



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 10:22 PM EDT

PDB ID : 3NO1  
Title : Crystal Structure of Mandelate racemase/muconate lactonizing enzyme from a Marine actinobacterium in complex with magnesium  
Authors : Satyanarayana, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2010-06-24  
Resolution : 2.16 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

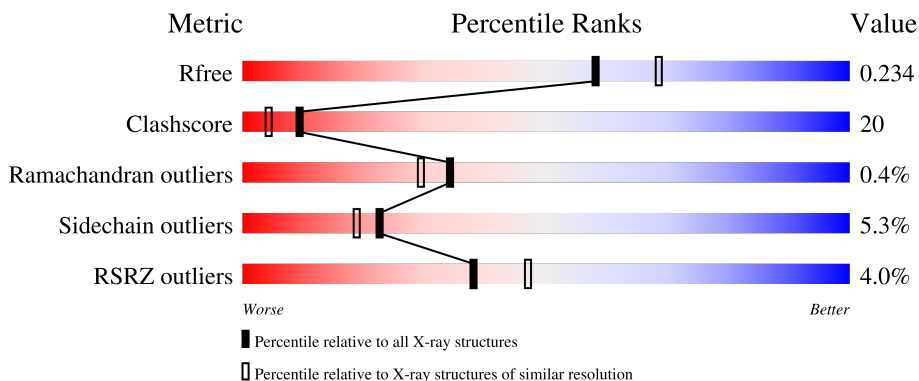
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 2.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



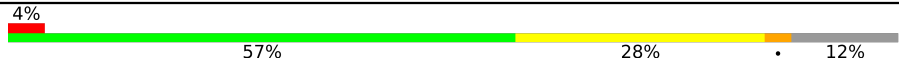
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	398	
1	B	398	
1	C	398	
1	D	398	
1	E	398	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	398	 <p>A horizontal bar chart showing the quality distribution of the chain. The bar is divided into four segments: a small red segment (4%), a large green segment (57%), a yellow segment (28%), and a small grey segment (12%).</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17170 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 Mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	355	2782	1757	488	522	5	10	0	0	0
1	B	349	2734	1726	477	516	5	10	0	0	0
1	C	357	2792	1762	490	525	5	10	0	0	0
1	D	350	2745	1732	481	517	5	10	0	0	0
1	E	353	2762	1742	484	521	5	10	0	0	0
1	F	349	2723	1718	476	514	5	10	0	0	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP A4AFX2
A	0	SER	-	expression tag	UNP A4AFX2
A	1	LEU	-	expression tag	UNP A4AFX2
A	389	GLU	-	expression tag	UNP A4AFX2
A	390	GLY	-	expression tag	UNP A4AFX2
A	391	HIS	-	expression tag	UNP A4AFX2
A	392	HIS	-	expression tag	UNP A4AFX2
A	393	HIS	-	expression tag	UNP A4AFX2
A	394	HIS	-	expression tag	UNP A4AFX2
A	395	HIS	-	expression tag	UNP A4AFX2
A	396	HIS	-	expression tag	UNP A4AFX2
B	-1	MSE	-	expression tag	UNP A4AFX2
B	0	SER	-	expression tag	UNP A4AFX2
B	1	LEU	-	expression tag	UNP A4AFX2
B	389	GLU	-	expression tag	UNP A4AFX2
B	390	GLY	-	expression tag	UNP A4AFX2
B	391	HIS	-	expression tag	UNP A4AFX2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	392	HIS	-	expression tag	UNP A4AFX2
B	393	HIS	-	expression tag	UNP A4AFX2
B	394	HIS	-	expression tag	UNP A4AFX2
B	395	HIS	-	expression tag	UNP A4AFX2
B	396	HIS	-	expression tag	UNP A4AFX2
C	-1	MSE	-	expression tag	UNP A4AFX2
C	0	SER	-	expression tag	UNP A4AFX2
C	1	LEU	-	expression tag	UNP A4AFX2
C	389	GLU	-	expression tag	UNP A4AFX2
C	390	GLY	-	expression tag	UNP A4AFX2
C	391	HIS	-	expression tag	UNP A4AFX2
C	392	HIS	-	expression tag	UNP A4AFX2
C	393	HIS	-	expression tag	UNP A4AFX2
C	394	HIS	-	expression tag	UNP A4AFX2
C	395	HIS	-	expression tag	UNP A4AFX2
C	396	HIS	-	expression tag	UNP A4AFX2
D	-1	MSE	-	expression tag	UNP A4AFX2
D	0	SER	-	expression tag	UNP A4AFX2
D	1	LEU	-	expression tag	UNP A4AFX2
D	389	GLU	-	expression tag	UNP A4AFX2
D	390	GLY	-	expression tag	UNP A4AFX2
D	391	HIS	-	expression tag	UNP A4AFX2
D	392	HIS	-	expression tag	UNP A4AFX2
D	393	HIS	-	expression tag	UNP A4AFX2
D	394	HIS	-	expression tag	UNP A4AFX2
D	395	HIS	-	expression tag	UNP A4AFX2
D	396	HIS	-	expression tag	UNP A4AFX2
E	-1	MSE	-	expression tag	UNP A4AFX2
E	0	SER	-	expression tag	UNP A4AFX2
E	1	LEU	-	expression tag	UNP A4AFX2
E	389	GLU	-	expression tag	UNP A4AFX2
E	390	GLY	-	expression tag	UNP A4AFX2
E	391	HIS	-	expression tag	UNP A4AFX2
E	392	HIS	-	expression tag	UNP A4AFX2
E	393	HIS	-	expression tag	UNP A4AFX2
E	394	HIS	-	expression tag	UNP A4AFX2
E	395	HIS	-	expression tag	UNP A4AFX2
E	396	HIS	-	expression tag	UNP A4AFX2
F	-1	MSE	-	expression tag	UNP A4AFX2
F	0	SER	-	expression tag	UNP A4AFX2
F	1	LEU	-	expression tag	UNP A4AFX2
F	389	GLU	-	expression tag	UNP A4AFX2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	390	GLY	-	expression tag	UNP A4AFX2
F	391	HIS	-	expression tag	UNP A4AFX2
F	392	HIS	-	expression tag	UNP A4AFX2
F	393	HIS	-	expression tag	UNP A4AFX2
F	394	HIS	-	expression tag	UNP A4AFX2
F	395	HIS	-	expression tag	UNP A4AFX2
F	396	HIS	-	expression tag	UNP A4AFX2

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

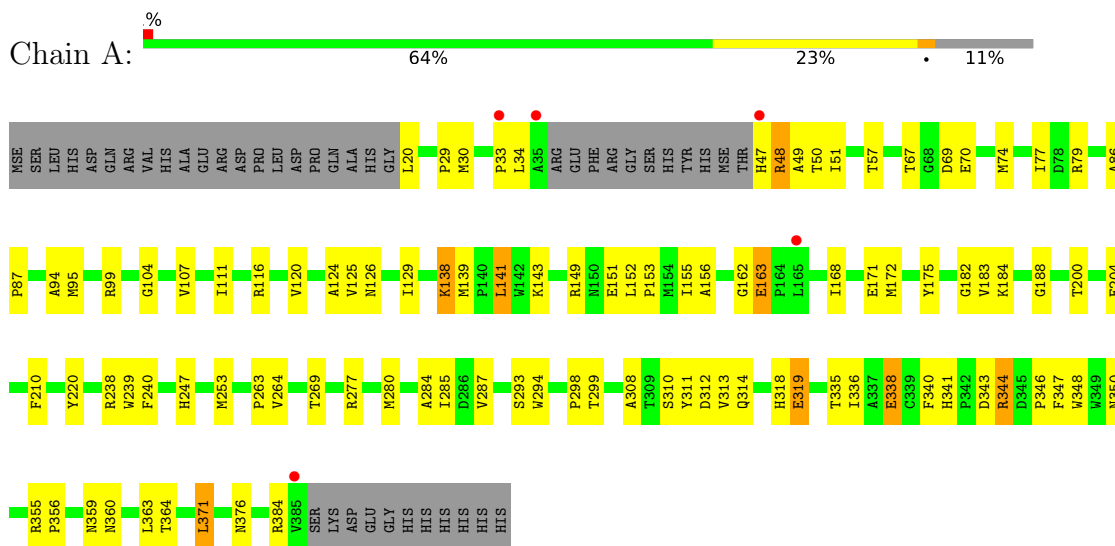
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	137	Total O 137 137	0	0
3	B	84	Total O 84 84	0	0
3	C	136	Total O 136 136	0	0
3	D	88	Total O 88 88	0	0
3	E	80	Total O 80 80	0	0
3	F	101	Total O 101 101	0	0

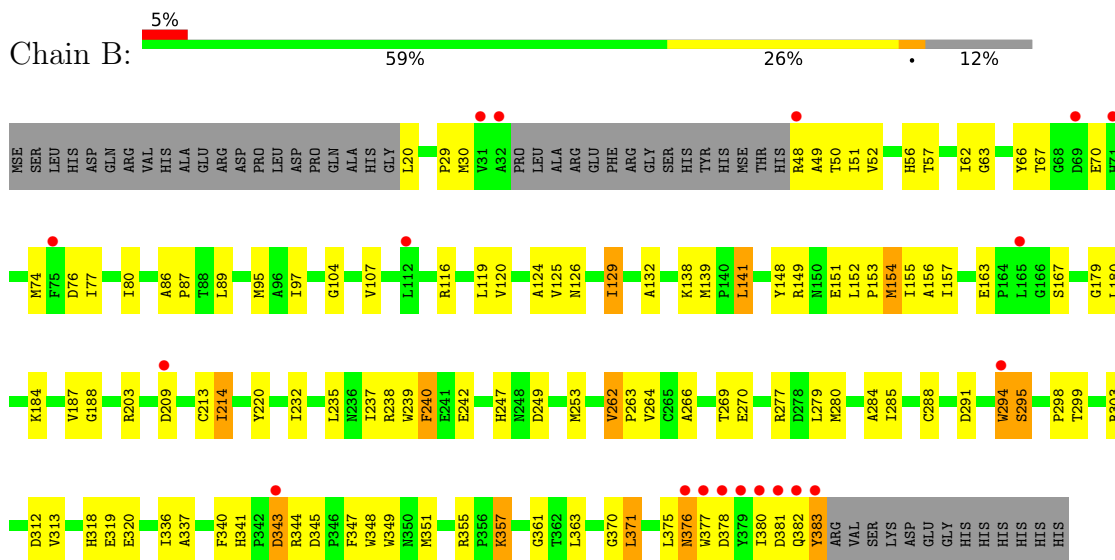
### 3 Residue-property plots [i](#)

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

- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

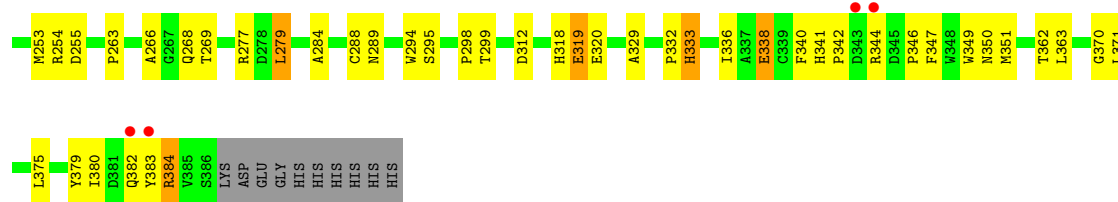


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

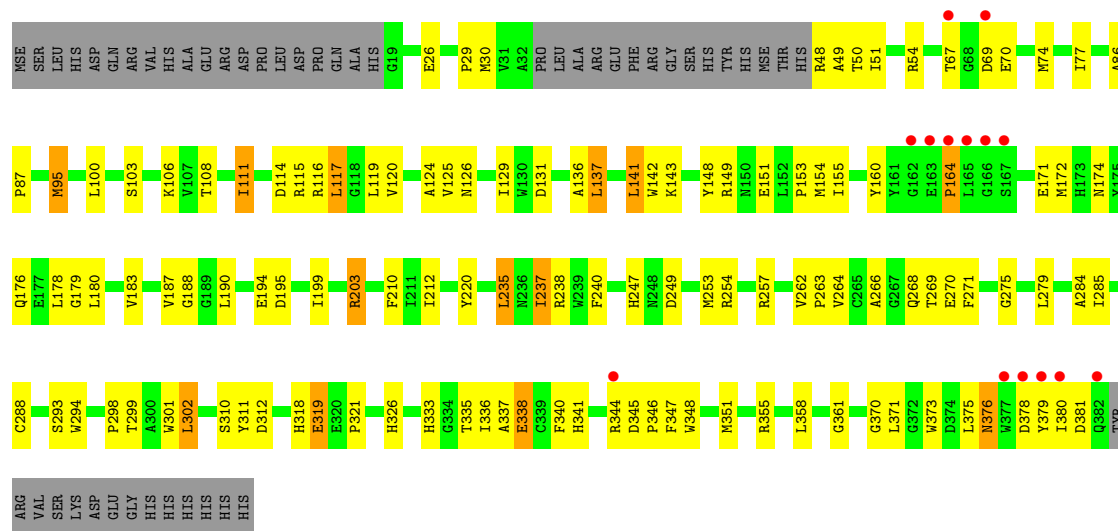








• Molecule 1: Mandelate racemase/muconate lactonizing enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.96Å 90.10Å 94.66Å 115.80° 109.75° 97.58°	Depositor
Resolution (Å)	42.51 – 2.16 42.51 – 2.16	Depositor EDS
% Data completeness (in resolution range)	96.0 (42.51-2.16) 96.1 (42.51-2.16)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.97 (at 2.16Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.207 , 0.240 0.202 , 0.234	Depositor DCC
$R_{free}$ test set	4670 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtrriage
Anisotropy	0.271	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17170	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0/2841	0.63	0/3851
1	B	0.33	0/2791	0.64	0/3782
1	C	0.34	0/2851	0.63	0/3864
1	D	0.33	0/2802	0.63	0/3796
1	E	0.32	0/2819	0.62	0/3819
1	F	0.36	0/2779	0.65	0/3765
All	All	0.34	0/16883	0.63	0/22877

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2782	0	2685	108	0
1	B	2734	0	2632	127	0
1	C	2792	0	2692	84	0
1	D	2745	0	2645	106	0
1	E	2762	0	2662	129	0
1	F	2723	0	2622	113	0
2	A	1	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	137	0	0	5	0
3	B	84	0	0	8	0
3	C	136	0	0	5	0
3	D	88	0	0	8	0
3	E	80	0	0	4	0
3	F	101	0	0	3	0
All	All	17170	0	15938	640	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 20.

All (640) 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:253:MSE:HE3	1:A:264:VAL:HG12	1.32	1.07
1:F:30:MSE:HE1	1:F:380:ILE:HG23	1.34	1.05
1:A:253:MSE:HE3	1:A:264:VAL:CG1	1.86	1.05
1:A:280:MSE:HE2	1:A:311:TYR:HB2	1.40	1.04
1:F:253:MSE:HE3	1:F:264:VAL:CG1	1.90	1.01
1:E:168:ILE:HD12	1:E:168:ILE:H	1.23	1.00
1:A:280:MSE:HE3	1:A:313:VAL:HB	1.42	0.99
1:A:280:MSE:CE	1:A:308:ALA:HA	1.94	0.98
1:A:280:MSE:HE1	1:A:308:ALA:HA	1.03	0.98
1:E:95:MSE:HE2	1:E:133:VAL:HG22	1.48	0.95
1:E:153:PRO:HG2	1:E:336:ILE:HG22	1.49	0.95
1:F:253:MSE:HE3	1:F:264:VAL:HG12	1.47	0.94
1:E:250:LYS:HG2	1:E:279:LEU:HD12	1.51	0.92
1:F:253:MSE:CE	1:F:285:ILE:HG22	2.01	0.90
1:B:253:MSE:HE3	1:B:264:VAL:CG1	2.02	0.90
1:B:341:HIS:HD1	1:B:343:ASP:H	1.18	0.88
1:F:30:MSE:H	1:F:74:MSE:HE1	1.37	0.88
1:B:253:MSE:HE1	1:B:285:ILE:HG22	1.53	0.86
1:C:303:ARG:O	1:C:307:ILE:HD13	1.74	0.86
1:C:384:ARG:HD3	3:C:423:HOH:O	1.74	0.86
1:E:351:MSE:HE3	1:E:375:LEU:HD22	1.56	0.86
1:E:277:ARG:HD2	1:F:311:TYR:CE2	2.11	0.86

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:ILE:HD12	1:F:111:ILE:H	1.38	0.85
1:B:163:GLU:OE1	1:B:167:SER:HA	1.76	0.85
1:B:348:TRP:O	1:B:355:ARG:HD3	1.76	0.85
1:A:280:MSE:HE1	1:A:308:ALA:CA	1.99	0.85
1:A:253:MSE:CE	1:A:285:ILE:HG22	2.06	0.84
1:A:20:LEU:HD12	1:A:20:LEU:O	1.78	0.83
1:A:253:MSE:HE2	1:A:285:ILE:HG22	1.59	0.83
1:F:253:MSE:HE1	1:F:285:ILE:HG22	1.59	0.83
1:E:155:ILE:HD12	1:E:336:ILE:HD13	1.59	0.82
1:B:277:ARG:HG2	1:B:277:ARG:HH11	1.44	0.82
1:D:204:GLU:HG2	3:D:420:HOH:O	1.79	0.82
1:B:156:ALA:HB2	1:B:180:LEU:HD13	1.62	0.82
1:B:253:MSE:HE3	1:B:264:VAL:HG12	1.60	0.80
1:E:67:THR:HG21	1:E:124:ALA:HA	1.64	0.80
1:F:30:MSE:CE	1:F:380:ILE:HG23	2.11	0.80
1:A:280:MSE:HE3	1:A:313:VAL:CB	2.12	0.80
1:F:103:SER:O	1:F:106:LYS:HE3	1.81	0.80
1:A:280:MSE:HE2	1:A:311:TYR:CB	2.11	0.80
1:E:277:ARG:HG2	1:E:277:ARG:HH11	1.46	0.79
1:A:50:THR:O	1:A:74:MSE:HE1	1.83	0.79
1:B:125:VAL:O	1:B:129:ILE:HG23	1.83	0.79
1:F:253:MSE:HE3	1:F:264:VAL:HG11	1.66	0.78
1:D:351:MSE:HE2	1:D:375:LEU:HD22	1.66	0.78
1:A:253:MSE:CE	1:A:264:VAL:HG12	2.12	0.78
1:B:253:MSE:CE	1:B:285:ILE:HG22	2.13	0.78
1:C:50:THR:N	1:C:74:MSE:HE1	2.00	0.77
1:A:153:PRO:HG2	1:A:336:ILE:HD12	1.66	0.77
1:E:235:LEU:HB2	1:E:237:ILE:HD11	1.66	0.77
1:F:29:PRO:HA	1:F:74:MSE:HE2	1.66	0.76
1:F:142:TRP:H	1:F:326:HIS:HD2	1.34	0.76
1:D:253:MSE:CE	1:D:285:ILE:HG23	2.16	0.76
1:E:151:GLU:HG2	1:E:362:THR:HG21	1.68	0.76
1:A:280:MSE:CE	1:A:311:TYR:HB2	2.15	0.76
1:A:67:THR:HG22	3:A:432:HOH:O	1.85	0.76
1:D:376:ASN:HD21	1:D:378:ASP:HB2	1.51	0.75
1:E:30:MSE:HE2	1:E:347:PHE:HE1	1.51	0.75
1:A:311:TYR:CE2	1:B:277:ARG:HD2	2.22	0.74
1:F:126:ASN:HD22	1:F:298:PRO:HD2	1.52	0.74
1:A:139:MSE:HE1	1:B:95:MSE:HG3	1.69	0.74
1:A:344:ARG:O	1:A:344:ARG:HD3	1.87	0.74
1:F:48:ARG:HG2	1:F:347:PHE:CE2	2.21	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:THR:HG22	1:F:119:LEU:HD12	1.70	0.73
1:A:280:MSE:CE	1:A:313:VAL:HB	2.17	0.73
1:D:253:MSE:HE3	1:D:285:ILE:HG23	1.69	0.73
1:D:190:LEU:HD23	1:D:194:GLU:HG2	1.71	0.72
1:E:95:MSE:CE	1:E:133:VAL:HG22	2.19	0.72
1:D:89:LEU:HD11	1:D:125:VAL:HG11	1.71	0.72
1:E:114:ASP:HB3	1:E:117:LEU:CD2	2.19	0.72
1:B:89:LEU:HD11	1:B:125:VAL:HG11	1.71	0.72
1:D:153:PRO:HG2	1:D:336:ILE:CD1	2.20	0.71
1:C:89:LEU:HD11	1:C:125:VAL:HG11	1.72	0.71
1:A:253:MSE:HE2	1:A:285:ILE:CG2	2.21	0.71
1:A:153:PRO:HG2	1:A:336:ILE:CD1	2.19	0.71
1:A:247:HIS:HE1	1:F:312:ASP:OD1	1.73	0.71
1:B:235:LEU:HB2	1:B:237:ILE:HD11	1.71	0.71
1:F:253:MSE:HE2	1:F:285:ILE:HG22	1.71	0.71
1:F:253:MSE:CE	1:F:264:VAL:HG12	2.19	0.71
1:C:250:LYS:HG2	1:C:279:LEU:HD12	1.73	0.70
1:F:174:ASN:HD21	1:F:341:HIS:HE2	1.39	0.69
1:B:253:MSE:HE3	1:B:264:VAL:HG11	1.74	0.69
1:B:344:ARG:HG2	1:B:344:ARG:HH11	1.57	0.69
1:C:336:ILE:HD11	3:C:501:HOH:O	1.91	0.69
1:E:126:ASN:HD21	1:E:299:THR:H	1.39	0.68
1:F:344:ARG:NH1	1:F:344:ARG:HB2	2.09	0.68
1:D:322:GLN:HG2	1:D:323:VAL:HG23	1.74	0.68
1:B:242:GLU:HG3	3:B:454:HOH:O	1.94	0.68
1:C:156:ALA:HB2	1:C:180:LEU:HD13	1.76	0.68
1:F:180:LEU:HD13	1:F:358:LEU:HD21	1.75	0.68
1:A:311:TYR:CZ	1:B:277:ARG:HD2	2.28	0.68
1:B:188:GLY:HA2	1:B:220:TYR:CZ	2.29	0.68
1:D:168:ILE:HG12	3:D:445:HOH:O	1.94	0.68
1:E:344:ARG:HG2	1:E:344:ARG:HH11	1.59	0.68
1:E:89:LEU:HD11	1:E:125:VAL:HG11	1.75	0.68
1:E:250:LYS:HG2	1:E:279:LEU:CD1	2.23	0.67
1:A:341:HIS:HD1	1:A:343:ASP:H	1.42	0.67
1:B:347:PHE:O	1:B:351:MSE:HB2	1.95	0.67
1:D:116:ARG:HD2	1:D:294:TRP:CD1	2.30	0.67
1:C:250:LYS:HG2	1:C:279:LEU:CD1	2.25	0.67
1:B:141:LEU:HD22	1:B:370:GLY:C	2.15	0.67
1:F:30:MSE:HE2	1:F:381:ASP:N	2.09	0.67
1:F:340:PHE:HB3	1:F:344:ARG:HG3	1.77	0.67
1:F:153:PRO:HG2	1:F:336:ILE:HD12	1.77	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:LEU:HD23	1:D:371:LEU:HD22	1.77	0.66
1:A:188:GLY:HA2	1:A:220:TYR:CZ	2.30	0.66
1:B:30:MSE:SE	3:B:455:HOH:O	2.63	0.66
1:B:97:ILE:HG12	1:B:129:ILE:HD11	1.77	0.66
1:C:48:ARG:HG3	1:C:48:ARG:HH11	1.60	0.66
1:D:131:ASP:HB2	1:D:371:LEU:HD23	1.77	0.66
1:E:50:THR:N	1:E:74:MSE:HE1	2.10	0.66
1:E:163:GLU:OE1	1:E:167:SER:HA	1.96	0.66
1:A:95:MSE:HE3	1:B:139:MSE:SE	2.46	0.66
1:F:270:GLU:OE1	1:F:279:LEU:HD21	1.96	0.66
1:F:50:THR:O	1:F:74:MSE:HE1	1.96	0.66
1:F:114:ASP:HB3	1:F:117:LEU:HD22	1.77	0.65
1:D:141:LEU:CD2	1:D:371:LEU:HD22	2.27	0.65
1:E:154:MSE:HE1	1:E:363:LEU:HD13	1.78	0.64
1:B:141:LEU:HD23	1:B:371:LEU:HD13	1.78	0.64
1:B:155:ILE:HG23	1:B:336:ILE:HG21	1.79	0.64
1:F:67:THR:OG1	1:F:293:SER:HB2	1.98	0.64
1:E:30:MSE:HE2	1:E:347:PHE:CE1	2.32	0.64
1:B:30:MSE:HE1	1:B:351:MSE:SE	2.48	0.64
1:E:174:ASN:HD21	1:E:341:HIS:HE2	1.46	0.64
1:B:247:HIS:HE1	1:C:312:ASP:OD1	1.80	0.63
1:C:162:GLY:C	1:C:163:GLU:HG2	2.18	0.63
1:F:131:ASP:HB2	1:F:371:LEU:HD23	1.79	0.63
1:B:312:ASP:OD1	1:E:247:HIS:HE1	1.82	0.63
1:C:188:GLY:HA2	1:C:220:TYR:CZ	2.34	0.63
1:B:340:PHE:HB2	1:B:345:ASP:HB3	1.80	0.63
1:C:253:MSE:HE3	1:C:285:ILE:HG23	1.81	0.63
1:E:336:ILE:HD12	1:E:336:ILE:O	1.98	0.63
1:B:238:ARG:O	1:B:263:PRO:HG2	1.98	0.63
1:D:195:ASP:O	1:D:199:ILE:HG12	1.99	0.63
1:A:253:MSE:HE3	1:A:264:VAL:HG11	1.76	0.63
1:E:99:ARG:HG3	1:F:148:TYR:O	1.98	0.63
1:F:171:GLU:HG2	1:F:172:MSE:HE2	1.81	0.63
1:B:270:GLU:OE1	1:B:279:LEU:HD21	1.98	0.63
1:F:48:ARG:HD2	1:F:346:PRO:HD2	1.81	0.63
1:F:238:ARG:O	1:F:263:PRO:HG2	1.99	0.63
1:E:86:ALA:O	1:E:90:ILE:HG12	1.98	0.62
1:D:383:TYR:HB3	3:D:401:HOH:O	2.00	0.62
1:F:30:MSE:HE2	1:F:381:ASP:H	1.64	0.62
1:F:346:PRO:HB2	1:F:379:TYR:OH	1.99	0.62
1:B:153:PRO:HG2	1:B:336:ILE:HG12	1.81	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:ARG:HG2	1:B:344:ARG:NH1	2.14	0.62
1:C:200:THR:O	1:C:204:GLU:HG2	1.99	0.62
1:D:151:GLU:OE1	1:D:362:THR:HG21	1.99	0.62
1:E:235:LEU:HB2	1:E:237:ILE:CD1	2.28	0.62
1:C:86:ALA:HB3	1:C:87:PRO:HD3	1.82	0.62
1:E:151:GLU:CG	1:E:362:THR:HG21	2.30	0.62
1:C:376:ASN:HD21	1:C:378:ASP:HB2	1.65	0.61
1:A:20:LEU:HD11	1:A:94:ALA:HB3	1.82	0.61
1:F:126:ASN:HD21	1:F:299:THR:H	1.47	0.61
1:E:277:ARG:HH11	1:E:277:ARG:CG	2.14	0.61
1:D:141:LEU:HD22	1:D:370:GLY:C	2.21	0.61
1:F:155:ILE:HD11	1:F:338:GLU:HB3	1.83	0.61
1:F:348:TRP:O	1:F:355:ARG:HD3	2.00	0.61
1:A:30:MSE:H	1:A:74:MSE:HE1	1.65	0.61
1:C:48:ARG:HG2	1:C:347:PHE:CE2	2.35	0.61
1:A:277:ARG:HH12	1:E:248:ASN:HD22	1.50	0.60
1:E:268:GLN:HE21	1:E:289:ASN:HD21	1.46	0.60
1:F:253:MSE:HE2	1:F:285:ILE:CG2	2.31	0.60
1:D:126:ASN:HD21	1:D:299:THR:H	1.49	0.60
1:E:103:SER:O	1:E:106:LYS:HG2	2.01	0.60
1:B:214:ILE:HD12	1:B:237:ILE:HG21	1.82	0.60
1:D:153:PRO:HG2	1:D:336:ILE:HD12	1.82	0.60
1:E:30:MSE:HB3	1:E:384:ARG:HA	1.84	0.60
1:E:27:THR:HG21	1:E:78:ASP:OD1	2.01	0.60
1:B:235:LEU:HB2	1:B:237:ILE:CD1	2.31	0.60
1:A:126:ASN:HD21	1:A:299:THR:H	1.49	0.59
1:D:187:VAL:HG11	1:D:199:ILE:HD11	1.84	0.59
1:E:27:THR:CG2	1:E:82:HIS:NE2	2.65	0.59
1:F:154:MSE:HE1	1:F:321:PRO:HB3	1.83	0.59
1:A:253:MSE:HE1	1:A:285:ILE:HG22	1.85	0.59
1:E:200:THR:O	1:E:204:GLU:HG2	2.02	0.59
1:B:253:MSE:CE	1:B:285:ILE:CG2	2.79	0.59
1:E:168:ILE:H	1:E:168:ILE:CD1	1.99	0.59
1:C:247:HIS:HE1	1:E:312:ASP:OD1	1.86	0.59
1:E:344:ARG:HG2	1:E:344:ARG:NH1	2.17	0.59
1:B:29:PRO:O	1:B:383:TYR:HB3	2.02	0.59
1:B:277:ARG:HH11	1:B:277:ARG:CG	2.13	0.59
1:E:141:LEU:CD2	1:E:370:GLY:HA2	2.33	0.59
1:E:277:ARG:HD3	1:F:310:SER:OG	2.02	0.59
1:B:20:LEU:HB2	1:B:95:MSE:CE	2.33	0.59
1:B:119:LEU:HB3	1:B:295:SER:HA	1.85	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:ILE:HD11	1:E:338:GLU:HB2	1.84	0.58
1:C:139:MSE:HE1	1:D:95:MSE:HG3	1.85	0.58
1:D:312:ASP:OD1	1:F:247:HIS:HE1	1.87	0.58
1:F:30:MSE:H	1:F:74:MSE:CE	2.11	0.58
1:A:200:THR:O	1:A:204:GLU:HG2	2.04	0.58
1:D:48:ARG:HG3	1:D:347:PHE:CE2	2.38	0.58
1:F:48:ARG:HG2	1:F:347:PHE:HE2	1.65	0.58
1:B:56:HIS:ND1	1:B:62:ILE:HD12	2.19	0.58
1:F:149:ARG:HD2	1:F:151:GLU:O	2.04	0.58
1:B:380:ILE:HA	3:B:455:HOH:O	2.03	0.58
1:F:351:MSE:HE2	1:F:375:LEU:HG	1.85	0.58
1:C:357:LYS:HD2	3:C:466:HOH:O	2.03	0.58
1:C:49:ALA:HB1	1:C:74:MSE:HE1	1.86	0.58
1:E:114:ASP:HB3	1:E:117:LEU:HD22	1.85	0.58
1:E:155:ILE:HD13	1:E:155:ILE:H	1.69	0.58
1:A:20:LEU:HD13	1:A:57:THR:CG2	2.33	0.57
1:F:160:TYR:HB2	1:F:164:PRO:HG3	1.85	0.57
1:B:214:ILE:HD13	1:B:239:TRP:O	2.03	0.57
1:A:126:ASN:HD22	1:A:298:PRO:HD2	1.68	0.57
1:A:50:THR:O	1:A:74:MSE:CE	2.53	0.57
1:A:95:MSE:HE3	1:B:139:MSE:CE	2.35	0.57
1:D:70:GLU:HG3	1:D:77:ILE:CD1	2.35	0.57
1:F:26:GLU:OE1	1:F:54:ARG:HD3	2.04	0.57
1:D:213:CYS:SG	1:D:238:ARG:HB3	2.45	0.57
1:B:30:MSE:HE2	1:B:52:VAL:HG23	1.87	0.57
1:E:182:GLY:HA2	1:E:210:PHE:CE1	2.38	0.57
1:F:253:MSE:CE	1:F:285:ILE:CG2	2.81	0.57
1:B:67:THR:HG22	3:B:599:HOH:O	2.03	0.57
1:D:190:LEU:HB3	1:D:194:GLU:HB3	1.86	0.57
1:B:29:PRO:O	1:B:383:TYR:CB	2.52	0.56
1:B:340:PHE:HB2	1:B:345:ASP:CB	2.35	0.56
1:C:232:ILE:HD12	1:C:237:ILE:HG13	1.87	0.56
1:D:50:THR:N	1:D:74:MSE:HE1	2.20	0.56
1:E:277:ARG:HD2	1:F:311:TYR:CZ	2.40	0.56
1:B:126:ASN:HD22	1:B:298:PRO:HD2	1.69	0.56
1:F:108:THR:CG2	1:F:119:LEU:HD12	2.33	0.56
1:B:240:PHE:HB2	1:B:262:VAL:CG2	2.35	0.56
1:D:49:ALA:O	1:D:69:ASP:HA	2.04	0.56
1:D:344:ARG:HH11	1:D:344:ARG:HG2	1.69	0.56
1:C:356:PRO:HG2	1:C:363:LEU:HG	1.88	0.56
1:C:49:ALA:HB1	1:C:74:MSE:CE	2.37	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:ASP:HB2	1:F:371:LEU:CD2	2.35	0.55
1:F:376:ASN:HD21	1:F:378:ASP:HB2	1.71	0.55
1:D:60:GLY:O	1:D:62:ILE:HD12	2.07	0.55
1:D:253:MSE:HE1	1:D:285:ILE:HG23	1.88	0.55
1:E:203:ARG:HG3	1:E:235:LEU:HB3	1.88	0.55
1:C:253:MSE:CE	1:C:279:LEU:HG	2.37	0.55
1:E:126:ASN:ND2	1:E:299:THR:H	2.04	0.55
1:E:138:LYS:HD3	1:E:138:LYS:N	2.21	0.55
1:E:237:ILE:HD12	1:E:237:ILE:N	2.22	0.55
1:B:20:LEU:HB2	1:B:95:MSE:HE2	1.88	0.55
1:E:347:PHE:O	1:E:351:MSE:HB2	2.06	0.55
1:B:50:THR:N	1:B:74:MSE:HE1	2.22	0.55
1:C:70:GLU:HG3	1:C:77:ILE:CD1	2.37	0.55
1:A:138:LYS:HE2	3:A:492:HOH:O	2.07	0.55
1:E:182:GLY:HA2	1:E:210:PHE:CZ	2.42	0.55
1:A:29:PRO:HA	1:A:74:MSE:HE2	1.88	0.55
1:A:348:TRP:CE2	1:A:355:ARG:HD3	2.41	0.55
1:B:253:MSE:CE	1:B:264:VAL:HG12	2.33	0.55
1:B:280:MSE:HG2	1:B:313:VAL:HG21	1.89	0.55
1:D:232:ILE:HD12	1:D:237:ILE:HG13	1.88	0.55
1:E:56:HIS:ND1	1:E:62:ILE:HD12	2.22	0.55
1:D:253:MSE:HE3	1:D:284:ALA:HB1	1.89	0.54
1:A:51:ILE:HG12	1:A:74:MSE:HE2	1.89	0.54
1:A:312:ASP:OD1	1:D:247:HIS:HE1	1.91	0.54
1:B:116:ARG:HD2	1:B:294:TRP:CD1	2.41	0.54
1:E:141:LEU:HD22	1:E:370:GLY:HA2	1.89	0.54
1:E:154:MSE:CE	1:E:363:LEU:HD13	2.37	0.54
1:B:351:MSE:HE3	1:B:375:LEU:HD22	1.89	0.54
1:E:51:ILE:HD11	1:E:74:MSE:HG3	1.89	0.54
1:B:303:ARG:HD2	3:B:448:HOH:O	2.07	0.54
1:E:238:ARG:O	1:E:263:PRO:HG2	2.07	0.54
1:A:310:SER:OG	1:B:277:ARG:HD3	2.08	0.54
1:A:360:ASN:N	3:A:461:HOH:O	2.39	0.54
1:B:253:MSE:HE1	1:B:285:ILE:CG2	2.32	0.54
1:C:104:GLY:O	1:C:107:VAL:HG22	2.08	0.54
1:D:268:GLN:HE21	1:D:289:ASN:HD21	1.55	0.54
1:F:188:GLY:HA2	1:F:220:TYR:CZ	2.43	0.54
1:A:30:MSE:HB3	1:A:384:ARG:HA	1.90	0.54
1:D:157:ILE:HD12	1:D:339:CYS:O	2.08	0.54
1:D:172:MSE:HG3	1:D:206:ALA:HB2	1.89	0.54
1:F:115:ARG:O	1:F:119:LEU:HD13	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:GLU:HG2	1:E:362:THR:CG2	2.36	0.53
1:E:172:MSE:HE2	1:E:172:MSE:HA	1.90	0.53
1:B:376:ASN:O	1:B:380:ILE:HG12	2.08	0.53
1:E:49:ALA:O	1:E:69:ASP:HA	2.08	0.53
1:F:301:TRP:HE3	1:F:302:LEU:HD13	1.74	0.53
1:B:67:THR:HG21	1:B:124:ALA:HA	1.89	0.53
1:C:97:ILE:HD13	1:C:130:TRP:CE2	2.42	0.53
1:E:48:ARG:HG3	1:E:347:PHE:CE2	2.44	0.53
1:C:341:HIS:HD1	1:C:343:ASP:H	1.57	0.53
1:A:20:LEU:CD1	1:A:94:ALA:HB3	2.38	0.53
1:D:344:ARG:HG2	1:D:344:ARG:O	2.07	0.53
1:E:149:ARG:HD2	1:E:151:GLU:O	2.08	0.53
1:C:31:VAL:HG22	1:C:385:VAL:HG11	1.89	0.53
1:C:153:PRO:HG2	1:C:336:ILE:HG12	1.90	0.53
1:C:238:ARG:O	1:C:263:PRO:HG2	2.08	0.53
1:A:20:LEU:HD13	1:A:57:THR:HG21	1.90	0.53
1:D:126:ASN:HD22	1:D:298:PRO:HD2	1.74	0.53
1:A:143:LYS:HD3	1:B:95:MSE:HB3	1.91	0.53
1:A:111:ILE:CD1	1:E:217:ASN:HB3	2.39	0.52
1:E:153:PRO:CG	1:E:336:ILE:HG22	2.32	0.52
1:A:269:THR:HG22	1:A:269:THR:O	2.08	0.52
1:B:237:ILE:HD12	1:B:237:ILE:N	2.24	0.52
1:C:148:TYR:O	1:D:99:ARG:NH1	2.42	0.52
1:D:153:PRO:HG2	1:D:336:ILE:HD13	1.91	0.52
1:E:171:GLU:HG2	1:E:175:TYR:CE2	2.44	0.52
1:F:190:LEU:HB3	1:F:194:GLU:OE2	2.08	0.52
1:C:126:ASN:HD22	1:C:298:PRO:HD2	1.74	0.52
1:C:253:MSE:HE3	1:C:284:ALA:HB1	1.92	0.52
1:D:138:LYS:HD3	1:D:138:LYS:N	2.24	0.52
1:E:188:GLY:HA2	1:E:220:TYR:CZ	2.44	0.52
1:F:126:ASN:ND2	1:F:299:THR:H	2.06	0.52
1:C:269:THR:HG22	1:C:269:THR:O	2.10	0.52
1:B:363:LEU:C	1:B:363:LEU:HD23	2.30	0.52
1:C:126:ASN:HD21	1:C:299:THR:H	1.58	0.52
1:C:253:MSE:HE1	1:C:266:ALA:HB3	1.91	0.52
1:D:189:GLY:O	1:D:190:LEU:HD12	2.09	0.52
1:E:155:ILE:HD11	1:E:338:GLU:HB3	1.91	0.52
1:F:155:ILE:CD1	1:F:338:GLU:HB3	2.40	0.52
1:E:157:ILE:HG23	1:E:186:LYS:HE2	1.92	0.52
1:B:232:ILE:HD12	1:B:237:ILE:HG12	1.92	0.52
1:B:253:MSE:HE2	1:B:284:ALA:O	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ASN:ND2	1:B:378:ASP:H	2.08	0.51
1:C:253:MSE:HE3	1:C:284:ALA:CB	2.40	0.51
1:B:157:ILE:HD12	1:B:184:LYS:HD2	1.92	0.51
1:D:360:ASN:ND2	3:D:561:HOH:O	2.43	0.51
1:F:154:MSE:HE2	1:F:338:GLU:C	2.31	0.51
1:A:104:GLY:O	1:A:107:VAL:HG22	2.11	0.51
1:C:29:PRO:HG2	1:C:385:VAL:O	2.10	0.51
1:C:183:VAL:HG22	1:C:184:LYS:N	2.26	0.51
1:C:319:GLU:HB2	3:C:462:HOH:O	2.11	0.51
1:D:380:ILE:O	1:D:384:ARG:HG2	2.10	0.51
1:C:376:ASN:C	1:C:376:ASN:HD22	2.14	0.51
1:A:340:PHE:HB3	1:A:344:ARG:HB3	1.93	0.51
1:D:70:GLU:HG3	1:D:77:ILE:HD11	1.93	0.51
1:A:253:MSE:CE	1:A:285:ILE:CG2	2.84	0.51
1:B:20:LEU:CB	1:B:95:MSE:HE2	2.40	0.51
1:B:149:ARG:HD2	1:B:151:GLU:O	2.11	0.51
1:D:89:LEU:CD1	1:D:125:VAL:HG11	2.40	0.51
1:B:126:ASN:HD21	1:B:299:THR:H	1.59	0.51
1:C:185:PHE:CD2	1:C:199:ILE:HD13	2.46	0.51
1:E:116:ARG:O	1:E:120:VAL:HG23	2.11	0.51
1:E:346:PRO:HB2	1:E:379:TYR:OH	2.10	0.51
1:F:338:GLU:HG3	3:F:449:HOH:O	2.10	0.51
1:B:213:CYS:SG	1:B:238:ARG:HB3	2.51	0.50
1:D:22:ILE:HD12	1:D:92:GLN:O	2.10	0.50
1:D:203:ARG:HD2	1:D:235:LEU:O	2.10	0.50
1:E:49:ALA:HB1	1:E:74:MSE:HE1	1.93	0.50
1:F:51:ILE:HG12	1:F:74:MSE:HE3	1.92	0.50
1:C:155:ILE:HD12	1:C:155:ILE:C	2.31	0.50
1:D:344:ARG:HG2	1:D:344:ARG:NH1	2.25	0.50
1:B:242:GLU:HG3	3:B:452:HOH:O	2.10	0.50
1:D:346:PRO:O	1:D:350:ASN:HB2	2.11	0.50
1:F:116:ARG:HG2	1:F:271:PHE:HE1	1.75	0.50
1:F:195:ASP:O	1:F:199:ILE:HG12	2.12	0.50
1:B:76:ASP:O	1:B:80:ILE:HG12	2.11	0.50
1:B:253:MSE:HE2	1:B:285:ILE:CG2	2.41	0.50
1:C:253:MSE:HE1	1:C:279:LEU:HG	1.92	0.50
1:D:249:ASP:O	1:D:253:MSE:HG2	2.11	0.50
1:F:67:THR:HG21	1:F:124:ALA:HA	1.94	0.50
1:A:238:ARG:O	1:A:263:PRO:HG2	2.10	0.50
1:D:49:ALA:HB1	1:D:74:MSE:HE1	1.94	0.50
1:A:48:ARG:HG2	1:A:347:PHE:CE2	2.46	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:MSE:HG3	1:B:284:ALA:HB1	1.94	0.50
1:E:338:GLU:HG3	3:E:424:HOH:O	2.12	0.50
1:C:340:PHE:HB2	1:C:345:ASP:HB3	1.94	0.50
1:D:253:MSE:CE	1:D:284:ALA:HB1	2.41	0.50
1:F:253:MSE:HE2	1:F:284:ALA:O	2.12	0.50
1:F:141:LEU:HD22	1:F:370:GLY:HA2	1.93	0.49
1:D:253:MSE:CE	1:D:285:ILE:CG2	2.89	0.49
1:D:253:MSE:HE3	1:D:284:ALA:CB	2.42	0.49
1:A:149:ARG:HD2	1:A:151:GLU:O	2.11	0.49
1:B:377:TRP:HA	1:B:380:ILE:HG12	1.94	0.49
1:E:141:LEU:HD23	1:E:370:GLY:C	2.32	0.49
1:D:156:ALA:HA	1:D:339:CYS:O	2.13	0.49
1:F:70:GLU:HG3	1:F:77:ILE:CD1	2.42	0.49
1:A:49:ALA:O	1:A:69:ASP:HA	2.13	0.49
1:D:250:LYS:HG2	1:D:279:LEU:CD1	2.43	0.49
1:C:162:GLY:O	1:C:163:GLU:HG2	2.11	0.49
1:F:126:ASN:ND2	1:F:298:PRO:HD2	2.25	0.49
1:F:344:ARG:HB2	1:F:344:ARG:HH11	1.78	0.49
1:A:48:ARG:HG3	1:A:48:ARG:HH11	1.77	0.49
1:D:253:MSE:HE1	1:D:285:ILE:CG2	2.43	0.49
1:D:253:MSE:HE2	1:D:279:LEU:CD1	2.42	0.49
1:E:99:ARG:HG3	1:E:99:ARG:HH11	1.77	0.49
1:E:172:MSE:HA	1:E:172:MSE:CE	2.43	0.49
1:C:28:ILE:HB	1:C:52:VAL:HB	1.95	0.49
1:F:50:THR:O	1:F:74:MSE:CE	2.60	0.49
1:D:383:TYR:C	3:D:401:HOH:O	2.52	0.48
1:F:51:ILE:HD11	1:F:74:MSE:HG3	1.94	0.48
1:B:277:ARG:CG	1:B:277:ARG:NH1	2.74	0.48
1:D:86:ALA:HB3	1:D:87:PRO:HD3	1.95	0.48
1:D:187:VAL:CG1	1:D:199:ILE:HD11	2.43	0.48
1:A:34:LEU:HD13	1:A:47:HIS:HA	1.95	0.48
1:A:239:TRP:HA	1:A:263:PRO:HG2	1.95	0.48
1:B:277:ARG:HG2	1:B:277:ARG:NH1	2.21	0.48
1:D:48:ARG:HG3	1:D:347:PHE:HE2	1.79	0.48
1:E:86:ALA:HB3	1:E:87:PRO:HD3	1.96	0.48
1:A:70:GLU:HG3	1:A:77:ILE:CD1	2.44	0.48
1:D:156:ALA:HB2	1:D:180:LEU:HD13	1.96	0.48
1:D:253:MSE:HG3	1:D:284:ALA:HB1	1.95	0.48
1:A:33:PRO:HA	1:A:47:HIS:ND1	2.27	0.48
1:E:89:LEU:CD1	1:E:125:VAL:HG11	2.43	0.48
1:B:77:ILE:HD13	1:B:120:VAL:HG11	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LYS:CD	1:B:357:LYS:H	2.26	0.48
1:D:103:SER:O	1:D:106:LYS:HG2	2.12	0.48
1:A:67:THR:OG1	1:A:293:SER:HB2	2.13	0.48
1:A:162:GLY:C	1:A:163:GLU:HG2	2.31	0.48
1:A:247:HIS:CE1	1:F:312:ASP:OD1	2.61	0.48
1:D:104:GLY:O	1:D:107:VAL:HG22	2.13	0.48
1:E:183:VAL:HG22	1:E:184:LYS:N	2.29	0.48
1:C:49:ALA:O	1:C:69:ASP:HA	2.13	0.48
1:C:195:ASP:O	1:C:199:ILE:HG12	2.13	0.48
1:D:136:ALA:O	1:D:138:LYS:HE2	2.14	0.48
1:D:183:VAL:HG22	1:D:184:LYS:N	2.28	0.48
1:E:172:MSE:SE	1:E:183:VAL:HG11	2.64	0.48
1:F:155:ILE:C	1:F:155:ILE:HD12	2.34	0.48
1:E:141:LEU:HD12	1:E:145:TRP:CE2	2.48	0.47
1:B:188:GLY:HA2	1:B:220:TYR:CE2	2.50	0.47
1:B:214:ILE:HD13	1:B:214:ILE:H	1.77	0.47
1:B:380:ILE:O	1:B:383:TYR:CD2	2.68	0.47
1:F:266:ALA:O	1:F:288:CYS:HA	2.14	0.47
1:F:142:TRP:N	1:F:326:HIS:HD2	2.08	0.47
1:A:277:ARG:HH12	1:E:248:ASN:ND2	2.11	0.47
1:B:104:GLY:O	1:B:107:VAL:HG22	2.14	0.47
1:A:344:ARG:HD3	1:A:344:ARG:C	2.33	0.47
1:C:141:LEU:HD22	1:C:370:GLY:C	2.34	0.47
1:E:76:ASP:O	1:E:80:ILE:HD13	2.15	0.47
1:D:67:THR:HG21	1:D:124:ALA:HA	1.95	0.47
1:E:269:THR:HG22	1:E:269:THR:O	2.15	0.47
1:F:269:THR:HG22	1:F:269:THR:O	2.14	0.47
1:B:89:LEU:HD11	1:B:125:VAL:CG1	2.43	0.47
1:B:214:ILE:CD1	1:B:240:PHE:HA	2.45	0.47
1:F:187:VAL:HG11	1:F:199:ILE:HD11	1.97	0.47
1:E:54:ARG:HA	1:E:63:GLY:O	2.15	0.47
1:E:70:GLU:O	1:E:74:MSE:HE3	2.15	0.47
1:E:155:ILE:HB	1:E:182:GLY:C	2.35	0.47
1:E:156:ALA:HB2	1:E:180:LEU:HD13	1.97	0.47
1:F:95:MSE:HE3	1:F:137:LEU:HD13	1.95	0.47
1:A:48:ARG:CZ	1:A:347:PHE:HD2	2.28	0.47
1:A:111:ILE:HD11	1:E:217:ASN:HB3	1.97	0.47
1:A:346:PRO:O	1:A:350:ASN:HB2	2.14	0.47
1:A:356:PRO:HG3	1:A:363:LEU:HD21	1.95	0.47
1:D:203:ARG:HG3	1:D:235:LEU:HB3	1.96	0.47
1:E:95:MSE:CE	1:E:95:MSE:HA	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ASP:HA	1:B:383:TYR:HE2	1.79	0.47
1:C:187:VAL:HG11	1:C:199:ILE:HD11	1.96	0.47
1:D:253:MSE:HE1	1:D:279:LEU:HG	1.96	0.47
1:D:311:TYR:O	1:D:312:ASP:HB2	2.15	0.47
1:E:380:ILE:O	1:E:384:ARG:HB3	2.15	0.47
1:B:357:LYS:H	1:B:357:LYS:HD2	1.80	0.46
1:D:152:LEU:HD12	1:D:152:LEU:O	2.15	0.46
1:D:363:LEU:C	1:D:363:LEU:HD23	2.34	0.46
1:E:340:PHE:CD1	1:E:344:ARG:HD3	2.51	0.46
1:F:153:PRO:HG2	1:F:336:ILE:CD1	2.44	0.46
1:B:154:MSE:HE3	3:B:439:HOH:O	2.14	0.46
1:C:268:GLN:HE21	1:C:289:ASN:HD21	1.64	0.46
1:A:67:THR:HG21	1:A:124:ALA:HA	1.97	0.46
1:D:188:GLY:HA2	1:D:220:TYR:CZ	2.51	0.46
1:D:209:ASP:CG	1:D:209:ASP:O	2.54	0.46
1:E:129:ILE:O	1:E:133:VAL:HG23	2.15	0.46
1:A:318:HIS:CD2	1:A:319:GLU:HG2	2.51	0.46
1:A:363:LEU:C	1:A:363:LEU:HD23	2.36	0.46
1:C:346:PRO:O	1:C:350:ASN:HB2	2.15	0.46
1:D:280:MSE:HG2	1:D:313:VAL:HG21	1.98	0.46
1:E:351:MSE:CE	1:E:375:LEU:HD22	2.38	0.46
1:A:183:VAL:HG22	1:A:184:LYS:N	2.30	0.46
1:B:249:ASP:O	1:B:253:MSE:HG2	2.16	0.46
1:C:99:ARG:HD3	1:D:148:TYR:O	2.16	0.46
1:E:31:VAL:O	1:E:383:TYR:HB3	2.16	0.46
1:F:183:VAL:HG12	1:F:212:ILE:HD13	1.98	0.46
1:B:357:LYS:HD2	1:B:357:LYS:N	2.31	0.45
1:E:106:LYS:HE2	1:E:106:LYS:HB3	1.72	0.45
1:E:277:ARG:CG	1:E:277:ARG:NH1	2.78	0.45
1:F:77:ILE:HD13	1:F:120:VAL:HG11	1.98	0.45
1:F:100:LEU:HD23	1:F:129:ILE:HD13	1.98	0.45
1:F:50:THR:HG22	1:F:347:PHE:CZ	2.52	0.45
1:F:351:MSE:CE	1:F:375:LEU:HG	2.45	0.45
1:E:27:THR:HG22	1:E:82:HIS:NE2	2.32	0.45
1:F:48:ARG:HD3	1:F:347:PHE:CD2	2.51	0.45
1:B:269:THR:O	1:B:269:THR:HG22	2.16	0.45
1:C:116:ARG:O	1:C:120:VAL:HG23	2.17	0.45
1:C:307:ILE:CD1	1:C:307:ILE:N	2.79	0.45
1:C:211:ILE:HD13	1:C:336:ILE:CD1	2.47	0.45
1:D:20:LEU:HB2	1:D:95:MSE:CE	2.46	0.45
1:E:203:ARG:HG2	1:E:212:ILE:HD12	1.98	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:PRO:HG3	1:E:349:TRP:CE2	2.52	0.45
1:F:86:ALA:N	1:F:87:PRO:HD2	2.32	0.45
1:F:235:LEU:HB3	1:F:237:ILE:HD11	1.99	0.45
1:F:318:HIS:HD2	3:F:415:HOH:O	1.99	0.45
1:A:126:ASN:ND2	1:A:299:THR:H	2.14	0.45
1:C:126:ASN:ND2	1:C:299:THR:H	2.15	0.45
1:D:242:GLU:HG3	3:D:465:HOH:O	2.17	0.45
1:E:126:ASN:HD22	1:E:298:PRO:HD2	1.81	0.45
1:F:142:TRP:H	1:F:326:HIS:CD2	2.23	0.45
1:C:174:ASN:HB3	3:C:455:HOH:O	2.16	0.45
1:E:266:ALA:O	1:E:288:CYS:HA	2.17	0.45
1:F:275:GLY:O	1:F:279:LEU:HD23	2.16	0.45
1:C:182:GLY:HA2	1:C:210:PHE:CE1	2.52	0.45
1:E:155:ILE:H	1:E:155:ILE:CD1	2.30	0.45
1:A:318:HIS:NE2	1:A:319:GLU:OE2	2.50	0.45
1:D:269:THR:O	1:D:269:THR:HG22	2.17	0.45
1:D:318:HIS:HD2	3:D:455:HOH:O	1.98	0.45
1:E:27:THR:HG21	1:E:82:HIS:NE2	2.31	0.45
1:A:363:LEU:HD23	1:A:364:THR:N	2.32	0.44
1:E:242:GLU:HG3	3:E:402:HOH:O	2.16	0.44
1:B:48:ARG:HG3	1:B:347:PHE:CE2	2.51	0.44
1:C:186:LYS:HD2	1:C:217:ASN:HD21	1.82	0.44
1:D:340:PHE:HB2	1:D:345:ASP:HB3	1.99	0.44
1:F:179:GLY:O	1:F:361:GLY:HA2	2.17	0.44
1:F:253:MSE:HG3	1:F:284:ALA:HB1	1.98	0.44
1:D:272:SER:HB2	3:D:411:HOH:O	2.17	0.44
1:E:151:GLU:CG	1:E:362:THR:CG2	2.95	0.44
1:A:20:LEU:HD12	1:A:20:LEU:C	2.35	0.44
1:B:179:GLY:O	1:B:361:GLY:HA2	2.17	0.44
1:B:266:ALA:O	1:B:288:CYS:HA	2.18	0.44
1:C:70:GLU:HG3	1:C:77:ILE:HD11	2.00	0.44
1:D:28:ILE:HB	1:D:52:VAL:HB	1.98	0.44
1:F:172:MSE:O	1:F:176:GLN:HG3	2.18	0.44
1:A:253:MSE:HG3	1:A:284:ALA:HB1	2.00	0.44
1:B:253:MSE:HE2	1:B:285:ILE:HG23	2.00	0.44
1:C:155:ILE:HD11	1:C:338:GLU:HB3	1.98	0.44
1:F:49:ALA:O	1:F:69:ASP:HA	2.17	0.44
1:A:77:ILE:HD13	1:A:120:VAL:HG11	1.99	0.44
1:C:157:ILE:HD12	1:C:184:LYS:HD2	1.99	0.44
1:D:342:PRO:HG3	1:D:349:TRP:CE2	2.52	0.44
1:E:155:ILE:CD1	1:E:336:ILE:HD13	2.39	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLU:HG3	3:A:417:HOH:O	2.17	0.44
1:E:254:ARG:HD2	1:E:255:ASP:OD2	2.17	0.44
1:B:86:ALA:HB3	1:B:87:PRO:HD3	1.99	0.44
1:E:148:TYR:CG	1:E:332:PRO:HA	2.53	0.44
1:F:237:ILE:N	1:F:237:ILE:CD1	2.81	0.44
1:F:254:ARG:O	1:F:257:ARG:HB3	2.17	0.44
1:B:345:ASP:O	1:B:349:TRP:HD1	2.01	0.44
1:F:235:LEU:HB3	1:F:237:ILE:CD1	2.48	0.44
1:B:318:HIS:HD2	3:B:433:HOH:O	2.00	0.43
1:E:61:ILE:O	1:E:62:ILE:HD13	2.17	0.43
1:A:51:ILE:HG12	1:A:74:MSE:CE	2.47	0.43
1:B:56:HIS:CG	1:B:62:ILE:HD12	2.54	0.43
1:B:377:TRP:HA	1:B:380:ILE:CG1	2.47	0.43
1:A:253:MSE:CG	1:A:284:ALA:HB1	2.49	0.43
1:B:20:LEU:HG	1:B:57:THR:HG21	1.99	0.43
1:B:29:PRO:O	1:B:383:TYR:HB2	2.18	0.43
1:D:182:GLY:HA2	1:D:210:PHE:CZ	2.53	0.43
1:E:363:LEU:HD23	1:E:363:LEU:C	2.39	0.43
1:B:240:PHE:HB2	1:B:262:VAL:HG21	1.99	0.43
1:C:103:SER:O	1:C:106:LYS:HG2	2.18	0.43
1:D:116:ARG:O	1:D:120:VAL:HG23	2.18	0.43
1:E:250:LYS:HE3	3:E:529:HOH:O	2.17	0.43
1:E:97:ILE:HD12	1:E:97:ILE:H	1.82	0.43
1:F:95:MSE:HE1	1:F:136:ALA:CB	2.48	0.43
1:A:99:ARG:HD3	1:B:148:TYR:O	2.19	0.43
1:B:336:ILE:HG22	1:B:337:ALA:O	2.19	0.43
1:C:253:MSE:HG3	1:C:284:ALA:HB1	2.01	0.43
1:D:30:MSE:HE2	1:D:347:PHE:HE1	1.84	0.43
1:E:319:GLU:HB2	1:E:320:GLU:H	1.63	0.43
1:B:129:ILE:C	1:B:129:ILE:HD12	2.39	0.43
1:B:383:TYR:CD2	1:B:383:TYR:N	2.85	0.43
1:A:79:ARG:CZ	1:A:79:ARG:HB2	2.48	0.43
1:B:20:LEU:HD22	1:B:95:MSE:HE1	2.01	0.43
1:E:104:GLY:O	1:E:107:VAL:HG22	2.19	0.43
1:A:287:VAL:HG22	1:A:314:GLN:HB2	2.00	0.43
1:B:381:ASP:HA	1:B:383:TYR:CE2	2.54	0.43
1:D:161:TYR:CE1	1:D:190:LEU:HD13	2.54	0.43
1:A:188:GLY:HA2	1:A:220:TYR:CE2	2.53	0.43
1:E:70:GLU:HG3	1:E:77:ILE:CD1	2.49	0.43
1:A:319:GLU:HB2	3:A:456:HOH:O	2.19	0.42
1:B:116:ARG:O	1:B:120:VAL:HG23	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:MSE:CE	1:B:284:ALA:O	2.67	0.42
1:B:30:MSE:HE3	1:B:50:THR:CG2	2.49	0.42
1:F:249:ASP:O	1:F:253:MSE:HG2	2.19	0.42
1:A:155:ILE:HG23	1:A:336:ILE:HG21	2.01	0.42
1:B:344:ARG:HG2	1:B:344:ARG:O	2.18	0.42
1:C:211:ILE:HD13	1:C:336:ILE:HD13	2.02	0.42
1:F:154:MSE:HE3	1:F:337:ALA:CB	2.49	0.42
1:A:168:ILE:O	1:A:172:MSE:HG2	2.19	0.42
1:B:156:ALA:HB2	1:B:180:LEU:CD1	2.42	0.42
1:B:382:GLN:H	1:B:383:TYR:HD2	1.67	0.42
1:C:33:PRO:HA	1:C:47:HIS:ND1	2.34	0.42
1:E:346:PRO:O	1:E:350:ASN:HB2	2.19	0.42
1:F:203:ARG:NH1	1:F:235:LEU:O	2.51	0.42
1:C:188:GLY:HA2	1:C:220:TYR:CE1	2.55	0.42
1:A:126:ASN:ND2	1:A:298:PRO:HD2	2.33	0.42
1:A:156:ALA:O	1:A:183:VAL:HG23	2.19	0.42
1:A:95:MSE:CE	1:B:139:MSE:SE	3.17	0.42
1:E:125:VAL:O	1:E:129:ILE:HG13	2.19	0.42
1:E:152:LEU:O	1:E:152:LEU:HD12	2.20	0.42
1:B:49:ALA:HB1	1:B:74:MSE:HE1	2.01	0.42
1:B:63:GLY:HA3	1:B:132:ALA:HB2	2.02	0.42
1:C:187:VAL:CG1	1:C:199:ILE:HD11	2.50	0.42
1:C:253:MSE:CG	1:C:284:ALA:HB1	2.49	0.42
1:D:20:LEU:HB2	1:D:95:MSE:HE2	2.01	0.42
1:E:333:HIS:ND1	1:E:333:HIS:N	2.68	0.42
1:F:125:VAL:O	1:F:129:ILE:HG13	2.19	0.42
1:C:31:VAL:HG22	1:C:385:VAL:CG1	2.50	0.42
1:D:131:ASP:CB	1:D:371:LEU:HD23	2.48	0.42
1:E:149:ARG:O	1:E:329:ALA:HB1	2.20	0.42
1:F:340:PHE:HB2	1:F:345:ASP:HB2	2.02	0.42
1:D:211:ILE:N	1:D:211:ILE:HD12	2.35	0.41
1:E:95:MSE:HE2	1:E:95:MSE:HA	2.02	0.41
1:F:142:TRP:CH2	1:F:143:LYS:HE3	2.55	0.41
1:F:210:PHE:HD2	1:F:212:ILE:HD11	1.85	0.41
1:B:51:ILE:O	1:B:66:TYR:HA	2.21	0.41
1:E:232:ILE:HD12	1:E:237:ILE:HG12	2.01	0.41
1:A:125:VAL:O	1:A:129:ILE:HG13	2.20	0.41
1:A:141:LEU:CD2	1:A:371:LEU:HD13	2.50	0.41
1:A:238:ARG:O	1:A:263:PRO:CG	2.68	0.41
1:C:157:ILE:HB	1:C:340:PHE:CD1	2.55	0.41
1:D:376:ASN:ND2	1:D:378:ASP:HB2	2.28	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:MSE:HE2	1:A:284:ALA:O	2.20	0.41
1:C:156:ALA:HA	1:C:339:CYS:O	2.21	0.41
1:C:253:MSE:CE	1:C:285:ILE:HG23	2.49	0.41
1:D:86:ALA:N	1:D:87:PRO:CD	2.84	0.41
1:F:178:LEU:HB3	1:F:180:LEU:HD23	2.03	0.41
1:F:347:PHE:O	1:F:351:MSE:HB2	2.20	0.41
1:B:318:HIS:O	1:B:319:GLU:HG2	2.21	0.41
1:C:48:ARG:HG2	1:C:347:PHE:CD2	2.55	0.41
1:F:51:ILE:HD13	1:F:74:MSE:HE2	2.01	0.41
1:B:126:ASN:ND2	1:B:298:PRO:HD2	2.33	0.41
1:B:291:ASP:HB2	1:B:318:HIS:HB3	2.03	0.41
1:D:340:PHE:CD1	1:D:344:ARG:HD3	2.56	0.41
1:E:190:LEU:HB3	1:E:194:GLU:OE2	2.20	0.41
1:E:336:ILE:HD12	1:E:336:ILE:C	2.41	0.41
1:C:30:MSE:HB3	1:C:384:ARG:HA	2.02	0.41
1:D:346:PRO:HB2	1:D:379:TYR:OH	2.21	0.41
1:A:86:ALA:HB3	1:A:87:PRO:HD3	2.02	0.41
1:C:266:ALA:O	1:C:288:CYS:HA	2.21	0.41
1:C:363:LEU:C	1:C:363:LEU:HD23	2.41	0.41
1:E:99:ARG:HG3	1:E:99:ARG:NH1	2.36	0.41
1:E:318:HIS:HD2	3:E:450:HOH:O	2.04	0.41
1:F:335:THR:O	1:F:336:ILE:HD13	2.21	0.41
1:A:116:ARG:O	1:A:120:VAL:HG23	2.20	0.41
1:A:171:GLU:HG2	1:A:175:TYR:CE2	2.56	0.41
1:A:335:THR:O	1:A:336:ILE:HD13	2.21	0.41
1:A:29:PRO:CA	1:A:74:MSE:HE2	2.51	0.40
1:A:50:THR:C	1:A:74:MSE:CE	2.90	0.40
1:B:319:GLU:HG3	1:B:320:GLU:HG2	2.03	0.40
1:C:48:ARG:HH11	1:C:48:ARG:CG	2.28	0.40
1:C:362:THR:CG2	1:C:363:LEU:N	2.84	0.40
1:D:50:THR:HG22	1:D:347:PHE:CZ	2.56	0.40
1:D:319:GLU:HB2	1:D:320:GLU:H	1.70	0.40
1:D:371:LEU:HB3	1:D:373:TRP:CD1	2.56	0.40
1:A:318:HIS:CE1	1:A:319:GLU:OE2	2.75	0.40
1:D:148:TYR:CG	1:D:332:PRO:HA	2.56	0.40
1:E:27:THR:O	1:E:27:THR:HG23	2.22	0.40
1:E:253:MSE:CG	1:E:284:ALA:HB1	2.51	0.40
1:F:371:LEU:HB3	1:F:373:TRP:CD1	2.56	0.40
1:A:182:GLY:HA2	1:A:210:PHE:CZ	2.56	0.40
1:B:70:GLU:HG3	1:B:77:ILE:CD1	2.51	0.40
1:D:157:ILE:CG2	1:D:186:LYS:HE2	2.51	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:GLU:HG2	1:D:175:TYR:CE2	2.57	0.40
1:C:111:ILE:HD12	1:C:111:ILE:N	2.37	0.40
1:F:319:GLU:HB2	3:F:613:HOH:O	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	351/398 (88%)	340 (97%)	10 (3%)	1 (0%)	41 37
1	B	345/398 (87%)	328 (95%)	16 (5%)	1 (0%)	41 37
1	C	353/398 (89%)	344 (98%)	8 (2%)	1 (0%)	41 37
1	D	346/398 (87%)	331 (96%)	14 (4%)	1 (0%)	41 37
1	E	349/398 (88%)	333 (95%)	14 (4%)	2 (1%)	25 18
1	F	345/398 (87%)	325 (94%)	18 (5%)	2 (1%)	25 18
All	All	2089/2388 (88%)	2001 (96%)	80 (4%)	8 (0%)	34 29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	319	GLU
1	A	319	GLU
1	F	319	GLU
1	B	187	VAL
1	C	319	GLU
1	D	110	ASP
1	E	187	VAL
1	F	164	PRO

### 5.3.2 Protein sidechains [i](#)

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	287/313 (92%)	275 (96%)	12 (4%)	30	28
1	B	282/313 (90%)	265 (94%)	17 (6%)	19	14
1	C	288/313 (92%)	277 (96%)	11 (4%)	33	31
1	D	283/313 (90%)	269 (95%)	14 (5%)	25	21
1	E	285/313 (91%)	265 (93%)	20 (7%)	15	10
1	F	280/313 (90%)	264 (94%)	16 (6%)	20	16
All	All	1705/1878 (91%)	1615 (95%)	90 (5%)	22	19

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	138	LYS
1	A	141	LEU
1	A	152	LEU
1	A	163	GLU
1	A	240	PHE
1	A	294	TRP
1	A	338	GLU
1	A	344	ARG
1	A	359	ASN
1	A	371	LEU
1	A	376	ASN
1	B	129	ILE
1	B	138	LYS
1	B	141	LEU
1	B	152	LEU
1	B	154	MSE
1	B	203	ARG
1	B	209	ASP
1	B	214	ILE
1	B	240	PHE
1	B	262	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	294	TRP
1	B	295	SER
1	B	343	ASP
1	B	357	LYS
1	B	371	LEU
1	B	376	ASN
1	B	383	TYR
1	C	48	ARG
1	C	141	LEU
1	C	152	LEU
1	C	172	MSE
1	C	221	LYS
1	C	279	LEU
1	C	294	TRP
1	C	307	ILE
1	C	338	GLU
1	C	344	ARG
1	C	376	ASN
1	D	138	LYS
1	D	141	LEU
1	D	152	LEU
1	D	163	GLU
1	D	172	MSE
1	D	194	GLU
1	D	203	ARG
1	D	228	LEU
1	D	240	PHE
1	D	279	LEU
1	D	295	SER
1	D	359	ASN
1	D	376	ASN
1	D	384	ARG
1	E	67	THR
1	E	95	MSE
1	E	99	ARG
1	E	138	LYS
1	E	141	LEU
1	E	152	LEU
1	E	155	ILE
1	E	163	GLU
1	E	172	MSE
1	E	203	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	221	LYS
1	E	240	PHE
1	E	279	LEU
1	E	294	TRP
1	E	295	SER
1	E	333	HIS
1	E	338	GLU
1	E	371	LEU
1	E	382	GLN
1	E	384	ARG
1	F	95	MSE
1	F	111	ILE
1	F	117	LEU
1	F	137	LEU
1	F	141	LEU
1	F	203	ARG
1	F	235	LEU
1	F	237	ILE
1	F	240	PHE
1	F	262	VAL
1	F	268	GLN
1	F	294	TRP
1	F	302	LEU
1	F	333	HIS
1	F	338	GLU
1	F	376	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	126	ASN
1	A	174	ASN
1	A	217	ASN
1	A	247	HIS
1	A	268	GLN
1	A	359	ASN
1	A	360	ASN
1	A	376	ASN
1	A	382	GLN
1	B	126	ASN
1	B	174	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	217	ASN
1	B	247	HIS
1	B	318	HIS
1	B	350	ASN
1	B	359	ASN
1	B	360	ASN
1	B	376	ASN
1	C	71	HIS
1	C	126	ASN
1	C	174	ASN
1	C	247	HIS
1	C	359	ASN
1	C	360	ASN
1	C	376	ASN
1	C	382	GLN
1	D	92	GLN
1	D	126	ASN
1	D	247	HIS
1	D	318	HIS
1	D	350	ASN
1	D	359	ASN
1	D	360	ASN
1	D	376	ASN
1	E	92	GLN
1	E	126	ASN
1	E	174	ASN
1	E	247	HIS
1	E	248	ASN
1	E	318	HIS
1	E	359	ASN
1	E	376	ASN
1	F	126	ASN
1	F	174	ASN
1	F	217	ASN
1	F	236	ASN
1	F	247	HIS
1	F	248	ASN
1	F	318	HIS
1	F	326	HIS
1	F	376	ASN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	345/398 (86%)	-0.18	5 (1%) 75 80	7, 16, 31, 41	0
1	B	339/398 (85%)	0.22	19 (5%) 24 33	8, 21, 38, 43	0
1	C	347/398 (87%)	-0.20	4 (1%) 79 83	7, 16, 31, 40	0
1	D	340/398 (85%)	0.26	26 (7%) 13 19	8, 21, 37, 44	0
1	E	343/398 (86%)	0.18	15 (4%) 34 43	10, 22, 37, 43	0
1	F	339/398 (85%)	0.21	14 (4%) 37 46	7, 22, 38, 48	0
All	All	2053/2388 (85%)	0.08	83 (4%) 38 47	7, 20, 36, 48	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	163	GLU	5.9
1	D	164	PRO	5.7
1	D	31	VAL	4.9
1	F	165	LEU	4.8
1	F	162	GLY	4.7
1	E	164	PRO	4.7
1	D	69	ASP	4.3
1	D	71	HIS	4.1
1	D	165	LEU	4.1
1	B	165	LEU	4.0
1	D	162	GLY	4.0
1	D	383	TYR	3.9
1	F	164	PRO	3.9
1	D	32	ALA	3.8
1	E	162	GLY	3.7
1	F	69	ASP	3.5
1	D	75	PHE	3.4
1	B	383	TYR	3.3
1	B	380	ILE	3.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	378	ASP	3.3
1	B	112	LEU	3.2
1	E	165	LEU	3.2
1	E	383	TYR	3.1
1	D	160	TYR	3.0
1	F	377	TRP	3.0
1	B	376	ASN	3.0
1	F	382	GLN	3.0
1	E	61	ILE	3.0
1	A	385	VAL	2.9
1	B	379	TYR	2.9
1	C	386	SER	2.9
1	B	343	ASP	2.9
1	F	166	GLY	2.9
1	F	380	ILE	2.9
1	D	163	GLU	2.9
1	D	72	GLU	2.9
1	F	379	TYR	2.8
1	B	381	ASP	2.8
1	D	357	LYS	2.8
1	E	204	GLU	2.8
1	B	32	ALA	2.7
1	D	344	ARG	2.7
1	A	47	HIS	2.7
1	E	62	ILE	2.7
1	E	168	ILE	2.7
1	B	69	ASP	2.6
1	A	165	LEU	2.6
1	D	166	GLY	2.6
1	B	31	VAL	2.6
1	D	350	ASN	2.6
1	E	209	ASP	2.6
1	A	35	ALA	2.6
1	B	294	TRP	2.5
1	A	33	PRO	2.5
1	D	382	GLN	2.4
1	B	377	TRP	2.4
1	C	47	HIS	2.4
1	E	234	ASP	2.4
1	D	48	ARG	2.4
1	C	112	LEU	2.4
1	D	343	ASP	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	382	GLN	2.3
1	D	380	ILE	2.3
1	D	379	TYR	2.3
1	B	75	PHE	2.3
1	E	60	GLY	2.3
1	B	71	HIS	2.2
1	B	209	ASP	2.2
1	E	344	ARG	2.2
1	F	344	ARG	2.2
1	D	49	ALA	2.2
1	C	209	ASP	2.1
1	D	381	ASP	2.1
1	E	138	LYS	2.1
1	F	378	ASP	2.1
1	B	48	ARG	2.1
1	B	382	GLN	2.1
1	D	204	GLU	2.1
1	F	167	SER	2.1
1	D	70	GLU	2.1
1	F	67	THR	2.0
1	E	343	ASP	2.0
1	D	346	PRO	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	F	397	1/1	0.91	0.12	26,26,26,26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	397	1/1	0.92	0.06	19,19,19,19	0
2	MG	D	397	1/1	0.93	0.07	24,24,24,24	0
2	MG	E	397	1/1	0.94	0.05	29,29,29,29	0
2	MG	B	397	1/1	0.94	0.08	25,25,25,25	0
2	MG	C	397	1/1	0.95	0.07	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.