1:C:137:LEU:HD21	2.48	0.43
1:C:265:ILE:HD13	1:D:265:ILE:HD12	2.00	0.43
1:E:119:PHE:CE1	1:E:125:ILE:HD13	2.52	0.43
1:E:173:ARG:HE	1:E:173:ARG:HB3	1.57	0.43
1:E:241:SER:O	1:E:244:ILE:HG22	2.18	0.43
1:F:113:LEU:HD23	1:F:113:LEU:HA	1.48	0.43
1:A:248:LYS:CE	1:G:214:ILE:HG21	2.44	0.43
1:C:104:LEU:HG	1:D:99:ALA:HB2	2.01	0.43
1:C:125:ILE:HD12	1:C:127:ILE:HG12	2.00	0.43
1:D:215:THR:HG23	1:E:240:ARG:HH12	1.83	0.43
1:E:19:GLY:O	1:E:22:LEU:HB3	2.17	0.43
1:E:215:THR:CB	1:E:225:THR:HG1	2.30	0.43
1:F:40:ARG:HB2	1:F:63:PHE:HD1	1.84	0.43
1:F:92:VAL:O	1:F:96:VAL:HG23	2.17	0.43
1:G:188:GLU:HA	1:G:191:HIS:CB	2.48	0.43
1:E:29:PHE:O	1:E:33:PHE:CB	2.66	0.43
1:F:125:ILE:HD12	1:F:127:ILE:HG12	2.01	0.43
1:F:177:TRP:CZ2	1:F:244:ILE:HD12	2.53	0.43
1:F:203:LYS:O	1:F:204:ILE:HG13	2.18	0.43
1:G:19:GLY:O	1:G:22:LEU:HB3	2.17	0.43
1:A:116:LEU:O	1:A:118:PRO:HD3	2.18	0.43
1:A:247:ILE:O	1:A:251:LEU:HB2	2.18	0.43
1:B:144:LEU:O	1:B:151:LEU:HA	2.19	0.43
1:D:103:TYR:O	1:D:106:SER:HB2	2.19	0.43
1:G:40:ARG:HB2	1:G:63:PHE:HD1	1.82	0.43
1:G:183:TYR:HD1	1:G:222:LEU:N	2.16	0.43
1:C:42:LYS:HE2	1:C:45:LYS:NZ	2.34	0.43
1:C:187:ILE:HG13	1:D:249:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:GLU:HA	1:D:191:HIS:HB2	1.99	0.43
1:E:140:PHE:CD1	1:E:140:PHE:N	2.85	0.43
1:A:97:ALA:HA	1:B:95:ALA:HB2	1.99	0.43
1:D:113:LEU:HD23	1:D:113:LEU:HA	1.66	0.43
1:F:164:ILE:H	1:F:164:ILE:HD12	1.83	0.43
1:A:145:ARG:CZ	1:G:170:THR:HG21	2.49	0.43
1:A:226:ILE:HG22	1:A:228:VAL:HG23	2.00	0.43
1:B:109:GLY:O	1:B:113:LEU:HG	2.18	0.43
1:B:112:ILE:CG1	1:C:140:PHE:CE2	3.02	0.43
1:B:154:LEU:N	1:B:154:LEU:HD12	2.34	0.43
1:B:183:TYR:OH	1:B:217:PHE:HD2	2.01	0.43
1:C:127:ILE:HD13	1:C:127:ILE:HA	1.74	0.43
1:D:86:ILE:HD12	1:E:84:SER:HA	2.00	0.43
1:B:18:PHE:CE1	1:B:21:ILE:HD11	2.54	0.43
1:B:27:ILE:O	1:B:31:ILE:HG13	2.18	0.43
1:B:29:PHE:HD2	1:B:30:CYS:HG	1.67	0.43
1:B:119:PHE:CZ	1:B:125:ILE:HD13	2.54	0.43
1:C:86:ILE:HD11	1:D:84:SER:HA	2.01	0.43
1:D:43:THR:HG21	1:D:58:VAL:O	2.18	0.43
1:A:235:GLY:HA2	1:A:239:VAL:HG23	2.00	0.43
1:F:214:ILE:HG21	1:G:248:LYS:CE	2.45	0.43
1:B:259:PRO:HB3	1:B:262:LYS:HZ1	1.82	0.42
1:C:265:ILE:HG21	1:D:265:ILE:HD12	2.01	0.42
1:F:44:MET:HE3	1:F:44:MET:HB3	1.82	0.42
1:F:112:ILE:HG13	1:G:140:PHE:HE2	1.84	0.42
1:G:43:THR:HG21	1:G:58:VAL:O	2.19	0.42
1:A:42:LYS:HG2	1:A:45:LYS:HE3	2.00	0.42
1:A:44:MET:HA	1:A:48:SER:HB3	2.00	0.42
1:A:104:LEU:HG	1:B:99:ALA:HB2	2.00	0.42
1:E:18:PHE:CE2	1:E:22:LEU:HD22	2.54	0.42
1:F:42:LYS:HE2	1:F:45:LYS:NZ	2.34	0.42
1:A:138:ASN:HD22	1:A:141:ASN:HB2	1.85	0.42
1:A:203:LYS:NZ	1:A:234:ASP:OD2	2.31	0.42
1:B:86:ILE:HD12	1:C:84:SER:HA	2.01	0.42
1:E:64:ILE:O	1:E:68:ILE:HG13	2.19	0.42
1:B:127:ILE:HD13	1:B:127:ILE:HA	1.73	0.42
1:C:235:GLY:O	1:C:236:ILE:C	2.63	0.42
1:A:140:PHE:CE2	1:G:112:ILE:HG13	2.51	0.42
1:B:43:THR:HG23	1:B:58:VAL:HG12	2.01	0.42
1:B:112:ILE:CG1	1:C:140:PHE:HE2	2.32	0.42
1:C:34:TYR:C	1:C:36:SER:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ILE:HD13	1:D:265:ILE:HD11	2.01	0.42
1:D:48:SER:O	1:D:49:LYS:HG2	2.18	0.42
1:E:97:ALA:HA	1:F:95:ALA:HB2	2.02	0.42
1:E:214:ILE:HG23	1:E:222:LEU:HD11	2.00	0.42
1:G:136:ALA:HB3	1:G:143:SER:CB	2.49	0.42
1:A:188:GLU:HA	1:A:191:HIS:HB3	2.00	0.42
1:A:265:ILE:HD13	1:B:265:ILE:CD1	2.50	0.42
1:C:188:GLU:HA	1:C:191:HIS:CB	2.49	0.42
1:C:214:ILE:HG23	1:C:222:LEU:CD1	2.50	0.42
1:D:228:VAL:HG12	1:D:229:TRP:N	2.35	0.42
1:E:113:LEU:HA	1:E:113:LEU:HD23	1.61	0.42
1:E:186:ASP:HB3	1:E:189:LEU:CG	2.40	0.42
1:E:203:LYS:O	1:E:204:ILE:HG13	2.19	0.42
1:F:19:GLY:O	1:F:22:LEU:HB3	2.20	0.42
1:F:241:SER:O	1:F:244:ILE:HG22	2.20	0.42
1:G:48:SER:HB2	1:G:55:ALA:HB1	2.01	0.42
1:D:104:LEU:HG	1:E:99:ALA:HB2	2.01	0.42
1:D:170:THR:OG1	1:E:151:LEU:HD21	2.18	0.42
1:E:83:THR:O	1:E:87:THR:OG1	2.37	0.42
1:B:64:ILE:O	1:B:68:ILE:HG13	2.20	0.42
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.42	0.42
1:C:124:ILE:HG22	1:C:133:LYS:HB2	2.00	0.42
1:E:98:LEU:HD23	1:E:98:LEU:HA	1.56	0.42
1:E:110:GLY:HA3	1:E:156:ASN:HD22	1.84	0.42
1:A:265:ILE:HD13	1:B:265:ILE:HD12	2.01	0.42
1:E:44:MET:CA	1:E:48:SER:HB3	2.44	0.42
1:E:105:SER:HB3	1:E:157:ARG:NH2	2.34	0.42
1:F:64:ILE:HG13	1:F:64:ILE:H	1.68	0.42
1:F:119:PHE:CE1	1:F:125:ILE:HD13	2.55	0.42
1:A:161:ASN:HD21	1:B:103:TYR:HE2	1.68	0.42
1:C:34:TYR:O	1:C:37:PHE:N	2.51	0.42
1:C:43:THR:HG21	1:C:58:VAL:O	2.20	0.42
1:C:177:TRP:CZ2	1:C:244:ILE:CD1	3.02	0.42
1:D:116:LEU:HD13	1:E:140:PHE:CD2	2.54	0.42
1:D:124:ILE:HG13	1:D:167:SER:HB2	2.00	0.42
1:F:161:ASN:ND2	1:G:103:TYR:HE2	2.17	0.42
1:F:227:ARG:HH12	1:G:236:ILE:HD11	1.84	0.42
1:G:171:ALA:O	1:G:232:ILE:HG13	2.20	0.42
1:A:125:ILE:HD12	1:A:127:ILE:HG12	2.02	0.41
1:B:173:ARG:HE	1:B:173:ARG:HB3	1.61	0.41
1:E:172:CYS:SG	1:E:208:MET:HE3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:THR:HG23	1:F:240:ARG:HH12	1.84	0.41
1:F:29:PHE:O	1:F:33:PHE:HB2	2.20	0.41
1:F:64:ILE:O	1:F:68:ILE:HG13	2.20	0.41
1:F:171:ALA:HA	1:F:232:ILE:HD12	2.01	0.41
1:G:42:LYS:HG2	1:G:45:LYS:HE3	2.02	0.41
1:A:142:THR:OG1	1:A:156:ASN:OD1	2.38	0.41
1:A:186:ASP:HB3	1:A:189:LEU:CG	2.43	0.41
1:C:177:TRP:HZ2	1:C:244:ILE:HD12	1.85	0.41
1:D:127:ILE:HD13	1:D:164:ILE:HA	2.03	0.41
1:D:251:LEU:HD22	1:D:256:ILE:HG21	2.02	0.41
1:A:29:PHE:O	1:A:33:PHE:CB	2.69	0.41
1:A:183:TYR:HD1	1:A:222:LEU:N	2.18	0.41
1:A:227:ARG:HH22	1:B:236:ILE:HD11	1.84	0.41
1:A:240:ARG:HH12	1:G:215:THR:HG23	1.85	0.41
1:B:43:THR:CG2	1:B:58:VAL:HG12	2.50	0.41
1:B:138:ASN:HD22	1:B:141:ASN:HB2	1.85	0.41
1:C:44:MET:HG2	1:C:59:ALA:HB2	2.01	0.41
1:D:42:LYS:NZ	1:D:46:LEU:HD11	2.36	0.41
1:D:171:ALA:O	1:D:232:ILE:HG13	2.21	0.41
1:F:72:ILE:HD11	1:F:85:ILE:HG22	2.02	0.41
1:F:228:VAL:HG12	1:F:229:TRP:N	2.36	0.41
1:C:217:PHE:CD1	1:D:248:LYS:NZ	2.88	0.41
1:E:116:LEU:HD13	1:F:140:PHE:CZ	2.56	0.41
1:E:214:ILE:HG21	1:E:214:ILE:HD13	1.88	0.41
1:F:65:LEU:HA	1:F:65:LEU:HD12	1.70	0.41
1:F:188:GLU:HA	1:F:191:HIS:HB3	2.01	0.41
1:A:72:ILE:HD11	1:A:85:ILE:HG22	2.02	0.41
1:B:62:THR:O	1:B:66:ILE:HG13	2.20	0.41
1:D:127:ILE:HG23	1:D:127:ILE:HD12	1.77	0.41
1:D:214:ILE:HG13	1:E:245:GLU:HG2	2.01	0.41
1:E:201:MET:HE1	1:E:246:ARG:HB2	2.02	0.41
1:B:242:GLU:O	1:B:245:GLU:N	2.53	0.41
1:C:180:GLY:HA2	1:C:222:LEU:O	2.21	0.41
1:C:228:VAL:HG12	1:C:229:TRP:N	2.35	0.41
1:F:201:MET:HB3	1:F:204:ILE:HD12	2.03	0.41
1:A:140:PHE:CE2	1:G:112:ILE:CG1	3.04	0.41
1:D:64:ILE:HG13	1:D:64:ILE:H	1.71	0.41
1:A:117:HIS:O	1:A:117:HIS:ND1	2.54	0.41
1:A:220:SER:CB	1:A:262:LYS:H	2.23	0.41
1:A:263:LEU:HD11	1:B:263:LEU:HD23	2.03	0.41
1:B:34:TYR:C	1:B:36:SER:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ILE:O	1:B:191:HIS:HB2	2.21	0.41
1:C:215:THR:CB	1:C:225:THR:HG1	2.31	0.41
1:F:208:MET:HA	1:F:209:PRO:HD3	1.96	0.41
1:G:65:LEU:O	1:G:69:ILE:HG13	2.20	0.41
1:G:127:ILE:HD13	1:G:127:ILE:HA	1.77	0.41
1:A:32:GLY:O	1:A:35:PHE:N	2.54	0.41
1:A:125:ILE:O	1:A:131:GLU:HG3	2.21	0.41
1:A:144:LEU:O	1:A:151:LEU:HA	2.19	0.41
1:A:178:VAL:HG12	1:A:223:ASN:HB3	2.02	0.41
1:B:38:PHE:O	1:B:42:LYS:HB2	2.21	0.41
1:B:109:GLY:HA2	1:C:103:TYR:CZ	2.56	0.41
1:C:220:SER:CB	1:C:262:LYS:H	2.21	0.41
1:E:26:VAL:H	1:E:26:VAL:HG23	1.60	0.41
1:F:114:ILE:HG13	1:F:137:LEU:HD21	2.02	0.41
1:F:124:ILE:HG22	1:F:133:LYS:HB2	2.01	0.41
1:G:29:PHE:O	1:G:33:PHE:CB	2.69	0.41
1:G:127:ILE:HD12	1:G:127:ILE:HG23	1.85	0.41
1:A:85:ILE:HD11	1:G:73:ILE:HD11	2.02	0.41
1:A:110:GLY:HA3	1:A:156:ASN:HD22	1.86	0.41
1:B:107:ILE:HG12	1:B:140:PHE:CE1	2.55	0.41
1:C:100:LEU:O	1:C:104:LEU:HB3	2.20	0.41
1:C:107:ILE:HG12	1:C:140:PHE:CD1	2.55	0.41
1:D:64:ILE:O	1:D:68:ILE:HG13	2.21	0.41
1:E:117:HIS:O	1:E:117:HIS:ND1	2.54	0.40
1:B:125:ILE:O	1:B:131:GLU:HG3	2.21	0.40
1:C:112:ILE:CG1	1:D:140:PHE:CE2	3.04	0.40
1:C:181:VAL:O	1:C:259:PRO:HD3	2.21	0.40
1:D:18:PHE:CD2	1:D:22:LEU:HD22	2.56	0.40
1:E:181:VAL:O	1:E:182:GLY:C	2.62	0.40
1:E:263:LEU:HD11	1:F:263:LEU:HB3	2.02	0.40
1:F:177:TRP:NE1	1:F:244:ILE:HD12	2.37	0.40
1:G:138:ASN:HD22	1:G:141:ASN:HB2	1.86	0.40
1:D:44:MET:HG2	1:D:59:ALA:HB2	2.03	0.40
1:F:251:LEU:HD23	1:F:251:LEU:HA	1.68	0.40
1:G:42:LYS:HE2	1:G:45:LYS:NZ	2.35	0.40
1:G:173:ARG:HE	1:G:173:ARG:HB3	1.53	0.40
1:G:214:ILE:HG12	1:G:224:PHE:CZ	2.56	0.40
1:A:215:THR:HG23	1:B:240:ARG:HH12	1.86	0.40
1:B:171:ALA:HA	1:B:232:ILE:HD12	2.02	0.40
1:G:142:THR:OG1	1:G:156:ASN:OD1	2.38	0.40
1:G:176:GLU:HA	1:G:226:ILE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:VAL:CG1	1:G:223:ASN:HB3	2.52	0.40
1:B:188:GLU:HA	1:B:191:HIS:HB2	2.02	0.40
1:C:65:LEU:HA	1:C:65:LEU:HD12	1.78	0.40
1:C:259:PRO:HB3	1:C:262:LYS:NZ	2.35	0.40
1:D:44:MET:HA	1:D:48:SER:HB3	2.04	0.40
1:D:173:ARG:HE	1:D:173:ARG:HB3	1.59	0.40
1:D:178:VAL:HG12	1:D:223:ASN:HB3	2.02	0.40
1:F:220:SER:HB2	1:F:262:LYS:N	2.16	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	251/309 (81%)	235 (94%)	15 (6%)	1 (0%)	30	65
1	B	251/309 (81%)	236 (94%)	14 (6%)	1 (0%)	30	65
1	C	251/309 (81%)	232 (92%)	17 (7%)	2 (1%)	16	52
1	D	251/309 (81%)	234 (93%)	16 (6%)	1 (0%)	30	65
1	E	251/309 (81%)	234 (93%)	16 (6%)	1 (0%)	30	65
1	F	251/309 (81%)	232 (92%)	18 (7%)	1 (0%)	30	65
1	G	251/309 (81%)	232 (92%)	17 (7%)	2 (1%)	16	52
All	All	1757/2163 (81%)	1635 (93%)	113 (6%)	9 (0%)	24	61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ILE
1	D	236	ILE
1	E	236	ILE

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Mol	Chain	Res	Type
1	F	236	ILE
1	G	236	ILE
1	C	236	ILE
1	G	138	ASN
1	B	237	PHE
1	C	118	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	A	220/272 (81%)	210 (96%)	10 (4%)	24	47
1	B	220/272 (81%)	208 (94%)	12 (6%)	19	43
1	C	220/272 (81%)	210 (96%)	10 (4%)	24	47
1	D	220/272 (81%)	213 (97%)	7 (3%)	34	56
1	E	220/272 (81%)	207 (94%)	13 (6%)	18	42
1	F	220/272 (81%)	210 (96%)	10 (4%)	24	47
1	G	220/272 (81%)	211 (96%)	9 (4%)	27	49
All	All	1540/1904 (81%)	1469 (95%)	71 (5%)	24	47

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	26	VAL
1	A	61	VAL
1	A	112	ILE
1	A	134	VAL
1	A	140	PHE
1	A	178	VAL
1	A	204	ILE
1	A	236	ILE
1	A	267	ILE
1	B	26	VAL

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Mol	Chain	Res	Type
1	B	50	LYS
1	B	61	VAL
1	B	92	VAL
1	B	112	ILE
1	B	134	VAL
1	B	140	PHE
1	B	178	VAL
1	B	204	ILE
1	B	236	ILE
1	B	244	ILE
1	B	267	ILE
1	C	26	VAL
1	C	47	LEU
1	C	61	VAL
1	C	112	ILE
1	C	134	VAL
1	C	178	VAL
1	C	204	ILE
1	C	222	LEU
1	C	236	ILE
1	C	267	ILE
1	D	26	VAL
1	D	61	VAL
1	D	112	ILE
1	D	134	VAL
1	D	178	VAL
1	D	204	ILE
1	D	267	ILE
1	E	26	VAL
1	E	48	SER
1	E	49	LYS
1	E	61	VAL
1	E	112	ILE
1	E	116	LEU
1	E	134	VAL
1	E	140	PHE
1	E	178	VAL
1	E	204	ILE
1	E	222	LEU
1	E	236	ILE
1	E	267	ILE
1	F	26	VAL

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Mol	Chain	Res	Type
1	F	61	VAL
1	F	112	ILE
1	F	134	VAL
1	F	140	PHE
1	F	178	VAL
1	F	204	ILE
1	F	233	GLU
1	F	236	ILE
1	F	267	ILE
1	G	26	VAL
1	G	61	VAL
1	G	86	ILE
1	G	92	VAL
1	G	112	ILE
1	G	134	VAL
1	G	178	VAL
1	G	204	ILE
1	G	267	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	138	ASN
1	A	270	GLN
1	B	138	ASN
1	B	191	HIS
1	B	270	GLN
1	C	81	GLN
1	C	138	ASN
1	C	169	ASN
1	C	270	GLN
1	D	81	GLN
1	D	138	ASN
1	D	191	HIS
1	D	270	GLN
1	E	81	GLN
1	E	138	ASN
1	E	191	HIS
1	E	238	ASN
1	E	270	GLN
1	F	138	ASN

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Mol	Chain	Res	Type
1	F	141	ASN
1	F	147	HIS
1	F	191	HIS
1	F	238	ASN
1	F	270	GLN
1	G	81	GLN
1	G	138	ASN
1	G	270	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	253/309 (81%)	-0.19	1 (0%) 88 76	46, 121, 198, 228	0
1	B	253/309 (81%)	-0.14	3 (1%) 76 60	52, 120, 196, 222	0
1	C	253/309 (81%)	-0.21	1 (0%) 88 76	52, 119, 191, 234	0
1	D	253/309 (81%)	-0.21	2 (0%) 82 67	55, 117, 190, 216	0
1	E	253/309 (81%)	-0.24	1 (0%) 88 76	55, 117, 191, 221	0
1	F	253/309 (81%)	-0.24	1 (0%) 88 76	54, 117, 189, 235	0
1	G	253/309 (81%)	-0.14	3 (1%) 76 60	53, 120, 188, 221	0
All	All	1771/2163 (81%)	-0.19	12 (0%) 84 69	46, 119, 194, 235	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	190	VAL	3.7
1	F	21	ILE	3.3
1	D	80	VAL	3.2
1	G	194	ILE	3.0
1	B	136	ALA	2.7
1	G	198	ILE	2.6
1	A	127	ILE	2.5
1	E	41	ASN	2.4
1	B	131	GLU	2.4
1	C	230	ALA	2.2
1	D	159	VAL	2.1
1	B	169	ASN	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.