



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:23 AM GMT

PDB ID : 3I4K  
Title : Crystal structure of Muconate lactonizing enzyme from *Corynebacterium glutamicum*  
Authors : Fedorov, A.A.; Fedorov, E.V.; Sauder, J.M.; Burley, S.K.; Gerlt, J.A.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2009-07-01  
Resolution : 2.20 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

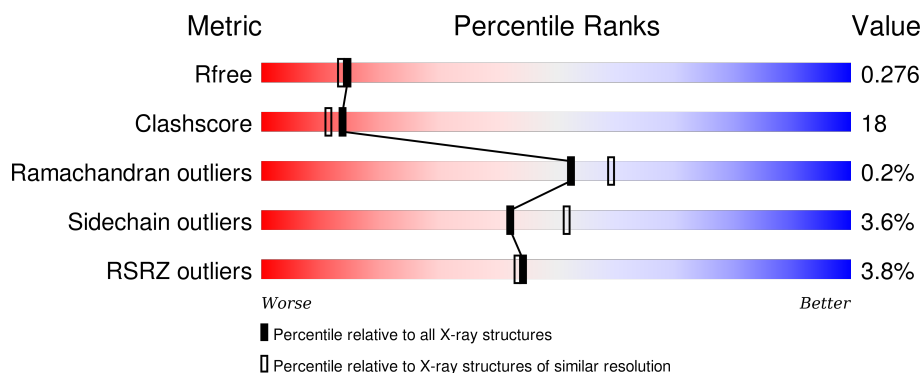
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	383	<div> <div>2%</div> <div>69%</div> <div>26%</div> <div>• •</div> </div>
1	B	383	<div> <div>2%</div> <div>67%</div> <div>27%</div> <div>• •</div> </div>
1	C	383	<div> <div>3%</div> <div>64%</div> <div>30%</div> <div>• •</div> </div>
1	D	383	<div> <div>4%</div> <div>69%</div> <div>25%</div> <div>• •</div> </div>
1	E	383	<div> <div>2%</div> <div>72%</div> <div>22%</div> <div>• •</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	383	<div><div></div><div>3%</div><div>69%</div><div>25%</div><div></div><div></div></div>
1	G	383	<div><div></div><div>8%</div><div>61%</div><div>34%</div><div></div><div></div></div>
1	H	383	<div><div></div><div>4%</div><div>65%</div><div>30%</div><div></div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23024 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 Muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	B	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	C	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	D	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	E	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	F	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	G	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			
1	H	370	Total	C	N	O	S	Se	0	0	0
			2809	1776	489	537	1	6			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q8NN12
A	2	SER	-	expression tag	UNP Q8NN12
A	3	LEU	-	expression tag	UNP Q8NN12
A	376	GLU	-	expression tag	UNP Q8NN12
A	377	GLY	-	expression tag	UNP Q8NN12
A	378	HIS	-	expression tag	UNP Q8NN12
A	379	HIS	-	expression tag	UNP Q8NN12
A	380	HIS	-	expression tag	UNP Q8NN12
A	381	HIS	-	expression tag	UNP Q8NN12
A	382	HIS	-	expression tag	UNP Q8NN12
A	383	HIS	-	expression tag	UNP Q8NN12
B	1	MSE	-	expression tag	UNP Q8NN12
B	2	SER	-	expression tag	UNP Q8NN12

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	LEU	-	expression tag	UNP Q8NN12
B	376	GLU	-	expression tag	UNP Q8NN12
B	377	GLY	-	expression tag	UNP Q8NN12
B	378	HIS	-	expression tag	UNP Q8NN12
B	379	HIS	-	expression tag	UNP Q8NN12
B	380	HIS	-	expression tag	UNP Q8NN12
B	381	HIS	-	expression tag	UNP Q8NN12
B	382	HIS	-	expression tag	UNP Q8NN12
B	383	HIS	-	expression tag	UNP Q8NN12
C	1	MSE	-	expression tag	UNP Q8NN12
C	2	SER	-	expression tag	UNP Q8NN12
C	3	LEU	-	expression tag	UNP Q8NN12
C	376	GLU	-	expression tag	UNP Q8NN12
C	377	GLY	-	expression tag	UNP Q8NN12
C	378	HIS	-	expression tag	UNP Q8NN12
C	379	HIS	-	expression tag	UNP Q8NN12
C	380	HIS	-	expression tag	UNP Q8NN12
C	381	HIS	-	expression tag	UNP Q8NN12
C	382	HIS	-	expression tag	UNP Q8NN12
C	383	HIS	-	expression tag	UNP Q8NN12
D	1	MSE	-	expression tag	UNP Q8NN12
D	2	SER	-	expression tag	UNP Q8NN12
D	3	LEU	-	expression tag	UNP Q8NN12
D	376	GLU	-	expression tag	UNP Q8NN12
D	377	GLY	-	expression tag	UNP Q8NN12
D	378	HIS	-	expression tag	UNP Q8NN12
D	379	HIS	-	expression tag	UNP Q8NN12
D	380	HIS	-	expression tag	UNP Q8NN12
D	381	HIS	-	expression tag	UNP Q8NN12
D	382	HIS	-	expression tag	UNP Q8NN12
D	383	HIS	-	expression tag	UNP Q8NN12
E	1	MSE	-	expression tag	UNP Q8NN12
E	2	SER	-	expression tag	UNP Q8NN12
E	3	LEU	-	expression tag	UNP Q8NN12
E	376	GLU	-	expression tag	UNP Q8NN12
E	377	GLY	-	expression tag	UNP Q8NN12
E	378	HIS	-	expression tag	UNP Q8NN12
E	379	HIS	-	expression tag	UNP Q8NN12
E	380	HIS	-	expression tag	UNP Q8NN12
E	381	HIS	-	expression tag	UNP Q8NN12
E	382	HIS	-	expression tag	UNP Q8NN12
E	383	HIS	-	expression tag	UNP Q8NN12

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MSE	-	expression tag	UNP Q8NN12
F	2	SER	-	expression tag	UNP Q8NN12
F	3	LEU	-	expression tag	UNP Q8NN12
F	376	GLU	-	expression tag	UNP Q8NN12
F	377	GLY	-	expression tag	UNP Q8NN12
F	378	HIS	-	expression tag	UNP Q8NN12
F	379	HIS	-	expression tag	UNP Q8NN12
F	380	HIS	-	expression tag	UNP Q8NN12
F	381	HIS	-	expression tag	UNP Q8NN12
F	382	HIS	-	expression tag	UNP Q8NN12
F	383	HIS	-	expression tag	UNP Q8NN12
G	1	MSE	-	expression tag	UNP Q8NN12
G	2	SER	-	expression tag	UNP Q8NN12
G	3	LEU	-	expression tag	UNP Q8NN12
G	376	GLU	-	expression tag	UNP Q8NN12
G	377	GLY	-	expression tag	UNP Q8NN12
G	378	HIS	-	expression tag	UNP Q8NN12
G	379	HIS	-	expression tag	UNP Q8NN12
G	380	HIS	-	expression tag	UNP Q8NN12
G	381	HIS	-	expression tag	UNP Q8NN12
G	382	HIS	-	expression tag	UNP Q8NN12
G	383	HIS	-	expression tag	UNP Q8NN12
H	1	MSE	-	expression tag	UNP Q8NN12
H	2	SER	-	expression tag	UNP Q8NN12
H	3	LEU	-	expression tag	UNP Q8NN12
H	376	GLU	-	expression tag	UNP Q8NN12
H	377	GLY	-	expression tag	UNP Q8NN12
H	378	HIS	-	expression tag	UNP Q8NN12
H	379	HIS	-	expression tag	UNP Q8NN12
H	380	HIS	-	expression tag	UNP Q8NN12
H	381	HIS	-	expression tag	UNP Q8NN12
H	382	HIS	-	expression tag	UNP Q8NN12
H	383	HIS	-	expression tag	UNP Q8NN12

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	F	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

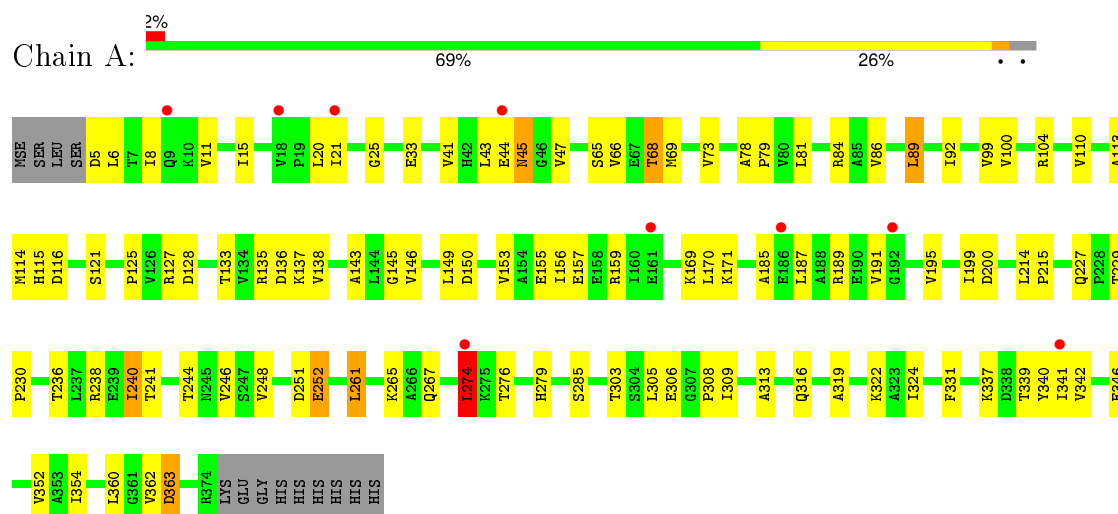
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total 73	O 73	0	0
4	B	75	Total 75	O 75	0	0
4	C	56	Total 56	O 56	0	0
4	D	72	Total 72	O 72	0	0
4	E	98	Total 98	O 98	0	0
4	F	65	Total 65	O 65	0	0
4	G	28	Total 28	O 28	0	0
4	H	45	Total 45	O 45	0	0



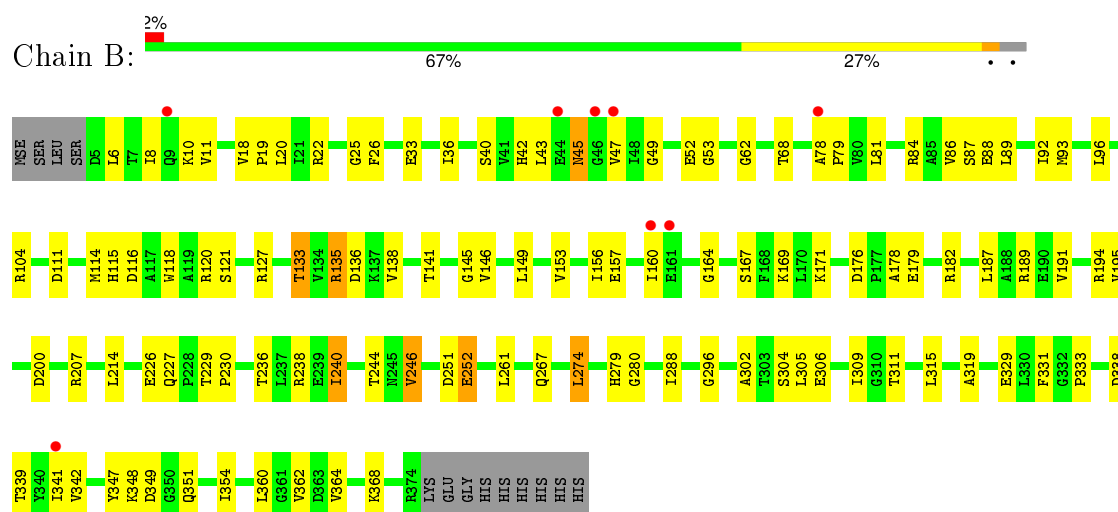
### 3 Residue-property plots

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

#### • Molecule 1: Muconate lactonizing enzyme

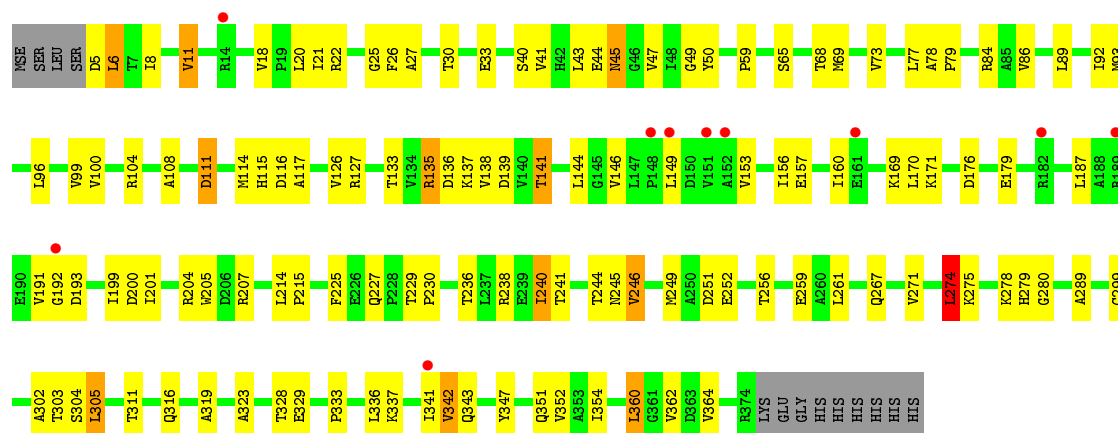


#### • Molecule 1: Muconate lactonizing enzyme

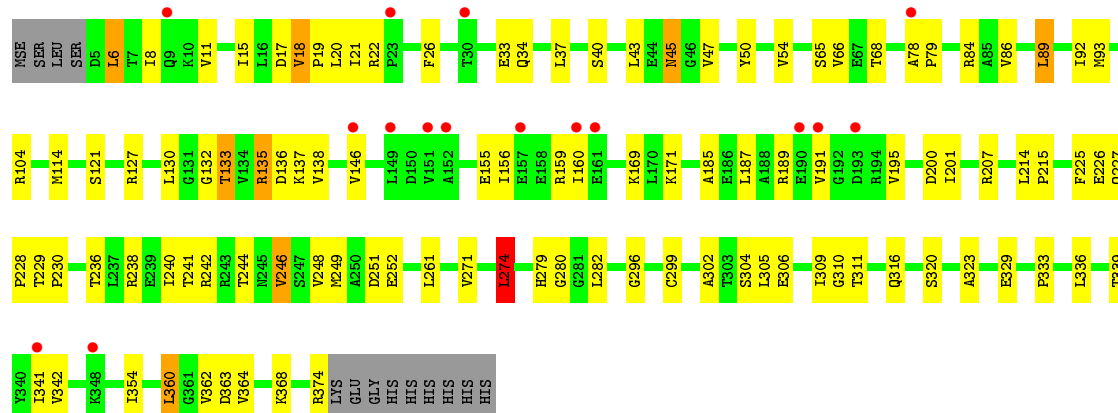


#### • Molecule 1: Muconate lactonizing enzyme

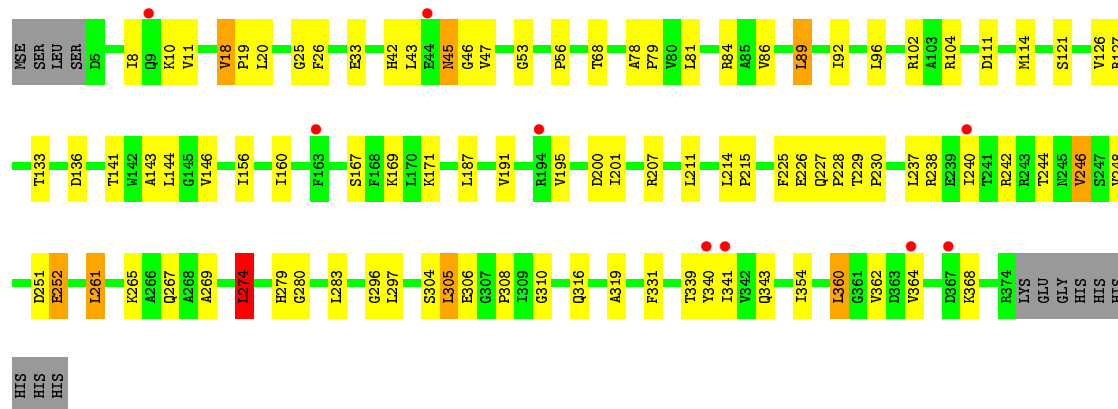




• Molecule 1: Muconate lactonizing enzyme

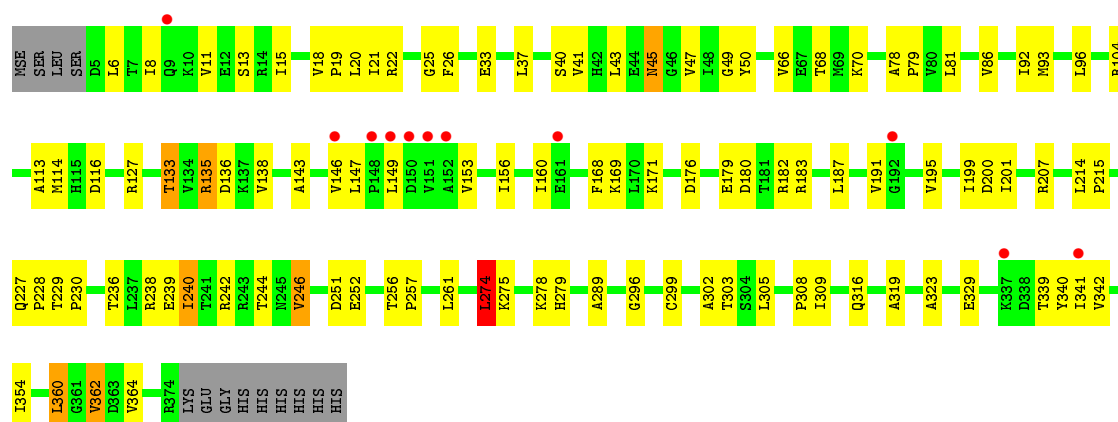


• Molecule 1: Muconate lactonizing enzyme

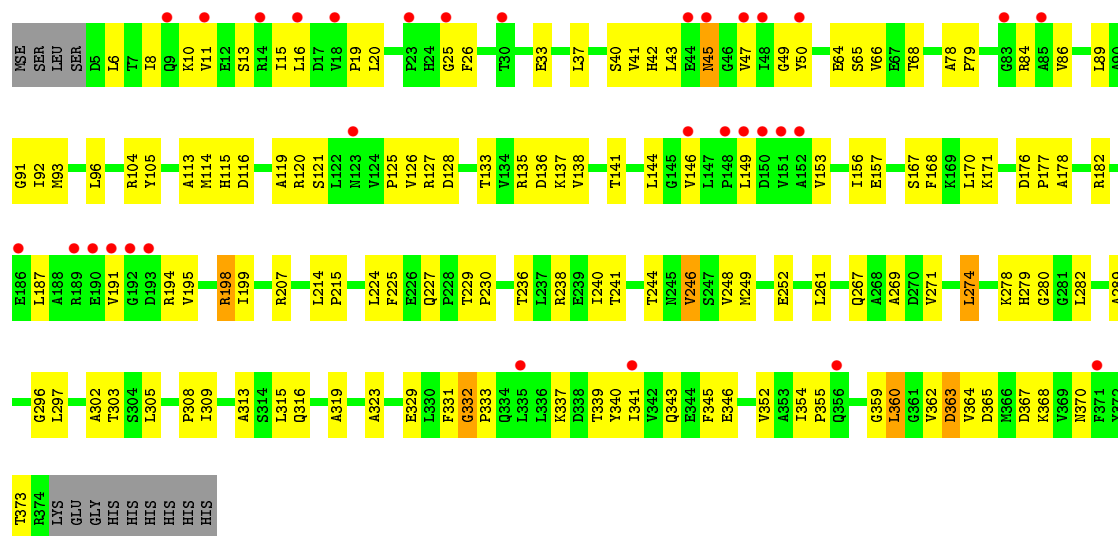


• Molecule 1: Muconate lactonizing enzyme

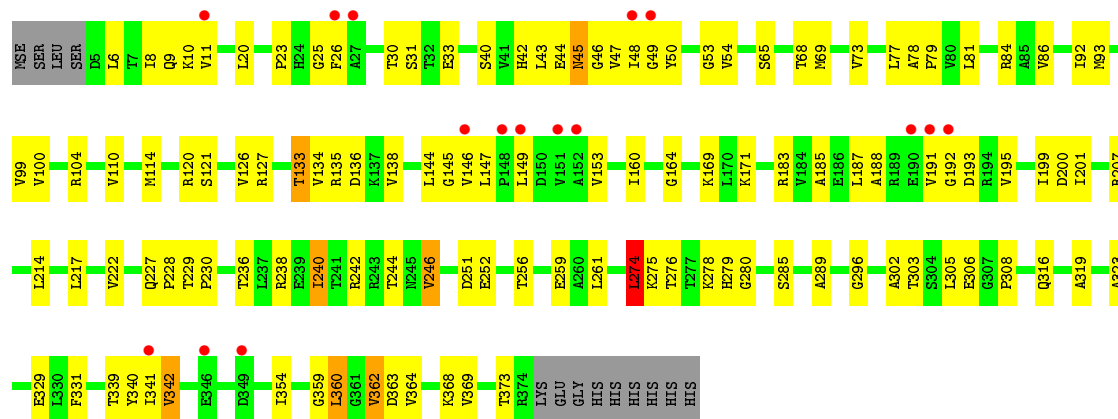




• Molecule 1: Muconate lactonizing enzyme



• Molecule 1: Muconate lactonizing enzyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.54Å 156.71Å 202.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.92 – 2.20 37.64 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.92-2.20) 99.3 (37.64-1.99)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.244 , 0.277 0.244 , 0.276	Depositor DCC
$R_{free}$ test set	8816 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 233128 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, 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	0/2853	0.64	2/3871 (0.1%)
1	B	0.34	0/2853	0.65	1/3871 (0.0%)
1	C	0.32	0/2853	0.62	1/3871 (0.0%)
1	D	0.33	0/2853	0.64	1/3871 (0.0%)
1	E	0.35	0/2853	0.65	2/3871 (0.1%)
1	F	0.34	0/2853	0.63	1/3871 (0.0%)
1	G	0.30	0/2853	0.60	0/3871
1	H	0.32	0/2853	0.62	2/3871 (0.1%)
All	All	0.33	0/22824	0.63	10/30968 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	LEU	CA-CB-CG	7.14	131.71	115.30
1	F	274	LEU	CA-CB-CG	6.42	130.07	115.30
1	A	274	LEU	CA-CB-CG	6.09	129.32	115.30
1	E	274	LEU	CA-CB-CG	5.75	128.52	115.30
1	H	274	LEU	CA-CB-CG	5.72	128.46	115.30
1	H	53	GLY	N-CA-C	-5.49	99.38	113.10
1	A	324	ILE	N-CA-C	-5.37	96.52	111.00
1	C	274	LEU	CA-CB-CG	5.29	127.47	115.30
1	E	53	GLY	N-CA-C	-5.09	100.38	113.10
1	B	53	GLY	N-CA-C	-5.02	100.55	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	2809	0	2829	102	0
1	B	2809	0	2829	111	0
1	C	2809	0	2829	107	0
1	D	2809	0	2829	98	0
1	E	2809	0	2829	96	0
1	F	2809	0	2829	99	0
1	G	2809	0	2829	125	0
1	H	2809	0	2829	110	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0
2	G	4	0	3	0	0
2	H	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	73	0	0	2	0
4	B	75	0	0	4	0
4	C	56	0	0	0	0
4	D	72	0	0	3	0
4	E	98	0	0	4	0
4	F	65	0	0	1	0
4	G	28	0	0	0	0
4	H	45	0	0	2	0
All	All	23024	0	22656	834	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 18.

All (834) 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:H:45:ASN:HD21	1:H:47:VAL:HG12	1.05	1.17
1:D:45:ASN:HD21	1:D:47:VAL:HG12	1.04	1.13
1:E:45:ASN:HD21	1:E:47:VAL:HG12	1.02	1.11
1:C:45:ASN:HD21	1:C:47:VAL:HG12	1.09	1.08
1:H:227:GLN:HG2	1:H:252:GLU:HG2	1.35	1.05
1:G:227:GLN:HG2	1:G:252:GLU:HG2	1.42	1.02
1:B:227:GLN:HG2	1:B:252:GLU:HG2	1.43	1.01
1:A:227:GLN:HG2	1:A:252:GLU:HG2	1.39	1.00
1:C:227:GLN:HG2	1:C:252:GLU:HG2	1.42	0.99
1:F:45:ASN:HD21	1:F:47:VAL:HG12	1.27	0.99
1:F:227:GLN:HG2	1:F:252:GLU:HG2	1.45	0.99
1:C:45:ASN:ND2	1:C:47:VAL:HG12	1.80	0.97
1:E:227:GLN:HG2	1:E:252:GLU:HG2	1.45	0.96
1:D:227:GLN:HG2	1:D:252:GLU:HG2	1.49	0.94
1:E:68:THR:HG22	4:E:452:HOH:O	1.68	0.93
1:B:45:ASN:HD21	1:B:47:VAL:HG12	1.33	0.92
1:C:92:ILE:HD12	1:C:114:MSE:HE1	1.51	0.92
1:A:45:ASN:ND2	1:A:47:VAL:HG12	1.85	0.92
1:E:45:ASN:ND2	1:E:47:VAL:HG12	1.85	0.90
1:A:15:ILE:HG23	1:A:66:VAL:HG21	1.54	0.89
1:D:45:ASN:ND2	1:D:47:VAL:HG12	1.88	0.87
1:G:45:ASN:HD21	1:G:47:VAL:HG12	1.40	0.86
1:A:45:ASN:HD21	1:A:47:VAL:HG12	1.40	0.86
1:G:141:THR:HG22	1:G:167:SER:OG	1.75	0.85
1:A:11:VAL:HG21	1:A:78:ALA:HB1	1.57	0.85
1:H:126:VAL:HG21	1:H:360:LEU:HD12	1.60	0.84
1:H:45:ASN:ND2	1:H:47:VAL:HG12	1.90	0.83
1:B:45:ASN:ND2	1:B:47:VAL:HG12	1.93	0.83
1:B:11:VAL:HG21	1:B:78:ALA:HB1	1.61	0.82
1:D:68:THR:HG22	4:D:390:HOH:O	1.80	0.82
1:G:227:GLN:HG2	1:G:252:GLU:CG	2.11	0.81
1:G:156:ILE:HG21	1:G:191:VAL:HG11	1.63	0.80
1:F:20:LEU:HD13	1:F:33:GLU:HA	1.62	0.80
1:E:92:ILE:HD13	1:E:114:MSE:HE1	1.62	0.80
1:B:141:THR:HG22	1:B:167:SER:OG	1.82	0.79
1:F:92:ILE:HD13	1:F:114:MSE:HE1	1.64	0.79
1:D:15:ILE:HG23	1:D:66:VAL:HG21	1.64	0.78
1:F:93:MSE:HE2	1:F:93:MSE:HA	1.65	0.77
1:E:43:LEU:HD12	1:E:47:VAL:CG1	2.14	0.77
1:D:86:VAL:HG23	1:D:114:MSE:HE2	1.66	0.77
1:B:11:VAL:CG2	1:B:78:ALA:HB1	2.15	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LEU:HD13	1:B:33:GLU:HA	1.67	0.76
1:A:11:VAL:CG2	1:A:78:ALA:HB1	2.15	0.76
1:F:227:GLN:HG2	1:F:252:GLU:CG	2.15	0.76
1:E:227:GLN:HG2	1:E:252:GLU:CG	2.16	0.76
1:G:45:ASN:ND2	1:G:47:VAL:HG12	2.00	0.76
1:B:127:ARG:HD2	1:B:133:THR:HG22	1.66	0.76
1:A:227:GLN:HG2	1:A:252:GLU:CG	2.14	0.75
1:E:45:ASN:HD21	1:E:47:VAL:CG1	1.91	0.75
1:E:127:ARG:HD2	1:E:133:THR:HG22	1.68	0.75
1:C:135:ARG:HD2	1:C:138:VAL:HG12	1.67	0.75
1:F:15:ILE:HG23	1:F:66:VAL:HG21	1.69	0.74
1:C:135:ARG:HB3	1:C:135:ARG:HH11	1.53	0.74
1:H:227:GLN:HG2	1:H:252:GLU:CG	2.15	0.73
1:B:341:ILE:HD12	1:B:364:VAL:HA	1.70	0.73
1:E:20:LEU:HD13	1:E:33:GLU:HA	1.71	0.73
1:D:227:GLN:HG2	1:D:252:GLU:CG	2.19	0.72
1:H:127:ARG:HH11	1:H:316:GLN:HE22	1.36	0.72
1:D:6:LEU:O	1:D:43:LEU:HD22	1.90	0.71
1:G:15:ILE:HG23	1:G:66:VAL:HG21	1.72	0.71
1:C:236:THR:O	1:C:240:ILE:HG23	1.89	0.71
1:C:20:LEU:HD13	1:C:33:GLU:HA	1.73	0.71
1:B:6:LEU:HG	1:B:86:VAL:HG12	1.72	0.71
1:D:11:VAL:HG21	1:D:78:ALA:HB1	1.71	0.71
1:B:227:GLN:HG2	1:B:252:GLU:CG	2.21	0.71
1:G:341:ILE:HG13	1:G:362:VAL:HG22	1.70	0.70
1:E:81:LEU:HD23	1:E:114:MSE:HE3	1.73	0.70
1:B:43:LEU:HB2	1:B:45:ASN:HD21	1.55	0.70
1:G:319:ALA:HB2	1:G:354:ILE:HG12	1.72	0.70
1:E:11:VAL:CG2	1:E:78:ALA:HB1	2.21	0.70
1:E:11:VAL:HG21	1:E:78:ALA:HB1	1.73	0.69
1:A:341:ILE:HG13	1:A:362:VAL:HG22	1.72	0.69
1:D:240:ILE:HD11	1:D:248:VAL:HG22	1.72	0.69
1:B:341:ILE:HG13	1:B:362:VAL:HG22	1.74	0.69
1:B:93:MSE:HA	1:B:93:MSE:HE2	1.73	0.69
1:G:240:ILE:HD11	1:G:248:VAL:HG22	1.74	0.69
1:A:20:LEU:HD13	1:A:33:GLU:HA	1.74	0.69
1:B:156:ILE:HG21	1:B:191:VAL:HG11	1.75	0.69
1:G:135:ARG:HD2	1:G:138:VAL:HG12	1.74	0.69
1:B:68:THR:HG22	4:B:430:HOH:O	1.93	0.68
1:B:156:ILE:O	1:B:160:ILE:HG13	1.92	0.68
1:B:339:THR:O	1:B:368:LYS:HD3	1.93	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ILE:O	1:C:160:ILE:HG13	1.93	0.68
1:C:341:ILE:HD12	1:C:364:VAL:HA	1.75	0.68
1:C:227:GLN:HG2	1:C:252:GLU:CG	2.20	0.68
1:D:20:LEU:HD13	1:D:33:GLU:HA	1.76	0.67
1:H:6:LEU:HG	1:H:86:VAL:HG12	1.76	0.67
1:E:171:LYS:HE3	4:E:407:HOH:O	1.94	0.67
1:D:11:VAL:CG2	1:D:78:ALA:HB1	2.24	0.67
1:B:214:LEU:HD13	1:B:240:ILE:HD12	1.77	0.67
1:G:41:VAL:HG23	1:G:113:ALA:HB1	1.77	0.67
1:F:341:ILE:HD12	1:F:364:VAL:HA	1.77	0.67
1:G:127:ARG:H	1:G:316:GLN:HE21	1.42	0.66
1:H:149:LEU:O	1:H:153:VAL:HG23	1.94	0.66
1:H:68:THR:HG22	4:H:403:HOH:O	1.94	0.66
1:E:26:PHE:CE1	1:E:171:LYS:HE2	2.31	0.66
1:D:341:ILE:HG13	1:D:362:VAL:HG22	1.77	0.66
1:H:127:ARG:HB3	1:H:316:GLN:HE21	1.59	0.66
1:H:11:VAL:HG21	1:H:78:ALA:HB1	1.78	0.65
1:G:10:LYS:HE3	1:G:42:HIS:CD2	2.31	0.65
1:E:339:THR:O	1:E:368:LYS:HD3	1.96	0.65
1:H:8:ILE:HD11	1:H:86:VAL:HB	1.77	0.65
1:G:127:ARG:H	1:G:316:GLN:NE2	1.94	0.65
1:E:341:ILE:HD12	1:E:364:VAL:HA	1.79	0.65
1:A:274:LEU:HD13	1:A:279:HIS:CD2	2.31	0.65
1:G:302:ALA:HA	1:G:329:GLU:HG2	1.79	0.65
1:F:227:GLN:CG	1:F:252:GLU:HG2	2.23	0.65
1:D:236:THR:O	1:D:240:ILE:HG23	1.96	0.65
1:F:11:VAL:CG2	1:F:78:ALA:HB1	2.27	0.64
1:G:65:SER:H	1:G:68:THR:HB	1.61	0.64
1:B:145:GLY:HA2	1:B:171:LYS:HD2	1.79	0.64
1:D:191:VAL:HG12	1:D:195:VAL:HG22	1.79	0.64
1:A:189:ARG:HG3	1:A:189:ARG:HH11	1.60	0.64
1:H:20:LEU:HD13	1:H:33:GLU:HA	1.78	0.64
1:H:244:THR:OG1	1:H:246:VAL:HG13	1.98	0.63
1:H:11:VAL:CG2	1:H:78:ALA:HB1	2.27	0.63
1:H:25:GLY:HA2	1:H:30:THR:HA	1.79	0.63
1:H:341:ILE:HG13	1:H:362:VAL:HG22	1.80	0.63
1:E:25:GLY:HA3	1:E:146:VAL:HG12	1.81	0.63
1:E:45:ASN:C	1:E:45:ASN:HD22	2.02	0.63
1:H:45:ASN:C	1:H:45:ASN:HD22	2.01	0.63
1:A:127:ARG:HD2	1:A:133:THR:HG22	1.80	0.63
1:G:19:PRO:HB2	1:G:337:LYS:HE3	1.81	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:ILE:HG13	1:D:241:THR:N	2.14	0.63
1:E:8:ILE:HD13	1:E:84:ARG:O	1.99	0.62
1:F:303:THR:HG22	1:F:329:GLU:HG3	1.80	0.62
1:H:339:THR:O	1:H:368:LYS:HD3	2.00	0.62
1:G:43:LEU:HD12	1:G:47:VAL:CG1	2.29	0.62
1:H:341:ILE:HD11	1:H:362:VAL:HG13	1.81	0.62
4:A:412:HOH:O	1:E:207:ARG:HD3	1.98	0.62
1:E:45:ASN:ND2	1:E:47:VAL:H	1.97	0.62
1:A:45:ASN:N	1:A:45:ASN:HD22	1.97	0.62
1:B:244:THR:OG1	1:B:246:VAL:HG13	2.00	0.62
1:D:341:ILE:HD12	1:D:364:VAL:HA	1.81	0.62
1:B:274:LEU:HD13	1:B:279:HIS:CD2	2.34	0.62
1:G:92:ILE:HD13	1:G:114:MSE:HE1	1.81	0.61
1:A:92:ILE:HD12	1:A:114:MSE:HE1	1.82	0.61
1:H:6:LEU:O	1:H:43:LEU:HD22	2.00	0.61
1:G:187:LEU:HD23	1:G:187:LEU:O	2.00	0.61
1:B:171:LYS:HE3	4:B:386:HOH:O	2.00	0.61
1:A:136:ASP:C	1:A:354:ILE:HD13	2.21	0.61
1:E:141:THR:HG22	1:E:167:SER:OG	2.01	0.61
1:H:227:GLN:CG	1:H:252:GLU:HG2	2.22	0.61
1:F:26:PHE:CE1	1:F:171:LYS:HE2	2.35	0.61
1:A:145:GLY:HA2	1:A:171:LYS:HD2	1.83	0.61
1:B:25:GLY:HA3	1:B:146:VAL:HG12	1.81	0.61
1:H:23:PRO:HA	1:H:31:SER:O	2.01	0.61
1:H:126:VAL:HG23	1:H:359:GLY:C	2.21	0.61
1:G:8:ILE:HD13	1:G:84:ARG:O	2.01	0.61
1:D:136:ASP:C	1:D:354:ILE:HD13	2.21	0.61
1:H:236:THR:O	1:H:240:ILE:HG23	2.01	0.61
1:A:339:THR:OG1	1:A:340:TYR:N	2.34	0.60
1:B:149:LEU:O	1:B:153:VAL:HG23	2.01	0.60
1:B:214:LEU:CD1	1:B:240:ILE:HD12	2.30	0.60
1:A:227:GLN:CG	1:A:252:GLU:HG2	2.24	0.60
1:G:93:MSE:HA	1:G:93:MSE:HE2	1.82	0.60
1:F:15:ILE:HG12	1:F:66:VAL:HG22	1.83	0.60
1:F:149:LEU:O	1:F:153:VAL:HG23	2.00	0.60
1:B:207:ARG:HD3	4:F:424:HOH:O	2.01	0.60
1:G:6:LEU:HG	1:G:86:VAL:HG12	1.83	0.60
1:F:40:SER:HA	1:F:49:GLY:O	2.01	0.60
1:E:237:LEU:O	1:E:240:ILE:HG12	2.02	0.60
1:H:50:TYR:CZ	1:H:364:VAL:HG21	2.37	0.60
1:H:187:LEU:HD23	1:H:187:LEU:O	2.01	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:HG23	1:A:100:VAL:HG23	1.83	0.59
1:H:191:VAL:O	1:H:193:ASP:N	2.35	0.59
1:A:153:VAL:O	1:A:157:GLU:HG2	2.02	0.59
1:F:21:ILE:HG22	1:F:22:ARG:HG3	1.84	0.59
1:D:45:ASN:ND2	1:D:47:VAL:H	2.00	0.59
1:H:341:ILE:O	1:H:342:VAL:HB	2.03	0.59
1:B:43:LEU:HB2	1:B:45:ASN:ND2	2.16	0.59
1:G:191:VAL:HG12	1:G:195:VAL:HG22	1.84	0.59
1:E:127:ARG:CD	1:E:133:THR:HG22	2.33	0.59
1:G:11:VAL:CG2	1:G:78:ALA:HB1	2.32	0.59
1:F:319:ALA:HB2	1:F:354:ILE:HG12	1.84	0.59
1:A:236:THR:O	1:A:240:ILE:HG23	2.02	0.59
1:E:211:LEU:HD23	1:E:240:ILE:HG22	1.85	0.59
1:G:153:VAL:O	1:G:157:GLU:HG2	2.02	0.59
1:B:127:ARG:CD	1:B:133:THR:HG22	2.33	0.59
1:G:274:LEU:HD13	1:G:279:HIS:CD2	2.38	0.59
1:E:89:LEU:HD12	1:E:283:LEU:HD11	1.85	0.59
1:A:229:THR:HB	1:A:230:PRO:HD2	1.85	0.59
1:B:319:ALA:HB2	1:B:354:ILE:HG12	1.85	0.58
1:B:10:LYS:HE3	1:B:42:HIS:CD2	2.38	0.58
1:C:240:ILE:HG13	1:C:241:THR:N	2.18	0.58
1:F:236:THR:O	1:F:240:ILE:HG23	2.03	0.58
1:A:8:ILE:HD13	1:A:84:ARG:O	2.03	0.58
1:A:261:LEU:HD22	1:A:265:LYS:HE3	1.85	0.58
1:D:43:LEU:HD12	1:D:47:VAL:CG1	2.33	0.58
1:C:43:LEU:HD12	1:C:47:VAL:CG1	2.34	0.58
1:F:43:LEU:HD12	1:F:47:VAL:CG1	2.33	0.58
1:H:341:ILE:CG1	1:H:362:VAL:HG22	2.33	0.58
1:F:274:LEU:HD13	1:F:279:HIS:CD2	2.39	0.58
1:C:176:ASP:OD2	1:C:179:GLU:HG3	2.03	0.58
1:H:81:LEU:HD23	1:H:114:MSE:HE3	1.84	0.58
1:A:191:VAL:HG12	1:A:195:VAL:HG22	1.86	0.58
1:G:47:VAL:HG11	1:G:121:SER:OG	2.04	0.58
1:G:149:LEU:O	1:G:153:VAL:HG23	2.02	0.58
1:A:170:LEU:HD11	1:A:187:LEU:HD22	1.86	0.58
1:E:26:PHE:HE1	1:E:171:LYS:HE2	1.68	0.57
1:F:43:LEU:HB2	1:F:47:VAL:HG12	1.86	0.57
1:D:15:ILE:HG12	1:D:66:VAL:HG22	1.86	0.57
1:B:136:ASP:C	1:B:354:ILE:HD13	2.25	0.57
1:E:10:LYS:HE3	1:E:42:HIS:CD2	2.38	0.57
1:C:116:ASP:CG	1:C:360:LEU:HD22	2.24	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HG	1:A:86:VAL:HG12	1.85	0.57
1:B:349:ASP:O	1:B:351:GLN:HG3	2.05	0.57
1:E:136:ASP:C	1:E:354:ILE:HD13	2.25	0.57
1:D:171:LYS:HE3	4:D:396:HOH:O	2.04	0.57
1:A:185:ALA:HB1	1:A:189:ARG:HH12	1.69	0.57
1:A:43:LEU:HB2	1:A:45:ASN:HD21	1.70	0.57
1:C:21:ILE:HG12	1:C:337:LYS:HA	1.87	0.57
1:H:341:ILE:HD12	1:H:364:VAL:HA	1.86	0.57
1:H:45:ASN:ND2	1:H:47:VAL:H	2.03	0.57
1:G:227:GLN:CG	1:G:252:GLU:HG2	2.25	0.57
1:B:26:PHE:CE1	1:B:171:LYS:HE2	2.39	0.57
1:B:153:VAL:O	1:B:157:GLU:HG2	2.04	0.57
1:C:229:THR:HB	1:C:230:PRO:HD2	1.87	0.57
1:A:189:ARG:HG3	1:A:189:ARG:NH1	2.19	0.56
1:F:302:ALA:HA	1:F:329:GLU:HG2	1.86	0.56
1:H:43:LEU:HD12	1:H:47:VAL:CG1	2.35	0.56
1:B:68:THR:HG23	1:E:68:THR:OG1	2.05	0.56
1:B:11:VAL:HG21	1:B:78:ALA:CB	2.35	0.56
1:G:144:LEU:HD21	1:G:156:ILE:HG13	1.87	0.56
1:H:274:LEU:HD13	1:H:279:HIS:CD2	2.40	0.56
1:C:26:PHE:CE1	1:C:171:LYS:HE2	2.41	0.56
1:E:227:GLN:CG	1:E:252:GLU:HG2	2.27	0.56
1:A:43:LEU:HD12	1:A:47:VAL:CG1	2.35	0.56
1:F:341:ILE:HG13	1:F:362:VAL:HG22	1.86	0.56
1:D:26:PHE:CE1	1:D:171:LYS:HE2	2.40	0.56
1:D:127:ARG:HE	1:D:133:THR:HG22	1.71	0.56
1:D:17:ASP:OD2	1:D:374:ARG:HB2	2.05	0.56
1:A:78:ALA:N	1:A:79:PRO:HD2	2.20	0.56
1:G:136:ASP:C	1:G:354:ILE:HD13	2.26	0.56
1:C:50:TYR:CZ	1:C:364:VAL:HG21	2.41	0.56
1:E:319:ALA:HB2	1:E:354:ILE:HG12	1.87	0.56
1:H:99:VAL:HG23	1:H:100:VAL:HG23	1.87	0.56
1:A:127:ARG:HE	1:A:133:THR:CG2	2.19	0.55
1:B:62:GLY:O	1:E:102:ARG:HD2	2.06	0.55
1:F:127:ARG:HD2	1:F:133:THR:HG22	1.88	0.55
1:F:169:LYS:HE3	1:F:200:ASP:HB2	1.88	0.55
1:H:104:ARG:O	1:H:280:GLY:HA2	2.06	0.55
1:E:308:PRO:HD2	1:E:340:TYR:CE1	2.42	0.55
1:D:18:VAL:HG22	1:D:336:LEU:HD22	1.89	0.55
1:H:199:ILE:C	1:H:199:ILE:HD12	2.26	0.55
1:F:6:LEU:HB3	1:F:86:VAL:HG12	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD21	1:A:110:VAL:HG13	1.87	0.55
1:B:341:ILE:CG1	1:B:362:VAL:HG22	2.36	0.55
1:G:19:PRO:CB	1:G:337:LYS:HE3	2.36	0.55
1:H:65:SER:O	1:H:69:MSE:HG3	2.07	0.55
1:C:137:LYS:HD2	1:C:351:GLN:NE2	2.22	0.55
1:A:229:THR:HB	1:A:230:PRO:CD	2.37	0.55
1:G:26:PHE:CE1	1:G:171:LYS:HE2	2.41	0.55
1:A:274:LEU:HD13	1:A:279:HIS:HD2	1.68	0.55
1:A:8:ILE:HD11	1:A:86:VAL:HB	1.89	0.55
1:C:311:THR:OG1	1:C:333:PRO:HD3	2.07	0.54
1:D:8:ILE:HD13	1:D:84:ARG:O	2.08	0.54
1:C:20:LEU:HD13	1:C:33:GLU:CA	2.37	0.54
1:G:11:VAL:HG21	1:G:78:ALA:HB1	1.90	0.54
1:C:78:ALA:N	1:C:79:PRO:HD2	2.22	0.54
1:G:308:PRO:HD2	1:G:340:TYR:CE1	2.42	0.54
1:E:191:VAL:HG12	1:E:195:VAL:HG22	1.89	0.54
1:B:236:THR:O	1:B:240:ILE:HG23	2.07	0.54
1:F:176:ASP:OD2	1:F:179:GLU:HG3	2.08	0.54
1:D:296:GLY:O	1:H:207:ARG:HB3	2.08	0.54
1:B:40:SER:HA	1:B:49:GLY:O	2.08	0.54
1:H:126:VAL:HG21	1:H:360:LEU:CD1	2.34	0.54
1:G:236:THR:O	1:G:240:ILE:HG23	2.06	0.54
1:G:127:ARG:HH11	1:G:316:GLN:HE22	1.56	0.54
1:B:25:GLY:C	1:B:146:VAL:HG12	2.28	0.54
1:H:92:ILE:HD13	1:H:114:MSE:HE1	1.88	0.54
1:F:13:SER:O	1:F:70:LYS:NZ	2.41	0.54
1:C:274:LEU:HD13	1:C:279:HIS:CD2	2.42	0.54
1:C:99:VAL:HG23	1:C:100:VAL:HG23	1.88	0.54
1:F:81:LEU:HD23	1:F:114:MSE:HE3	1.90	0.54
1:C:135:ARG:HB3	1:C:135:ARG:NH1	2.21	0.54
1:A:341:ILE:HG13	1:A:362:VAL:CG2	2.38	0.54
1:F:135:ARG:HD2	1:F:138:VAL:HG12	1.89	0.54
1:C:153:VAL:O	1:C:157:GLU:HG2	2.07	0.53
1:C:187:LEU:HD23	1:C:187:LEU:O	2.08	0.53
1:F:45:ASN:HD21	1:F:47:VAL:CG1	2.11	0.53
1:H:144:LEU:N	1:H:144:LEU:HD12	2.23	0.53
1:C:5:ASP:O	1:C:44:GLU:HB3	2.09	0.53
1:B:135:ARG:HD2	1:B:138:VAL:HG12	1.91	0.53
1:G:8:ILE:HD11	1:G:86:VAL:HB	1.90	0.53
1:H:339:THR:OG1	1:H:340:TYR:N	2.41	0.53
1:A:319:ALA:HB2	1:A:354:ILE:HG12	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:214:LEU:HD13	1:H:240:ILE:HD12	1.89	0.53
1:F:25:GLY:C	1:F:146:VAL:HG12	2.29	0.53
1:F:156:ILE:HG21	1:F:191:VAL:HG11	1.90	0.53
1:B:187:LEU:O	1:B:187:LEU:HD23	2.08	0.53
1:B:68:THR:HG23	1:E:68:THR:HG23	1.89	0.53
1:A:45:ASN:HD21	1:A:47:VAL:CG1	2.15	0.53
1:F:45:ASN:ND2	1:F:47:VAL:H	2.06	0.53
1:G:13:SER:HB2	1:G:37:LEU:HD11	1.89	0.53
1:D:127:ARG:HE	1:D:133:THR:CG2	2.21	0.53
1:A:25:GLY:C	1:A:146:VAL:HG12	2.29	0.53
1:C:89:LEU:HD21	1:C:115:HIS:CD2	2.44	0.53
1:G:341:ILE:HD11	1:G:362:VAL:HG13	1.90	0.53
1:D:20:LEU:HD13	1:D:33:GLU:CA	2.37	0.53
1:D:156:ILE:HG21	1:D:191:VAL:HG11	1.91	0.53
1:A:127:ARG:CD	1:A:133:THR:HG22	2.39	0.53
1:A:187:LEU:C	1:A:187:LEU:HD23	2.29	0.53
1:F:136:ASP:C	1:F:354:ILE:HD13	2.29	0.53
1:H:274:LEU:HD13	1:H:279:HIS:HD2	1.73	0.53
1:G:92:ILE:HG22	1:G:93:MSE:CE	2.39	0.53
1:C:137:LYS:CE	1:C:351:GLN:HE22	2.22	0.53
1:B:120:ARG:HH11	1:B:120:ARG:HG2	1.72	0.52
1:F:15:ILE:HG12	1:F:66:VAL:CG2	2.39	0.52
1:G:354:ILE:HD12	1:G:354:ILE:N	2.24	0.52
1:A:156:ILE:HG21	1:A:191:VAL:HG11	1.91	0.52
1:E:43:LEU:HD12	1:E:47:VAL:HG11	1.89	0.52
1:C:341:ILE:HG13	1:C:362:VAL:HG22	1.90	0.52
1:F:41:VAL:HG23	1:F:113:ALA:HB1	1.91	0.52
1:H:10:LYS:HE3	1:H:42:HIS:CD2	2.45	0.52
1:B:227:GLN:CG	1:B:252:GLU:HG2	2.29	0.52
1:D:137:LYS:N	1:D:354:ILE:HD13	2.25	0.52
1:F:207:ARG:HD3	4:H:476:HOH:O	2.09	0.52
1:C:227:GLN:CG	1:C:252:GLU:HG2	2.29	0.52
1:C:137:LYS:N	1:C:354:ILE:HD13	2.25	0.52
1:H:147:LEU:H	1:H:183:ARG:NH1	2.08	0.52
1:D:40:SER:HB3	1:D:50:TYR:CE1	2.44	0.52
1:A:5:ASP:O	1:A:44:GLU:HB3	2.10	0.52
1:A:47:VAL:HG11	1:A:121:SER:OG	2.09	0.52
1:H:81:LEU:HD21	1:H:110:VAL:HG13	1.91	0.52
1:F:127:ARG:HE	1:F:133:THR:CG2	2.23	0.52
1:B:238:ARG:HD3	1:B:267:GLN:O	2.10	0.52
1:B:189:ARG:HG3	1:B:189:ARG:HH11	1.73	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ASP:HB3	1:A:252:GLU:OE2	2.10	0.52
1:F:20:LEU:HD13	1:F:33:GLU:CA	2.36	0.52
1:H:341:ILE:O	1:H:363:ASP:O	2.28	0.52
1:G:64:GLU:OE1	1:G:105:TYR:HB2	2.10	0.52
1:A:45:ASN:N	1:A:45:ASN:ND2	2.58	0.51
1:E:11:VAL:HG21	1:E:78:ALA:CB	2.38	0.51
1:H:185:ALA:O	1:H:188:ALA:HB3	2.09	0.51
1:B:169:LYS:HE3	1:B:200:ASP:HB2	1.93	0.51
1:D:201:ILE:HB	1:D:228:PRO:HA	1.92	0.51
1:B:104:ARG:O	1:B:280:GLY:HA2	2.10	0.51
1:B:47:VAL:HG11	1:B:121:SER:OG	2.10	0.51
1:A:45:ASN:ND2	1:A:45:ASN:H	2.08	0.51
1:B:20:LEU:HD13	1:B:33:GLU:CA	2.39	0.51
1:H:9:GLN:HE21	1:H:44:GLU:HB2	1.76	0.51
1:D:45:ASN:C	1:D:45:ASN:HD22	2.14	0.51
1:G:126:VAL:HG21	1:G:360:LEU:HD13	1.92	0.51
1:D:187:LEU:HD23	1:D:187:LEU:O	2.11	0.51
1:H:217:LEU:HB3	1:H:222:VAL:HG21	1.92	0.51
1:D:65:SER:H	1:D:68:THR:HB	1.76	0.51
1:G:333:PRO:HG2	1:G:345:PHE:CE2	2.45	0.51
1:D:244:THR:OG1	1:D:246:VAL:HG13	2.10	0.51
1:G:91:GLY:HA2	1:H:134:VAL:HG22	1.92	0.51
1:H:8:ILE:HD11	1:H:86:VAL:CB	2.41	0.51
1:D:240:ILE:HD11	1:D:248:VAL:CG2	2.38	0.51
1:A:65:SER:H	1:A:68:THR:HB	1.76	0.51
1:D:274:LEU:HD13	1:D:279:HIS:CD2	2.46	0.51
1:F:11:VAL:HG23	1:F:78:ALA:HB1	1.91	0.51
1:H:302:ALA:HA	1:H:329:GLU:HG2	1.91	0.51
1:C:50:TYR:CE2	1:C:364:VAL:HG21	2.46	0.51
1:C:65:SER:H	1:C:68:THR:HB	1.76	0.51
1:A:125:PRO:HD2	1:A:128:ASP:OD2	2.11	0.51
1:E:126:VAL:HG21	1:E:360:LEU:CD1	2.40	0.51
1:E:43:LEU:HD12	1:E:47:VAL:HG13	1.92	0.50
1:F:40:SER:HB3	1:F:50:TYR:CE1	2.46	0.50
1:F:199:ILE:C	1:F:199:ILE:HD12	2.31	0.50
1:D:6:LEU:HG	1:D:86:VAL:HG12	1.91	0.50
1:B:127:ARG:HE	1:B:133:THR:CG2	2.24	0.50
1:B:111:ASP:O	1:B:115:HIS:HD2	1.95	0.50
1:C:6:LEU:HG	1:C:86:VAL:HG12	1.92	0.50
1:E:341:ILE:HG13	1:E:362:VAL:HG22	1.94	0.50
1:B:25:GLY:CA	1:B:146:VAL:HG12	2.41	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:THR:HB	1:F:230:PRO:CD	2.42	0.50
1:F:244:THR:OG1	1:F:246:VAL:HG13	2.11	0.50
1:H:229:THR:HB	1:H:230:PRO:HD2	1.93	0.50
1:B:178:ALA:O	1:B:182:ARG:HD3	2.11	0.50
1:G:115:HIS:CD2	1:G:282:LEU:HD12	2.46	0.50
1:G:229:THR:HB	1:G:230:PRO:HD2	1.92	0.50
1:C:27:ALA:CB	1:C:204:ARG:HG3	2.41	0.50
1:B:338:ASP:CG	1:B:339:THR:H	2.15	0.50
1:E:242:ARG:NH2	4:E:715:HOH:O	2.45	0.50
1:D:185:ALA:O	1:D:189:ARG:HG3	2.11	0.50
1:H:8:ILE:N	1:H:8:ILE:HD12	2.27	0.50
1:D:309:ILE:HD11	1:D:364:VAL:HG12	1.93	0.50
1:G:170:LEU:HD11	1:G:187:LEU:HD22	1.94	0.50
1:F:135:ARG:HB3	1:F:135:ARG:HH11	1.76	0.50
1:C:238:ARG:HD3	1:C:267:GLN:O	2.12	0.50
1:F:339:THR:OG1	1:F:340:TYR:N	2.44	0.50
1:D:251:ASP:HB3	1:D:252:GLU:OE2	2.12	0.49
1:H:276:THR:HA	1:H:285:SER:OG	2.12	0.49
1:E:45:ASN:HD22	1:E:47:VAL:H	1.59	0.49
1:E:127:ARG:HE	1:E:133:THR:CG2	2.25	0.49
1:B:187:LEU:C	1:B:187:LEU:HD23	2.33	0.49
1:D:229:THR:HB	1:D:230:PRO:HD2	1.94	0.49
1:G:25:GLY:C	1:G:146:VAL:HG12	2.33	0.49
1:F:43:LEU:HD12	1:F:47:VAL:HG11	1.95	0.49
1:F:8:ILE:HD11	1:F:86:VAL:HB	1.92	0.49
1:G:229:THR:HB	1:G:230:PRO:CD	2.42	0.49
1:D:169:LYS:HE3	1:D:200:ASP:HB2	1.93	0.49
1:C:139:ASP:HA	1:C:351:GLN:HG2	1.93	0.49
1:H:145:GLY:HA2	1:H:171:LYS:HD2	1.93	0.49
1:B:274:LEU:HD13	1:B:279:HIS:HD2	1.76	0.49
1:F:116:ASP:CG	1:F:360:LEU:HD22	2.33	0.49
1:C:303:THR:HG22	1:C:329:GLU:HG3	1.93	0.49
1:C:92:ILE:HD12	1:C:114:MSE:CE	2.33	0.49
1:E:8:ILE:HD11	1:E:86:VAL:CA	2.42	0.49
1:H:147:LEU:H	1:H:183:ARG:HH12	1.61	0.49
1:H:54:VAL:HG11	1:H:306:GLU:HA	1.94	0.49
1:F:11:VAL:HG21	1:F:78:ALA:HB1	1.93	0.49
1:B:191:VAL:HG12	1:B:195:VAL:HG22	1.93	0.49
1:F:229:THR:HB	1:F:230:PRO:HD2	1.93	0.49
1:A:21:ILE:HG12	1:A:337:LYS:HA	1.95	0.49
1:F:341:ILE:CG1	1:F:362:VAL:HG22	2.42	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:PRO:HD3	1:C:65:SER:HB3	1.95	0.49
1:G:26:PHE:HE1	1:G:171:LYS:HE2	1.77	0.49
1:F:25:GLY:HA3	1:F:146:VAL:HG12	1.94	0.49
1:B:88:GLU:O	1:B:92:ILE:HG13	2.13	0.49
1:G:238:ARG:HD3	1:G:267:GLN:O	2.13	0.49
1:F:187:LEU:HD23	1:F:187:LEU:C	2.33	0.49
1:G:313:ALA:HA	1:G:360:LEU:HD12	1.94	0.49
1:D:127:ARG:HH11	1:D:316:GLN:HE22	1.61	0.49
1:A:25:GLY:O	1:A:146:VAL:HG12	2.12	0.48
1:F:45:ASN:ND2	1:F:47:VAL:HG12	2.11	0.48
1:B:274:LEU:C	1:B:274:LEU:HD12	2.33	0.48
1:A:308:PRO:HD2	1:A:340:TYR:CE1	2.48	0.48
1:A:116:ASP:OD1	1:A:360:LEU:HD22	2.14	0.48
1:B:311:THR:O	1:B:315:LEU:HG	2.14	0.48
1:D:47:VAL:HG11	1:D:121:SER:OG	2.13	0.48
1:D:227:GLN:CG	1:D:252:GLU:HG2	2.34	0.48
1:C:11:VAL:CG2	1:C:78:ALA:HB1	2.43	0.48
1:E:143:ALA:HB3	1:E:331:PHE:CZ	2.48	0.48
1:F:37:LEU:HB2	1:F:66:VAL:HG23	1.95	0.48
1:H:127:ARG:HB3	1:H:316:GLN:NE2	2.28	0.48
1:A:240:ILE:HG13	1:A:241:THR:N	2.27	0.48
1:E:225:PHE:CE2	1:E:246:VAL:HG11	2.49	0.48
1:E:78:ALA:N	1:E:79:PRO:HD2	2.29	0.48
1:B:93:MSE:HE1	1:B:96:LEU:HD11	1.96	0.48
1:F:135:ARG:HB3	1:F:135:ARG:NH1	2.29	0.48
1:G:176:ASP:OD2	1:G:178:ALA:HB3	2.14	0.48
1:B:116:ASP:OD1	1:B:360:LEU:HD22	2.13	0.48
1:E:229:THR:HB	1:E:230:PRO:HD2	1.95	0.48
1:C:199:ILE:C	1:C:199:ILE:HD12	2.34	0.48
1:C:201:ILE:HD13	1:C:205:TRP:CD2	2.49	0.48
1:B:251:ASP:HB3	1:B:252:GLU:OE2	2.13	0.48
1:F:45:ASN:C	1:F:45:ASN:HD22	2.16	0.48
1:G:198:ARG:HG3	1:G:224:LEU:HB3	1.94	0.48
1:F:78:ALA:N	1:F:79:PRO:HD2	2.29	0.48
1:F:93:MSE:HE1	1:F:96:LEU:HD11	1.96	0.48
1:F:127:ARG:CD	1:F:133:THR:HG22	2.44	0.48
1:D:187:LEU:C	1:D:187:LEU:HD23	2.34	0.48
1:G:92:ILE:CD1	1:G:114:MSE:HE1	2.43	0.48
1:E:8:ILE:N	1:E:8:ILE:HD12	2.29	0.48
1:H:40:SER:HA	1:H:49:GLY:O	2.13	0.48
1:A:137:LYS:N	1:A:354:ILE:HD13	2.29	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:SER:O	1:D:305:LEU:HB2	2.13	0.47
1:F:18:VAL:O	1:F:33:GLU:HB2	2.15	0.47
1:A:125:PRO:HB3	1:A:127:ARG:NH1	2.29	0.47
1:A:11:VAL:HG21	1:A:78:ALA:CB	2.35	0.47
1:G:187:LEU:HD23	1:G:187:LEU:C	2.35	0.47
1:B:157:GLU:OE1	1:B:194:ARG:NH2	2.45	0.47
1:C:187:LEU:HD23	1:C:187:LEU:C	2.35	0.47
1:C:104:ARG:O	1:C:280:GLY:HA2	2.14	0.47
1:D:339:THR:O	1:D:368:LYS:HD3	2.13	0.47
1:E:187:LEU:HD23	1:E:187:LEU:C	2.34	0.47
1:G:240:ILE:HD11	1:G:248:VAL:CG2	2.43	0.47
1:E:84:ARG:HD2	4:E:443:HOH:O	2.14	0.47
1:H:110:VAL:O	1:H:114:MSE:HG3	2.14	0.47
1:A:276:THR:HA	1:A:285:SER:OG	2.15	0.47
1:F:341:ILE:O	1:F:342:VAL:HB	2.14	0.47
1:A:127:ARG:HE	1:A:133:THR:HG22	1.80	0.47
1:B:43:LEU:HD12	1:B:47:VAL:CG1	2.44	0.47
1:A:11:VAL:HG12	1:A:41:VAL:HG22	1.96	0.47
1:G:144:LEU:N	1:G:144:LEU:HD12	2.29	0.47
1:G:341:ILE:O	1:G:363:ASP:O	2.33	0.47
1:B:93:MSE:CA	1:B:93:MSE:HE2	2.42	0.47
1:C:229:THR:HB	1:C:230:PRO:CD	2.45	0.47
1:G:125:PRO:HD2	1:G:128:ASP:OD2	2.15	0.47
1:H:369:VAL:O	1:H:373:THR:OG1	2.29	0.47
1:F:239:GLU:HA	1:F:242:ARG:HE	1.80	0.47
1:E:8:ILE:HD11	1:E:86:VAL:CB	2.45	0.47
1:F:156:ILE:O	1:F:160:ILE:HG13	2.14	0.47
1:B:120:ARG:NH1	1:B:120:ARG:HG2	2.30	0.47
1:H:45:ASN:C	1:H:45:ASN:ND2	2.67	0.47
1:B:127:ARG:HE	1:B:133:THR:HG21	1.79	0.47
1:F:299:CYS:HB2	1:F:323:ALA:O	2.14	0.47
1:B:229:THR:HB	1:B:230:PRO:HD2	1.97	0.47
1:C:141:THR:HG23	1:C:328:THR:O	2.14	0.47
1:H:238:ARG:HE	1:H:242:ARG:HH11	1.61	0.47
1:D:299:CYS:HB2	1:D:323:ALA:O	2.14	0.47
1:C:137:LYS:HD2	1:C:351:GLN:HE22	1.80	0.47
1:G:341:ILE:HD12	1:G:364:VAL:HA	1.97	0.47
1:G:137:LYS:N	1:G:354:ILE:HD13	2.30	0.47
1:C:149:LEU:O	1:C:153:VAL:HG23	2.15	0.47
1:C:256:THR:OG1	1:C:259:GLU:HG3	2.15	0.47
1:D:156:ILE:O	1:D:160:ILE:HG13	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ILE:HD12	1:D:228:PRO:CB	2.45	0.46
1:C:69:MSE:O	1:C:73:VAL:HG23	2.15	0.46
1:G:104:ARG:O	1:G:280:GLY:HA2	2.15	0.46
1:C:144:LEU:N	1:C:144:LEU:HD12	2.30	0.46
1:E:238:ARG:HD3	1:E:267:GLN:O	2.15	0.46
1:G:289:ALA:HB1	1:G:323:ALA:HB3	1.96	0.46
1:C:68:THR:OG1	1:H:68:THR:HG23	2.15	0.46
1:D:18:VAL:CG2	1:D:336:LEU:HD22	2.46	0.46
1:D:229:THR:HB	1:D:230:PRO:CD	2.44	0.46
1:B:36:ILE:CG2	1:B:52:GLU:HG2	2.46	0.46
1:C:319:ALA:HB2	1:C:354:ILE:HG12	1.97	0.46
1:B:189:ARG:NH1	1:B:189:ARG:HG3	2.30	0.46
1:D:8:ILE:HD11	1:D:86:VAL:CA	2.45	0.46
1:F:92:ILE:CD1	1:F:114:MSE:HE1	2.41	0.46
1:B:45:ASN:N	1:B:45:ASN:HD22	2.12	0.46
1:E:308:PRO:HD2	1:E:340:TYR:CZ	2.51	0.46
1:G:339:THR:OG1	1:G:340:TYR:N	2.49	0.46
1:E:126:VAL:HG21	1:E:360:LEU:HD12	1.97	0.46
1:G:49:GLY:HA2	1:G:116:ASP:OD2	2.16	0.46
1:B:11:VAL:HG23	1:B:78:ALA:HB1	1.95	0.46
1:B:179:GLU:HG2	1:B:182:ARG:NH2	2.30	0.46
1:C:302:ALA:HA	1:C:329:GLU:HG2	1.98	0.46
1:D:214:LEU:N	1:D:215:PRO:CD	2.78	0.46
1:H:319:ALA:HB2	1:H:354:ILE:HG12	1.97	0.46
1:G:225:PHE:CE2	1:G:246:VAL:CG1	2.99	0.46
1:E:81:LEU:HG	1:E:92:ILE:HG21	1.98	0.46
1:B:160:ILE:O	1:B:164:GLY:HA2	2.16	0.46
1:H:191:VAL:HG12	1:H:195:VAL:HG22	1.97	0.46
1:E:229:THR:HB	1:E:230:PRO:CD	2.44	0.46
1:D:54:VAL:HG11	1:D:306:GLU:HA	1.98	0.46
1:A:322:LYS:O	1:A:322:LYS:HD3	2.16	0.46
1:G:37:LEU:HB2	1:G:66:VAL:HG23	1.97	0.46
1:E:339:THR:OG1	1:E:340:TYR:N	2.49	0.46
1:G:214:LEU:N	1:G:215:PRO:CD	2.79	0.46
1:G:92:ILE:HG22	1:G:93:MSE:HE2	1.97	0.46
1:F:127:ARG:HE	1:F:133:THR:HG22	1.79	0.46
1:E:274:LEU:HD13	1:E:279:HIS:CD2	2.51	0.46
1:C:135:ARG:HH11	1:C:135:ARG:CB	2.23	0.46
1:G:240:ILE:HG13	1:G:241:THR:N	2.31	0.46
1:G:41:VAL:HG23	1:G:113:ALA:CB	2.46	0.46
1:G:16:LEU:HD23	1:G:373:THR:HA	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:VAL:HB	1:G:316:GLN:HG3	1.98	0.45
1:G:20:LEU:HD13	1:G:33:GLU:HA	1.97	0.45
1:C:207:ARG:HB3	1:G:296:GLY:O	2.16	0.45
1:H:45:ASN:HD22	1:H:46:GLY:N	2.14	0.45
1:D:43:LEU:HB2	1:D:47:VAL:HG12	1.98	0.45
1:F:93:MSE:CE	1:F:93:MSE:HA	2.42	0.45
1:C:169:LYS:HE3	1:C:200:ASP:HB2	1.97	0.45
1:E:201:ILE:HB	1:E:228:PRO:HA	1.98	0.45
1:H:289:ALA:HB1	1:H:323:ALA:HB3	1.98	0.45
1:B:8:ILE:HD13	1:B:84:ARG:O	2.16	0.45
1:D:26:PHE:HE1	1:D:171:LYS:HE2	1.81	0.45
1:C:11:VAL:HG12	1:C:41:VAL:HG22	1.97	0.45
1:A:155:GLU:O	1:A:159:ARG:HG2	2.16	0.45
1:F:309:ILE:HD11	1:F:341:ILE:HD11	1.98	0.45
1:E:8:ILE:HD11	1:E:86:VAL:HB	1.98	0.45
1:G:370:ASN:N	1:G:370:ASN:HD22	2.13	0.45
1:H:8:ILE:HD13	1:H:84:ARG:O	2.16	0.45
1:A:240:ILE:HD11	1:A:248:VAL:HG22	1.99	0.45
1:H:47:VAL:HG22	1:H:48:ILE:N	2.32	0.45
1:B:68:THR:HG23	1:E:68:THR:CG2	2.46	0.45
1:C:127:ARG:HH11	1:C:316:GLN:HE22	1.65	0.45
1:A:214:LEU:N	1:A:215:PRO:CD	2.80	0.45
1:C:40:SER:HA	1:C:49:GLY:O	2.17	0.45
1:E:146:VAL:HG13	1:E:146:VAL:O	2.15	0.45
1:C:27:ALA:HB3	1:C:204:ARG:HG3	1.98	0.45
1:G:194:ARG:HG3	1:G:194:ARG:HH11	1.81	0.45
1:D:21:ILE:HG22	1:D:22:ARG:HG3	1.98	0.45
1:H:78:ALA:N	1:H:79:PRO:HD2	2.32	0.45
1:D:130:LEU:HD11	1:D:282:LEU:HD13	1.98	0.45
1:E:251:ASP:HB3	1:E:252:GLU:OE2	2.17	0.45
1:G:91:GLY:CA	1:H:134:VAL:HG22	2.47	0.45
1:F:214:LEU:N	1:F:215:PRO:CD	2.80	0.45
1:F:251:ASP:HB3	1:F:252:GLU:OE2	2.17	0.45
1:E:226:GLU:O	1:E:227:GLN:C	2.56	0.45
1:G:309:ILE:HG12	1:G:341:ILE:HD13	1.99	0.45
1:C:93:MSE:HA	1:C:93:MSE:HE2	1.97	0.45
1:A:43:LEU:HD12	1:A:47:VAL:HG11	1.99	0.44
1:C:341:ILE:CG1	1:C:362:VAL:HG22	2.46	0.44
1:H:256:THR:OG1	1:H:259:GLU:HG3	2.17	0.44
1:E:306:GLU:HB3	1:E:310:GLY:HA3	1.99	0.44
1:D:155:GLU:O	1:D:159:ARG:HG2	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:HB2	1:A:47:VAL:CG1	2.48	0.44
1:H:120:ARG:HH11	1:H:120:ARG:HG2	1.82	0.44
1:G:303:THR:HG22	1:G:329:GLU:HG3	2.00	0.44
1:C:304:SER:O	1:C:305:LEU:HB2	2.17	0.44
1:A:303:THR:OG1	1:A:306:GLU:OE1	2.29	0.44
1:E:127:ARG:NE	1:E:133:THR:HG22	2.32	0.44
1:B:309:ILE:HD11	1:B:341:ILE:HD11	1.99	0.44
1:B:194:ARG:HH11	1:B:194:ARG:HG3	1.81	0.44
1:A:240:ILE:HD11	1:A:248:VAL:CG2	2.48	0.44
1:C:126:VAL:HG21	1:C:360:LEU:HD13	1.99	0.44
1:C:274:LEU:HD12	1:C:274:LEU:C	2.37	0.44
1:C:170:LEU:HD11	1:C:187:LEU:HD22	1.98	0.44
1:D:132:GLY:O	1:D:320:SER:HB3	2.18	0.44
1:D:302:ALA:HA	1:D:329:GLU:HG2	2.00	0.44
1:H:146:VAL:HG13	1:H:146:VAL:O	2.16	0.44
1:A:143:ALA:HB3	1:A:331:PHE:CZ	2.53	0.44
1:H:47:VAL:HG11	1:H:121:SER:OG	2.17	0.44
1:C:45:ASN:HD21	1:C:47:VAL:CG1	2.01	0.44
1:G:198:ARG:HD2	1:G:198:ARG:N	2.33	0.44
1:B:169:LYS:HE3	1:B:200:ASP:CB	2.48	0.44
1:F:187:LEU:HD23	1:F:187:LEU:O	2.17	0.44
1:D:146:VAL:O	1:D:146:VAL:HG13	2.17	0.44
1:B:304:SER:HB2	1:B:306:GLU:OE2	2.16	0.44
1:C:251:ASP:HB3	1:C:252:GLU:OE2	2.17	0.44
1:C:138:VAL:HG13	1:C:354:ILE:HD11	2.00	0.44
1:B:176:ASP:OD2	1:B:179:GLU:HG3	2.17	0.44
1:D:135:ARG:HD2	1:D:138:VAL:HG12	1.98	0.44
1:A:69:MSE:O	1:A:73:VAL:HG23	2.18	0.44
1:D:11:VAL:HG21	1:D:78:ALA:CB	2.45	0.44
1:A:127:ARG:NE	1:A:133:THR:HG22	2.32	0.44
1:B:25:GLY:HA3	1:B:146:VAL:CG1	2.47	0.44
1:F:143:ALA:HA	1:F:169:LYS:O	2.18	0.44
1:A:116:ASP:CG	1:A:360:LEU:HD22	2.37	0.44
1:G:86:VAL:HG23	1:G:114:MSE:HE2	2.00	0.44
1:D:242:ARG:NH2	4:D:772:HOH:O	2.51	0.44
1:C:146:VAL:O	1:C:146:VAL:HG13	2.17	0.44
1:H:251:ASP:HB3	1:H:252:GLU:OE2	2.18	0.44
1:A:41:VAL:HG23	1:A:113:ALA:HB1	2.00	0.44
1:B:311:THR:OG1	1:B:333:PRO:HD3	2.18	0.44
1:A:244:THR:OG1	1:A:246:VAL:HG13	2.18	0.44
1:H:42:HIS:HD1	1:H:48:ILE:HG12	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ASN:C	1:E:45:ASN:ND2	2.71	0.43
1:D:78:ALA:N	1:D:79:PRO:HD2	2.32	0.43
1:A:309:ILE:CD1	1:A:341:ILE:HD11	2.48	0.43
1:H:169:LYS:HE3	1:H:200:ASP:HB2	1.99	0.43
1:A:15:ILE:HG12	1:A:66:VAL:CG2	2.48	0.43
1:B:341:ILE:HG23	1:B:341:ILE:O	2.18	0.43
1:B:26:PHE:HE1	1:B:171:LYS:HE2	1.83	0.43
1:B:22:ARG:HH11	1:B:22:ARG:HG2	1.83	0.43
1:H:42:HIS:CE1	1:H:48:ILE:HD13	2.53	0.43
1:B:341:ILE:O	1:B:342:VAL:HB	2.18	0.43
1:G:309:ILE:HD11	1:G:341:ILE:HD11	2.00	0.43
1:C:11:VAL:HG21	1:C:78:ALA:HB1	2.01	0.43
1:C:225:PHE:CE2	1:C:246:VAL:HG11	2.54	0.43
1:C:249:MSE:HA	1:C:271:VAL:O	2.19	0.43
1:D:89:LEU:HD22	1:D:114:MSE:HB3	2.00	0.43
1:C:341:ILE:O	1:C:341:ILE:HG23	2.18	0.43
1:F:341:ILE:O	1:F:341:ILE:HG23	2.18	0.43
1:A:81:LEU:HD21	1:A:110:VAL:CG1	2.48	0.43
1:E:156:ILE:HG21	1:E:191:VAL:HG11	2.00	0.43
1:H:303:THR:HG22	1:H:329:GLU:OE2	2.18	0.43
1:G:269:ALA:O	1:G:297:LEU:HD22	2.18	0.43
1:C:8:ILE:HD12	1:C:84:ARG:O	2.19	0.43
1:E:127:ARG:HE	1:E:133:THR:HG22	1.83	0.43
1:F:127:ARG:NE	1:F:133:THR:HG22	2.34	0.43
1:H:229:THR:HB	1:H:230:PRO:CD	2.48	0.43
1:E:104:ARG:O	1:E:280:GLY:HA2	2.18	0.43
1:G:365:ASP:OD1	1:G:367:ASP:HB2	2.17	0.43
1:H:11:VAL:HG23	1:H:78:ALA:HB1	2.01	0.43
1:A:86:VAL:HA	1:A:114:MSE:HE3	2.00	0.43
1:E:156:ILE:O	1:E:160:ILE:HG13	2.18	0.43
1:H:217:LEU:HB3	1:H:222:VAL:CG2	2.48	0.43
1:C:18:VAL:HG13	1:C:336:LEU:HD22	2.00	0.43
1:H:331:PHE:C	1:H:331:PHE:CD1	2.90	0.43
1:D:8:ILE:N	1:D:8:ILE:HD12	2.33	0.43
1:A:8:ILE:HD11	1:A:86:VAL:CB	2.48	0.43
1:G:278:LYS:HE3	1:G:279:HIS:CE1	2.54	0.43
1:F:274:LEU:HD13	1:F:279:HIS:HD2	1.80	0.43
1:F:8:ILE:HD11	1:F:86:VAL:CB	2.49	0.43
1:G:339:THR:O	1:G:368:LYS:HD3	2.19	0.43
1:E:244:THR:OG1	1:E:246:VAL:HG13	2.18	0.43
1:C:77:LEU:HD22	1:C:96:LEU:HD13	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:ARG:HD2	1:H:138:VAL:HG12	2.01	0.43
1:G:156:ILE:HG23	1:G:168:PHE:CE2	2.53	0.43
1:A:20:LEU:HD13	1:A:33:GLU:CA	2.45	0.43
1:B:207:ARG:HB3	1:F:296:GLY:O	2.18	0.43
1:E:240:ILE:HD11	1:E:248:VAL:HG21	2.00	0.43
1:E:304:SER:O	1:E:305:LEU:HB2	2.17	0.43
1:B:331:PHE:C	1:B:331:PHE:CD1	2.92	0.43
1:A:135:ARG:HD2	1:A:138:VAL:HG12	2.01	0.43
1:D:43:LEU:HD12	1:D:47:VAL:HG11	1.99	0.43
1:G:119:ALA:HB3	1:G:359:GLY:HA2	2.01	0.43
1:G:120:ARG:HG3	1:G:359:GLY:HA3	1.99	0.43
1:A:8:ILE:HD12	1:A:8:ILE:N	2.34	0.43
1:F:127:ARG:H	1:F:316:GLN:HE21	1.66	0.43
1:F:179:GLU:HG2	1:F:182:ARG:NH2	2.34	0.43
1:G:40:SER:HA	1:G:49:GLY:O	2.19	0.43
1:F:180:ASP:OD1	1:F:183:ARG:NH2	2.45	0.43
1:C:86:VAL:HA	1:C:114:MSE:HE3	2.01	0.43
1:C:8:ILE:CD1	1:C:84:ARG:O	2.67	0.43
1:C:137:LYS:CD	1:C:351:GLN:HE22	2.32	0.43
1:H:341:ILE:CD1	1:H:362:VAL:HG13	2.47	0.43
1:H:26:PHE:CE1	1:H:171:LYS:HE2	2.54	0.43
1:G:249:MSE:HA	1:G:271:VAL:O	2.19	0.43
1:F:201:ILE:HB	1:F:228:PRO:HA	2.01	0.43
1:H:8:ILE:HD11	1:H:86:VAL:CA	2.49	0.42
1:A:43:LEU:HB2	1:A:47:VAL:HG13	2.00	0.42
1:H:127:ARG:HD2	1:H:133:THR:HG22	2.00	0.42
1:A:127:ARG:H	1:A:316:GLN:NE2	2.17	0.42
1:F:303:THR:HG22	1:F:329:GLU:CG	2.48	0.42
1:H:308:PRO:HD2	1:H:340:TYR:CE1	2.54	0.42
1:G:11:VAL:HG23	1:G:78:ALA:HB1	1.99	0.42
1:A:169:LYS:HE3	1:A:200:ASP:HB2	2.01	0.42
1:A:238:ARG:HD3	1:A:267:GLN:O	2.19	0.42
1:C:244:THR:O	1:C:245:ASN:HB2	2.20	0.42
1:E:144:LEU:HD12	1:E:144:LEU:N	2.33	0.42
1:C:289:ALA:HB1	1:C:323:ALA:HB3	2.01	0.42
1:G:6:LEU:HD11	1:G:121:SER:CB	2.50	0.42
1:C:136:ASP:C	1:C:354:ILE:HD13	2.39	0.42
1:E:341:ILE:O	1:E:341:ILE:HG23	2.18	0.42
1:F:104:ARG:HE	1:F:256:THR:HG22	1.84	0.42
1:A:89:LEU:HD21	1:A:115:HIS:CD2	2.54	0.42
1:B:296:GLY:O	1:D:207:ARG:HB3	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASN:ND2	1:B:45:ASN:N	2.66	0.42
1:C:8:ILE:HD11	1:C:86:VAL:CA	2.49	0.42
1:H:73:VAL:HA	1:H:77:LEU:HB2	2.00	0.42
1:A:313:ALA:HA	1:A:360:LEU:HD12	2.01	0.42
1:C:214:LEU:N	1:C:215:PRO:CD	2.82	0.42
1:H:160:ILE:O	1:H:164:GLY:HA2	2.18	0.42
1:B:226:GLU:O	1:B:227:GLN:C	2.58	0.42
1:G:225:PHE:CE2	1:G:246:VAL:HG13	2.54	0.42
1:F:168:PHE:HE2	1:F:195:VAL:HG11	1.85	0.42
1:G:89:LEU:HD13	1:G:114:MSE:CB	2.49	0.42
1:D:37:LEU:HB2	1:D:66:VAL:HG23	2.01	0.42
1:E:341:ILE:HD11	1:E:362:VAL:HG13	2.02	0.42
1:A:8:ILE:HD11	1:A:86:VAL:CA	2.49	0.42
1:G:78:ALA:N	1:G:79:PRO:HD2	2.34	0.42
1:D:274:LEU:HD13	1:D:279:HIS:HD2	1.85	0.42
1:H:354:ILE:N	1:H:354:ILE:HD12	2.34	0.42
1:B:93:MSE:HA	1:B:93:MSE:CE	2.47	0.42
1:E:225:PHE:CE2	1:E:246:VAL:CG1	3.02	0.42
1:C:49:GLY:HA3	1:C:117:ALA:HB2	2.00	0.42
1:C:299:CYS:HB2	1:C:323:ALA:O	2.18	0.42
1:A:104:ARG:CZ	4:A:391:HOH:O	2.68	0.42
1:C:25:GLY:HA2	1:C:30:THR:HA	2.00	0.42
1:E:261:LEU:HD13	1:E:265:LYS:HE3	2.02	0.42
1:H:201:ILE:HB	1:H:228:PRO:HA	2.01	0.42
1:E:47:VAL:HG11	1:E:121:SER:OG	2.19	0.42
1:G:93:MSE:HE1	1:G:96:LEU:HD11	2.02	0.42
1:B:78:ALA:N	1:B:79:PRO:HD2	2.34	0.42
1:E:92:ILE:O	1:E:96:LEU:HG	2.20	0.42
1:B:141:THR:HG23	4:B:404:HOH:O	2.19	0.42
1:B:229:THR:HB	1:B:230:PRO:CD	2.49	0.42
1:C:225:PHE:CE2	1:C:246:VAL:CG1	3.02	0.42
1:C:347:TYR:CD1	1:C:352:VAL:HB	2.55	0.42
1:D:8:ILE:HD11	1:D:86:VAL:HA	2.02	0.42
1:E:45:ASN:HD22	1:E:46:GLY:N	2.18	0.42
1:G:89:LEU:HD13	1:G:114:MSE:HB2	2.01	0.42
1:A:341:ILE:O	1:A:342:VAL:HB	2.19	0.42
1:G:45:ASN:HD22	1:G:45:ASN:C	2.24	0.42
1:G:141:THR:HG21	1:G:198:ARG:NH1	2.34	0.42
1:G:15:ILE:HG12	1:G:66:VAL:HG22	2.01	0.42
1:E:244:THR:OG1	1:E:246:VAL:CG1	2.68	0.42
1:C:108:ALA:HB2	1:C:280:GLY:HA2	2.02	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:ASP:C	1:H:354:ILE:HD13	2.40	0.42
1:D:306:GLU:HB3	1:D:310:GLY:HA3	2.01	0.42
1:D:249:MSE:HA	1:D:271:VAL:O	2.20	0.42
1:C:45:ASN:N	1:C:45:ASN:HD22	2.16	0.42
1:A:341:ILE:O	1:A:363:ASP:O	2.38	0.42
1:F:8:ILE:HD11	1:F:86:VAL:CA	2.49	0.42
1:C:111:ASP:O	1:C:115:HIS:HD2	2.02	0.42
1:H:238:ARG:HE	1:H:242:ARG:NH1	2.18	0.42
1:G:315:LEU:HD13	1:G:355:PRO:HD3	2.02	0.42
1:E:214:LEU:N	1:E:215:PRO:CD	2.83	0.42
1:C:275:LYS:HB2	1:C:278:LYS:HB3	2.01	0.42
1:C:43:LEU:HD12	1:C:47:VAL:HG13	2.02	0.41
1:G:127:ARG:N	1:G:316:GLN:HE21	2.12	0.41
1:C:191:VAL:O	1:C:193:ASP:N	2.53	0.41
1:E:18:VAL:HA	1:E:19:PRO:HD3	1.84	0.41
1:G:331:PHE:O	1:G:332:GLY:C	2.59	0.41
1:G:43:LEU:HD12	1:G:47:VAL:HG11	2.01	0.41
1:B:11:VAL:HG11	1:B:81:LEU:HD22	2.01	0.41
1:F:207:ARG:HB3	1:H:296:GLY:O	2.21	0.41
1:D:45:ASN:ND2	1:D:45:ASN:C	2.73	0.41
1:D:8:ILE:HG12	1:D:114:MSE:HE3	2.01	0.41
1:D:92:ILE:HG22	1:D:93:MSE:HE2	2.02	0.41
1:F:45:ASN:C	1:F:45:ASN:ND2	2.73	0.41
1:G:89:LEU:O	1:G:93:MSE:HG2	2.21	0.41
1:C:341:ILE:O	1:C:341:ILE:HG13	2.20	0.41
1:F:135:ARG:HD2	1:F:138:VAL:CG1	2.49	0.41
1:B:115:HIS:HE1	4:B:434:HOH:O	2.03	0.41
1:B:92:ILE:CD1	1:B:114:MSE:HE1	2.50	0.41
1:E:269:ALA:O	1:E:297:LEU:HD22	2.20	0.41
1:C:8:ILE:HD11	1:C:86:VAL:HA	2.03	0.41
1:F:11:VAL:HG12	1:F:41:VAL:HG22	2.03	0.41
1:A:149:LEU:O	1:A:153:VAL:HG23	2.20	0.41
1:F:146:VAL:O	1:F:147:LEU:HD23	2.21	0.41
1:C:342:VAL:HB	1:C:343:GLN:OE1	2.20	0.41
1:D:311:THR:OG1	1:D:333:PRO:HD3	2.21	0.41
1:E:296:GLY:O	1:G:207:ARG:HB3	2.20	0.41
1:A:341:ILE:HG23	1:A:341:ILE:O	2.20	0.41
1:H:341:ILE:O	1:H:342:VAL:CB	2.65	0.41
1:D:18:VAL:HA	1:D:19:PRO:HD3	1.83	0.41
1:D:225:PHE:CE2	1:D:246:VAL:CG1	3.03	0.41
1:E:169:LYS:HE3	1:E:200:ASP:HB2	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:HIS:CG	1:B:288:ILE:HG13	2.55	0.41
1:E:211:LEU:CD2	1:E:240:ILE:HG22	2.51	0.41
1:H:69:MSE:O	1:H:73:VAL:HG23	2.20	0.41
1:D:34:GLN:HE21	1:D:305:LEU:HB3	1.84	0.41
1:D:92:ILE:CD1	1:D:114:MSE:HE1	2.50	0.41
1:B:8:ILE:HG21	1:B:81:LEU:HB3	2.01	0.41
1:G:176:ASP:HA	1:G:177:PRO:HD3	1.93	0.41
1:G:244:THR:OG1	1:G:246:VAL:HG13	2.21	0.41
1:A:43:LEU:HB2	1:A:45:ASN:ND2	2.33	0.41
1:F:18:VAL:HA	1:F:19:PRO:HD3	1.85	0.41
1:D:11:VAL:HG23	1:D:78:ALA:HB1	2.01	0.41
1:B:274:LEU:CD1	1:B:274:LEU:C	2.89	0.41
1:F:289:ALA:HB1	1:F:323:ALA:HB3	2.03	0.41
1:E:56:PRO:HG3	1:E:304:SER:HA	2.02	0.41
1:D:104:ARG:O	1:D:280:GLY:HA2	2.20	0.41
1:B:347:TYR:O	1:B:348:LYS:HB3	2.20	0.41
1:D:360:LEU:HD12	1:D:360:LEU:HA	1.89	0.41
1:B:302:ALA:HA	1:B:329:GLU:HG2	2.02	0.41
1:D:309:ILE:HD11	1:D:341:ILE:HD11	2.03	0.41
1:A:125:PRO:HB2	1:A:127:ARG:HG2	2.03	0.41
1:F:25:GLY:CA	1:F:146:VAL:HG12	2.51	0.41
1:H:201:ILE:HD12	1:H:228:PRO:CB	2.50	0.41
1:C:347:TYR:CE1	1:C:352:VAL:HB	2.55	0.41
1:A:199:ILE:C	1:A:199:ILE:HD12	2.41	0.41
1:H:93:MSE:HE2	1:H:93:MSE:HA	2.02	0.41
1:C:341:ILE:HG12	1:C:362:VAL:HG13	2.03	0.41
1:D:341:ILE:O	1:D:363:ASP:O	2.39	0.41
1:E:341:ILE:O	1:E:343:GLN:N	2.51	0.41
1:D:225:PHE:CE2	1:D:246:VAL:HG11	2.56	0.41
1:A:346:GLU:O	1:A:352:VAL:HA	2.21	0.41
1:G:8:ILE:HD11	1:G:86:VAL:CB	2.51	0.40
1:G:313:ALA:HA	1:G:360:LEU:CD1	2.51	0.40
1:H:341:ILE:HG12	1:H:362:VAL:CG2	2.51	0.40
1:D:226:GLU:CD	1:D:249:MSE:HE3	2.41	0.40
1:G:47:VAL:HG11	1:G:121:SER:HG	1.85	0.40
1:G:343:GLN:NE2	1:G:363:ASP:OD1	2.54	0.40
1:G:50:TYR:CZ	1:G:364:VAL:HG21	2.56	0.40
1:F:238:ARG:HG3	1:F:242:ARG:CZ	2.51	0.40
1:B:18:VAL:HA	1:B:19:PRO:HD3	1.86	0.40
1:B:87:SER:HA	1:B:118:TRP:CZ2	2.57	0.40
1:A:274:LEU:HD12	1:A:274:LEU:C	2.42	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ALA:O	1:A:189:ARG:NH1	2.55	0.40
1:E:240:ILE:HD11	1:E:248:VAL:CG2	2.51	0.40
1:H:275:LYS:HB2	1:H:278:LYS:HB3	2.03	0.40
1:E:127:ARG:HH11	1:E:316:GLN:HE22	1.70	0.40
1:G:126:VAL:HG23	1:G:359:GLY:C	2.42	0.40
1:F:308:PRO:HD2	1:F:340:TYR:CE1	2.57	0.40
1:G:346:GLU:O	1:G:352:VAL:HA	2.21	0.40
1:F:275:LYS:HB2	1:F:278:LYS:HB3	2.04	0.40
1:G:127:ARG:HG2	1:G:316:GLN:HE22	1.87	0.40
1:D:341:ILE:O	1:D:342:VAL:HB	2.21	0.40
1:G:274:LEU:C	1:G:274:LEU:HD12	2.41	0.40
1:D:238:ARG:NH2	1:H:242:ARG:HH21	2.19	0.40
1:G:199:ILE:C	1:G:199:ILE:HD12	2.42	0.40
1:C:22:ARG:HH11	1:C:22:ARG:HG2	1.87	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	368/383 (96%)	350 (95%)	18 (5%)	0	100	100
1	B	368/383 (96%)	349 (95%)	19 (5%)	0	100	100
1	C	368/383 (96%)	344 (94%)	22 (6%)	2 (0%)	34	35
1	D	368/383 (96%)	346 (94%)	22 (6%)	0	100	100
1	E	368/383 (96%)	350 (95%)	18 (5%)	0	100	100
1	F	368/383 (96%)	344 (94%)	24 (6%)	0	100	100
1	G	368/383 (96%)	340 (92%)	27 (7%)	1 (0%)	46	50
1	H	368/383 (96%)	343 (93%)	23 (6%)	2 (0%)	34	35
All	All	2944/3064 (96%)	2766 (94%)	173 (6%)	5 (0%)	52	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	192	GLY
1	H	192	GLY
1	G	332	GLY
1	H	342	VAL
1	C	342	VAL

### 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	291/296 (98%)	281 (97%)	10 (3%)	44	54
1	B	291/296 (98%)	281 (97%)	10 (3%)	44	54
1	C	291/296 (98%)	278 (96%)	13 (4%)	34	41
1	D	291/296 (98%)	281 (97%)	10 (3%)	44	54
1	E	291/296 (98%)	281 (97%)	10 (3%)	44	54
1	F	291/296 (98%)	279 (96%)	12 (4%)	37	45
1	G	291/296 (98%)	281 (97%)	10 (3%)	44	54
1	H	291/296 (98%)	282 (97%)	9 (3%)	47	59
All	All	2328/2368 (98%)	2244 (96%)	84 (4%)	42	52

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	68	THR
1	A	89	LEU
1	A	150	ASP
1	A	240	ILE
1	A	252	GLU
1	A	261	LEU
1	A	274	LEU
1	A	305	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	363	ASP
1	B	45	ASN
1	B	89	LEU
1	B	133	THR
1	B	135	ARG
1	B	240	ILE
1	B	246	VAL
1	B	252	GLU
1	B	261	LEU
1	B	274	LEU
1	B	305	LEU
1	C	6	LEU
1	C	11	VAL
1	C	45	ASN
1	C	111	ASP
1	C	133	THR
1	C	135	ARG
1	C	141	THR
1	C	240	ILE
1	C	246	VAL
1	C	261	LEU
1	C	274	LEU
1	C	305	LEU
1	C	360	LEU
1	D	6	LEU
1	D	18	VAL
1	D	45	ASN
1	D	89	LEU
1	D	133	THR
1	D	135	ARG
1	D	246	VAL
1	D	261	LEU
1	D	274	LEU
1	D	360	LEU
1	E	18	VAL
1	E	45	ASN
1	E	89	LEU
1	E	111	ASP
1	E	246	VAL
1	E	252	GLU
1	E	261	LEU
1	E	274	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	305	LEU
1	E	360	LEU
1	F	45	ASN
1	F	68	THR
1	F	133	THR
1	F	135	ARG
1	F	240	ILE
1	F	246	VAL
1	F	257	PRO
1	F	261	LEU
1	F	274	LEU
1	F	305	LEU
1	F	360	LEU
1	F	362	VAL
1	G	45	ASN
1	G	133	THR
1	G	182	ARG
1	G	198	ARG
1	G	246	VAL
1	G	261	LEU
1	G	274	LEU
1	G	305	LEU
1	G	360	LEU
1	G	363	ASP
1	H	45	ASN
1	H	133	THR
1	H	240	ILE
1	H	246	VAL
1	H	261	LEU
1	H	274	LEU
1	H	305	LEU
1	H	360	LEU
1	H	362	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	45	ASN
1	A	115	HIS
1	A	316	GLN
1	A	351	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	370	ASN
1	B	45	ASN
1	B	115	HIS
1	B	316	GLN
1	B	370	ASN
1	C	45	ASN
1	C	115	HIS
1	C	316	GLN
1	C	351	GLN
1	C	370	ASN
1	D	45	ASN
1	D	115	HIS
1	D	316	GLN
1	D	370	ASN
1	E	9	GLN
1	E	45	ASN
1	E	115	HIS
1	E	316	GLN
1	E	370	ASN
1	F	45	ASN
1	F	115	HIS
1	F	316	GLN
1	F	370	ASN
1	G	45	ASN
1	G	115	HIS
1	G	316	GLN
1	G	370	ASN
1	H	9	GLN
1	H	45	ASN
1	H	115	HIS
1	H	316	GLN
1	H	370	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ACY	A	384	3	1,3,3	1.74	0	0,3,3	0.00	-
2	ACY	B	384	3	1,3,3	1.28	0	0,3,3	0.00	-
2	ACY	C	384	3	1,3,3	1.30	0	0,3,3	0.00	-
2	ACY	D	384	3	1,3,3	2.30	1 (100%)	0,3,3	0.00	-
2	ACY	E	384	3	1,3,3	0.94	0	0,3,3	0.00	-
2	ACY	F	384	3	1,3,3	2.30	1 (100%)	0,3,3	0.00	-
2	ACY	G	384	3	1,3,3	1.80	0	0,3,3	0.00	-
2	ACY	H	384	3	1,3,3	1.78	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACY	A	384	3	-	0/0/0/0	0/0/0/0
2	ACY	B	384	3	-	0/0/0/0	0/0/0/0
2	ACY	C	384	3	-	0/0/0/0	0/0/0/0
2	ACY	D	384	3	-	0/0/0/0	0/0/0/0
2	ACY	E	384	3	-	0/0/0/0	0/0/0/0
2	ACY	F	384	3	-	0/0/0/0	0/0/0/0
2	ACY	G	384	3	-	0/0/0/0	0/0/0/0
2	ACY	H	384	3	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	384	ACY	CH3-C	2.30	1.52	1.48
2	F	384	ACY	CH3-C	2.30	1.52	1.48

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	364/383 (95%)	0.09	9 (2%) 61 60	26, 44, 64, 71	0
1	B	364/383 (95%)	0.07	8 (2%) 65 64	25, 43, 65, 77	0
1	C	364/383 (95%)	0.10	10 (2%) 58 57	25, 46, 70, 80	0
1	D	364/383 (95%)	0.21	16 (4%) 38 37	27, 45, 74, 86	0
1	E	364/383 (95%)	0.03	9 (2%) 61 60	23, 40, 61, 71	0
1	F	364/383 (95%)	0.09	11 (3%) 54 53	27, 45, 69, 80	0
1	G	364/383 (95%)	0.45	32 (8%) 12 11	30, 54, 79, 87	0
1	H	364/383 (95%)	0.25	16 (4%) 38 37	28, 48, 73, 85	0
All	All	2912/3064 (95%)	0.16	111 (3%) 44 43	23, 45, 72, 87	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	152	ALA	6.7
1	H	151	VAL	5.6
1	G	341	ILE	4.6
1	D	191	VAL	4.3
1	D	151	VAL	3.8
1	D	341	ILE	3.8
1	G	9	GLN	3.8
1	D	9	GLN	3.7
1	F	151	VAL	3.6
1	B	341	ILE	3.5
1	F	146	VAL	3.4
1	F	192	GLY	3.4
1	C	151	VAL	3.3
1	H	346	GLU	3.1
1	F	148	PRO	3.1
1	G	356	GLN	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	152	ALA	3.0
1	H	190	GLU	3.0
1	F	149	LEU	3.0
1	A	44	GLU	3.0
1	H	48	ILE	3.0
1	F	9	GLN	3.0
1	A	186	GLU	2.9
1	E	9	GLN	2.9
1	G	123	ASN	2.9
1	F	337	LYS	2.9
1	D	152	ALA	2.9
1	H	11	VAL	2.9
1	G	25	GLY	2.8
1	G	83	GLY	2.8
1	H	26	PHE	2.8
1	A	341	ILE	2.8
1	F	152	ALA	2.8
1	G	152	ALA	2.8
1	D	160	ILE	2.8
1	A	21	ILE	2.8
1	H	146	VAL	2.7
1	H	49	GLY	2.7
1	G	16	LEU	2.7
1	H	148	PRO	2.7
1	B	161	GLU	2.7
1	H	27	ALA	2.7
1	G	23	PRO	2.7
1	G	146	VAL	2.6
1	G	149	LEU	2.6
1	G	47	VAL	2.6
1	B	9	GLN	2.6
1	C	341	ILE	2.6
1	A	161	GLU	2.5
1	H	341	ILE	2.5
1	G	191	VAL	2.5
1	G	148	PRO	2.5
1	G	50	TYR	2.5
1	D	190	GLU	2.5
1	G	48	ILE	2.5
1	H	349	ASP	2.5
1	H	192	GLY	2.5
1	C	14	ARG	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	163	PHE	2.5
1	A	9	GLN	2.4
1	G	193	ASP	2.4
1	C	149	LEU	2.4
1	D	146	VAL	2.4
1	D	161	GLU	2.4
1	E	44	GLU	2.4
1	G	151	VAL	2.4
1	G	371	PHE	2.4
1	C	161	GLU	2.4
1	B	78	ALA	2.4
1	G	45	ASN	2.3
1	D	30	THR	2.3
1	B	46	GLY	2.3
1	C	189	ARG	2.3
1	D	78	ALA	2.3
1	A	192	GLY	2.3
1	D	348	LYS	2.3
1	G	30	THR	2.3
1	B	47	VAL	2.2
1	D	157	GLU	2.2
1	E	341	ILE	2.2
1	F	150	ASP	2.2
1	B	44	GLU	2.2
1	C	192	GLY	2.2
1	D	23	PRO	2.2
1	G	189	ARG	2.2
1	F	161	GLU	2.2
1	G	190	GLU	2.2
1	G	150	ASP	2.1
1	A	18	VAL	2.1
1	G	192	GLY	2.1
1	G	186	GLU	2.1
1	G	85	ALA	2.1
1	G	14	ARG	2.1
1	G	11	VAL	2.1
1	C	182	ARG	2.1
1	E	340	TYR	2.1
1	C	148	PRO	2.1
1	F	341	ILE	2.1
1	D	149	LEU	2.1
1	B	160	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	193	ASP	2.1
1	E	367	ASP	2.1
1	E	240	ILE	2.1
1	E	364	VAL	2.1
1	H	191	VAL	2.1
1	G	335	LEU	2.0
1	A	274	LEU	2.0
1	H	149	LEU	2.0
1	G	18	VAL	2.0
1	G	44	GLU	2.0
1	E	194	ARG	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	H	385	1/1	0.95	0.21	1.70	35,35,35,35	0
3	MG	C	385	1/1	0.93	0.18	1.69	31,31,31,31	0
3	MG	G	385	1/1	0.92	0.18	1.42	38,38,38,38	0
3	MG	F	385	1/1	0.98	0.15	1.37	31,31,31,31	0
3	MG	A	385	1/1	0.98	0.18	1.17	28,28,28,28	0
2	ACY	B	384	4/4	0.93	0.17	0.62	28,28,29,29	0
3	MG	D	385	1/1	0.93	0.17	0.45	33,33,33,33	0
2	ACY	D	384	4/4	0.90	0.16	0.06	44,45,46,46	0
2	ACY	H	384	4/4	0.94	0.14	-0.35	41,42,45,45	0
2	ACY	E	384	4/4	0.97	0.11	-0.35	31,31,32,32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	E	385	1/1	0.97	0.10	-0.62	24,24,24,24	0
3	MG	B	385	1/1	0.99	0.12	-0.74	25,25,25,25	0
2	ACY	F	384	4/4	0.94	0.12	-0.90	39,39,40,40	0
2	ACY	G	384	4/4	0.95	0.12	-1.11	48,49,49,50	0
2	ACY	C	384	4/4	0.97	0.10	-1.14	40,40,40,41	0
2	ACY	A	384	4/4	0.96	0.10	-1.26	32,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.