



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:55 PM GMT

PDB ID : 4U96  
Title : Coupling of remote alternating-access transport mechanisms for protons and substrates in the multidrug efflux pump AcrB  
Authors : Pos, K.M.  
Deposited on : 2014-08-05  
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

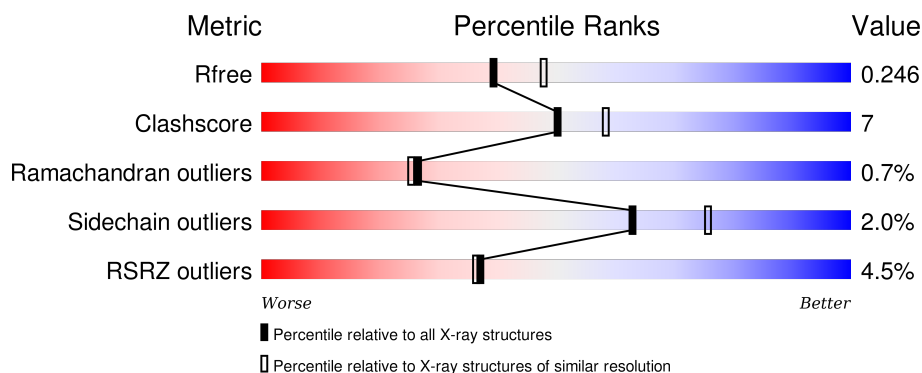
# 1 Overall quality at a glance

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	1057	<div> <div>10%</div> <div>79%18%..</div> </div>
1	B	1057	<div> <div>2%</div> <div>84%13%..</div> </div>
1	C	1057	<div> <div>%</div> <div>85%11%..</div> </div>
2	D	169	<div> <div>%</div> <div>88%5%8%</div> </div>
2	E	169	<div> <div>9%</div> <div>74%14%•10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LMT	A	1101	-	-	-	X
3	LMT	A	1102	-	-	-	X
3	LMT	A	1103	-	-	-	X
3	LMT	B	1101	-	-	-	X
3	LMT	B	1102	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28556 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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7937	5103	1312	1478	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7843	5049	1292	1458	44			
1	C	1033	Total	C	N	O	S	0	0	0
			7843	5049	1292	1458	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	971	ALA	ARG	engineered mutation	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224
B	971	ALA	ARG	engineered mutation	UNP P31224
B	1050	LEU	-	expression tag	UNP P31224
B	1051	GLU	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
B	1054	HIS	-	expression tag	UNP P31224
B	1055	HIS	-	expression tag	UNP P31224
B	1056	HIS	-	expression tag	UNP P31224
B	1057	HIS	-	expression tag	UNP P31224
C	971	ALA	ARG	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

*Continued on next page...*

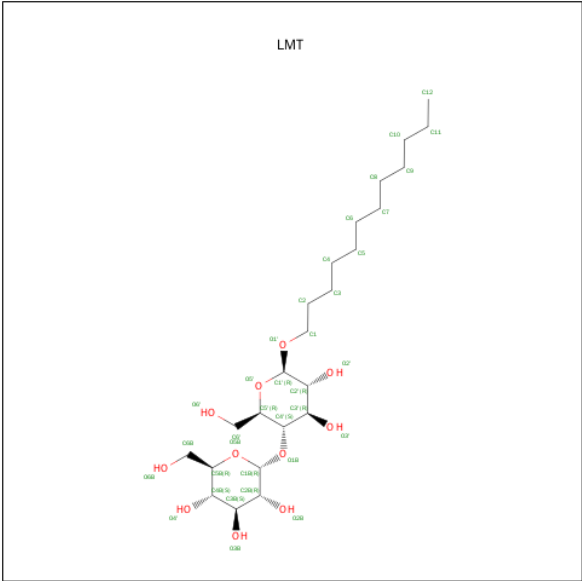
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	E	152	Total	C	N	O	S	0	0	0
			1151	726	202	222	1			

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			27	16	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

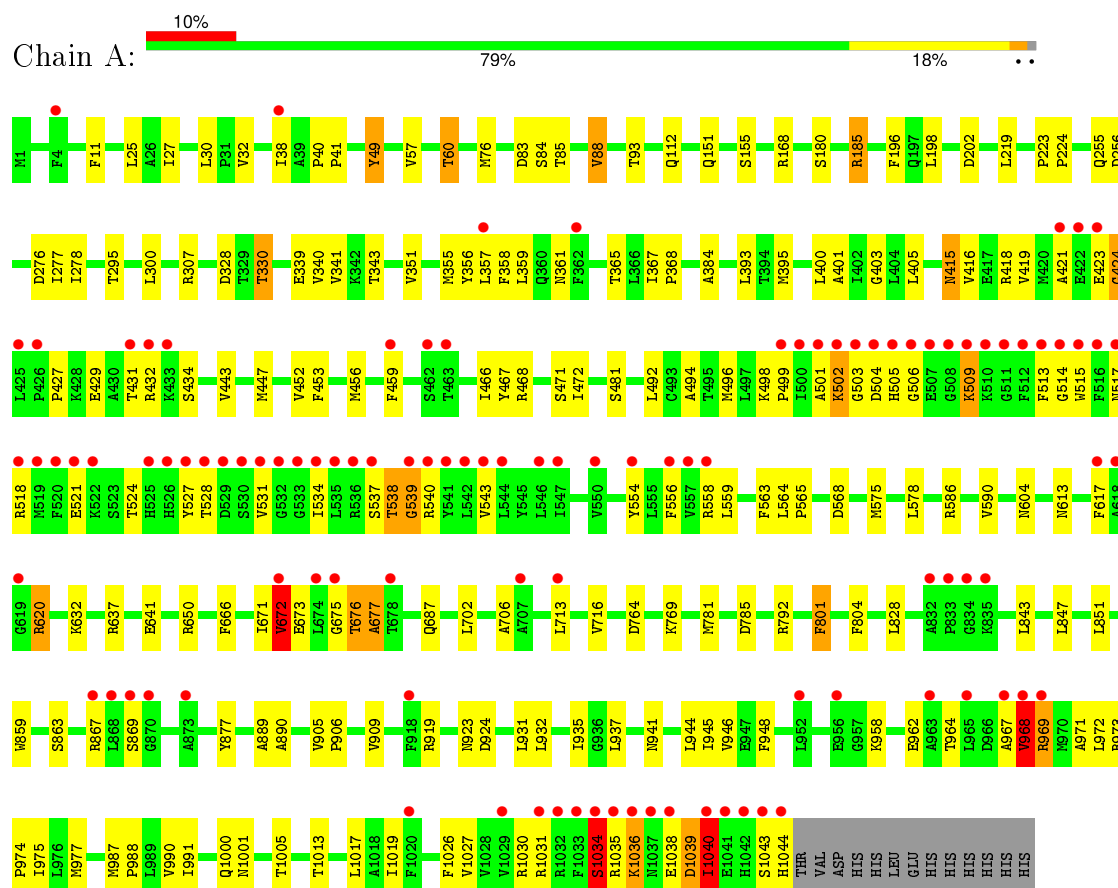
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	710	Total	O	0	0
			710	710		
4	B	668	Total	O	0	0
			668	668		
4	C	785	Total	O	0	0
			785	785		
4	D	111	Total	O	0	0
			111	111		
4	E	94	Total	O	0	0
			94	94		

### 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: Multidrug efflux pump subunit AcrB







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.79Å 160.77Å 246.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.90 – 2.20 49.14 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.90-2.20) 99.3 (49.14-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.196 , 0.246 0.197 , 0.246	Depositor DCC
$R_{free}$ test set	14502 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 290078 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	28556	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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: LMT

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	0.42	0/8089	0.58	2/10984 (0.0%)
1	B	0.40	0/7993	0.55	0/10856
1	C	0.45	0/7993	0.58	0/10856
2	D	0.36	0/1196	0.51	0/1626
2	E	0.32	0/1170	0.50	0/1591
All	All	0.42	0/26441	0.56	2/35913 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	VAL	CB-CA-C	-5.39	101.15	111.40
1	A	185	ARG	NE-CZ-NH2	-5.15	117.72	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1040	ILE	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	969	ARG	Peptide
1	C	509	LYS	Peptide

## 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	7937	0	8076	163	0
1	B	7843	0	7993	104	0
1	C	7843	0	7993	96	0
2	D	1177	0	1159	4	0
2	E	1151	0	1136	18	0
3	A	97	0	119	10	0
3	B	70	0	92	3	0
3	C	70	0	92	3	0
4	A	710	0	0	9	0
4	B	668	0	0	19	0
4	C	785	0	0	16	0
4	D	111	0	0	2	0
4	E	94	0	0	5	0
All	All	28556	0	26660	369	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 7.

All (369) 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:B:405:LEU:HD21	1:B:477:ALA:HB1	1.53	0.91
1:A:968:VAL:O	1:A:969:ARG:NH1	2.07	0.88
1:A:945:ILE:HG12	1:A:969:ARG:HH12	1.41	0.85
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.57	0.85
1:C:575:MET:HE1	1:C:617:PHE:H	1.44	0.82
1:A:641:GLU:O	1:A:650:ARG:NH2	2.12	0.82
1:A:276:ASP:OD2	1:A:620:ARG:NH1	2.13	0.81
1:A:527:TYR:OH	1:A:1019:ILE:O	1.99	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:876:LEU:HD21	1:C:932:LEU:HD11	1.63	0.80
1:A:675:GLY:O	1:A:677:ALA:N	2.16	0.79
1:C:904:VAL:HG13	1:C:938:SER:HB3	1.62	0.79
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.66	0.78
1:B:904:VAL:HG11	1:B:942:ALA:HB2	1.63	0.78
1:A:447:MET:SD	4:A:1777:HOH:O	2.41	0.78
1:A:423:GLU:HG3	1:A:424:GLY:H	1.47	0.78
1:A:890:ALA:HB2	1:C:14:VAL:HG21	1.66	0.77
2:E:15:GLY:N	4:E:254:HOH:O	2.18	0.75
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.69	0.75
1:B:968:VAL:HG11	1:B:1023:PRO:HG3	1.67	0.74
3:B:1101:LMT:H6E	3:B:1101:LMT:H5B	1.71	0.73
1:C:578:LEU:HD22	1:C:587:THR:HG22	1.70	0.72
1:A:513:PHE:O	1:A:517:ASN:ND2	2.23	0.72
1:A:969:ARG:HB3	1:A:972:LEU:HB2	1.69	0.72
1:A:568:ASP:OD2	1:A:637:ARG:NH2	2.23	0.70
1:B:919:ARG:NH1	4:B:1543:HOH:O	2.26	0.68
1:A:429:GLU:HG3	1:A:432:ARG:HH21	1.57	0.68
1:C:950:LYS:NZ	4:C:1520:HOH:O	2.27	0.68
1:A:785:ASP:OD1	4:A:1201:HOH:O	2.12	0.67
1:A:456:MET:HB2	1:A:459:PHE:HE2	1.59	0.67
1:B:168:ARG:NH1	4:B:1588:HOH:O	2.20	0.67
1:C:867:ARG:NH1	4:C:1386:HOH:O	2.28	0.67
1:C:688:ALA:O	4:C:1363:HOH:O	2.13	0.67
1:A:49:TYR:HE2	1:A:60:THR:HG21	1.58	0.67
1:B:1001:ASN:O	1:B:1005:THR:HG23	1.94	0.66
1:B:463:THR:HG22	1:B:563:PHE:HE1	1.61	0.66
1:B:919:ARG:NE	4:B:1495:HOH:O	2.29	0.66
1:A:935:ILE:HG21	3:A:1102:LMT:H111	1.78	0.66
1:A:531:VAL:HA	1:A:534:ILE:HG12	1.78	0.65
1:A:958:LYS:HE3	1:A:962:GLU:OE2	1.97	0.65
1:A:202:ASP:OD2	1:A:792:ARG:NH2	2.29	0.64
1:A:673:GLU:OE1	4:A:1407:HOH:O	2.14	0.64
1:C:587:THR:HG21	1:C:623:ASN:HA	1.79	0.64
1:C:404:LEU:HD21	1:C:937:LEU:HD21	1.79	0.64
1:A:502:LYS:O	1:A:504:ASP:N	2.31	0.64
1:A:456:MET:HB2	1:A:459:PHE:CE2	2.33	0.64
1:A:453:PHE:O	1:A:456:MET:HG2	1.98	0.64
1:A:343:THR:HB	1:A:988:PRO:HB2	1.80	0.63
1:B:396:PHE:CZ	1:B:1003:VAL:HG11	2.33	0.63
1:C:1033:PHE:O	4:C:1855:HOH:O	2.15	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:867:ARG:NH2	4:C:1424:HOH:O	2.32	0.63
1:A:554:TYR:OH	1:A:558:ARG:NH1	2.31	0.62
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.82	0.62
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.81	0.62
1:A:964:THR:O	1:A:968:VAL:N	2.28	0.62
3:A:1103:LMT:H6D	3:A:1103:LMT:H2B	1.81	0.61
1:A:456:MET:SD	1:A:932:LEU:HD13	2.40	0.61
1:A:351:VAL:O	1:A:355:MET:HG2	2.01	0.61
2:E:127:GLU:HG2	4:E:212:HOH:O	2.01	0.60
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.82	0.60
1:B:363:ARG:NH1	1:B:496:MET:O	2.35	0.60
1:A:969:ARG:HB3	1:A:972:LEU:CB	2.31	0.60
1:A:468:ARG:O	1:A:472:ILE:HG12	2.02	0.60
1:A:328:ASP:OD1	1:A:330:THR:HB	2.02	0.60
1:C:575:MET:SD	4:C:1618:HOH:O	2.57	0.60
1:C:901:VAL:O	1:C:904:VAL:HG12	2.02	0.60
1:A:418:ARG:HA	1:A:421:ALA:HB3	1.83	0.59
1:A:405:LEU:HD22	1:A:481:SER:HB2	1.85	0.59
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.84	0.59
1:B:248:LYS:NZ	4:B:1414:HOH:O	2.35	0.59
1:B:669:PRO:HB3	1:B:676:THR:H	1.67	0.58
1:A:559:LEU:HD23	1:A:923:ASN:HB2	1.85	0.58
1:A:671:ILE:HG22	1:A:672:VAL:O	2.04	0.58
1:B:247:GLY:HA2	1:B:268:ILE:HD13	1.85	0.58
1:B:416:VAL:O	1:B:420:MET:HG3	2.04	0.58
1:C:34:GLN:O	1:C:392:THR:HB	2.04	0.58
1:C:168:ARG:HD2	4:C:1388:HOH:O	2.04	0.57
1:C:498:LYS:HG3	1:C:499:PRO:HD2	1.85	0.57
1:A:877:TYR:CZ	3:A:1102:LMT:H41	2.38	0.57
1:A:1027:VAL:O	1:A:1031:ARG:HG3	2.04	0.57
2:E:21:ALA:HA	2:E:26:ARG:HD2	1.86	0.57
1:A:527:TYR:HE2	1:A:969:ARG:CG	2.17	0.57
1:C:151:GLN:NE2	1:C:279:ALA:O	2.38	0.57
1:A:49:TYR:CE2	1:A:60:THR:HG21	2.39	0.56
1:C:671:ILE:H	1:C:862:MET:HE1	1.69	0.56
1:A:415:ASN:HB3	1:A:434:SER:OG	2.05	0.56
1:B:414:GLU:HG3	1:B:977:MET:CE	2.35	0.56
1:A:946:VAL:HG13	1:A:1026:PHE:CE2	2.41	0.56
1:A:969:ARG:CB	1:A:972:LEU:HB2	2.36	0.56
1:A:41:PRO:HB3	1:A:295:THR:HG21	1.87	0.55
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LYS:NZ	4:B:1635:HOH:O	2.40	0.55
1:A:990:VAL:HG23	1:A:991:ILE:HG23	1.89	0.55
1:C:527:TYR:CE2	1:C:968:VAL:HG13	2.41	0.55
1:C:563:PHE:O	1:C:924:ASP:HB2	2.06	0.55
1:B:940:LYS:NZ	4:B:1565:HOH:O	2.40	0.55
1:C:867:ARG:NE	4:C:1424:HOH:O	2.40	0.55
1:A:343:THR:HG21	1:A:1000:GLN:OE1	2.06	0.55
1:B:335:ILE:O	1:B:339:GLU:HG2	2.06	0.55
1:A:941:ASN:HB3	1:A:975:ILE:HD13	1.90	0.54
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.88	0.54
1:C:369:THR:O	1:C:372:VAL:HG13	2.07	0.54
1:A:537:SER:OG	1:A:538:THR:N	2.39	0.54
1:B:259:ARG:NH2	4:B:1421:HOH:O	2.38	0.54
1:C:764:ASP:HB3	1:C:769:LYS:HD2	1.88	0.54
1:A:30:LEU:HD21	1:A:384:ALA:HA	1.89	0.54
1:C:151:GLN:HG2	4:C:1553:HOH:O	2.08	0.54
1:C:808:ARG:NH1	1:C:810:GLU:OE2	2.42	0.53
1:C:336:SER:O	1:C:340:VAL:HG23	2.09	0.53
1:C:64:VAL:O	1:C:67:GLN:HG2	2.08	0.53
1:A:32:VAL:HG21	3:A:1101:LMT:H11	1.91	0.53
1:A:1001:ASN:O	1:A:1005:THR:HG23	2.08	0.53
1:A:416:VAL:HG22	1:A:431:THR:HA	1.90	0.53
1:B:571:VAL:HG12	1:B:630:SER:HA	1.91	0.53
1:A:969:ARG:CG	1:A:972:LEU:HB2	2.39	0.53
1:A:419:VAL:O	1:A:423:GLU:HG2	2.08	0.53
1:B:835:LYS:O	4:B:1530:HOH:O	2.19	0.52
1:B:420:MET:HE1	1:B:499:PRO:HA	1.90	0.52
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.90	0.52
1:B:892:TYR:O	1:B:950:LYS:HE3	2.09	0.52
2:D:94:GLU:HG2	4:D:263:HOH:O	2.08	0.52
1:C:440:GLY:HA2	3:C:1102:LMT:O2'	2.10	0.52
1:A:202:ASP:CG	1:A:792:ARG:HH22	2.13	0.52
1:A:356:TYR:HA	1:A:365:THR:HG21	1.91	0.52
2:E:92:HIS:O	2:E:96:VAL:HG23	2.09	0.52
1:A:946:VAL:HG13	1:A:1026:PHE:HE2	1.75	0.52
1:B:459:PHE:O	1:B:464:GLY:HA3	2.09	0.52
1:C:799:VAL:HG23	1:C:804:PHE:HE2	1.75	0.52
1:B:510:LYS:HD2	1:B:510:LYS:H	1.74	0.52
1:A:527:TYR:CE2	1:A:969:ARG:CG	2.92	0.52
1:A:1038:GLU:HG2	1:A:1039:ASP:H	1.74	0.52
1:A:968:VAL:C	1:A:969:ARG:HD2	2.31	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.40	0.51
1:C:259:ARG:NH1	2:E:155:ASN:OD1	2.43	0.51
1:C:254:ASN:HB2	1:C:258:SER:HB3	1.93	0.51
1:B:388:PHE:CE1	1:B:472:ILE:HD12	2.46	0.51
1:C:10:ILE:HG13	1:C:11:PHE:N	2.26	0.51
1:B:979:SER:OG	1:B:1015:THR:HG21	2.11	0.51
1:A:863:SER:O	1:A:867:ARG:HG3	2.12	0.51
1:A:968:VAL:HG13	1:A:969:ARG:HD2	1.93	0.50
1:A:423:GLU:HG3	1:A:424:GLY:N	2.22	0.50
1:A:568:ASP:CG	1:A:637:ARG:HH22	2.13	0.50
1:B:764:ASP:HB3	1:B:769:LYS:HD2	1.92	0.50
1:B:445:ILE:HD13	1:B:940:LYS:HG3	1.92	0.50
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.45	0.50
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.93	0.50
1:C:57:VAL:HG13	1:C:82:SER:HB3	1.94	0.50
1:A:524:THR:O	1:A:528:THR:HG23	2.12	0.50
1:B:64:VAL:HG11	1:B:117:LEU:HB2	1.94	0.50
1:B:428:LYS:HE2	1:B:429:GLU:OE2	2.11	0.49
1:A:877:TYR:CD1	3:A:1102:LMT:H81	2.47	0.49
1:A:431:THR:HG21	1:A:494:ALA:HB2	1.94	0.49
2:E:28:ASP:O	2:E:32:ILE:HG12	2.12	0.49
1:A:38:ILE:HD11	1:A:671:ILE:HD13	1.94	0.49
1:A:307:ARG:NE	4:A:1398:HOH:O	2.42	0.49
1:B:979:SER:HA	1:B:1011:MET:HE1	1.94	0.49
2:D:163:GLU:OE2	4:D:244:HOH:O	2.20	0.49
1:A:514:GLY:HA2	1:A:517:ASN:HD22	1.78	0.48
1:A:527:TYR:CE2	1:A:969:ARG:HG3	2.48	0.48
1:C:361:ASN:C	1:C:361:ASN:OD1	2.50	0.48
1:A:604:ASN:OD1	4:A:1202:HOH:O	2.20	0.48
1:B:346:GLU:HA	1:B:349:ILE:HD12	1.95	0.48
1:A:672:VAL:O	1:A:673:GLU:HB2	2.13	0.48
1:A:1038:GLU:HG2	1:A:1039:ASP:N	2.28	0.48
1:B:1011:MET:O	1:B:1015:THR:HG23	2.13	0.48
1:C:394:THR:HG22	1:C:395:MET:HE3	1.94	0.48
1:A:575:MET:HG3	1:A:617:PHE:HD2	1.79	0.48
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.96	0.48
2:E:98:VAL:O	2:E:102:ASN:ND2	2.42	0.48
1:B:370:ILE:O	1:B:373:PRO:HD2	2.13	0.48
2:E:34:MET:CE	2:E:40:VAL:HG12	2.42	0.48
1:C:85:THR:OG1	1:C:87:THR:HG22	2.14	0.48
1:A:889:ALA:O	1:C:10:ILE:HD11	2.12	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:GLU:N	4:E:243:HOH:O	2.46	0.48
1:C:370:ILE:O	1:C:373:PRO:HD2	2.13	0.48
1:C:903:LEU:O	1:C:906:PRO:HD2	2.13	0.48
1:A:801:PHE:HA	1:A:804:PHE:CZ	2.49	0.48
1:C:447:MET:SD	1:C:887:CYS:HB3	2.53	0.48
1:A:359:LEU:HB2	1:A:365:THR:HG22	1.96	0.48
1:A:716:VAL:HA	1:A:828:LEU:O	2.13	0.48
1:A:403:GLY:HA3	1:A:937:LEU:HD11	1.96	0.48
1:A:401:ALA:O	1:A:405:LEU:HG	2.13	0.47
1:C:671:ILE:N	1:C:862:MET:HE1	2.28	0.47
1:B:982:PHE:CD2	1:B:1011:MET:HG3	2.49	0.47
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.14	0.47
1:C:898:PRO:O	1:C:902:MET:HG2	2.13	0.47
1:C:919:ARG:NH2	4:C:1754:HOH:O	2.47	0.47
1:C:456:MET:HG3	1:C:467:TYR:HB3	1.97	0.47
1:B:418:ARG:HD3	4:B:1329:HOH:O	2.13	0.47
2:E:73:VAL:HG13	2:E:74:ASN:OD1	2.15	0.47
1:C:968:VAL:HG21	1:C:1023:PRO:HG3	1.96	0.47
1:A:341:VAL:HG21	3:A:1101:LMT:H41	1.97	0.47
1:A:540:ARG:HA	1:A:543:VAL:HG23	1.96	0.47
1:B:225:VAL:HG13	1:C:781:MET:HG3	1.97	0.47
1:A:339:GLU:O	1:A:343:THR:HG23	2.15	0.47
1:C:128:SER:HB2	1:C:130:GLU:OE1	2.13	0.47
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.96	0.47
1:C:120:GLN:HG2	4:C:1715:HOH:O	2.15	0.47
1:A:575:MET:HG3	1:A:617:PHE:CD2	2.50	0.47
1:A:84:SER:HB2	4:A:1537:HOH:O	2.13	0.47
1:B:396:PHE:HZ	1:B:1003:VAL:HG11	1.79	0.47
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.97	0.47
1:B:342:LYS:O	1:B:346:GLU:HG2	2.16	0.46
1:B:115:MET:HB2	1:B:116:PRO:HD3	1.97	0.46
1:A:255:GLN:CD	1:A:255:GLN:H	2.19	0.46
1:A:1039:ASP:O	1:A:1040:ILE:HB	2.15	0.46
2:E:105:ASP:HB3	2:E:108:ALA:HB2	1.97	0.46
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.97	0.46
1:B:937:LEU:HA	1:B:937:LEU:HD23	1.76	0.46
1:C:372:VAL:HG22	1:C:373:PRO:HD3	1.98	0.46
1:A:255:GLN:HG2	1:A:256:ASP:H	1.80	0.46
1:A:969:ARG:HE	1:A:972:LEU:CA	2.28	0.46
1:A:969:ARG:HH21	1:A:972:LEU:HA	1.80	0.46
1:A:617:PHE:CZ	1:A:666:PHE:HZ	2.33	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:75:ALA:O	2:E:83:PRO:HD3	2.14	0.46
1:C:7:ASP:OD1	1:C:432:ARG:NH2	2.47	0.46
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.96	0.46
1:A:357:LEU:HD12	1:A:513:PHE:HE1	1.79	0.46
2:E:34:MET:HE2	2:E:40:VAL:HG12	1.96	0.46
2:E:40:VAL:HG13	4:E:277:HOH:O	2.16	0.46
1:C:452:VAL:HG13	1:C:884:VAL:HG21	1.96	0.46
1:A:515:TRP:HD1	1:A:518:ARG:NH2	2.13	0.46
1:B:464:GLY:O	1:B:468:ARG:HB2	2.15	0.46
2:D:100:LEU:HD11	2:D:132:LEU:HD23	1.98	0.46
1:A:987:MET:O	1:A:991:ILE:HG12	2.16	0.46
1:A:1034:SER:HB3	1:A:1036:LYS:HE3	1.98	0.45
1:C:70:ASN:HB3	4:C:1933:HOH:O	2.15	0.45
1:A:427:PRO:O	1:A:431:THR:HG22	2.15	0.45
1:B:174:ASP:HA	1:C:70:ASN:ND2	2.31	0.45
1:B:108:GLN:HE22	1:C:108:GLN:HE21	1.62	0.45
1:A:537:SER:O	1:A:539:GLY:N	2.42	0.45
1:C:414:GLU:OE1	1:C:973:ARG:HD3	2.15	0.45
1:A:358:PHE:CG	1:A:977:MET:HG2	2.51	0.45
1:C:392:THR:HG23	1:C:396:PHE:CE2	2.52	0.45
1:C:904:VAL:HG23	1:C:907:LEU:HD12	1.99	0.45
1:A:27:ILE:HD13	3:A:1101:LMT:H72	1.99	0.45
1:C:185:ARG:HB2	1:C:269:GLU:O	2.16	0.45
1:A:521:GLU:O	1:A:524:THR:HB	2.16	0.45
1:A:687:GLN:NE2	4:A:1727:HOH:O	2.50	0.45
1:B:420:MET:CE	1:B:499:PRO:HA	2.46	0.45
1:A:563:PHE:O	1:A:924:ASP:HB2	2.16	0.45
1:A:578:LEU:HD11	1:A:590:VAL:HG21	1.99	0.45
1:A:151:GLN:HE21	1:A:278:ILE:HA	1.81	0.45
1:A:969:ARG:HE	1:A:972:LEU:HB2	1.80	0.44
1:B:219:LEU:HD23	1:C:754:TRP:HZ3	1.82	0.44
1:C:852:PRO:HG2	4:C:1370:HOH:O	2.18	0.44
1:C:185:ARG:HD3	1:C:185:ARG:HA	1.75	0.44
1:C:332:PHE:HA	1:C:335:ILE:HG22	2.00	0.44
1:A:361:ASN:O	1:A:365:THR:HG23	2.17	0.44
1:C:254:ASN:N	1:C:258:SER:O	2.45	0.44
1:C:467:TYR:OH	1:C:928:GLN:OE1	2.33	0.44
1:A:905:VAL:O	1:A:909:VAL:HG23	2.17	0.44
1:B:401:ALA:O	1:B:405:LEU:HG	2.18	0.44
1:A:948:PHE:CE2	1:A:971:ALA:HB2	2.53	0.44
1:B:904:VAL:HG11	1:B:942:ALA:CB	2.43	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:PHE:CE1	1:C:395:MET:HE1	2.53	0.44
1:B:1022:VAL:HG22	1:B:1023:PRO:HD3	1.99	0.43
1:A:556:PHE:CZ	3:A:1102:LMT:H21	2.53	0.43
1:C:358:PHE:CG	1:C:977:MET:HG2	2.53	0.43
1:A:859:TRP:HB2	1:A:867:ARG:CZ	2.48	0.43
1:A:604:ASN:O	1:A:632:LYS:HD2	2.18	0.43
1:B:173:GLY:HA2	1:C:71:GLY:HA3	2.00	0.43
1:A:443:VAL:HG12	4:A:1777:HOH:O	2.18	0.43
1:B:429:GLU:H	1:B:429:GLU:CD	2.21	0.43
1:B:1:MET:N	4:B:1818:HOH:O	2.38	0.43
1:B:420:MET:HE2	4:B:1335:HOH:O	2.18	0.43
1:A:919:ARG:HD2	1:A:1005:THR:HG21	2.00	0.43
1:B:181:GLN:HG3	1:B:769:LYS:HG2	2.00	0.43
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.99	0.43
1:C:338:HIS:ND1	4:C:1940:HOH:O	2.36	0.43
1:A:586:ARG:HB3	4:A:1870:HOH:O	2.16	0.43
2:D:46:VAL:O	2:D:77:ASP:HB2	2.18	0.43
1:A:676:THR:O	1:A:677:ALA:HB3	2.19	0.43
1:A:168:ARG:HG2	1:B:69:MET:O	2.19	0.43
1:B:534:ILE:HD11	3:B:1101:LMT:H12	2.01	0.43
1:A:453:PHE:O	1:A:471:SER:OG	2.35	0.43
1:A:83:ASP:OD1	1:A:85:THR:HB	2.19	0.43
1:A:40:PRO:HA	1:A:41:PRO:HD3	1.84	0.43
1:B:637:ARG:O	1:B:643:LYS:HE3	2.19	0.43
1:B:197:GLN:NE2	4:B:1742:HOH:O	2.51	0.43
1:B:228:GLN:OE1	1:C:781:MET:HB3	2.19	0.43
1:B:167:SER:HB3	1:C:70:ASN:HB3	2.00	0.43
1:B:187:TRP:HB3	1:B:776:GLU:HG2	2.01	0.43
1:C:892:TYR:HD1	3:C:1102:LMT:H6'2	1.84	0.42
1:A:556:PHE:HZ	3:A:1102:LMT:H21	1.84	0.42
1:C:423:GLU:HB3	1:C:425:LEU:HD13	2.01	0.42
1:B:498:LYS:HG2	4:B:1277:HOH:O	2.19	0.42
1:A:76:MET:HE2	1:A:93:THR:HG22	2.00	0.42
1:A:702:LEU:HD13	1:A:851:LEU:HD11	2.01	0.42
1:A:517:ASN:O	1:A:521:GLU:HG2	2.19	0.42
1:C:950:LYS:HE2	1:C:951:ASP:OD1	2.19	0.42
1:C:443:VAL:HG12	1:C:447:MET:HE3	2.00	0.42
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.49	0.42
1:C:694:LYS:HA	1:C:694:LYS:HD3	1.87	0.42
1:C:867:ARG:CZ	4:C:1424:HOH:O	2.66	0.42
1:A:877:TYR:CE1	3:A:1102:LMT:H41	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:940:LYS:HB3	1:B:940:LYS:HE2	1.83	0.42
1:A:393:LEU:HD11	1:A:466:ILE:HG13	2.00	0.42
1:A:492:LEU:O	1:A:496:MET:HB2	2.19	0.42
1:B:851:LEU:HD23	1:B:851:LEU:HA	1.74	0.42
1:B:463:THR:HG22	1:B:563:PHE:CE1	2.47	0.42
2:E:94:GLU:O	4:E:243:HOH:O	2.22	0.42
1:B:281:PHE:CE2	1:B:324:VAL:HG11	2.55	0.42
1:A:459:PHE:CD2	1:A:467:TYR:HB2	2.55	0.42
1:B:174:ASP:HA	1:C:70:ASN:HD21	1.84	0.42
1:A:196:PHE:O	1:A:198:LEU:HG	2.19	0.42
1:A:355:MET:HB3	1:A:365:THR:HB	2.01	0.42
1:A:367:ILE:HB	1:A:368:PRO:HD3	2.02	0.42
1:A:155:SER:HB3	1:A:180:SER:H	1.85	0.42
1:B:1031:ARG:NH2	4:B:1202:HOH:O	2.53	0.42
1:A:706:ALA:HB1	1:A:716:VAL:HG11	2.02	0.42
1:A:931:LEU:HD23	1:A:931:LEU:HA	1.67	0.42
1:A:781:MET:HB3	1:C:228:GLN:OE1	2.19	0.42
1:A:969:ARG:HE	1:A:972:LEU:CB	2.33	0.42
1:B:808:ARG:NH1	4:B:1279:HOH:O	2.51	0.42
1:B:813:SER:HA	1:B:814:PRO:HD3	1.82	0.42
1:A:944:LEU:HD12	1:A:944:LEU:HA	1.84	0.41
1:A:969:ARG:NH2	1:A:975:ILE:HD12	2.35	0.41
1:B:973:ARG:HG2	1:B:977:MET:CE	2.50	0.41
1:A:498:LYS:HA	1:A:499:PRO:HD3	1.91	0.41
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.54	0.41
1:B:309:GLU:OE1	4:B:1822:HOH:O	2.21	0.41
1:B:149:MET:O	4:B:1736:HOH:O	2.21	0.41
1:B:919:ARG:HH11	1:B:921:LEU:HD11	1.85	0.41
1:A:859:TRP:CD1	1:A:867:ARG:HD3	2.55	0.41
1:B:287:SER:OG	1:B:288:GLY:N	2.52	0.41
1:C:937:LEU:HD23	1:C:937:LEU:HA	1.90	0.41
1:B:185:ARG:HD3	1:B:185:ARG:HA	1.93	0.41
1:C:587:THR:HG21	1:C:622:GLN:O	2.20	0.41
1:A:300:LEU:HD23	1:A:330:THR:HG23	2.03	0.41
1:A:400:LEU:HA	1:A:400:LEU:HD23	1.79	0.41
1:A:185:ARG:HD3	1:A:185:ARG:HA	1.69	0.41
1:B:159:ALA:HB2	1:B:177:LEU:HD22	2.02	0.41
1:C:324:VAL:HG13	1:C:326:PRO:HD3	2.03	0.41
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.84	0.41
1:A:1026:PHE:O	1:A:1030:ARG:HG2	2.20	0.41
1:A:713:LEU:HG	1:A:843:LEU:HD23	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:PHE:N	4:B:1285:HOH:O	2.53	0.41
1:B:103:ALA:O	1:B:107:VAL:HG23	2.20	0.41
1:C:584:GLN:HG2	4:C:1460:HOH:O	2.20	0.41
1:C:950:LYS:CE	3:C:1102:LMT:H6'1	2.51	0.41
1:C:889:ALA:HA	1:C:898:PRO:HG2	2.02	0.41
1:B:395:MET:O	1:B:399:VAL:HG13	2.21	0.41
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	2.03	0.41
1:B:952:LEU:HD22	1:B:958:LYS:HD2	2.02	0.41
1:C:446:ALA:HB2	1:C:482:VAL:HG13	2.03	0.41
1:A:25:LEU:HD23	3:B:1102:LMT:H21	2.03	0.41
1:A:277:ILE:HA	1:A:613:ASN:O	2.21	0.41
2:E:127:GLU:H	2:E:127:GLU:HG2	1.64	0.41
1:B:185:ARG:HD2	4:B:1232:HOH:O	2.21	0.41
2:E:89:HIS:HE1	2:E:123:ARG:CZ	2.34	0.41
1:C:438:ILE:O	1:C:442:LEU:HG	2.21	0.41
1:A:1043:SER:O	1:A:1044:HIS:CB	2.69	0.41
1:B:602:GLU:HB3	1:B:606:VAL:HG23	2.02	0.41
1:A:967:ALA:O	1:A:968:VAL:C	2.60	0.40
1:A:456:MET:CE	1:A:467:TYR:HB3	2.51	0.40
1:A:843:LEU:O	1:A:847:LEU:HG	2.20	0.40
1:A:564:LEU:HA	1:A:565:PRO:HD3	1.88	0.40
1:B:923:ASN:OD1	1:B:927:PHE:HD2	2.05	0.40
1:B:11:PHE:O	1:B:11:PHE:HD2	2.02	0.40
1:B:428:LYS:HE3	1:B:432:ARG:HH22	1.86	0.40
1:C:154:ILE:O	1:C:158:VAL:HG13	2.21	0.40
1:A:219:LEU:HD23	1:B:754:TRP:CZ3	2.56	0.40
1:B:400:LEU:HD11	1:B:1003:VAL:HG21	2.02	0.40
1:B:669:PRO:CB	1:B:676:THR:H	2.33	0.40
1:B:425:LEU:HA	1:B:426:PRO:HD3	1.93	0.40
1:A:509:LYS:O	1:A:509:LYS:NZ	2.42	0.40
1:A:968:VAL:HG13	1:A:969:ARG:CD	2.51	0.40
2:E:91:GLY:HA2	2:E:128:ILE:HD12	2.03	0.40
1:C:544:LEU:HA	1:C:544:LEU:HD13	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1042/1057 (99%)	984 (94%)	39 (4%)	19 (2%)	11	7
1	B	1031/1057 (98%)	1001 (97%)	26 (2%)	4 (0%)	39	42
1	C	1031/1057 (98%)	1000 (97%)	31 (3%)	0	100	100
2	D	154/169 (91%)	151 (98%)	3 (2%)	0	100	100
2	E	150/169 (89%)	147 (98%)	1 (1%)	2 (1%)	15	11
All	All	3408/3509 (97%)	3283 (96%)	100 (3%)	25 (1%)	26	25

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	503	GLY
1	A	506	GLY
1	A	538	THR
1	A	672	VAL
1	A	676	THR
1	A	1034	SER
1	A	1035	ARG
1	A	1036	LYS
1	A	1039	ASP
1	B	659	LYS
1	B	676	THR
1	A	502	LYS
1	A	869	SER
1	A	509	LYS
1	A	1040	ILE
1	B	675	GLY
2	E	26	ARG
1	A	501	ALA
1	A	677	ALA
2	E	105	ASP
1	A	424	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	620	ARG
1	A	539	GLY
1	A	968	VAL
1	B	994	GLY

### 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	849/862 (98%)	837 (99%)	12 (1%)	74	85
1	B	838/862 (97%)	822 (98%)	16 (2%)	65	77
1	C	838/862 (97%)	816 (97%)	22 (3%)	54	66
2	D	120/132 (91%)	118 (98%)	2 (2%)	68	81
2	E	117/132 (89%)	114 (97%)	3 (3%)	54	66
All	All	2762/2850 (97%)	2707 (98%)	55 (2%)	63	76

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	49	TYR
1	A	60	THR
1	A	112	GLN
1	A	330	THR
1	A	415	ASN
1	A	452	VAL
1	A	505	HIS
1	A	672	VAL
1	A	801	PHE
1	A	968	VAL
1	A	1034	SER
1	B	11	PHE
1	B	30	LEU
1	B	48	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	49	TYR
1	B	81	ASN
1	B	128	SER
1	B	132	SER
1	B	261	LEU
1	B	293	LEU
1	B	324	VAL
1	B	365	THR
1	B	472	ILE
1	B	510	LYS
1	B	530	SER
1	B	976	LEU
1	B	987	MET
1	C	10	ILE
1	C	11	PHE
1	C	49	TYR
1	C	87	THR
1	C	152	GLU
1	C	324	VAL
1	C	361	ASN
1	C	392	THR
1	C	394	THR
1	C	448	VAL
1	C	452	VAL
1	C	482	VAL
1	C	483	LEU
1	C	510	LYS
1	C	540	ARG
1	C	584	GLN
1	C	587	THR
1	C	641	GLU
1	C	676	THR
1	C	876	LEU
1	C	968	VAL
1	C	993	THR
2	D	45	VAL
2	D	139	VAL
2	E	28	ASP
2	E	45	VAL
2	E	139	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	112	GLN
1	A	360	GLN
1	A	517	ASN
1	A	726	GLN
1	B	81	ASN
1	B	108	GLN
1	C	124	GLN
1	C	569	GLN
2	E	89	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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	$\# Z  > 2$
3	LMT	A	1101	-	36,36,36	0.36	0	47,47,47	1.09	4 (8%)
3	LMT	A	1102	-	36,36,36	0.52	1 (2%)	47,47,47	1.18	6 (12%)
3	LMT	A	1103	-	28,28,36	0.50	0	39,39,47	1.41	5 (12%)
3	LMT	B	1101	-	36,36,36	0.39	0	47,47,47	1.00	3 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LMT	B	1102	-	36,36,36	0.50	0	47,47,47	1.38	4 (8%)
3	LMT	C	1101	-	36,36,36	0.43	0	47,47,47	0.92	2 (4%)
3	LMT	C	1102	-	36,36,36	0.55	1 (2%)	47,47,47	1.03	2 (4%)

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
3	LMT	A	1101	-	-	0/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	0/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	0/13/53/61	0/2/2/2
3	LMT	B	1101	-	-	0/21/61/61	0/2/2/2
3	LMT	B	1102	-	-	0/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	0/21/61/61	0/2/2/2
3	LMT	C	1102	-	-	0/21/61/61	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	LMT	O1'-C1'	2.02	1.43	1.40
3	C	1102	LMT	O1'-C1'	2.17	1.44	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	LMT	C1'-O5'-C5'	-2.70	108.51	113.75
3	A	1103	LMT	O5'-C5'-C4'	-2.51	104.44	109.75
3	A	1101	LMT	C1B-O1B-C4'	-2.46	111.57	118.01
3	A	1103	LMT	O5'-C1'-O1'	-2.32	104.46	110.05
3	A	1101	LMT	O5'-C1'-O1'	-2.29	104.54	110.05
3	B	1102	LMT	O5'-C1'-C2'	-2.27	105.61	110.28
3	B	1101	LMT	C4B-C3B-C2B	-2.15	106.77	110.79
3	C	1101	LMT	C1B-O1B-C4'	-2.11	112.50	118.01
3	A	1102	LMT	O5B-C5B-C4B	2.03	113.49	109.68
3	A	1102	LMT	C2'-C3'-C4'	2.04	114.08	109.60
3	B	1101	LMT	O1B-C1B-C2B	2.04	113.08	108.10
3	C	1101	LMT	O1'-C1'-C2'	2.18	110.80	108.04
3	B	1101	LMT	O5B-C5B-C4B	2.23	113.87	109.68
3	A	1103	LMT	C6'-C5'-C4'	2.26	119.82	113.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	LMT	O1'-C1'-C2'	2.27	110.91	108.04
3	B	1102	LMT	C1B-C2B-C3B	2.27	114.45	109.97
3	A	1102	LMT	O5B-C5B-C6B	2.31	112.18	106.36
3	A	1103	LMT	O1'-C1'-C2'	2.34	110.99	108.04
3	A	1102	LMT	O5'-C5'-C6'	2.47	112.60	106.36
3	A	1101	LMT	C3B-C4B-C5B	2.50	114.55	110.20
3	A	1102	LMT	C1'-C2'-C3'	2.52	114.94	109.97
3	C	1102	LMT	O1B-C1B-C2B	2.98	115.36	108.10
3	A	1102	LMT	C1B-O5B-C5B	3.44	120.42	113.75
3	C	1102	LMT	O1'-C1'-C2'	3.62	112.61	108.04
3	A	1103	LMT	O1B-C4'-C5'	4.85	122.06	109.32
3	B	1102	LMT	O1'-C1'-C2'	6.67	116.47	108.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	LMT	3	0
3	A	1102	LMT	6	0
3	A	1103	LMT	1	0
3	B	1101	LMT	2	0
3	B	1102	LMT	1	0
3	C	1102	LMT	3	0

## 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	1044/1057 (98%)	0.16	106 (10%) <b>9</b> <b>8</b>	15, 42, 110, 164	0
1	B	1033/1057 (97%)	-0.37	18 (1%) <b>73</b> <b>72</b>	16, 37, 59, 92	0
1	C	1033/1057 (97%)	-0.45	11 (1%) <b>82</b> <b>82</b>	16, 30, 55, 104	0
2	D	156/169 (92%)	-0.34	2 (1%) <b>79</b> <b>78</b>	27, 38, 66, 99	0
2	E	152/169 (89%)	0.32	16 (10%) <b>8</b> <b>7</b>	36, 50, 82, 94	0
All	All	3418/3509 (97%)	-0.20	153 (4%) <b>37</b> <b>36</b>	15, 37, 82, 164	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	506	GLY	10.2
1	A	509	LYS	9.7
1	A	512	PHE	9.6
1	A	508	GLY	9.1
1	A	505	HIS	8.6
1	A	507	GLU	8.2
1	A	513	PHE	8.0
1	A	503	GLY	7.9
1	A	540	ARG	7.9
1	A	534	ILE	7.3
1	A	511	GLY	7.1
1	A	501	ALA	7.1
1	A	515	TRP	7.0
1	A	543	VAL	6.6
1	A	541	TYR	6.3
1	A	421	ALA	6.2
1	A	510	LYS	6.2
1	A	1035	ARG	6.0
1	A	516	PHE	5.8
1	A	869	SER	5.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	514	GLY	5.6
2	D	11	GLY	5.4
1	A	529	ASP	5.4
1	A	519	MET	5.3
1	A	1029	VAL	5.2
1	A	518	ARG	5.2
1	A	539	GLY	5.2
1	A	504	ASP	5.2
1	A	870	GLY	5.0
1	A	1037	ASN	4.8
1	A	502	LYS	4.5
1	A	554	TYR	4.4
1	A	422	GLU	4.4
1	A	433	LYS	4.4
1	A	542	LEU	4.3
1	A	678	THR	4.2
1	A	500	ILE	4.2
1	A	536	ARG	4.1
1	A	968	VAL	4.0
1	A	531	VAL	3.9
1	A	517	ASN	3.9
1	A	425	LEU	3.9
1	A	672	VAL	3.9
1	A	619	GLY	3.8
1	C	362	PHE	3.8
1	A	1036	LYS	3.8
1	A	533	GLY	3.8
1	B	499	PRO	3.6
1	A	462	SER	3.6
1	A	520	PHE	3.5
1	A	535	LEU	3.5
1	A	423	GLU	3.5
1	B	498	LYS	3.5
1	A	868	LEU	3.5
1	A	617	PHE	3.5
2	E	35	ALA	3.5
1	A	550	VAL	3.4
2	E	68	LYS	3.4
1	A	1044	HIS	3.3
1	A	4	PHE	3.2
1	A	963	ALA	3.2
1	A	1034	SER	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	833	PRO	3.2
1	A	1038	GLU	3.2
1	A	499	PRO	3.2
1	A	873	ALA	3.2
1	B	501	ALA	3.2
1	A	965	LEU	3.1
1	A	1031	ARG	3.1
1	A	918	PHE	3.1
1	A	38	ILE	3.1
1	B	508	GLY	3.1
1	A	459	PHE	3.1
1	A	1033	PHE	3.1
1	A	431	THR	3.0
1	A	1042	HIS	3.0
1	A	952	LEU	3.0
1	A	558	ARG	3.0
1	A	526	HIS	3.0
2	E	32	ILE	3.0
1	A	530	SER	3.0
1	A	834	GLY	3.0
1	A	832	ALA	2.9
1	B	653	ARG	2.9
1	C	1032	ARG	2.9
1	A	522	LYS	2.9
1	A	527	TYR	2.9
2	D	12	SER	2.9
1	A	525	HIS	2.9
2	E	66	LEU	2.8
1	A	1040	ILE	2.8
1	A	546	LEU	2.8
1	A	967	ALA	2.8
2	E	166	GLN	2.8
1	A	713	LEU	2.7
1	A	1020	PHE	2.7
1	C	510	LYS	2.7
1	A	362	PHE	2.7
1	B	514	GLY	2.7
2	E	37	GLY	2.7
2	E	138	ASP	2.6
1	A	537	SER	2.6
1	B	510	LYS	2.6
1	C	428	LYS	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	544	LEU	2.6
2	E	31	ARG	2.6
1	A	1041	GLU	2.6
2	E	165	LEU	2.5
1	B	674	LEU	2.5
1	A	426	PRO	2.5
2	E	28	ASP	2.5
1	C	618	ALA	2.5
1	A	432	ARG	2.5
1	B	955	LYS	2.4
1	B	511	GLY	2.4
1	A	956	GLU	2.4
1	A	835	LYS	2.4
2	E	139	VAL	2.4
1	A	618	ALA	2.3
1	B	554	TYR	2.3
1	B	660	ASP	2.3
1	A	556	PHE	2.3
1	B	659	LYS	2.3
2	E	100	LEU	2.3
1	A	969	ARG	2.3
1	C	429	GLU	2.3
1	A	532	GLY	2.3
1	A	707	ALA	2.3
1	A	674	LEU	2.3
1	A	1043	SER	2.2
1	B	600	THR	2.2
1	A	521	GLU	2.2
2	E	97	GLU	2.2
2	E	36	ASN	2.2
1	C	811	TYR	2.2
1	B	957	GLY	2.2
1	A	557	VAL	2.2
1	A	1032	ARG	2.2
1	A	357	LEU	2.2
1	A	547	ILE	2.1
1	B	558	ARG	2.1
1	C	797	GLN	2.1
1	B	557	VAL	2.1
2	E	67	LEU	2.1
1	C	619	GLY	2.1
1	C	512	PHE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	463	THR	2.1
1	A	528	THR	2.1
1	C	498	LYS	2.1
2	E	141	ALA	2.0
1	B	657	GLN	2.0
1	A	867	ARG	2.0
1	A	675	GLY	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	LMT	A	1103	27/35	0.85	0.17	3.88	69,82,90,92	0
3	LMT	A	1101	35/35	0.91	0.16	3.39	27,55,81,90	0
3	LMT	A	1102	35/35	0.62	0.43	3.02	100,114,125,127	0
3	LMT	B	1102	35/35	0.86	0.23	3.00	40,67,83,88	0
3	LMT	B	1101	35/35	0.92	0.18	2.69	48,58,83,86	0
3	LMT	C	1101	35/35	0.94	0.14	1.72	38,59,68,75	0
3	LMT	C	1102	35/35	0.86	0.14	0.93	37,85,101,111	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.