



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:09 am GMT

PDB ID : 2OAU  
Title : Mechanosensitive Channel of Small Conductance (MscS)  
Authors : Rees, D.C.; Bass, R.B.; Steinbacher, S.; Strop, P.; Barclay, M.T.  
Deposited on : 2006-12-17  
Resolution : 3.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

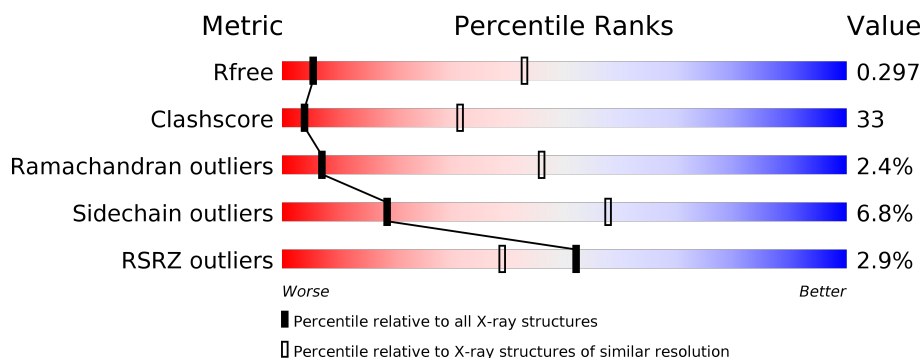
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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))
$R_{free}$	100719	1234 (3.90-3.50)
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)
RSRZ outliers	101464	1262 (3.90-3.50)

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. 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	306	<div> <div>0%</div> <div> <div>38%</div> <div>40%</div> <div>5%</div> <div>17%</div> </div> </div>
1	B	306	<div> <div>2%</div> <div> <div>39%</div> <div>39%</div> <div>5%</div> <div>17%</div> </div> </div>
1	C	306	<div> <div>3%</div> <div> <div>41%</div> <div>38%</div> <div>5%</div> <div>17%</div> </div> </div>
1	D	306	<div> <div>2%</div> <div> <div>36%</div> <div>42%</div> <div>5%</div> <div>17%</div> </div> </div>
1	E	306	<div> <div>2%</div> <div> <div>44%</div> <div>34%</div> <div>5%</div> <div>17%</div> </div> </div>
1	F	306	<div> <div>7%</div> <div> <div>41%</div> <div>36%</div> <div>6%</div> <div>17%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	306	<div><div></div><div>42%</div><div>35%</div><div>6%</div><div>17%</div></div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13573 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 Small-conductance mechanosensitive channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1939	1245	339	349	6			
1	B	254	Total	C	N	O	S	0	0	0
			1939	1245	339	349	6			
1	C	254	Total	C	N	O	S	0	0	0
			1939	1245	339	349	6			
1	D	254	Total	C	N	O	S	0	0	0
			1939	1245	339	349	6			
1	E	254	Total	C	N	O	S	0	0	0
			1939	1245	339	349	6			
1	F	254	Total	C	N	O	S	0	0	0
			1939	1245	339	349	6			
1	G	254	Total	C	N	O	S	0	0	0
			1939	1245	339	349	6			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	SEE REMARK 999	UNP P0C0S1
A	-18	GLY	-	SEE REMARK 999	UNP P0C0S1
A	-17	SER	-	SEE REMARK 999	UNP P0C0S1
A	-16	SER	-	SEE REMARK 999	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	-	SEE REMARK 999	UNP P0C0S1
A	-8	SER	-	SEE REMARK 999	UNP P0C0S1
A	-7	GLY	-	SEE REMARK 999	UNP P0C0S1
A	-6	LEU	-	SEE REMARK 999	UNP P0C0S1
A	-5	VAL	-	SEE REMARK 999	UNP P0C0S1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	SEE REMARK 999	UNP P0C0S1
A	-3	ARG	-	SEE REMARK 999	UNP P0C0S1
A	-2	GLY	-	SEE REMARK 999	UNP P0C0S1
A	-1	SER	-	SEE REMARK 999	UNP P0C0S1
A	0	HIS	-	SEE REMARK 999	UNP P0C0S1
B	-19	MET	-	SEE REMARK 999	UNP P0C0S1
B	-18	GLY	-	SEE REMARK 999	UNP P0C0S1
B	-17	SER	-	SEE REMARK 999	UNP P0C0S1
B	-16	SER	-	SEE REMARK 999	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	-	SEE REMARK 999	UNP P0C0S1
B	-8	SER	-	SEE REMARK 999	UNP P0C0S1
B	-7	GLY	-	SEE REMARK 999	UNP P0C0S1
B	-6	LEU	-	SEE REMARK 999	UNP P0C0S1
B	-5	VAL	-	SEE REMARK 999	UNP P0C0S1
B	-4	PRO	-	SEE REMARK 999	UNP P0C0S1
B	-3	ARG	-	SEE REMARK 999	UNP P0C0S1
B	-2	GLY	-	SEE REMARK 999	UNP P0C0S1
B	-1	SER	-	SEE REMARK 999	UNP P0C0S1
B	0	HIS	-	SEE REMARK 999	UNP P0C0S1
C	-19	MET	-	SEE REMARK 999	UNP P0C0S1
C	-18	GLY	-	SEE REMARK 999	UNP P0C0S1
C	-17	SER	-	SEE REMARK 999	UNP P0C0S1
C	-16	SER	-	SEE REMARK 999	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	-	SEE REMARK 999	UNP P0C0S1
C	-8	SER	-	SEE REMARK 999	UNP P0C0S1
C	-7	GLY	-	SEE REMARK 999	UNP P0C0S1
C	-6	LEU	-	SEE REMARK 999	UNP P0C0S1
C	-5	VAL	-	SEE REMARK 999	UNP P0C0S1
C	-4	PRO	-	SEE REMARK 999	UNP P0C0S1
C	-3	ARG	-	SEE REMARK 999	UNP P0C0S1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	SEE REMARK 999	UNP P0C0S1
C	-1	SER	-	SEE REMARK 999	UNP P0C0S1
C	0	HIS	-	SEE REMARK 999	UNP P0C0S1
D	-19	MET	-	SEE REMARK 999	UNP P0C0S1
D	-18	GLY	-	SEE REMARK 999	UNP P0C0S1
D	-17	SER	-	SEE REMARK 999	UNP P0C0S1
D	-16	SER	-	SEE REMARK 999	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	-	SEE REMARK 999	UNP P0C0S1
D	-8	SER	-	SEE REMARK 999	UNP P0C0S1
D	-7	GLY	-	SEE REMARK 999	UNP P0C0S1
D	-6	LEU	-	SEE REMARK 999	UNP P0C0S1
D	-5	VAL	-	SEE REMARK 999	UNP P0C0S1
D	-4	PRO	-	SEE REMARK 999	UNP P0C0S1
D	-3	ARG	-	SEE REMARK 999	UNP P0C0S1
D	-2	GLY	-	SEE REMARK 999	UNP P0C0S1
D	-1	SER	-	SEE REMARK 999	UNP P0C0S1
D	0	HIS	-	SEE REMARK 999	UNP P0C0S1
E	-19	MET	-	SEE REMARK 999	UNP P0C0S1
E	-18	GLY	-	SEE REMARK 999	UNP P0C0S1
E	-17	SER	-	SEE REMARK 999	UNP P0C0S1
E	-16	SER	-	SEE REMARK 999	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	-	SEE REMARK 999	UNP P0C0S1
E	-8	SER	-	SEE REMARK 999	UNP P0C0S1
E	-7	GLY	-	SEE REMARK 999	UNP P0C0S1
E	-6	LEU	-	SEE REMARK 999	UNP P0C0S1
E	-5	VAL	-	SEE REMARK 999	UNP P0C0S1
E	-4	PRO	-	SEE REMARK 999	UNP P0C0S1
E	-3	ARG	-	SEE REMARK 999	UNP P0C0S1
E	-2	GLY	-	SEE REMARK 999	UNP P0C0S1
E	-1	SER	-	SEE REMARK 999	UNP P0C0S1

*Continued on next page...*

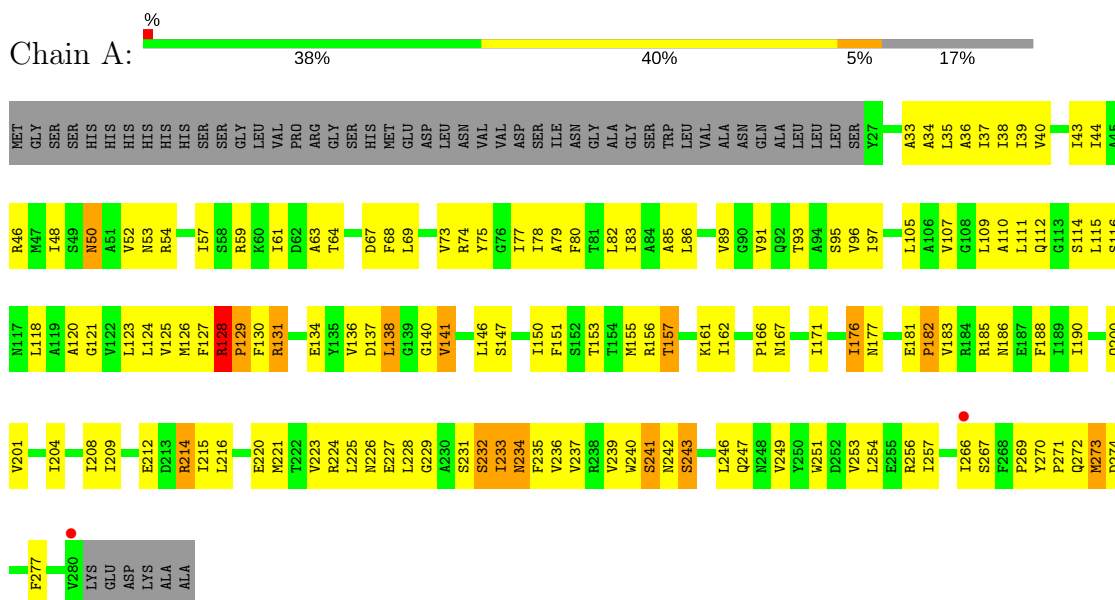
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	SEE REMARK 999	UNP P0C0S1
F	-19	MET	-	SEE REMARK 999	UNP P0C0S1
F	-18	GLY	-	SEE REMARK 999	UNP P0C0S1
F	-17	SER	-	SEE REMARK 999	UNP P0C0S1
F	-16	SER	-	SEE REMARK 999	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	-	SEE REMARK 999	UNP P0C0S1
F	-8	SER	-	SEE REMARK 999	UNP P0C0S1
F	-7	GLY	-	SEE REMARK 999	UNP P0C0S1
F	-6	LEU	-	SEE REMARK 999	UNP P0C0S1
F	-5	VAL	-	SEE REMARK 999	UNP P0C0S1
F	-4	PRO	-	SEE REMARK 999	UNP P0C0S1
F	-3	ARG	-	SEE REMARK 999	UNP P0C0S1
F	-2	GLY	-	SEE REMARK 999	UNP P0C0S1
F	-1	SER	-	SEE REMARK 999	UNP P0C0S1
F	0	HIS	-	SEE REMARK 999	UNP P0C0S1
G	-19	MET	-	SEE REMARK 999	UNP P0C0S1
G	-18	GLY	-	SEE REMARK 999	UNP P0C0S1
G	-17	SER	-	SEE REMARK 999	UNP P0C0S1
G	-16	SER	-	SEE REMARK 999	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	-	SEE REMARK 999	UNP P0C0S1
G	-8	SER	-	SEE REMARK 999	UNP P0C0S1
G	-7	GLY	-	SEE REMARK 999	UNP P0C0S1
G	-6	LEU	-	SEE REMARK 999	UNP P0C0S1
G	-5	VAL	-	SEE REMARK 999	UNP P0C0S1
G	-4	PRO	-	SEE REMARK 999	UNP P0C0S1
G	-3	ARG	-	SEE REMARK 999	UNP P0C0S1
G	-2	GLY	-	SEE REMARK 999	UNP P0C0S1
G	-1	SER	-	SEE REMARK 999	UNP P0C0S1
G	0	HIS	-	SEE REMARK 999	UNP P0C0S1

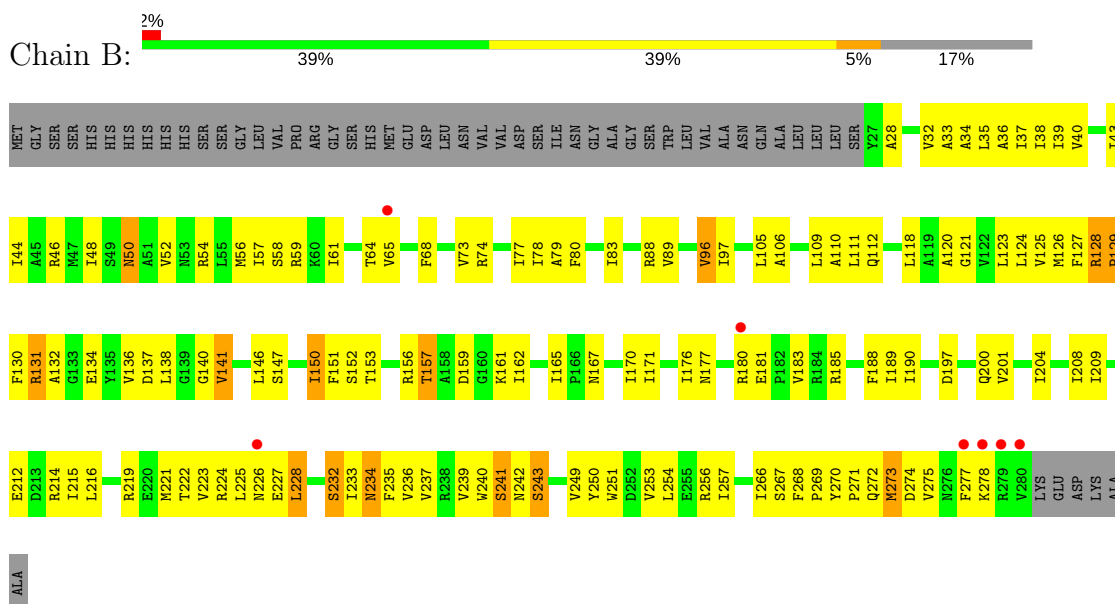
### 3 Residue-property plots

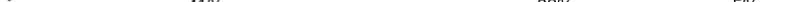
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

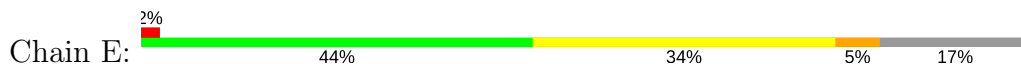
- Molecule 1: Small-conductance mechanosensitive channel



- Molecule 1: Small-conductance mechanosensitive channel

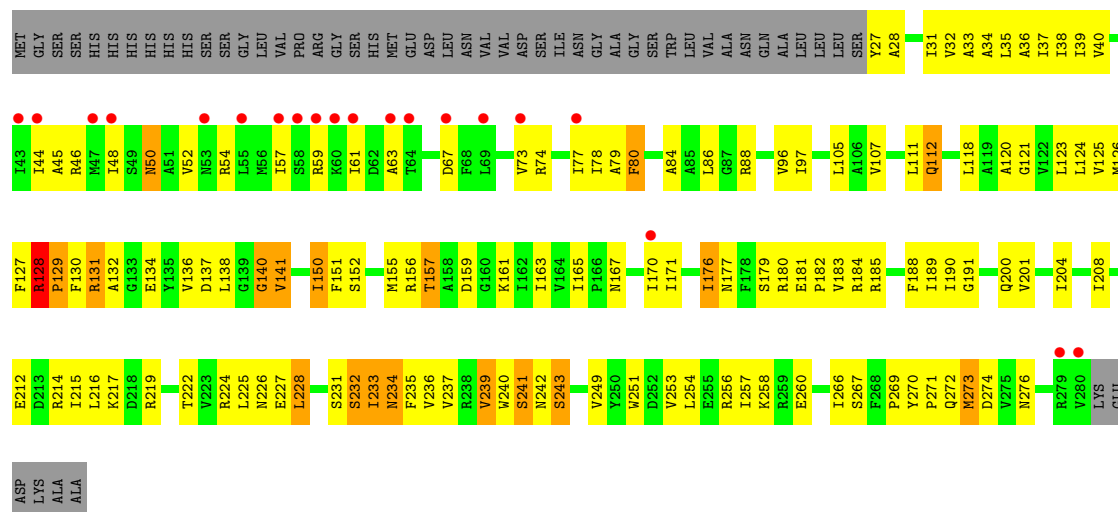
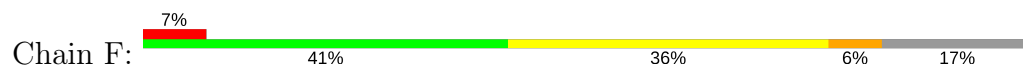


Chain C: 

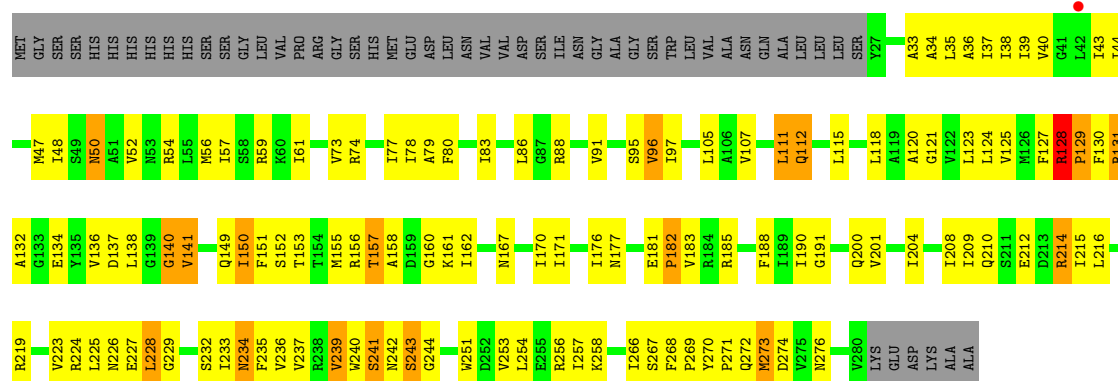




• Molecule 1: Small-conductance mechanosensitive channel



• Molecule 1: Small-conductance mechanosensitive channel



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.27Å 184.27Å 260.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.70 48.39 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.70) 99.9 (48.39-3.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 3.67Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.293 , 0.321 0.274 , 0.297	Depositor DCC
$R_{free}$ test set	2429 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	123.8	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	13573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 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	0.49	0/1964	0.77	2/2663 (0.1%)
1	B	0.49	0/1964	0.76	2/2663 (0.1%)
1	C	0.46	0/1964	0.73	2/2663 (0.1%)
1	D	0.48	0/1964	0.75	2/2663 (0.1%)
1	E	0.50	0/1964	0.77	2/2663 (0.1%)
1	F	0.55	0/1964	0.78	3/2663 (0.1%)
1	G	0.54	0/1964	0.80	3/2663 (0.1%)
All	All	0.50	0/13748	0.77	16/18641 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	G	128	ARG	N-CA-C	8.47	133.86	111.00
1	D	128	ARG	N-CA-C	8.39	133.65	111.00
1	E	128	ARG	N-CA-C	7.48	131.21	111.00
1	C	128	ARG	N-CA-C	7.15	130.29	111.00
1	F	128	ARG	N-CA-C	6.80	129.37	111.00
1	A	128	ARG	N-CA-C	6.59	128.80	111.00
1	B	128	ARG	N-CA-C	6.18	127.68	111.00
1	G	140	GLY	N-CA-C	-5.71	98.82	113.10
1	A	233	ILE	N-CA-C	-5.43	96.33	111.00
1	G	268	PHE	N-CA-C	-5.39	96.43	111.00
1	B	268	PHE	N-CA-C	-5.37	96.50	111.00
1	E	140	GLY	N-CA-C	-5.24	100.00	113.10
1	D	140	GLY	N-CA-C	-5.24	100.01	113.10
1	C	140	GLY	N-CA-C	-5.13	100.27	113.10
1	F	233	ILE	N-CA-C	-5.04	97.39	111.00
1	F	140	GLY	N-CA-C	-5.03	100.54	113.10

There are no chirality outliers.

There are no planarity outliers.

## 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	1939	0	2032	158	0
1	B	1939	0	2032	157	0
1	C	1939	0	2032	153	0
1	D	1939	0	2032	173	0
1	E	1939	0	2032	132	0
1	F	1939	0	2032	145	0
1	G	1939	0	2032	160	0
All	All	13573	0	14224	923	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 33.

All (923) 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:A:126:MET:HB3	1:B:65:VAL:HG21	1.22	1.15
1:B:180:ARG:HD3	1:C:162:ILE:HG21	1.28	1.10
1:C:124:LEU:O	1:C:128:ARG:HB3	1.58	1.01
1:A:124:LEU:O	1:A:128:ARG:HB3	1.59	1.01
1:D:137:ASP:HB3	1:D:176:ILE:HG23	1.43	1.00
1:B:126:MET:HB3	1:C:65:VAL:HG21	1.40	1.00
1:E:137:ASP:HB3	1:E:176:ILE:HG23	1.41	1.00
1:G:124:LEU:O	1:G:128:ARG:HB3	1.62	0.98
1:G:137:ASP:HB3	1:G:176:ILE:HG23	1.47	0.95
1:B:124:LEU:O	1:B:128:ARG:HB3	1.65	0.95
1:G:150:ILE:H	1:G:150:ILE:HD12	1.33	0.93
1:F:157:THR:HG21	1:F:161:LYS:HB2	1.51	0.93
1:B:157:THR:HG21	1:B:161:LYS:HB2	1.50	0.93
1:F:124:LEU:O	1:F:128:ARG:HB3	1.69	0.93
1:B:57:ILE:HA	1:B:61:ILE:HB	1.52	0.92
1:B:176:ILE:HD11	1:C:161:LYS:HD2	1.49	0.91
1:C:128:ARG:O	1:C:128:ARG:HD2	1.68	0.91
1:B:137:ASP:HB3	1:B:176:ILE:HG23	1.53	0.91
1:D:86:LEU:HB3	1:D:91:VAL:HB	1.53	0.91
1:D:105:LEU:HD13	1:E:105:LEU:HD23	1.54	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:LEU:HD13	1:F:105:LEU:HD23	1.56	0.88
1:B:136:VAL:HG12	1:B:177:ASN:HA	1.56	0.88
1:A:137:ASP:HB3	1:A:176:ILE:HG23	1.55	0.87
1:A:123:LEU:O	1:A:127:PHE:HB2	1.75	0.86
1:C:226:ASN:HB2	1:C:236:VAL:HG12	1.56	0.86
1:E:228:LEU:HD22	1:F:254:LEU:HD11	1.58	0.86
1:C:123:LEU:O	1:C:127:PHE:HB2	1.76	0.85
1:E:157:THR:HG21	1:E:161:LYS:HB2	1.57	0.85
1:A:157:THR:HG21	1:A:161:LYS:HB2	1.58	0.85
1:B:97:ILE:HD12	1:C:95:SER:HA	1.57	0.85
1:G:57:ILE:HA	1:G:61:ILE:HB	1.56	0.85
1:G:129:PRO:HG2	1:G:130:PHE:H	1.41	0.85
1:C:57:ILE:HA	1:C:61:ILE:HB	1.57	0.85
1:C:137:ASP:HB3	1:C:176:ILE:HG23	1.57	0.85
1:B:129:PRO:HG2	1:B:130:PHE:H	1.41	0.84
1:C:129:PRO:HG2	1:C:130:PHE:H	1.42	0.84
1:A:57:ILE:HA	1:A:61:ILE:HB	1.58	0.83
1:D:123:LEU:O	1:D:127:PHE:HB2	1.78	0.82
1:A:129:PRO:HG2	1:A:130:PHE:H	1.44	0.82
1:E:123:LEU:O	1:E:127:PHE:HB2	1.79	0.82
1:E:137:ASP:HB3	1:E:176:ILE:CG2	2.09	0.82
1:F:137:ASP:HB3	1:F:176:ILE:HG23	1.61	0.82
1:D:157:THR:HG21	1:D:161:LYS:HB2	1.62	0.81
1:F:157:THR:CG2	1:F:161:LYS:HB2	2.10	0.81
1:E:124:LEU:O	1:E:128:ARG:HB3	1.80	0.81
1:D:121:GLY:O	1:D:125:VAL:HG23	1.81	0.81
1:F:228:LEU:HD22	1:G:254:LEU:HD11	1.62	0.81
1:D:83:ILE:HG23	1:D:93:THR:HG21	1.63	0.81
1:G:215:ILE:HG23	1:G:239:VAL:HG13	1.63	0.81
1:B:123:LEU:O	1:B:127:PHE:HB2	1.81	0.80
1:G:226:ASN:HB2	1:G:236:VAL:HG12	1.62	0.80
1:F:57:ILE:HA	1:F:61:ILE:HB	1.62	0.80
1:E:57:ILE:HA	1:E:61:ILE:HB	1.64	0.79
1:F:123:LEU:O	1:F:127:PHE:HB2	1.82	0.79
1:G:123:LEU:O	1:G:127:PHE:HB2	1.82	0.79
1:D:57:ILE:HA	1:D:61:ILE:HB	1.64	0.78
1:F:136:VAL:HG12	1:F:177:ASN:HA	1.65	0.78
1:B:157:THR:HG23	1:B:161:LYS:H	1.48	0.78
1:F:176:ILE:HD11	1:G:161:LYS:HD2	1.63	0.78
1:A:157:THR:CG2	1:A:161:LYS:HB2	2.14	0.78
1:G:121:GLY:O	1:G:125:VAL:HG23	1.83	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:ILE:HD11	1:F:161:LYS:HD2	1.66	0.78
1:A:151:PHE:CE1	1:G:123:LEU:HD21	2.19	0.78
1:B:83:ILE:HG12	1:B:96:VAL:HG11	1.64	0.77
1:B:157:THR:CG2	1:B:161:LYS:HB2	2.14	0.77
1:C:105:LEU:HD13	1:D:105:LEU:HD23	1.66	0.77
1:A:115:LEU:HB3	1:B:110:ALA:HB2	1.67	0.77
1:D:136:VAL:HG12	1:D:177:ASN:HA	1.66	0.76
1:C:150:ILE:HD12	1:C:150:ILE:H	1.49	0.76
1:D:181:GLU:OE1	1:D:181:GLU:HA	1.85	0.76
1:D:157:THR:CG2	1:D:161:LYS:HB2	2.16	0.75
1:D:226:ASN:HB2	1:D:236:VAL:HG12	1.68	0.75
1:D:137:ASP:HB3	1:D:176:ILE:CG2	2.16	0.75
1:F:224:ARG:HD3	1:G:251:TRP:CD2	2.21	0.75
1:A:105:LEU:HD23	1:G:105:LEU:HD13	1.68	0.75
1:A:36:ALA:O	1:A:40:VAL:HG23	1.88	0.74
1:D:83:ILE:HG23	1:D:93:THR:CG2	2.18	0.74
1:G:136:VAL:HG12	1:G:177:ASN:HA	1.70	0.73
1:E:128:ARG:HD3	1:E:128:ARG:O	1.87	0.73
1:A:226:ASN:HB2	1:A:236:VAL:HG12	1.69	0.73
1:G:181:GLU:OE2	1:G:182:PRO:HD2	1.89	0.72
1:G:183:VAL:HG23	1:G:241:SER:O	1.90	0.72
1:D:253:VAL:O	1:D:257:ILE:HG13	1.88	0.72
1:C:157:THR:HG21	1:C:161:LYS:HB2	1.70	0.72
1:B:204:ILE:HD12	1:B:266:ILE:HD11	1.71	0.72
1:F:267:SER:O	1:F:269:PRO:HD3	1.91	0.71
1:B:137:ASP:HB3	1:B:176:ILE:CG2	2.20	0.71
1:C:124:LEU:O	1:C:128:ARG:CB	2.35	0.71
1:F:84:ALA:HB1	1:G:91:VAL:HG13	1.73	0.71
1:C:225:LEU:HD11	1:C:233:ILE:HG12	1.72	0.71
1:G:157:THR:HG21	1:G:161:LYS:HB2	1.73	0.71
1:F:180:ARG:HD3	1:G:162:ILE:HG21	1.72	0.70
1:D:36:ALA:O	1:D:40:VAL:HG23	1.90	0.70
1:E:157:THR:CG2	1:E:161:LYS:HB2	2.20	0.70
1:E:273:MET:HE3	1:F:273:MET:HE2	1.72	0.70
1:B:36:ALA:O	1:B:40:VAL:HG23	1.90	0.70
1:A:114:SER:HB3	1:G:123:LEU:HD11	1.72	0.70
1:F:129:PRO:HG2	1:F:130:PHE:H	1.56	0.70
1:A:114:SER:HB3	1:G:123:LEU:CD1	2.22	0.70
1:A:270:TYR:HB3	1:A:271:PRO:CD	2.22	0.70
1:A:126:MET:CB	1:B:65:VAL:HG21	2.13	0.70
1:G:225:LEU:HD11	1:G:233:ILE:HG12	1.73	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:PRO:HG2	1:D:130:PHE:H	1.57	0.69
1:E:36:ALA:O	1:E:40:VAL:HG23	1.92	0.69
1:C:36:ALA:O	1:C:40:VAL:HG23	1.92	0.69
1:E:129:PRO:HG2	1:E:130:PHE:H	1.57	0.68
1:G:137:ASP:HB3	1:G:176:ILE:CG2	2.21	0.68
1:F:226:ASN:HB2	1:F:236:VAL:HG12	1.75	0.68
1:A:95:SER:HA	1:G:97:ILE:HD12	1.76	0.68
1:C:107:VAL:O	1:C:111:LEU:HB2	1.93	0.68
1:G:208:ILE:HG23	1:G:256:ARG:HG2	1.75	0.68
1:B:97:ILE:CD1	1:C:95:SER:HA	2.22	0.68
1:D:181:GLU:HG3	1:D:182:PRO:CD	2.23	0.68
1:B:249:VAL:O	1:B:253:VAL:HG23	1.93	0.68
1:C:97:ILE:HD12	1:D:95:SER:HA	1.76	0.68
1:A:126:MET:HB3	1:B:65:VAL:CG2	2.14	0.67
1:D:227:GLU:HB3	1:D:234:ASN:OD1	1.93	0.67
1:F:233:ILE:O	1:F:233:ILE:HG23	1.94	0.67
1:E:121:GLY:O	1:E:125:VAL:HG23	1.94	0.67
1:D:204:ILE:HD12	1:D:266:ILE:HD11	1.75	0.67
1:E:128:ARG:HH21	1:E:131:ARG:NH2	1.93	0.67
1:A:225:LEU:HD11	1:A:233:ILE:HG12	1.75	0.67
1:G:200:GLN:O	1:G:204:ILE:HG13	1.95	0.67
1:C:136:VAL:HG12	1:C:177:ASN:HA	1.74	0.67
1:G:190:ILE:HG12	1:G:257:ILE:HG21	1.77	0.66
1:B:129:PRO:HG2	1:B:130:PHE:N	2.10	0.66
1:C:253:VAL:O	1:C:257:ILE:HG13	1.95	0.66
1:G:36:ALA:O	1:G:40:VAL:HG23	1.95	0.66
1:C:121:GLY:O	1:C:125:VAL:HG23	1.96	0.66
1:B:185:ARG:HB2	1:B:240:TRP:CD2	2.29	0.66
1:A:274:ASP:HB2	1:B:272:GLN:NE2	2.09	0.66
1:C:227:GLU:HB3	1:C:234:ASN:OD1	1.94	0.66
1:A:151:PHE:HE1	1:G:123:LEU:HD21	1.56	0.66
1:C:200:GLN:O	1:C:204:ILE:HG13	1.96	0.66
1:D:105:LEU:HD13	1:E:105:LEU:CD2	2.27	0.65
1:A:95:SER:HA	1:G:97:ILE:CD1	2.25	0.65
1:E:136:VAL:HG12	1:E:177:ASN:HA	1.79	0.65
1:B:185:ARG:HB2	1:B:240:TRP:CE2	2.32	0.65
1:E:249:VAL:O	1:E:253:VAL:HG23	1.96	0.65
1:B:118:LEU:HB2	1:B:151:PHE:CE2	2.32	0.64
1:B:157:THR:HG23	1:B:161:LYS:N	2.12	0.64
1:C:233:ILE:HG23	1:C:233:ILE:O	1.96	0.64
1:D:233:ILE:O	1:D:233:ILE:HG23	1.97	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:LEU:HD11	1:D:114:SER:HB3	1.80	0.64
1:G:157:THR:OG1	1:G:158:ALA:N	2.30	0.64
1:E:233:ILE:HG23	1:E:233:ILE:O	1.96	0.64
1:A:190:ILE:HG12	1:A:257:ILE:HG21	1.80	0.64
1:D:48:ILE:HD12	1:D:77:ILE:HD13	1.78	0.64
1:F:225:LEU:HD11	1:F:233:ILE:HG12	1.80	0.64
1:G:83:ILE:HG12	1:G:96:VAL:HG11	1.80	0.64
1:G:157:THR:CG2	1:G:161:LYS:HB2	2.27	0.64
1:A:121:GLY:O	1:A:125:VAL:HG23	1.98	0.64
1:E:274:ASP:HB2	1:F:272:GLN:NE2	2.12	0.64
1:A:201:VAL:HG11	1:A:235:PHE:CD2	2.33	0.64
1:G:152:SER:HA	1:G:167:ASN:ND2	2.12	0.64
1:F:97:ILE:CD1	1:G:95:SER:HA	2.28	0.63
1:B:233:ILE:HG23	1:B:233:ILE:O	1.98	0.63
1:C:226:ASN:HB2	1:C:236:VAL:CG1	2.29	0.63
1:A:272:GLN:NE2	1:G:274:ASP:HB2	2.13	0.63
1:A:188:PHE:HB2	1:A:237:VAL:HB	1.81	0.63
1:B:183:VAL:HG23	1:B:241:SER:O	1.98	0.63
1:C:115:LEU:HB3	1:D:110:ALA:HB2	1.79	0.63
1:D:224:ARG:HD3	1:E:251:TRP:CD2	2.34	0.63
1:A:82:LEU:O	1:A:86:LEU:HG	1.99	0.63
1:B:156:ARG:HH11	1:B:156:ARG:HG2	1.62	0.63
1:C:137:ASP:HB3	1:C:176:ILE:CG2	2.27	0.63
1:C:97:ILE:CD1	1:D:95:SER:HA	2.28	0.63
1:F:36:ALA:O	1:F:40:VAL:HG23	1.99	0.63
1:D:272:GLN:HG3	1:E:270:TYR:CZ	2.34	0.62
1:F:121:GLY:O	1:F:125:VAL:HG23	1.99	0.62
1:G:253:VAL:O	1:G:257:ILE:HG13	1.99	0.62
1:C:273:MET:HE3	1:D:273:MET:HE2	1.81	0.62
1:A:137:ASP:HB3	1:A:176:ILE:CG2	2.29	0.62
1:B:126:MET:SD	1:C:65:VAL:HG11	2.40	0.62
1:B:33:ALA:O	1:B:37:ILE:HG13	2.00	0.62
1:F:216:LEU:H	1:F:216:LEU:HD12	1.63	0.62
1:A:274:ASP:HB2	1:B:272:GLN:HE22	1.64	0.62
1:F:274:ASP:HB2	1:G:272:GLN:NE2	2.15	0.62
1:E:189:ILE:HG22	1:E:189:ILE:O	1.98	0.62
1:B:224:ARG:HD3	1:C:251:TRP:CD2	2.35	0.61
1:C:273:MET:HE3	1:D:273:MET:CE	2.29	0.61
1:D:33:ALA:O	1:D:37:ILE:HG13	2.00	0.61
1:C:157:THR:CG2	1:C:161:LYS:HB2	2.29	0.61
1:C:183:VAL:HG23	1:C:241:SER:O	1.99	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ILE:HD12	1:B:77:ILE:HD13	1.82	0.61
1:F:215:ILE:HD13	1:F:239:VAL:HG21	1.82	0.61
1:G:78:ILE:HG13	1:G:79:ALA:N	2.15	0.61
1:E:216:LEU:H	1:E:216:LEU:HD12	1.66	0.61
1:D:274:ASP:HB2	1:E:272:GLN:NE2	2.16	0.61
1:G:185:ARG:HB2	1:G:240:TRP:CE2	2.35	0.61
1:C:157:THR:HG22	1:C:161:LYS:O	2.01	0.61
1:C:171:ILE:O	1:D:166:PRO:HG2	2.00	0.61
1:D:124:LEU:O	1:D:128:ARG:HB3	2.01	0.61
1:D:200:GLN:O	1:D:204:ILE:HG13	2.01	0.61
1:G:212:GLU:HG3	1:G:215:ILE:HG13	1.83	0.60
1:D:118:LEU:HD12	1:D:151:PHE:CE2	2.36	0.60
1:E:176:ILE:HB	1:F:163:ILE:HG12	1.83	0.60
1:F:185:ARG:HB2	1:F:240:TRP:CE2	2.35	0.60
1:G:73:VAL:O	1:G:77:ILE:HG13	2.00	0.60
1:B:121:GLY:O	1:B:125:VAL:HG23	2.02	0.60
1:F:124:LEU:O	1:F:128:ARG:CB	2.45	0.60
1:G:34:ALA:O	1:G:38:ILE:HG13	2.01	0.60
1:B:270:TYR:HB3	1:B:271:PRO:CD	2.31	0.60
1:F:33:ALA:O	1:F:37:ILE:HG13	2.00	0.60
1:E:157:THR:HG23	1:E:161:LYS:H	1.67	0.60
1:E:78:ILE:HG13	1:E:79:ALA:N	2.16	0.60
1:A:140:GLY:O	1:A:141:VAL:C	2.40	0.60
1:C:48:ILE:HD12	1:C:77:ILE:HD13	1.83	0.60
1:E:183:VAL:HG23	1:E:241:SER:O	2.02	0.60
1:F:204:ILE:HD12	1:F:266:ILE:HD11	1.84	0.60
1:B:150:ILE:HD12	1:B:150:ILE:H	1.67	0.60
1:E:256:ARG:NH1	1:E:256:ARG:HG2	2.15	0.60
1:G:270:TYR:HB3	1:G:271:PRO:CD	2.31	0.60
1:A:208:ILE:HG23	1:A:256:ARG:HG2	1.84	0.60
1:A:74:ARG:O	1:A:78:ILE:HG23	2.01	0.60
1:B:123:LEU:HD21	1:C:151:PHE:CE1	2.37	0.60
1:B:253:VAL:O	1:B:257:ILE:HG13	2.01	0.59
1:B:89:VAL:HG12	1:B:89:VAL:O	2.02	0.59
1:C:128:ARG:HD2	1:C:128:ARG:C	2.23	0.59
1:E:181:GLU:OE2	1:E:181:GLU:HA	2.01	0.59
1:G:190:ILE:HD12	1:G:190:ILE:N	2.16	0.59
1:D:210:GLN:O	1:D:217:LYS:HE2	2.02	0.59
1:F:137:ASP:HB3	1:F:176:ILE:CG2	2.33	0.59
1:G:124:LEU:O	1:G:128:ARG:CB	2.46	0.59
1:C:78:ILE:HG13	1:C:79:ALA:N	2.18	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:PHE:CZ	1:G:86:LEU:HD13	2.38	0.59
1:E:118:LEU:HB2	1:E:151:PHE:CE2	2.37	0.59
1:E:157:THR:HG23	1:E:161:LYS:N	2.18	0.59
1:F:219:ARG:HG3	1:F:219:ARG:HH11	1.67	0.59
1:A:138:LEU:HD22	1:A:155:MET:CE	2.32	0.59
1:A:231:SER:HB3	1:A:272:GLN:H	1.66	0.59
1:A:33:ALA:O	1:A:37:ILE:HG13	2.01	0.59
1:D:181:GLU:HG3	1:D:182:PRO:HD2	1.85	0.59
1:D:225:LEU:HD11	1:D:233:ILE:HG12	1.85	0.59
1:F:233:ILE:O	1:F:233:ILE:CG2	2.51	0.59
1:D:140:GLY:O	1:D:141:VAL:C	2.42	0.58
1:E:188:PHE:HB2	1:E:237:VAL:HB	1.85	0.58
1:E:33:ALA:O	1:E:37:ILE:HG13	2.03	0.58
1:F:190:ILE:HG12	1:F:257:ILE:HG21	1.85	0.58
1:A:126:MET:HG3	1:A:127:PHE:HD1	1.69	0.58
1:E:185:ARG:HB2	1:E:240:TRP:CE2	2.39	0.58
1:E:232:SER:OG	1:E:233:ILE:N	2.35	0.58
1:A:73:VAL:O	1:A:77:ILE:HG13	2.02	0.58
1:B:188:PHE:HB2	1:B:237:VAL:HB	1.85	0.58
1:C:123:LEU:HD21	1:D:151:PHE:CE1	2.37	0.58
1:D:48:ILE:O	1:D:52:VAL:HG23	2.03	0.58
1:E:216:LEU:CD1	1:E:241:SER:HA	2.33	0.58
1:D:249:VAL:O	1:D:253:VAL:HG23	2.03	0.58
1:D:105:LEU:CD1	1:E:105:LEU:HD23	2.31	0.58
1:F:185:ARG:HB2	1:F:240:TRP:CD2	2.37	0.58
1:F:40:VAL:O	1:F:44:ILE:HG12	2.03	0.58
1:F:157:THR:HG23	1:F:161:LYS:H	1.68	0.58
1:B:74:ARG:O	1:B:78:ILE:HG23	2.03	0.58
1:E:185:ARG:HB2	1:E:240:TRP:CD2	2.39	0.58
1:A:46:ARG:HD2	1:A:74:ARG:HD2	1.84	0.58
1:B:228:LEU:HD22	1:C:254:LEU:HD11	1.84	0.58
1:D:124:LEU:O	1:D:128:ARG:HG3	2.03	0.58
1:E:157:THR:HG22	1:E:161:LYS:O	2.03	0.58
1:E:48:ILE:HD12	1:E:77:ILE:HD13	1.84	0.58
1:B:73:VAL:O	1:B:77:ILE:HG13	2.03	0.58
1:F:273:MET:HE3	1:G:273:MET:HE2	1.85	0.58
1:F:48:ILE:O	1:F:52:VAL:HG23	2.03	0.58
1:A:227:GLU:HB3	1:A:234:ASN:OD1	2.04	0.58
1:A:201:VAL:HG11	1:A:235:PHE:CE2	2.39	0.58
1:F:73:VAL:O	1:F:77:ILE:HG13	2.04	0.58
1:D:78:ILE:HG13	1:D:79:ALA:N	2.17	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:233:ILE:HG23	1:G:233:ILE:O	2.04	0.58
1:A:78:ILE:HG13	1:A:79:ALA:N	2.18	0.57
1:C:267:SER:O	1:C:269:PRO:HD3	2.04	0.57
1:G:141:VAL:HG23	1:G:141:VAL:O	2.03	0.57
1:G:188:PHE:CZ	1:G:253:VAL:HB	2.40	0.57
1:E:74:ARG:O	1:E:78:ILE:HG23	2.05	0.57
1:G:225:LEU:HA	1:G:235:PHE:CD1	2.39	0.57
1:A:272:GLN:HE22	1:G:274:ASP:HB2	1.67	0.57
1:C:120:ALA:HB1	1:C:171:ILE:HD12	1.86	0.57
1:C:140:GLY:O	1:C:141:VAL:C	2.42	0.57
1:G:48:ILE:O	1:G:52:VAL:HG23	2.04	0.57
1:B:138:LEU:HD23	1:B:170:ILE:HD13	1.87	0.57
1:C:125:VAL:O	1:C:128:ARG:HG3	2.05	0.57
1:E:256:ARG:HG2	1:E:256:ARG:HH11	1.70	0.57
1:F:200:GLN:O	1:F:204:ILE:HG13	2.05	0.57
1:A:156:ARG:HH11	1:A:156:ARG:HG2	1.68	0.57
1:A:185:ARG:HB2	1:A:240:TRP:CE2	2.40	0.57
1:B:88:ARG:HH11	1:B:88:ARG:HG2	1.70	0.57
1:D:215:ILE:HD13	1:D:239:VAL:HG21	1.85	0.57
1:F:216:LEU:CD1	1:F:241:SER:HA	2.35	0.57
1:A:254:LEU:HD11	1:G:228:LEU:HD22	1.86	0.56
1:A:253:VAL:O	1:A:257:ILE:HG13	2.04	0.56
1:C:233:ILE:HD12	1:D:258:LYS:HE2	1.86	0.56
1:C:272:GLN:HG3	1:D:270:TYR:CZ	2.39	0.56
1:A:267:SER:O	1:A:269:PRO:HD3	2.05	0.56
1:C:33:ALA:O	1:C:37:ILE:HG13	2.05	0.56
1:D:83:ILE:HG23	1:D:93:THR:CB	2.36	0.56
1:E:129:PRO:HG2	1:E:130:PHE:N	2.20	0.56
1:F:183:VAL:HG23	1:F:241:SER:O	2.05	0.56
1:G:33:ALA:O	1:G:37:ILE:HG13	2.04	0.56
1:B:78:ILE:HG13	1:B:79:ALA:N	2.20	0.56
1:B:278:LYS:HD2	1:C:276:ASN:OD1	2.05	0.56
1:F:105:LEU:HD13	1:G:105:LEU:HD23	1.87	0.56
1:F:276:ASN:HB2	1:G:274:ASP:OD1	2.05	0.56
1:A:274:ASP:OD1	1:G:276:ASN:HB2	2.06	0.56
1:C:176:ILE:HD11	1:D:161:LYS:HD2	1.86	0.56
1:E:48:ILE:O	1:E:52:VAL:HG23	2.05	0.56
1:C:181:GLU:HG3	1:C:182:PRO:HD2	1.87	0.56
1:C:48:ILE:O	1:C:52:VAL:HG23	2.06	0.56
1:C:115:LEU:HB3	1:D:110:ALA:CB	2.34	0.56
1:B:227:GLU:HB3	1:B:234:ASN:OD1	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LEU:HD22	1:C:155:MET:CE	2.35	0.56
1:G:150:ILE:H	1:G:150:ILE:CD1	2.06	0.56
1:B:126:MET:HG3	1:B:127:PHE:HD1	1.70	0.56
1:C:129:PRO:HG2	1:C:130:PHE:N	2.16	0.56
1:A:129:PRO:HG2	1:A:130:PHE:N	2.16	0.56
1:C:190:ILE:HG12	1:C:257:ILE:HG21	1.88	0.56
1:E:224:ARG:HD3	1:F:251:TRP:CD2	2.41	0.56
1:A:126:MET:SD	1:B:65:VAL:HG11	2.46	0.56
1:B:209:ILE:HD12	1:B:221:MET:CE	2.36	0.56
1:D:73:VAL:O	1:D:77:ILE:HG13	2.05	0.56
1:E:176:ILE:CD1	1:F:161:LYS:HD2	2.34	0.56
1:B:165:ILE:HB	1:B:170:ILE:HD11	1.88	0.55
1:E:140:GLY:O	1:E:141:VAL:C	2.43	0.55
1:A:86:LEU:HB3	1:A:91:VAL:HB	1.88	0.55
1:B:131:ARG:HG3	1:B:131:ARG:HH11	1.71	0.55
1:B:209:ILE:HD12	1:B:221:MET:HE2	1.89	0.55
1:G:138:LEU:HD22	1:G:155:MET:HE1	1.88	0.55
1:D:83:ILE:CG2	1:D:93:THR:HG21	2.34	0.55
1:F:188:PHE:CZ	1:F:253:VAL:HB	2.41	0.55
1:B:200:GLN:O	1:B:204:ILE:HG13	2.07	0.55
1:C:84:ALA:HB1	1:D:91:VAL:CG1	2.37	0.55
1:D:115:LEU:HB3	1:E:110:ALA:HB2	1.87	0.55
1:B:152:SER:HA	1:B:167:ASN:ND2	2.21	0.55
1:F:157:THR:HG22	1:F:161:LYS:O	2.07	0.55
1:A:251:TRP:CD2	1:G:224:ARG:HD3	2.41	0.55
1:A:83:ILE:HG23	1:A:93:THR:HG21	1.88	0.55
1:B:190:ILE:HG12	1:B:257:ILE:HG21	1.88	0.55
1:D:273:MET:HE1	1:E:273:MET:CE	2.37	0.55
1:E:267:SER:O	1:E:269:PRO:HD3	2.06	0.55
1:B:97:ILE:CD1	1:C:95:SER:CA	2.85	0.55
1:D:120:ALA:O	1:D:124:LEU:HB2	2.07	0.55
1:D:74:ARG:O	1:D:78:ILE:HG23	2.07	0.55
1:E:73:VAL:O	1:E:77:ILE:HG13	2.07	0.55
1:A:231:SER:CB	1:A:272:GLN:H	2.20	0.55
1:E:188:PHE:CZ	1:E:253:VAL:HB	2.42	0.55
1:C:73:VAL:O	1:C:77:ILE:HG13	2.06	0.55
1:D:204:ILE:O	1:D:208:ILE:HG13	2.07	0.55
1:G:232:SER:OG	1:G:233:ILE:N	2.40	0.55
1:A:224:ARG:HD3	1:B:251:TRP:CD2	2.42	0.54
1:B:140:GLY:O	1:B:141:VAL:C	2.46	0.54
1:C:46:ARG:HD2	1:C:74:ARG:HD2	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ILE:HD12	1:D:266:ILE:CD1	2.37	0.54
1:C:176:ILE:CD1	1:D:161:LYS:HD2	2.37	0.54
1:A:110:ALA:HB2	1:G:115:LEU:HB3	1.89	0.54
1:C:216:LEU:CD1	1:C:241:SER:HA	2.37	0.54
1:F:140:GLY:O	1:F:141:VAL:C	2.45	0.54
1:F:48:ILE:HD12	1:F:77:ILE:HD13	1.89	0.54
1:C:188:PHE:CZ	1:C:253:VAL:HB	2.43	0.54
1:C:233:ILE:O	1:C:233:ILE:CG2	2.55	0.54
1:D:40:VAL:O	1:D:44:ILE:HG12	2.08	0.54
1:F:46:ARG:HD2	1:F:74:ARG:HD2	1.88	0.54
1:A:157:THR:HG23	1:A:161:LYS:H	1.73	0.54
1:C:152:SER:HA	1:C:167:ASN:ND2	2.23	0.54
1:D:226:ASN:HB2	1:D:236:VAL:CG1	2.36	0.54
1:A:200:GLN:O	1:A:204:ILE:HG13	2.07	0.54
1:B:189:ILE:O	1:B:189:ILE:HG22	2.06	0.54
1:C:118:LEU:HD12	1:C:151:PHE:CE2	2.43	0.54
1:C:272:GLN:HG3	1:D:270:TYR:CE1	2.44	0.54
1:C:40:VAL:O	1:C:44:ILE:HG12	2.07	0.54
1:C:228:LEU:HD22	1:D:254:LEU:HD11	1.90	0.54
1:G:140:GLY:O	1:G:141:VAL:C	2.45	0.54
1:C:190:ILE:N	1:C:190:ILE:HD12	2.22	0.53
1:D:272:GLN:HG3	1:E:270:TYR:CE1	2.42	0.53
1:A:136:VAL:HG12	1:A:177:ASN:HA	1.91	0.53
1:F:120:ALA:HB1	1:F:171:ILE:HD12	1.90	0.53
1:D:267:SER:O	1:D:269:PRO:HD3	2.08	0.53
1:G:185:ARG:HB2	1:G:240:TRP:CD2	2.42	0.53
1:A:185:ARG:HB2	1:A:240:TRP:CD2	2.43	0.53
1:B:208:ILE:HG23	1:B:256:ARG:HG2	1.90	0.53
1:A:190:ILE:N	1:A:190:ILE:HD12	2.24	0.53
1:C:224:ARG:HD3	1:D:251:TRP:CD2	2.44	0.53
1:C:273:MET:CE	1:D:273:MET:HE2	2.37	0.53
1:A:233:ILE:HG23	1:A:233:ILE:O	2.08	0.53
1:C:141:VAL:HG23	1:C:141:VAL:O	2.09	0.53
1:C:88:ARG:HG2	1:D:90:GLY:O	2.08	0.53
1:E:225:LEU:HD11	1:E:233:ILE:HG12	1.89	0.53
1:F:97:ILE:HD12	1:G:95:SER:HA	1.90	0.53
1:B:157:THR:HG22	1:B:161:LYS:O	2.08	0.53
1:E:226:ASN:HB2	1:E:236:VAL:HG12	1.89	0.53
1:D:273:MET:HE1	1:E:273:MET:HE2	1.90	0.53
1:F:215:ILE:HG21	1:F:239:VAL:HG22	1.91	0.53
1:A:157:THR:HG23	1:A:161:LYS:N	2.24	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:PHE:CZ	1:D:253:VAL:HB	2.44	0.53
1:F:126:MET:HG3	1:F:127:PHE:HD1	1.74	0.53
1:C:74:ARG:O	1:C:78:ILE:HG23	2.09	0.53
1:D:233:ILE:O	1:D:233:ILE:CG2	2.57	0.53
1:G:215:ILE:HD13	1:G:239:VAL:HG11	1.92	0.52
1:C:232:SER:OG	1:C:233:ILE:N	2.42	0.52
1:A:249:VAL:O	1:A:253:VAL:HG23	2.10	0.52
1:A:89:VAL:O	1:A:89:VAL:HG12	2.10	0.52
1:F:128:ARG:O	1:F:128:ARG:HD2	2.09	0.52
1:F:157:THR:HG23	1:F:161:LYS:N	2.25	0.52
1:C:212:GLU:HG3	1:C:215:ILE:HG13	1.92	0.52
1:F:270:TYR:HB3	1:F:271:PRO:CD	2.40	0.52
1:G:129:PRO:HG2	1:G:130:PHE:N	2.17	0.52
1:C:219:ARG:HH11	1:C:219:ARG:HG3	1.75	0.52
1:D:138:LEU:HD23	1:D:170:ILE:HD13	1.91	0.52
1:D:190:ILE:HG12	1:D:257:ILE:HG21	1.92	0.52
1:D:274:ASP:HB2	1:E:272:GLN:HE22	1.74	0.52
1:A:242:ASN:O	1:A:243:SER:C	2.48	0.52
1:A:95:SER:CA	1:G:97:ILE:CD1	2.86	0.52
1:C:37:ILE:CD1	1:D:91:VAL:HG22	2.40	0.52
1:D:188:PHE:HB2	1:D:237:VAL:HB	1.91	0.52
1:E:79:ALA:O	1:E:83:ILE:HG13	2.09	0.52
1:F:150:ILE:H	1:F:150:ILE:HD12	1.74	0.52
1:F:253:VAL:O	1:F:257:ILE:HG13	2.10	0.52
1:F:273:MET:CE	1:G:273:MET:HE2	2.39	0.52
1:A:138:LEU:HD22	1:A:155:MET:HE3	1.91	0.52
1:B:219:ARG:HH11	1:B:219:ARG:HG3	1.75	0.52
1:F:232:SER:OG	1:F:233:ILE:N	2.43	0.52
1:A:232:SER:OG	1:A:233:ILE:N	2.43	0.51
1:A:79:ALA:O	1:A:83:ILE:HG13	2.10	0.51
1:D:138:LEU:HD22	1:D:155:MET:CE	2.40	0.51
1:E:124:LEU:O	1:E:128:ARG:CB	2.55	0.51
1:G:256:ARG:NH1	1:G:256:ARG:HG2	2.25	0.51
1:D:201:VAL:HG11	1:D:235:PHE:CD2	2.46	0.51
1:A:183:VAL:HG23	1:A:241:SER:O	2.10	0.51
1:B:225:LEU:HD11	1:B:233:ILE:HG12	1.92	0.51
1:B:129:PRO:CG	1:B:130:PHE:H	2.17	0.51
1:B:146:LEU:HD12	1:B:146:LEU:N	2.25	0.51
1:C:129:PRO:CG	1:C:130:PHE:H	2.19	0.51
1:C:37:ILE:HD11	1:D:91:VAL:HG22	1.91	0.51
1:D:83:ILE:HG12	1:D:96:VAL:HG11	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PRO:CG	1:A:130:PHE:H	2.21	0.51
1:C:157:THR:HG23	1:C:161:LYS:H	1.76	0.51
1:E:208:ILE:HG23	1:E:256:ARG:HG2	1.92	0.51
1:A:118:LEU:HB2	1:A:151:PHE:CE2	2.45	0.51
1:D:129:PRO:HG2	1:D:130:PHE:N	2.24	0.51
1:F:152:SER:HA	1:F:167:ASN:ND2	2.25	0.51
1:A:110:ALA:CB	1:G:115:LEU:HB3	2.40	0.51
1:A:48:ILE:O	1:A:52:VAL:HG23	2.10	0.51
1:B:267:SER:O	1:B:269:PRO:HD3	2.11	0.51
1:D:118:LEU:HD12	1:D:151:PHE:CZ	2.46	0.51
1:F:125:VAL:O	1:F:128:ARG:HG3	2.11	0.51
1:C:123:LEU:CD1	1:D:114:SER:HB3	2.40	0.51
1:D:83:ILE:CD1	1:D:96:VAL:HG11	2.41	0.51
1:F:270:TYR:HB3	1:F:271:PRO:HD2	1.93	0.51
1:A:141:VAL:O	1:A:141:VAL:HG23	2.11	0.51
1:A:188:PHE:CZ	1:A:253:VAL:HB	2.46	0.51
1:A:186:ASN:ND2	1:A:246:LEU:HG	2.25	0.51
1:A:109:LEU:HD23	1:B:109:LEU:HD13	1.93	0.51
1:B:216:LEU:CD1	1:B:241:SER:HA	2.41	0.51
1:D:146:LEU:O	1:D:147:SER:HB3	2.11	0.51
1:G:188:PHE:HB2	1:G:237:VAL:HB	1.92	0.51
1:A:118:LEU:HB2	1:A:151:PHE:CZ	2.46	0.51
1:A:176:ILE:HA	1:B:162:ILE:O	2.11	0.51
1:A:228:LEU:HD22	1:B:254:LEU:HD11	1.91	0.51
1:E:209:ILE:HD12	1:E:221:MET:CE	2.40	0.51
1:F:189:ILE:HG22	1:F:189:ILE:O	2.11	0.51
1:G:149:GLN:HB3	1:G:150:ILE:HD12	1.93	0.51
1:A:212:GLU:OE2	1:A:214:ARG:HB2	2.10	0.50
1:E:181:GLU:HG3	1:E:182:PRO:HD2	1.93	0.50
1:A:157:THR:HG22	1:A:161:LYS:O	2.12	0.50
1:B:40:VAL:O	1:B:44:ILE:HG12	2.12	0.50
1:C:34:ALA:O	1:C:38:ILE:HG13	2.11	0.50
1:G:118:LEU:HD12	1:G:151:PHE:HE2	1.77	0.50
1:E:274:ASP:HB2	1:F:272:GLN:HE22	1.76	0.50
1:G:223:VAL:O	1:G:224:ARG:HG3	2.11	0.50
1:A:273:MET:HE2	1:G:273:MET:HE1	1.94	0.50
1:D:232:SER:OG	1:D:233:ILE:N	2.44	0.50
1:A:128:ARG:CD	1:A:128:ARG:N	2.74	0.50
1:A:48:ILE:HD12	1:A:77:ILE:HD13	1.92	0.50
1:B:120:ALA:O	1:B:124:LEU:HB2	2.11	0.50
1:D:215:ILE:CD1	1:D:239:VAL:HG11	2.42	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:ASP:O	1:D:249:VAL:HG23	2.12	0.50
1:E:223:VAL:O	1:E:224:ARG:HG3	2.11	0.50
1:F:208:ILE:HG23	1:F:256:ARG:HG2	1.93	0.50
1:G:229:GLY:HA3	1:G:232:SER:O	2.12	0.50
1:G:48:ILE:HD12	1:G:77:ILE:HD13	1.94	0.50
1:F:274:ASP:HB2	1:G:272:GLN:HE22	1.77	0.50
1:G:40:VAL:O	1:G:44:ILE:HG12	2.12	0.50
1:A:109:LEU:HD23	1:B:109:LEU:CD1	2.42	0.49
1:B:153:THR:N	1:B:167:ASN:HD21	2.10	0.49
1:B:222:THR:O	1:B:237:VAL:HA	2.11	0.49
1:G:226:ASN:HB2	1:G:236:VAL:CG1	2.36	0.49
1:A:183:VAL:HG21	1:A:216:LEU:HD22	1.94	0.49
1:D:225:LEU:HA	1:D:235:PHE:CD1	2.47	0.49
1:D:201:VAL:HG11	1:D:235:PHE:CE2	2.48	0.49
1:G:128:ARG:NH2	1:G:131:ARG:HH21	2.10	0.49
1:E:223:VAL:HG22	1:E:237:VAL:HG22	1.94	0.49
1:G:219:ARG:HH11	1:G:219:ARG:HG3	1.77	0.49
1:A:226:ASN:HB2	1:A:236:VAL:CG1	2.38	0.49
1:G:129:PRO:CG	1:G:130:PHE:H	2.20	0.49
1:E:176:ILE:HD11	1:F:161:LYS:HB3	1.95	0.49
1:G:229:GLY:CA	1:G:232:SER:O	2.60	0.49
1:B:223:VAL:O	1:B:224:ARG:HG3	2.13	0.49
1:D:83:ILE:HG23	1:D:93:THR:HB	1.94	0.49
1:A:270:TYR:HB3	1:A:271:PRO:HD3	1.94	0.49
1:G:130:PHE:HA	1:G:134:GLU:OE1	2.11	0.49
1:G:157:THR:HG23	1:G:161:LYS:H	1.77	0.49
1:A:95:SER:CA	1:G:97:ILE:HD11	2.43	0.49
1:C:181:GLU:OE2	1:C:181:GLU:HA	2.13	0.49
1:C:105:LEU:CD1	1:D:105:LEU:HD23	2.38	0.49
1:D:107:VAL:O	1:D:111:LEU:HB2	2.13	0.49
1:E:190:ILE:N	1:E:190:ILE:HD12	2.28	0.49
1:E:233:ILE:CG2	1:E:233:ILE:O	2.60	0.49
1:A:273:MET:HE2	1:G:273:MET:CE	2.43	0.49
1:A:40:VAL:O	1:A:44:ILE:HG12	2.12	0.48
1:G:138:LEU:HD22	1:G:155:MET:CE	2.43	0.48
1:G:201:VAL:HG11	1:G:235:PHE:CD2	2.48	0.48
1:C:138:LEU:HD22	1:C:155:MET:HE3	1.94	0.48
1:C:274:ASP:HB2	1:D:272:GLN:NE2	2.27	0.48
1:E:222:THR:O	1:E:237:VAL:HA	2.13	0.48
1:G:181:GLU:CD	1:G:182:PRO:HD2	2.32	0.48
1:B:50:ASN:O	1:B:54:ARG:HG3	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:VAL:HG11	1:C:235:PHE:CD2	2.48	0.48
1:C:215:ILE:HD13	1:C:239:VAL:HG21	1.95	0.48
1:C:204:ILE:HD12	1:C:266:ILE:HD11	1.96	0.48
1:C:97:ILE:CD1	1:D:95:SER:CA	2.91	0.48
1:G:157:THR:HG23	1:G:161:LYS:N	2.28	0.48
1:G:204:ILE:O	1:G:208:ILE:HG13	2.13	0.48
1:A:183:VAL:HG13	1:A:183:VAL:O	2.13	0.48
1:B:190:ILE:N	1:B:190:ILE:HD12	2.28	0.48
1:B:197:ASP:HB3	1:B:200:GLN:HB3	1.95	0.48
1:C:216:LEU:HD12	1:C:216:LEU:H	1.78	0.48
1:D:208:ILE:HG23	1:D:256:ARG:HG2	1.96	0.48
1:E:34:ALA:O	1:E:38:ILE:HG13	2.13	0.48
1:E:35:LEU:O	1:E:39:ILE:HG13	2.13	0.48
1:G:225:LEU:HD11	1:G:233:ILE:CG1	2.42	0.48
1:A:225:LEU:HD11	1:A:233:ILE:CG1	2.42	0.48
1:B:35:LEU:O	1:B:39:ILE:HG13	2.13	0.48
1:G:52:VAL:O	1:G:56:MET:HG2	2.14	0.48
1:C:201:VAL:HG11	1:C:235:PHE:CE2	2.49	0.48
1:D:150:ILE:HD12	1:D:150:ILE:H	1.78	0.48
1:D:118:LEU:HB2	1:D:151:PHE:CE2	2.49	0.48
1:E:231:SER:HB3	1:E:272:GLN:H	1.79	0.48
1:A:105:LEU:HD13	1:B:105:LEU:CD2	2.44	0.48
1:E:253:VAL:O	1:E:257:ILE:HG13	2.13	0.48
1:E:40:VAL:O	1:E:44:ILE:HG12	2.13	0.48
1:F:159:ASP:OD1	1:F:161:LYS:HG3	2.13	0.48
1:F:273:MET:HE3	1:G:273:MET:CE	2.43	0.48
1:D:43:ILE:HG13	1:D:44:ILE:N	2.29	0.48
1:E:120:ALA:O	1:E:124:LEU:HB2	2.14	0.48
1:G:227:GLU:HB3	1:G:234:ASN:OD1	2.13	0.48
1:B:46:ARG:HD2	1:B:74:ARG:HD2	1.96	0.47
1:D:190:ILE:HD12	1:D:190:ILE:N	2.29	0.47
1:D:222:THR:O	1:D:237:VAL:HA	2.13	0.47
1:E:190:ILE:HG12	1:E:257:ILE:HG21	1.95	0.47
1:E:29:VAL:HG11	1:F:27:TYR:CE2	2.49	0.47
1:F:78:ILE:HG13	1:F:79:ALA:N	2.28	0.47
1:G:216:LEU:CD1	1:G:241:SER:HA	2.44	0.47
1:A:239:VAL:HG12	1:A:239:VAL:O	2.13	0.47
1:B:181:GLU:OE2	1:B:181:GLU:HA	2.14	0.47
1:C:256:ARG:NH1	1:C:256:ARG:HG2	2.29	0.47
1:D:156:ARG:HH11	1:D:156:ARG:HG2	1.79	0.47
1:D:46:ARG:HD2	1:D:74:ARG:HD2	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:ILE:HD12	1:E:266:ILE:HD11	1.96	0.47
1:E:227:GLU:HB3	1:E:234:ASN:OD1	2.14	0.47
1:F:227:GLU:HB3	1:F:234:ASN:OD1	2.14	0.47
1:A:233:ILE:CG2	1:A:233:ILE:O	2.63	0.47
1:B:226:ASN:HB2	1:B:236:VAL:HG12	1.96	0.47
1:C:208:ILE:HG23	1:C:256:ARG:HG2	1.97	0.47
1:E:216:LEU:N	1:E:216:LEU:HD12	2.29	0.47
1:A:273:MET:CE	1:G:273:MET:HE1	2.45	0.47
1:B:40:VAL:O	1:B:44:ILE:HG23	2.15	0.47
1:E:46:ARG:HD2	1:E:74:ARG:HD2	1.97	0.47
1:B:219:ARG:HG3	1:B:219:ARG:NH1	2.29	0.47
1:D:124:LEU:O	1:D:128:ARG:CB	2.63	0.47
1:C:43:ILE:HG13	1:C:44:ILE:N	2.30	0.47
1:B:233:ILE:CG2	1:B:233:ILE:O	2.62	0.47
1:D:35:LEU:O	1:D:39:ILE:HG13	2.15	0.47
1:F:215:ILE:CD1	1:F:239:VAL:HG11	2.45	0.47
1:A:114:SER:HB3	1:G:123:LEU:HD12	1.96	0.47
1:A:201:VAL:HG22	1:A:266:ILE:HD13	1.96	0.47
1:D:212:GLU:OE2	1:D:214:ARG:HB2	2.15	0.47
1:D:31:ILE:O	1:D:35:LEU:HG	2.15	0.47
1:F:118:LEU:HD12	1:F:151:PHE:HE2	1.80	0.47
1:F:242:ASN:O	1:F:243:SER:C	2.53	0.47
1:G:233:ILE:CG2	1:G:233:ILE:O	2.63	0.47
1:G:256:ARG:HG2	1:G:256:ARG:HH11	1.80	0.47
1:B:118:LEU:HD12	1:B:151:PHE:HE2	1.80	0.47
1:B:256:ARG:NH1	1:B:256:ARG:HG2	2.29	0.47
1:E:272:GLN:HG3	1:F:270:TYR:CZ	2.50	0.47
1:G:204:ILE:HD12	1:G:266:ILE:HD11	1.97	0.47
1:A:130:PHE:HA	1:A:134:GLU:OE1	2.15	0.46
1:C:185:ARG:HB2	1:C:240:TRP:CD2	2.50	0.46
1:C:242:ASN:O	1:C:243:SER:C	2.53	0.46
1:E:272:GLN:HG3	1:F:270:TYR:CE1	2.50	0.46
1:F:222:THR:O	1:F:237:VAL:HA	2.15	0.46
1:C:50:ASN:O	1:C:54:ARG:HG3	2.15	0.46
1:D:40:VAL:HA	1:D:43:ILE:HD11	1.97	0.46
1:G:118:LEU:HD12	1:G:151:PHE:CE2	2.49	0.46
1:A:273:MET:HE3	1:B:273:MET:HE2	1.98	0.46
1:D:28:ALA:O	1:D:32:VAL:HG23	2.15	0.46
1:G:111:LEU:HD12	1:G:111:LEU:HA	1.68	0.46
1:G:191:GLY:HA2	1:G:234:ASN:HB3	1.97	0.46
1:A:176:ILE:CD1	1:B:161:LYS:HB3	2.45	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:VAL:O	1:C:253:VAL:HG23	2.14	0.46
1:C:85:ALA:O	1:C:89:VAL:HG23	2.15	0.46
1:D:231:SER:HB3	1:D:272:GLN:H	1.81	0.46
1:G:112:GLN:HE21	1:G:112:GLN:HB3	1.50	0.46
1:A:128:ARG:N	1:A:128:ARG:HD3	2.30	0.46
1:D:157:THR:HG23	1:D:161:LYS:N	2.30	0.46
1:D:215:ILE:HG12	1:D:239:VAL:CG1	2.46	0.46
1:D:183:VAL:HG23	1:D:241:SER:O	2.16	0.46
1:C:233:ILE:CD1	1:D:258:LYS:HE2	2.44	0.46
1:F:107:VAL:O	1:F:111:LEU:HB2	2.16	0.46
1:F:231:SER:HB3	1:F:272:GLN:H	1.80	0.46
1:G:128:ARG:NH2	1:G:131:ARG:NH2	2.64	0.46
1:G:156:ARG:HG2	1:G:156:ARG:HH11	1.80	0.46
1:A:225:LEU:HA	1:A:235:PHE:CD1	2.50	0.46
1:A:256:ARG:HG2	1:A:256:ARG:NH1	2.30	0.46
1:E:236:VAL:O	1:E:236:VAL:HG13	2.14	0.46
1:A:277:PHE:CZ	1:B:277:PHE:HZ	2.34	0.46
1:A:115:LEU:CD2	1:B:106:ALA:HB1	2.46	0.46
1:D:140:GLY:O	1:D:141:VAL:O	2.33	0.46
1:D:247:GLN:HG3	1:D:251:TRP:CZ3	2.51	0.46
1:E:85:ALA:O	1:E:89:VAL:HG23	2.15	0.46
1:A:128:ARG:HH21	1:A:131:ARG:NH2	2.14	0.46
1:A:223:VAL:O	1:A:224:ARG:HG3	2.15	0.46
1:E:112:GLN:HG2	1:E:112:GLN:O	2.16	0.46
1:G:74:ARG:O	1:G:78:ILE:HG23	2.16	0.46
1:B:273:MET:HE3	1:C:273:MET:HE2	1.97	0.46
1:C:84:ALA:HB1	1:D:91:VAL:HG12	1.98	0.46
1:F:219:ARG:HG3	1:F:219:ARG:NH1	2.31	0.46
1:F:249:VAL:O	1:F:253:VAL:HG23	2.15	0.46
1:B:224:ARG:HG2	1:B:224:ARG:NH1	2.31	0.46
1:F:31:ILE:O	1:F:35:LEU:HG	2.16	0.46
1:A:107:VAL:O	1:A:111:LEU:HB2	2.16	0.45
1:A:43:ILE:HG13	1:A:44:ILE:N	2.31	0.45
1:E:152:SER:HA	1:E:167:ASN:ND2	2.31	0.45
1:E:153:THR:N	1:E:167:ASN:HD21	2.13	0.45
1:F:190:ILE:HD12	1:F:190:ILE:N	2.31	0.45
1:G:153:THR:HB	1:G:170:ILE:HD11	1.98	0.45
1:B:48:ILE:O	1:B:52:VAL:HG23	2.16	0.45
1:D:112:GLN:HG2	1:D:112:GLN:O	2.15	0.45
1:D:188:PHE:CZ	1:D:250:TYR:HA	2.52	0.45
1:G:167:ASN:N	1:G:167:ASN:HD22	2.13	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PRO:CG	1:A:130:PHE:N	2.78	0.45
1:A:35:LEU:O	1:A:39:ILE:HG13	2.16	0.45
1:F:224:ARG:CD	1:G:251:TRP:CE3	2.98	0.45
1:G:125:VAL:O	1:G:128:ARG:HG3	2.16	0.45
1:G:50:ASN:O	1:G:54:ARG:HG3	2.16	0.45
1:B:183:VAL:O	1:B:183:VAL:HG13	2.16	0.45
1:B:215:ILE:HG23	1:B:239:VAL:HG13	1.99	0.45
1:B:123:LEU:HD11	1:C:151:PHE:HE1	1.81	0.45
1:D:176:ILE:CD1	1:E:161:LYS:HD2	2.46	0.45
1:A:162:ILE:HA	1:A:162:ILE:HD13	1.76	0.45
1:B:224:ARG:HH11	1:B:224:ARG:HG2	1.81	0.45
1:C:126:MET:HG3	1:C:127:PHE:HD1	1.82	0.45
1:D:270:TYR:HB3	1:D:271:PRO:CD	2.46	0.45
1:E:31:ILE:O	1:E:35:LEU:HG	2.17	0.45
1:F:128:ARG:CZ	1:F:131:ARG:HH21	2.29	0.45
1:F:215:ILE:HD13	1:F:239:VAL:CG2	2.46	0.45
1:C:128:ARG:CB	1:C:129:PRO:HD2	2.46	0.45
1:D:128:ARG:CB	1:D:129:PRO:HD2	2.44	0.45
1:D:171:ILE:O	1:E:166:PRO:HG2	2.16	0.45
1:D:216:LEU:HD12	1:D:216:LEU:N	2.31	0.45
1:D:83:ILE:HD13	1:D:96:VAL:HG11	1.99	0.45
1:G:270:TYR:HB3	1:G:271:PRO:HD2	1.98	0.45
1:B:118:LEU:HD12	1:B:151:PHE:CE2	2.51	0.45
1:B:28:ALA:O	1:B:32:VAL:HG23	2.16	0.45
1:D:152:SER:HA	1:D:167:ASN:ND2	2.31	0.45
1:G:79:ALA:O	1:G:83:ILE:HG13	2.16	0.45
1:B:242:ASN:O	1:B:243:SER:C	2.55	0.45
1:D:157:THR:HG22	1:D:161:LYS:O	2.17	0.45
1:D:242:ASN:O	1:D:243:SER:C	2.54	0.45
1:F:35:LEU:O	1:F:39:ILE:HG13	2.17	0.45
1:A:270:TYR:CD2	1:G:272:GLN:HB3	2.52	0.45
1:B:162:ILE:HD13	1:B:162:ILE:HA	1.70	0.45
1:E:118:LEU:HD12	1:E:151:PHE:CE2	2.52	0.45
1:E:215:ILE:HG21	1:E:239:VAL:HG22	1.99	0.45
1:A:40:VAL:O	1:A:44:ILE:HG23	2.17	0.45
1:B:180:ARG:HD3	1:C:162:ILE:CG2	2.21	0.45
1:C:120:ALA:O	1:C:124:LEU:HB2	2.16	0.45
1:C:276:ASN:HB2	1:D:274:ASP:OD1	2.17	0.45
1:D:34:ALA:O	1:D:38:ILE:HG13	2.17	0.45
1:D:50:ASN:O	1:D:54:ARG:HG3	2.17	0.45
1:F:138:LEU:HD23	1:F:170:ILE:HD13	2.00	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:GLN:HG3	1:G:270:TYR:CZ	2.51	0.45
1:F:28:ALA:O	1:F:32:VAL:HG23	2.17	0.45
1:A:112:GLN:O	1:A:116:SER:HB2	2.16	0.44
1:E:156:ARG:HH11	1:E:156:ARG:HG2	1.82	0.44
1:E:197:ASP:HB3	1:E:200:GLN:HB3	1.98	0.44
1:F:120:ALA:O	1:F:124:LEU:HB2	2.16	0.44
1:F:188:PHE:HB2	1:F:237:VAL:HB	1.98	0.44
1:G:35:LEU:O	1:G:39:ILE:HG13	2.17	0.44
1:A:128:ARG:O	1:A:128:ARG:HD3	2.17	0.44
1:A:146:LEU:O	1:A:147:SER:HB3	2.16	0.44
1:B:111:LEU:HA	1:B:111:LEU:HD12	1.75	0.44
1:B:43:ILE:HG13	1:B:44:ILE:N	2.32	0.44
1:D:115:LEU:HB3	1:E:110:ALA:CB	2.47	0.44
1:A:186:ASN:HD21	1:A:246:LEU:HG	1.80	0.44
1:B:212:GLU:HB3	1:B:215:ILE:HD12	1.98	0.44
1:B:274:ASP:HB2	1:C:272:GLN:NE2	2.32	0.44
1:E:118:LEU:HD12	1:E:151:PHE:HE2	1.83	0.44
1:E:185:ARG:HG2	1:E:186:ASN:N	2.31	0.44
1:B:188:PHE:CE2	1:B:250:TYR:CD1	3.05	0.44
1:D:205:LEU:O	1:D:209:ILE:HG12	2.17	0.44
1:D:86:LEU:HB3	1:D:91:VAL:CB	2.38	0.44
1:E:205:LEU:O	1:E:209:ILE:HG12	2.18	0.44
1:B:204:ILE:O	1:B:208:ILE:HG13	2.18	0.44
1:B:275:VAL:HG22	1:C:275:VAL:HG12	1.99	0.44
1:C:185:ARG:HB2	1:C:240:TRP:CE2	2.53	0.44
1:D:219:ARG:HH11	1:D:219:ARG:HG3	1.82	0.44
1:A:209:ILE:HD12	1:A:221:MET:CE	2.47	0.44
1:A:111:LEU:HA	1:A:111:LEU:HD12	1.78	0.44
1:A:153:THR:N	1:A:167:ASN:HD21	2.16	0.44
1:B:156:ARG:HA	1:B:162:ILE:HD13	2.00	0.44
1:B:201:VAL:HG11	1:B:235:PHE:CD2	2.53	0.44
1:D:183:VAL:HG13	1:D:183:VAL:O	2.17	0.44
1:F:212:GLU:OE2	1:F:214:ARG:HB2	2.18	0.44
1:F:233:ILE:HD12	1:G:258:LYS:HE2	1.99	0.44
1:F:256:ARG:HG2	1:F:256:ARG:NH1	2.31	0.44
1:F:50:ASN:O	1:F:54:ARG:HG3	2.18	0.44
1:A:181:GLU:HG3	1:A:182:PRO:HD2	2.00	0.44
1:B:159:ASP:OD2	1:B:161:LYS:HE2	2.18	0.44
1:F:129:PRO:CG	1:F:130:PHE:H	2.30	0.44
1:F:165:ILE:HB	1:F:170:ILE:HD11	1.99	0.44
1:F:260:GLU:OE2	1:F:260:GLU:HA	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:ALA:HB1	1:F:74:ARG:HG3	2.00	0.44
1:A:64:THR:O	1:A:68:PHE:HB2	2.18	0.43
1:F:226:ASN:HB2	1:F:236:VAL:CG1	2.46	0.43
1:G:208:ILE:CG2	1:G:256:ARG:HG2	2.45	0.43
1:C:35:LEU:O	1:C:39:ILE:HG13	2.18	0.43
1:C:40:VAL:HA	1:C:43:ILE:HD11	2.00	0.43
1:A:97:ILE:HD13	1:A:97:ILE:HA	1.86	0.43
1:B:215:ILE:CD1	1:B:239:VAL:HG11	2.48	0.43
1:C:157:THR:HG23	1:C:161:LYS:N	2.32	0.43
1:D:130:PHE:HA	1:D:134:GLU:OE1	2.18	0.43
1:E:270:TYR:HB3	1:E:271:PRO:CD	2.48	0.43
1:F:131:ARG:N	1:F:134:GLU:OE1	2.38	0.43
1:F:274:ASP:CB	1:G:272:GLN:HE22	2.32	0.43
1:F:86:LEU:HD23	1:F:86:LEU:HA	1.91	0.43
1:G:157:THR:HG22	1:G:161:LYS:O	2.18	0.43
1:B:270:TYR:HB3	1:B:271:PRO:HD2	2.00	0.43
1:C:204:ILE:O	1:C:208:ILE:HG13	2.18	0.43
1:E:150:ILE:HD12	1:E:150:ILE:H	1.84	0.43
1:E:209:ILE:HD12	1:E:221:MET:HE2	1.99	0.43
1:F:112:GLN:HB3	1:F:112:GLN:HE21	1.53	0.43
1:F:181:GLU:CD	1:F:182:PRO:HD2	2.39	0.43
1:A:212:GLU:HG3	1:A:215:ILE:HG13	2.00	0.43
1:B:232:SER:OG	1:B:233:ILE:N	2.51	0.43
1:C:40:VAL:O	1:C:44:ILE:HG23	2.18	0.43
1:B:97:ILE:HD11	1:C:95:SER:HB2	2.00	0.43
1:D:134:GLU:O	1:D:145:VAL:HG23	2.17	0.43
1:C:274:ASP:HB2	1:D:272:GLN:HE22	1.84	0.43
1:F:191:GLY:HA2	1:F:234:ASN:HB3	1.99	0.43
1:G:140:GLY:O	1:G:141:VAL:O	2.36	0.43
1:G:209:ILE:HG13	1:G:210:GLN:N	2.34	0.43
1:G:97:ILE:HD13	1:G:97:ILE:HA	1.75	0.43
1:B:97:ILE:HD12	1:C:95:SER:CA	2.39	0.43
1:D:270:TYR:HB3	1:D:271:PRO:HD2	1.99	0.43
1:E:40:VAL:HA	1:E:43:ILE:HD11	2.00	0.43
1:F:129:PRO:HG2	1:F:130:PHE:N	2.27	0.43
1:F:204:ILE:HD12	1:F:266:ILE:CD1	2.48	0.43
1:E:274:ASP:CB	1:F:272:GLN:HE22	2.31	0.43
1:B:272:GLN:HG3	1:C:270:TYR:CZ	2.53	0.43
1:D:163:ILE:HG22	1:D:164:VAL:N	2.34	0.43
1:D:223:VAL:HG22	1:D:237:VAL:HG22	2.01	0.43
1:E:245:ASP:O	1:E:249:VAL:HG23	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:ARG:HG2	1:G:160:GLY:HA3	2.00	0.43
1:F:224:ARG:HD3	1:G:251:TRP:CG	2.53	0.43
1:A:53:ASN:O	1:A:57:ILE:HG22	2.18	0.43
1:B:146:LEU:O	1:B:147:SER:HB3	2.19	0.43
1:F:118:LEU:HD12	1:F:151:PHE:CE2	2.54	0.43
1:A:215:ILE:CD1	1:A:239:VAL:HG11	2.48	0.43
1:A:50:ASN:O	1:A:54:ARG:HG3	2.19	0.43
1:C:153:THR:N	1:C:167:ASN:HD21	2.16	0.43
1:E:128:ARG:HA	1:E:129:PRO:HD3	1.83	0.43
1:F:216:LEU:N	1:F:216:LEU:HD12	2.30	0.43
1:G:162:ILE:HD13	1:G:162:ILE:HA	1.82	0.43
1:G:204:ILE:HD12	1:G:266:ILE:CD1	2.48	0.43
1:B:228:LEU:HA	1:B:228:LEU:HD12	1.85	0.42
1:D:111:LEU:HA	1:D:111:LEU:HD12	1.78	0.42
1:D:105:LEU:CD1	1:E:105:LEU:CD2	2.96	0.42
1:E:112:GLN:HB3	1:E:112:GLN:HE21	1.61	0.42
1:F:165:ILE:HG22	1:F:170:ILE:HG13	2.00	0.42
1:F:84:ALA:HB1	1:G:91:VAL:CG1	2.44	0.42
1:B:223:VAL:HG22	1:B:237:VAL:HG22	2.01	0.42
1:D:153:THR:N	1:D:167:ASN:HD21	2.16	0.42
1:F:141:VAL:HG23	1:F:141:VAL:O	2.19	0.42
1:G:107:VAL:O	1:G:111:LEU:HB2	2.19	0.42
1:A:166:PRO:HG2	1:G:171:ILE:O	2.20	0.42
1:B:204:ILE:HD12	1:B:266:ILE:CD1	2.43	0.42
1:A:274:ASP:CB	1:B:272:GLN:HE22	2.29	0.42
1:C:140:GLY:O	1:C:141:VAL:O	2.36	0.42
1:C:150:ILE:H	1:C:150:ILE:CD1	2.18	0.42
1:D:185:ARG:HB2	1:D:240:TRP:CD2	2.54	0.42
1:D:39:ILE:O	1:D:43:ILE:HG12	2.20	0.42
1:E:111:LEU:HA	1:E:111:LEU:HD12	1.71	0.42
1:G:215:ILE:CD1	1:G:239:VAL:HG11	2.49	0.42
1:G:43:ILE:O	1:G:47:MET:HG3	2.19	0.42
1:B:152:SER:C	1:B:167:ASN:HD21	2.22	0.42
1:C:219:ARG:HG3	1:C:219:ARG:NH1	2.33	0.42
1:A:34:ALA:O	1:A:38:ILE:HG13	2.19	0.42
1:A:256:ARG:HG2	1:A:256:ARG:HH11	1.84	0.42
1:B:34:ALA:O	1:B:38:ILE:HG13	2.19	0.42
1:D:126:MET:HG3	1:D:127:PHE:HD1	1.84	0.42
1:D:223:VAL:O	1:D:224:ARG:HG3	2.20	0.42
1:D:225:LEU:HD11	1:D:233:ILE:CG1	2.47	0.42
1:D:63:ALA:O	1:D:67:ASP:HB2	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ILE:O	1:E:43:ILE:HG12	2.20	0.42
1:F:156:ARG:HG2	1:F:156:ARG:HH11	1.84	0.42
1:F:97:ILE:HD11	1:G:95:SER:CA	2.49	0.42
1:G:43:ILE:HG13	1:G:44:ILE:N	2.35	0.42
1:F:224:ARG:HD3	1:G:251:TRP:CE3	2.52	0.42
1:E:52:VAL:O	1:E:56:MET:HG2	2.19	0.42
1:G:124:LEU:HD12	1:G:124:LEU:HA	1.79	0.42
1:G:243:SER:O	1:G:244:GLY:C	2.58	0.42
1:B:97:ILE:HD13	1:B:97:ILE:HA	1.78	0.42
1:C:146:LEU:N	1:C:146:LEU:HD12	2.34	0.42
1:C:64:THR:O	1:C:68:PHE:HB2	2.20	0.42
1:D:128:ARG:NH1	1:D:131:ARG:HH21	2.18	0.42
1:E:204:ILE:HD12	1:E:266:ILE:CD1	2.50	0.42
1:E:64:THR:O	1:E:68:PHE:HB2	2.19	0.42
1:F:111:LEU:HA	1:F:111:LEU:HD12	1.75	0.42
1:F:231:SER:CB	1:F:272:GLN:H	2.33	0.42
1:G:215:ILE:CG2	1:G:239:VAL:HG13	2.43	0.42
1:A:85:ALA:O	1:A:89:VAL:HG23	2.19	0.42
1:B:156:ARG:CG	1:B:156:ARG:HH11	2.28	0.42
1:A:176:ILE:HD11	1:B:161:LYS:HB3	2.02	0.42
1:B:57:ILE:HG23	1:B:58:SER:N	2.35	0.42
1:D:83:ILE:CG1	1:D:96:VAL:HG11	2.49	0.42
1:E:129:PRO:CG	1:E:130:PHE:N	2.83	0.42
1:F:134:GLU:HG2	1:F:179:SER:HB2	2.02	0.42
1:G:128:ARG:CD	1:G:128:ARG:O	2.67	0.42
1:G:219:ARG:NH1	1:G:219:ARG:HG3	2.34	0.42
1:A:105:LEU:CD1	1:B:105:LEU:CD2	2.98	0.41
1:B:128:ARG:HA	1:B:129:PRO:HD3	1.79	0.41
1:C:118:LEU:HB2	1:C:151:PHE:CE2	2.55	0.41
1:D:112:GLN:HB3	1:D:112:GLN:HE21	1.55	0.41
1:E:215:ILE:HD13	1:E:239:VAL:HG21	2.01	0.41
1:F:216:LEU:HD12	1:F:241:SER:HA	2.01	0.41
1:A:246:LEU:HD23	1:A:246:LEU:C	2.40	0.41
1:B:201:VAL:HG11	1:B:235:PHE:CE2	2.55	0.41
1:D:124:LEU:O	1:D:128:ARG:CG	2.67	0.41
1:F:138:LEU:HD22	1:F:155:MET:CE	2.50	0.41
1:F:222:THR:HG21	1:G:251:TRP:CH2	2.55	0.41
1:C:191:GLY:HA2	1:C:234:ASN:HB3	2.02	0.41
1:G:128:ARG:CB	1:G:129:PRO:HD2	2.44	0.41
1:G:242:ASN:O	1:G:243:SER:C	2.58	0.41
1:A:120:ALA:HB1	1:A:171:ILE:HD12	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:ILE:HD12	1:E:221:MET:HE1	2.02	0.41
1:A:69:LEU:O	1:A:73:VAL:HG23	2.21	0.41
1:B:130:PHE:HA	1:B:134:GLU:OE1	2.21	0.41
1:B:216:LEU:HD13	1:B:241:SER:HA	2.02	0.41
1:C:112:GLN:HB3	1:C:112:GLN:HE21	1.61	0.41
1:B:123:LEU:HD11	1:C:151:PHE:CE1	2.56	0.41
1:C:146:LEU:HD11	1:C:156:ARG:HB3	2.01	0.41
1:C:52:VAL:O	1:C:56:MET:HG2	2.21	0.41
1:C:79:ALA:O	1:C:83:ILE:HG13	2.20	0.41
1:D:118:LEU:HD12	1:D:151:PHE:HE2	1.82	0.41
1:D:277:PHE:CZ	1:E:277:PHE:HZ	2.39	0.41
1:G:183:VAL:HG23	1:G:241:SER:C	2.40	0.41
1:A:273:MET:HE3	1:B:273:MET:CE	2.51	0.41
1:B:212:GLU:HG3	1:B:215:ILE:HG13	2.02	0.41
1:B:188:PHE:CZ	1:B:250:TYR:HA	2.56	0.41
1:B:57:ILE:CA	1:B:61:ILE:HB	2.38	0.41
1:C:204:ILE:HD12	1:C:266:ILE:CD1	2.51	0.41
1:D:141:VAL:HG23	1:D:141:VAL:O	2.21	0.41
1:F:97:ILE:HA	1:F:97:ILE:HD13	1.83	0.41
1:G:214:ARG:O	1:G:241:SER:HB3	2.21	0.41
1:G:208:ILE:HG23	1:G:256:ARG:NH1	2.36	0.41
1:A:75:TYR:O	1:A:78:ILE:HG12	2.20	0.41
1:B:256:ARG:HG2	1:B:256:ARG:HH11	1.86	0.41
1:C:215:ILE:HG23	1:C:239:VAL:HG13	2.03	0.41
1:D:191:GLY:HA2	1:D:234:ASN:HB3	2.01	0.41
1:F:74:ARG:O	1:F:78:ILE:HG23	2.20	0.41
1:A:40:VAL:HA	1:A:43:ILE:HD11	2.02	0.41
1:B:52:VAL:O	1:B:56:MET:HG2	2.20	0.41
1:C:131:ARG:O	1:C:132:ALA:C	2.58	0.41
1:C:97:ILE:HD13	1:C:97:ILE:HA	1.85	0.41
1:D:216:LEU:H	1:D:216:LEU:HD12	1.84	0.41
1:D:43:ILE:O	1:D:47:MET:HG3	2.21	0.41
1:E:107:VAL:O	1:E:111:LEU:HB2	2.21	0.41
1:E:233:ILE:HD12	1:F:258:LYS:HE2	2.03	0.41
1:G:162:ILE:HD12	1:G:162:ILE:HG23	1.78	0.41
1:A:39:ILE:O	1:A:43:ILE:HG12	2.21	0.41
1:E:128:ARG:HD3	1:E:128:ARG:C	2.34	0.41
1:G:120:ALA:O	1:G:124:LEU:HB2	2.21	0.41
1:A:176:ILE:HD11	1:B:161:LYS:HD2	2.03	0.41
1:A:95:SER:HB2	1:G:97:ILE:HD11	2.02	0.41
1:C:270:TYR:HB3	1:C:271:PRO:CD	2.50	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLY:HA3	1:D:106:ALA:HB2	2.02	0.41
1:D:228:LEU:HD12	1:D:228:LEU:HA	1.79	0.41
1:E:226:ASN:HB2	1:E:236:VAL:CG1	2.51	0.41
1:E:188:PHE:CE2	1:E:253:VAL:HB	2.55	0.41
1:F:215:ILE:O	1:F:217:LYS:HE3	2.20	0.41
1:A:181:GLU:HG3	1:A:182:PRO:CD	2.51	0.40
1:D:109:LEU:HD23	1:E:109:LEU:HD13	2.03	0.40
1:D:138:LEU:HD22	1:D:155:MET:HE1	2.03	0.40
1:E:162:ILE:HD13	1:E:162:ILE:HA	1.77	0.40
1:E:50:ASN:O	1:E:54:ARG:HG3	2.21	0.40
1:F:201:VAL:HG11	1:F:235:PHE:CD2	2.57	0.40
1:A:247:GLN:NE2	1:A:251:TRP:CD2	2.83	0.40
1:A:63:ALA:O	1:A:67:ASP:HB2	2.21	0.40
1:C:156:ARG:HG2	1:C:156:ARG:HH11	1.86	0.40
1:C:165:ILE:HA	1:C:166:PRO:HD3	1.92	0.40
1:C:28:ALA:O	1:C:32:VAL:HG23	2.21	0.40
1:F:232:SER:OG	1:F:234:ASN:ND2	2.54	0.40
1:G:131:ARG:O	1:G:132:ALA:C	2.59	0.40
1:G:167:ASN:ND2	1:G:167:ASN:N	2.68	0.40
1:G:267:SER:O	1:G:269:PRO:HD3	2.21	0.40
1:A:247:GLN:NE2	1:A:251:TRP:CE2	2.90	0.40
1:B:165:ILE:HG21	1:B:170:ILE:HG12	2.03	0.40
1:B:180:ARG:CD	1:C:162:ILE:HG21	2.21	0.40
1:C:188:PHE:CZ	1:C:250:TYR:HA	2.57	0.40
1:D:163:ILE:HG22	1:D:165:ILE:HG13	2.04	0.40
1:E:228:LEU:HA	1:E:228:LEU:HD12	1.80	0.40
1:F:228:LEU:HD12	1:F:228:LEU:HA	1.91	0.40
1:A:216:LEU:CD1	1:A:241:SER:HA	2.51	0.40
1:B:123:LEU:HD11	1:C:114:SER:HB3	2.04	0.40
1:B:239:VAL:HG12	1:B:239:VAL:O	2.20	0.40
1:C:63:ALA:O	1:C:67:ASP:HB2	2.21	0.40
1:D:157:THR:HG23	1:D:161:LYS:H	1.85	0.40
1:E:138:LEU:HD22	1:E:155:MET:CE	2.52	0.40
1:F:138:LEU:CD1	1:F:138:LEU:N	2.84	0.40
1:F:34:ALA:O	1:F:38:ILE:HG13	2.21	0.40
1:A:162:ILE:HG22	1:A:162:ILE:O	2.21	0.40
1:A:216:LEU:HD13	1:A:241:SER:HA	2.03	0.40
1:B:156:ARG:CG	1:B:156:ARG:NH1	2.84	0.40
1:B:64:THR:O	1:B:68:PHE:HB2	2.21	0.40
1:D:83:ILE:HD13	1:D:96:VAL:CG1	2.52	0.40
1:E:112:GLN:O	1:E:116:SER:HB2	2.22	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:ALA:O	1:F:67:ASP:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	252/306 (82%)	228 (90%)	16 (6%)	8 (3%)	5	40
1	B	252/306 (82%)	227 (90%)	19 (8%)	6 (2%)	7	46
1	C	252/306 (82%)	226 (90%)	19 (8%)	7 (3%)	6	43
1	D	252/306 (82%)	227 (90%)	19 (8%)	6 (2%)	7	46
1	E	252/306 (82%)	229 (91%)	18 (7%)	5 (2%)	9	50
1	F	252/306 (82%)	233 (92%)	14 (6%)	5 (2%)	9	50
1	G	252/306 (82%)	229 (91%)	17 (7%)	6 (2%)	7	46
All	All	1764/2142 (82%)	1599 (91%)	122 (7%)	43 (2%)	7	46

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	VAL
1	A	182	PRO
1	B	141	VAL
1	C	141	VAL
1	D	141	VAL
1	D	182	PRO
1	E	141	VAL
1	F	141	VAL
1	G	141	VAL
1	A	59	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	229	GLY
1	B	59	ARG
1	C	59	ARG
1	D	59	ARG
1	D	229	GLY
1	E	59	ARG
1	E	182	PRO
1	F	59	ARG
1	G	59	ARG
1	A	243	SER
1	B	129	PRO
1	D	243	SER
1	E	243	SER
1	G	129	PRO
1	B	214	ARG
1	C	182	PRO
1	G	214	ARG
1	G	243	SER
1	B	132	ALA
1	B	243	SER
1	C	129	PRO
1	C	214	ARG
1	C	229	GLY
1	C	243	SER
1	D	181	GLU
1	E	129	PRO
1	F	243	SER
1	G	182	PRO
1	A	214	ARG
1	A	220	GLU
1	F	132	ALA
1	A	129	PRO
1	F	129	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	206/248 (83%)	193 (94%)	13 (6%)	21	60
1	B	206/248 (83%)	193 (94%)	13 (6%)	21	60
1	C	206/248 (83%)	195 (95%)	11 (5%)	26	65
1	D	206/248 (83%)	191 (93%)	15 (7%)	16	55
1	E	206/248 (83%)	191 (93%)	15 (7%)	16	55
1	F	206/248 (83%)	190 (92%)	16 (8%)	15	52
1	G	206/248 (83%)	191 (93%)	15 (7%)	16	55
All	All	1442/1736 (83%)	1344 (93%)	98 (7%)	18	58

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	80	PHE
1	A	96	VAL
1	A	128	ARG
1	A	131	ARG
1	A	138	LEU
1	A	150	ILE
1	A	157	THR
1	A	176	ILE
1	A	232	SER
1	A	234	ASN
1	A	241	SER
1	A	273	MET
1	B	50	ASN
1	B	80	PHE
1	B	96	VAL
1	B	112	GLN
1	B	131	ARG
1	B	150	ILE
1	B	157	THR
1	B	171	ILE
1	B	228	LEU
1	B	232	SER
1	B	234	ASN
1	B	241	SER
1	B	273	MET
1	C	50	ASN
1	C	80	PHE
1	C	88	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	96	VAL
1	C	111	LEU
1	C	112	GLN
1	C	131	ARG
1	C	228	LEU
1	C	234	ASN
1	C	239	VAL
1	C	273	MET
1	D	50	ASN
1	D	80	PHE
1	D	88	ARG
1	D	96	VAL
1	D	112	GLN
1	D	128	ARG
1	D	131	ARG
1	D	150	ILE
1	D	157	THR
1	D	171	ILE
1	D	176	ILE
1	D	181	GLU
1	D	232	SER
1	D	234	ASN
1	D	273	MET
1	E	50	ASN
1	E	80	PHE
1	E	88	ARG
1	E	96	VAL
1	E	112	GLN
1	E	128	ARG
1	E	131	ARG
1	E	157	THR
1	E	171	ILE
1	E	228	LEU
1	E	232	SER
1	E	234	ASN
1	E	239	VAL
1	E	241	SER
1	E	273	MET
1	F	50	ASN
1	F	80	PHE
1	F	88	ARG
1	F	96	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	112	GLN
1	F	128	ARG
1	F	131	ARG
1	F	150	ILE
1	F	157	THR
1	F	176	ILE
1	F	228	LEU
1	F	232	SER
1	F	234	ASN
1	F	239	VAL
1	F	241	SER
1	F	273	MET
1	G	50	ASN
1	G	80	PHE
1	G	88	ARG
1	G	96	VAL
1	G	111	LEU
1	G	112	GLN
1	G	128	ARG
1	G	131	ARG
1	G	150	ILE
1	G	157	THR
1	G	228	LEU
1	G	234	ASN
1	G	239	VAL
1	G	241	SER
1	G	273	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	112	GLN
1	A	167	ASN
1	A	234	ASN
1	A	272	GLN
1	B	50	ASN
1	B	112	GLN
1	B	167	ASN
1	B	234	ASN
1	B	272	GLN
1	C	50	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	112	GLN
1	C	167	ASN
1	C	272	GLN
1	D	50	ASN
1	D	112	GLN
1	D	167	ASN
1	D	272	GLN
1	E	50	ASN
1	E	112	GLN
1	E	167	ASN
1	E	234	ASN
1	E	272	GLN
1	F	50	ASN
1	F	112	GLN
1	F	167	ASN
1	F	234	ASN
1	F	272	GLN
1	G	50	ASN
1	G	112	GLN
1	G	167	ASN
1	G	272	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 carbohydrates 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

### 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	254/306 (83%)	-0.22	2 (0%) 86 77	49, 93, 232, 245	0
1	B	254/306 (83%)	-0.16	7 (2%) 53 41	57, 92, 234, 245	0
1	C	254/306 (83%)	-0.10	9 (3%) 44 33	58, 98, 233, 244	0
1	D	254/306 (83%)	-0.11	5 (1%) 65 53	54, 96, 238, 247	0
1	E	254/306 (83%)	-0.05	7 (2%) 53 41	53, 96, 234, 246	0
1	F	254/306 (83%)	0.16	20 (7%) 13 10	44, 85, 237, 249	0
1	G	254/306 (83%)	-0.24	1 (0%) 92 88	47, 86, 234, 244	0
All	All	1778/2142 (83%)	-0.10	51 (2%) 52 39	44, 93, 237, 249	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	58	SER	8.6
1	F	63	ALA	5.9
1	F	57	ILE	5.2
1	D	42	LEU	4.8
1	F	59	ARG	4.6
1	C	51	ALA	4.5
1	C	56	MET	4.3
1	F	43	ILE	4.0
1	D	45	ALA	4.0
1	B	279	ARG	4.0
1	E	130	PHE	3.9
1	F	60	LYS	3.9
1	C	55	LEU	3.8
1	C	52	VAL	3.8
1	F	73	VAL	3.8
1	D	38	ILE	3.8
1	D	41	GLY	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	280	VAL	3.3
1	B	278	LYS	2.9
1	D	162	ILE	2.8
1	F	69	LEU	2.8
1	F	280	VAL	2.8
1	F	61	ILE	2.8
1	C	65	VAL	2.7
1	F	279	ARG	2.7
1	G	42	LEU	2.7
1	F	67	ASP	2.6
1	E	131	ARG	2.5
1	E	57	ILE	2.5
1	F	48	ILE	2.5
1	C	92	GLN	2.4
1	F	44	ILE	2.4
1	C	91	VAL	2.3
1	F	170	ILE	2.2
1	C	177	ASN	2.2
1	B	180	ARG	2.2
1	B	277	PHE	2.2
1	A	280	VAL	2.2
1	C	130	PHE	2.2
1	B	226	ASN	2.1
1	B	65	VAL	2.1
1	F	77	ILE	2.1
1	E	39	ILE	2.1
1	F	53	ASN	2.1
1	F	47	MET	2.1
1	E	92	GLN	2.1
1	F	55	LEU	2.1
1	A	266	ILE	2.0
1	E	279	ARG	2.0
1	F	64	THR	2.0
1	E	280	VAL	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 [i](#)

There are no carbohydrates 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.