



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:46 AM GMT

PDB ID : 4HWA  
Title : Crystal Structure of Escherichia coli MscS Wildtype (Open State)  
Authors : Lai, J.Y.; Poon, Y.S.; Kaiser, J.; Rees, D.C.  
Deposited on : 2012-11-07  
Resolution : 4.37 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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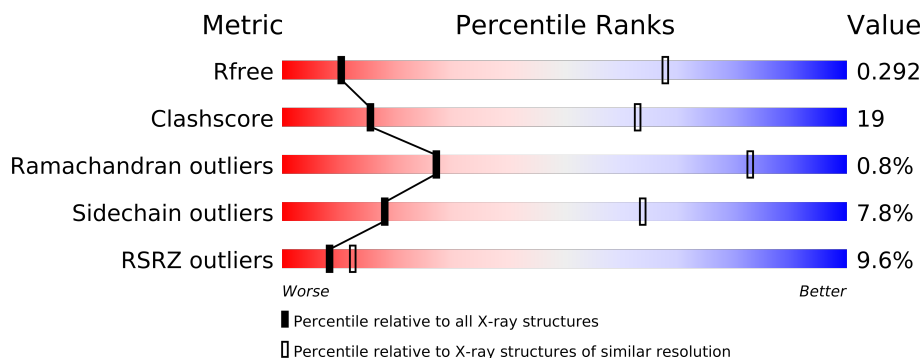
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 4.37 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))
$R_{free}$	66092	1019 (5.26-3.50)
Clashscore	79885	1284 (5.26-3.50)
Ramachandran outliers	78287	1214 (5.26-3.50)
Sidechain outliers	78261	1195 (5.26-3.50)
RSRZ outliers	66119	1019 (5.26-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	306	
1	B	306	
1	C	306	
1	D	306	
1	E	306	
1	F	306	
1	G	306	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13678 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called Small-conductance mechanosensitive channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	1
			1954	1254	342	352	6			
1	B	257	Total	C	N	O	S	0	0	1
			1954	1254	342	352	6			
1	C	257	Total	C	N	O	S	0	0	1
			1954	1254	342	352	6			
1	D	257	Total	C	N	O	S	0	0	1
			1954	1254	342	352	6			
1	E	257	Total	C	N	O	S	0	0	1
			1954	1254	342	352	6			
1	F	257	Total	C	N	O	S	0	0	1
			1954	1254	342	352	6			
1	G	257	Total	C	N	O	S	0	0	1
			1954	1254	342	352	6			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P0C0S1
A	-18	GLY	-	EXPRESSION TAG	UNP P0C0S1
A	-17	SER	-	EXPRESSION TAG	UNP P0C0S1
A	-16	SER	-	EXPRESSION TAG	UNP P0C0S1
A	-15	HIS	-	EXPRESSION TAG	UNP P0C0S1
A	-14	HIS	-	EXPRESSION TAG	UNP P0C0S1
A	-13	HIS	-	EXPRESSION TAG	UNP P0C0S1
A	-12	HIS	-	EXPRESSION TAG	UNP P0C0S1
A	-11	HIS	-	EXPRESSION TAG	UNP P0C0S1
A	-10	HIS	-	EXPRESSION TAG	UNP P0C0S1
A	-9	SER	-	EXPRESSION TAG	UNP P0C0S1
A	-8	SER	-	EXPRESSION TAG	UNP P0C0S1
A	-7	GLY	-	EXPRESSION TAG	UNP P0C0S1
A	-6	LEU	-	EXPRESSION TAG	UNP P0C0S1
A	-5	VAL	-	EXPRESSION TAG	UNP P0C0S1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	EXPRESSION TAG	UNP P0C0S1
A	-3	ARG	-	EXPRESSION TAG	UNP P0C0S1
A	-2	GLY	-	EXPRESSION TAG	UNP P0C0S1
A	-1	SER	-	EXPRESSION TAG	UNP P0C0S1
A	0	HIS	-	EXPRESSION TAG	UNP P0C0S1
B	-19	MET	-	EXPRESSION TAG	UNP P0C0S1
B	-18	GLY	-	EXPRESSION TAG	UNP P0C0S1
B	-17	SER	-	EXPRESSION TAG	UNP P0C0S1
B	-16	SER	-	EXPRESSION TAG	UNP P0C0S1
B	-15	HIS	-	EXPRESSION TAG	UNP P0C0S1
B	-14	HIS	-	EXPRESSION TAG	UNP P0C0S1
B	-13	HIS	-	EXPRESSION TAG	UNP P0C0S1
B	-12	HIS	-	EXPRESSION TAG	UNP P0C0S1
B	-11	HIS	-	EXPRESSION TAG	UNP P0C0S1
B	-10	HIS	-	EXPRESSION TAG	UNP P0C0S1
B	-9	SER	-	EXPRESSION TAG	UNP P0C0S1
B	-8	SER	-	EXPRESSION TAG	UNP P0C0S1
B	-7	GLY	-	EXPRESSION TAG	UNP P0C0S1
B	-6	LEU	-	EXPRESSION TAG	UNP P0C0S1
B	-5	VAL	-	EXPRESSION TAG	UNP P0C0S1
B	-4	PRO	-	EXPRESSION TAG	UNP P0C0S1
B	-3	ARG	-	EXPRESSION TAG	UNP P0C0S1
B	-2	GLY	-	EXPRESSION TAG	UNP P0C0S1
B	-1	SER	-	EXPRESSION TAG	UNP P0C0S1
B	0	HIS	-	EXPRESSION TAG	UNP P0C0S1
C	-19	MET	-	EXPRESSION TAG	UNP P0C0S1
C	-18	GLY	-	EXPRESSION TAG	UNP P0C0S1
C	-17	SER	-	EXPRESSION TAG	UNP P0C0S1
C	-16	SER	-	EXPRESSION TAG	UNP P0C0S1
C	-15	HIS	-	EXPRESSION TAG	UNP P0C0S1
C	-14	HIS	-	EXPRESSION TAG	UNP P0C0S1
C	-13	HIS	-	EXPRESSION TAG	UNP P0C0S1
C	-12	HIS	-	EXPRESSION TAG	UNP P0C0S1
C	-11	HIS	-	EXPRESSION TAG	UNP P0C0S1
C	-10	HIS	-	EXPRESSION TAG	UNP P0C0S1
C	-9	SER	-	EXPRESSION TAG	UNP P0C0S1
C	-8	SER	-	EXPRESSION TAG	UNP P0C0S1
C	-7	GLY	-	EXPRESSION TAG	UNP P0C0S1
C	-6	LEU	-	EXPRESSION TAG	UNP P0C0S1
C	-5	VAL	-	EXPRESSION TAG	UNP P0C0S1
C	-4	PRO	-	EXPRESSION TAG	UNP P0C0S1
C	-3	ARG	-	EXPRESSION TAG	UNP P0C0S1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP P0C0S1
C	-1	SER	-	EXPRESSION TAG	UNP P0C0S1
C	0	HIS	-	EXPRESSION TAG	UNP P0C0S1
D	-19	MET	-	EXPRESSION TAG	UNP P0C0S1
D	-18	GLY	-	EXPRESSION TAG	UNP P0C0S1
D	-17	SER	-	EXPRESSION TAG	UNP P0C0S1
D	-16	SER	-	EXPRESSION TAG	UNP P0C0S1
D	-15	HIS	-	EXPRESSION TAG	UNP P0C0S1
D	-14	HIS	-	EXPRESSION TAG	UNP P0C0S1
D	-13	HIS	-	EXPRESSION TAG	UNP P0C0S1
D	-12	HIS	-	EXPRESSION TAG	UNP P0C0S1
D	-11	HIS	-	EXPRESSION TAG	UNP P0C0S1
D	-10	HIS	-	EXPRESSION TAG	UNP P0C0S1
D	-9	SER	-	EXPRESSION TAG	UNP P0C0S1
D	-8	SER	-	EXPRESSION TAG	UNP P0C0S1
D	-7	GLY	-	EXPRESSION TAG	UNP P0C0S1
D	-6	LEU	-	EXPRESSION TAG	UNP P0C0S1
D	-5	VAL	-	EXPRESSION TAG	UNP P0C0S1
D	-4	PRO	-	EXPRESSION TAG	UNP P0C0S1
D	-3	ARG	-	EXPRESSION TAG	UNP P0C0S1
D	-2	GLY	-	EXPRESSION TAG	UNP P0C0S1
D	-1	SER	-	EXPRESSION TAG	UNP P0C0S1
D	0	HIS	-	EXPRESSION TAG	UNP P0C0S1
E	-19	MET	-	EXPRESSION TAG	UNP P0C0S1
E	-18	GLY	-	EXPRESSION TAG	UNP P0C0S1
E	-17	SER	-	EXPRESSION TAG	UNP P0C0S1
E	-16	SER	-	EXPRESSION TAG	UNP P0C0S1
E	-15	HIS	-	EXPRESSION TAG	UNP P0C0S1
E	-14	HIS	-	EXPRESSION TAG	UNP P0C0S1
E	-13	HIS	-	EXPRESSION TAG	UNP P0C0S1
E	-12	HIS	-	EXPRESSION TAG	UNP P0C0S1
E	-11	HIS	-	EXPRESSION TAG	UNP P0C0S1
E	-10	HIS	-	EXPRESSION TAG	UNP P0C0S1
E	-9	SER	-	EXPRESSION TAG	UNP P0C0S1
E	-8	SER	-	EXPRESSION TAG	UNP P0C0S1
E	-7	GLY	-	EXPRESSION TAG	UNP P0C0S1
E	-6	LEU	-	EXPRESSION TAG	UNP P0C0S1
E	-5	VAL	-	EXPRESSION TAG	UNP P0C0S1
E	-4	PRO	-	EXPRESSION TAG	UNP P0C0S1
E	-3	ARG	-	EXPRESSION TAG	UNP P0C0S1
E	-2	GLY	-	EXPRESSION TAG	UNP P0C0S1
E	-1	SER	-	EXPRESSION TAG	UNP P0C0S1

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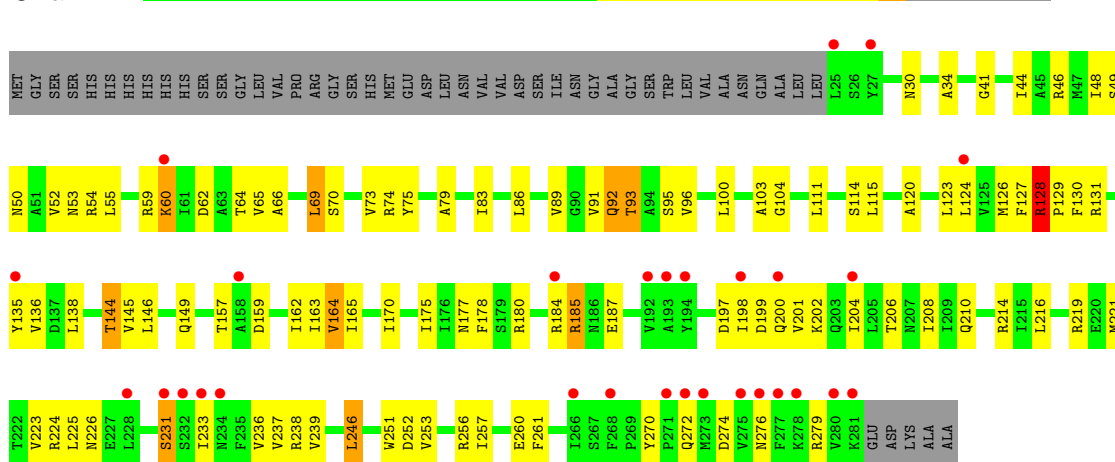
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	EXPRESSION TAG	UNP P0C0S1
F	-19	MET	-	EXPRESSION TAG	UNP P0C0S1
F	-18	GLY	-	EXPRESSION TAG	UNP P0C0S1
F	-17	SER	-	EXPRESSION TAG	UNP P0C0S1
F	-16	SER	-	EXPRESSION TAG	UNP P0C0S1
F	-15	HIS	-	EXPRESSION TAG	UNP P0C0S1
F	-14	HIS	-	EXPRESSION TAG	UNP P0C0S1
F	-13	HIS	-	EXPRESSION TAG	UNP P0C0S1
F	-12	HIS	-	EXPRESSION TAG	UNP P0C0S1
F	-11	HIS	-	EXPRESSION TAG	UNP P0C0S1
F	-10	HIS	-	EXPRESSION TAG	UNP P0C0S1
F	-9	SER	-	EXPRESSION TAG	UNP P0C0S1
F	-8	SER	-	EXPRESSION TAG	UNP P0C0S1
F	-7	GLY	-	EXPRESSION TAG	UNP P0C0S1
F	-6	LEU	-	EXPRESSION TAG	UNP P0C0S1
F	-5	VAL	-	EXPRESSION TAG	UNP P0C0S1
F	-4	PRO	-	EXPRESSION TAG	UNP P0C0S1
F	-3	ARG	-	EXPRESSION TAG	UNP P0C0S1
F	-2	GLY	-	EXPRESSION TAG	UNP P0C0S1
F	-1	SER	-	EXPRESSION TAG	UNP P0C0S1
F	0	HIS	-	EXPRESSION TAG	UNP P0C0S1
G	-19	MET	-	EXPRESSION TAG	UNP P0C0S1
G	-18	GLY	-	EXPRESSION TAG	UNP P0C0S1
G	-17	SER	-	EXPRESSION TAG	UNP P0C0S1
G	-16	SER	-	EXPRESSION TAG	UNP P0C0S1
G	-15	HIS	-	EXPRESSION TAG	UNP P0C0S1
G	-14	HIS	-	EXPRESSION TAG	UNP P0C0S1
G	-13	HIS	-	EXPRESSION TAG	UNP P0C0S1
G	-12	HIS	-	EXPRESSION TAG	UNP P0C0S1
G	-11	HIS	-	EXPRESSION TAG	UNP P0C0S1
G	-10	HIS	-	EXPRESSION TAG	UNP P0C0S1
G	-9	SER	-	EXPRESSION TAG	UNP P0C0S1
G	-8	SER	-	EXPRESSION TAG	UNP P0C0S1
G	-7	GLY	-	EXPRESSION TAG	UNP P0C0S1
G	-6	LEU	-	EXPRESSION TAG	UNP P0C0S1
G	-5	VAL	-	EXPRESSION TAG	UNP P0C0S1
G	-4	PRO	-	EXPRESSION TAG	UNP P0C0S1
G	-3	ARG	-	EXPRESSION TAG	UNP P0C0S1
G	-2	GLY	-	EXPRESSION TAG	UNP P0C0S1
G	-1	SER	-	EXPRESSION TAG	UNP P0C0S1
G	0	HIS	-	EXPRESSION TAG	UNP P0C0S1

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

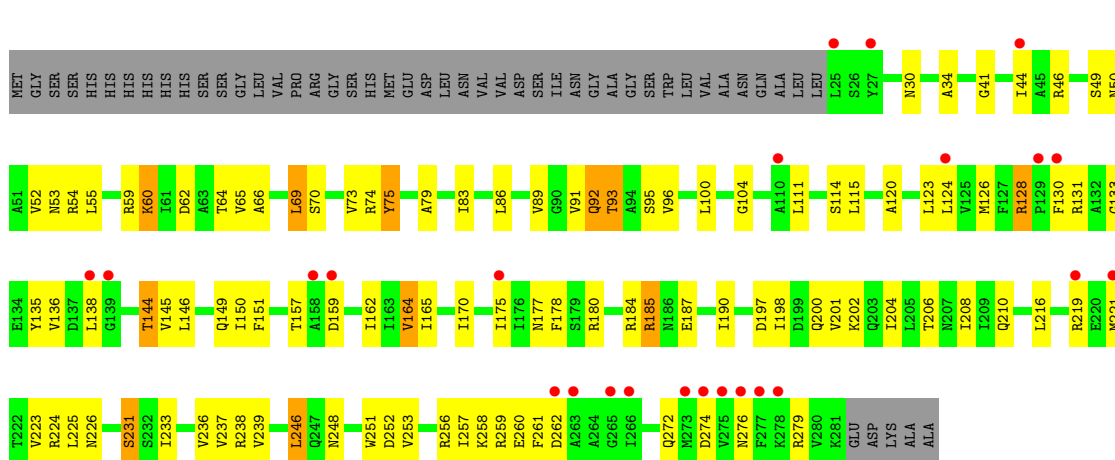
- Molecule 1: Small-conductance mechanosensitive channel

Chain A:



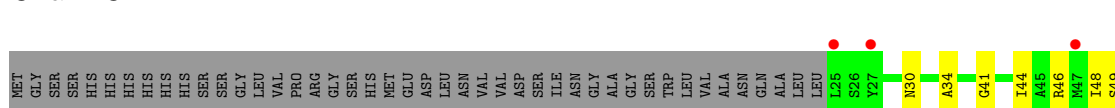
- Molecule 1: Small-conductance mechanosensitive channel

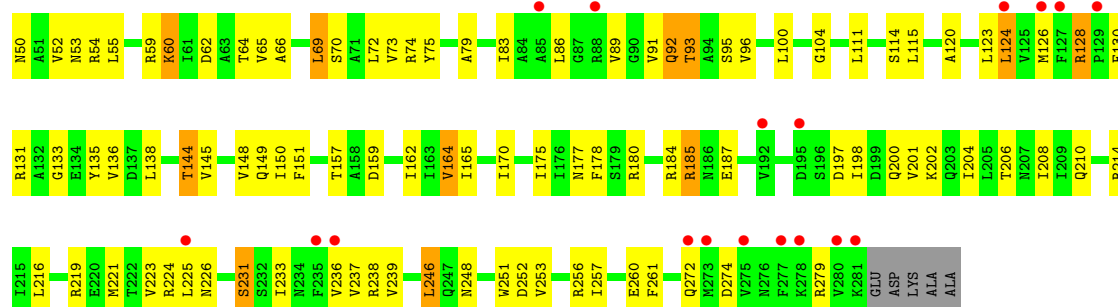
Chain B:



- Molecule 1: Small-conductance mechanosensitive channel

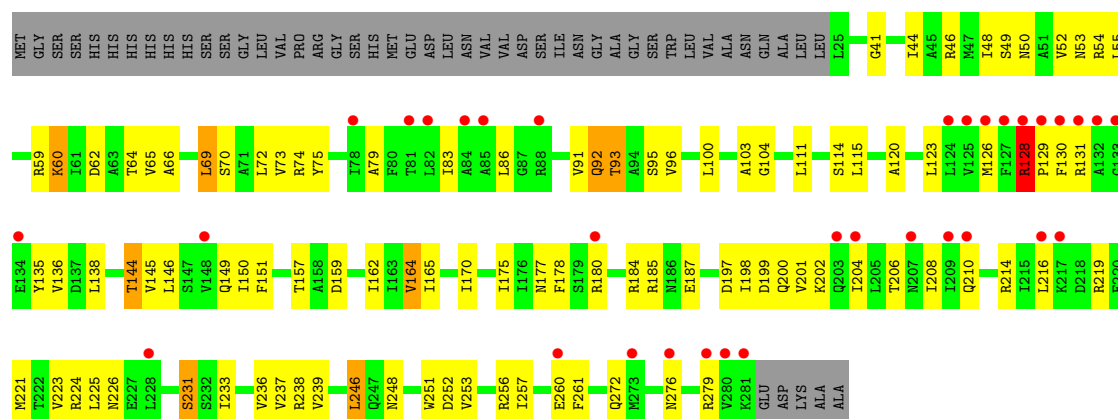
Chain C:





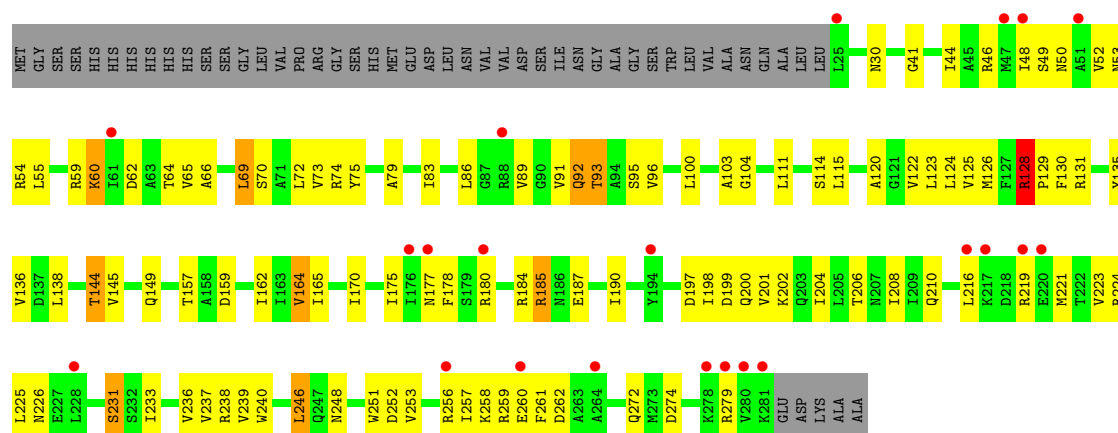
- Molecule 1: Small-conductance mechanosensitive channel

Chain D:



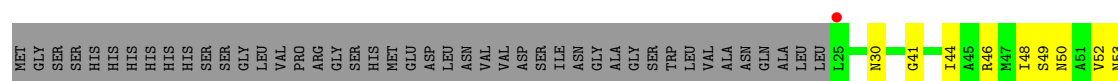
- Molecule 1: Small-conductance mechanosensitive channel

Chain E:

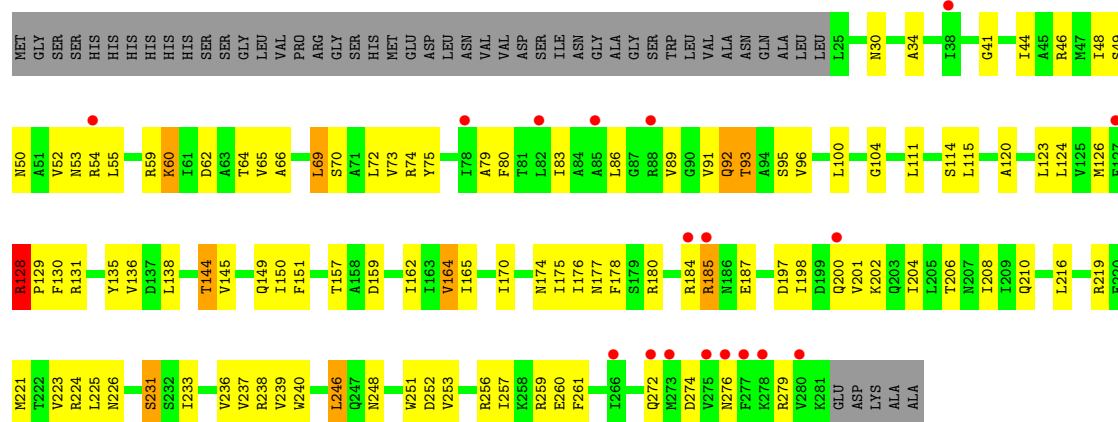


- Molecule 1: Small-conductance mechanosensitive channel

Chain F:







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.24Å 149.97Å 175.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.91 – 4.37 46.58 – 4.37	Depositor EDS
% Data completeness (in resolution range)	94.8 (37.91-4.37) 99.6 (46.58-4.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.28 (at 4.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)	Depositor
R, $R_{free}$	0.267 , 0.288 0.268 , 0.292	Depositor DCC
$R_{free}$ test set	1149 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	199.0	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 60.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 22481 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	13678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.33	0/1979	0.57	0/2684
1	B	0.31	0/1979	0.56	0/2684
1	C	0.32	0/1979	0.57	0/2684
1	D	0.32	0/1979	0.57	0/2684
1	E	0.35	0/1979	0.56	0/2684
1	F	0.33	0/1979	0.57	0/2684
1	G	0.32	0/1979	0.57	0/2684
All	All	0.33	0/13853	0.57	0/18788

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1954	0	2048	89	0
1	B	1954	0	2048	80	0
1	C	1954	0	2048	82	0
1	D	1954	0	2048	82	0
1	E	1954	0	2048	83	0
1	F	1954	0	2048	82	0
1	G	1954	0	2048	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13678	0	14336	521	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (521) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:164:VAL:HG23	1:G:175:ILE:HB	1.48	0.92
1:F:175:ILE:HB	1:G:164:VAL:HG23	1.53	0.90
1:C:175:ILE:HB	1:D:164:VAL:HG23	1.54	0.90
1:E:49:SER:HB3	1:E:74:ARG:HB2	1.57	0.87
1:G:185:ARG:HH21	1:G:238:ARG:HD3	1.40	0.86
1:D:49:SER:HB3	1:D:74:ARG:HB2	1.58	0.86
1:F:49:SER:HB3	1:F:74:ARG:HB2	1.59	0.84
1:C:49:SER:HB3	1:C:74:ARG:HB2	1.58	0.84
1:A:49:SER:HB3	1:A:74:ARG:HB2	1.59	0.84
1:G:49:SER:HB3	1:G:74:ARG:HB2	1.58	0.84
1:B:185:ARG:HH21	1:B:238:ARG:HD3	1.43	0.83
1:A:185:ARG:HH21	1:A:238:ARG:HD3	1.44	0.83
1:C:185:ARG:HH21	1:C:238:ARG:HD3	1.43	0.83
1:E:175:ILE:HB	1:F:164:VAL:HG23	1.62	0.82
1:D:185:ARG:HH21	1:D:238:ARG:HD3	1.44	0.81
1:A:175:ILE:HB	1:B:164:VAL:HG23	1.62	0.81
1:B:49:SER:HB3	1:B:74:ARG:HB2	1.59	0.81
1:F:185:ARG:HH21	1:F:238:ARG:HD3	1.46	0.81
1:E:185:ARG:HH21	1:E:238:ARG:HD3	1.45	0.81
1:B:175:ILE:HB	1:C:164:VAL:HG23	1.62	0.80
1:D:279:ARG:HH12	1:E:279:ARG:HH21	1.30	0.80
1:C:131:ARG:HH21	1:C:180:ARG:HD2	1.47	0.79
1:A:231:SER:HB3	1:A:272:GLN:H	1.48	0.79
1:A:279:ARG:HH12	1:B:279:ARG:HH21	1.30	0.79
1:G:231:SER:HB3	1:G:272:GLN:H	1.48	0.78
1:D:175:ILE:HB	1:E:164:VAL:HG23	1.63	0.78
1:B:131:ARG:HH21	1:B:180:ARG:HD2	1.47	0.78
1:C:231:SER:HB3	1:C:272:GLN:H	1.47	0.78
1:D:131:ARG:HH21	1:D:180:ARG:HD2	1.48	0.78
1:F:231:SER:HB3	1:F:272:GLN:H	1.49	0.78
1:B:231:SER:HB3	1:B:272:GLN:H	1.49	0.77
1:D:231:SER:HB3	1:D:272:GLN:H	1.49	0.77
1:F:131:ARG:HH21	1:F:180:ARG:HD2	1.49	0.77
1:G:131:ARG:HH21	1:G:180:ARG:HD2	1.48	0.77
1:A:131:ARG:HH21	1:A:180:ARG:HD2	1.48	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:231:SER:HB3	1:E:272:GLN:H	1.50	0.76
1:A:46:ARG:HH21	1:A:74:ARG:HH21	1.35	0.75
1:F:224:ARG:NH2	1:G:252:ASP:OD1	2.20	0.74
1:E:131:ARG:HH21	1:E:180:ARG:HD2	1.50	0.73
1:E:279:ARG:HH12	1:F:279:ARG:HH21	1.36	0.73
1:B:120:ALA:HA	1:B:123:LEU:HB2	1.70	0.72
1:A:120:ALA:HA	1:A:123:LEU:HB2	1.71	0.72
1:G:120:ALA:HA	1:G:123:LEU:HB2	1.71	0.72
1:F:46:ARG:HH21	1:F:74:ARG:HH21	1.38	0.72
1:E:120:ALA:HA	1:E:123:LEU:HB2	1.72	0.71
1:D:46:ARG:HH21	1:D:74:ARG:HH21	1.38	0.71
1:C:46:ARG:HH21	1:C:74:ARG:HH21	1.38	0.71
1:F:224:ARG:HD3	1:G:251:TRP:HB3	1.72	0.71
1:G:46:ARG:HH21	1:G:74:ARG:HH21	1.39	0.71
1:C:279:ARG:HH12	1:D:279:ARG:HH21	1.36	0.70
1:B:46:ARG:HH21	1:B:74:ARG:HH21	1.37	0.70
1:C:120:ALA:HA	1:C:123:LEU:HB2	1.72	0.70
1:F:120:ALA:HA	1:F:123:LEU:HB2	1.74	0.69
1:D:120:ALA:HA	1:D:123:LEU:HB2	1.74	0.68
1:E:46:ARG:HH21	1:E:74:ARG:HH21	1.39	0.68
1:C:52:VAL:HG21	1:C:73:VAL:HG11	1.79	0.65
1:E:52:VAL:HG21	1:E:73:VAL:HG11	1.80	0.64
1:C:180:ARG:HH12	1:D:162:ILE:HG21	1.63	0.64
1:E:86:LEU:HB3	1:E:91:VAL:HB	1.80	0.64
1:B:52:VAL:HG21	1:B:73:VAL:HG11	1.80	0.64
1:A:52:VAL:HG21	1:A:73:VAL:HG11	1.80	0.63
1:F:86:LEU:HB3	1:F:91:VAL:HB	1.81	0.63
1:D:52:VAL:HG21	1:D:73:VAL:HG11	1.79	0.63
1:F:52:VAL:HG21	1:F:73:VAL:HG11	1.81	0.62
1:A:279:ARG:HH21	1:G:279:ARG:HH12	1.47	0.62
1:G:52:VAL:HG21	1:G:73:VAL:HG11	1.81	0.62
1:F:180:ARG:HH12	1:G:162:ILE:HG21	1.63	0.62
1:F:279:ARG:HH12	1:G:279:ARG:HH21	1.46	0.62
1:G:86:LEU:HB3	1:G:91:VAL:HB	1.82	0.61
1:G:223:VAL:HG22	1:G:237:VAL:HG22	1.82	0.61
1:D:86:LEU:HB3	1:D:91:VAL:HB	1.82	0.61
1:F:206:THR:O	1:F:210:GLN:HG2	2.01	0.61
1:G:208:ILE:HG23	1:G:256:ARG:HD2	1.82	0.61
1:A:86:LEU:HB3	1:A:91:VAL:HB	1.81	0.61
1:F:223:VAL:HG22	1:F:237:VAL:HG22	1.81	0.60
1:F:208:ILE:HG23	1:F:256:ARG:HD2	1.83	0.60
1:G:206:THR:O	1:G:210:GLN:HG2	2.00	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:206:THR:O	1:A:210:GLN:HG2	2.01	0.60
1:D:53:ASN:HB3	1:D:70:SER:HB3	1.84	0.60
1:D:49:SER:CB	1:D:74:ARG:HB2	2.31	0.60
1:B:136:VAL:HG12	1:B:177:ASN:HA	1.83	0.60
1:E:206:THR:O	1:E:210:GLN:HG2	2.01	0.60
1:D:279:ARG:HH12	1:E:279:ARG:NH2	2.00	0.60
1:D:136:VAL:HG12	1:D:177:ASN:HA	1.84	0.60
1:D:206:THR:O	1:D:210:GLN:HG2	2.01	0.60
1:C:223:VAL:HG22	1:C:237:VAL:HG22	1.82	0.60
1:E:198:ILE:HD12	1:E:198:ILE:H	1.67	0.60
1:C:206:THR:O	1:C:210:GLN:HG2	2.02	0.60
1:C:185:ARG:NH2	1:C:238:ARG:HD3	2.17	0.60
1:F:136:VAL:HG12	1:F:177:ASN:HA	1.83	0.59
1:C:86:LEU:HB3	1:C:91:VAL:HB	1.83	0.59
1:G:53:ASN:HB3	1:G:70:SER:HB3	1.84	0.59
1:B:86:LEU:HB3	1:B:91:VAL:HB	1.82	0.59
1:A:136:VAL:HG12	1:A:177:ASN:HA	1.84	0.59
1:E:49:SER:CB	1:E:74:ARG:HB2	2.31	0.59
1:D:223:VAL:HG22	1:D:237:VAL:HG22	1.84	0.59
1:B:53:ASN:HB3	1:B:70:SER:HB3	1.83	0.59
1:E:53:ASN:HB3	1:E:70:SER:HB3	1.84	0.59
1:C:208:ILE:HG23	1:C:256:ARG:HD2	1.84	0.59
1:G:49:SER:CB	1:G:74:ARG:HB2	2.31	0.59
1:E:223:VAL:HG22	1:E:237:VAL:HG22	1.84	0.59
1:B:185:ARG:NH2	1:B:238:ARG:HD3	2.16	0.59
1:A:279:ARG:HH12	1:B:279:ARG:NH2	1.98	0.59
1:D:180:ARG:HH12	1:E:162:ILE:HG21	1.66	0.59
1:F:199:ASP:OD2	1:G:259:ARG:NH1	2.34	0.59
1:A:53:ASN:HB3	1:A:70:SER:HB3	1.84	0.59
1:E:224:ARG:HD3	1:F:251:TRP:HB3	1.85	0.59
1:A:208:ILE:HG23	1:A:256:ARG:HD2	1.85	0.59
1:A:223:VAL:HG22	1:A:237:VAL:HG22	1.84	0.59
1:E:86:LEU:HD22	1:E:91:VAL:HG21	1.85	0.59
1:E:208:ILE:HG23	1:E:256:ARG:HD2	1.85	0.59
1:G:136:VAL:HG12	1:G:177:ASN:HA	1.84	0.58
1:C:136:VAL:HG12	1:C:177:ASN:HA	1.84	0.58
1:B:53:ASN:HB2	1:B:66:ALA:HB1	1.86	0.58
1:B:206:THR:O	1:B:210:GLN:HG2	2.02	0.58
1:C:130:PHE:HE1	1:C:145:VAL:HG11	1.67	0.58
1:B:198:ILE:H	1:B:198:ILE:HD12	1.68	0.58
1:E:136:VAL:HG12	1:E:177:ASN:HA	1.85	0.58
1:G:130:PHE:HE1	1:G:145:VAL:HG11	1.68	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:53:ASN:HB2	1:E:66:ALA:HB1	1.86	0.58
1:C:53:ASN:HB3	1:C:70:SER:HB3	1.85	0.58
1:F:49:SER:CB	1:F:74:ARG:HB2	2.33	0.58
1:D:224:ARG:HD3	1:E:251:TRP:HB3	1.84	0.58
1:B:208:ILE:HG23	1:B:256:ARG:HD2	1.84	0.58
1:A:198:ILE:HD12	1:A:198:ILE:H	1.69	0.57
1:A:162:ILE:HG21	1:G:180:ARG:HH12	1.69	0.57
1:A:138:LEU:HD13	1:A:170:ILE:HG12	1.86	0.57
1:F:53:ASN:HB3	1:F:70:SER:HB3	1.85	0.57
1:A:83:ILE:HG12	1:A:96:VAL:HG11	1.86	0.57
1:A:53:ASN:HB2	1:A:66:ALA:HB1	1.87	0.57
1:G:83:ILE:HG12	1:G:96:VAL:HG11	1.86	0.57
1:D:86:LEU:HD22	1:D:91:VAL:HG21	1.87	0.57
1:C:53:ASN:HB2	1:C:66:ALA:HB1	1.86	0.57
1:A:41:GLY:HA2	1:A:44:ILE:HG22	1.87	0.57
1:C:123:LEU:HD11	1:D:114:SER:OG	2.05	0.57
1:A:185:ARG:NH2	1:A:238:ARG:HD3	2.17	0.57
1:E:123:LEU:HD11	1:F:114:SER:OG	2.05	0.57
1:A:49:SER:CB	1:A:74:ARG:HB2	2.32	0.56
1:D:53:ASN:HB2	1:D:66:ALA:HB1	1.87	0.56
1:D:41:GLY:HA2	1:D:44:ILE:HG22	1.87	0.56
1:B:130:PHE:HE1	1:B:145:VAL:HG11	1.69	0.56
1:C:41:GLY:HA2	1:C:44:ILE:HG22	1.88	0.56
1:C:157:THR:C	1:C:159:ASP:H	2.08	0.56
1:C:124:LEU:HD21	1:C:170:ILE:HG21	1.87	0.56
1:E:180:ARG:HH12	1:F:162:ILE:HG21	1.69	0.56
1:F:138:LEU:HD13	1:F:170:ILE:HG12	1.86	0.56
1:G:53:ASN:HB2	1:G:66:ALA:HB1	1.87	0.56
1:F:53:ASN:HB2	1:F:66:ALA:HB1	1.87	0.56
1:B:41:GLY:HA2	1:B:44:ILE:HG22	1.87	0.56
1:G:138:LEU:HD13	1:G:170:ILE:HG12	1.87	0.56
1:C:49:SER:CB	1:C:74:ARG:HB2	2.32	0.56
1:F:41:GLY:HA2	1:F:44:ILE:HG22	1.88	0.56
1:G:198:ILE:H	1:G:198:ILE:HD12	1.70	0.56
1:F:157:THR:C	1:F:159:ASP:H	2.09	0.56
1:A:130:PHE:HE1	1:A:145:VAL:HG11	1.71	0.56
1:B:223:VAL:HG22	1:B:237:VAL:HG22	1.87	0.56
1:B:138:LEU:HD13	1:B:170:ILE:HG12	1.88	0.56
1:E:224:ARG:NH2	1:F:252:ASP:OD1	2.39	0.56
1:G:157:THR:C	1:G:159:ASP:H	2.09	0.56
1:E:130:PHE:HE1	1:E:145:VAL:HG11	1.71	0.56
1:D:224:ARG:NH2	1:E:252:ASP:OD1	2.37	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:124:LEU:HD11	1:A:170:ILE:HG21	1.88	0.55
1:G:86:LEU:HD22	1:G:91:VAL:HG21	1.87	0.55
1:A:157:THR:C	1:A:159:ASP:H	2.08	0.55
1:A:46:ARG:HH21	1:A:74:ARG:NH2	2.04	0.55
1:D:198:ILE:HD12	1:D:198:ILE:H	1.70	0.55
1:F:253:VAL:O	1:F:257:ILE:HG13	2.07	0.55
1:G:185:ARG:NH2	1:G:238:ARG:HD3	2.16	0.55
1:B:157:THR:C	1:B:159:ASP:H	2.10	0.55
1:C:198:ILE:HD12	1:C:198:ILE:H	1.70	0.55
1:E:138:LEU:HD13	1:E:170:ILE:HG12	1.87	0.55
1:F:198:ILE:HD12	1:F:198:ILE:H	1.70	0.55
1:G:41:GLY:HA2	1:G:44:ILE:HG22	1.88	0.55
1:D:130:PHE:HE1	1:D:145:VAL:HG11	1.72	0.55
1:D:208:ILE:HG23	1:D:256:ARG:HD2	1.87	0.55
1:C:138:LEU:HD13	1:C:170:ILE:HG12	1.88	0.55
1:F:86:LEU:HD22	1:F:91:VAL:HG21	1.89	0.55
1:A:224:ARG:NH2	1:B:252:ASP:OD1	2.40	0.55
1:E:253:VAL:O	1:E:257:ILE:HG13	2.07	0.54
1:F:130:PHE:HE1	1:F:145:VAL:HG11	1.71	0.54
1:A:135:TYR:HD1	1:A:144:THR:HG23	1.73	0.54
1:E:41:GLY:HA2	1:E:44:ILE:HG22	1.88	0.54
1:D:46:ARG:HH21	1:D:74:ARG:NH2	2.06	0.54
1:D:225:LEU:HD11	1:D:233:ILE:HG23	1.89	0.54
1:G:253:VAL:O	1:G:257:ILE:HG13	2.08	0.54
1:E:157:THR:C	1:E:159:ASP:H	2.10	0.54
1:F:135:TYR:HD1	1:F:144:THR:HG23	1.73	0.54
1:A:252:ASP:OD1	1:G:224:ARG:NH2	2.41	0.54
1:E:185:ARG:NH2	1:E:238:ARG:HD3	2.18	0.54
1:D:157:THR:C	1:D:159:ASP:H	2.10	0.53
1:E:279:ARG:HH12	1:F:279:ARG:NH2	2.05	0.53
1:A:180:ARG:HH12	1:B:162:ILE:HG21	1.73	0.53
1:B:86:LEU:HD22	1:B:91:VAL:HG21	1.90	0.53
1:E:225:LEU:HD11	1:E:233:ILE:HG23	1.90	0.53
1:B:83:ILE:HG12	1:B:96:VAL:HG11	1.90	0.53
1:A:225:LEU:HD11	1:A:233:ILE:HG23	1.90	0.53
1:D:135:TYR:HD1	1:D:144:THR:HG23	1.73	0.53
1:C:83:ILE:HG12	1:C:96:VAL:HG11	1.89	0.53
1:G:225:LEU:HD11	1:G:233:ILE:HG23	1.90	0.53
1:D:123:LEU:HD11	1:E:114:SER:OG	2.08	0.53
1:B:253:VAL:O	1:B:257:ILE:HG13	2.09	0.53
1:F:225:LEU:HD11	1:F:233:ILE:HG23	1.91	0.53
1:B:49:SER:CB	1:B:74:ARG:HB2	2.33	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:138:LEU:HD13	1:D:170:ILE:HG12	1.89	0.53
1:A:114:SER:OG	1:G:123:LEU:HD11	2.08	0.53
1:F:185:ARG:NH2	1:F:238:ARG:HD3	2.20	0.53
1:F:201:VAL:HG13	1:F:261:PHE:CZ	2.43	0.53
1:A:253:VAL:O	1:A:257:ILE:HG13	2.08	0.53
1:A:251:TRP:HB3	1:G:224:ARG:HD3	1.91	0.53
1:C:224:ARG:NH2	1:D:252:ASP:OD1	2.42	0.53
1:B:225:LEU:HD11	1:B:233:ILE:HG23	1.90	0.53
1:F:201:VAL:HG13	1:F:261:PHE:HZ	1.74	0.52
1:A:224:ARG:HD3	1:B:251:TRP:HB3	1.90	0.52
1:E:83:ILE:HG12	1:E:96:VAL:HG11	1.90	0.52
1:G:170:ILE:HG23	1:G:175:ILE:HD11	1.91	0.52
1:B:59:ARG:O	1:B:60:LYS:HG3	2.09	0.52
1:D:83:ILE:HG12	1:D:96:VAL:HG11	1.90	0.52
1:B:46:ARG:HH21	1:B:74:ARG:NH2	2.06	0.52
1:C:201:VAL:HG13	1:C:261:PHE:CZ	2.45	0.52
1:B:180:ARG:HH12	1:C:162:ILE:HG21	1.74	0.52
1:G:135:TYR:HD1	1:G:144:THR:HG23	1.74	0.52
1:F:123:LEU:HD11	1:G:114:SER:OG	2.10	0.52
1:A:86:LEU:HD22	1:A:91:VAL:HG21	1.91	0.52
1:F:83:ILE:HG12	1:F:96:VAL:HG11	1.91	0.52
1:C:224:ARG:HD3	1:D:251:TRP:HB3	1.92	0.52
1:C:253:VAL:O	1:C:257:ILE:HG13	2.09	0.51
1:C:120:ALA:O	1:C:124:LEU:HB2	2.10	0.51
1:C:86:LEU:HD22	1:C:91:VAL:HG21	1.93	0.51
1:E:135:TYR:HD1	1:E:144:THR:HG23	1.74	0.51
1:G:221:MET:HG3	1:G:239:VAL:HG12	1.92	0.51
1:D:185:ARG:NH2	1:D:238:ARG:HD3	2.18	0.51
1:F:257:ILE:O	1:F:261:PHE:HB2	2.11	0.51
1:A:201:VAL:HG13	1:A:261:PHE:CZ	2.45	0.51
1:D:62:ASP:HB3	1:D:65:VAL:HB	1.92	0.51
1:C:62:ASP:HB3	1:C:65:VAL:HB	1.93	0.51
1:E:124:LEU:HD11	1:E:170:ILE:HG21	1.92	0.51
1:F:59:ARG:O	1:F:60:LYS:HG3	2.11	0.51
1:A:138:LEU:HD11	1:A:165:ILE:HD13	1.92	0.51
1:B:201:VAL:HG13	1:B:261:PHE:HZ	1.76	0.51
1:C:225:LEU:HD11	1:C:233:ILE:HG23	1.92	0.51
1:E:62:ASP:HB3	1:E:65:VAL:HB	1.92	0.51
1:G:201:VAL:HG13	1:G:261:PHE:CZ	2.46	0.51
1:B:135:TYR:HD1	1:B:144:THR:HG23	1.76	0.51
1:E:50:ASN:O	1:E:54:ARG:HB2	2.11	0.51
1:C:135:TYR:HD1	1:C:144:THR:HG23	1.74	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:253:VAL:O	1:D:257:ILE:HG13	2.10	0.51
1:F:170:ILE:HG23	1:F:175:ILE:HD11	1.93	0.51
1:D:138:LEU:HD11	1:D:165:ILE:HD13	1.92	0.51
1:G:257:ILE:O	1:G:261:PHE:HB2	2.11	0.51
1:G:62:ASP:HB3	1:G:65:VAL:HB	1.92	0.51
1:D:50:ASN:O	1:D:54:ARG:HB2	2.11	0.51
1:A:201:VAL:HG13	1:A:261:PHE:HZ	1.75	0.51
1:G:138:LEU:HD11	1:G:165:ILE:HD13	1.92	0.50
1:G:50:ASN:O	1:G:54:ARG:HB2	2.12	0.50
1:A:62:ASP:HB3	1:A:65:VAL:HB	1.93	0.50
1:F:138:LEU:HD11	1:F:165:ILE:HD13	1.94	0.50
1:E:46:ARG:HH21	1:E:74:ARG:NH2	2.07	0.50
1:B:138:LEU:HD11	1:B:165:ILE:HD13	1.94	0.50
1:B:257:ILE:O	1:B:261:PHE:HB2	2.11	0.50
1:C:257:ILE:O	1:C:261:PHE:HB2	2.12	0.50
1:C:59:ARG:O	1:C:60:LYS:HG3	2.11	0.50
1:G:46:ARG:HH21	1:G:74:ARG:NH2	2.07	0.50
1:D:199:ASP:OD2	1:E:259:ARG:NH1	2.44	0.50
1:A:50:ASN:O	1:A:54:ARG:HB2	2.11	0.50
1:B:170:ILE:HG23	1:B:175:ILE:HD11	1.93	0.50
1:A:177:ASN:ND2	1:A:180:ARG:HB2	2.27	0.50
1:D:257:ILE:O	1:D:261:PHE:HB2	2.12	0.50
1:B:279:ARG:HH12	1:C:279:ARG:HH21	1.60	0.50
1:G:201:VAL:HG13	1:G:261:PHE:HZ	1.76	0.50
1:C:201:VAL:HG13	1:C:261:PHE:HZ	1.75	0.50
1:B:201:VAL:HG13	1:B:261:PHE:CZ	2.46	0.49
1:F:62:ASP:HB3	1:F:65:VAL:HB	1.93	0.49
1:G:216:LEU:HD22	1:G:219:ARG:HD2	1.93	0.49
1:E:138:LEU:HD11	1:E:165:ILE:HD13	1.94	0.49
1:E:170:ILE:HG23	1:E:175:ILE:HD11	1.94	0.49
1:F:216:LEU:HD22	1:F:219:ARG:HD2	1.94	0.49
1:C:46:ARG:HH21	1:C:74:ARG:NH2	2.07	0.49
1:D:170:ILE:HG23	1:D:175:ILE:HD11	1.94	0.49
1:E:59:ARG:O	1:E:60:LYS:HG3	2.12	0.49
1:A:170:ILE:HG23	1:A:175:ILE:HD11	1.93	0.49
1:G:210:GLN:OE1	1:G:210:GLN:HA	2.13	0.49
1:A:103:ALA:HB1	1:G:72:LEU:HD22	1.95	0.49
1:E:201:VAL:HG13	1:E:261:PHE:HZ	1.76	0.49
1:C:138:LEU:HD11	1:C:165:ILE:HD13	1.93	0.49
1:F:224:ARG:HD3	1:G:251:TRP:CB	2.42	0.49
1:E:201:VAL:HG13	1:E:261:PHE:CZ	2.47	0.49
1:F:50:ASN:O	1:F:54:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:162:ILE:O	1:G:177:ASN:N	2.41	0.49
1:D:201:VAL:HG13	1:D:261:PHE:CZ	2.48	0.49
1:A:59:ARG:O	1:A:60:LYS:HG3	2.12	0.49
1:C:216:LEU:HD22	1:C:219:ARG:HD2	1.95	0.49
1:E:257:ILE:O	1:E:261:PHE:HB2	2.13	0.49
1:F:130:PHE:CD1	1:F:145:VAL:HG21	2.48	0.49
1:D:216:LEU:HD22	1:D:219:ARG:HD2	1.94	0.49
1:E:216:LEU:HD22	1:E:219:ARG:HD2	1.94	0.49
1:B:276:ASN:HB2	1:C:274:ASP:OD1	2.13	0.49
1:D:59:ARG:O	1:D:60:LYS:HG3	2.13	0.49
1:A:257:ILE:O	1:A:261:PHE:HB2	2.12	0.49
1:A:123:LEU:HD11	1:B:114:SER:OG	2.13	0.48
1:B:62:ASP:HB3	1:B:65:VAL:HB	1.94	0.48
1:G:59:ARG:O	1:G:60:LYS:HG3	2.12	0.48
1:F:210:GLN:OE1	1:F:210:GLN:HA	2.12	0.48
1:F:221:MET:HG3	1:F:239:VAL:HG12	1.95	0.48
1:C:170:ILE:HG23	1:C:175:ILE:HD11	1.95	0.48
1:A:221:MET:HG3	1:A:239:VAL:HG12	1.95	0.48
1:D:210:GLN:HA	1:D:210:GLN:OE1	2.13	0.48
1:C:256:ARG:HG2	1:C:260:GLU:HG3	1.96	0.48
1:B:221:MET:HG3	1:B:239:VAL:HG12	1.96	0.48
1:B:130:PHE:CE1	1:B:145:VAL:HG11	2.49	0.48
1:B:50:ASN:O	1:B:54:ARG:HB2	2.12	0.48
1:B:216:LEU:HD22	1:B:219:ARG:HD2	1.95	0.48
1:A:216:LEU:HD22	1:A:219:ARG:HD2	1.94	0.48
1:C:72:LEU:HD22	1:D:103:ALA:HB1	1.96	0.48
1:F:46:ARG:HH21	1:F:74:ARG:NH2	2.07	0.48
1:D:201:VAL:HG13	1:D:261:PHE:HZ	1.79	0.48
1:A:163:ILE:HG12	1:G:176:ILE:HG12	1.95	0.48
1:C:124:LEU:HB3	1:C:148:VAL:HG11	1.96	0.48
1:A:198:ILE:O	1:A:202:LYS:HG3	2.14	0.48
1:B:210:GLN:HA	1:B:210:GLN:OE1	2.13	0.47
1:B:198:ILE:O	1:B:202:LYS:HG3	2.14	0.47
1:D:55:LEU:O	1:D:59:ARG:HG2	2.14	0.47
1:C:50:ASN:O	1:C:54:ARG:HB2	2.14	0.47
1:G:198:ILE:O	1:G:202:LYS:HG3	2.14	0.47
1:E:177:ASN:ND2	1:E:180:ARG:H	2.13	0.47
1:A:100:LEU:O	1:A:104:GLY:N	2.44	0.47
1:B:100:LEU:O	1:B:104:GLY:N	2.43	0.47
1:C:221:MET:HG3	1:C:239:VAL:HG12	1.95	0.47
1:C:130:PHE:CE1	1:C:145:VAL:HG11	2.48	0.47
1:G:100:LEU:O	1:G:104:GLY:N	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:256:ARG:HG2	1:F:260:GLU:HG3	1.97	0.47
1:A:210:GLN:OE1	1:A:210:GLN:HA	2.14	0.47
1:E:198:ILE:O	1:E:202:LYS:HG3	2.15	0.47
1:D:256:ARG:HG2	1:D:260:GLU:HG3	1.97	0.47
1:B:79:ALA:O	1:B:83:ILE:HG13	2.15	0.47
1:E:55:LEU:O	1:E:59:ARG:HG2	2.15	0.47
1:G:55:LEU:O	1:G:59:ARG:HG2	2.15	0.47
1:C:184:ARG:HB2	1:C:246:LEU:HD13	1.97	0.47
1:G:184:ARG:HB2	1:G:246:LEU:HD13	1.96	0.47
1:C:133:GLY:N	1:C:145:VAL:O	2.46	0.47
1:F:198:ILE:O	1:F:202:LYS:HG3	2.15	0.47
1:E:79:ALA:O	1:E:83:ILE:HG13	2.14	0.47
1:E:128:ARG:HA	1:E:129:PRO:HD2	1.76	0.47
1:F:128:ARG:HA	1:F:129:PRO:HD2	1.72	0.47
1:B:55:LEU:O	1:B:59:ARG:HG2	2.16	0.46
1:D:221:MET:HG3	1:D:239:VAL:HG12	1.97	0.46
1:A:92:GLN:HB3	1:A:95:SER:OG	2.15	0.46
1:D:100:LEU:O	1:D:104:GLY:N	2.47	0.46
1:E:100:LEU:O	1:E:104:GLY:N	2.44	0.46
1:E:210:GLN:HA	1:E:210:GLN:OE1	2.15	0.46
1:F:55:LEU:O	1:F:59:ARG:HG2	2.15	0.46
1:E:256:ARG:HG2	1:E:260:GLU:HG3	1.96	0.46
1:C:130:PHE:CD1	1:C:145:VAL:HG21	2.51	0.46
1:A:157:THR:C	1:A:159:ASP:N	2.69	0.46
1:C:210:GLN:OE1	1:C:210:GLN:HA	2.15	0.46
1:C:198:ILE:O	1:C:202:LYS:HG3	2.16	0.46
1:C:55:LEU:O	1:C:59:ARG:HG2	2.16	0.46
1:F:200:GLN:O	1:F:204:ILE:HG13	2.15	0.46
1:E:226:ASN:HB2	1:E:236:VAL:HG12	1.97	0.46
1:E:221:MET:HG3	1:E:239:VAL:HG12	1.98	0.46
1:B:124:LEU:HA	1:B:124:LEU:HD23	1.78	0.46
1:F:79:ALA:O	1:F:83:ILE:HG13	2.15	0.46
1:G:177:ASN:ND2	1:G:180:ARG:HB2	2.31	0.46
1:B:123:LEU:HD11	1:C:114:SER:OG	2.16	0.46
1:A:79:ALA:O	1:A:83:ILE:HG13	2.15	0.46
1:A:130:PHE:CD1	1:A:145:VAL:HG21	2.51	0.46
1:D:198:ILE:O	1:D:202:LYS:HG3	2.16	0.46
1:F:197:ASP:HB3	1:F:200:GLN:HB3	1.98	0.46
1:B:224:ARG:HD3	1:C:251:TRP:HB3	1.98	0.46
1:B:177:ASN:ND2	1:B:180:ARG:HB2	2.31	0.45
1:C:200:GLN:O	1:C:204:ILE:HG13	2.16	0.45
1:B:187:GLU:HG3	1:B:238:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:165:ILE:HG23	1:G:174:ASN:OD1	2.15	0.45
1:A:256:ARG:HG2	1:A:260:GLU:HG3	1.98	0.45
1:F:157:THR:C	1:F:159:ASP:N	2.69	0.45
1:F:184:ARG:HB2	1:F:246:LEU:HD13	1.98	0.45
1:A:55:LEU:O	1:A:59:ARG:HG2	2.16	0.45
1:D:53:ASN:HB3	1:D:70:SER:CB	2.46	0.45
1:D:200:GLN:O	1:D:204:ILE:HG13	2.17	0.45
1:A:200:GLN:O	1:A:204:ILE:HG13	2.17	0.45
1:F:91:VAL:O	1:F:93:THR:N	2.50	0.45
1:F:130:PHE:CE1	1:F:145:VAL:HG11	2.51	0.45
1:E:258:LYS:NZ	1:E:262:ASP:OD2	2.41	0.45
1:B:130:PHE:CD1	1:B:145:VAL:HG21	2.51	0.45
1:E:72:LEU:HD22	1:F:103:ALA:HB1	1.98	0.45
1:G:53:ASN:HB3	1:G:70:SER:CB	2.47	0.45
1:G:130:PHE:CE1	1:G:145:VAL:HG11	2.49	0.45
1:A:130:PHE:CE1	1:A:145:VAL:HG11	2.51	0.45
1:G:200:GLN:O	1:G:204:ILE:HG13	2.17	0.45
1:E:184:ARG:HB2	1:E:246:LEU:HD13	1.98	0.45
1:E:91:VAL:O	1:E:93:THR:N	2.49	0.45
1:D:79:ALA:O	1:D:83:ILE:HG13	2.16	0.45
1:B:91:VAL:O	1:B:93:THR:N	2.50	0.45
1:B:224:ARG:NH2	1:C:252:ASP:OD1	2.50	0.45
1:G:30:ASN:HB3	1:G:89:VAL:HA	1.99	0.45
1:D:226:ASN:HB2	1:D:236:VAL:HG12	2.00	0.45
1:C:100:LEU:O	1:C:104:GLY:N	2.44	0.45
1:D:177:ASN:ND2	1:D:180:ARG:HB2	2.31	0.44
1:C:79:ALA:O	1:C:83:ILE:HG13	2.18	0.44
1:G:130:PHE:CD1	1:G:145:VAL:HG21	2.51	0.44
1:B:133:GLY:N	1:B:145:VAL:O	2.45	0.44
1:E:130:PHE:CD1	1:E:145:VAL:HG21	2.51	0.44
1:A:197:ASP:HB3	1:A:200:GLN:HB3	1.99	0.44
1:F:276:ASN:HB2	1:G:274:ASP:OD1	2.16	0.44
1:C:187:GLU:HG3	1:C:238:ARG:HG2	2.00	0.44
1:G:79:ALA:O	1:G:83:ILE:HG13	2.18	0.44
1:D:130:PHE:CE1	1:D:145:VAL:HG11	2.52	0.44
1:G:256:ARG:HG2	1:G:260:GLU:HG3	2.00	0.44
1:E:157:THR:C	1:E:159:ASP:N	2.71	0.44
1:B:65:VAL:O	1:B:69:LEU:HB2	2.18	0.44
1:F:100:LEU:O	1:F:104:GLY:N	2.45	0.44
1:G:187:GLU:HG3	1:G:238:ARG:HG2	2.00	0.44
1:A:91:VAL:O	1:A:93:THR:N	2.50	0.44
1:A:53:ASN:HB3	1:A:70:SER:CB	2.47	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:157:THR:C	1:G:159:ASP:N	2.70	0.44
1:D:130:PHE:CD1	1:D:145:VAL:HG21	2.52	0.44
1:D:184:ARG:HB2	1:D:246:LEU:HD13	2.00	0.44
1:G:124:LEU:HD11	1:G:170:ILE:HG21	2.00	0.44
1:C:157:THR:C	1:C:159:ASP:N	2.70	0.44
1:D:150:ILE:HG13	1:D:151:PHE:N	2.32	0.44
1:E:53:ASN:HB3	1:E:70:SER:CB	2.48	0.44
1:F:44:ILE:O	1:F:48:ILE:HG13	2.18	0.44
1:B:184:ARG:HB2	1:B:246:LEU:HD13	2.00	0.44
1:A:274:ASP:OD1	1:G:276:ASN:HB2	2.18	0.44
1:C:226:ASN:HB2	1:C:236:VAL:HG12	2.00	0.43
1:B:200:GLN:O	1:B:204:ILE:HG13	2.17	0.43
1:D:91:VAL:O	1:D:93:THR:N	2.51	0.43
1:D:157:THR:C	1:D:159:ASP:N	2.71	0.43
1:A:270:TYR:HD2	1:F:276:ASN:ND2	2.16	0.43
1:F:226:ASN:HB2	1:F:236:VAL:HG12	2.00	0.43
1:F:53:ASN:HB3	1:F:70:SER:CB	2.48	0.43
1:G:92:GLN:HB3	1:G:95:SER:OG	2.18	0.43
1:B:226:ASN:HB2	1:B:236:VAL:HG12	1.99	0.43
1:D:187:GLU:HG3	1:D:238:ARG:HG2	2.00	0.43
1:A:86:LEU:HD13	1:G:80:PHE:CE2	2.54	0.43
1:C:92:GLN:HB3	1:C:95:SER:OG	2.17	0.43
1:B:258:LYS:NZ	1:B:262:ASP:OD2	2.37	0.43
1:E:197:ASP:HB3	1:E:200:GLN:HB3	1.99	0.43
1:E:200:GLN:O	1:E:204:ILE:HG13	2.18	0.43
1:B:53:ASN:HB3	1:B:70:SER:CB	2.47	0.43
1:E:130:PHE:CE1	1:E:145:VAL:HG11	2.51	0.43
1:C:197:ASP:HB3	1:C:200:GLN:HB3	1.99	0.43
1:D:128:ARG:HA	1:D:129:PRO:HD2	1.71	0.43
1:B:256:ARG:HG2	1:B:260:GLU:HG3	1.99	0.43
1:B:157:THR:C	1:B:159:ASP:N	2.71	0.43
1:G:135:TYR:HD2	1:G:178:PHE:CD1	2.36	0.43
1:D:150:ILE:HD12	1:D:151:PHE:CE1	2.53	0.43
1:A:279:ARG:NH2	1:G:279:ARG:HH12	2.15	0.43
1:F:92:GLN:HB3	1:F:95:SER:OG	2.18	0.43
1:F:135:TYR:HD2	1:F:178:PHE:CD1	2.37	0.43
1:E:187:GLU:HG3	1:E:238:ARG:HG2	2.00	0.43
1:F:177:ASN:ND2	1:F:180:ARG:HB2	2.33	0.43
1:D:72:LEU:HD22	1:E:103:ALA:HB1	2.00	0.43
1:B:197:ASP:HB3	1:B:200:GLN:HB3	2.00	0.43
1:A:214:ARG:HB2	1:A:214:ARG:HE	1.68	0.43
1:F:124:LEU:HD11	1:F:170:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:91:VAL:O	1:G:93:THR:N	2.51	0.42
1:D:197:ASP:HB3	1:D:200:GLN:HB3	2.01	0.42
1:E:92:GLN:HB3	1:E:95:SER:OG	2.19	0.42
1:B:30:ASN:HB3	1:B:89:VAL:HA	2.02	0.42
1:F:187:GLU:HG3	1:F:238:ARG:HG2	2.00	0.42
1:F:65:VAL:O	1:F:69:LEU:HB2	2.20	0.42
1:D:92:GLN:HB3	1:D:95:SER:OG	2.19	0.42
1:D:214:ARG:HB2	1:D:214:ARG:HE	1.67	0.42
1:C:91:VAL:O	1:C:93:THR:N	2.52	0.42
1:G:128:ARG:HA	1:G:129:PRO:HD2	1.73	0.42
1:G:44:ILE:O	1:G:48:ILE:HG13	2.19	0.42
1:D:65:VAL:O	1:D:69:LEU:HB2	2.19	0.42
1:E:135:TYR:HD2	1:E:178:PHE:CD1	2.37	0.42
1:A:65:VAL:O	1:A:69:LEU:HB2	2.19	0.42
1:A:184:ARG:HB2	1:A:246:LEU:HD13	2.00	0.42
1:C:30:ASN:HB3	1:C:89:VAL:HA	2.01	0.42
1:C:124:LEU:HA	1:C:124:LEU:HD12	1.76	0.42
1:A:138:LEU:CD1	1:A:165:ILE:HD13	2.50	0.42
1:A:44:ILE:O	1:A:48:ILE:HG13	2.20	0.42
1:D:44:ILE:O	1:D:48:ILE:HG13	2.19	0.42
1:C:214:ARG:HB2	1:C:214:ARG:HE	1.66	0.42
1:G:226:ASN:HB2	1:G:236:VAL:HG12	2.01	0.42
1:D:135:TYR:HD2	1:D:178:PHE:CD1	2.38	0.42
1:G:65:VAL:O	1:G:69:LEU:HB2	2.20	0.42
1:A:30:ASN:HB3	1:A:89:VAL:HA	2.02	0.42
1:A:187:GLU:HG3	1:A:238:ARG:HG2	2.02	0.41
1:E:65:VAL:O	1:E:69:LEU:HB2	2.20	0.41
1:A:199:ASP:OD2	1:B:259:ARG:NH1	2.51	0.41
1:B:75:TYR:HA	1:B:75:TYR:HD1	1.74	0.41
1:D:276:ASN:HB2	1:E:274:ASP:OD1	2.19	0.41
1:B:92:GLN:HB3	1:B:95:SER:OG	2.19	0.41
1:E:199:ASP:OD2	1:F:259:ARG:NH1	2.50	0.41
1:C:177:ASN:ND2	1:C:180:ARG:HB2	2.34	0.41
1:B:135:TYR:HD2	1:B:178:PHE:CD1	2.38	0.41
1:G:83:ILE:HG12	1:G:96:VAL:CG1	2.50	0.41
1:A:226:ASN:HB2	1:A:236:VAL:HG12	2.02	0.41
1:E:30:ASN:HB3	1:E:89:VAL:HA	2.01	0.41
1:G:150:ILE:HD12	1:G:151:PHE:CE1	2.55	0.41
1:C:53:ASN:HB3	1:C:70:SER:CB	2.48	0.41
1:G:150:ILE:HG13	1:G:151:PHE:N	2.35	0.41
1:F:30:ASN:HB3	1:F:89:VAL:HA	2.02	0.41
1:E:185:ARG:HB2	1:E:240:TRP:CG	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:44:ILE:O	1:C:48:ILE:HG13	2.20	0.41
1:E:44:ILE:O	1:E:48:ILE:HG13	2.20	0.41
1:G:197:ASP:HB3	1:G:200:GLN:HB3	2.02	0.41
1:A:276:ASN:HB2	1:B:274:ASP:OD1	2.21	0.41
1:F:122:VAL:O	1:F:125:VAL:HG22	2.20	0.41
1:A:135:TYR:HD2	1:A:178:PHE:CD1	2.39	0.41
1:B:150:ILE:HD12	1:B:151:PHE:CE1	2.56	0.41
1:A:128:ARG:HA	1:A:129:PRO:HD2	1.74	0.41
1:C:65:VAL:O	1:C:69:LEU:HB2	2.20	0.41
1:C:135:TYR:HD2	1:C:178:PHE:CD1	2.38	0.41
1:A:34:ALA:HB2	1:A:89:VAL:CG2	2.51	0.41
1:G:138:LEU:CD1	1:G:165:ILE:HD13	2.51	0.40
1:A:83:ILE:HG12	1:A:96:VAL:CG1	2.50	0.40
1:G:34:ALA:HB2	1:G:89:VAL:CG2	2.51	0.40
1:E:122:VAL:O	1:E:125:VAL:HG22	2.21	0.40
1:F:49:SER:HB3	1:F:74:ARG:CB	2.42	0.40
1:A:126:MET:O	1:A:127:PHE:HB2	2.21	0.40
1:C:279:ARG:HH12	1:D:279:ARG:NH2	2.09	0.40
1:C:150:ILE:HG13	1:C:151:PHE:N	2.37	0.40
1:G:185:ARG:HB2	1:G:240:TRP:CG	2.57	0.40
1:D:138:LEU:CD1	1:D:165:ILE:HD13	2.52	0.40
1:C:34:ALA:HB2	1:C:89:VAL:CG2	2.51	0.40
1:D:150:ILE:HD12	1:D:151:PHE:CD1	2.56	0.40
1:B:34:ALA:HB2	1:B:89:VAL:CG2	2.52	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	255/306 (83%)	234 (92%)	19 (8%)	2 (1%)	27 83
1	B	255/306 (83%)	233 (91%)	20 (8%)	2 (1%)	27 83
1	C	255/306 (83%)	233 (91%)	20 (8%)	2 (1%)	27 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	255/306 (83%)	233 (91%)	19 (8%)	3 (1%)	19	77
1	E	255/306 (83%)	233 (91%)	20 (8%)	2 (1%)	27	83
1	F	255/306 (83%)	231 (91%)	22 (9%)	2 (1%)	27	83
1	G	255/306 (83%)	234 (92%)	19 (8%)	2 (1%)	27	83
All	All	1785/2142 (83%)	1631 (91%)	139 (8%)	15 (1%)	27	83

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	B	92	GLN
1	C	92	GLN
1	D	92	GLN
1	E	92	GLN
1	F	92	GLN
1	G	92	GLN
1	D	146	LEU
1	C	128	ARG
1	E	128	ARG
1	F	128	ARG
1	A	128	ARG
1	B	128	ARG
1	D	128	ARG
1	G	128	ARG

### 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	208/248 (84%)	193 (93%)	15 (7%)	21	67
1	B	208/248 (84%)	190 (91%)	18 (9%)	15	58
1	C	208/248 (84%)	191 (92%)	17 (8%)	17	61
1	D	208/248 (84%)	193 (93%)	15 (7%)	21	67
1	E	208/248 (84%)	191 (92%)	17 (8%)	17	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	208/248 (84%)	192 (92%)	16 (8%)	18	64
1	G	208/248 (84%)	192 (92%)	16 (8%)	18	64
All	All	1456/1736 (84%)	1342 (92%)	114 (8%)	18	64

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	64	THR
1	A	69	LEU
1	A	75	TYR
1	A	93	THR
1	A	111	LEU
1	A	115	LEU
1	A	128	ARG
1	A	144	THR
1	A	146	LEU
1	A	149	GLN
1	A	164	VAL
1	A	185	ARG
1	A	231	SER
1	A	246	LEU
1	B	60	LYS
1	B	64	THR
1	B	69	LEU
1	B	75	TYR
1	B	93	THR
1	B	111	LEU
1	B	115	LEU
1	B	126	MET
1	B	128	ARG
1	B	144	THR
1	B	146	LEU
1	B	149	GLN
1	B	164	VAL
1	B	185	ARG
1	B	190	ILE
1	B	231	SER
1	B	246	LEU
1	B	248	ASN
1	C	60	LYS

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Mol	Chain	Res	Type
1	C	64	THR
1	C	69	LEU
1	C	75	TYR
1	C	93	THR
1	C	111	LEU
1	C	115	LEU
1	C	124	LEU
1	C	126	MET
1	C	128	ARG
1	C	144	THR
1	C	149	GLN
1	C	164	VAL
1	C	185	ARG
1	C	231	SER
1	C	246	LEU
1	C	248	ASN
1	D	60	LYS
1	D	64	THR
1	D	69	LEU
1	D	75	TYR
1	D	93	THR
1	D	111	LEU
1	D	115	LEU
1	D	126	MET
1	D	128	ARG
1	D	144	THR
1	D	149	GLN
1	D	164	VAL
1	D	231	SER
1	D	246	LEU
1	D	248	ASN
1	E	60	LYS
1	E	64	THR
1	E	69	LEU
1	E	75	TYR
1	E	93	THR
1	E	111	LEU
1	E	115	LEU
1	E	126	MET
1	E	128	ARG
1	E	144	THR
1	E	149	GLN

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Mol	Chain	Res	Type
1	E	164	VAL
1	E	185	ARG
1	E	190	ILE
1	E	231	SER
1	E	246	LEU
1	E	248	ASN
1	F	60	LYS
1	F	64	THR
1	F	69	LEU
1	F	75	TYR
1	F	93	THR
1	F	111	LEU
1	F	115	LEU
1	F	126	MET
1	F	128	ARG
1	F	144	THR
1	F	149	GLN
1	F	164	VAL
1	F	185	ARG
1	F	231	SER
1	F	246	LEU
1	F	248	ASN
1	G	60	LYS
1	G	64	THR
1	G	69	LEU
1	G	75	TYR
1	G	93	THR
1	G	111	LEU
1	G	115	LEU
1	G	126	MET
1	G	128	ARG
1	G	144	THR
1	G	149	GLN
1	G	164	VAL
1	G	185	ARG
1	G	231	SER
1	G	246	LEU
1	G	248	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	177	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	257/306 (83%)	0.73	29 (11%) 6 9	64, 108, 146, 200	0
1	B	257/306 (83%)	0.70	24 (9%) 9 13	60, 106, 139, 176	0
1	C	257/306 (83%)	0.48	21 (8%) 12 15	67, 101, 132, 187	0
1	D	257/306 (83%)	0.79	33 (12%) 4 7	67, 114, 148, 168	0
1	E	257/306 (83%)	0.62	22 (8%) 11 14	75, 122, 153, 174	0
1	F	257/306 (83%)	0.65	25 (9%) 8 12	73, 115, 146, 166	0
1	G	257/306 (83%)	0.54	18 (7%) 16 18	76, 110, 140, 162	0
All	All	1799/2142 (83%)	0.64	172 (9%) 8 12	60, 111, 146, 200	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	281	LYS	10.7
1	F	281	LYS	7.6
1	E	280	VAL	6.6
1	A	231	SER	6.0
1	D	131	ARG	5.8
1	A	281	LYS	5.6
1	F	280	VAL	5.3
1	F	258	LYS	5.2
1	D	128	ARG	5.1
1	D	88	ARG	4.8
1	G	273	MET	4.8
1	A	276	ASN	4.8
1	F	268	PHE	4.8
1	F	278	LYS	4.7
1	A	194	TYR	4.5
1	F	266	ILE	4.4
1	F	265	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	130	PHE	4.3
1	E	47	MET	4.3
1	B	277	PHE	4.1
1	C	25	LEU	4.1
1	E	219	ARG	4.1
1	A	272	GLN	4.0
1	B	25	LEU	4.0
1	E	278	LYS	3.9
1	B	273	MET	3.8
1	G	278	LYS	3.8
1	D	126	MET	3.7
1	E	217	LYS	3.6
1	D	132	ALA	3.6
1	D	81	THR	3.6
1	A	273	MET	3.5
1	B	276	ASN	3.5
1	A	275	VAL	3.5
1	E	260	GLU	3.5
1	B	27	TYR	3.5
1	C	27	TYR	3.5
1	B	274	ASP	3.4
1	D	134	GLU	3.4
1	A	192	VAL	3.3
1	D	217	LYS	3.3
1	A	124	LEU	3.3
1	A	193	ALA	3.3
1	F	264	ALA	3.3
1	F	277	PHE	3.2
1	D	125	VAL	3.2
1	C	277	PHE	3.2
1	C	225	LEU	3.2
1	E	194	TYR	3.2
1	D	124	LEU	3.1
1	B	263	ALA	3.1
1	E	51	ALA	3.1
1	A	266	ILE	3.1
1	G	38	ILE	3.1
1	A	233	ILE	3.1
1	F	275	VAL	3.1
1	G	88	ARG	3.1
1	B	175	ILE	3.1
1	C	88	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	185	ARG	3.1
1	B	129	PRO	3.1
1	D	127	PHE	3.0
1	D	216	LEU	3.0
1	B	275	VAL	3.0
1	C	235	PHE	3.0
1	C	272	GLN	2.9
1	G	280	VAL	2.9
1	G	275	VAL	2.9
1	B	262	ASP	2.9
1	F	262	ASP	2.9
1	F	25	LEU	2.9
1	D	180	ARG	2.9
1	E	88	ARG	2.9
1	C	85	ALA	2.8
1	G	85	ALA	2.8
1	C	273	MET	2.8
1	D	281	LYS	2.8
1	A	60	LYS	2.8
1	B	219	ARG	2.8
1	A	268	PHE	2.8
1	D	203	GLN	2.8
1	A	278	LYS	2.7
1	B	266	ILE	2.7
1	C	195	ASP	2.7
1	C	275	VAL	2.7
1	A	158	ALA	2.7
1	B	221	MET	2.7
1	B	278	LYS	2.7
1	D	280	VAL	2.7
1	G	200	GLN	2.7
1	F	260	GLU	2.7
1	B	138	LEU	2.7
1	D	85	ALA	2.7
1	E	220	GLU	2.6
1	B	139	GLY	2.6
1	G	184	ARG	2.6
1	D	129	PRO	2.6
1	A	25	LEU	2.6
1	E	228	LEU	2.5
1	E	25	LEU	2.5
1	A	228	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	232	SER	2.5
1	C	280	VAL	2.5
1	F	273	MET	2.5
1	B	44	ILE	2.5
1	D	84	ALA	2.5
1	A	280	VAL	2.5
1	A	277	PHE	2.5
1	C	129	PRO	2.5
1	F	276	ASN	2.5
1	E	279	ARG	2.5
1	G	127	PHE	2.5
1	B	130	PHE	2.4
1	F	110	ALA	2.4
1	E	216	LEU	2.4
1	D	210	GLN	2.4
1	F	274	ASP	2.4
1	D	82	LEU	2.4
1	F	261	PHE	2.4
1	D	273	MET	2.4
1	B	110	ALA	2.4
1	C	127	PHE	2.4
1	F	148	VAL	2.4
1	F	279	ARG	2.4
1	G	54	ARG	2.4
1	G	277	PHE	2.3
1	B	158	ALA	2.3
1	E	176	ILE	2.3
1	E	177	ASN	2.3
1	C	126	MET	2.3
1	A	135	TYR	2.3
1	F	162	ILE	2.3
1	D	209	ILE	2.3
1	C	278	LYS	2.3
1	D	207	ASN	2.3
1	D	204	ILE	2.2
1	C	281	LYS	2.2
1	G	266	ILE	2.2
1	F	267	SER	2.2
1	E	256	ARG	2.2
1	D	148	VAL	2.2
1	B	265	GLY	2.2
1	D	276	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	61	ILE	2.2
1	A	271	PRO	2.1
1	C	47	MET	2.1
1	A	204	ILE	2.1
1	G	78	ILE	2.1
1	D	260	GLU	2.1
1	F	133	GLY	2.1
1	F	270	TYR	2.1
1	G	276	ASN	2.1
1	B	159	ASP	2.1
1	C	192	VAL	2.1
1	B	124	LEU	2.1
1	F	146	LEU	2.1
1	D	279	ARG	2.1
1	E	48	ILE	2.1
1	E	180	ARG	2.1
1	G	272	GLN	2.0
1	A	200	GLN	2.0
1	A	198	ILE	2.0
1	C	124	LEU	2.0
1	C	236	VAL	2.0
1	D	228	LEU	2.0
1	E	264	ALA	2.0
1	D	133	GLY	2.0
1	A	27	TYR	2.0
1	G	82	LEU	2.0
1	D	78	ILE	2.0
1	A	184	ARG	2.0
1	A	234	ASN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.