



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 07:20 am BST

PDB ID : 4ZIV  
Title : Crystal structure of AcrB triple mutant in P21 space group  
Authors : Ababou, A.; Koronakis, V.  
Deposited on : 2015-04-28  
Resolution : 3.16 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

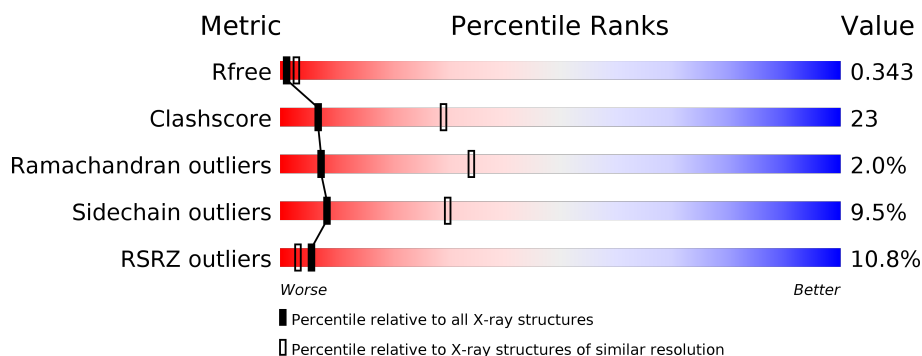
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.16 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1049	<div> <div>8%</div> <div>52%</div> <div>43%</div> <div>• •</div> </div>
1	B	1049	<div> <div>7%</div> <div>53%</div> <div>39%</div> <div>6% •</div> </div>
1	C	1049	<div> <div>11%</div> <div>53%</div> <div>41%</div> <div>6%</div> </div>
1	D	1049	<div> <div>11%</div> <div>53%</div> <div>41%</div> <div>• •</div> </div>
1	E	1049	<div> <div>12%</div> <div>48%</div> <div>43%</div> <div>7% •</div> </div>
1	F	1049	<div> <div>15%</div> <div>52%</div> <div>43%</div> <div>•</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
2	LMT	B	1101	X	-	-	-
2	LMT	C	1101	X	-	-	-
2	LMT	E	1101	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 47736 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	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	B	1046	Total	C	N	O	S	0	0	0
			7939	5099	1314	1483	43			
1	C	1044	Total	C	N	O	S	0	0	0
			7924	5090	1312	1479	43			
1	D	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	F	1046	Total	C	N	O	S	0	0	0
			7939	5099	1314	1483	43			

There are 18 discrepancies between the modelled and reference sequences:

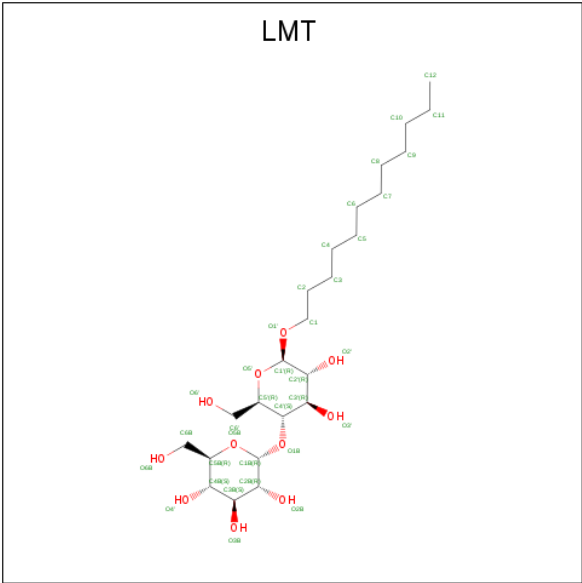
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	ALA	PHE	engineered mutation	UNP P31224
A	617	ALA	PHE	engineered mutation	UNP P31224
A	620	ALA	ARG	engineered mutation	UNP P31224
B	615	ALA	PHE	engineered mutation	UNP P31224
B	617	ALA	PHE	engineered mutation	UNP P31224
B	620	ALA	ARG	engineered mutation	UNP P31224
C	615	ALA	PHE	engineered mutation	UNP P31224
C	617	ALA	PHE	engineered mutation	UNP P31224
C	620	ALA	ARG	engineered mutation	UNP P31224
D	615	ALA	PHE	engineered mutation	UNP P31224
D	617	ALA	PHE	engineered mutation	UNP P31224
D	620	ALA	ARG	engineered mutation	UNP P31224
E	615	ALA	PHE	engineered mutation	UNP P31224
E	617	ALA	PHE	engineered mutation	UNP P31224
E	620	ALA	ARG	engineered mutation	UNP P31224
F	615	ALA	PHE	engineered mutation	UNP P31224
F	617	ALA	PHE	engineered mutation	UNP P31224

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Chain	Residue	Modelled	Actual	Comment	Reference
F	620	ALA	ARG	engineered mutation	UNP P31224

- Molecule 2 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
2	A	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	C	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		

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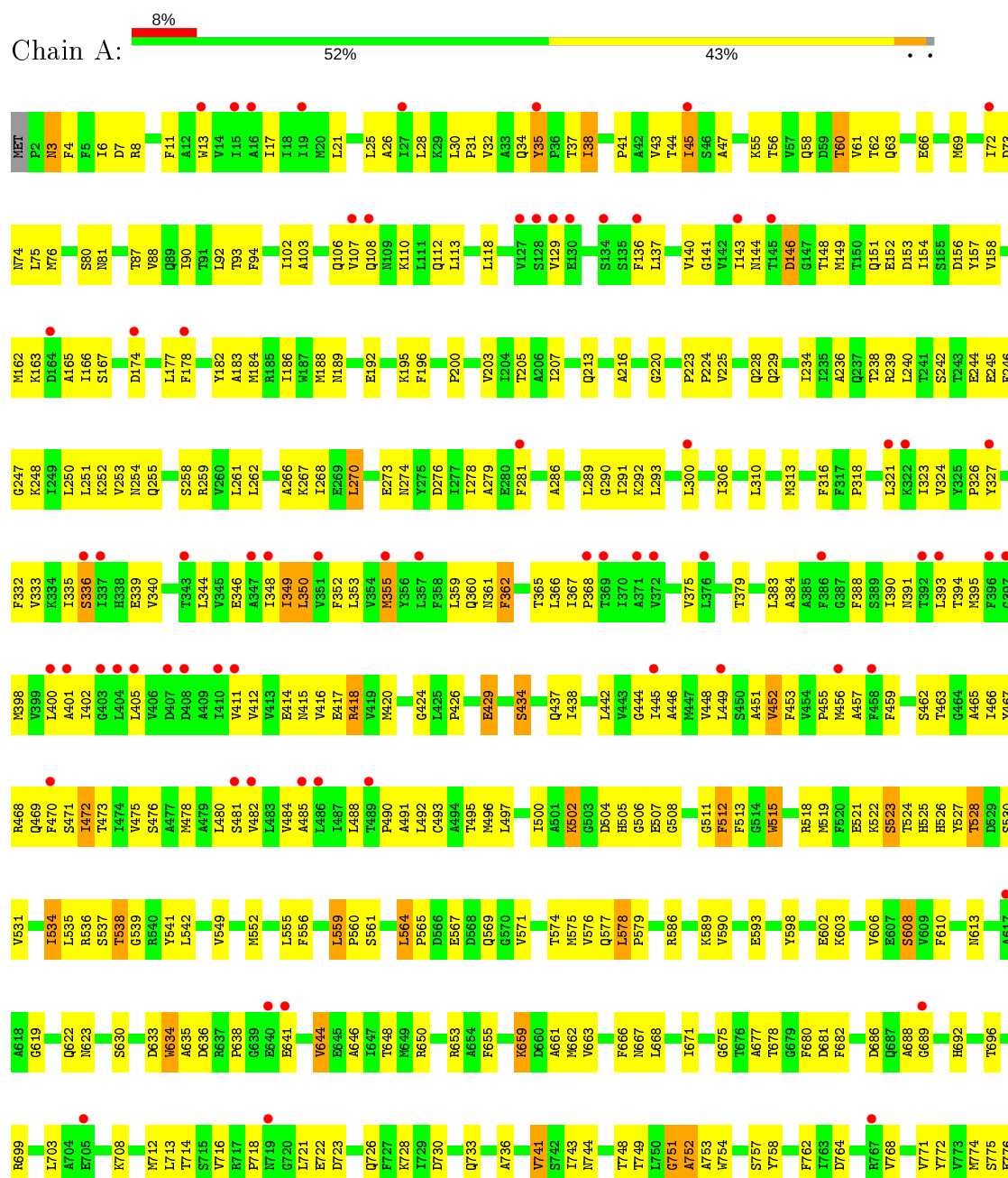
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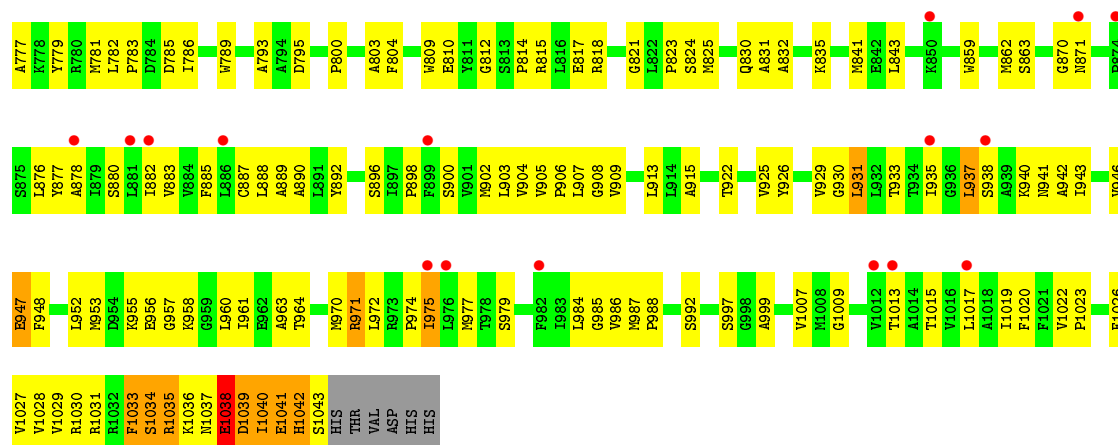
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Ni	0	0
			1	1		

### 3 Residue-property plots

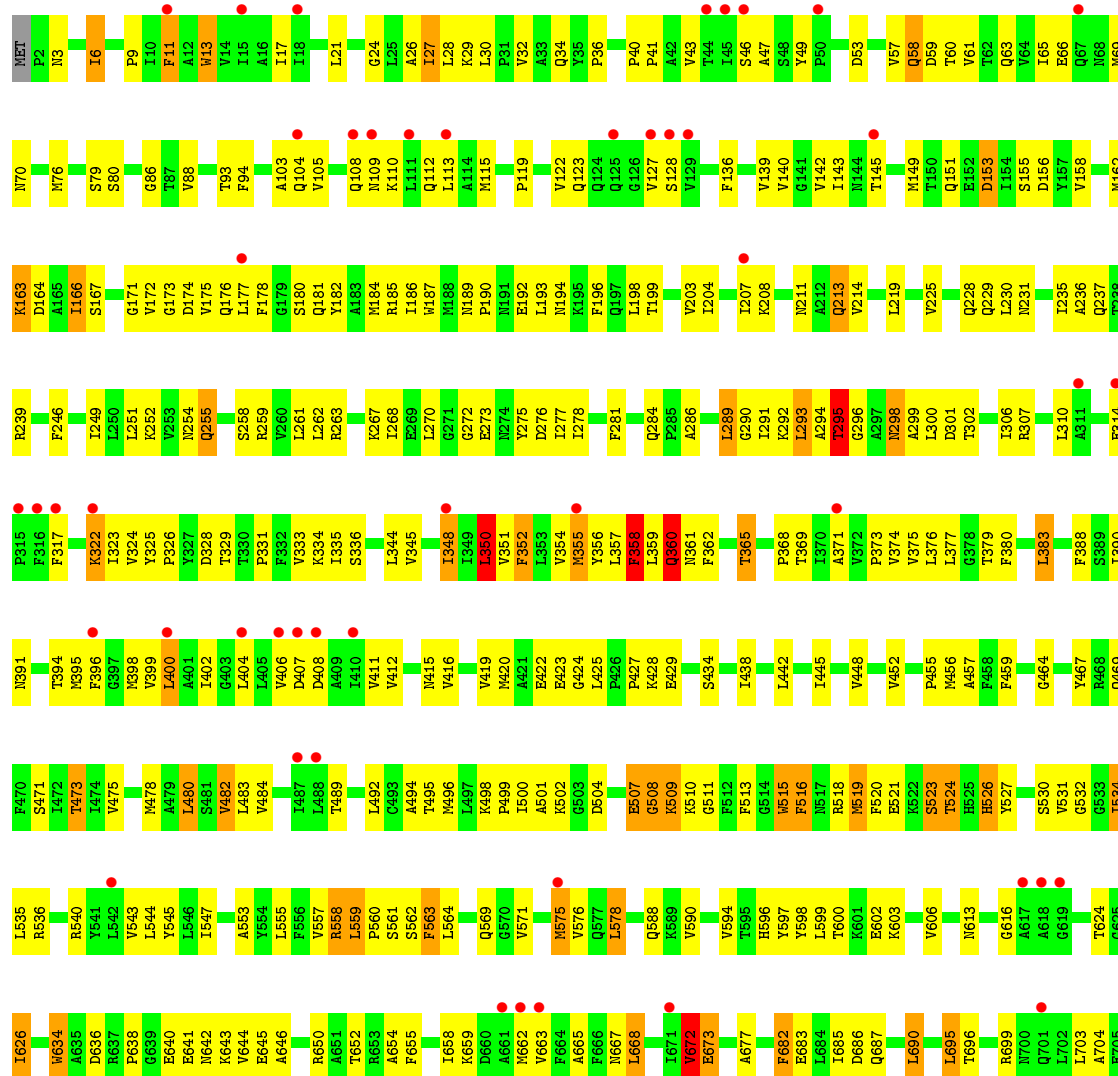
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Multidrug efflux pump subunit AcrB

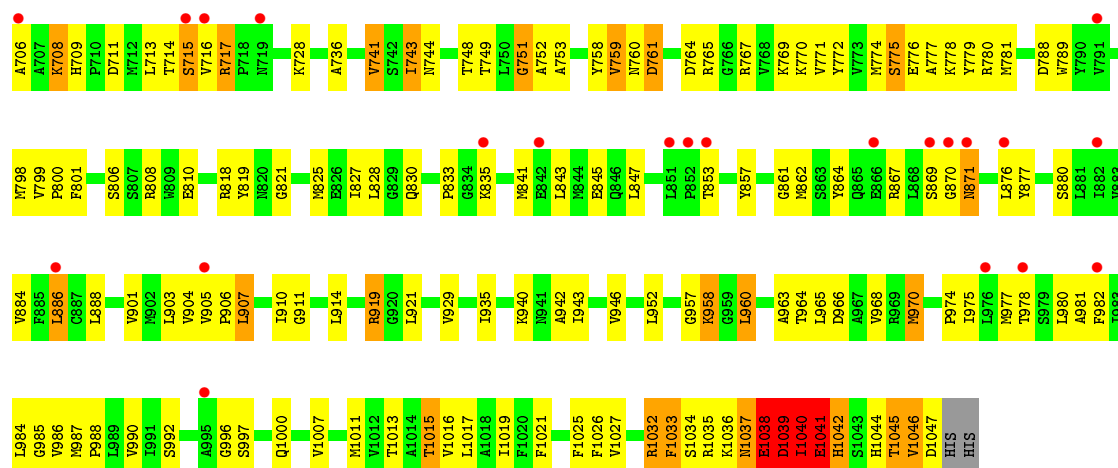




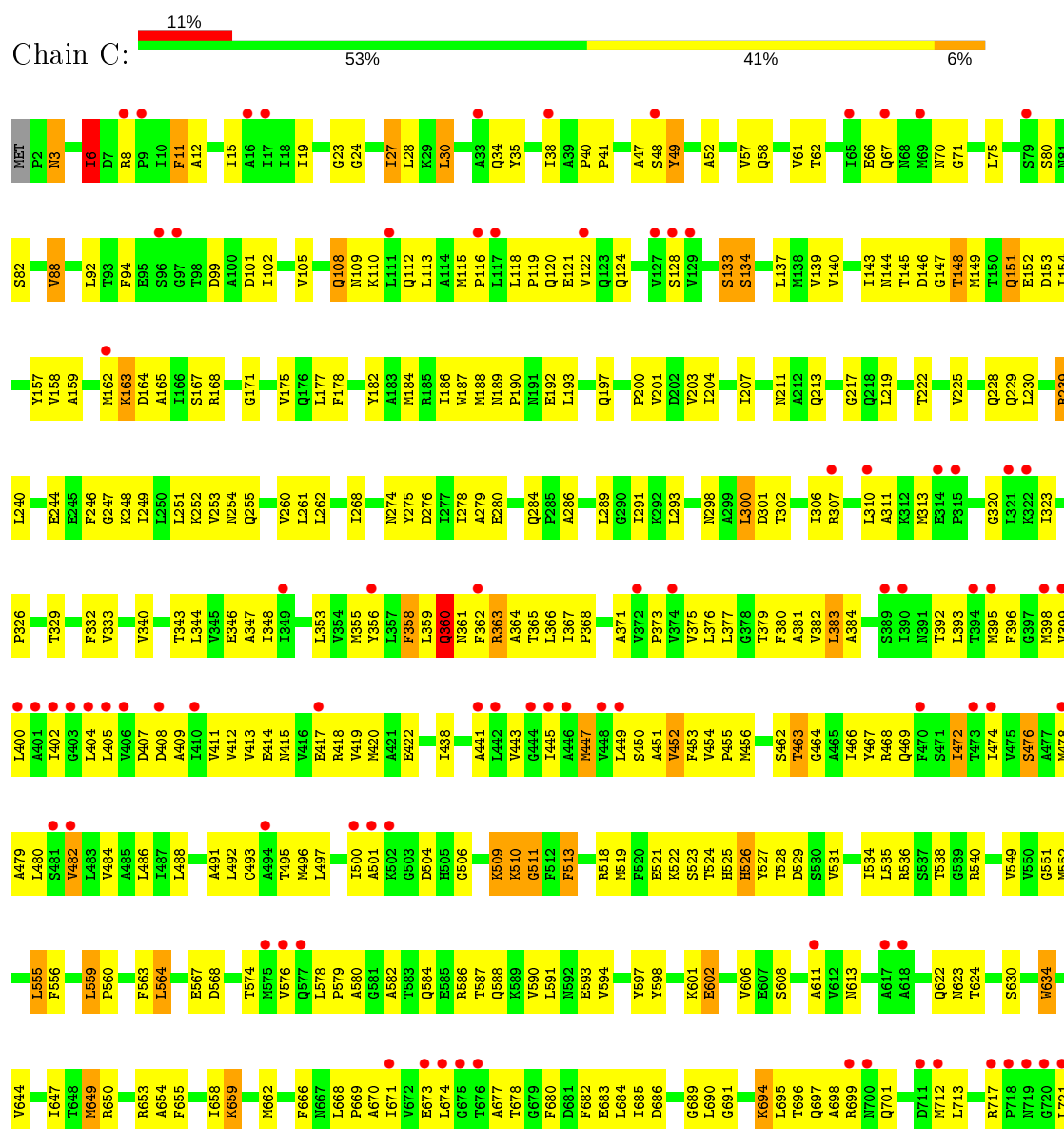
• Molecule 1: Multidrug efflux pump subunit AcrB

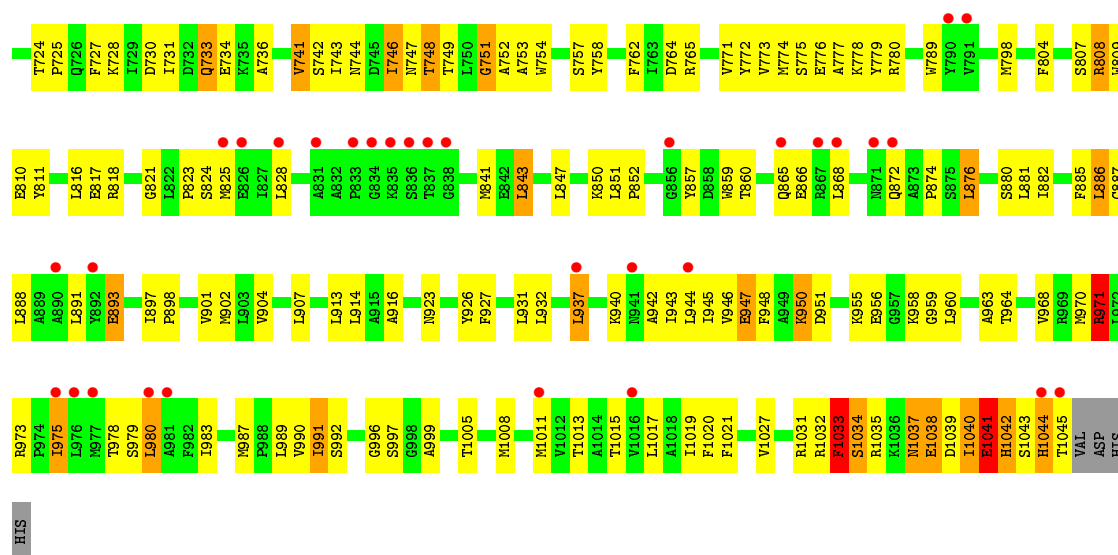




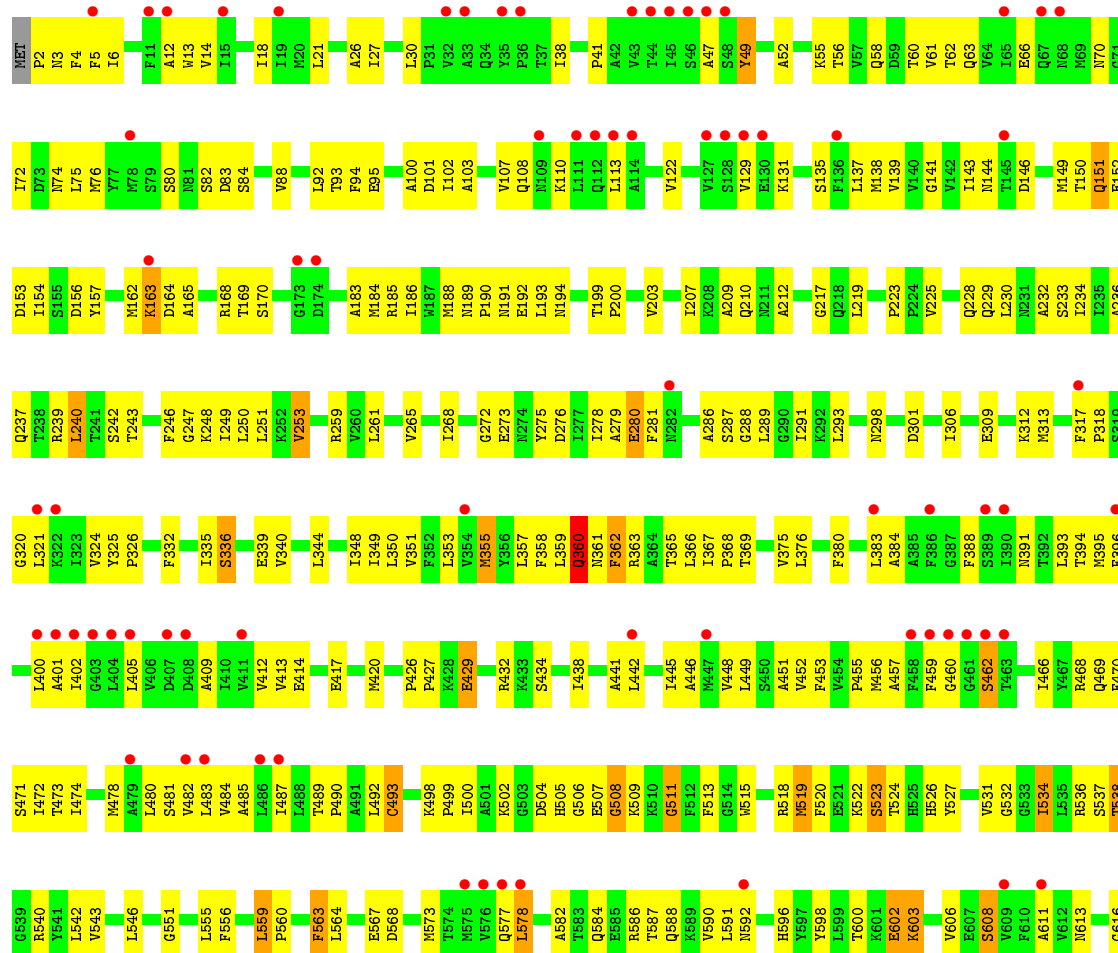


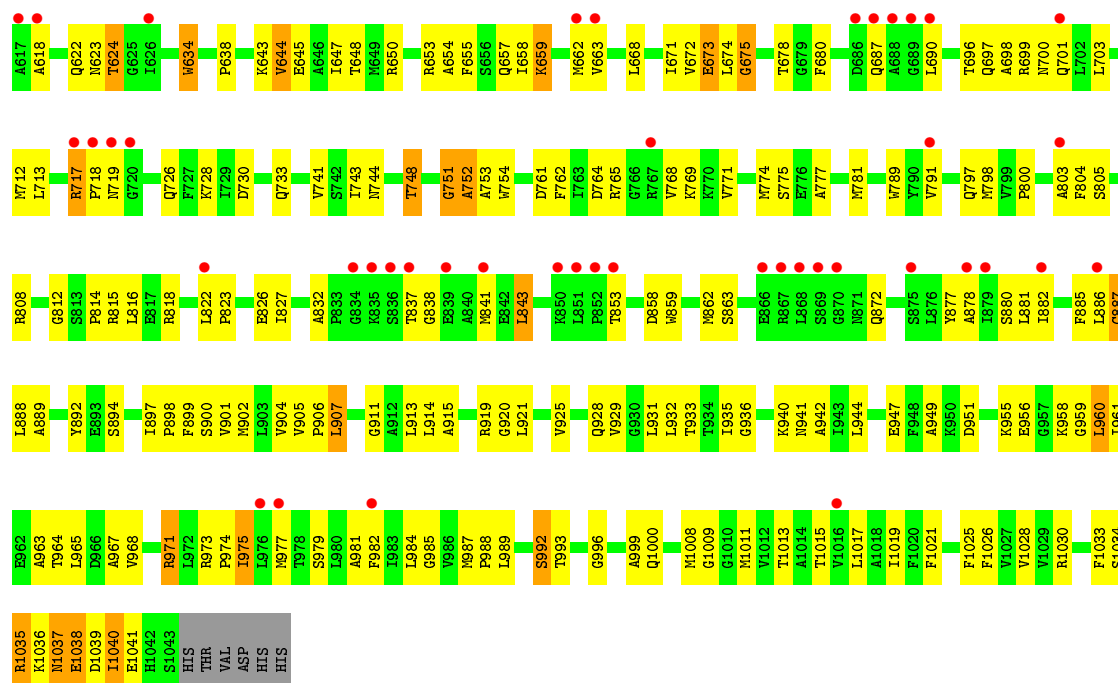
• Molecule 1: Multidrug efflux pump subunit AcrB



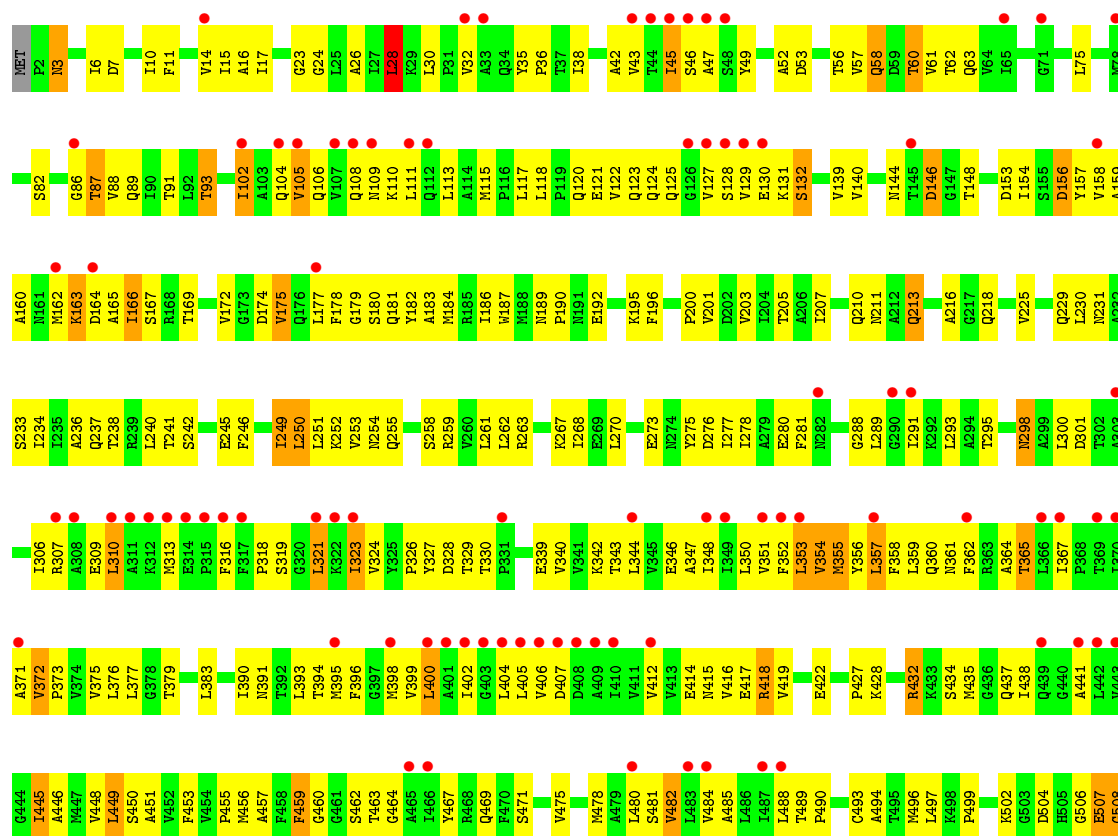


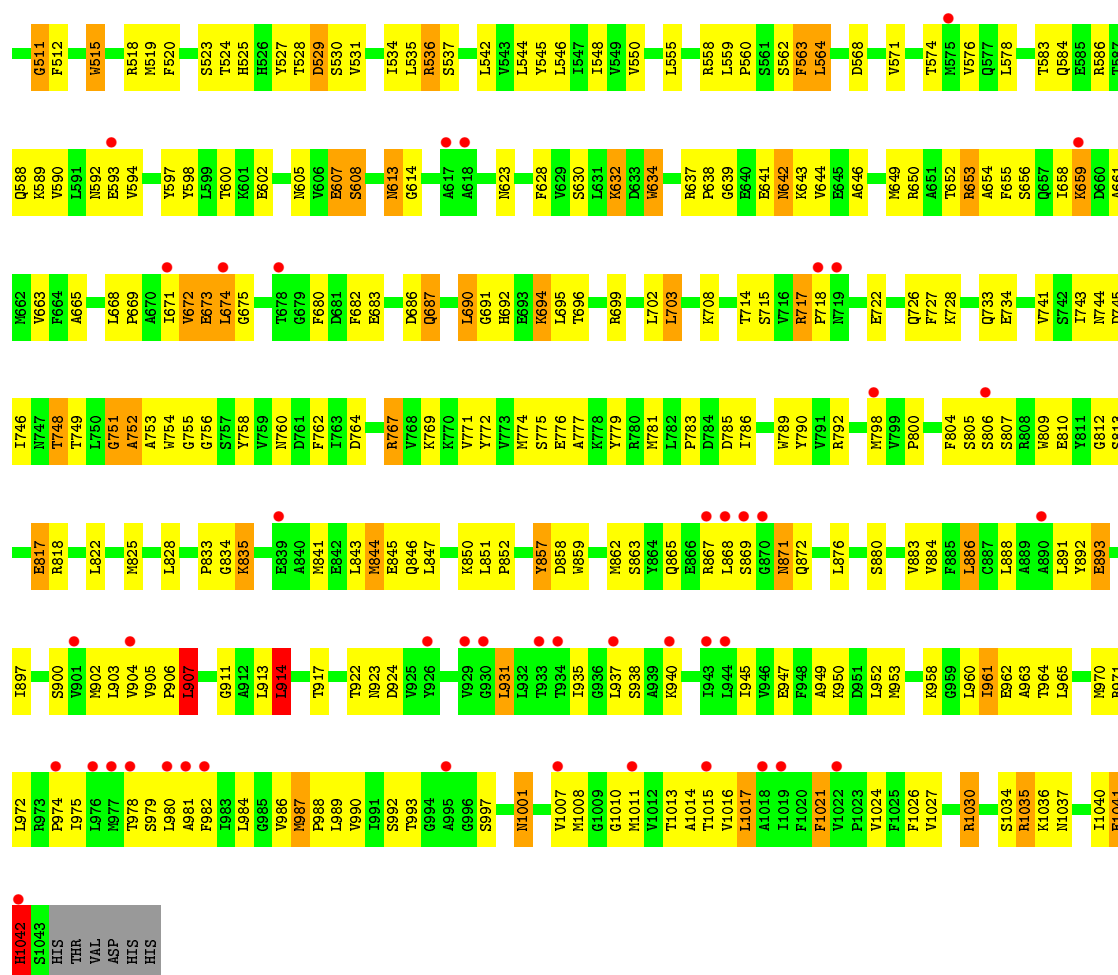
### • Molecule 1: Multidrug efflux pump subunit AcrB



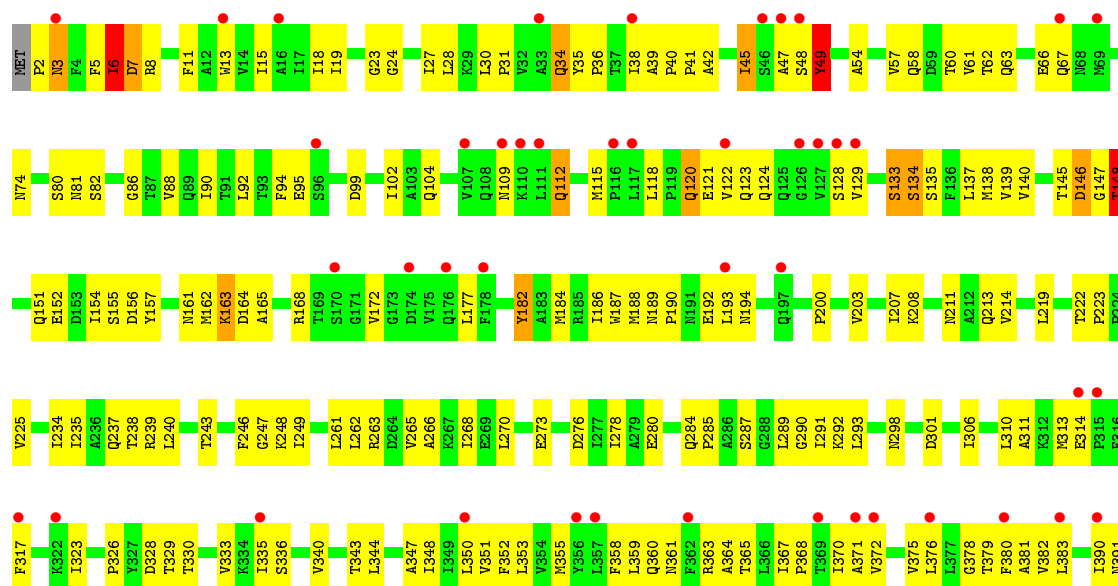


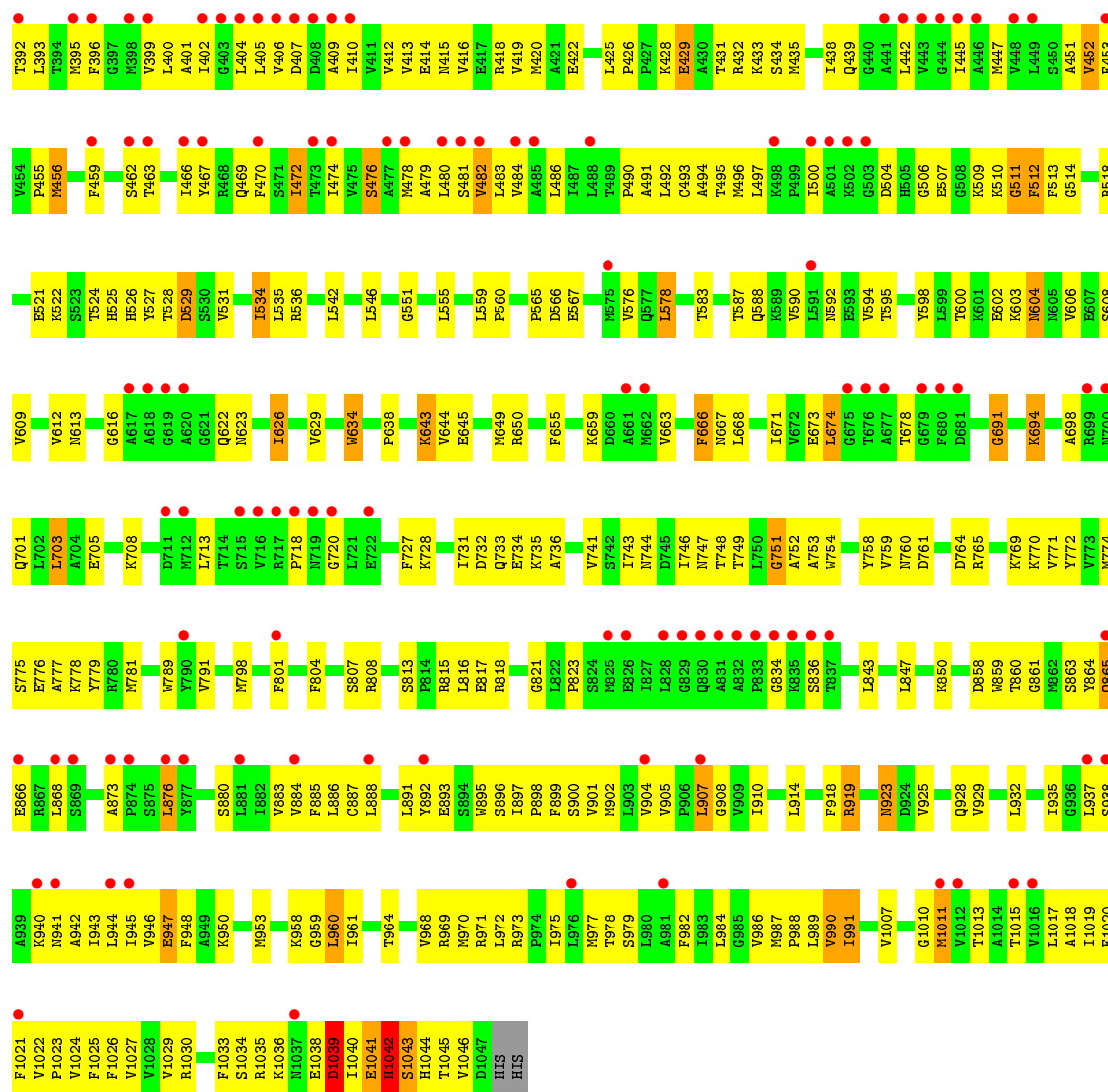
### • Molecule 1: Multidrug efflux pump subunit AcrB





• Molecule 1: Multidrug efflux pump subunit AcrB





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.28Å 157.49Å 219.16Å 90.00° 92.74° 90.00°	Depositor
Resolution (Å)	19.98 – 3.16 109.45 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.98-3.16) 97.7 (109.45-3.16)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, $R_{free}$	0.270 , 0.335 0.280 , 0.343	Depositor DCC
$R_{free}$ test set	8816 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 63.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.075 for -k,-h,-l 0.095 for k,h,-l 0.089 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	47736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.6875e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 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	0.61	1/8056 (0.0%)	0.83	5/10940 (0.0%)
1	B	0.63	1/8089 (0.0%)	0.86	6/10986 (0.1%)
1	C	0.63	0/8074	0.89	16/10965 (0.1%)
1	D	0.56	2/8056 (0.0%)	0.82	8/10940 (0.1%)
1	E	0.57	2/8056 (0.0%)	0.83	9/10940 (0.1%)
1	F	0.58	0/8089	0.85	7/10986 (0.1%)
All	All	0.60	6/48420 (0.0%)	0.85	51/65757 (0.1%)

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	C	0	1
1	D	0	2
1	F	0	2
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	TRP	CB-CG	7.82	1.64	1.50
1	E	515	TRP	CB-CG	6.85	1.62	1.50
1	D	515	TRP	CB-CG	6.71	1.62	1.50
1	B	515	TRP	CB-CG	6.47	1.61	1.50
1	E	493	CYS	CB-SG	-6.06	1.72	1.82
1	D	887	CYS	CB-SG	-5.98	1.72	1.81

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	529	ASP	CB-CG-OD1	9.33	126.69	118.30
1	E	914	LEU	CA-CB-CG	7.93	133.55	115.30
1	A	972	LEU	CA-CB-CG	7.92	133.50	115.30
1	E	529	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	357	LEU	CA-CB-CG	7.55	132.67	115.30
1	D	914	LEU	CA-CB-CG	7.17	131.80	115.30
1	B	350	LEU	CA-CB-CG	-7.07	99.04	115.30
1	C	529	ASP	CB-CG-OD1	7.07	124.66	118.30
1	B	483	LEU	CA-CB-CG	7.05	131.51	115.30
1	C	383	LEU	CA-CB-CG	6.78	130.90	115.30
1	E	357	LEU	CA-CB-CG	6.60	130.49	115.30
1	E	843	LEU	CA-CB-CG	6.46	130.17	115.30
1	C	1033	PHE	C-N-CA	6.43	137.77	121.70
1	A	937	LEU	CA-CB-CG	-6.41	100.55	115.30
1	E	293	LEU	CA-CB-CG	6.23	129.62	115.30
1	D	944	LEU	CA-CB-CG	-6.16	101.13	115.30
1	F	1041	GLU	C-N-CA	6.13	137.03	121.70
1	E	250	LEU	CA-CB-CG	6.09	129.31	115.30
1	C	971	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	1034	SER	C-N-CA	5.72	136.00	121.70
1	C	366	LEU	CA-CB-CG	5.69	128.39	115.30
1	C	937	LEU	CA-CB-CG	-5.59	102.43	115.30
1	F	691	GLY	N-CA-C	5.59	127.07	113.10
1	C	30	LEU	CA-CB-CG	5.58	128.12	115.30
1	B	1039	ASP	N-CA-C	5.55	125.98	111.00
1	C	113	LEU	CA-CB-CG	5.51	127.98	115.30
1	C	1041	GLU	N-CA-C	-5.38	96.46	111.00
1	C	529	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	21	LEU	CA-CB-CG	5.35	127.61	115.30
1	E	511	GLY	N-CA-C	5.34	126.45	113.10
1	E	28	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	300	LEU	CA-CB-CG	5.27	127.43	115.30
1	C	1041	GLU	C-N-CA	5.27	134.88	121.70
1	F	834	GLY	N-CA-C	-5.27	99.92	113.10
1	B	519	MET	CB-CG-SD	5.27	128.20	112.40
1	D	21	LEU	CA-CB-CG	-5.26	103.20	115.30
1	A	534	ILE	CG1-CB-CG2	-5.22	99.91	111.40
1	C	1041	GLU	CA-C-N	5.22	128.68	117.20
1	F	49	TYR	CA-CB-CG	5.21	123.31	113.40
1	E	1041	GLU	C-N-CA	5.20	134.69	121.70
1	C	1033	PHE	CA-C-N	5.19	128.62	117.20
1	D	673	GLU	N-CA-C	5.19	125.00	111.00
1	D	511	GLY	N-CA-C	5.18	126.06	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	529	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	D	240	LEU	CA-CB-CG	5.16	127.16	115.30
1	C	8	ARG	N-CA-C	-5.15	97.09	111.00
1	F	919	ARG	N-CA-C	-5.11	97.19	111.00
1	D	534	ILE	CG1-CB-CG2	-5.09	100.21	111.40
1	A	35	TYR	C-N-CD	5.08	139.06	128.40
1	C	980	LEU	CA-CB-CG	-5.08	103.62	115.30
1	D	519	MET	CB-CG-SD	5.01	127.43	112.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	6	ILE	Peptide
1	D	1034	SER	Peptide
1	D	992	SER	Peptide
1	F	1036	LYS	Peptide
1	F	1039	ASP	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	7907	0	8050	393	0
1	B	7939	0	8077	355	0
1	C	7924	0	8064	396	0
1	D	7907	0	8050	369	0
1	E	7907	0	8050	414	1
1	F	7939	0	8077	397	1
2	A	35	0	46	4	0
2	B	35	0	46	3	0
2	C	35	0	46	4	0
2	D	35	0	46	1	0
2	E	35	0	46	4	0
2	F	35	0	46	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
All	All	47736	0	48644	2245	1

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 23.

All (2245) 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:D:446:ALA:HB2	1:D:482:VAL:HG21	1.39	0.99
1:A:957:GLY:HA2	1:A:1042:HIS:HB2	1.41	0.99
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.46	0.98
1:D:536:ARG:NH2	2:D:1101:LMT:O3B	1.97	0.97
1:F:578:LEU:HG	1:F:587:THR:HG22	1.46	0.95
1:F:135:SER:HB3	1:F:673:GLU:HB3	1.49	0.94
1:E:196:PHE:O	1:E:252:LYS:NZ	2.04	0.91
1:D:457:ALA:O	1:D:468:ARG:NE	2.03	0.90
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.54	0.90
1:F:35:TYR:HB3	1:F:38:ILE:HD12	1.54	0.89
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.54	0.89
1:E:159:ALA:O	1:E:767:ARG:NH2	2.07	0.88
1:E:354:VAL:HG11	1:E:980:LEU:HB3	1.55	0.88
1:C:1041:GLU:HB3	1:C:1042:HIS:HB2	1.53	0.88
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.54	0.88
1:F:1041:GLU:HB3	1:F:1042:HIS:HB3	1.56	0.88
1:F:452:VAL:HG12	1:F:880:SER:HB3	1.56	0.88
1:D:578:LEU:HD21	1:D:590:VAL:HG21	1.56	0.87
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.56	0.87
1:D:41:PRO:HG2	1:D:94:PHE:HB2	1.57	0.87
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.09	0.86
1:B:919:ARG:NH2	1:B:990:VAL:O	2.09	0.86
1:B:399:VAL:O	1:B:402:ILE:HG13	1.76	0.86
1:F:616:GLY:HA2	1:F:626:ILE:HD13	1.57	0.85
1:A:350:LEU:HD22	1:A:984:LEU:HB3	1.58	0.85
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.58	0.85
1:C:38:ILE:HG23	1:C:462:SER:HB2	1.57	0.85
1:A:400:LEU:HD23	1:A:929:VAL:HG12	1.59	0.84
1:E:56:THR:O	1:E:60:THR:OG1	1.95	0.84
1:A:619:GLY:HA3	1:A:815:ARG:HH22	1.40	0.84
1:F:559:LEU:HD22	1:F:560:PRO:HD2	1.60	0.84
1:C:112:GLN:HA	1:C:115:MET:HB2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:992:SER:O	1:B:997:SER:OG	1.96	0.83
1:B:559:LEU:HD22	1:B:560:PRO:HD2	1.59	0.83
1:C:940:LYS:HZ1	1:C:978:THR:HG21	1.44	0.83
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.14	0.82
1:F:340:VAL:HG11	1:F:395:MET:HB3	1.59	0.82
1:E:58:GLN:OE1	1:E:818:ARG:NH1	2.12	0.82
1:B:156:ASP:OD1	1:B:765:ARG:NH2	2.11	0.82
1:A:38:ILE:HG12	1:A:462:SER:HB2	1.62	0.81
1:E:692:HIS:NE2	1:E:813:SER:OG	2.13	0.81
1:D:170:SER:HB2	1:E:75:LEU:H	1.42	0.81
1:D:219:LEU:HD23	1:E:754:TRP:HZ3	1.45	0.81
1:E:702:LEU:HD11	1:E:847:LEU:HB3	1.60	0.81
1:E:508:GLY:HA3	1:E:518:ARG:HE	1.46	0.81
1:B:156:ASP:OD2	1:B:769:LYS:NZ	2.13	0.80
1:A:986:VAL:HG21	1:A:1007:VAL:HG11	1.63	0.80
1:A:196:PHE:O	1:A:252:LYS:NZ	2.14	0.80
1:C:536:ARG:NH2	2:C:1101:LMT:O3B	2.13	0.80
1:B:186:ILE:HG12	1:B:268:ILE:HG12	1.63	0.80
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.62	0.80
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.62	0.80
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.64	0.80
1:C:3:ASN:N	1:C:3:ASN:OD1	2.13	0.80
1:E:156:ASP:OD1	1:E:769:LYS:NZ	2.15	0.80
1:E:261:LEU:HD12	1:E:263:ARG:HH12	1.46	0.79
1:E:236:ALA:O	1:F:728:LYS:NZ	2.15	0.79
1:A:146:ASP:OD2	1:A:146:ASP:N	2.16	0.79
1:A:248:LYS:HA	1:A:261:LEU:HD13	1.64	0.79
1:B:508:GLY:HA2	1:B:518:ARG:HH21	1.47	0.79
1:F:510:LYS:HA	1:F:518:ARG:HH12	1.45	0.79
1:A:564:LEU:HD13	1:A:671:ILE:HD11	1.64	0.79
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.63	0.79
1:A:56:THR:O	1:A:60:THR:OG1	1.98	0.79
1:B:1013:THR:O	1:B:1017:LEU:HB2	1.83	0.79
1:F:986:VAL:HG21	1:F:1007:VAL:HG11	1.63	0.78
1:C:452:VAL:HG12	1:C:880:SER:HB3	1.65	0.78
1:E:42:ALA:HB2	1:E:93:THR:HG23	1.64	0.78
1:F:509:LYS:O	1:F:518:ARG:NH1	2.16	0.78
1:E:555:LEU:HD22	1:E:913:LEU:HB3	1.64	0.78
1:F:944:LEU:HB3	1:F:971:ARG:HE	1.49	0.78
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.66	0.78
1:C:356:TYR:HA	1:C:365:THR:HG21	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ARG:HH12	1:A:823:PRO:HG3	1.46	0.78
1:A:885:PHE:HD1	1:A:902:MET:HE1	1.48	0.78
1:B:350:LEU:HD22	1:B:984:LEU:HB3	1.64	0.78
1:C:940:LYS:NZ	1:C:978:THR:HG21	1.98	0.78
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.66	0.77
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.66	0.77
1:E:559:LEU:HD22	1:E:560:PRO:HD2	1.65	0.77
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.64	0.77
1:D:58:GLN:O	1:D:63:GLN:HG3	1.85	0.77
1:E:326:PRO:O	1:E:630:SER:OG	2.01	0.77
1:F:536:ARG:NH1	2:F:1101:LMT:O4'	2.16	0.77
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.66	0.77
1:B:602:GLU:OE2	1:B:650:ARG:NH1	2.17	0.77
1:B:957:GLY:O	1:B:1041:GLU:HA	1.83	0.77
1:B:6:ILE:O	1:B:428:LYS:NZ	2.17	0.77
1:D:426:PRO:HD2	1:D:429:GLU:HG3	1.67	0.77
1:A:108:GLN:NE2	1:B:109:ASN:O	2.17	0.77
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.67	0.77
1:D:183:ALA:HB2	1:D:273:GLU:HG3	1.66	0.77
1:B:196:PHE:O	1:B:252:LYS:NZ	2.17	0.77
1:F:298:ASN:ND2	1:F:301:ASP:OD2	2.17	0.77
1:B:362:PHE:O	1:B:365:THR:HG22	1.84	0.77
1:C:602:GLU:OE2	1:C:650:ARG:NH1	2.18	0.77
1:B:9:PRO:HB3	1:B:495:THR:HG21	1.68	0.76
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.51	0.76
1:D:448:VAL:HG22	1:D:887:CYS:HB3	1.67	0.76
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.68	0.76
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.66	0.75
1:D:507:GLU:O	1:D:509:LYS:N	2.19	0.75
1:D:61:VAL:HG21	1:D:122:VAL:HG21	1.68	0.75
1:E:907:LEU:HG	1:E:1017:LEU:HB3	1.68	0.75
1:F:705:GLU:HA	1:F:708:LYS:HE3	1.68	0.75
1:C:527:TYR:OH	1:C:1019:ILE:O	2.03	0.75
1:A:236:ALA:O	1:B:728:LYS:NZ	2.18	0.74
1:A:405:LEU:HD22	1:A:481:SER:HB2	1.69	0.74
1:C:671:ILE:HD13	1:C:674:LEU:HD12	1.68	0.74
1:F:525:HIS:HA	1:F:528:THR:HG22	1.69	0.74
1:D:375:VAL:HB	1:D:405:LEU:HD13	1.67	0.74
1:E:1026:PHE:O	1:E:1030:ARG:HB2	1.88	0.74
1:F:23:GLY:HA2	1:F:381:ALA:HB2	1.69	0.74
1:B:108:GLN:HE22	1:C:112:GLN:HB3	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:LEU:HD13	1:C:611:ALA:HB1	1.69	0.74
1:F:588:GLN:O	1:F:592:ASN:ND2	2.18	0.74
1:D:72:ILE:HD13	1:D:107:VAL:HG22	1.68	0.74
1:F:944:LEU:HB3	1:F:971:ARG:NE	2.03	0.74
1:A:1039:ASP:OD1	1:A:1039:ASP:N	2.20	0.74
1:B:163:LYS:HA	1:B:289:LEU:HD11	1.70	0.74
1:E:637:ARG:HB3	1:E:642:ASN:HB3	1.68	0.74
1:A:712:MET:HB3	1:A:713:LEU:HD22	1.69	0.73
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.69	0.73
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.51	0.73
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.70	0.73
1:D:248:LYS:HA	1:D:261:LEU:HD13	1.70	0.73
1:E:146:ASP:N	1:E:146:ASP:OD2	2.19	0.73
1:A:362:PHE:O	1:A:365:THR:HG22	1.88	0.73
1:E:61:VAL:HA	1:E:118:LEU:HD22	1.70	0.73
1:F:344:LEU:HD22	1:F:402:ILE:HD11	1.69	0.73
1:E:602:GLU:OE2	1:E:650:ARG:NH1	2.21	0.73
1:B:139:VAL:O	1:B:326:PRO:HD2	1.87	0.73
1:B:345:VAL:O	1:B:348:ILE:HG22	1.89	0.73
1:C:1043:SER:OG	1:C:1044:HIS:N	2.21	0.73
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.69	0.73
1:D:144:ASN:HA	1:D:320:GLY:O	1.89	0.73
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.71	0.73
1:E:986:VAL:HG21	1:E:1007:VAL:HG11	1.69	0.73
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.71	0.72
1:E:157:TYR:OH	1:E:316:PHE:O	2.05	0.72
1:F:733:GLN:HE22	1:F:743:ILE:HG21	1.55	0.72
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.70	0.72
1:F:380:PHE:HD2	1:F:383:LEU:HD12	1.54	0.72
1:A:26:ALA:O	1:A:30:LEU:HB2	1.90	0.72
1:B:58:GLN:O	1:B:63:GLN:HG3	1.88	0.72
1:E:162:MET:O	1:E:164:ASP:N	2.17	0.72
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.72	0.72
1:B:508:GLY:O	1:B:510:LYS:N	2.22	0.72
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.71	0.72
1:D:455:PRO:HG2	1:D:880:SER:HB2	1.70	0.72
1:E:520:PHE:O	1:E:523:SER:OG	2.05	0.72
1:E:578:LEU:HD21	1:E:590:VAL:HG21	1.71	0.72
1:B:236:ALA:O	1:C:728:LYS:NZ	2.19	0.72
1:E:189:ASN:HB3	1:E:192:GLU:HB2	1.72	0.72
1:C:240:LEU:HB2	1:C:246:PHE:HE1	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:971:ARG:HH21	1:F:975:ILE:HD11	1.55	0.72
1:F:972:LEU:HA	1:F:975:ILE:HD12	1.71	0.71
1:A:417:GLU:O	1:A:420:MET:N	2.24	0.71
1:B:26:ALA:O	1:B:30:LEU:HB2	1.89	0.71
1:B:871:ASN:N	1:B:871:ASN:OD1	2.23	0.71
1:C:278:ILE:HG13	1:C:613:ASN:HB3	1.72	0.71
1:D:375:VAL:HG22	1:D:484:VAL:HG21	1.72	0.71
1:E:353:LEU:O	1:E:355:MET:N	2.21	0.71
1:B:428:LYS:HD3	1:B:494:ALA:HB1	1.70	0.71
1:B:907:LEU:HG	1:B:1017:LEU:HD23	1.72	0.71
1:A:25:LEU:HA	1:A:28:LEU:HD12	1.72	0.71
1:D:971:ARG:NH1	1:D:971:ARG:H	1.88	0.71
1:F:1041:GLU:CB	1:F:1042:HIS:HB3	2.21	0.71
1:D:555:LEU:HD22	1:D:913:LEU:HB3	1.73	0.71
1:E:658:ILE:O	1:E:659:LYS:NZ	2.22	0.71
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.55	0.70
1:A:555:LEU:HD22	1:A:913:LEU:HB3	1.74	0.70
1:E:508:GLY:HA3	1:E:518:ARG:NE	2.06	0.70
1:B:1037:ASN:H	1:B:1038:GLU:HB3	1.55	0.70
1:B:527:TYR:O	1:B:531:VAL:HG23	1.90	0.70
1:C:193:LEU:HD13	1:C:200:PRO:HD3	1.73	0.70
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.27	0.70
1:E:291:ILE:HD13	1:E:306:ILE:HD13	1.73	0.70
1:C:578:LEU:HD13	1:C:579:PRO:HD2	1.73	0.70
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.73	0.70
1:C:682:PHE:CE1	1:C:857:TYR:HB2	2.26	0.70
1:D:18:ILE:HG13	1:E:886:LEU:HD23	1.74	0.70
1:A:186:ILE:HG12	1:A:268:ILE:HG12	1.74	0.70
1:B:60:THR:HG22	1:B:119:PRO:HD3	1.74	0.70
1:C:1033:PHE:H	1:C:1034:SER:CB	2.03	0.70
1:E:45:ILE:HG23	1:E:129:VAL:HG22	1.73	0.70
1:F:317:PHE:HE2	1:F:323:ILE:HD11	1.57	0.70
1:F:278:ILE:HG13	1:F:613:ASN:HB3	1.73	0.70
1:F:668:LEU:H	1:F:668:LEU:HD23	1.56	0.70
1:F:211:ASN:O	1:F:760:ASN:ND2	2.24	0.70
1:B:383:LEU:HD13	1:B:388:PHE:HD1	1.57	0.69
1:B:845:GLU:OE2	1:B:867:ARG:NH1	2.24	0.69
1:D:318:PRO:HD2	1:D:321:LEU:HD12	1.71	0.69
1:E:463:THR:O	1:E:467:TYR:HD1	1.75	0.69
1:E:422:GLU:O	1:E:502:LYS:NZ	2.25	0.69
1:F:284:GLN:HG3	1:F:285:PRO:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:971:ARG:NH2	1:F:975:ILE:HD11	2.07	0.69
1:A:519:MET:O	1:A:523:SER:OG	2.09	0.69
1:E:203:VAL:O	1:E:207:ILE:HG13	1.92	0.69
1:A:35:TYR:CE2	1:A:564:LEU:HD21	2.27	0.69
1:D:243:THR:HG23	1:D:268:ILE:HG22	1.73	0.69
1:E:211:ASN:OD1	1:E:760:ASN:ND2	2.26	0.69
1:E:441:ALA:HA	1:E:891:LEU:HD21	1.74	0.69
1:E:971:ARG:O	1:E:975:ILE:HG12	1.91	0.69
1:A:721:LEU:HB3	1:A:814:PRO:HG2	1.75	0.69
1:A:129:VAL:O	1:B:110:LYS:NZ	2.22	0.69
1:F:383:LEU:HD23	1:F:472:ILE:HD13	1.75	0.69
1:F:731:ILE:HD13	1:F:746:ILE:HD11	1.74	0.69
1:E:534:ILE:HG22	2:E:1101:LMT:H1'	1.74	0.68
1:F:971:ARG:HB3	1:F:971:ARG:NH1	2.08	0.68
1:C:556:PHE:HD1	1:C:913:LEU:HD21	1.59	0.68
1:E:169:THR:HG21	1:E:306:ILE:HG13	1.73	0.68
1:F:420:MET:HB3	1:F:500:ILE:HB	1.74	0.68
1:F:604:ASN:OD1	1:F:604:ASN:N	2.26	0.68
1:D:298:ASN:HB3	1:D:301:ASP:HB2	1.74	0.68
1:D:564:LEU:HD13	1:D:671:ILE:HD13	1.76	0.68
1:D:189:ASN:HB3	1:D:192:GLU:HB2	1.75	0.68
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.75	0.68
1:C:201:VAL:HA	1:C:204:ILE:HD12	1.74	0.68
1:E:157:TYR:CZ	1:E:318:PRO:HD3	2.29	0.67
1:A:411:VAL:HG22	1:A:971:ARG:HH22	1.60	0.67
1:D:151:GLN:H	1:D:151:GLN:CD	1.97	0.67
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.76	0.67
1:E:613:ASN:HD22	1:E:614:GLY:N	1.92	0.67
1:A:1034:SER:OG	1:A:1035:ARG:O	2.12	0.67
1:B:225:VAL:HG12	1:C:777:ALA:HB1	1.75	0.67
1:D:225:VAL:HG22	1:E:781:MET:HE2	1.75	0.67
1:F:186:ILE:HG12	1:F:268:ILE:HG12	1.76	0.67
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.75	0.67
1:C:298:ASN:ND2	1:C:301:ASP:OD2	2.23	0.67
1:D:967:ALA:O	1:D:971:ARG:NH1	2.27	0.67
1:A:696:THR:HG23	1:A:699:ARG:HH12	1.57	0.67
1:C:249:ILE:HB	1:C:262:LEU:HB2	1.77	0.67
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.76	0.67
1:C:944:LEU:HB3	1:C:971:ARG:HD2	1.77	0.67
1:A:203:VAL:O	1:A:207:ILE:HG13	1.95	0.67
1:D:979:SER:OG	1:D:1015:THR:HG21	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:VAL:HA	1:A:931:LEU:HD21	1.77	0.67
1:B:986:VAL:HG21	1:B:1007:VAL:HG11	1.75	0.67
1:D:191:ASN:O	1:D:194:ASN:N	2.27	0.67
1:D:393:LEU:HD11	1:D:466:ILE:HD13	1.75	0.67
1:E:445:ILE:HG12	1:E:940:LYS:HE3	1.76	0.67
1:F:146:ASP:O	1:F:148:THR:N	2.27	0.67
1:A:564:LEU:HD23	1:A:565:PRO:HD2	1.75	0.67
1:C:987:MET:O	1:C:990:VAL:N	2.26	0.67
1:E:166:ILE:HD11	1:E:310:LEU:HD13	1.76	0.67
1:E:546:LEU:O	1:E:550:VAL:HG23	1.94	0.67
1:E:451:ALA:HB1	1:E:883:VAL:HG13	1.75	0.67
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.77	0.67
1:C:587:THR:HG21	1:C:622:GLN:O	1.93	0.67
1:D:344:LEU:HD13	1:D:376:LEU:HD13	1.77	0.66
1:D:982:PHE:O	1:D:985:GLY:N	2.28	0.66
1:B:142:VAL:HG21	1:B:162:MET:HE1	1.78	0.66
1:F:34:GLN:HG2	1:F:333:VAL:HG22	1.76	0.66
1:B:469:GLN:O	1:B:473:THR:OG1	2.14	0.66
1:F:139:VAL:HG22	1:F:290:GLY:HA2	1.78	0.66
1:B:249:ILE:HD11	1:B:262:LEU:HD22	1.78	0.66
1:B:396:PHE:O	1:B:400:LEU:HB2	1.95	0.66
1:B:108:GLN:OE1	1:C:112:GLN:HG3	1.96	0.66
1:D:190:PRO:HB3	1:D:789:TRP:CE2	2.30	0.66
1:C:531:VAL:O	1:C:534:ILE:HG13	1.95	0.66
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.78	0.66
1:E:525:HIS:HA	1:E:528:THR:HG22	1.77	0.66
1:A:1030:ARG:HH12	1:A:1033:PHE:HB3	1.61	0.66
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.76	0.66
1:E:653:ARG:O	1:E:656:SER:OG	2.14	0.66
1:A:251:LEU:HD11	1:A:262:LEU:HA	1.78	0.65
1:B:176:GLN:O	1:B:289:LEU:HD23	1.95	0.65
1:D:82:SER:HB2	1:D:816:LEU:HB2	1.77	0.65
1:F:329:THR:O	1:F:333:VAL:HG23	1.96	0.65
1:F:401:ALA:HB2	1:F:474:ILE:HG12	1.78	0.65
1:F:38:ILE:HG23	1:F:462:SER:HB2	1.78	0.65
1:C:11:PHE:O	1:C:11:PHE:HD2	1.78	0.65
1:F:1040:ILE:HA	1:F:1041:GLU:HB2	1.77	0.65
1:F:400:LEU:HB3	1:F:474:ILE:HD11	1.79	0.65
1:A:527:TYR:OH	1:A:1019:ILE:O	2.09	0.65
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.78	0.65
1:B:558:ARG:HA	1:B:558:ARG:HE	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:GLY:O	1:F:27:ILE:HG12	1.96	0.65
1:F:534:ILE:HD11	1:F:1024:VAL:HG22	1.77	0.65
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.27	0.65
1:C:947:GLU:HG3	1:C:948:PHE:HD1	1.61	0.65
1:A:455:PRO:HG2	1:A:880:SER:HB2	1.79	0.65
1:A:979:SER:OG	1:A:1015:THR:HG21	1.96	0.65
1:B:578:LEU:HD21	1:B:590:VAL:HG21	1.78	0.65
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.78	0.65
1:D:584:GLN:HB2	1:D:622:GLN:HG2	1.78	0.65
1:E:641:GLU:HA	1:E:646:ALA:HB3	1.80	0.65
1:F:58:GLN:HA	1:F:62:THR:HB	1.79	0.65
1:E:120:GLN:OE1	1:E:123:GLN:NE2	2.30	0.64
1:C:146:ASP:O	1:C:148:THR:N	2.30	0.64
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.79	0.64
1:B:901:VAL:HG12	1:B:946:VAL:HG21	1.78	0.64
1:C:66:GLU:OE1	1:C:821:GLY:HA2	1.97	0.64
1:D:332:PHE:O	1:D:336:SER:HB3	1.98	0.64
1:B:576:VAL:HG22	1:B:663:VAL:HG22	1.79	0.64
1:E:1013:THR:O	1:E:1017:LEU:HB2	1.97	0.64
1:E:703:LEU:HD11	1:E:718:PRO:HG3	1.78	0.64
1:C:248:LYS:HA	1:C:261:LEU:HD13	1.79	0.64
1:E:733:GLN:NE2	1:E:743:ILE:HG21	2.13	0.64
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.80	0.64
1:C:420:MET:HB3	1:C:500:ILE:HB	1.80	0.64
1:D:699:ARG:HG3	1:D:827:ILE:HD11	1.79	0.64
1:C:23:GLY:HA2	1:C:381:ALA:HB2	1.80	0.64
1:C:27:ILE:HA	1:C:30:LEU:HD22	1.80	0.63
1:C:555:LEU:HD22	1:C:913:LEU:HB3	1.79	0.63
1:D:388:PHE:HE2	1:D:472:ILE:HG21	1.64	0.63
1:F:509:LYS:HG2	1:F:513:PHE:HB2	1.79	0.63
1:F:57:VAL:HG23	1:F:82:SER:HB3	1.81	0.63
1:B:272:GLY:N	1:B:275:TYR:OH	2.30	0.63
1:E:184:MET:HB3	1:E:771:VAL:HG13	1.81	0.63
1:F:291:ILE:HD13	1:F:306:ILE:HD13	1.79	0.63
1:B:171:GLY:O	1:B:294:ALA:N	2.30	0.63
1:F:935:ILE:O	1:F:938:SER:OG	2.16	0.63
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.27	0.63
1:D:568:ASP:O	1:D:634:TRP:HZ3	1.82	0.63
1:F:1021:PHE:HB3	1:F:1025:PHE:CE1	2.32	0.63
1:A:400:LEU:HD21	1:A:930:GLY:HA2	1.78	0.63
1:A:941:ASN:HB3	1:A:975:ILE:HD13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:LEU:HB3	1:C:478:MET:SD	2.39	0.63
1:D:452:VAL:HA	1:D:880:SER:OG	1.99	0.63
1:A:183:ALA:HB2	1:A:273:GLU:HG3	1.81	0.63
1:B:13:TRP:CH2	1:B:492:LEU:HD21	2.33	0.63
1:A:832:ALA:HB3	1:A:835:LYS:HD3	1.81	0.63
1:B:459:PHE:CE1	1:B:876:LEU:HD12	2.34	0.63
1:C:746:ILE:HG13	1:C:747:ASN:N	2.14	0.63
1:D:567:GLU:OE1	1:D:996:GLY:HA2	1.99	0.63
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.81	0.62
1:E:144:ASN:ND2	1:E:319:SER:O	2.30	0.62
1:D:591:LEU:HD13	1:D:611:ALA:HB1	1.81	0.62
1:E:949:ALA:HB3	1:E:1026:PHE:HE2	1.64	0.62
1:E:945:ILE:HD12	1:E:971:ARG:HD3	1.81	0.62
1:A:531:VAL:O	1:A:535:LEU:HG	1.99	0.62
1:A:445:ILE:HD13	1:A:940:LYS:HE2	1.82	0.62
1:C:535:LEU:HD13	1:C:1027:VAL:HG21	1.81	0.62
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.80	0.62
1:D:358:PHE:CD1	1:D:977:MET:HG2	2.35	0.62
1:F:187:TRP:HA	1:F:774:MET:O	1.99	0.62
1:F:203:VAL:O	1:F:207:ILE:HG13	1.99	0.62
1:A:449:LEU:HD22	1:A:453:PHE:HE1	1.64	0.62
1:E:471:SER:O	1:E:475:VAL:HG23	2.00	0.62
1:F:120:GLN:HG3	1:F:123:GLN:HB2	1.81	0.62
1:C:536:ARG:HH21	2:C:1101:LMT:H3O1	1.43	0.62
1:D:280:GLU:OE2	1:D:588:GLN:NE2	2.32	0.62
1:D:360:GLN:NE2	1:D:513:PHE:O	2.31	0.62
1:A:246:PHE:HB3	1:A:268:ILE:HD13	1.80	0.62
1:A:359:LEU:O	1:A:361:ASN:N	2.32	0.62
1:A:492:LEU:O	1:A:496:MET:HG2	1.99	0.62
1:C:450:SER:O	1:C:454:VAL:HG23	2.00	0.62
1:D:445:ILE:O	1:D:449:LEU:HB2	1.98	0.62
1:F:1043:SER:OG	1:F:1044:HIS:N	2.32	0.62
1:F:602:GLU:OE2	1:F:650:ARG:NH1	2.32	0.62
1:B:298:ASN:HB3	1:B:301:ASP:HB2	1.81	0.62
1:B:442:LEU:O	1:B:445:ILE:HG13	2.00	0.62
1:C:950:LYS:HG3	1:C:951:ASP:N	2.14	0.62
1:B:531:VAL:HA	1:B:534:ILE:HG23	1.82	0.62
1:C:712:MET:HB3	1:C:713:LEU:HD12	1.82	0.62
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.82	0.62
1:F:698:ALA:O	1:F:701:GLN:HB3	1.99	0.62
1:C:144:ASN:HA	1:C:320:GLY:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:MET:O	1:C:164:ASP:N	2.33	0.62
1:E:751:GLY:O	1:E:753:ALA:N	2.33	0.62
1:F:733:GLN:NE2	1:F:743:ILE:HG21	2.14	0.62
1:A:216:ALA:HB1	1:A:234:ILE:HG22	1.82	0.61
1:C:380:PHE:HD2	1:C:383:LEU:HD12	1.64	0.61
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.35	0.61
1:F:5:PHE:O	1:F:7:ASP:N	2.25	0.61
1:A:445:ILE:HD13	1:A:940:LYS:CE	2.30	0.61
1:B:658:ILE:O	1:B:659:LYS:HD2	1.99	0.61
1:B:219:LEU:HD23	1:C:754:TRP:HZ3	1.64	0.61
1:E:186:ILE:HD13	1:E:262:LEU:HD21	1.80	0.61
1:E:717:ARG:HH21	1:E:828:LEU:HB3	1.63	0.61
1:F:365:THR:O	1:F:368:PRO:HD2	1.98	0.61
1:A:375:VAL:HG11	1:A:481:SER:HB2	1.82	0.61
1:B:919:ARG:HB3	1:B:921:LEU:HD23	1.82	0.61
1:C:584:GLN:HB2	1:C:622:GLN:HG2	1.82	0.61
1:C:960:LEU:O	1:C:964:THR:HG23	2.00	0.61
1:F:1039:ASP:HB3	1:F:1040:ILE:HA	1.83	0.61
1:F:919:ARG:NH2	1:F:990:VAL:O	2.33	0.61
1:D:281:PHE:CZ	1:D:608:SER:HB2	2.34	0.61
1:E:960:LEU:HD13	1:E:1030:ARG:HG2	1.81	0.61
1:E:441:ALA:O	1:E:445:ILE:HG23	1.99	0.61
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.82	0.61
1:F:187:TRP:HB3	1:F:776:GLU:HG2	1.81	0.61
1:C:47:ALA:HB3	1:C:88:VAL:HG13	1.81	0.61
1:F:340:VAL:CG1	1:F:395:MET:HB3	2.31	0.61
1:C:252:LYS:NZ	1:C:254:ASN:OD1	2.33	0.61
1:D:388:PHE:CE2	1:D:472:ILE:HG21	2.34	0.61
1:E:692:HIS:CD2	1:E:813:SER:HG	2.16	0.61
1:A:703:LEU:HD21	1:A:718:PRO:HD3	1.83	0.61
1:C:897:ILE:HD12	1:C:946:VAL:CG1	2.31	0.61
1:C:731:ILE:HD13	1:C:746:ILE:HD11	1.81	0.61
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.82	0.61
1:F:66:GLU:OE2	1:F:80:SER:OG	2.13	0.61
1:F:470:PHE:CD1	1:F:929:VAL:HG11	2.36	0.61
1:C:482:VAL:O	1:C:486:LEU:HG	2.01	0.61
1:F:559:LEU:HD12	1:F:923:ASN:HB2	1.83	0.61
1:B:706:ALA:HB3	1:B:716:VAL:HG11	1.81	0.60
1:C:115:MET:HB3	1:C:116:PRO:HD3	1.81	0.60
1:E:354:VAL:HG12	1:E:354:VAL:O	2.00	0.60
1:A:154:ILE:O	1:A:157:TYR:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLN:HE21	1:A:63:GLN:HE21	1.49	0.60
1:C:578:LEU:HG	1:C:587:THR:HG22	1.83	0.60
1:C:623:ASN:N	1:C:623:ASN:OD1	2.34	0.60
1:C:668:LEU:H	1:C:668:LEU:HD23	1.65	0.60
1:A:157:TYR:OH	1:A:316:PHE:O	2.20	0.60
1:A:326:PRO:HA	1:A:630:SER:OG	2.01	0.60
1:F:375:VAL:HB	1:F:405:LEU:HD22	1.82	0.60
1:C:817:GLU:HB2	1:C:824:SER:O	2.01	0.60
1:E:251:LEU:HD11	1:E:262:LEU:HA	1.83	0.60
1:F:350:LEU:HD23	1:F:984:LEU:HB3	1.84	0.60
1:A:681:ASP:HB2	1:A:862:MET:HE3	1.82	0.60
1:E:216:ALA:HB1	1:E:234:ILE:HG22	1.83	0.60
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.02	0.60
1:D:519:MET:O	1:D:523:SER:OG	2.17	0.60
1:F:248:LYS:HA	1:F:261:LEU:HD13	1.84	0.60
1:B:171:GLY:HA3	1:B:302:THR:OG1	2.00	0.60
1:D:278:ILE:HG13	1:D:613:ASN:HB3	1.83	0.60
1:D:904:VAL:HG21	1:D:942:ALA:HB2	1.83	0.60
1:D:228:GLN:HB3	1:E:583:THR:HG21	1.83	0.60
1:F:527:TYR:O	1:F:531:VAL:HG23	2.02	0.60
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.84	0.60
1:C:559:LEU:HD23	1:C:560:PRO:HD2	1.84	0.60
1:C:563:PHE:CE2	1:C:564:LEU:HD22	2.36	0.60
1:E:140:VAL:N	1:E:289:LEU:O	2.35	0.60
1:F:542:LEU:O	1:F:546:LEU:HG	2.02	0.60
1:C:1040:ILE:HG12	1:C:1041:GLU:N	2.16	0.59
1:C:38:ILE:CG2	1:C:462:SER:HB2	2.29	0.59
1:D:70:ASN:O	1:D:110:LYS:NZ	2.36	0.59
1:E:111:LEU:HD11	1:E:127:VAL:HB	1.84	0.59
1:A:379:THR:HG23	1:A:476:SER:OG	2.02	0.59
1:A:943:ILE:O	1:A:947:GLU:HB3	2.02	0.59
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.84	0.59
1:D:958:LYS:HB3	1:D:963:ALA:HB2	1.83	0.59
1:F:45:ILE:HG23	1:F:129:VAL:HG22	1.82	0.59
1:F:429:GLU:O	1:F:433:LYS:HB2	2.02	0.59
1:A:906:PRO:O	1:A:908:GLY:N	2.35	0.59
1:B:203:VAL:O	1:B:207:ILE:HG13	2.02	0.59
1:F:58:GLN:OE1	1:F:818:ARG:NH1	2.33	0.59
1:A:518:ARG:O	1:A:522:LYS:HG3	2.03	0.59
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.84	0.59
1:F:82:SER:HB2	1:F:816:LEU:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:HG12	1:A:207:ILE:HD11	1.83	0.59
1:B:682:PHE:O	1:B:827:ILE:N	2.22	0.59
1:E:211:ASN:ND2	1:E:240:LEU:H	2.00	0.59
1:F:61:VAL:HA	1:F:118:LEU:HD22	1.85	0.59
1:F:455:PRO:HG2	1:F:880:SER:HA	1.83	0.59
1:A:960:LEU:O	1:A:964:THR:HG23	2.02	0.59
1:B:369:THR:O	1:B:373:PRO:HG2	2.03	0.59
1:C:959:GLY:HA2	1:C:1041:GLU:O	2.03	0.59
1:E:353:LEU:C	1:E:355:MET:H	2.06	0.59
1:F:462:SER:OG	1:F:865:GLN:HG2	2.03	0.59
1:A:680:PHE:HB2	1:A:859:TRP:HZ3	1.67	0.59
1:B:354:VAL:O	1:B:358:PHE:HB2	2.03	0.59
1:D:699:ARG:NE	1:D:718:PRO:HB3	2.18	0.59
1:C:634:TRP:N	1:C:634:TRP:CD1	2.71	0.59
1:E:979:SER:HB3	1:E:1015:THR:HG21	1.85	0.59
1:E:562:SER:OG	1:E:563:PHE:N	2.33	0.59
1:F:587:THR:HG21	1:F:622:GLN:O	2.03	0.59
1:A:577:GLN:O	1:A:661:ALA:HB1	2.03	0.59
1:A:696:THR:HG23	1:A:699:ARG:NH1	2.18	0.59
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.84	0.59
1:C:443:VAL:O	1:C:447:MET:HB3	2.02	0.59
1:A:394:THR:HG23	1:A:469:GLN:HB3	1.84	0.58
1:B:162:MET:O	1:B:164:ASP:N	2.36	0.58
1:B:213:GLN:HE22	1:C:52:ALA:HA	1.68	0.58
1:C:518:ARG:O	1:C:522:LYS:HG3	2.02	0.58
1:C:66:GLU:OE2	1:C:80:SER:OG	2.15	0.58
1:A:953:MET:HE2	1:A:963:ALA:HB3	1.85	0.58
1:B:744:ASN:O	1:B:748:THR:HG23	2.03	0.58
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.34	0.58
1:E:703:LEU:HD21	1:E:718:PRO:HD3	1.85	0.58
1:E:752:ALA:O	1:E:774:MET:HA	2.04	0.58
1:F:982:PHE:HD2	1:F:1011:MET:HG2	1.67	0.58
1:A:904:VAL:HG12	1:A:938:SER:HB2	1.84	0.58
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.03	0.58
1:B:104:GLN:HG2	1:C:109:ASN:ND2	2.18	0.58
1:B:173:GLY:HA2	1:C:71:GLY:HA3	1.85	0.58
1:B:351:VAL:HG22	1:B:981:ALA:HB1	1.85	0.58
1:C:751:GLY:O	1:C:753:ALA:N	2.35	0.58
1:D:751:GLY:O	1:D:753:ALA:N	2.36	0.58
1:E:166:ILE:HG13	1:E:309:GLU:HB3	1.86	0.58
1:E:394:THR:HG23	1:E:469:GLN:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:TRP:HH2	1:F:370:ILE:HD13	1.69	0.58
1:F:368:PRO:HG3	1:F:413:VAL:HG21	1.85	0.58
1:F:492:LEU:HA	1:F:495:THR:OG1	2.03	0.58
1:F:551:GLY:O	1:F:555:LEU:HB2	2.03	0.58
1:A:459:PHE:CZ	1:A:876:LEU:HD12	2.39	0.58
1:A:733:GLN:NE2	1:A:743:ILE:HG21	2.18	0.58
1:B:511:GLY:HA2	1:B:515:TRP:HE1	1.69	0.58
1:C:371:ALA:O	1:C:375:VAL:HG23	2.04	0.58
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.85	0.58
1:D:696:THR:HG23	1:D:699:ARG:HH12	1.68	0.58
1:B:685:ILE:HD11	1:B:819:TYR:HD2	1.68	0.58
1:E:871:ASN:N	1:E:871:ASN:OD1	2.37	0.58
1:F:351:VAL:HG11	1:F:406:VAL:HG11	1.85	0.58
1:E:14:VAL:HG22	1:F:886:LEU:HD12	1.84	0.58
1:A:906:PRO:O	1:A:909:VAL:N	2.37	0.58
1:F:380:PHE:HA	1:F:383:LEU:HD12	1.85	0.58
1:A:960:LEU:HD23	1:A:1031:ARG:CZ	2.34	0.58
1:A:146:ASP:HB2	1:A:148:THR:HG23	1.85	0.58
1:A:140:VAL:HG11	1:A:310:LEU:HD21	1.86	0.58
1:B:189:ASN:HB3	1:B:192:GLU:HB2	1.86	0.58
1:D:897:ILE:HG12	1:D:1030:ARG:HD2	1.85	0.58
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.67	0.58
1:D:230:LEU:HD21	1:E:809:TRP:HH2	1.68	0.58
1:F:1040:ILE:CA	1:F:1041:GLU:HB2	2.33	0.58
1:D:113:LEU:HD11	1:F:128:SER:HB3	1.84	0.58
1:A:94:PHE:CE1	1:A:103:ALA:HB1	2.39	0.58
1:A:137:LEU:HB2	1:A:293:LEU:HB2	1.85	0.58
1:F:164:ASP:O	1:F:168:ARG:NH1	2.36	0.58
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.85	0.58
1:A:400:LEU:CD2	1:A:929:VAL:HG12	2.33	0.57
1:B:167:SER:OG	1:C:70:ASN:ND2	2.37	0.57
1:C:1039:ASP:HB3	1:C:1040:ILE:HA	1.85	0.57
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.85	0.57
1:C:414:GLU:OE1	1:C:973:ARG:NH1	2.36	0.57
1:D:383:LEU:HD22	1:D:388:PHE:HD2	1.69	0.57
1:D:674:LEU:HD23	1:D:675:GLY:N	2.19	0.57
1:D:971:ARG:C	1:D:974:PRO:HD2	2.23	0.57
1:C:578:LEU:CD1	1:C:579:PRO:HD2	2.33	0.57
1:D:420:MET:HB3	1:D:500:ILE:HB	1.85	0.57
1:E:166:ILE:HG23	1:E:306:ILE:HG12	1.87	0.57
1:E:869:SER:O	1:E:869:SER:OG	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.38	0.57
1:F:81:ASN:HD21	1:F:815:ARG:HH22	1.52	0.57
1:F:66:GLU:OE1	1:F:821:GLY:HA2	2.04	0.57
1:A:590:VAL:O	1:A:593:GLU:HB2	2.04	0.57
1:D:448:VAL:HG22	1:D:887:CYS:CB	2.34	0.57
1:E:162:MET:C	1:E:164:ASP:H	2.04	0.57
1:A:13:TRP:O	1:A:17:ILE:HG13	2.04	0.57
1:C:521:GLU:O	1:C:524:THR:HG22	2.03	0.57
1:C:525:HIS:HA	1:C:528:THR:HG22	1.87	0.57
1:C:326:PRO:O	1:C:630:SER:HB2	2.04	0.57
1:D:989:LEU:HB3	1:D:1000:GLN:O	2.04	0.57
1:E:931:LEU:O	1:E:935:ILE:HG13	2.03	0.57
1:F:426:PRO:HD2	1:F:429:GLU:HG2	1.85	0.57
1:A:165:ALA:HB3	1:A:313:MET:HE1	1.85	0.57
1:A:832:ALA:O	1:A:835:LYS:HB2	2.05	0.57
1:A:947:GLU:HG3	1:A:948:PHE:HD1	1.69	0.57
1:D:154:ILE:O	1:D:157:TYR:N	2.37	0.57
1:D:52:ALA:HB1	1:D:56:THR:HB	1.86	0.57
1:D:728:LYS:HG2	1:D:808:ARG:NH1	2.19	0.57
1:F:612:VAL:HB	1:F:626:ILE:HG22	1.85	0.57
1:E:535:LEU:O	1:E:537:SER:N	2.38	0.57
1:A:465:ALA:O	1:A:469:GLN:HG2	2.04	0.57
1:A:971:ARG:C	1:A:974:PRO:HD2	2.25	0.57
1:B:172:VAL:HG22	1:B:306:ILE:HD11	1.86	0.57
1:E:911:GLY:HA3	1:E:1013:THR:OG1	2.05	0.57
1:E:359:LEU:O	1:E:361:ASN:N	2.37	0.57
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.87	0.57
1:F:744:ASN:O	1:F:748:THR:HG23	2.04	0.57
1:A:254:ASN:HB2	1:A:258:SER:O	2.05	0.57
1:A:515:TRP:O	1:A:519:MET:HG3	2.05	0.57
1:A:744:ASN:O	1:A:748:THR:HG23	2.04	0.57
1:C:418:ARG:O	1:C:422:GLU:HB2	2.05	0.57
1:E:987:MET:O	1:E:990:VAL:N	2.35	0.57
1:A:344:LEU:HD11	1:A:398:MET:HB3	1.85	0.57
1:A:414:GLU:HG3	1:A:977:MET:HE1	1.87	0.57
1:C:171:GLY:HA3	1:C:302:THR:OG1	2.04	0.57
1:D:344:LEU:CD2	1:D:402:ILE:HD11	2.34	0.57
1:D:781:MET:HE2	1:F:225:VAL:HG22	1.86	0.57
1:E:344:LEU:HD23	1:E:402:ILE:HD11	1.86	0.57
1:E:634:TRP:N	1:E:634:TRP:CD1	2.71	0.57
1:E:699:ARG:NH2	1:E:722:GLU:OE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:VAL:HG22	1:A:971:ARG:NH2	2.20	0.56
1:A:4:PHE:O	1:A:8:ARG:HD2	2.04	0.56
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.87	0.56
1:B:540:ARG:O	1:B:543:VAL:HB	2.05	0.56
1:C:6:ILE:CG2	1:C:12:ALA:HB2	2.35	0.56
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.87	0.56
1:E:841:MET:HE1	1:E:867:ARG:HB2	1.87	0.56
1:F:694:LYS:H	1:F:694:LYS:HD2	1.70	0.56
1:B:535:LEU:HD13	1:B:1027:VAL:HG21	1.86	0.56
1:B:686:ASP:HB2	1:B:695:LEU:HD23	1.88	0.56
1:B:181:GLN:NE2	1:B:769:LYS:HG2	2.19	0.56
1:D:350:LEU:HD13	1:D:984:LEU:O	2.05	0.56
1:E:399:VAL:O	1:E:402:ILE:HG13	2.05	0.56
1:F:336:SER:O	1:F:340:VAL:HG23	2.04	0.56
1:A:69:MET:SD	1:A:72:ILE:HD11	2.45	0.56
1:D:485:ALA:O	1:D:490:PRO:HD3	2.04	0.56
1:D:527:TYR:O	1:D:531:VAL:HG23	2.05	0.56
1:E:355:MET:SD	1:E:365:THR:HA	2.44	0.56
1:F:1039:ASP:OD2	1:F:1041:GLU:HG3	2.05	0.56
1:F:713:LEU:HD11	1:F:843:LEU:HD12	1.87	0.56
1:A:947:GLU:HG3	1:A:948:PHE:N	2.19	0.56
1:B:400:LEU:HG	1:B:929:VAL:HG12	1.87	0.56
1:D:350:LEU:HD22	1:D:984:LEU:HB3	1.88	0.56
1:E:542:LEU:O	1:E:546:LEU:HG	2.05	0.56
1:B:713:LEU:HD11	1:B:843:LEU:HD12	1.86	0.56
1:C:958:LYS:HB3	1:C:963:ALA:HB2	1.88	0.56
1:D:1013:THR:O	1:D:1017:LEU:HB2	2.05	0.56
1:F:420:MET:HG2	1:F:425:LEU:O	2.06	0.56
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.87	0.56
1:A:157:TYR:CZ	1:A:318:PRO:HD3	2.40	0.56
1:A:395:MET:O	1:A:398:MET:HB2	2.06	0.56
1:A:564:LEU:HD22	1:A:671:ILE:HG13	1.87	0.56
1:B:194:ASN:HA	1:B:798:MET:HE1	1.88	0.56
1:D:184:MET:HB3	1:D:771:VAL:HG13	1.87	0.56
1:D:932:LEU:HD23	1:D:935:ILE:HD12	1.87	0.56
1:F:137:LEU:HB2	1:F:293:LEU:HB2	1.87	0.56
1:F:156:ASP:OD1	1:F:765:ARG:NH2	2.38	0.56
1:F:414:GLU:OE1	1:F:973:ARG:HD3	2.06	0.56
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.86	0.56
1:F:455:PRO:HG3	1:F:883:VAL:HG21	1.87	0.56
1:A:512:PHE:HB3	1:A:513:PHE:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:979:SER:HB3	1:C:1015:THR:HG21	1.87	0.56
1:C:356:TYR:HE1	1:C:362:PHE:HA	1.70	0.56
1:D:391:ASN:O	1:D:395:MET:HG2	2.05	0.56
1:D:393:LEU:HD13	1:D:466:ILE:HA	1.88	0.56
1:D:507:GLU:C	1:D:509:LYS:H	2.09	0.56
1:F:99:ASP:O	1:F:102:ILE:HB	2.05	0.56
1:A:332:PHE:O	1:A:336:SER:HB3	2.05	0.56
1:A:549:VAL:O	1:A:552:MET:HB3	2.04	0.56
1:A:623:ASN:OD1	1:A:623:ASN:N	2.36	0.56
1:D:375:VAL:HG11	1:D:405:LEU:HD22	1.88	0.56
1:E:347:ALA:HB1	1:E:402:ILE:HG21	1.88	0.56
1:E:367:ILE:HG12	1:E:496:MET:SD	2.45	0.56
1:A:751:GLY:O	1:A:753:ALA:N	2.39	0.56
1:B:652:THR:CG2	1:B:665:ALA:H	2.19	0.56
1:C:968:VAL:HA	1:C:971:ARG:HH12	1.71	0.56
1:C:40:PRO:HD2	1:C:674:LEU:HD11	1.88	0.56
1:C:6:ILE:HG21	1:C:12:ALA:HB2	1.87	0.56
1:D:955:LYS:O	1:D:956:GLU:HG2	2.06	0.56
1:E:459:PHE:CB	1:E:464:GLY:HA2	2.36	0.56
1:E:589:LYS:HA	1:E:592:ASN:HD22	1.70	0.56
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.71	0.56
1:E:699:ARG:O	1:E:703:LEU:HB2	2.05	0.56
1:F:743:ILE:O	1:F:746:ILE:HG13	2.06	0.56
1:D:251:LEU:HD11	1:D:265:VAL:HG21	1.88	0.56
1:D:643:LYS:NZ	1:D:993:THR:HG23	2.21	0.56
1:D:66:GLU:OE2	1:D:80:SER:OG	2.14	0.56
1:E:42:ALA:HB3	1:E:132:SER:HB3	1.87	0.56
1:E:524:THR:O	1:E:527:TYR:HB3	2.06	0.56
1:F:409:ALA:O	1:F:413:VAL:HG23	2.06	0.56
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.41	0.55
1:B:399:VAL:HG13	1:B:402:ILE:HD11	1.88	0.55
1:B:456:MET:HG3	1:B:471:SER:OG	2.06	0.55
1:C:947:GLU:HG3	1:C:948:PHE:CD1	2.41	0.55
1:D:699:ARG:HE	1:D:703:LEU:HD11	1.70	0.55
1:E:751:GLY:O	1:E:754:TRP:N	2.39	0.55
1:F:350:LEU:HD23	1:F:984:LEU:HD22	1.88	0.55
1:F:671:ILE:HG21	1:F:674:LEU:HB2	1.87	0.55
1:C:187:TRP:HA	1:C:774:MET:O	2.05	0.55
1:D:38:ILE:HG23	1:D:462:SER:OG	2.06	0.55
1:A:736:ALA:HB1	1:A:741:VAL:HG23	1.88	0.55
1:A:220:GLY:HA2	1:B:781:MET:HE3	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLN:O	1:C:112:GLN:HG2	2.06	0.55
1:C:121:GLU:O	1:C:124:GLN:HG2	2.06	0.55
1:D:185:ARG:NE	1:D:272:GLY:O	2.39	0.55
1:D:366:LEU:HA	1:D:369:THR:HB	1.87	0.55
1:B:1011:MET:O	1:B:1015:THR:HG23	2.05	0.55
1:B:861:GLY:O	1:B:864:TYR:HB3	2.07	0.55
1:F:359:LEU:O	1:F:361:ASN:N	2.39	0.55
1:A:166:ILE:HD12	1:A:306:ILE:HG12	1.87	0.55
1:C:441:ALA:HB2	1:C:948:PHE:HE1	1.72	0.55
1:C:775:SER:HB2	1:C:789:TRP:CZ2	2.42	0.55
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.72	0.55
1:D:456:MET:HG3	1:D:471:SER:HB2	1.89	0.55
1:E:534:ILE:CG2	2:E:1101:LMT:H1'	2.36	0.55
1:E:668:LEU:HD23	1:E:668:LEU:H	1.71	0.55
1:E:692:HIS:CE1	1:E:813:SER:HG	2.15	0.55
1:F:135:SER:HB3	1:F:673:GLU:CB	2.31	0.55
1:C:363:ARG:HB3	1:C:363:ARG:HH11	1.71	0.55
1:C:355:MET:SD	1:C:368:PRO:HB2	2.46	0.55
1:C:654:ALA:O	1:C:658:ILE:HG12	2.07	0.55
1:B:230:LEU:HD21	1:C:809:TRP:HH2	1.71	0.55
1:D:449:LEU:HB3	1:D:478:MET:SD	2.47	0.55
1:F:703:LEU:HD11	1:F:718:PRO:HD3	1.87	0.55
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.42	0.55
1:B:377:LEU:O	1:B:380:PHE:HB2	2.06	0.55
1:C:375:VAL:HA	1:C:480:LEU:HD13	1.89	0.55
1:C:568:ASP:O	1:C:634:TRP:HZ3	1.89	0.55
1:C:758:TYR:HB2	1:C:772:TYR:CZ	2.41	0.55
1:D:75:LEU:HD11	1:D:92:LEU:HD23	1.88	0.55
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.89	0.55
1:B:375:VAL:O	1:B:379:THR:OG1	2.23	0.55
1:E:775:SER:HB2	1:E:789:TRP:CZ2	2.42	0.55
1:A:453:PHE:O	1:A:471:SER:OG	2.13	0.55
1:C:279:ALA:HB3	1:C:286:ALA:O	2.07	0.55
1:C:464:GLY:O	1:C:468:ARG:HB2	2.06	0.55
1:C:590:VAL:HA	1:C:593:GLU:OE1	2.07	0.55
1:D:253:VAL:HG12	1:D:259:ARG:HG2	1.88	0.55
1:D:4:PHE:HB2	1:D:5:PHE:CD1	2.42	0.55
1:D:668:LEU:H	1:D:668:LEU:HD23	1.70	0.55
1:A:318:PRO:HD2	1:A:321:LEU:HD12	1.89	0.55
1:B:456:MET:O	1:B:467:TYR:HB3	2.07	0.55
1:D:480:LEU:O	1:D:484:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:987:MET:HB3	1:D:988:PRO:HD3	1.89	0.55
1:E:254:ASN:HB2	1:E:258:SER:O	2.06	0.55
1:A:144:ASN:OD1	1:A:148:THR:OG1	2.25	0.54
1:A:244:GLU:O	1:A:247:GLY:N	2.36	0.54
1:A:136:PHE:HE2	1:A:290:GLY:HA3	1.72	0.54
1:A:327:TYR:HA	1:A:571:VAL:HG11	1.89	0.54
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.88	0.54
1:A:521:GLU:O	1:A:524:THR:HG22	2.07	0.54
1:B:616:GLY:HA3	1:B:624:THR:HB	1.87	0.54
1:E:140:VAL:O	1:E:289:LEU:N	2.39	0.54
1:E:669:PRO:HB3	1:E:674:LEU:HD12	1.89	0.54
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.88	0.54
1:F:623:ASN:OD1	1:F:623:ASN:N	2.40	0.54
1:B:1037:ASN:N	1:B:1038:GLU:HB3	2.23	0.54
1:D:169:THR:HG21	1:D:306:ILE:HG13	1.90	0.54
1:D:647:ILE:HG12	1:D:650:ARG:HH12	1.72	0.54
1:E:376:LEU:O	1:E:379:THR:N	2.39	0.54
1:E:568:ASP:O	1:E:634:TRP:HZ3	1.90	0.54
1:B:317:PHE:CE2	1:B:323:ILE:HD11	2.43	0.54
1:E:139:VAL:O	1:E:326:PRO:HD2	2.06	0.54
1:E:459:PHE:HB2	1:E:464:GLY:HA2	1.89	0.54
1:E:950:LYS:HA	1:E:953:MET:HE3	1.89	0.54
1:F:145:THR:HA	1:F:284:GLN:HE22	1.73	0.54
1:A:531:VAL:O	1:A:534:ILE:HG13	2.07	0.54
1:B:685:ILE:HD11	1:B:819:TYR:CD2	2.41	0.54
1:D:394:THR:HG22	1:D:473:THR:OG1	2.07	0.54
1:F:189:ASN:HB3	1:F:192:GLU:HB2	1.88	0.54
1:F:940:LYS:NZ	1:F:978:THR:HG21	2.23	0.54
1:B:545:TYR:CE2	1:B:1025:PHE:HZ	2.26	0.54
1:E:104:GLN:HB2	1:E:131:LYS:HD2	1.90	0.54
1:E:181:GLN:HG2	1:E:182:TYR:N	2.23	0.54
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.90	0.54
1:E:201:VAL:HG21	1:E:745:ASP:HB3	1.90	0.54
1:F:184:MET:HB3	1:F:771:VAL:HG13	1.88	0.54
1:C:412:VAL:HG22	1:C:438:ILE:HD12	1.89	0.54
1:C:504:ASP:OD1	1:C:506:GLY:N	2.35	0.54
1:C:808:ARG:NH1	1:C:810:GLU:OE2	2.41	0.54
1:D:1017:LEU:O	1:D:1021:PHE:HB2	2.08	0.54
1:D:728:LYS:HA	1:F:235:ILE:HB	1.89	0.54
1:F:139:VAL:O	1:F:326:PRO:HD2	2.08	0.54
1:A:34:GLN:HA	1:A:333:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:VAL:HG13	1:B:291:ILE:HG23	1.90	0.54
1:B:294:ALA:O	1:B:296:GLY:N	2.40	0.54
1:B:600:THR:O	1:B:603:LYS:HB2	2.08	0.54
1:B:66:GLU:OE2	1:B:818:ARG:HD3	2.08	0.54
1:C:187:TRP:HB3	1:C:776:GLU:HG2	1.90	0.54
1:A:781:MET:HE1	1:C:225:VAL:H	1.72	0.54
1:C:668:LEU:HB2	1:C:669:PRO:HD2	1.90	0.54
1:A:641:GLU:HB2	1:A:650:ARG:HH22	1.72	0.54
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.89	0.54
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.43	0.54
1:C:24:GLY:HA2	1:C:27:ILE:HG23	1.89	0.54
1:C:598:TYR:HB3	1:C:606:VAL:HG21	1.88	0.54
1:C:61:VAL:HG11	1:C:88:VAL:HG11	1.89	0.54
1:C:971:ARG:HH11	1:C:971:ARG:HB3	1.72	0.54
1:E:213:GLN:HA	1:E:237:GLN:O	2.08	0.54
1:E:179:GLY:HA2	1:E:277:ILE:HD11	1.90	0.54
1:E:776:GLU:HB3	1:E:779:TYR:CD1	2.42	0.54
1:F:249:ILE:HB	1:F:262:LEU:HB2	1.90	0.54
1:B:530:SER:OG	2:B:1101:LMT:H12	2.07	0.54
1:C:393:LEU:HD13	1:C:466:ILE:HA	1.88	0.54
1:C:669:PRO:HD3	1:C:677:ALA:C	2.28	0.54
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.42	0.54
1:E:165:ALA:HB3	1:E:313:MET:CE	2.38	0.54
1:A:401:ALA:O	1:A:405:LEU:HG	2.08	0.54
1:A:699:ARG:NH2	1:A:722:GLU:OE1	2.37	0.54
1:B:553:ALA:O	1:B:557:VAL:HG23	2.08	0.54
1:B:596:HIS:O	1:B:600:THR:OG1	2.18	0.54
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.43	0.54
1:E:121:GLU:O	1:E:125:GLN:HB2	2.08	0.54
1:E:351:VAL:HG22	1:E:981:ALA:HB1	1.90	0.54
1:F:428:LYS:O	1:F:432:ARG:HG3	2.08	0.54
1:A:434:SER:O	1:A:438:ILE:HG12	2.08	0.53
1:B:448:VAL:O	1:B:452:VAL:HG13	2.08	0.53
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.37	0.53
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.90	0.53
1:D:889:ALA:HA	1:D:894:SER:O	2.09	0.53
1:E:1041:GLU:HB3	1:E:1042:HIS:CB	2.39	0.53
1:F:145:THR:HA	1:F:284:GLN:NE2	2.22	0.53
1:B:174:ASP:HB3	1:B:292:LYS:HD2	1.90	0.53
1:C:587:THR:HA	1:C:590:VAL:HG23	1.91	0.53
1:D:225:VAL:O	1:D:228:GLN:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:LEU:O	1:D:361:ASN:N	2.41	0.53
1:E:165:ALA:HB3	1:E:313:MET:HE3	1.90	0.53
1:F:527:TYR:OH	1:F:1019:ILE:O	2.21	0.53
1:F:960:LEU:HD21	1:F:1027:VAL:HA	1.91	0.53
1:B:239:ARG:NH1	1:B:761:ASP:HB3	2.23	0.53
1:D:1038:GLU:OE1	1:D:1038:GLU:HA	2.09	0.53
1:D:459:PHE:O	1:D:468:ARG:NH2	2.41	0.53
1:E:7:ASP:OD2	1:E:432:ARG:NH2	2.41	0.53
1:F:355:MET:HB3	1:F:365:THR:HG23	1.90	0.53
1:A:225:VAL:HG22	1:B:781:MET:HE2	1.91	0.53
1:A:888:LEU:HD22	1:A:892:TYR:CE2	2.43	0.53
1:D:885:PHE:CE1	1:D:898:PRO:HB2	2.43	0.53
1:E:669:PRO:CB	1:E:674:LEU:HD12	2.38	0.53
1:F:368:PRO:O	1:F:371:ALA:HB3	2.08	0.53
1:A:186:ILE:HD13	1:A:262:LEU:HD21	1.91	0.53
1:B:398:MET:HG3	1:B:473:THR:HG22	1.91	0.53
1:B:652:THR:HG22	1:B:665:ALA:H	1.73	0.53
1:D:414:GLU:HG3	1:D:974:PRO:HG3	1.90	0.53
1:E:158:VAL:HG13	1:E:162:MET:HB2	1.91	0.53
1:E:559:LEU:HD12	1:E:923:ASN:HB2	1.90	0.53
1:F:187:TRP:CB	1:F:776:GLU:HG2	2.38	0.53
1:A:200:PRO:HA	1:A:203:VAL:HG23	1.91	0.53
1:B:307:ARG:HG2	1:B:325:TYR:OH	2.08	0.53
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.43	0.53
1:D:234:ILE:HD11	1:E:754:TRP:CE3	2.44	0.53
1:D:94:PHE:CE2	1:D:103:ALA:HB1	2.43	0.53
1:E:1041:GLU:HB3	1:E:1042:HIS:HB3	1.90	0.53
1:F:758:TYR:HB2	1:F:772:TYR:CZ	2.43	0.53
1:C:376:LEU:HD22	1:C:398:MET:SD	2.49	0.53
1:C:594:VAL:HG22	1:C:655:PHE:CE2	2.44	0.53
1:D:726:GLN:CD	1:D:812:GLY:HA3	2.29	0.53
1:E:157:TYR:CE1	1:E:318:PRO:HD3	2.44	0.53
1:E:675:GLY:HA3	1:E:862:MET:SD	2.49	0.53
1:A:598:TYR:HB3	1:A:606:VAL:HG21	1.89	0.53
1:B:34:GLN:HG3	1:B:333:VAL:HG22	1.90	0.53
1:D:335:ILE:O	1:D:339:GLU:HG2	2.09	0.53
1:E:639:GLY:O	1:E:643:LYS:HG3	2.09	0.53
1:F:27:ILE:HA	1:F:30:LEU:HD22	1.91	0.53
1:A:43:VAL:HG23	1:A:94:PHE:HE1	1.74	0.53
1:B:751:GLY:O	1:B:753:ALA:N	2.42	0.53
1:C:3:ASN:O	1:C:6:ILE:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.44	0.53
1:D:556:PHE:HD1	1:D:913:LEU:HD21	1.72	0.53
1:D:754:TRP:HZ3	1:F:219:LEU:HD23	1.73	0.53
1:E:1035:ARG:HB3	1:E:1035:ARG:CZ	2.39	0.53
1:E:445:ILE:HD12	1:E:449:LEU:HG	1.91	0.53
1:F:186:ILE:HD13	1:F:262:LEU:HD21	1.90	0.53
1:F:378:GLY:HA3	1:F:480:LEU:HD11	1.91	0.53
1:C:298:ASN:HB3	1:C:301:ASP:HB2	1.91	0.53
1:D:602:GLU:HB3	1:D:606:VAL:HG23	1.90	0.53
1:D:396:PHE:HE1	1:D:999:ALA:HB1	1.74	0.53
1:E:190:PRO:HB3	1:E:789:TRP:CE2	2.43	0.53
1:E:343:THR:HG21	1:E:399:VAL:HG13	1.91	0.53
1:F:152:GLU:HA	1:F:155:SER:HB2	1.90	0.53
1:F:352:PHE:HD2	1:F:353:LEU:HD23	1.73	0.53
1:F:378:GLY:O	1:F:382:VAL:HG23	2.08	0.53
1:F:643:LYS:HE2	1:F:645:GLU:CG	2.39	0.53
1:C:743:ILE:HD12	1:C:743:ILE:H	1.74	0.52
1:E:38:ILE:HG22	1:E:462:SER:HB3	1.92	0.52
1:D:886:LEU:HD13	1:F:18:ILE:HG13	1.91	0.52
1:A:1034:SER:HA	1:A:1035:ARG:HB2	1.91	0.52
1:A:952:LEU:O	1:A:956:GLU:HB2	2.09	0.52
1:B:36:PRO:HD3	1:B:391:ASN:OD1	2.09	0.52
1:B:516:PHE:HA	1:B:519:MET:HB2	1.91	0.52
1:B:594:VAL:HG22	1:B:655:PHE:CE2	2.44	0.52
1:D:412:VAL:HG22	1:D:438:ILE:CD1	2.39	0.52
1:D:442:LEU:O	1:D:445:ILE:HG13	2.10	0.52
1:D:744:ASN:O	1:D:748:THR:HG23	2.09	0.52
1:E:124:GLN:HE21	1:E:758:TYR:HD2	1.56	0.52
1:E:237:GLN:OE1	1:F:747:ASN:ND2	2.39	0.52
1:A:712:MET:HG2	1:A:843:LEU:HG	1.91	0.52
1:A:955:LYS:O	1:A:956:GLU:HG2	2.10	0.52
1:C:396:PHE:O	1:C:400:LEU:HB2	2.08	0.52
1:C:694:LYS:HE3	1:C:694:LYS:H	1.74	0.52
1:C:449:LEU:HD11	1:C:937:LEU:HD21	1.91	0.52
1:C:968:VAL:HA	1:C:971:ARG:NH1	2.24	0.52
1:D:577:GLN:OE1	1:D:624:THR:HG23	2.09	0.52
1:E:111:LEU:O	1:E:115:MET:HG2	2.10	0.52
1:E:415:ASN:O	1:E:419:VAL:HG23	2.09	0.52
1:E:418:ARG:HD2	1:E:422:GLU:OE1	2.09	0.52
1:E:817:GLU:OE1	1:E:825:MET:HA	2.09	0.52
1:C:310:LEU:HD23	1:C:323:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:VAL:O	1:C:417:GLU:HG2	2.10	0.52
1:C:818:ARG:NH2	1:C:821:GLY:O	2.43	0.52
1:D:58:GLN:HA	1:D:62:THR:HB	1.92	0.52
1:E:960:LEU:HD21	1:E:1027:VAL:HA	1.90	0.52
1:A:1020:PHE:CE2	2:A:1101:LMT:H22	2.44	0.52
1:C:456:MET:HB3	1:C:876:LEU:HD21	1.90	0.52
1:C:393:LEU:HD11	1:C:466:ILE:HD13	1.92	0.52
1:D:230:LEU:HD21	1:E:809:TRP:CH2	2.43	0.52
1:E:35:TYR:HD2	1:E:393:LEU:HG	1.74	0.52
1:F:764:ASP:OD1	1:F:765:ARG:HG3	2.09	0.52
1:F:947:GLU:HG3	1:F:948:PHE:N	2.24	0.52
1:A:451:ALA:HB1	1:A:883:VAL:HG12	1.92	0.52
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.44	0.52
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.89	0.52
1:A:781:MET:CE	1:C:225:VAL:H	2.23	0.52
1:E:987:MET:HB3	1:E:988:PRO:HD3	1.91	0.52
1:F:165:ALA:HB3	1:F:313:MET:HE1	1.91	0.52
1:F:412:VAL:HG22	1:F:438:ILE:HD12	1.92	0.52
1:F:447:MET:SD	1:F:891:LEU:HD22	2.50	0.52
1:B:415:ASN:O	1:B:419:VAL:HG23	2.09	0.52
1:E:536:ARG:CZ	2:E:1101:LMT:H4B	2.39	0.52
1:E:949:ALA:HB3	1:E:1026:PHE:CE2	2.45	0.52
1:F:379:THR:HG23	1:F:476:SER:OG	2.09	0.52
1:A:350:LEU:CD2	1:A:984:LEU:HB3	2.36	0.52
1:C:682:PHE:HE1	1:C:857:TYR:HB2	1.73	0.52
1:C:898:PRO:O	1:C:901:VAL:HG12	2.10	0.52
1:D:14:VAL:HG13	1:E:886:LEU:HG	1.91	0.52
1:E:371:ALA:O	1:E:375:VAL:HG23	2.09	0.52
1:A:768:VAL:HG12	1:B:63:GLN:NE2	2.24	0.52
1:B:149:MET:HB3	1:B:153:ASP:HB3	1.92	0.52
1:B:516:PHE:O	1:B:520:PHE:N	2.43	0.52
1:C:551:GLY:O	1:C:555:LEU:HB2	2.10	0.52
1:C:893:GLU:HG3	1:C:893:GLU:O	2.09	0.52
1:E:783:PRO:HA	1:E:786:ILE:HG12	1.91	0.52
1:F:743:ILE:H	1:F:743:ILE:HD12	1.74	0.52
1:A:375:VAL:HG21	1:A:481:SER:HA	1.92	0.52
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.44	0.52
1:A:743:ILE:HD12	1:A:743:ILE:H	1.75	0.52
1:B:641:GLU:O	1:B:650:ARG:NH2	2.24	0.52
1:D:355:MET:HB3	1:D:365:THR:OG1	2.10	0.52
1:D:540:ARG:O	1:D:543:VAL:HB	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:435:MET:SD	1:E:490:PRO:HB3	2.50	0.52
1:E:445:ILE:HB	1:E:940:LYS:HG3	1.92	0.52
1:E:588:GLN:O	1:E:592:ASN:ND2	2.42	0.52
1:E:576:VAL:HG22	1:E:663:VAL:HG22	1.91	0.52
1:E:846:GLN:O	1:E:850:LYS:HG2	2.11	0.52
1:E:57:VAL:HG11	1:E:86:GLY:HA2	1.92	0.52
1:F:491:ALA:O	1:F:495:THR:HG23	2.10	0.52
1:F:63:GLN:OE1	1:F:67:GLN:NE2	2.43	0.52
1:F:925:VAL:HA	1:F:928:GLN:OE1	2.09	0.52
1:F:407:ASP:OD1	1:F:978:THR:HG23	2.09	0.52
1:A:586:ARG:O	1:A:589:LYS:HB3	2.10	0.51
1:A:817:GLU:HB2	1:A:824:SER:O	2.10	0.51
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.92	0.51
1:D:394:THR:HG23	1:D:469:GLN:HB3	1.92	0.51
1:D:13:TRP:CZ2	1:D:492:LEU:HD21	2.45	0.51
1:D:445:ILE:HG12	1:D:940:LYS:HE3	1.92	0.51
1:E:347:ALA:CB	1:E:402:ILE:HG21	2.40	0.51
1:F:531:VAL:O	1:F:535:LEU:HG	2.10	0.51
1:F:463:THR:HG23	1:F:925:VAL:HG22	1.92	0.51
1:A:508:GLY:O	1:A:511:GLY:N	2.42	0.51
1:A:957:GLY:HA2	1:A:1042:HIS:CB	2.28	0.51
1:B:544:LEU:HA	1:B:547:ILE:HD12	1.91	0.51
1:B:654:ALA:O	1:B:658:ILE:HG12	2.10	0.51
1:D:587:THR:HB	1:D:613:ASN:HD21	1.74	0.51
1:E:691:GLY:N	1:E:694:LYS:HD3	2.25	0.51
1:E:743:ILE:H	1:E:743:ILE:HD12	1.75	0.51
1:E:762:PHE:CE1	1:E:764:ASP:HB2	2.45	0.51
1:F:1035:ARG:HB2	1:F:1038:GLU:HB2	1.92	0.51
1:F:456:MET:HE3	1:F:932:LEU:HD12	1.93	0.51
1:F:888:LEU:HD11	1:F:943:ILE:HD11	1.91	0.51
1:A:58:GLN:NE2	1:A:63:GLN:HE21	2.08	0.51
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.91	0.51
1:A:47:ALA:O	1:A:87:THR:HA	2.11	0.51
1:B:356:TYR:C	1:B:358:PHE:H	2.13	0.51
1:D:360:GLN:NE2	1:D:513:PHE:HB3	2.25	0.51
1:F:412:VAL:CG2	1:F:442:LEU:HD11	2.41	0.51
1:A:238:THR:HG23	1:B:728:LYS:NZ	2.26	0.51
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.44	0.51
1:A:888:LEU:HD22	1:A:892:TYR:HE2	1.75	0.51
1:C:742:SER:O	1:C:746:ILE:HG23	2.10	0.51
1:D:219:LEU:HD23	1:E:754:TRP:CZ3	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:527:TYR:O	1:E:530:SER:HB3	2.10	0.51
1:E:527:TYR:CE2	1:E:972:LEU:HG	2.46	0.51
1:F:192:GLU:HB3	1:F:265:VAL:HA	1.92	0.51
1:F:504:ASP:C	1:F:506:GLY:H	2.12	0.51
1:F:525:HIS:HA	1:F:528:THR:CG2	2.40	0.51
1:A:958:LYS:HB3	1:A:963:ALA:HB2	1.92	0.51
1:B:143:ILE:HG21	1:B:281:PHE:CD2	2.46	0.51
1:B:231:ASN:HD22	1:C:622:GLN:CD	2.13	0.51
1:B:65:ILE:O	1:B:69:MET:HG2	2.11	0.51
1:D:2:PRO:O	1:D:6:ILE:HG23	2.10	0.51
1:D:717:ARG:O	1:D:827:ILE:HG23	2.10	0.51
1:E:457:ALA:HB2	1:E:471:SER:CB	2.40	0.51
1:F:594:VAL:HG22	1:F:655:PHE:CE2	2.45	0.51
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.92	0.51
1:C:736:ALA:HB1	1:C:741:VAL:HG23	1.92	0.51
1:D:559:LEU:HD23	1:D:560:PRO:HD2	1.92	0.51
1:F:1034:SER:OG	1:F:1035:ARG:N	2.43	0.51
1:F:162:MET:O	1:F:164:ASP:N	2.43	0.51
1:F:479:ALA:O	1:F:483:LEU:HD23	2.10	0.51
1:F:566:ASP:CG	1:F:678:THR:HG23	2.31	0.51
1:F:945:ILE:HA	1:F:971:ARG:NH1	2.25	0.51
1:F:973:ARG:HG2	1:F:977:MET:HE3	1.91	0.51
1:B:575:MET:HB3	1:B:626:ILE:HG13	1.92	0.51
1:B:715:SER:O	1:B:715:SER:OG	2.29	0.51
1:D:393:LEU:HD12	1:D:469:GLN:HG3	1.92	0.51
1:D:777:ALA:HB1	1:F:225:VAL:HG12	1.91	0.51
1:E:776:GLU:HB3	1:E:779:TYR:CE1	2.44	0.51
1:F:873:ALA:HB2	1:F:928:GLN:NE2	2.25	0.51
1:F:947:GLU:HG3	1:F:948:PHE:HD1	1.75	0.51
1:A:904:VAL:CG1	1:A:938:SER:HB2	2.40	0.51
1:C:82:SER:HB2	1:C:816:LEU:HB2	1.92	0.51
1:D:616:GLY:HA3	1:D:624:THR:HG22	1.93	0.51
1:E:696:THR:HG23	1:E:699:ARG:NH1	2.25	0.51
1:F:376:LEU:O	1:F:379:THR:N	2.44	0.51
1:F:400:LEU:HD11	1:F:1007:VAL:HG21	1.93	0.51
1:F:598:TYR:HB3	1:F:606:VAL:HG21	1.92	0.51
1:F:720:GLY:HA3	1:F:817:GLU:OE1	2.11	0.51
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.93	0.51
1:A:355:MET:HB3	1:A:365:THR:OG1	2.10	0.51
1:A:726:GLN:OE1	1:A:812:GLY:HA3	2.11	0.51
1:A:775:SER:HB2	1:A:789:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:GLU:O	1:B:502:LYS:NZ	2.44	0.51
1:B:267:LYS:HD3	1:B:776:GLU:OE2	2.11	0.51
1:C:408:ASP:O	1:C:412:VAL:HG23	2.11	0.51
1:C:40:PRO:HG2	1:C:674:LEU:HD21	1.91	0.51
1:D:1026:PHE:CE2	1:D:1030:ARG:HG3	2.46	0.51
1:D:941:ASN:HB3	1:D:975:ILE:HD13	1.93	0.51
1:E:203:VAL:HG12	1:E:207:ILE:HD11	1.93	0.51
1:E:46:SER:OG	1:E:89:GLN:HG2	2.10	0.51
1:B:295:THR:O	1:B:295:THR:OG1	2.25	0.51
1:C:149:MET:HB2	1:C:153:ASP:HB3	1.91	0.51
1:F:27:ILE:HG22	1:F:380:PHE:HB3	1.93	0.51
1:C:576:VAL:HG21	1:C:591:LEU:HD23	1.93	0.50
1:C:751:GLY:O	1:C:754:TRP:N	2.44	0.50
1:C:888:LEU:HD11	1:C:943:ILE:HD11	1.93	0.50
1:D:532:GLY:O	1:D:536:ARG:HG3	2.11	0.50
1:E:167:SER:HB2	1:E:175:VAL:HG11	1.93	0.50
1:E:183:ALA:HB2	1:E:273:GLU:HG3	1.93	0.50
1:F:344:LEU:HA	1:F:399:VAL:HG22	1.93	0.50
1:C:139:VAL:O	1:C:326:PRO:HD2	2.11	0.50
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.94	0.50
1:C:683:GLU:HB3	1:C:685:ILE:HD11	1.94	0.50
1:D:775:SER:HB2	1:D:789:TRP:HZ2	1.76	0.50
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.93	0.50
1:A:72:ILE:HD13	1:A:107:VAL:HG22	1.93	0.50
1:A:144:ASN:HD22	1:A:321:LEU:HD23	1.76	0.50
1:A:467:TYR:HE2	1:A:925:VAL:HG13	1.76	0.50
1:B:352:PHE:CD2	1:B:352:PHE:C	2.85	0.50
1:B:36:PRO:HG3	1:B:469:GLN:HG3	1.93	0.50
1:B:877:TYR:HA	1:B:880:SER:HB3	1.93	0.50
1:B:966:ASP:O	1:B:970:MET:HG2	2.10	0.50
1:F:182:TYR:O	1:F:769:LYS:HD3	2.11	0.50
1:F:372:VAL:HG22	1:F:405:LEU:HD11	1.93	0.50
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.93	0.50
1:A:391:ASN:O	1:A:395:MET:HG2	2.10	0.50
1:B:267:LYS:N	1:B:267:LYS:HD2	2.25	0.50
1:D:401:ALA:O	1:D:405:LEU:HG	2.12	0.50
1:D:892:TYR:CD2	1:D:897:ILE:HG22	2.47	0.50
1:E:102:ILE:O	1:E:106:GLN:HG3	2.11	0.50
1:E:190:PRO:HB3	1:E:789:TRP:CD2	2.46	0.50
1:F:431:THR:HG21	1:F:490:PRO:O	2.12	0.50
1:C:112:GLN:OE1	1:C:115:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:VAL:O	1:C:207:ILE:HG13	2.12	0.50
1:C:744:ASN:O	1:C:748:THR:HG23	2.12	0.50
1:D:634:TRP:CD1	1:D:634:TRP:N	2.80	0.50
1:E:362:PHE:O	1:E:365:THR:HG22	2.11	0.50
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.94	0.50
1:B:412:VAL:HG22	1:B:438:ILE:HD11	1.93	0.50
1:E:16:ALA:HB2	1:E:488:LEU:HD13	1.94	0.50
1:E:298:ASN:HB3	1:E:301:ASP:HB2	1.92	0.50
1:E:339:GLU:HA	1:E:342:LYS:HB2	1.93	0.50
1:F:404:LEU:HB3	1:F:478:MET:SD	2.51	0.50
1:F:896:SER:HB3	1:F:1033:PHE:CE1	2.47	0.50
1:F:987:MET:HB3	1:F:988:PRO:HD3	1.93	0.50
1:A:878:ALA:O	1:A:882:ILE:HG12	2.12	0.50
1:A:896:SER:HB3	1:A:1033:PHE:CD1	2.47	0.50
1:B:531:VAL:O	1:B:534:ILE:HG23	2.12	0.50
1:C:359:LEU:O	1:C:361:ASN:N	2.43	0.50
1:D:191:ASN:O	1:D:193:LEU:N	2.44	0.50
1:E:1016:VAL:HG12	1:E:1016:VAL:O	2.11	0.50
1:F:372:VAL:HA	1:F:405:LEU:HD13	1.93	0.50
1:F:5:PHE:CE2	1:F:8:ARG:HD2	2.46	0.50
1:F:959:GLY:HA3	1:F:1042:HIS:O	2.12	0.50
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.46	0.50
1:D:563:PHE:C	1:D:564:LEU:HD12	2.32	0.50
1:D:563:PHE:O	1:D:564:LEU:HD12	2.11	0.50
1:D:598:TYR:HB3	1:D:606:VAL:HG11	1.93	0.50
1:A:985:GLY:O	1:A:988:PRO:HD2	2.12	0.50
1:C:343:THR:HA	1:C:346:GLU:OE1	2.12	0.50
1:C:597:TYR:CD1	1:C:601:LYS:HD2	2.47	0.50
1:D:907:LEU:HD21	1:D:1021:PHE:CB	2.41	0.50
1:E:163:LYS:O	1:E:163:LYS:HG2	2.12	0.50
1:E:240:LEU:HB2	1:E:246:PHE:CE1	2.47	0.50
1:E:668:LEU:HD12	1:E:672:VAL:HG12	1.94	0.50
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.12	0.50
1:A:692:HIS:HE2	1:A:723:ASP:CG	2.15	0.49
1:A:62:THR:OG1	1:A:88:VAL:HG21	2.12	0.49
1:B:383:LEU:HD11	1:B:473:THR:HG23	1.94	0.49
1:C:1020:PHE:CD1	2:C:1101:LMT:H41	2.47	0.49
1:C:730:ASP:CG	1:C:808:ARG:HH21	2.15	0.49
1:D:162:MET:HA	1:D:313:MET:SD	2.52	0.49
1:D:414:GLU:CG	1:D:974:PRO:HG3	2.42	0.49
1:F:133:SER:OG	1:F:293:LEU:O	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:ASN:OD1	1:F:798:MET:HG3	2.12	0.49
1:B:478:MET:O	1:B:482:VAL:HG12	2.12	0.49
1:B:696:THR:HG23	1:B:699:ARG:NH1	2.27	0.49
1:C:979:SER:CB	1:C:1015:THR:HG21	2.43	0.49
1:D:362:PHE:O	1:D:365:THR:HG22	2.11	0.49
1:E:46:SER:HA	1:E:88:VAL:O	2.12	0.49
1:E:3:ASN:HA	1:E:6:ILE:HD12	1.93	0.49
1:F:969:ARG:HH11	1:F:970:MET:HB3	1.77	0.49
1:A:452:VAL:HA	1:A:880:SER:OG	2.13	0.49
1:B:151:GLN:OE1	1:B:278:ILE:HA	2.12	0.49
1:B:184:MET:HB3	1:B:771:VAL:HA	1.94	0.49
1:B:425:LEU:HD13	1:B:429:GLU:HG3	1.93	0.49
1:B:544:LEU:O	1:B:547:ILE:HB	2.12	0.49
1:B:185:ARG:HH22	1:B:774:MET:HE3	1.76	0.49
1:A:17:ILE:CG2	1:B:886:LEU:HD21	2.42	0.49
1:E:987:MET:HA	1:E:1008:MET:HE3	1.94	0.49
1:E:484:VAL:HG13	1:E:488:LEU:HB3	1.93	0.49
1:F:139:VAL:HA	1:F:289:LEU:O	2.12	0.49
1:F:435:MET:CE	1:F:490:PRO:HB3	2.43	0.49
1:A:228:GLN:HG3	1:A:229:GLN:N	2.27	0.49
1:B:527:TYR:OH	1:B:1019:ILE:O	2.19	0.49
1:B:155:SER:O	1:B:158:VAL:HB	2.12	0.49
1:B:47:ALA:HB2	1:B:127:VAL:HG13	1.94	0.49
1:C:144:ASN:HB3	1:C:148:THR:HG23	1.95	0.49
1:D:623:ASN:OD1	1:D:623:ASN:N	2.45	0.49
1:D:83:ASP:OD1	1:D:815:ARG:HD3	2.13	0.49
1:E:654:ALA:O	1:E:658:ILE:HG12	2.11	0.49
1:F:344:LEU:CD2	1:F:402:ILE:HD11	2.42	0.49
1:A:1037:ASN:HA	1:A:1038:GLU:O	2.12	0.49
1:A:1040:ILE:HG12	1:A:1041:GLU:H	1.77	0.49
1:B:61:VAL:HG21	1:B:122:VAL:HG21	1.95	0.49
1:B:905:VAL:HG13	1:B:935:ILE:HG23	1.94	0.49
1:C:35:TYR:HB3	1:C:38:ILE:HD12	1.94	0.49
1:C:968:VAL:CA	1:C:971:ARG:HH12	2.26	0.49
1:E:343:THR:OG1	1:E:989:LEU:HD21	2.13	0.49
1:F:480:LEU:O	1:F:484:VAL:HG23	2.13	0.49
1:A:348:ILE:HG22	1:A:349:ILE:HD13	1.94	0.49
1:A:644:VAL:HG11	1:A:667:ASN:HB2	1.94	0.49
1:C:534:ILE:HD12	1:C:535:LEU:HD23	1.94	0.49
1:D:156:ASP:OD1	1:D:765:ARG:NH2	2.45	0.49
1:D:236:ALA:O	1:E:728:LYS:NZ	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:VAL:HG22	1:E:306:ILE:HD11	1.93	0.49
1:E:42:ALA:O	1:E:132:SER:N	2.27	0.49
1:E:904:VAL:HG12	1:E:938:SER:OG	2.11	0.49
1:B:394:THR:O	1:B:473:THR:HG21	2.12	0.49
1:B:508:GLY:C	1:B:510:LYS:H	2.14	0.49
1:B:668:LEU:HD23	1:B:668:LEU:H	1.77	0.49
1:C:1033:PHE:N	1:C:1034:SER:OG	2.27	0.49
1:F:940:LYS:HZ1	1:F:978:THR:HG21	1.78	0.49
1:A:17:ILE:HG22	1:B:886:LEU:HD21	1.95	0.49
1:A:484:VAL:HG13	1:A:488:LEU:HB3	1.93	0.49
1:B:562:SER:OG	1:B:563:PHE:N	2.46	0.49
1:B:736:ALA:HB1	1:B:741:VAL:HG23	1.94	0.49
1:C:154:ILE:O	1:C:157:TYR:N	2.45	0.49
1:C:904:VAL:HG21	1:C:942:ALA:HB2	1.94	0.49
1:C:945:ILE:HG12	1:C:971:ARG:CZ	2.43	0.49
1:D:445:ILE:HD13	1:D:940:LYS:HE3	1.95	0.49
1:E:979:SER:CB	1:E:1015:THR:HG21	2.42	0.49
1:E:32:VAL:HA	1:E:390:ILE:O	2.13	0.49
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.94	0.49
1:A:534:ILE:HG22	1:A:541:TYR:OH	2.13	0.49
1:A:776:GLU:HG2	1:A:777:ALA:H	1.77	0.49
1:C:244:GLU:O	1:C:247:GLY:N	2.46	0.49
1:D:163:LYS:O	1:D:163:LYS:HG2	2.12	0.49
1:D:696:THR:HG23	1:D:699:ARG:NH1	2.28	0.49
1:E:507:GLU:OE1	1:E:518:ARG:HG2	2.13	0.49
1:C:904:VAL:O	1:C:907:LEU:HB2	2.12	0.49
1:D:859:TRP:HE3	1:D:863:SER:HG	1.59	0.49
1:F:163:LYS:O	1:F:163:LYS:HG2	2.13	0.49
1:F:968:VAL:O	1:F:972:LEU:HB2	2.13	0.49
1:B:76:MET:HB2	1:B:93:THR:O	2.13	0.48
1:D:531:VAL:O	1:D:534:ILE:HG13	2.13	0.48
1:D:643:LYS:HZ2	1:D:993:THR:HG23	1.77	0.48
1:F:112:GLN:HA	1:F:115:MET:HB2	1.94	0.48
1:D:754:TRP:CZ3	1:F:219:LEU:HD23	2.48	0.48
1:F:154:ILE:HG22	1:F:287:SER:HB3	1.94	0.48
1:F:459:PHE:CE1	1:F:876:LEU:HG	2.48	0.48
1:F:941:ASN:CG	1:F:975:ILE:HG23	2.34	0.48
1:A:574:THR:HG21	1:A:598:TYR:CE2	2.43	0.48
1:A:76:MET:HB2	1:A:93:THR:O	2.13	0.48
1:B:199:THR:HB	1:B:749:THR:HG21	1.95	0.48
1:B:307:ARG:HG2	1:B:325:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:672:VAL:O	1:B:673:GLU:HB3	2.13	0.48
1:C:527:TYR:HE2	1:C:968:VAL:HG13	1.77	0.48
1:C:885:PHE:HD2	1:C:886:LEU:HD13	1.78	0.48
1:D:445:ILE:CD1	1:D:940:LYS:HE3	2.43	0.48
1:A:393:LEU:CD1	1:A:466:ILE:HA	2.43	0.48
1:A:752:ALA:O	1:A:774:MET:HA	2.13	0.48
1:B:532:GLY:O	1:B:536:ARG:N	2.46	0.48
1:B:758:TYR:HB2	1:B:772:TYR:CZ	2.48	0.48
1:E:733:GLN:HE22	1:E:743:ILE:HG21	1.78	0.48
1:E:744:ASN:O	1:E:748:THR:HG23	2.13	0.48
1:E:922:THR:O	1:E:924:ASP:N	2.43	0.48
1:F:358:PHE:O	1:F:973:ARG:NH2	2.45	0.48
1:A:751:GLY:O	1:A:754:TRP:N	2.45	0.48
1:B:383:LEU:HD13	1:B:388:PHE:CD1	2.44	0.48
1:C:380:PHE:CD2	1:C:383:LEU:HD12	2.48	0.48
1:C:504:ASP:C	1:C:506:GLY:H	2.17	0.48
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.95	0.48
1:D:445:ILE:CG1	1:D:940:LYS:HE3	2.44	0.48
1:E:982:PHE:CD2	1:E:1011:MET:HG3	2.49	0.48
1:E:261:LEU:HD12	1:E:263:ARG:NH1	2.24	0.48
1:E:776:GLU:HG2	1:E:777:ALA:H	1.78	0.48
1:A:536:ARG:HD2	2:A:1101:LMT:O4'	2.13	0.48
1:B:110:LYS:HD3	1:B:113:LEU:HD12	1.96	0.48
1:B:158:VAL:HA	1:B:162:MET:HE2	1.95	0.48
1:B:24:GLY:O	1:B:27:ILE:HG22	2.14	0.48
1:D:911:GLY:HA3	1:D:1013:THR:OG1	2.13	0.48
1:D:470:PHE:CD2	1:D:929:VAL:HG21	2.48	0.48
1:F:733:GLN:OE1	1:F:743:ILE:HG12	2.14	0.48
1:A:141:GLY:O	1:A:323:ILE:HA	2.14	0.48
1:A:412:VAL:O	1:A:416:VAL:HG23	2.13	0.48
1:A:655:PHE:HB3	1:A:663:VAL:HB	1.95	0.48
1:B:423:GLU:O	1:B:502:LYS:HD2	2.14	0.48
1:B:76:MET:SD	1:B:864:TYR:HE2	2.37	0.48
1:C:58:GLN:HA	1:C:62:THR:HB	1.96	0.48
1:C:197:GLN:HA	1:C:798:MET:SD	2.53	0.48
1:D:279:ALA:HB3	1:D:286:ALA:O	2.14	0.48
1:D:348:ILE:HG22	1:D:349:ILE:HD12	1.94	0.48
1:E:902:MET:O	1:E:905:VAL:HG23	2.14	0.48
1:F:456:MET:HB3	1:F:876:LEU:HD21	1.96	0.48
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.49	0.48
1:A:279:ALA:HB3	1:A:286:ALA:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLN:HG3	1:C:82:SER:OG	2.14	0.48
1:D:647:ILE:HG12	1:D:650:ARG:NH1	2.29	0.48
1:E:26:ALA:O	1:E:30:LEU:HB2	2.13	0.48
1:F:602:GLU:HB3	1:F:606:VAL:HG23	1.95	0.48
1:A:887:CYS:O	1:A:890:ALA:HB3	2.14	0.48
1:B:11:PHE:O	1:B:11:PHE:HD2	1.97	0.48
1:B:136:PHE:CD2	1:B:290:GLY:HA3	2.49	0.48
1:B:527:TYR:O	1:B:530:SER:HB3	2.14	0.48
1:C:182:TYR:HD2	1:C:765:ARG:NH2	2.12	0.48
1:D:137:LEU:HB2	1:D:293:LEU:HB2	1.96	0.48
1:D:141:GLY:HA3	1:D:324:VAL:HG12	1.95	0.48
1:D:453:PHE:O	1:D:471:SER:OG	2.21	0.48
1:E:527:TYR:O	1:E:531:VAL:HG23	2.14	0.48
1:E:586:ARG:O	1:E:589:LYS:HB3	2.14	0.48
1:A:902:MET:O	1:A:905:VAL:HG23	2.13	0.48
1:B:208:LYS:HE3	1:B:759:VAL:HG22	1.95	0.48
1:B:501:ALA:O	1:B:504:ASP:HB2	2.14	0.48
1:B:985:GLY:O	1:B:988:PRO:HD2	2.14	0.48
1:C:901:VAL:HG23	1:C:942:ALA:CB	2.44	0.48
1:E:210:GLN:O	1:E:237:GLN:NE2	2.44	0.48
1:E:844:MET:HA	1:E:844:MET:CE	2.44	0.48
1:F:351:VAL:O	1:F:355:MET:HE2	2.14	0.48
1:F:941:ASN:HA	1:F:944:LEU:HD12	1.94	0.48
1:A:110:LYS:HA	1:A:110:LYS:HD3	1.59	0.48
1:A:216:ALA:HB1	1:A:234:ILE:CG2	2.44	0.48
1:B:153:ASP:OD2	1:B:182:TYR:OH	2.26	0.48
1:B:888:LEU:HD21	1:B:943:ILE:HD11	1.95	0.48
1:C:375:VAL:HB	1:C:405:LEU:HD22	1.96	0.48
1:D:191:ASN:C	1:D:193:LEU:H	2.17	0.48
1:E:291:ILE:HG21	1:E:306:ILE:HD11	1.96	0.48
1:E:504:ASP:C	1:E:506:GLY:H	2.16	0.48
1:F:380:PHE:O	1:F:383:LEU:HB2	2.14	0.48
1:F:452:VAL:O	1:F:455:PRO:HD2	2.14	0.48
1:A:446:ALA:CB	1:A:482:VAL:HG21	2.36	0.47
1:B:845:GLU:HG2	1:B:857:TYR:CE1	2.48	0.47
1:C:1032:ARG:O	1:C:1033:PHE:HD1	1.97	0.47
1:C:479:ALA:O	1:C:482:VAL:HG23	2.14	0.47
1:D:233:SER:O	1:E:726:GLN:HB2	2.14	0.47
1:E:414:GLU:HG3	1:E:974:PRO:HB3	1.96	0.47
1:F:47:ALA:HB1	1:F:122:VAL:HG13	1.96	0.47
1:F:600:THR:C	1:F:602:GLU:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:TYR:HB2	1:A:772:TYR:CZ	2.49	0.47
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.97	0.47
1:C:649:MET:SD	1:C:653:ARG:NH2	2.87	0.47
1:C:960:LEU:HB2	1:C:1040:ILE:HG13	1.95	0.47
1:D:49:TYR:CE1	1:D:60:THR:HG21	2.48	0.47
1:E:318:PRO:HG2	1:E:321:LEU:HB2	1.96	0.47
1:F:987:MET:O	1:F:990:VAL:HG23	2.14	0.47
1:C:400:LEU:HD23	1:C:474:ILE:HD11	1.95	0.47
1:C:992:SER:HB3	1:C:997:SER:HB2	1.96	0.47
1:D:542:LEU:O	1:D:546:LEU:HG	2.14	0.47
1:D:644:VAL:HG12	1:D:645:GLU:N	2.30	0.47
1:F:659:LYS:HD3	1:F:659:LYS:HA	1.63	0.47
1:A:444:GLY:O	1:A:448:VAL:HG23	2.13	0.47
1:A:420:MET:HB3	1:A:500:ILE:HB	1.96	0.47
1:A:641:GLU:HB2	1:A:650:ARG:NH2	2.29	0.47
1:A:841:MET:HG2	1:A:859:TRP:CH2	2.49	0.47
1:B:189:ASN:OD1	1:B:190:PRO:HD2	2.14	0.47
1:B:600:THR:C	1:B:602:GLU:H	2.17	0.47
1:B:789:TRP:O	1:B:801:PHE:HD2	1.97	0.47
1:B:960:LEU:O	1:B:964:THR:HG23	2.14	0.47
1:C:186:ILE:HG22	1:C:773:VAL:HG23	1.96	0.47
1:C:409:ALA:O	1:C:413:VAL:HG23	2.14	0.47
1:D:586:ARG:O	1:D:590:VAL:HG23	2.14	0.47
1:E:11:PHE:HE2	1:E:15:ILE:HD11	1.78	0.47
1:E:535:LEU:O	1:E:536:ARG:C	2.51	0.47
1:E:597:TYR:OH	1:E:650:ARG:HG3	2.14	0.47
1:F:343:THR:HG21	1:F:989:LEU:CD2	2.44	0.47
1:A:166:ILE:HD11	1:A:310:LEU:HD13	1.97	0.47
1:A:276:ASP:HA	1:C:222:THR:HG21	1.96	0.47
1:B:270:LEU:HA	1:B:270:LEU:HD12	1.67	0.47
1:B:521:GLU:HA	1:B:524:THR:HG23	1.97	0.47
1:B:767:ARG:HH11	1:B:767:ARG:HG2	1.79	0.47
1:C:143:ILE:HG22	1:C:286:ALA:CB	2.43	0.47
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.96	0.47
1:C:447:MET:SD	1:C:891:LEU:HD22	2.54	0.47
1:D:355:MET:HG3	1:D:359:LEU:HD12	1.96	0.47
1:E:542:LEU:O	1:E:545:TYR:HB3	2.15	0.47
1:E:961:ILE:HG13	1:E:962:GLU:N	2.28	0.47
1:F:727:PHE:CZ	1:F:807:SER:HB2	2.49	0.47
1:A:567:GLU:O	1:A:569:GLN:HG3	2.14	0.47
1:A:728:LYS:HB2	1:A:810:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:PHE:N	1:B:827:ILE:O	2.47	0.47
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.45	0.47
1:C:382:VAL:HG12	1:C:472:ILE:HD11	1.95	0.47
1:C:944:LEU:C	1:C:971:ARG:HD2	2.34	0.47
1:D:100:ALA:HB1	1:D:131:LYS:HD2	1.96	0.47
1:D:508:GLY:H	1:D:518:ARG:HG3	1.79	0.47
1:D:984:LEU:HD23	1:D:984:LEU:HA	1.71	0.47
1:D:987:MET:HA	1:D:1008:MET:HE1	1.96	0.47
1:E:544:LEU:O	1:E:548:ILE:HG13	2.15	0.47
1:F:901:VAL:HG22	1:F:942:ALA:HB1	1.96	0.47
1:B:728:LYS:HB2	1:B:810:GLU:OE1	2.15	0.47
1:C:177:LEU:HD23	1:C:178:PHE:N	2.29	0.47
1:C:137:LEU:HD22	1:C:293:LEU:HD23	1.97	0.47
1:C:329:THR:O	1:C:332:PHE:HB3	2.14	0.47
1:C:340:VAL:HG12	1:C:395:MET:HE3	1.96	0.47
1:C:881:LEU:HD22	1:C:902:MET:HE1	1.97	0.47
1:D:137:LEU:HD13	1:D:293:LEU:HB2	1.97	0.47
1:D:933:THR:O	1:D:936:GLY:N	2.47	0.47
1:E:104:GLN:OE1	1:E:131:LYS:HD3	2.14	0.47
1:E:376:LEU:HD22	1:E:398:MET:HE3	1.96	0.47
1:E:858:ASP:OD1	1:E:859:TRP:N	2.48	0.47
1:E:911:GLY:HA2	1:E:914:LEU:HD22	1.96	0.47
1:F:904:VAL:HG21	1:F:1022:VAL:HG22	1.96	0.47
1:A:818:ARG:HH22	1:A:823:PRO:HD3	1.79	0.47
1:B:428:LYS:HE2	1:B:494:ALA:O	2.14	0.47
1:B:459:PHE:O	1:B:464:GLY:HA3	2.13	0.47
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.62	0.47
1:B:588:GLN:HB2	1:B:613:ASN:HD22	1.79	0.47
1:C:574:THR:HG21	1:C:598:TYR:HE2	1.80	0.47
1:C:647:ILE:HG12	1:C:650:ARG:HH12	1.80	0.47
1:D:1040:ILE:HG23	1:D:1041:GLU:N	2.30	0.47
1:D:137:LEU:HG	1:D:138:MET:HE3	1.96	0.47
1:D:582:ALA:HA	1:D:586:ARG:HH21	1.79	0.47
1:E:478:MET:O	1:E:482:VAL:HG12	2.14	0.47
1:E:886:LEU:HA	1:E:886:LEU:HD12	1.72	0.47
1:E:350:LEU:HD21	1:E:984:LEU:HB2	1.95	0.47
1:F:509:LYS:HB3	1:F:514:GLY:HA3	1.96	0.47
1:A:783:PRO:HA	1:A:786:ILE:HG12	1.97	0.47
1:B:317:PHE:HE2	1:B:323:ILE:HD11	1.79	0.47
1:B:520:PHE:O	1:B:524:THR:HG22	2.14	0.47
1:B:910:ILE:HG23	1:B:911:GLY:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1037:ASN:O	1:C:1038:GLU:HB2	2.15	0.47
1:C:61:VAL:HG13	1:C:118:LEU:HD13	1.96	0.47
1:F:776:GLU:HB2	1:F:779:TYR:CD1	2.50	0.47
1:F:937:LEU:HD13	1:F:1011:MET:SD	2.54	0.47
1:A:394:THR:HG22	1:A:473:THR:OG1	2.15	0.47
1:A:47:ALA:HB3	1:A:88:VAL:CG1	2.44	0.47
1:B:46:SER:HA	1:B:88:VAL:O	2.15	0.47
1:C:990:VAL:HG13	1:C:1005:THR:OG1	2.14	0.47
1:D:250:LEU:HD13	1:D:261:LEU:HD23	1.95	0.47
1:D:728:LYS:HG2	1:D:808:ARG:CZ	2.45	0.47
1:E:588:GLN:NE2	1:E:592:ASN:OD1	2.47	0.47
1:F:858:ASP:OD2	1:F:859:TRP:N	2.48	0.47
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.50	0.47
1:A:225:VAL:HG12	1:B:777:ALA:HB1	1.97	0.47
1:C:407:ASP:OD2	1:C:940:LYS:HD2	2.15	0.47
1:D:317:PHE:HA	1:D:318:PRO:HD3	1.60	0.47
1:D:518:ARG:O	1:D:522:LYS:HG3	2.15	0.47
1:F:451:ALA:HB3	1:F:884:VAL:HG22	1.97	0.47
1:A:383:LEU:HD11	1:A:473:THR:HG23	1.97	0.46
1:A:892:TYR:OH	1:A:943:ILE:HA	2.15	0.46
1:C:363:ARG:O	1:C:367:ILE:HG13	2.14	0.46
1:C:907:LEU:HD21	1:C:1021:PHE:CB	2.44	0.46
1:D:162:MET:O	1:D:164:ASP:N	2.48	0.46
1:D:645:GLU:O	1:D:648:THR:OG1	2.30	0.46
1:D:719:ASN:HB3	1:D:826:GLU:HG2	1.97	0.46
1:D:199:THR:CG2	1:D:791:VAL:HA	2.45	0.46
1:E:1001:ASN:HD22	1:E:1001:ASN:N	2.12	0.46
1:F:986:VAL:HG11	1:F:1007:VAL:HG12	1.97	0.46
1:F:13:TRP:CH2	1:F:370:ILE:HD13	2.48	0.46
1:F:214:VAL:HG23	1:F:237:GLN:HB2	1.97	0.46
1:F:425:LEU:HD13	1:F:429:GLU:HG3	1.96	0.46
1:F:898:PRO:O	1:F:902:MET:HG2	2.15	0.46
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.96	0.46
1:A:680:PHE:HB2	1:A:859:TRP:CZ3	2.48	0.46
1:B:164:ASP:HA	1:B:167:SER:HB3	1.96	0.46
1:B:182:TYR:O	1:B:769:LYS:HD3	2.14	0.46
1:B:254:ASN:HB2	1:B:258:SER:O	2.15	0.46
1:B:402:ILE:O	1:B:406:VAL:HG23	2.15	0.46
1:D:587:THR:OG1	1:D:622:GLN:O	2.14	0.46
1:D:168:ARG:HB3	1:E:75:LEU:HD22	1.97	0.46
1:A:45:ILE:HD12	1:A:90:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ALA:HB2	1:A:471:SER:OG	2.15	0.46
1:A:648:THR:HG21	1:A:666:PHE:HA	1.97	0.46
1:C:343:THR:HG21	1:C:989:LEU:HD21	1.97	0.46
1:C:364:ALA:O	1:C:368:PRO:HD3	2.15	0.46
1:C:527:TYR:O	1:C:531:VAL:HG23	2.15	0.46
1:B:235:ILE:HB	1:C:728:LYS:HA	1.98	0.46
1:D:841:MET:HG2	1:D:859:TRP:CH2	2.50	0.46
1:A:1027:VAL:O	1:A:1031:ARG:HG3	2.15	0.46
1:A:445:ILE:HD12	1:A:446:ALA:N	2.30	0.46
1:B:571:VAL:HG12	1:B:668:LEU:HD21	1.98	0.46
1:C:480:LEU:O	1:C:484:VAL:HG23	2.15	0.46
1:D:900:SER:HA	1:D:1025:PHE:HB3	1.97	0.46
1:D:108:GLN:OE1	1:D:129:VAL:HB	2.15	0.46
1:D:26:ALA:O	1:D:30:LEU:HB2	2.15	0.46
1:E:715:SER:O	1:E:715:SER:OG	2.31	0.46
1:F:156:ASP:OD2	1:F:769:LYS:NZ	2.47	0.46
1:F:576:VAL:HG22	1:F:663:VAL:HG22	1.97	0.46
1:F:736:ALA:HB1	1:F:741:VAL:HG23	1.97	0.46
1:A:335:ILE:O	1:A:339:GLU:HG2	2.16	0.46
1:A:525:HIS:HA	1:A:528:THR:HG22	1.96	0.46
1:A:524:THR:O	1:A:527:TYR:HB3	2.16	0.46
1:B:536:ARG:NH1	2:B:1101:LMT:O4'	2.48	0.46
1:B:140:VAL:HG11	1:B:310:LEU:HD21	1.96	0.46
1:B:261:LEU:HD12	1:B:263:ARG:NH1	2.31	0.46
1:B:776:GLU:O	1:B:780:ARG:HG2	2.16	0.46
1:B:57:VAL:HG11	1:B:86:GLY:O	2.15	0.46
1:C:61:VAL:HG21	1:C:122:VAL:HG21	1.98	0.46
1:D:979:SER:CB	1:D:1015:THR:HG21	2.46	0.46
1:E:160:ALA:HA	1:E:767:ARG:NH2	2.31	0.46
1:E:987:MET:O	1:E:990:VAL:HG23	2.16	0.46
1:F:818:ARG:HH12	1:F:823:PRO:HG3	1.80	0.46
1:F:897:ILE:HG23	1:F:946:VAL:CG1	2.44	0.46
1:A:162:MET:HA	1:A:313:MET:SD	2.56	0.46
1:A:538:THR:O	1:A:542:LEU:HD13	2.15	0.46
1:B:753:ALA:O	1:B:775:SER:HB3	2.16	0.46
1:D:225:VAL:HG13	1:E:781:MET:SD	2.56	0.46
1:E:418:ARG:HD3	1:E:970:MET:HB2	1.98	0.46
1:F:751:GLY:O	1:F:753:ALA:N	2.49	0.46
1:A:906:PRO:HA	1:A:909:VAL:HB	1.96	0.46
1:B:1032:ARG:O	1:B:1033:PHE:HB2	2.15	0.46
1:B:597:TYR:OH	1:B:650:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:TYR:CE2	1:C:968:VAL:HG13	2.50	0.46
1:C:668:LEU:HA	1:C:677:ALA:HA	1.97	0.46
1:D:135:SER:HB3	1:D:672:VAL:HG11	1.98	0.46
1:D:965:LEU:HA	1:D:965:LEU:HD23	1.63	0.46
1:E:1041:GLU:HB3	1:E:1042:HIS:C	2.36	0.46
1:E:291:ILE:HG21	1:E:306:ILE:CD1	2.45	0.46
1:E:903:LEU:O	1:E:906:PRO:HD2	2.15	0.46
1:A:539:GLY:O	1:A:542:LEU:HB2	2.15	0.46
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.96	0.46
1:B:261:LEU:HD12	1:B:263:ARG:HH12	1.81	0.46
1:B:459:PHE:CD1	1:B:876:LEU:HD12	2.50	0.46
1:B:767:ARG:HG2	1:B:767:ARG:NH1	2.31	0.46
1:C:167:SER:HA	1:C:175:VAL:HG21	1.98	0.46
1:C:35:TYR:HE1	1:C:670:ALA:HB1	1.80	0.46
1:C:415:ASN:O	1:C:419:VAL:HG23	2.15	0.46
1:D:194:ASN:HA	1:D:798:MET:HE1	1.97	0.46
1:E:225:VAL:HG13	1:F:781:MET:SD	2.55	0.46
1:E:356:TYR:HE1	1:E:362:PHE:N	2.13	0.46
1:E:520:PHE:O	1:E:524:THR:HG23	2.16	0.46
1:E:978:THR:O	1:E:982:PHE:N	2.47	0.46
1:F:1020:PHE:CZ	2:F:1101:LMT:H31	2.51	0.46
1:F:361:ASN:HB3	1:F:364:ALA:CB	2.46	0.46
1:F:415:ASN:O	1:F:419:VAL:HG23	2.16	0.46
1:F:452:VAL:HG13	1:F:884:VAL:HG23	1.98	0.46
1:A:504:ASP:O	1:A:506:GLY:N	2.49	0.46
1:B:412:VAL:O	1:B:416:VAL:HG23	2.15	0.46
1:B:415:ASN:HB3	1:B:434:SER:OG	2.16	0.46
1:C:144:ASN:O	1:C:148:THR:HG23	2.16	0.46
1:C:937:LEU:HD23	1:C:937:LEU:HA	1.50	0.46
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.97	0.46
1:E:200:PRO:HB2	1:E:749:THR:HG22	1.97	0.46
1:B:27:ILE:HD12	1:B:27:ILE:HA	1.66	0.46
1:B:509:LYS:HE2	1:B:509:LYS:HB3	1.63	0.46
1:C:898:PRO:HA	1:C:901:VAL:HG12	1.98	0.46
1:E:589:LYS:O	1:E:592:ASN:HB2	2.15	0.46
1:F:959:GLY:HA3	1:F:1043:SER:HA	1.98	0.46
1:F:80:SER:HB3	1:F:90:ILE:HG23	1.97	0.46
1:F:940:LYS:HZ1	1:F:978:THR:CG2	2.29	0.46
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.46	0.45
1:A:523:SER:O	1:A:526:HIS:HB2	2.16	0.45
1:B:1026:PHE:CD2	1:B:1026:PHE:C	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:MET:O	1:C:523:SER:OG	2.26	0.45
1:C:778:LYS:HG3	1:C:779:TYR:CE1	2.51	0.45
1:D:58:GLN:OE1	1:D:63:GLN:NE2	2.49	0.45
1:D:592:ASN:O	1:D:596:HIS:HB2	2.15	0.45
1:E:231:ASN:HB2	1:F:583:THR:HG22	1.97	0.45
1:E:348:ILE:HG12	1:E:372:VAL:HG21	1.97	0.45
1:E:594:VAL:HG22	1:E:655:PHE:CE2	2.52	0.45
1:F:445:ILE:HG23	1:F:940:LYS:HG3	1.98	0.45
1:A:174:ASP:HB3	1:A:292:LYS:HB2	1.99	0.45
1:B:1038:GLU:CG	1:B:1039:ASP:H	2.29	0.45
1:C:158:VAL:HG22	1:C:162:MET:HE2	1.98	0.45
1:C:730:ASP:OD2	1:C:808:ARG:NH2	2.49	0.45
1:C:947:GLU:HG3	1:C:948:PHE:N	2.30	0.45
1:D:596:HIS:O	1:D:600:THR:OG1	2.25	0.45
1:D:602:GLU:OE2	1:D:650:ARG:NH1	2.50	0.45
1:D:680:PHE:HB2	1:D:859:TRP:HZ3	1.82	0.45
1:E:162:MET:C	1:E:164:ASP:N	2.67	0.45
1:A:244:GLU:O	1:A:246:PHE:N	2.49	0.45
1:A:30:LEU:HD11	1:A:384:ALA:HA	1.97	0.45
1:A:491:ALA:O	1:A:495:THR:OG1	2.22	0.45
1:B:139:VAL:HG13	1:B:178:PHE:CE1	2.52	0.45
1:C:493:CYS:O	1:C:497:LEU:HB2	2.17	0.45
1:D:74:ASN:HB3	1:D:95:GLU:CG	2.46	0.45
1:D:899:PHE:HA	1:D:902:MET:HE2	1.98	0.45
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.98	0.45
1:F:410:ILE:HD13	1:F:977:MET:HG2	1.99	0.45
1:A:281:PHE:HD1	1:A:610:PHE:HD1	1.63	0.45
1:A:650:ARG:O	1:A:653:ARG:HB3	2.16	0.45
1:B:181:GLN:HG2	1:B:182:TYR:N	2.30	0.45
1:B:273:GLU:CD	1:B:770:LYS:HD2	2.36	0.45
1:B:277:ILE:HG13	1:B:277:ILE:H	1.68	0.45
1:B:903:LEU:O	1:B:906:PRO:HD2	2.16	0.45
1:D:414:GLU:CD	1:D:974:PRO:HG3	2.36	0.45
1:D:412:VAL:HG22	1:D:438:ILE:HD12	1.97	0.45
1:D:520:PHE:HE2	1:D:973:ARG:HG3	1.80	0.45
1:D:960:LEU:O	1:D:964:THR:HG23	2.16	0.45
1:E:412:VAL:O	1:E:416:VAL:HG23	2.16	0.45
1:E:613:ASN:HD22	1:E:614:GLY:H	1.64	0.45
1:F:1022:VAL:HA	1:F:1025:PHE:HD1	1.82	0.45
1:F:1025:PHE:O	1:F:1029:VAL:HG23	2.16	0.45
1:E:105:VAL:HG23	1:F:109:ASN:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:PHE:CD2	1:F:383:LEU:HD12	2.42	0.45
1:F:2:PRO:HB2	1:F:3:ASN:H	1.59	0.45
1:A:459:PHE:CE2	1:A:876:LEU:HD12	2.52	0.45
1:B:198:LEU:HA	1:B:198:LEU:HD23	1.79	0.45
1:B:758:TYR:OH	1:B:761:ASP:OD1	2.35	0.45
1:C:1011:MET:O	1:C:1015:THR:HG23	2.17	0.45
1:C:368:PRO:HA	1:C:409:ALA:HB1	1.98	0.45
1:C:699:ARG:HD3	1:C:825:MET:SD	2.56	0.45
1:D:527:TYR:OH	1:D:1019:ILE:O	2.19	0.45
1:D:538:THR:HG21	1:D:1028:VAL:HG22	1.98	0.45
1:D:752:ALA:O	1:D:774:MET:HA	2.16	0.45
1:E:230:LEU:HG	1:E:231:ASN:N	2.30	0.45
1:F:1018:ALA:O	1:F:1022:VAL:HG23	2.16	0.45
1:F:1030:ARG:HH11	1:F:1033:PHE:HD2	1.64	0.45
1:F:30:LEU:HA	1:F:31:PRO:HD3	1.88	0.45
1:F:363:ARG:O	1:F:367:ILE:HG13	2.17	0.45
1:A:692:HIS:NE2	1:A:723:ASP:OD1	2.50	0.45
1:B:457:ALA:HB2	1:B:471:SER:CB	2.46	0.45
1:B:743:ILE:HG13	1:B:743:ILE:H	1.65	0.45
1:B:919:ARG:HB3	1:B:921:LEU:CD2	2.46	0.45
1:C:1034:SER:O	1:C:1035:ARG:HG2	2.16	0.45
1:C:149:MET:HB2	1:C:153:ASP:CB	2.47	0.45
1:D:13:TRP:CE2	1:D:492:LEU:HD21	2.51	0.45
1:D:368:PRO:HG3	1:D:413:VAL:HG21	1.99	0.45
1:D:344:LEU:HD23	1:D:402:ILE:HD11	1.97	0.45
1:D:959:GLY:CA	1:D:1039:ASP:HA	2.47	0.45
1:E:574:THR:HG21	1:E:598:TYR:HE2	1.81	0.45
1:F:11:PHE:HE2	1:F:15:ILE:HD11	1.81	0.45
1:F:34:GLN:CG	1:F:333:VAL:HG22	2.47	0.45
1:F:38:ILE:CG2	1:F:462:SER:HB2	2.43	0.45
1:F:497:LEU:HD12	1:F:497:LEU:HA	1.50	0.45
1:F:507:GLU:HG2	1:F:518:ARG:HG3	1.99	0.45
1:E:225:VAL:HG12	1:F:777:ALA:HB1	1.98	0.45
1:F:893:GLU:O	1:F:893:GLU:HG3	2.16	0.45
1:B:519:MET:O	1:B:523:SER:OG	2.33	0.45
1:B:764:ASP:OD1	1:B:765:ARG:HG3	2.17	0.45
1:B:799:VAL:HG12	1:B:800:PRO:O	2.16	0.45
1:B:974:PRO:HA	1:B:977:MET:HE2	1.99	0.45
1:C:1044:HIS:HB2	1:C:1045:THR:H	1.45	0.45
1:C:733:GLN:OE1	1:C:743:ILE:HG21	2.16	0.45
1:D:191:ASN:C	1:D:193:LEU:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:ALA:HB2	1:E:471:SER:OG	2.17	0.45
1:F:11:PHE:CE2	1:F:15:ILE:HD11	2.51	0.45
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.52	0.45
1:F:595:THR:HG23	1:F:609:VAL:HB	1.98	0.45
1:A:424:GLY:HA3	1:A:502:LYS:CG	2.37	0.45
1:A:393:LEU:HD13	1:A:466:ILE:HA	1.99	0.45
1:A:449:LEU:HB3	1:A:478:MET:SD	2.57	0.45
1:A:75:LEU:HD11	1:A:92:LEU:HB3	1.99	0.45
1:B:13:TRP:CE3	1:B:13:TRP:HA	2.52	0.45
1:B:300:LEU:CD2	1:B:334:LYS:HG3	2.47	0.45
1:C:189:ASN:O	1:C:193:LEU:N	2.49	0.45
1:D:441:ALA:HB2	1:D:947:GLU:CD	2.37	0.45
1:F:375:VAL:HG11	1:F:405:LEU:HB3	1.99	0.45
1:F:850:LYS:O	1:F:850:LYS:HG3	2.17	0.45
1:A:542:LEU:HD11	1:A:1028:VAL:HG21	1.98	0.45
1:A:1034:SER:HA	1:A:1035:ARG:CB	2.46	0.45
1:A:200:PRO:HB2	1:A:749:THR:HG22	1.99	0.45
1:B:344:LEU:HD11	1:B:398:MET:CE	2.47	0.45
1:B:767:ARG:NH2	1:C:67:GLN:HE22	2.14	0.45
1:E:1021:PHE:HA	1:E:1024:VAL:HG23	1.98	0.45
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.99	0.45
1:E:361:ASN:O	1:E:365:THR:HB	2.17	0.45
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.52	0.45
1:F:789:TRP:O	1:F:801:PHE:HD2	2.00	0.45
1:F:885:PHE:HE1	1:F:899:PHE:CE2	2.35	0.45
1:F:910:ILE:O	1:F:914:LEU:HB2	2.17	0.45
1:A:108:GLN:O	1:A:112:GLN:HG2	2.17	0.45
1:A:497:LEU:HA	1:A:497:LEU:HD12	1.83	0.45
1:A:703:LEU:CD2	1:A:718:PRO:HD3	2.46	0.45
1:B:682:PHE:CD2	1:B:827:ILE:HD12	2.52	0.45
1:C:684:LEU:HD11	1:C:851:LEU:HD11	1.99	0.45
1:C:686:ASP:HB3	1:C:823:PRO:O	2.17	0.45
1:C:717:ARG:NH2	1:C:828:LEU:HD13	2.32	0.45
1:D:223:PRO:HD3	1:E:275:TYR:CD1	2.52	0.45
1:E:310:LEU:CD1	1:E:323:ILE:HG12	2.46	0.45
1:E:687:GLN:HG3	1:E:822:LEU:HD13	1.99	0.45
1:F:371:ALA:O	1:F:375:VAL:HG23	2.17	0.45
1:F:486:LEU:O	1:F:490:PRO:HG2	2.17	0.45
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.53	0.44
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.99	0.44
1:B:185:ARG:HD3	1:B:772:TYR:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:THR:HA	1:B:284:GLN:OE1	2.17	0.44
1:C:11:PHE:CD2	1:C:11:PHE:C	2.91	0.44
1:D:239:ARG:HD2	1:D:761:ASP:O	2.16	0.44
1:E:115:MET:HE3	1:E:123:GLN:HG2	1.98	0.44
1:E:47:ALA:O	1:E:87:THR:HA	2.18	0.44
1:F:746:ILE:HG22	1:F:791:VAL:HG21	1.99	0.44
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.21	0.44
1:A:785:ASP:O	1:A:789:TRP:HD1	2.00	0.44
1:A:793:ALA:HB3	1:A:795:ASP:OD2	2.17	0.44
1:B:507:GLU:O	1:B:509:LYS:N	2.50	0.44
1:C:200:PRO:CG	1:C:749:THR:HG22	2.47	0.44
1:D:498:LYS:HG3	1:D:499:PRO:HD2	1.99	0.44
1:D:460:GLY:H	1:D:872:GLN:HE22	1.65	0.44
1:F:121:GLU:O	1:F:124:GLN:HG2	2.17	0.44
1:B:843:LEU:HD13	1:B:847:LEU:HG	2.00	0.44
1:B:904:VAL:O	1:B:907:LEU:HB2	2.18	0.44
1:C:1041:GLU:HB3	1:C:1042:HIS:CB	2.36	0.44
1:C:841:MET:HG2	1:C:859:TRP:CH2	2.51	0.44
1:D:212:ALA:HA	1:D:239:ARG:HD3	1.99	0.44
1:E:417:GLU:HG2	1:E:497:LEU:HD21	2.00	0.44
1:E:542:LEU:HD23	1:E:542:LEU:HA	1.68	0.44
1:E:659:LYS:HE3	1:E:659:LYS:HB3	1.60	0.44
1:F:587:THR:HG21	1:F:623:ASN:HA	1.98	0.44
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.98	0.44
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.74	0.44
1:A:400:LEU:HG	1:A:933:THR:OG1	2.18	0.44
1:A:442:LEU:O	1:A:445:ILE:HG13	2.17	0.44
1:A:776:GLU:HB3	1:A:779:TYR:CD1	2.53	0.44
1:A:66:GLU:OE1	1:A:821:GLY:HA2	2.18	0.44
1:A:971:ARG:O	1:A:975:ILE:HG13	2.17	0.44
1:B:996:GLY:O	1:B:1000:GLN:HG3	2.17	0.44
1:B:228:GLN:HG3	1:B:229:GLN:H	1.82	0.44
1:B:143:ILE:HG22	1:B:286:ALA:HB2	2.00	0.44
1:B:398:MET:HE3	1:B:398:MET:HB3	1.60	0.44
1:B:686:ASP:OD1	1:B:690:LEU:HG	2.17	0.44
1:D:982:PHE:HD2	1:D:1011:MET:HG3	1.82	0.44
1:D:915:ALA:HB2	1:D:1009:GLY:HA3	1.99	0.44
1:E:607:GLU:HG3	1:E:607:GLU:O	2.17	0.44
1:E:327:TYR:HB2	1:E:628:PHE:CE2	2.53	0.44
1:E:892:TYR:O	1:E:893:GLU:HB2	2.16	0.44
1:F:479:ALA:O	1:F:482:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASN:OD1	1:A:276:ASP:HB2	2.17	0.44
1:A:34:GLN:HB2	1:A:333:VAL:HG22	1.98	0.44
1:A:352:PHE:HD2	1:A:353:LEU:HD23	1.82	0.44
1:A:579:PRO:HD3	1:A:661:ALA:HB2	2.00	0.44
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.52	0.44
1:B:1045:THR:HB	1:B:1047:ASP:H	1.82	0.44
1:B:211:ASN:ND2	1:B:760:ASN:HD22	2.16	0.44
1:B:228:GLN:HG3	1:B:229:GLN:N	2.32	0.44
1:D:242:SER:O	1:D:246:PHE:HD1	2.00	0.44
1:D:165:ALA:HB3	1:D:313:MET:HE3	1.99	0.44
1:E:1034:SER:HB3	1:E:1035:ARG:H	1.59	0.44
1:E:600:THR:C	1:E:602:GLU:H	2.21	0.44
1:E:674:LEU:HB3	1:E:675:GLY:H	1.40	0.44
1:F:892:TYR:CD1	1:F:897:ILE:HG21	2.53	0.44
1:A:960:LEU:HD21	1:A:1027:VAL:HG13	1.99	0.44
1:A:366:LEU:HA	1:A:366:LEU:HD23	1.63	0.44
1:B:545:TYR:HB2	1:B:1021:PHE:CE2	2.53	0.44
1:B:119:PRO:O	1:B:123:GLN:HG3	2.18	0.44
1:B:211:ASN:O	1:B:760:ASN:ND2	2.44	0.44
1:B:293:LEU:HG	1:B:299:ALA:HA	1.99	0.44
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.82	0.44
1:B:982:PHE:O	1:B:985:GLY:N	2.50	0.44
1:C:152:GLU:H	1:C:152:GLU:CD	2.20	0.44
1:C:188:MET:SD	1:C:200:PRO:HG3	2.58	0.44
1:C:713:LEU:HD11	1:C:843:LEU:HD12	1.99	0.44
1:E:448:VAL:HG13	1:E:884:VAL:HG13	2.00	0.44
1:E:762:PHE:HD2	1:E:771:VAL:HG22	1.83	0.44
1:F:908:GLY:O	1:F:1010:GLY:HA2	2.18	0.44
1:D:55:LYS:NZ	1:F:238:THR:OG1	2.23	0.44
1:F:54:ALA:HB1	1:F:816:LEU:HG	2.00	0.44
1:A:536:ARG:NH1	2:A:1101:LMT:O3B	2.51	0.44
1:A:158:VAL:HA	1:A:162:MET:HE2	1.99	0.44
1:A:177:LEU:HD23	1:A:178:PHE:N	2.32	0.44
1:A:216:ALA:HB3	1:A:234:ILE:O	2.17	0.44
1:A:818:ARG:NH1	1:A:823:PRO:HG3	2.25	0.44
1:A:47:ALA:HB3	1:A:88:VAL:HG13	1.99	0.44
1:D:193:LEU:HD13	1:D:200:PRO:HD3	2.00	0.44
1:D:438:ILE:O	1:D:441:ALA:HB3	2.17	0.44
1:D:877:TYR:O	1:D:881:LEU:HB2	2.17	0.44
1:E:246:PHE:O	1:E:249:ILE:HG23	2.18	0.44
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:428:LYS:HG2	1:E:494:ALA:HB1	1.99	0.44
1:E:727:PHE:CZ	1:E:807:SER:HB2	2.53	0.44
2:F:1101:LMT:H72	2:F:1101:LMT:H101	1.40	0.44
1:F:964:THR:O	1:F:968:VAL:HB	2.17	0.44
1:A:708:LYS:HE3	1:A:708:LYS:HB3	1.73	0.44
1:B:300:LEU:HD23	1:B:334:LYS:HG3	2.00	0.44
1:B:643:LYS:O	1:B:645:GLU:N	2.51	0.44
1:B:204:ILE:HG23	1:B:759:VAL:HG21	2.00	0.44
1:C:307:ARG:NH2	1:C:311:ALA:HB2	2.32	0.44
1:C:344:LEU:HD11	1:C:376:LEU:HD11	1.98	0.44
1:C:647:ILE:HG12	1:C:650:ARG:NH1	2.33	0.44
1:C:746:ILE:HG13	1:C:747:ASN:H	1.81	0.44
1:D:60:THR:HG23	1:D:61:VAL:HG23	2.00	0.44
1:E:115:MET:HE1	1:E:123:GLN:HA	1.99	0.44
1:E:166:ILE:HG12	1:E:306:ILE:HG23	1.99	0.44
1:E:327:TYR:HB2	1:E:628:PHE:CZ	2.53	0.44
1:E:515:TRP:O	1:E:519:MET:HG3	2.17	0.44
1:E:637:ARG:HD2	1:E:642:ASN:O	2.18	0.44
1:E:952:LEU:HB2	1:E:963:ALA:HB1	2.00	0.44
1:F:200:PRO:HB2	1:F:749:THR:HG22	2.00	0.44
1:F:492:LEU:O	1:F:496:MET:HG2	2.18	0.44
1:F:521:GLU:O	1:F:524:THR:HG22	2.17	0.44
1:F:603:LYS:HB2	1:F:603:LYS:HE3	1.80	0.44
2:A:1101:LMT:H21	2:A:1101:LMT:H51	1.66	0.44
1:A:21:LEU:HA	1:A:21:LEU:HD13	1.71	0.44
1:B:190:PRO:HG3	1:B:779:TYR:HB3	2.00	0.44
1:B:143:ILE:HG12	1:B:322:LYS:O	2.18	0.44
1:B:952:LEU:HD13	1:B:966:ASP:HB3	2.00	0.44
1:C:472:ILE:O	1:C:476:SER:HB3	2.18	0.44
1:D:139:VAL:HA	1:D:289:LEU:O	2.18	0.44
1:D:188:MET:HB2	1:D:188:MET:HE2	1.82	0.44
1:D:504:ASP:C	1:D:506:GLY:H	2.22	0.44
1:D:805:SER:OG	1:D:805:SER:O	2.35	0.44
1:E:343:THR:HA	1:E:346:GLU:OE1	2.18	0.44
1:A:184:MET:HB3	1:A:771:VAL:HG13	2.00	0.43
1:A:622:GLN:NE2	1:C:222:THR:HG22	2.33	0.43
1:A:659:LYS:HD3	1:A:659:LYS:HA	1.48	0.43
1:B:1040:ILE:HG23	1:B:1041:GLU:H	1.83	0.43
1:B:361:ASN:OD1	1:B:498:LYS:HD2	2.17	0.43
1:B:958:LYS:HB3	1:B:963:ALA:HB2	2.00	0.43
1:C:983:ILE:HG23	1:C:1008:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ASN:O	1:C:284:GLN:NE2	2.50	0.43
1:C:524:THR:O	1:C:527:TYR:HB3	2.18	0.43
1:C:580:ALA:HB1	1:C:724:THR:HG22	2.00	0.43
1:D:228:GLN:HG3	1:D:229:GLN:N	2.33	0.43
1:D:413:VAL:O	1:D:417:GLU:HG2	2.18	0.43
1:E:61:VAL:HG21	1:E:122:VAL:HG21	2.00	0.43
1:E:178:PHE:HD1	1:E:288:GLY:HA3	1.82	0.43
1:E:182:TYR:O	1:E:769:LYS:HD3	2.17	0.43
1:E:459:PHE:HD1	1:E:467:TYR:CG	2.36	0.43
1:E:47:ALA:HB3	1:E:88:VAL:HB	1.98	0.43
1:F:504:ASP:C	1:F:506:GLY:N	2.71	0.43
1:A:166:ILE:HD13	1:A:166:ILE:HA	1.65	0.43
1:A:346:GLU:O	1:A:349:ILE:N	2.51	0.43
1:A:870:GLY:O	1:A:871:ASN:HB2	2.18	0.43
1:A:7:ASP:O	1:A:8:ARG:HG3	2.18	0.43
1:B:344:LEU:HD11	1:B:398:MET:HE3	1.99	0.43
1:C:694:LYS:HA	1:C:697:GLN:OE1	2.18	0.43
1:D:108:GLN:NE2	1:E:109:ASN:HB3	2.32	0.43
1:D:259:ARG:NH1	1:E:734:GLU:OE2	2.51	0.43
1:D:460:GLY:N	1:D:872:GLN:HE22	2.15	0.43
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.47	0.43
1:E:578:LEU:HB2	1:E:623:ASN:O	2.18	0.43
1:F:452:VAL:C	1:F:455:PRO:HD2	2.38	0.43
1:F:667:ASN:O	1:F:678:THR:OG1	2.22	0.43
1:A:225:VAL:H	1:B:781:MET:CE	2.31	0.43
1:A:270:LEU:HA	1:A:270:LEU:HD12	1.72	0.43
1:A:534:ILE:HG22	1:A:541:TYR:CZ	2.53	0.43
1:A:66:GLU:OE2	1:A:80:SER:OG	2.30	0.43
1:B:112:GLN:HA	1:B:115:MET:HG2	2.00	0.43
1:B:706:ALA:CB	1:B:716:VAL:HG11	2.46	0.43
1:B:76:MET:HG2	1:B:864:TYR:OH	2.18	0.43
1:C:1034:SER:OG	1:C:1035:ARG:N	2.48	0.43
1:C:492:LEU:HA	1:C:495:THR:HG1	1.83	0.43
1:C:509:LYS:HD2	1:C:509:LYS:HA	1.70	0.43
1:C:690:LEU:O	1:C:694:LYS:HB2	2.19	0.43
1:C:698:ALA:O	1:C:701:GLN:HB3	2.18	0.43
1:C:888:LEU:HA	1:C:888:LEU:HD23	1.75	0.43
1:C:944:LEU:HB3	1:C:971:ARG:CD	2.45	0.43
1:D:449:LEU:O	1:D:453:PHE:HD1	2.02	0.43
1:E:132:SER:O	1:E:132:SER:OG	2.27	0.43
1:E:241:THR:N	1:E:245:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:986:VAL:HG12	1:E:1008:MET:HE3	2.00	0.43
1:F:2:PRO:O	1:F:5:PHE:HB3	2.18	0.43
1:F:42:ALA:HA	1:F:92:LEU:O	2.17	0.43
1:C:163:LYS:O	1:C:163:LYS:HG2	2.17	0.43
1:C:492:LEU:HA	1:C:495:THR:OG1	2.18	0.43
1:C:757:SER:O	1:C:772:TYR:HA	2.17	0.43
1:C:559:LEU:HD11	1:C:916:ALA:HB1	1.99	0.43
1:D:247:GLY:O	1:D:261:LEU:HB3	2.19	0.43
1:D:904:VAL:HG21	1:D:942:ALA:CB	2.47	0.43
1:E:690:LEU:HB2	1:E:694:LYS:HB2	2.00	0.43
1:A:448:VAL:O	1:A:451:ALA:HB3	2.19	0.43
1:A:459:PHE:CE1	1:A:876:LEU:HD12	2.53	0.43
1:A:818:ARG:NH2	1:A:823:PRO:HD3	2.33	0.43
1:B:1033:PHE:HA	1:B:1034:SER:HA	1.78	0.43
1:B:211:ASN:ND2	1:B:246:PHE:HZ	2.17	0.43
1:B:424:GLY:HA3	1:B:502:LYS:HB2	2.01	0.43
1:B:520:PHE:O	1:B:523:SER:OG	2.36	0.43
1:D:272:GLY:N	1:D:275:TYR:OH	2.50	0.43
1:D:393:LEU:HD22	1:D:470:PHE:HE1	1.84	0.43
1:D:698:ALA:O	1:D:701:GLN:HB3	2.18	0.43
1:D:743:ILE:HD12	1:D:743:ILE:H	1.83	0.43
1:E:166:ILE:O	1:E:169:THR:HB	2.19	0.43
1:E:686:ASP:HB2	1:E:695:LEU:HD21	1.99	0.43
1:D:217:GLY:HA2	1:E:755:GLY:CA	2.48	0.43
1:F:379:THR:O	1:F:382:VAL:HB	2.18	0.43
1:F:671:ILE:CG2	1:F:674:LEU:HB2	2.48	0.43
1:F:135:SER:CB	1:F:673:GLU:HB3	2.35	0.43
1:F:560:PRO:HB2	1:F:836:SER:OG	2.18	0.43
1:A:250:LEU:HD11	1:A:259:ARG:HD2	2.00	0.43
1:A:485:ALA:O	1:A:490:PRO:HD3	2.18	0.43
1:A:900:SER:HB3	1:A:1029:VAL:HG21	2.01	0.43
1:A:903:LEU:HD23	1:A:903:LEU:HA	1.65	0.43
1:A:75:LEU:CD1	1:A:92:LEU:HB3	2.49	0.43
1:A:926:TYR:HE1	1:A:999:ALA:HB1	1.83	0.43
1:B:480:LEU:O	1:B:484:VAL:HG23	2.18	0.43
1:C:1032:ARG:O	1:C:1033:PHE:CD1	2.71	0.43
1:D:904:VAL:O	1:D:907:LEU:HB2	2.18	0.43
1:D:925:VAL:HA	1:D:928:GLN:OE1	2.17	0.43
1:E:52:ALA:HB3	1:E:57:VAL:HG12	2.01	0.43
1:F:565:PRO:O	1:F:567:GLU:HG2	2.19	0.43
1:A:634:TRP:CD1	1:A:634:TRP:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:SER:O	1:A:772:TYR:HA	2.19	0.43
1:A:862:MET:HG3	1:A:863:SER:H	1.84	0.43
1:B:136:PHE:HD2	1:B:290:GLY:HA3	1.82	0.43
1:C:1027:VAL:O	1:C:1031:ARG:HG3	2.19	0.43
1:C:363:ARG:CZ	1:C:363:ARG:H	2.32	0.43
1:C:523:SER:HA	1:C:526:HIS:HB2	2.00	0.43
1:C:549:VAL:O	1:C:552:MET:HB3	2.18	0.43
1:C:955:LYS:O	1:C:956:GLU:HG2	2.18	0.43
1:D:971:ARG:NH1	1:D:971:ARG:N	2.64	0.43
1:E:743:ILE:O	1:E:746:ILE:HB	2.19	0.43
1:E:455:PRO:O	1:E:876:LEU:HD13	2.18	0.43
1:F:140:VAL:HG11	1:F:310:LEU:CD2	2.49	0.43
1:F:405:LEU:HD12	1:F:406:VAL:N	2.34	0.43
1:F:54:ALA:HB3	1:F:813:SER:O	2.18	0.43
1:A:1040:ILE:HG23	1:A:1041:GLU:N	2.33	0.43
1:A:668:LEU:H	1:A:668:LEU:HD23	1.84	0.43
1:A:686:ASP:OD1	1:A:689:GLY:N	2.48	0.43
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.71	0.43
1:B:709:HIS:CE1	1:B:847:LEU:HD21	2.54	0.43
1:B:350:LEU:HD13	1:B:984:LEU:O	2.18	0.43
1:C:881:LEU:HD22	1:C:902:MET:CE	2.48	0.43
1:D:203:VAL:O	1:D:207:ILE:HG13	2.19	0.43
1:D:678:THR:HA	1:D:837:THR:OG1	2.19	0.43
1:E:177:LEU:HA	1:E:289:LEU:HD23	2.00	0.43
1:E:702:LEU:HA	1:E:702:LEU:HD12	1.81	0.43
1:E:888:LEU:HD23	1:E:888:LEU:HA	1.70	0.43
1:F:270:LEU:HA	1:F:270:LEU:HD12	1.89	0.43
1:F:396:PHE:O	1:F:400:LEU:HB2	2.19	0.43
1:A:156:ASP:OD2	1:A:182:TYR:HB2	2.19	0.43
1:A:359:LEU:C	1:A:361:ASN:H	2.21	0.43
1:A:641:GLU:HA	1:A:646:ALA:HB3	1.99	0.43
1:B:214:VAL:HG23	1:B:237:GLN:HB3	2.00	0.43
1:B:331:PRO:O	1:B:335:ILE:HD13	2.19	0.43
1:B:641:GLU:HA	1:B:646:ALA:HB3	2.01	0.43
1:B:704:ALA:O	1:B:708:LYS:HE3	2.19	0.43
1:C:102:ILE:HD13	1:C:102:ILE:HA	1.89	0.43
1:E:583:THR:HG22	1:E:584:GLN:N	2.33	0.43
1:E:571:VAL:HG13	1:E:628:PHE:HE1	1.83	0.43
1:E:880:SER:O	1:E:884:VAL:HG23	2.19	0.43
1:F:157:TYR:O	1:F:161:ASN:HB2	2.18	0.43
1:F:239:ARG:CZ	1:F:761:ASP:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:343:THR:HG21	1:F:989:LEU:HD23	2.00	0.43
1:F:3:ASN:ND2	1:F:486:LEU:HD22	2.33	0.43
1:F:598:TYR:CE2	1:F:629:VAL:HG21	2.53	0.43
1:A:259:ARG:NH2	1:A:261:LEU:HD11	2.34	0.43
1:A:394:THR:HG22	1:A:473:THR:HG1	1.82	0.43
1:B:187:TRP:HA	1:B:774:MET:O	2.19	0.43
1:B:523:SER:O	1:B:526:HIS:HB2	2.19	0.43
1:C:907:LEU:HD21	1:C:1021:PHE:HB3	2.01	0.43
1:D:1040:ILE:HG12	1:D:1041:GLU:H	1.84	0.43
1:D:49:TYR:HE1	1:D:60:THR:HG21	1.84	0.43
1:D:973:ARG:HB3	1:D:974:PRO:HD3	2.01	0.43
1:E:180:SER:OG	1:E:273:GLU:N	2.52	0.43
1:F:188:MET:HA	1:F:266:ALA:HB2	1.99	0.43
1:F:361:ASN:HB3	1:F:364:ALA:HB3	2.00	0.43
1:F:511:GLY:O	1:F:512:PHE:CD2	2.72	0.43
1:F:534:ILE:HG22	2:F:1101:LMT:H5'	1.99	0.43
1:F:583:THR:O	1:F:587:THR:HG23	2.19	0.43
1:F:752:ALA:O	1:F:774:MET:HA	2.19	0.43
1:A:167:SER:O	1:B:70:ASN:HB2	2.19	0.42
1:A:225:VAL:HG11	1:B:778:LYS:HA	2.01	0.42
1:C:110:LYS:HA	1:C:110:LYS:HD3	1.86	0.42
1:C:659:LYS:HD3	1:C:659:LYS:HA	1.39	0.42
1:C:943:ILE:O	1:C:947:GLU:HB3	2.19	0.42
1:D:351:VAL:HG22	1:D:981:ALA:HB1	2.01	0.42
1:D:654:ALA:O	1:D:658:ILE:HG12	2.18	0.42
1:E:43:VAL:HA	1:E:130:GLU:O	2.19	0.42
1:E:652:THR:OG1	1:E:665:ALA:HB3	2.18	0.42
1:E:869:SER:HB2	1:E:872:GLN:NE2	2.33	0.42
1:F:979:SER:HA	1:F:1011:MET:HE3	2.01	0.42
1:D:75:LEU:HD23	1:F:168:ARG:HB3	2.01	0.42
1:F:15:ILE:O	1:F:19:ILE:HG13	2.19	0.42
1:F:463:THR:HG22	1:F:467:TYR:CZ	2.55	0.42
1:F:751:GLY:O	1:F:754:TRP:N	2.52	0.42
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.59	0.42
1:A:58:GLN:O	1:A:63:GLN:HG3	2.19	0.42
1:A:712:MET:O	1:A:832:ALA:N	2.50	0.42
1:A:699:ARG:NH1	1:A:825:MET:SD	2.91	0.42
1:A:885:PHE:CD1	1:A:902:MET:HE1	2.40	0.42
1:B:277:ILE:HD12	1:B:277:ILE:O	2.18	0.42
1:B:668:LEU:CD2	1:B:668:LEU:H	2.33	0.42
1:C:851:LEU:HB3	1:C:852:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:904:VAL:HG12	1:C:904:VAL:O	2.18	0.42
1:D:655:PHE:HB3	1:D:663:VAL:HB	2.01	0.42
1:D:919:ARG:HG2	1:D:920:GLY:H	1.83	0.42
1:D:949:ALA:HA	1:D:967:ALA:HB2	2.01	0.42
1:E:187:TRP:HA	1:E:774:MET:O	2.19	0.42
1:E:53:ASP:O	1:E:57:VAL:HG13	2.18	0.42
1:D:768:VAL:HG12	1:E:63:GLN:OE1	2.19	0.42
1:E:965:LEU:HD23	1:E:965:LEU:HA	1.86	0.42
1:F:311:ALA:HA	1:F:314:GLU:HG3	2.01	0.42
1:F:39:ALA:HA	1:F:40:PRO:HD2	1.87	0.42
1:A:633:ASP:OD1	1:A:635:ALA:HB3	2.19	0.42
1:B:1016:VAL:HG13	2:B:1101:LMT:H102	2.01	0.42
1:B:13:TRP:HE3	1:B:13:TRP:HA	1.83	0.42
1:B:455:PRO:HG2	1:B:880:SER:HB2	2.01	0.42
1:C:101:ASP:O	1:C:105:VAL:HG23	2.19	0.42
1:C:133:SER:O	1:C:134:SER:HB2	2.19	0.42
1:C:213:GLN:HG2	1:C:239:ARG:HG3	2.02	0.42
1:C:274:ASN:OD1	1:C:276:ASP:HB2	2.20	0.42
1:C:182:TYR:HD2	1:C:765:ARG:HH22	1.67	0.42
1:C:897:ILE:HB	1:C:898:PRO:HD3	2.01	0.42
1:D:367:ILE:HD13	1:D:493:CYS:HA	2.01	0.42
1:D:690:LEU:HD11	1:D:853:THR:O	2.18	0.42
1:D:858:ASP:OD2	1:D:859:TRP:N	2.50	0.42
1:E:102:ILE:HD12	1:E:102:ILE:HA	1.73	0.42
1:E:30:LEU:HA	1:E:30:LEU:HD12	1.83	0.42
1:E:728:LYS:HB2	1:E:810:GLU:OE1	2.19	0.42
1:E:897:ILE:O	1:E:900:SER:OG	2.27	0.42
1:F:1022:VAL:N	1:F:1023:PRO:HD2	2.34	0.42
1:F:247:GLY:O	1:F:261:LEU:HB3	2.19	0.42
1:F:261:LEU:HD12	1:F:263:ARG:NH1	2.33	0.42
1:F:588:GLN:OE1	1:F:592:ASN:ND2	2.42	0.42
1:F:634:TRP:CD1	1:F:634:TRP:N	2.82	0.42
1:F:731:ILE:HG13	1:F:731:ILE:O	2.19	0.42
1:F:991:ILE:O	1:F:991:ILE:HG23	2.19	0.42
1:A:242:SER:OG	1:A:245:GLU:HG2	2.19	0.42
1:B:368:PRO:HA	1:B:371:ALA:HB3	2.00	0.42
1:B:448:VAL:HG13	1:B:884:VAL:HG22	2.01	0.42
1:A:622:GLN:HE21	1:C:222:THR:HG22	1.84	0.42
1:C:356:TYR:C	1:C:358:PHE:H	2.23	0.42
1:E:1010:GLY:O	1:E:1014:ALA:HB2	2.20	0.42
1:E:1034:SER:O	1:E:1035:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:VAL:CG2	1:E:122:VAL:HG21	2.49	0.42
1:E:434:SER:O	1:E:438:ILE:HG12	2.20	0.42
1:F:189:ASN:OD1	1:F:190:PRO:HD2	2.20	0.42
1:A:41:PRO:HG2	1:A:94:PHE:CB	2.41	0.42
1:A:889:ALA:N	1:A:898:PRO:HG3	2.34	0.42
1:B:575:MET:HB3	1:B:626:ILE:CG1	2.49	0.42
1:B:576:VAL:HG22	1:B:663:VAL:CG2	2.49	0.42
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.76	0.42
1:C:364:ALA:HA	1:C:367:ILE:CD1	2.49	0.42
1:C:492:LEU:O	1:C:496:MET:HG2	2.19	0.42
1:C:536:ARG:NH2	2:C:1101:LMT:H3O1	2.09	0.42
1:C:762:PHE:CE1	1:C:764:ASP:HB2	2.54	0.42
1:C:923:ASN:HA	1:C:927:PHE:CD2	2.55	0.42
1:D:151:GLN:H	1:D:151:GLN:NE2	2.17	0.42
1:D:186:ILE:HG12	1:D:268:ILE:HG12	2.02	0.42
1:D:751:GLY:O	1:D:754:TRP:N	2.53	0.42
1:D:838:GLY:O	1:D:841:MET:HB2	2.20	0.42
1:F:348:ILE:HG13	1:F:402:ILE:HD13	2.01	0.42
1:F:355:MET:SD	1:F:368:PRO:HB2	2.60	0.42
1:F:863:SER:HA	1:F:866:GLU:HB3	2.01	0.42
1:F:905:VAL:HG13	1:F:935:ILE:HG12	2.01	0.42
1:A:151:GLN:HG2	1:A:152:GLU:N	2.34	0.42
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.50	0.42
1:B:66:GLU:OE1	1:B:821:GLY:HA2	2.18	0.42
1:C:11:PHE:C	1:C:11:PHE:HD2	2.23	0.42
1:E:460:GLY:O	1:E:463:THR:OG1	2.38	0.42
1:D:225:VAL:HG12	1:E:777:ALA:HB1	2.01	0.42
1:E:448:VAL:HG13	1:E:884:VAL:HG22	2.01	0.42
1:F:134:SER:H	1:F:292:LYS:HD3	1.84	0.42
1:F:753:ALA:HA	1:F:775:SER:HB3	2.02	0.42
1:A:537:SER:O	1:A:537:SER:OG	2.23	0.42
1:A:831:ALA:HB1	1:A:835:LYS:HB3	2.02	0.42
1:B:61:VAL:CG2	1:B:122:VAL:HG21	2.50	0.42
1:B:139:VAL:HG13	1:B:178:PHE:HE1	1.85	0.42
1:B:281:PHE:O	1:B:284:GLN:HB2	2.20	0.42
1:A:75:LEU:CD2	1:C:168:ARG:HD3	2.50	0.42
1:C:958:LYS:CB	1:C:963:ALA:HB2	2.50	0.42
1:D:344:LEU:HD13	1:D:376:LEU:CD1	2.46	0.42
1:D:563:PHE:CE2	1:D:674:LEU:HD22	2.55	0.42
1:D:76:MET:HB2	1:D:93:THR:O	2.20	0.42
1:E:189:ASN:ND2	1:E:192:GLU:OE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:649:MET:O	1:E:653:ARG:HB2	2.20	0.42
1:E:758:TYR:HB2	1:E:772:TYR:CZ	2.54	0.42
1:F:163:LYS:HD2	1:F:177:LEU:HD12	2.02	0.42
1:A:30:LEU:HA	1:A:31:PRO:HD3	1.89	0.42
1:A:457:ALA:HB1	1:A:468:ARG:HG3	2.00	0.42
1:A:809:TRP:HH2	1:C:230:LEU:HD21	1.85	0.42
1:B:300:LEU:HD11	1:B:333:VAL:HG12	2.01	0.42
1:B:355:MET:HG3	1:B:359:LEU:HD12	2.01	0.42
1:C:252:LYS:O	1:C:260:VAL:HG23	2.20	0.42
1:C:356:TYR:HD1	1:C:365:THR:HG21	1.85	0.42
1:C:379:THR:HG23	1:C:476:SER:OG	2.19	0.42
1:E:324:VAL:HG12	1:E:326:PRO:HD3	2.01	0.42
1:F:249:ILE:O	1:F:262:LEU:N	2.52	0.42
1:F:588:GLN:HB2	1:F:613:ASN:HD22	1.85	0.42
1:F:892:TYR:HD1	1:F:897:ILE:HG21	1.84	0.42
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.96	0.42
1:B:911:GLY:O	1:B:914:LEU:HB3	2.20	0.42
1:C:447:MET:O	1:C:451:ALA:HB2	2.20	0.42
1:C:587:THR:HG21	1:C:623:ASN:HA	2.02	0.42
1:C:567:GLU:OE1	1:C:996:GLY:HA2	2.19	0.42
1:D:138:MET:HG2	1:D:291:ILE:HB	2.01	0.42
1:D:489:THR:O	1:D:493:CYS:HB2	2.19	0.42
1:E:536:ARG:NH1	2:E:1101:LMT:H4B	2.35	0.42
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.61	0.42
1:E:960:LEU:O	1:E:964:THR:HG23	2.19	0.42
1:F:138:MET:HE3	1:F:328:ASP:OD1	2.20	0.42
1:F:778:LYS:HG3	1:F:779:TYR:CE1	2.55	0.42
1:F:953:MET:HE3	1:F:953:MET:HB2	1.90	0.42
1:A:781:MET:HE2	1:C:225:VAL:HG22	2.02	0.42
1:A:937:LEU:HA	1:A:937:LEU:HD23	1.53	0.42
1:B:634:TRP:N	1:B:634:TRP:CD1	2.79	0.42
1:C:445:ILE:HG23	1:C:940:LYS:HG3	2.01	0.42
1:C:940:LYS:O	1:C:943:ILE:HB	2.19	0.42
1:D:453:PHE:CE2	1:D:474:ILE:HG21	2.54	0.42
1:D:534:ILE:HG13	1:D:534:ILE:H	1.66	0.42
1:D:818:ARG:HH12	1:D:823:PRO:HG3	1.85	0.42
1:D:971:ARG:C	1:D:971:ARG:CZ	2.88	0.42
1:E:270:LEU:HA	1:E:270:LEU:HD12	1.87	0.42
1:E:508:GLY:N	1:E:518:ARG:HG3	2.35	0.42
1:E:834:GLY:O	1:E:835:LYS:HE2	2.20	0.42
1:E:851:LEU:HB3	1:E:852:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:GLU:CD	1:F:770:LYS:HD2	2.39	0.42
1:F:36:PRO:HD3	1:F:391:ASN:ND2	2.35	0.42
1:A:300:LEU:HD11	1:A:333:VAL:HG11	2.02	0.41
1:A:471:SER:O	1:A:475:VAL:HG23	2.20	0.41
1:B:445:ILE:HG21	1:B:940:LYS:HG3	2.02	0.41
1:C:885:PHE:CD1	1:C:898:PRO:HB3	2.55	0.41
1:D:520:PHE:O	1:D:524:THR:HG22	2.20	0.41
1:D:764:ASP:HB3	1:D:769:LYS:HD2	2.02	0.41
1:D:862:MET:HG3	1:D:863:SER:H	1.85	0.41
1:D:556:PHE:CD1	1:D:913:LEU:HD21	2.54	0.41
1:E:1041:GLU:HB3	1:E:1042:HIS:CA	2.50	0.41
1:E:267:LYS:HD3	1:E:776:GLU:OE2	2.20	0.41
1:E:281:PHE:CE1	1:E:608:SER:HB2	2.54	0.41
1:E:564:LEU:CD1	1:E:671:ILE:HD12	2.50	0.41
1:E:726:GLN:CD	1:E:812:GLY:HA3	2.40	0.41
1:E:790:TYR:CE1	1:E:800:PRO:HB3	2.55	0.41
1:E:892:TYR:CD2	1:E:897:ILE:HG22	2.55	0.41
1:F:182:TYR:HD1	1:F:182:TYR:HA	1.73	0.41
1:F:777:ALA:O	1:F:781:MET:HG2	2.20	0.41
1:F:49:TYR:N	1:F:86:GLY:O	2.41	0.41
1:A:102:ILE:HD12	1:C:101:ASP:HB3	2.02	0.41
1:A:1035:ARG:C	1:A:1037:ASN:H	2.23	0.41
1:B:177:LEU:HD23	1:B:178:PHE:N	2.36	0.41
1:B:36:PRO:HD3	1:B:391:ASN:CG	2.39	0.41
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.51	0.41
1:B:420:MET:HB3	1:B:500:ILE:HB	2.02	0.41
1:C:159:ALA:HB2	1:C:177:LEU:HD11	2.02	0.41
1:C:15:ILE:O	1:C:19:ILE:HG13	2.20	0.41
1:C:228:GLN:HG3	1:C:229:GLN:N	2.36	0.41
1:C:211:ASN:ND2	1:C:246:PHE:HZ	2.18	0.41
1:C:280:GLU:OE2	1:C:588:GLN:NE2	2.49	0.41
1:C:360:GLN:HB3	1:C:513:PHE:CE2	2.55	0.41
1:C:30:LEU:HD13	1:C:384:ALA:HB2	2.02	0.41
1:C:75:LEU:HA	1:C:94:PHE:HD2	1.85	0.41
1:D:219:LEU:HD12	1:D:232:ALA:HB3	2.02	0.41
1:E:58:GLN:O	1:E:62:THR:HB	2.19	0.41
1:F:193:LEU:HD23	1:F:193:LEU:HA	1.76	0.41
1:F:23:GLY:O	1:F:27:ILE:HG23	2.19	0.41
1:A:141:GLY:O	1:A:323:ILE:HG23	2.20	0.41
1:A:244:GLU:C	1:A:246:PHE:N	2.73	0.41
1:A:456:MET:HB3	1:A:877:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:SER:O	1:A:997:SER:HB2	2.20	0.41
1:B:251:LEU:HD21	1:B:262:LEU:HD13	2.02	0.41
1:B:420:MET:HG2	1:B:425:LEU:O	2.21	0.41
1:B:888:LEU:HA	1:B:888:LEU:HD23	1.71	0.41
1:C:931:LEU:HD23	1:C:931:LEU:HA	1.68	0.41
1:D:1008:MET:HB2	1:D:1008:MET:HE3	1.90	0.41
1:D:163:LYS:HG3	1:D:289:LEU:HD21	2.01	0.41
1:D:700:ASN:HA	1:D:703:LEU:HD12	2.02	0.41
1:D:775:SER:HB2	1:D:789:TRP:CZ2	2.54	0.41
1:E:785:ASP:OD1	1:E:785:ASP:N	2.54	0.41
1:F:208:LYS:HE3	1:F:759:VAL:HG13	2.02	0.41
1:F:311:ALA:HA	1:F:314:GLU:CD	2.41	0.41
1:A:149:MET:CE	1:A:153:ASP:HB3	2.50	0.41
1:A:149:MET:HE2	1:A:153:ASP:HB3	2.03	0.41
1:A:457:ALA:O	1:A:468:ARG:NE	2.28	0.41
1:A:782:LEU:HA	1:A:783:PRO:HD3	1.85	0.41
1:A:905:VAL:HG13	1:A:935:ILE:HD13	2.01	0.41
1:A:946:VAL:HG22	1:A:1026:PHE:HB2	2.03	0.41
1:B:1038:GLU:HG3	1:B:1039:ASP:H	1.85	0.41
1:B:249:ILE:HD13	1:B:249:ILE:HG21	1.83	0.41
1:B:390:ILE:HG23	1:B:395:MET:CG	2.51	0.41
1:C:151:GLN:N	1:C:151:GLN:OE1	2.54	0.41
1:C:189:ASN:O	1:C:193:LEU:HG	2.21	0.41
1:D:618:ALA:O	1:D:815:ARG:NH2	2.54	0.41
1:D:602:GLU:OE1	1:D:647:ILE:HG23	2.20	0.41
1:D:190:PRO:HB3	1:D:789:TRP:CZ2	2.54	0.41
1:E:148:THR:HG21	1:E:319:SER:OG	2.20	0.41
1:E:402:ILE:HG22	1:E:406:VAL:HG23	2.01	0.41
1:E:482:VAL:O	1:E:485:ALA:HB3	2.20	0.41
1:E:907:LEU:HD21	1:E:1021:PHE:HB3	2.02	0.41
1:D:781:MET:CE	1:F:225:VAL:H	2.33	0.41
1:F:418:ARG:O	1:F:422:GLU:HB2	2.20	0.41
1:A:463:THR:O	1:A:466:ILE:HB	2.20	0.41
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.73	0.41
1:A:575:MET:O	1:A:575:MET:HG3	2.18	0.41
1:A:678:THR:OG1	1:A:678:THR:O	2.36	0.41
1:A:3:ASN:O	1:A:6:ILE:HG13	2.20	0.41
1:B:407:ASP:O	1:B:411:VAL:HG23	2.20	0.41
1:C:121:GLU:N	1:C:121:GLU:OE1	2.49	0.41
1:D:26:ALA:HB1	1:D:384:ALA:CB	2.50	0.41
1:D:5:PHE:HD2	1:D:12:ALA:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ASN:HB3	1:D:95:GLU:HG3	2.03	0.41
1:E:364:ALA:HB2	1:E:497:LEU:HD11	2.01	0.41
1:E:578:LEU:HD13	1:E:661:ALA:HB2	2.03	0.41
1:E:184:MET:HB2	1:E:762:PHE:CE2	2.56	0.41
1:E:783:PRO:O	1:E:786:ILE:HB	2.20	0.41
1:E:841:MET:O	1:E:845:GLU:HG3	2.20	0.41
1:F:352:PHE:CD2	1:F:353:LEU:HD23	2.53	0.41
1:F:602:GLU:OE2	1:F:650:ARG:HD2	2.20	0.41
1:F:666:PHE:CD1	1:F:666:PHE:N	2.88	0.41
1:F:900:SER:OG	1:F:1026:PHE:HD1	2.04	0.41
1:F:953:MET:HE1	1:F:960:LEU:HA	2.02	0.41
1:A:576:VAL:HG22	1:A:663:VAL:HG22	2.02	0.41
1:A:58:GLN:NE2	1:A:818:ARG:NH1	2.69	0.41
1:B:255:GLN:HG3	1:B:255:GLN:H	1.29	0.41
1:D:27:ILE:HD11	1:D:380:PHE:CD1	2.56	0.41
1:D:393:LEU:HB3	1:D:470:PHE:CE1	2.55	0.41
1:D:603:LYS:HB3	1:D:603:LYS:HE2	1.91	0.41
1:D:921:LEU:HA	1:D:921:LEU:HD13	1.84	0.41
1:F:982:PHE:CD2	1:F:1011:MET:HG2	2.52	0.41
1:A:143:ILE:HG22	1:A:286:ALA:HB2	2.02	0.41
1:A:182:TYR:HA	1:A:182:TYR:HD1	1.66	0.41
1:A:714:THR:HB	1:A:830:GLN:HB2	2.03	0.41
1:B:373:PRO:O	1:B:376:LEU:HB2	2.20	0.41
1:B:524:THR:O	1:B:527:TYR:HB3	2.20	0.41
1:C:725:PRO:HG3	1:C:811:TYR:HE1	1.85	0.41
1:D:61:VAL:CG2	1:D:122:VAL:HG21	2.42	0.41
1:D:822:LEU:HA	1:D:823:PRO:HD3	1.95	0.41
1:D:932:LEU:HD23	1:D:932:LEU:HA	1.75	0.41
1:E:108:GLN:HA	1:E:129:VAL:HG21	2.03	0.41
1:E:357:LEU:O	1:E:358:PHE:HD1	2.04	0.41
1:E:868:LEU:HD23	1:E:868:LEU:HA	1.73	0.41
1:F:45:ILE:H	1:F:45:ILE:HG13	1.54	0.41
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	2.03	0.41
1:A:158:VAL:HG22	1:A:162:MET:HE1	2.02	0.41
1:A:475:VAL:HA	1:A:478:MET:CE	2.51	0.41
1:B:1038:GLU:HG3	1:B:1040:ILE:HB	2.01	0.41
1:B:166:ILE:CD1	1:B:310:LEU:HD13	2.51	0.41
1:B:80:SER:HB3	1:B:818:ARG:HB2	2.03	0.41
1:B:682:PHE:HB3	1:B:827:ILE:HB	2.02	0.41
1:C:453:PHE:CD2	1:C:456:MET:HE2	2.56	0.41
1:C:504:ASP:C	1:C:506:GLY:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:THR:H	1:C:587:THR:HG23	1.62	0.41
1:C:944:LEU:HD13	1:C:975:ILE:HG12	2.03	0.41
1:D:959:GLY:HA2	1:D:1039:ASP:HA	2.02	0.41
1:D:531:VAL:HB	1:D:965:LEU:HD21	2.02	0.41
1:D:659:LYS:HD3	1:D:659:LYS:HA	1.76	0.41
1:D:888:LEU:HD13	1:D:898:PRO:O	2.21	0.41
1:E:353:LEU:C	1:E:355:MET:N	2.72	0.41
1:E:6:ILE:HG23	1:E:494:ALA:HB2	2.03	0.41
1:D:225:VAL:H	1:E:781:MET:CE	2.34	0.41
1:F:1041:GLU:OE1	1:F:1044:HIS:ND1	2.54	0.41
1:D:754:TRP:CE3	1:F:234:ILE:HD11	2.56	0.41
1:F:559:LEU:HA	1:F:560:PRO:HD2	1.80	0.41
1:A:375:VAL:CG2	1:A:481:SER:HA	2.51	0.41
1:A:728:LYS:HE3	1:A:730:ASP:HB2	2.03	0.41
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.53	0.41
1:A:957:GLY:O	1:A:1041:GLU:HA	2.21	0.41
1:B:3:ASN:O	1:B:6:ILE:HB	2.21	0.41
1:C:563:PHE:HB2	1:C:866:GLU:CG	2.50	0.41
1:C:882:ILE:HG22	1:C:886:LEU:HD22	2.02	0.41
1:D:185:ARG:HA	1:D:185:ARG:HD3	1.95	0.41
1:D:189:ASN:OD1	1:D:190:PRO:HD2	2.21	0.41
1:D:209:ALA:O	1:D:237:GLN:NE2	2.53	0.41
1:D:340:VAL:HG22	1:D:396:PHE:CE2	2.56	0.41
1:E:949:ALA:CB	1:E:1026:PHE:HE2	2.32	0.41
1:E:407:ASP:OD2	1:E:940:LYS:HD3	2.20	0.41
1:E:43:VAL:HG13	1:E:130:GLU:O	2.21	0.41
1:F:393:LEU:HD12	1:F:469:GLN:HG3	2.02	0.41
1:F:6:ILE:C	1:F:8:ARG:H	2.23	0.41
1:F:905:VAL:CG1	1:F:935:ILE:HG12	2.50	0.41
1:A:81:ASN:O	1:A:88:VAL:HA	2.21	0.41
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	2.02	0.41
1:B:1041:GLU:HB2	1:B:1042:HIS:H	1.71	0.41
1:B:108:GLN:HE22	1:C:112:GLN:CB	2.29	0.41
1:B:448:VAL:HG13	1:B:884:VAL:HG13	2.03	0.41
1:B:375:VAL:HG22	1:B:484:VAL:HG21	2.02	0.41
1:C:373:PRO:O	1:C:377:LEU:N	2.49	0.41
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.55	0.41
1:C:850:LYS:O	1:C:850:LYS:HG3	2.21	0.41
1:D:405:LEU:HD22	1:D:481:SER:HB2	2.02	0.41
1:D:800:PRO:HG2	1:D:803:ALA:HB2	2.02	0.41
1:D:84:SER:HB3	1:D:814:PRO:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:878:ALA:O	1:D:882:ILE:HG12	2.19	0.41
1:E:249:ILE:HD13	1:E:262:LEU:HD22	2.03	0.41
1:E:162:MET:CE	1:E:323:ILE:HD11	2.51	0.41
1:E:682:PHE:CE1	1:E:857:TYR:HB2	2.56	0.41
1:F:462:SER:O	1:F:466:ILE:HG12	2.21	0.41
1:F:463:THR:HG23	1:F:925:VAL:CG2	2.50	0.41
1:F:746:ILE:HG13	1:F:747:ASN:H	1.86	0.41
1:A:1042:HIS:HB3	1:A:1043:SER:H	1.75	0.41
1:A:188:MET:HA	1:A:266:ALA:HB2	2.03	0.41
1:A:393:LEU:HB3	1:A:470:PHE:CE1	2.56	0.41
1:B:415:ASN:HD22	1:B:434:SER:CB	2.33	0.41
1:B:695:LEU:HD12	1:B:825:MET:HG3	2.02	0.41
1:C:188:MET:HB3	1:C:193:LEU:HD11	2.02	0.41
1:C:449:LEU:HD11	1:C:937:LEU:CD2	2.50	0.41
1:D:188:MET:HE3	1:D:789:TRP:CH2	2.56	0.41
1:D:325:TYR:HA	1:D:326:PRO:HD2	1.88	0.41
1:D:361:ASN:HD21	1:D:363:ARG:HG2	1.85	0.41
1:D:451:ALA:O	1:D:880:SER:OG	2.32	0.41
1:D:455:PRO:HG2	1:D:880:SER:CB	2.47	0.41
1:D:687:GLN:HA	1:D:822:LEU:HD13	2.03	0.41
1:E:445:ILE:HG13	1:E:446:ALA:N	2.35	0.41
1:E:605:ASN:O	1:E:632:LYS:HG3	2.21	0.41
1:F:1041:GLU:HB3	1:F:1042:HIS:CB	2.39	0.41
1:F:732:ASP:HB3	1:F:735:LYS:HG3	2.02	0.41
1:F:776:GLU:HB2	1:F:779:TYR:HD1	1.84	0.41
1:A:525:HIS:CD2	1:A:525:HIS:O	2.74	0.40
1:B:166:ILE:HA	1:B:166:ILE:HD12	1.71	0.40
1:B:207:ILE:HG12	1:B:249:ILE:CD1	2.50	0.40
1:B:682:PHE:C	1:B:682:PHE:CD2	2.95	0.40
1:B:905:VAL:HB	1:B:906:PRO:HD3	2.03	0.40
1:C:407:ASP:O	1:C:411:VAL:HG23	2.21	0.40
1:C:454:VAL:HB	1:C:455:PRO:HD3	2.03	0.40
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.87	0.40
1:D:150:THR:HB	1:D:151:GLN:NE2	2.36	0.40
1:D:309:GLU:O	1:D:312:LYS:HB2	2.21	0.40
1:E:242:SER:O	1:E:246:PHE:HD1	2.04	0.40
1:E:252:LYS:HE2	1:E:252:LYS:HB3	1.83	0.40
1:E:47:ALA:N	1:E:88:VAL:O	2.46	0.40
1:F:172:VAL:HG13	1:F:291:ILE:HG23	2.03	0.40
1:F:445:ILE:HG12	1:F:940:LYS:HG3	2.03	0.40
1:A:244:GLU:C	1:A:246:PHE:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:CD2	1:A:565:PRO:HD2	2.47	0.40
1:B:360:GLN:HB3	1:B:513:PHE:CZ	2.56	0.40
1:B:108:GLN:CD	1:C:112:GLN:HG3	2.42	0.40
1:C:61:VAL:HG22	1:C:119:PRO:HD2	2.01	0.40
1:A:781:MET:SD	1:C:225:VAL:HG13	2.61	0.40
1:C:344:LEU:HA	1:C:399:VAL:HG22	2.02	0.40
1:C:872:GLN:C	1:C:874:PRO:HD2	2.41	0.40
1:C:932:LEU:HA	1:C:932:LEU:HD23	1.81	0.40
1:D:149:MET:HB2	1:D:153:ASP:HB3	2.04	0.40
1:D:210:GLN:OE1	1:D:249:ILE:HG23	2.20	0.40
1:D:6:ILE:CD1	1:D:432:ARG:HE	2.34	0.40
1:D:5:PHE:CD2	1:D:487:ILE:HG23	2.56	0.40
1:D:913:LEU:HA	1:D:913:LEU:HD23	1.96	0.40
1:E:756:GLY:HA2	1:E:774:MET:HG3	2.03	0.40
1:F:120:GLN:HA	1:F:123:GLN:HB2	2.03	0.40
1:F:412:VAL:O	1:F:416:VAL:HG23	2.21	0.40
1:F:453:PHE:CD1	1:F:453:PHE:N	2.89	0.40
1:F:453:PHE:HD1	1:F:453:PHE:N	2.19	0.40
1:A:1040:ILE:HG23	1:A:1041:GLU:H	1.86	0.40
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.53	0.40
1:A:538:THR:HG23	1:A:542:LEU:HD13	2.03	0.40
1:B:307:ARG:NH1	1:B:328:ASP:OD2	2.50	0.40
1:B:58:GLN:HG2	1:B:59:ASP:OD1	2.21	0.40
1:B:717:ARG:HD2	1:B:828:LEU:HB2	2.04	0.40
1:B:699:ARG:HH11	1:B:825:MET:HE1	1.86	0.40
1:B:841:MET:O	1:B:845:GLU:HG3	2.21	0.40
1:C:189:ASN:OD1	1:C:190:PRO:HD2	2.21	0.40
1:C:201:VAL:O	1:C:204:ILE:HB	2.21	0.40
1:C:488:LEU:O	1:C:491:ALA:HB3	2.21	0.40
1:C:671:ILE:HG21	1:C:674:LEU:HD12	2.03	0.40
1:D:409:ALA:O	1:D:413:VAL:HG23	2.22	0.40
1:D:429:GLU:HG2	1:D:429:GLU:H	1.44	0.40
1:D:47:ALA:HB3	1:D:88:VAL:CG1	2.52	0.40
1:D:551:GLY:O	1:D:555:LEU:HB2	2.21	0.40
1:D:650:ARG:O	1:D:653:ARG:HB3	2.21	0.40
1:D:888:LEU:CB	1:D:898:PRO:HB3	2.51	0.40
1:E:167:SER:OG	1:E:175:VAL:HG21	2.22	0.40
1:E:189:ASN:HB3	1:E:192:GLU:CB	2.47	0.40
1:E:24:GLY:O	1:E:28:LEU:HB2	2.20	0.40
1:E:680:PHE:HB2	1:E:863:SER:OG	2.21	0.40
1:E:992:SER:O	1:E:997:SER:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:746:ILE:HG22	1:F:791:VAL:HG11	2.03	0.40
1:A:492:LEU:HD22	1:A:496:MET:SD	2.62	0.40
1:A:74:ASN:O	1:A:94:PHE:HD2	2.04	0.40
1:B:492:LEU:O	1:B:496:MET:HG2	2.21	0.40
1:C:725:PRO:HG3	1:C:811:TYR:CE1	2.57	0.40
1:D:199:THR:HG21	1:D:791:VAL:HA	2.03	0.40
1:E:383:LEU:HA	1:E:383:LEU:HD23	1.83	0.40
1:E:588:GLN:HG3	1:E:592:ASN:HD21	1.86	0.40
1:E:602:GLU:OE1	1:E:650:ARG:HD2	2.22	0.40
1:E:805:SER:OG	1:E:805:SER:O	2.37	0.40
1:F:58:GLN:HG3	1:F:82:SER:OG	2.21	0.40
1:F:674:LEU:CD2	1:F:861:GLY:HA2	2.51	0.40
1:A:909:VAL:HG22	1:A:931:LEU:HD21	2.04	0.40
1:B:427:PRO:CD	1:B:499:PRO:HB3	2.52	0.40
1:C:165:ALA:HB3	1:C:313:MET:CE	2.50	0.40
1:C:246:PHE:O	1:C:249:ILE:HG13	2.22	0.40
1:C:501:ALA:O	1:C:504:ASP:HB2	2.20	0.40
1:C:510:LYS:HG2	1:C:511:GLY:N	2.37	0.40
1:C:948:PHE:HB3	1:C:970:MET:CE	2.52	0.40
1:C:991:ILE:O	1:C:991:ILE:HD13	2.21	0.40
1:C:926:TYR:HE1	1:C:999:ALA:HA	1.87	0.40
1:D:287:SER:OG	1:D:288:GLY:N	2.50	0.40
1:D:537:SER:O	1:D:537:SER:OG	2.38	0.40
1:D:712:MET:O	1:D:832:ALA:N	2.46	0.40
1:D:730:ASP:HB2	1:D:808:ARG:NH2	2.37	0.40
1:D:964:THR:O	1:D:967:ALA:HB3	2.22	0.40
1:E:1017:LEU:HD12	1:E:1017:LEU:HA	1.70	0.40
1:E:154:ILE:O	1:E:157:TYR:N	2.55	0.40
1:E:162:MET:HA	1:E:313:MET:HE1	2.03	0.40
1:E:36:PRO:HD3	1:E:391:ASN:CG	2.42	0.40
1:E:396:PHE:O	1:E:400:LEU:HB2	2.20	0.40
1:E:415:ASN:ND2	1:E:437:GLN:OE1	2.47	0.40
1:E:453:PHE:HB3	1:E:475:VAL:HG22	2.02	0.40
1:E:792:ARG:HB2	1:E:798:MET:SD	2.61	0.40
1:E:834:GLY:C	1:E:835:LYS:HE2	2.42	0.40
1:E:445:ILE:CG1	1:E:940:LYS:HE3	2.48	0.40
1:F:222:THR:HA	1:F:223:PRO:HA	1.90	0.40
1:F:435:MET:HE1	1:F:490:PRO:HB3	2.04	0.40
1:F:522:LYS:O	1:F:525:HIS:N	2.54	0.40
1:F:535:LEU:HA	1:F:535:LEU:HD23	1.72	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-



metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:529:ASP:OD1	1:F:529:ASP:OD2[2_555]	2.08	0.12

## 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	1040/1049 (99%)	939 (90%)	82 (8%)	19 (2%)	8	37
1	B	1044/1049 (100%)	925 (89%)	92 (9%)	27 (3%)	5	28
1	C	1042/1049 (99%)	931 (89%)	91 (9%)	20 (2%)	8	36
1	D	1040/1049 (99%)	941 (90%)	83 (8%)	16 (2%)	10	41
1	E	1040/1049 (99%)	919 (88%)	97 (9%)	24 (2%)	6	31
1	F	1044/1049 (100%)	936 (90%)	87 (8%)	21 (2%)	7	34
All	All	6250/6294 (99%)	5591 (90%)	532 (8%)	127 (2%)	7	34

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	675	GLY
1	A	1038	GLU
1	B	163	LYS
1	B	360	GLN
1	B	509	LYS
1	B	516	PHE
1	B	644	VAL
1	B	673	GLU
1	B	677	ALA
1	B	1033	PHE
1	B	1038	GLU
1	B	1040	ILE

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Mol	Chain	Res	Type
1	B	1041	GLU
1	B	1046	VAL
1	C	134	SER
1	C	147	GLY
1	C	163	LYS
1	C	360	GLN
1	C	509	LYS
1	C	691	GLY
1	C	1034	SER
1	C	1038	GLU
1	D	163	LYS
1	D	360	GLN
1	D	508	GLY
1	D	511	GLY
1	D	644	VAL
1	D	1035	ARG
1	D	1037	ASN
1	E	163	LYS
1	E	354	VAL
1	E	360	GLN
1	E	536	ARG
1	E	632	LYS
1	E	644	VAL
1	E	673	GLU
1	E	674	LEU
1	E	893	GLU
1	E	1035	ARG
1	F	134	SER
1	F	147	GLY
1	F	360	GLN
1	F	644	VAL
1	F	691	GLY
1	F	1039	ASP
1	F	1042	HIS
1	F	1045	THR
1	F	1046	VAL
1	A	507	GLU
1	A	644	VAL
1	A	677	ALA
1	A	751	GLY
1	A	1040	ILE
1	B	295	THR

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Mol	Chain	Res	Type
1	B	508	GLY
1	B	751	GLY
1	B	1037	ASN
1	C	133	SER
1	C	644	VAL
1	C	689	GLY
1	C	751	GLY
1	C	752	ALA
1	C	893	GLU
1	C	1042	HIS
1	D	675	GLY
1	D	751	GLY
1	D	752	ALA
1	D	992	SER
1	D	1033	PHE
1	D	1040	ILE
1	E	132	SER
1	E	508	GLY
1	E	672	VAL
1	E	751	GLY
1	E	1040	ILE
1	F	6	ILE
1	F	163	LYS
1	F	751	GLY
1	F	1043	SER
1	A	37	THR
1	A	752	ALA
1	A	907	LEU
1	A	1035	ARG
1	B	41	PRO
1	B	358	PHE
1	B	638	PRO
1	B	672	VAL
1	B	833	PRO
1	B	960	LEU
1	C	1033	PHE
1	C	1037	ASN
1	C	1041	GLU
1	D	960	LEU
1	E	752	ALA
1	E	907	LEU
1	E	993	THR

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Mol	Chain	Res	Type
1	F	133	SER
1	F	146	ASP
1	F	148	THR
1	A	163	LYS
1	A	505	HIS
1	A	688	ALA
1	A	1033	PHE
1	B	1044	HIS
1	D	907	LEU
1	E	195	LYS
1	E	1042	HIS
1	F	638	PRO
1	F	907	LEU
1	B	40	PRO
1	B	752	ALA
1	E	638	PRO
1	E	1037	ASN
1	F	960	LEU
1	A	195	LYS
1	A	418	ARG
1	A	638	PRO
1	B	907	LEU
1	E	353	LEU
1	F	923	ASN
1	B	870	GLY
1	C	511	GLY
1	E	833	PRO
1	C	217	GLY
1	D	638	PRO
1	F	511	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	845/852 (99%)	789 (93%)	56 (7%)	16	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	849/852 (100%)	735 (87%)	114 (13%)	4	17
1	C	847/852 (99%)	769 (91%)	78 (9%)	9	31
1	D	845/852 (99%)	786 (93%)	59 (7%)	15	45
1	E	845/852 (99%)	735 (87%)	110 (13%)	4	18
1	F	849/852 (100%)	783 (92%)	66 (8%)	12	40
All	All	5080/5112 (99%)	4597 (90%)	483 (10%)	8	30

All (483) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	11	PHE
1	A	38	ILE
1	A	44	THR
1	A	45	ILE
1	A	60	THR
1	A	146	ASP
1	A	205	THR
1	A	253	VAL
1	A	255	GLN
1	A	267	LYS
1	A	270	LEU
1	A	336	SER
1	A	349	ILE
1	A	350	LEU
1	A	355	MET
1	A	362	PHE
1	A	429	GLU
1	A	434	SER
1	A	437	GLN
1	A	452	VAL
1	A	472	ILE
1	A	493	CYS
1	A	502	LYS
1	A	512	PHE
1	A	523	SER
1	A	528	THR
1	A	530	SER
1	A	538	THR
1	A	559	LEU

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Mol	Chain	Res	Type
1	A	561	SER
1	A	564	LEU
1	A	578	LEU
1	A	602	GLU
1	A	603	LYS
1	A	608	SER
1	A	634	TRP
1	A	636	ASP
1	A	659	LYS
1	A	662	MET
1	A	682	PHE
1	A	716	VAL
1	A	741	VAL
1	A	804	PHE
1	A	922	THR
1	A	931	LEU
1	A	947	GLU
1	A	961	ILE
1	A	970	MET
1	A	971	ARG
1	A	975	ILE
1	A	1036	LYS
1	A	1038	GLU
1	A	1039	ASP
1	A	1041	GLU
1	A	1042	HIS
1	B	6	ILE
1	B	11	PHE
1	B	13	TRP
1	B	17	ILE
1	B	27	ILE
1	B	28	LEU
1	B	29	LYS
1	B	32	VAL
1	B	43	VAL
1	B	49	TYR
1	B	53	ASP
1	B	58	GLN
1	B	79	SER
1	B	105	VAL
1	B	128	SER
1	B	153	ASP

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Mol	Chain	Res	Type
1	B	166	ILE
1	B	175	VAL
1	B	180	SER
1	B	213	GLN
1	B	255	GLN
1	B	259	ARG
1	B	276	ASP
1	B	289	LEU
1	B	293	LEU
1	B	295	THR
1	B	298	ASN
1	B	314	GLU
1	B	322	LYS
1	B	329	THR
1	B	336	SER
1	B	348	ILE
1	B	350	LEU
1	B	352	PHE
1	B	355	MET
1	B	358	PHE
1	B	360	GLN
1	B	365	THR
1	B	374	VAL
1	B	383	LEU
1	B	400	LEU
1	B	404	LEU
1	B	473	THR
1	B	475	VAL
1	B	480	LEU
1	B	482	VAL
1	B	489	THR
1	B	507	GLU
1	B	523	SER
1	B	524	THR
1	B	526	HIS
1	B	534	ILE
1	B	555	LEU
1	B	558	ARG
1	B	559	LEU
1	B	561	SER
1	B	563	PHE
1	B	564	LEU

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Mol	Chain	Res	Type
1	B	569	GLN
1	B	575	MET
1	B	578	LEU
1	B	599	LEU
1	B	626	ILE
1	B	634	TRP
1	B	636	ASP
1	B	640	GLU
1	B	642	ASN
1	B	662	MET
1	B	667	ASN
1	B	668	LEU
1	B	672	VAL
1	B	682	PHE
1	B	683	GLU
1	B	687	GLN
1	B	690	LEU
1	B	695	LEU
1	B	703	LEU
1	B	708	LYS
1	B	711	ASP
1	B	715	SER
1	B	717	ARG
1	B	741	VAL
1	B	743	ILE
1	B	759	VAL
1	B	761	ASP
1	B	775	SER
1	B	788	ASP
1	B	806	SER
1	B	808	ARG
1	B	835	LYS
1	B	853	THR
1	B	862	MET
1	B	869	SER
1	B	871	ASN
1	B	886	LEU
1	B	919	ARG
1	B	958	LYS
1	B	965	LEU
1	B	968	VAL
1	B	970	MET

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Mol	Chain	Res	Type
1	B	975	ILE
1	B	978	THR
1	B	980	LEU
1	B	1015	THR
1	B	1032	ARG
1	B	1035	ARG
1	B	1036	LYS
1	B	1038	GLU
1	B	1039	ASP
1	B	1040	ILE
1	B	1041	GLU
1	B	1042	HIS
1	B	1045	THR
1	B	1046	VAL
1	C	3	ASN
1	C	6	ILE
1	C	11	PHE
1	C	27	ILE
1	C	28	LEU
1	C	48	SER
1	C	49	TYR
1	C	88	VAL
1	C	92	LEU
1	C	108	GLN
1	C	120	GLN
1	C	145	THR
1	C	148	THR
1	C	151	GLN
1	C	239	ARG
1	C	253	VAL
1	C	255	GLN
1	C	275	TYR
1	C	300	LEU
1	C	353	LEU
1	C	358	PHE
1	C	360	GLN
1	C	363	ARG
1	C	392	THR
1	C	447	MET
1	C	452	VAL
1	C	463	THR
1	C	472	ILE

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Mol	Chain	Res	Type
1	C	476	SER
1	C	482	VAL
1	C	510	LYS
1	C	513	PHE
1	C	526	HIS
1	C	538	THR
1	C	540	ARG
1	C	555	LEU
1	C	559	LEU
1	C	564	LEU
1	C	602	GLU
1	C	608	SER
1	C	624	THR
1	C	634	TRP
1	C	649	MET
1	C	659	LYS
1	C	662	MET
1	C	666	PHE
1	C	673	GLU
1	C	678	THR
1	C	694	LYS
1	C	695	LEU
1	C	696	THR
1	C	721	LEU
1	C	733	GLN
1	C	734	GLU
1	C	741	VAL
1	C	746	ILE
1	C	748	THR
1	C	804	PHE
1	C	808	ARG
1	C	843	LEU
1	C	847	LEU
1	C	860	THR
1	C	865	GLN
1	C	868	LEU
1	C	876	LEU
1	C	886	LEU
1	C	887	CYS
1	C	914	LEU
1	C	947	GLU
1	C	950	LYS

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Mol	Chain	Res	Type
1	C	971	ARG
1	C	975	ILE
1	C	980	LEU
1	C	991	ILE
1	C	1033	PHE
1	C	1040	ILE
1	C	1041	GLU
1	C	1044	HIS
1	D	3	ASN
1	D	49	TYR
1	D	101	ASP
1	D	102	ILE
1	D	146	ASP
1	D	151	GLN
1	D	152	GLU
1	D	253	VAL
1	D	276	ASP
1	D	280	GLU
1	D	336	SER
1	D	353	LEU
1	D	355	MET
1	D	357	LEU
1	D	360	GLN
1	D	362	PHE
1	D	400	LEU
1	D	429	GLU
1	D	434	SER
1	D	462	SER
1	D	483	LEU
1	D	493	CYS
1	D	502	LYS
1	D	505	HIS
1	D	523	SER
1	D	526	HIS
1	D	538	THR
1	D	559	LEU
1	D	563	PHE
1	D	573	MET
1	D	578	LEU
1	D	602	GLU
1	D	603	LYS
1	D	608	SER

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Mol	Chain	Res	Type
1	D	624	THR
1	D	634	TRP
1	D	657	GLN
1	D	659	LYS
1	D	662	MET
1	D	673	GLU
1	D	697	GLN
1	D	717	ARG
1	D	733	GLN
1	D	741	VAL
1	D	748	THR
1	D	797	GLN
1	D	804	PHE
1	D	843	LEU
1	D	901	VAL
1	D	931	LEU
1	D	951	ASP
1	D	961	ILE
1	D	968	VAL
1	D	971	ARG
1	D	975	ILE
1	D	1035	ARG
1	D	1036	LYS
1	D	1037	ASN
1	D	1038	GLU
1	E	3	ASN
1	E	10	ILE
1	E	17	ILE
1	E	28	LEU
1	E	45	ILE
1	E	49	TYR
1	E	58	GLN
1	E	60	THR
1	E	82	SER
1	E	87	THR
1	E	91	THR
1	E	93	THR
1	E	102	ILE
1	E	105	VAL
1	E	110	LYS
1	E	113	LEU
1	E	117	LEU

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Mol	Chain	Res	Type
1	E	128	SER
1	E	146	ASP
1	E	153	ASP
1	E	156	ASP
1	E	166	ILE
1	E	174	ASP
1	E	175	VAL
1	E	205	THR
1	E	213	GLN
1	E	218	GLN
1	E	229	GLN
1	E	233	SER
1	E	238	THR
1	E	249	ILE
1	E	250	LEU
1	E	253	VAL
1	E	255	GLN
1	E	259	ARG
1	E	268	ILE
1	E	276	ASP
1	E	280	GLU
1	E	295	THR
1	E	298	ASN
1	E	300	LEU
1	E	310	LEU
1	E	321	LEU
1	E	323	ILE
1	E	329	THR
1	E	330	THR
1	E	352	PHE
1	E	355	MET
1	E	365	THR
1	E	372	VAL
1	E	400	LEU
1	E	404	LEU
1	E	418	ARG
1	E	432	ARG
1	E	445	ILE
1	E	449	LEU
1	E	450	SER
1	E	456	MET
1	E	459	PHE

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Mol	Chain	Res	Type
1	E	480	LEU
1	E	482	VAL
1	E	507	GLU
1	E	512	PHE
1	E	558	ARG
1	E	563	PHE
1	E	564	LEU
1	E	593	GLU
1	E	607	GLU
1	E	608	SER
1	E	613	ASN
1	E	634	TRP
1	E	642	ASN
1	E	653	ARG
1	E	659	LYS
1	E	673	GLU
1	E	683	GLU
1	E	687	GLN
1	E	690	LEU
1	E	694	LYS
1	E	703	LEU
1	E	708	LYS
1	E	714	THR
1	E	717	ARG
1	E	741	VAL
1	E	748	THR
1	E	767	ARG
1	E	804	PHE
1	E	806	SER
1	E	817	GLU
1	E	835	LYS
1	E	844	MET
1	E	857	TYR
1	E	865	GLN
1	E	871	ASN
1	E	886	LEU
1	E	907	LEU
1	E	914	LEU
1	E	917	THR
1	E	931	LEU
1	E	937	LEU
1	E	947	GLU

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Mol	Chain	Res	Type
1	E	958	LYS
1	E	961	ILE
1	E	987	MET
1	E	1001	ASN
1	E	1017	LEU
1	E	1021	PHE
1	E	1030	ARG
1	E	1036	LYS
1	E	1042	HIS
1	F	3	ASN
1	F	6	ILE
1	F	7	ASP
1	F	28	LEU
1	F	34	GLN
1	F	45	ILE
1	F	48	SER
1	F	49	TYR
1	F	60	THR
1	F	104	GLN
1	F	112	GLN
1	F	120	GLN
1	F	148	THR
1	F	151	GLN
1	F	182	TYR
1	F	243	THR
1	F	276	ASP
1	F	280	GLU
1	F	330	THR
1	F	335	ILE
1	F	392	THR
1	F	429	GLU
1	F	434	SER
1	F	439	GLN
1	F	452	VAL
1	F	456	MET
1	F	472	ILE
1	F	476	SER
1	F	481	SER
1	F	482	VAL
1	F	493	CYS
1	F	512	PHE
1	F	526	HIS

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Mol	Chain	Res	Type
1	F	534	ILE
1	F	578	LEU
1	F	604	ASN
1	F	608	SER
1	F	626	ILE
1	F	634	TRP
1	F	643	LYS
1	F	649	MET
1	F	666	PHE
1	F	674	LEU
1	F	694	LYS
1	F	703	LEU
1	F	734	GLU
1	F	804	PHE
1	F	808	ARG
1	F	847	LEU
1	F	860	THR
1	F	864	TYR
1	F	865	GLN
1	F	868	LEU
1	F	876	LEU
1	F	887	CYS
1	F	895	TRP
1	F	918	PHE
1	F	947	GLU
1	F	950	LYS
1	F	958	LYS
1	F	961	ILE
1	F	990	VAL
1	F	991	ILE
1	F	1011	MET
1	F	1015	THR
1	F	1042	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	231	ASN
1	A	584	GLN
1	B	63	GLN
1	B	108	GLN

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Mol	Chain	Res	Type
1	B	189	ASN
1	B	213	GLN
1	B	584	GLN
1	B	709	HIS
1	B	760	ASN
1	B	865	GLN
1	B	1037	ASN
1	C	67	GLN
1	C	70	ASN
1	C	928	GLN
1	D	151	GLN
1	D	505	HIS
1	E	34	GLN
1	E	112	GLN
1	E	123	GLN
1	E	125	GLN
1	E	189	ASN
1	E	211	ASN
1	E	588	GLN
1	E	592	ASN
1	E	613	ASN
1	E	760	ASN
1	F	63	GLN
1	F	67	GLN
1	F	70	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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	LMT	F	1101	-	36,36,36	1.97	10 (27%)	47,47,47	1.43	7 (14%)
2	LMT	B	1101	-	36,36,36	1.81	9 (25%)	47,47,47	1.32	8 (17%)
2	LMT	C	1101	-	36,36,36	1.75	7 (19%)	47,47,47	1.59	9 (19%)
2	LMT	E	1101	-	36,36,36	1.85	11 (30%)	47,47,47	1.46	6 (12%)
2	LMT	A	1101	-	36,36,36	1.85	10 (27%)	47,47,47	1.24	5 (10%)
2	LMT	D	1101	-	36,36,36	1.77	10 (27%)	47,47,47	1.37	6 (12%)

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	LMT	F	1101	-	-	15/21/61/61	0/2/2/2
2	LMT	B	1101	-	1/1/10/10	12/21/61/61	0/2/2/2
2	LMT	C	1101	-	1/1/10/10	14/21/61/61	0/2/2/2
2	LMT	E	1101	-	-	10/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	8/21/61/61	0/2/2/2
2	LMT	D	1101	-	-	16/21/61/61	0/2/2/2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1101	LMT	O5'-C5'	4.73	1.55	1.44
2	F	1101	LMT	O1'-C1'	4.59	1.48	1.40
2	A	1101	LMT	O5'-C5'	4.41	1.55	1.44
2	E	1101	LMT	O5'-C5'	4.10	1.54	1.44
2	E	1101	LMT	O1'-C1'	4.05	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1101	LMT	O5B-C1B	3.98	1.52	1.41
2	F	1101	LMT	O5'-C1'	3.83	1.51	1.41
2	B	1101	LMT	O1'-C1'	3.82	1.46	1.40
2	C	1101	LMT	O5'-C5'	3.81	1.53	1.44
2	B	1101	LMT	O5B-C1B	3.80	1.51	1.41
2	B	1101	LMT	O5'-C5'	3.78	1.53	1.44
2	C	1101	LMT	O5B-C1B	3.77	1.51	1.41
2	D	1101	LMT	O5'-C5'	3.68	1.53	1.44
2	D	1101	LMT	C6'-C5'	-3.62	1.39	1.51
2	A	1101	LMT	O5B-C1B	3.59	1.51	1.41
2	C	1101	LMT	O1'-C1'	3.58	1.46	1.40
2	C	1101	LMT	C6'-C5'	-3.52	1.40	1.51
2	E	1101	LMT	O5B-C1B	3.45	1.50	1.41
2	D	1101	LMT	O5B-C1B	3.38	1.50	1.41
2	B	1101	LMT	C6'-C5'	-3.34	1.40	1.51
2	E	1101	LMT	O5'-C1'	3.29	1.50	1.41
2	B	1101	LMT	O3B-C3B	3.27	1.50	1.43
2	F	1101	LMT	C6'-C5'	-3.25	1.40	1.51
2	A	1101	LMT	C6'-C5'	-3.18	1.41	1.51
2	A	1101	LMT	O5'-C1'	3.14	1.49	1.41
2	C	1101	LMT	O5'-C1'	3.12	1.49	1.41
2	A	1101	LMT	C3'-C2'	-3.10	1.44	1.52
2	C	1101	LMT	C3'-C2'	-3.09	1.44	1.52
2	B	1101	LMT	O5'-C1'	3.06	1.49	1.41
2	D	1101	LMT	O5'-C1'	3.03	1.49	1.41
2	E	1101	LMT	C6'-C5'	-3.02	1.41	1.51
2	D	1101	LMT	O1'-C1'	2.87	1.45	1.40
2	A	1101	LMT	O1'-C1'	2.86	1.45	1.40
2	D	1101	LMT	C3B-C2B	-2.84	1.45	1.52
2	F	1101	LMT	O3B-C3B	2.78	1.49	1.43
2	A	1101	LMT	O3B-C3B	2.66	1.49	1.43
2	C	1101	LMT	O3B-C3B	2.66	1.49	1.43
2	E	1101	LMT	O3B-C3B	2.65	1.49	1.43
2	D	1101	LMT	O3B-C3B	2.64	1.49	1.43
2	E	1101	LMT	C3B-C2B	-2.63	1.45	1.52
2	D	1101	LMT	C3'-C2'	-2.53	1.45	1.52
2	E	1101	LMT	C3'-C2'	-2.44	1.46	1.52
2	F	1101	LMT	C3'-C2'	-2.40	1.46	1.52
2	F	1101	LMT	C3B-C2B	-2.40	1.46	1.52
2	B	1101	LMT	C3'-C2'	-2.33	1.46	1.52
2	F	1101	LMT	O2'-C2'	2.28	1.48	1.43
2	E	1101	LMT	O3'-C3'	2.19	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	LMT	O2'-C2'	2.15	1.48	1.43
2	A	1101	LMT	O3'-C3'	2.14	1.48	1.43
2	A	1101	LMT	C5-C4	2.09	1.63	1.51
2	F	1101	LMT	C5-C4	2.09	1.63	1.51
2	E	1101	LMT	O2'-C2'	2.08	1.47	1.43
2	E	1101	LMT	C5-C4	2.08	1.63	1.51
2	A	1101	LMT	O2'-C2'	2.01	1.47	1.43
2	B	1101	LMT	O3'-C3'	2.01	1.47	1.43
2	D	1101	LMT	C5-C4	2.01	1.62	1.51
2	D	1101	LMT	O2'-C2'	2.01	1.47	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	LMT	C4B-C3B-C2B	4.91	119.39	110.82
2	E	1101	LMT	O5B-C5B-C4B	4.50	117.86	109.69
2	D	1101	LMT	O3B-C3B-C2B	-4.04	101.01	110.35
2	A	1101	LMT	C1B-O1B-C4'	-4.03	107.99	117.96
2	F	1101	LMT	O5B-C5B-C4B	4.02	116.99	109.69
2	E	1101	LMT	C3B-C4B-C5B	3.85	117.10	110.24
2	D	1101	LMT	C1B-O1B-C4'	-3.84	108.46	117.96
2	C	1101	LMT	O5B-C5B-C4B	-3.66	103.05	109.69
2	F	1101	LMT	C1B-O5B-C5B	3.60	120.76	113.69
2	B	1101	LMT	C1-O1'-C1'	3.52	119.67	113.84
2	C	1101	LMT	C3B-C4B-C5B	3.27	116.07	110.24
2	B	1101	LMT	O5B-C5B-C6B	3.07	114.07	106.44
2	C	1101	LMT	C1B-C2B-C3B	3.07	116.38	110.00
2	C	1101	LMT	O5B-C5B-C6B	2.98	113.85	106.44
2	F	1101	LMT	C1'-O5'-C5'	2.97	119.52	113.69
2	F	1101	LMT	C1-O1'-C1'	2.95	118.73	113.84
2	D	1101	LMT	O5B-C5B-C4B	2.89	114.93	109.69
2	A	1101	LMT	C1'-C2'-C3'	-2.84	104.09	110.00
2	F	1101	LMT	O1'-C1'-C2'	2.79	112.66	108.30
2	F	1101	LMT	C1B-O1B-C4'	-2.76	111.13	117.96
2	C	1101	LMT	O3'-C3'-C2'	-2.73	104.04	110.35
2	E	1101	LMT	C1B-O1B-C4'	-2.66	111.37	117.96
2	E	1101	LMT	C1-O1'-C1'	2.53	118.03	113.84
2	E	1101	LMT	C1'-C2'-C3'	2.44	115.08	110.00
2	D	1101	LMT	C4B-C3B-C2B	2.40	115.02	110.82
2	E	1101	LMT	C6B-C5B-C4B	-2.40	107.39	113.00
2	D	1101	LMT	O2B-C2B-C3B	-2.36	104.90	110.35
2	B	1101	LMT	C2'-C3'-C4'	2.35	115.04	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	LMT	C3B-C4B-C5B	2.34	114.42	110.24
2	B	1101	LMT	C1'-C2'-C3'	2.34	114.87	110.00
2	B	1101	LMT	O1'-C1'-C2'	2.31	111.91	108.30
2	A	1101	LMT	O5B-C1B-C2B	2.30	115.21	110.35
2	B	1101	LMT	C6B-C5B-C4B	-2.21	107.83	113.00
2	A	1101	LMT	C4B-C3B-C2B	2.20	114.67	110.82
2	F	1101	LMT	O5'-C5'-C4'	2.12	114.23	109.75
2	C	1101	LMT	O1'-C1'-C2'	2.10	111.58	108.30
2	C	1101	LMT	O4'-C4B-C3B	-2.08	105.54	110.35
2	B	1101	LMT	O2'-C2'-C3'	-2.06	105.58	110.35
2	D	1101	LMT	C3B-C4B-C5B	2.04	113.89	110.24
2	A	1101	LMT	C1B-C2B-C3B	2.02	114.20	110.00
2	C	1101	LMT	O6'-C6'-C5'	-2.01	104.38	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1101	LMT	C3B
2	C	1101	LMT	C3B

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	LMT	O5'-C1'-O1'-C1
2	C	1101	LMT	C2'-C1'-O1'-C1
2	C	1101	LMT	O5'-C1'-O1'-C1
2	E	1101	LMT	C2'-C1'-O1'-C1
2	B	1101	LMT	O5B-C5B-C6B-O6B
2	D	1101	LMT	O5'-C5'-C6'-O6'
2	A	1101	LMT	C2-C3-C4-C5
2	F	1101	LMT	O5B-C5B-C6B-O6B
2	C	1101	LMT	O5B-C5B-C6B-O6B
2	C	1101	LMT	C4B-C5B-C6B-O6B
2	D	1101	LMT	C4'-C5'-C6'-O6'
2	F	1101	LMT	C4'-C5'-C6'-O6'
2	B	1101	LMT	C4B-C5B-C6B-O6B
2	F	1101	LMT	C7-C8-C9-C10
2	B	1101	LMT	C4'-C5'-C6'-O6'
2	E	1101	LMT	O5B-C5B-C6B-O6B
2	F	1101	LMT	C4B-C5B-C6B-O6B
2	A	1101	LMT	C4'-C5'-C6'-O6'
2	B	1101	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
2	D	1101	LMT	O5B-C5B-C6B-O6B
2	E	1101	LMT	O5'-C1'-O1'-C1
2	F	1101	LMT	O5'-C5'-C6'-O6'
2	C	1101	LMT	C4'-C5'-C6'-O6'
2	E	1101	LMT	C4B-C5B-C6B-O6B
2	B	1101	LMT	C2'-C1'-O1'-C1
2	D	1101	LMT	C4B-C5B-C6B-O6B
2	E	1101	LMT	C5-C6-C7-C8
2	A	1101	LMT	O5'-C5'-C6'-O6'
2	E	1101	LMT	C4'-C5'-C6'-O6'
2	C	1101	LMT	O1'-C1-C2-C3
2	A	1101	LMT	O1'-C1-C2-C3
2	B	1101	LMT	O1'-C1-C2-C3
2	E	1101	LMT	O1'-C1-C2-C3
2	F	1101	LMT	O1'-C1-C2-C3
2	B	1101	LMT	C3-C4-C5-C6
2	F	1101	LMT	C3-C4-C5-C6
2	A	1101	LMT	C6-C7-C8-C9
2	A	1101	LMT	C5-C6-C7-C8
2	D	1101	LMT	C2'-C1'-O1'-C1
2	F	1101	LMT	C4-C5-C6-C7
2	B	1101	LMT	C4-C5-C6-C7
2	D	1101	LMT	C3-C4-C5-C6
2	C	1101	LMT	O5'-C5'-C6'-O6'
2	D	1101	LMT	C7-C8-C9-C10
2	C	1101	LMT	C6-C7-C8-C9
2	C	1101	LMT	C2-C1-O1'-C1'
2	D	1101	LMT	C2-C1-O1'-C1'
2	E	1101	LMT	C1-C2-C3-C4
2	F	1101	LMT	C6-C7-C8-C9
2	C	1101	LMT	C11-C10-C9-C8
2	D	1101	LMT	C4-C5-C6-C7
2	D	1101	LMT	C5-C6-C7-C8
2	D	1101	LMT	C11-C10-C9-C8
2	C	1101	LMT	C7-C8-C9-C10
2	B	1101	LMT	C11-C10-C9-C8
2	D	1101	LMT	O5'-C1'-O1'-C1
2	F	1101	LMT	C9-C10-C11-C12
2	C	1101	LMT	C2-C3-C4-C5
2	F	1101	LMT	C1-C2-C3-C4
2	F	1101	LMT	C2-C3-C4-C5
2	D	1101	LMT	C6-C7-C8-C9

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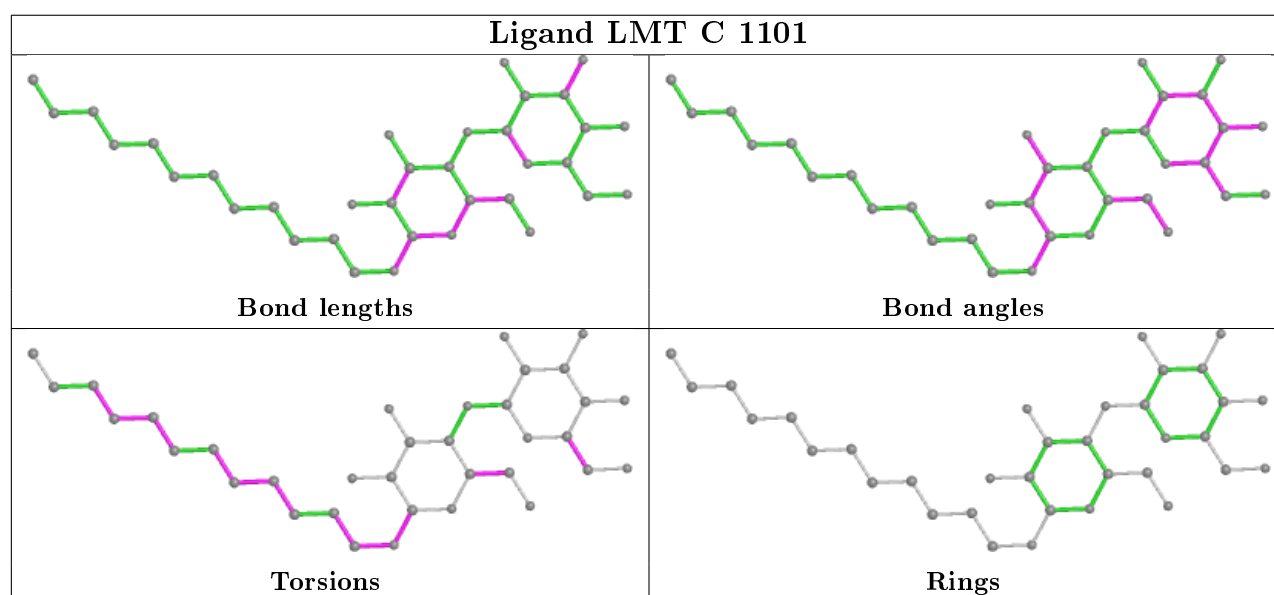
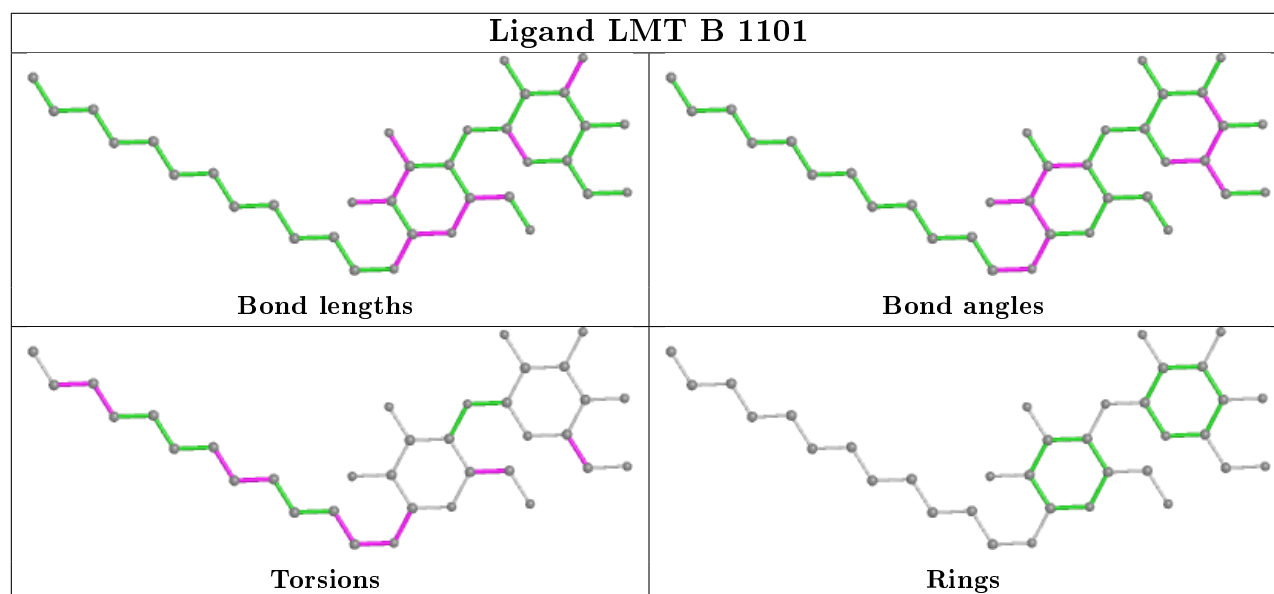
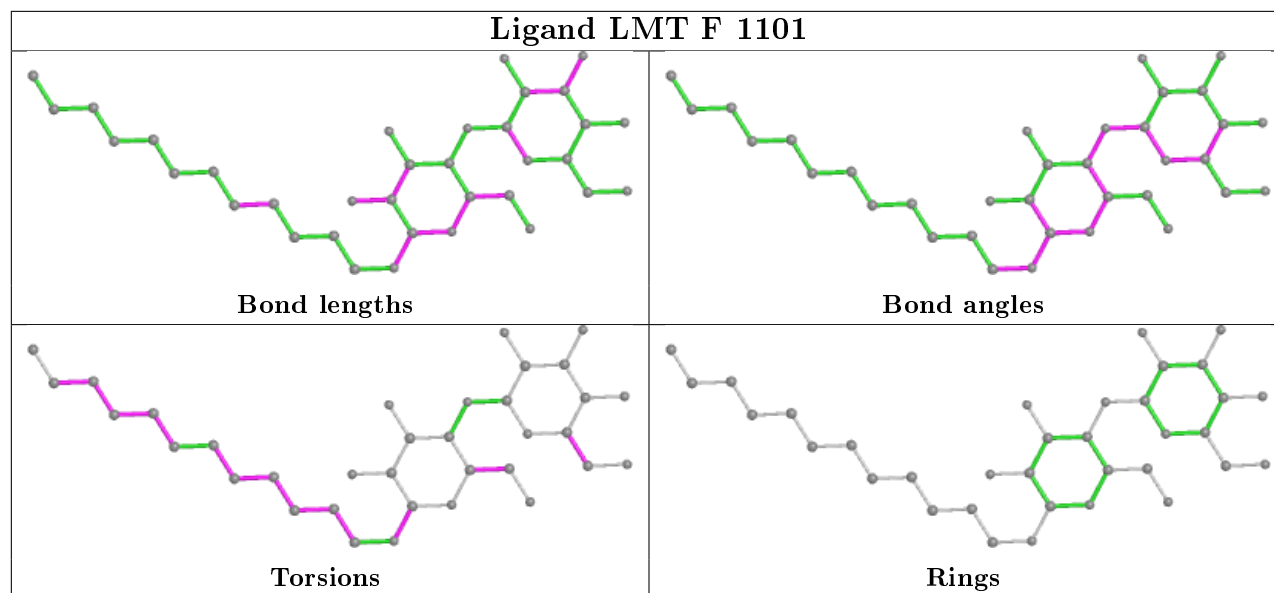
Mol	Chain	Res	Type	Atoms
2	D	1101	LMT	C1-C2-C3-C4
2	E	1101	LMT	O5'-C5'-C6'-O6'
2	A	1101	LMT	C4-C5-C6-C7
2	F	1101	LMT	C2'-C1'-O1'-C1
2	D	1101	LMT	C2-C3-C4-C5
2	D	1101	LMT	O1'-C1-C2-C3
2	B	1101	LMT	C9-C10-C11-C12
2	A	1101	LMT	C3-C4-C5-C6
2	F	1101	LMT	C11-C10-C9-C8
2	E	1101	LMT	C9-C10-C11-C12
2	C	1101	LMT	C4-C5-C6-C7
2	C	1101	LMT	C3-C4-C5-C6
2	B	1101	LMT	C2-C1-O1'-C1'
2	F	1101	LMT	O5'-C1'-O1'-C1

There are no ring outliers.

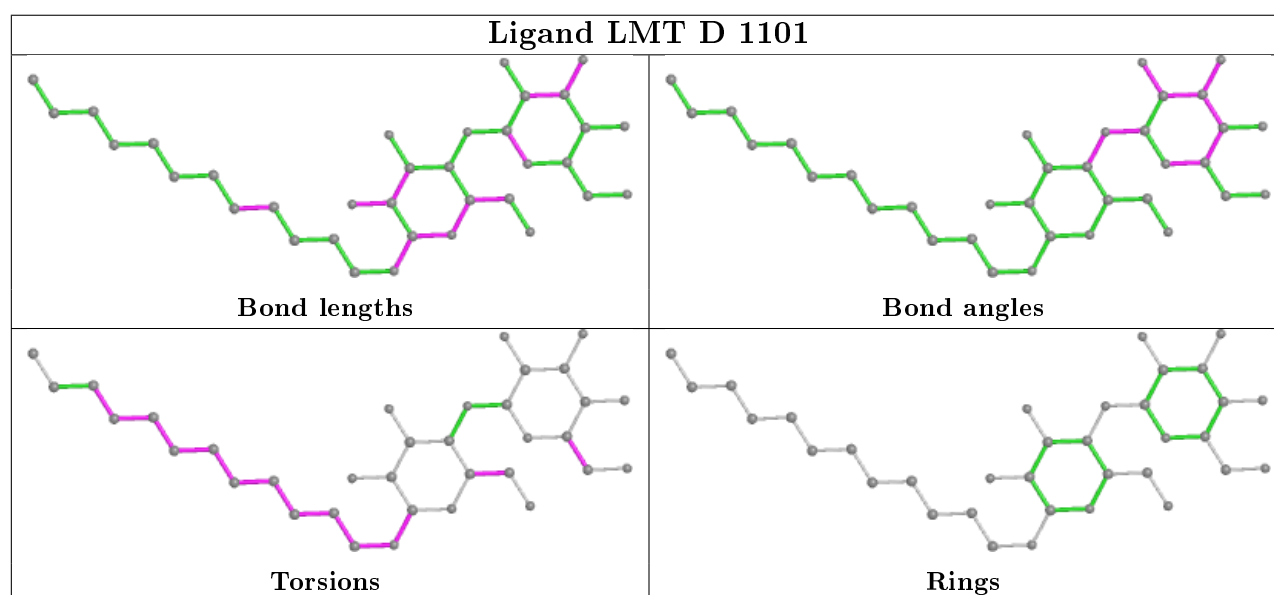
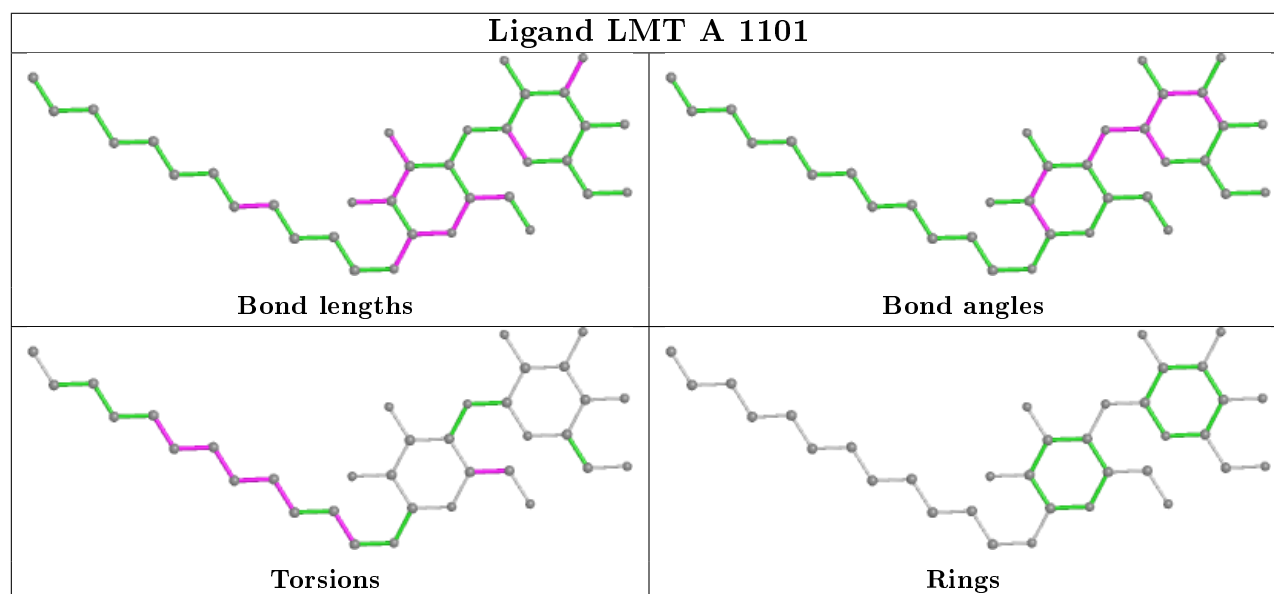
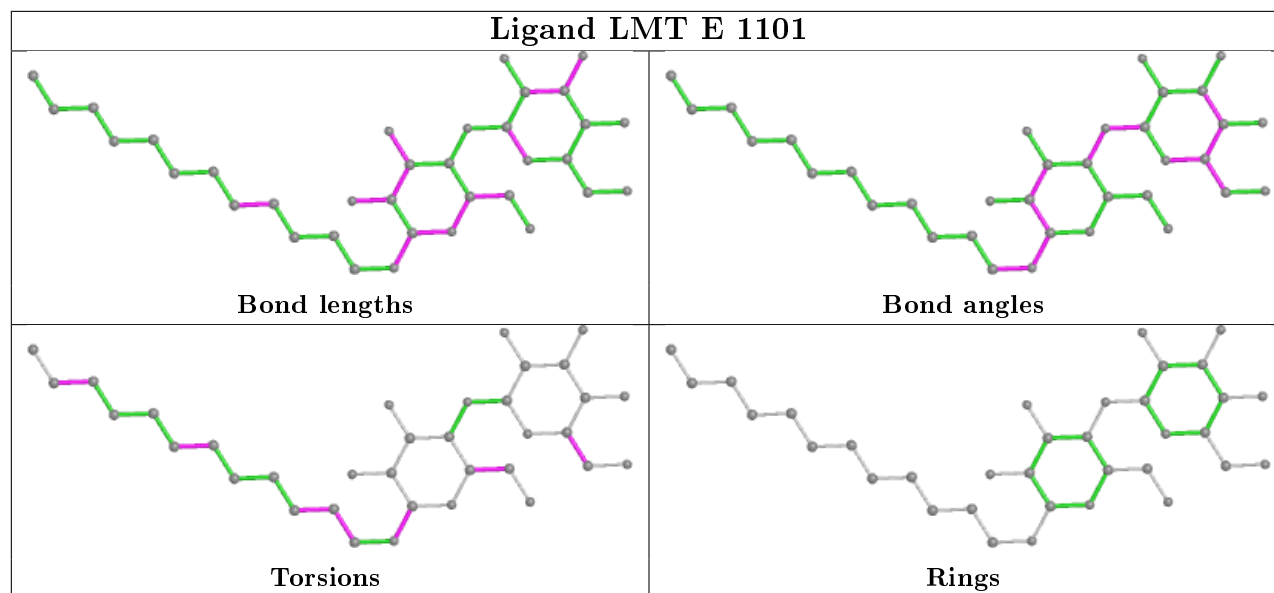
6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1101	LMT	4	0
2	B	1101	LMT	3	0
2	C	1101	LMT	4	0
2	E	1101	LMT	4	0
2	A	1101	LMT	4	0
2	D	1101	LMT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1042/1049 (99%)	0.32	86 (8%) 11 6	28, 63, 113, 139	0
1	B	1046/1049 (99%)	0.18	70 (6%) 17 9	26, 57, 100, 161	0
1	C	1044/1049 (99%)	0.46	117 (11%) 5 3	17, 56, 98, 173	0
1	D	1042/1049 (99%)	0.45	115 (11%) 5 3	21, 81, 133, 168	0
1	E	1042/1049 (99%)	0.53	131 (12%) 3 2	38, 77, 119, 154	0
1	F	1046/1049 (99%)	0.62	155 (14%) 2 1	29, 73, 120, 143	0
All	All	6262/6294 (99%)	0.43	674 (10%) 5 3	17, 68, 116, 173	0

All (674) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	314	GLU	16.2
1	E	315	PRO	15.9
1	D	869	SER	14.3
1	F	481	SER	12.3
1	E	128	SER	12.1
1	C	720	GLY	11.7
1	B	315	PRO	11.3
1	C	719	ASN	10.8
1	F	676	THR	10.7
1	F	442	LEU	10.6
1	F	719	ASN	10.3
1	F	941	ASN	10.3
1	B	314	GLU	10.2
1	F	836	SER	9.9
1	E	129	VAL	9.3
1	F	406	VAL	9.0
1	F	127	VAL	8.8
1	F	128	SER	8.7
1	D	689	GLY	8.6

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Mol	Chain	Res	Type	RSRZ
1	B	869	SER	8.5
1	D	322	LYS	8.5
1	D	461	GLY	8.4
1	E	311	ALA	8.4
1	F	829	GLY	8.4
1	C	402	ILE	7.8
1	F	403	GLY	7.8
1	E	44	THR	7.8
1	E	348	ILE	7.5
1	F	441	ALA	7.5
1	E	408	ASP	7.4
1	D	459	PHE	7.4
1	D	719	ASN	7.3
1	C	403	GLY	7.2
1	F	402	ILE	7.1
1	F	828	LEU	7.1
1	E	405	LEU	7.0
1	F	407	ASP	7.0
1	F	618	ALA	7.0
1	A	369	THR	7.0
1	C	837	THR	6.9
1	F	46	SER	6.9
1	E	310	LEU	6.8
1	A	404	LEU	6.8
1	F	720	GLY	6.7
1	D	720	GLY	6.7
1	F	445	ILE	6.7
1	E	978	THR	6.6
1	A	396	PHE	6.5
1	E	307	ARG	6.5
1	C	826	GLU	6.4
1	F	410	ILE	6.4
1	F	617	ALA	6.4
1	C	314	GLU	6.4
1	A	35	TYR	6.3
1	E	409	ALA	6.2
1	E	487	ILE	6.2
1	F	675	GLY	6.2
1	A	372	VAL	6.1
1	E	164	ASP	6.1
1	A	408	ASP	6.0
1	A	482	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	481	SER	6.0
1	B	617	ALA	6.0
1	E	406	VAL	5.9
1	C	445	ILE	5.9
1	E	443	VAL	5.9
1	E	105	VAL	5.8
1	A	174	ASP	5.8
1	E	322	LYS	5.8
1	F	700	ASN	5.7
1	E	977	MET	5.7
1	D	460	GLY	5.6
1	D	690	LEU	5.6
1	F	111	LEU	5.6
1	F	449	LEU	5.6
1	C	406	VAL	5.6
1	D	617	ALA	5.5
1	E	869	SER	5.5
1	D	868	LEU	5.5
1	F	937	LEU	5.5
1	F	405	LEU	5.5
1	C	501	ALA	5.4
1	F	448	VAL	5.4
1	F	446	ALA	5.3
1	C	618	ALA	5.3
1	D	851	LEU	5.3
1	F	711	ASP	5.3
1	A	371	ALA	5.3
1	E	308	ALA	5.3
1	C	721	LEU	5.3
1	F	837	THR	5.3
1	F	362	PHE	5.3
1	D	128	SER	5.3
1	D	282	ASN	5.2
1	C	835	LYS	5.2
1	E	317	PHE	5.2
1	E	46	SER	5.2
1	F	718	PRO	5.2
1	E	981	ALA	5.2
1	F	834	GLY	5.2
1	C	676	THR	5.1
1	C	48	SER	5.1
1	A	486	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	449	LEU	5.0
1	C	838	GLY	5.1
1	C	322	LYS	5.0
1	E	108	GLN	5.0
1	F	873	ALA	5.0
1	F	835	LYS	5.0
1	D	486	LEU	5.0
1	C	856	GLY	4.9
1	F	474	ILE	4.9
1	A	368	PRO	4.9
1	F	826	GLU	4.9
1	C	448	VAL	4.9
1	E	933	THR	4.9
1	E	442	LEU	4.9
1	D	174	ASP	4.9
1	F	48	SER	4.9
1	A	400	LEU	4.8
1	F	47	ALA	4.8
1	A	376	LEU	4.8
1	C	127	VAL	4.8
1	E	47	ALA	4.8
1	E	352	PHE	4.8
1	C	129	VAL	4.8
1	A	935	ILE	4.8
1	F	315	PRO	4.8
1	F	944	LEU	4.8
1	E	410	ILE	4.8
1	A	321	LEU	4.8
1	C	446	ALA	4.7
1	A	976	LEU	4.7
1	E	316	PHE	4.7
1	F	717	ARG	4.7
1	D	400	LEU	4.7
1	C	717	ARG	4.6
1	E	398	MET	4.6
1	E	944	LEU	4.6
1	E	982	PHE	4.6
1	F	408	ASP	4.6
1	C	405	LEU	4.6
1	A	405	LEU	4.6
1	C	442	LEU	4.6
1	E	370	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	33	ALA	4.6
1	F	699	ARG	4.6
1	D	401	ALA	4.6
1	D	839	GLU	4.6
1	D	575	MET	4.5
1	E	929	VAL	4.5
1	A	881	LEU	4.5
1	E	349	ILE	4.5
1	B	322	LYS	4.5
1	D	688	ALA	4.5
1	C	674	LEU	4.5
1	E	362	PHE	4.5
1	F	109	ASN	4.5
1	D	145	THR	4.5
1	C	500	ILE	4.5
1	F	372	VAL	4.5
1	C	394	THR	4.4
1	D	408	ASP	4.4
1	E	488	LEU	4.4
1	F	404	LEU	4.4
1	C	831	ALA	4.4
1	E	130	GLU	4.4
1	C	836	SER	4.4
1	E	104	GLN	4.4
1	E	127	VAL	4.4
1	F	500	ILE	4.4
1	A	899	PHE	4.4
1	E	1019	ILE	4.4
1	E	402	ILE	4.3
1	E	404	LEU	4.3
1	F	874	PRO	4.3
1	D	853	THR	4.3
1	A	128	SER	4.3
1	F	110	LYS	4.3
1	F	502	LYS	4.3
1	E	369	THR	4.3
1	C	398	MET	4.3
1	F	129	VAL	4.2
1	B	316	PHE	4.2
1	E	111	LEU	4.2
1	A	411	VAL	4.2
1	F	444	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	938	SER	4.2
1	C	718	PRO	4.2
1	D	404	LEU	4.1
1	D	687	GLN	4.1
1	F	712	MET	4.1
1	E	483	LEU	4.1
1	D	836	SER	4.1
1	E	367	ILE	4.1
1	A	15	ILE	4.1
1	A	640	GLU	4.1
1	F	888	LEU	4.1
1	D	136	PHE	4.1
1	D	458	PHE	4.1
1	E	678	THR	4.1
1	A	485	ALA	4.0
1	E	366	LEU	4.0
1	E	109	ASN	4.0
1	D	411	VAL	4.0
1	A	355	MET	4.0
1	D	576	VAL	4.0
1	C	390	ILE	4.0
1	D	487	ILE	4.0
1	F	904	VAL	4.0
1	A	882	ILE	4.0
1	F	662	MET	4.0
1	A	322	LYS	4.0
1	C	502	LYS	4.0
1	F	322	LYS	4.0
1	F	482	VAL	3.9
1	F	117	LEU	3.9
1	D	866	GLU	3.9
1	C	79	SER	3.9
1	D	386	PHE	3.9
1	C	441	ALA	3.9
1	D	15	ILE	3.9
1	F	501	ALA	3.9
1	A	1017	LEU	3.9
1	F	1016	VAL	3.9
1	D	791	VAL	3.9
1	C	128	SER	3.9
1	D	482	VAL	3.9
1	C	372	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	129	VAL	3.9
1	D	852	PRO	3.9
1	A	407	ASP	3.9
1	F	33	ALA	3.8
1	B	348	ILE	3.8
1	E	400	LEU	3.8
1	A	719	ASN	3.8
1	C	410	ILE	3.8
1	C	408	ASP	3.8
1	E	395	MET	3.8
1	F	976	LEU	3.8
1	A	410	ILE	3.8
1	C	712	MET	3.8
1	C	315	PRO	3.8
1	A	470	PHE	3.8
1	A	16	ALA	3.7
1	D	870	GLY	3.7
1	A	878	ALA	3.7
1	E	466	ILE	3.7
1	F	484	VAL	3.7
1	F	443	VAL	3.7
1	E	617	ALA	3.7
1	D	462	SER	3.7
1	D	875	SER	3.7
1	C	33	ALA	3.7
1	F	398	MET	3.7
1	E	282	ASN	3.7
1	A	392	THR	3.6
1	A	129	VAL	3.6
1	B	406	VAL	3.6
1	E	904	VAL	3.6
1	E	43	VAL	3.6
1	E	974	PRO	3.6
1	D	44	THR	3.6
1	D	835	LYS	3.6
1	E	868	LEU	3.6
1	F	376	LEU	3.6
1	D	611	ALA	3.6
1	B	111	LEU	3.6
1	D	867	ARG	3.5
1	C	941	ASN	3.5
1	E	407	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	404	LEU	3.5
1	A	456	MET	3.5
1	F	865	GLN	3.5
1	D	321	LEU	3.5
1	F	715	SER	3.5
1	B	317	PHE	3.5
1	F	16	ALA	3.5
1	D	396	PHE	3.4
1	A	871	ASN	3.4
1	B	177	LEU	3.4
1	A	403	GLY	3.4
1	C	474	ILE	3.4
1	F	409	ALA	3.4
1	E	980	LEU	3.4
1	D	383	LEU	3.4
1	E	291	ILE	3.4
1	E	937	LEU	3.4
1	F	399	VAL	3.4
1	C	307	ARG	3.4
1	E	484	VAL	3.4
1	A	136	PHE	3.4
1	E	321	LEU	3.4
1	B	842	GLU	3.4
1	D	113	LEU	3.4
1	C	494	ALA	3.4
1	A	1013	THR	3.4
1	C	1044	HIS	3.4
1	F	1015	THR	3.3
1	D	718	PRO	3.3
1	F	356	TYR	3.3
1	B	371	ALA	3.3
1	C	711	ASP	3.3
1	F	591	LEU	3.3
1	A	351	VAL	3.3
1	C	833	PRO	3.3
1	B	663	VAL	3.3
1	D	111	LEU	3.3
1	F	69	MET	3.3
1	B	671	ILE	3.3
1	F	945	ILE	3.3
1	B	113	LEU	3.3
1	B	542	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	395	MET	3.3
1	C	69	MET	3.3
1	E	126	GLY	3.3
1	F	477	ALA	3.3
1	F	193	LEU	3.3
1	E	107	VAL	3.2
1	A	481	SER	3.2
1	F	470	PHE	3.2
1	D	850	LYS	3.2
1	D	112	GLN	3.2
1	A	982	PHE	3.2
1	E	86	GLY	3.2
1	D	11	PHE	3.2
1	D	618	ALA	3.2
1	C	38	ILE	3.2
1	B	871	ASN	3.2
1	E	303	ALA	3.2
1	A	617	ALA	3.1
1	C	401	ALA	3.1
1	C	868	LEU	3.1
1	A	938	SER	3.1
1	B	408	ASP	3.1
1	E	718	PRO	3.1
1	F	881	LEU	3.1
1	C	400	LEU	3.1
1	E	940	LYS	3.1
1	C	478	MET	3.1
1	C	321	LEU	3.1
1	E	618	ALA	3.1
1	C	473	THR	3.1
1	A	348	ILE	3.1
1	E	313	MET	3.1
1	E	290	GLY	3.1
1	D	886	LEU	3.1
1	E	177	LEU	3.1
1	D	67	GLN	3.0
1	D	483	LEU	3.0
1	D	129	VAL	3.0
1	D	463	THR	3.0
1	F	473	THR	3.0
1	E	351	VAL	3.0
1	A	19	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	877	TYR	3.0
1	C	9	PRO	3.0
1	C	791	VAL	3.0
1	B	128	SER	3.0
1	C	444	GLY	3.0
1	C	981	ALA	3.0
1	E	401	ALA	3.0
1	B	311	ALA	3.0
1	A	445	ILE	3.0
1	C	611	ALA	3.0
1	D	35	TYR	3.0
1	E	1018	ALA	3.0
1	F	892	TYR	3.0
1	E	403	GLY	2.9
1	C	699	ARG	2.9
1	F	940	LYS	2.9
1	C	576	VAL	2.9
1	F	831	ALA	2.9
1	E	312	LYS	2.9
1	A	336	SER	2.9
1	B	109	ASN	2.9
1	F	833	PRO	2.9
1	A	178	PHE	2.9
1	F	396	PHE	2.9
1	F	981	ALA	2.9
1	B	905	VAL	2.9
1	C	122	VAL	2.9
1	C	828	LEU	2.9
1	C	1011	MET	2.9
1	D	701	GLN	2.9
1	E	465	ALA	2.9
1	F	369	THR	2.9
1	C	162	MET	2.9
1	F	1012	VAL	2.9
1	C	362	PHE	2.9
1	F	869	SER	2.9
1	B	876	LEU	2.9
1	C	17	ILE	2.9
1	E	162	MET	2.9
1	C	675	GLY	2.9
1	D	803	ALA	2.9
1	E	719	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	995	ALA	2.8
1	F	3	ASN	2.8
1	F	197	GLN	2.8
1	B	44	THR	2.8
1	B	487	ILE	2.8
1	C	65	ILE	2.8
1	C	834	GLY	2.8
1	E	1022	VAL	2.8
1	D	577	GLN	2.8
1	B	791	VAL	2.8
1	A	145	THR	2.8
1	B	835	LYS	2.8
1	B	870	GLY	2.8
1	C	310	LEU	2.8
1	F	1037	ASN	2.8
1	C	617	ALA	2.8
1	C	865	GLN	2.8
1	B	661	ALA	2.8
1	F	126	GLY	2.8
1	F	178	PHE	2.8
1	E	870	GLY	2.8
1	D	32	VAL	2.8
1	E	65	ILE	2.8
1	D	114	ALA	2.8
1	D	977	MET	2.7
1	F	96	SER	2.7
1	E	45	ILE	2.7
1	F	116	PRO	2.7
1	E	930	GLY	2.7
1	B	18	ILE	2.7
1	E	943	ILE	2.7
1	D	407	ASP	2.7
1	D	837	THR	2.7
1	C	97	GLY	2.7
1	E	71	GLY	2.7
1	D	46	SER	2.7
1	F	335	ILE	2.7
1	C	872	GLN	2.7
1	F	619	GLY	2.7
1	F	122	VAL	2.7
1	F	357	LEU	2.7
1	F	680	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	488	LEU	2.7
1	F	907	LEU	2.7
1	B	866	GLU	2.7
1	D	65	ILE	2.7
1	A	108	GLN	2.7
1	A	397	GLY	2.7
1	E	32	VAL	2.7
1	B	853	THR	2.7
1	D	976	LEU	2.7
1	E	1015	THR	2.7
1	D	173	GLY	2.7
1	E	48	SER	2.7
1	D	767	ARG	2.7
1	F	478	MET	2.7
1	F	314	GLU	2.7
1	C	577	GLN	2.6
1	E	839	GLU	2.6
1	F	462	SER	2.6
1	A	164	ASP	2.6
1	F	176	GLN	2.6
1	B	400	LEU	2.6
1	C	395	MET	2.6
1	C	575	MET	2.6
1	D	717	ARG	2.6
1	C	389	SER	2.6
1	F	13	TRP	2.6
1	A	347	ALA	2.6
1	C	944	LEU	2.6
1	E	1042	HIS	2.6
1	B	355	MET	2.6
1	F	67	GLN	2.6
1	C	111	LEU	2.6
1	D	390	ILE	2.6
1	D	36	PRO	2.6
1	A	13	TRP	2.6
1	A	886	LEU	2.6
1	D	109	ASN	2.6
1	B	852	PRO	2.6
1	D	663	VAL	2.6
1	A	401	ALA	2.6
1	E	441	ALA	2.6
1	A	449	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	453	PHE	2.6
1	F	876	LEU	2.6
1	B	575	MET	2.6
1	C	8	ARG	2.6
1	C	976	LEU	2.6
1	F	480	LEU	2.6
1	D	43	VAL	2.5
1	E	480	LEU	2.5
1	F	463	THR	2.5
1	C	671	ILE	2.5
1	A	1012	VAL	2.5
1	C	937	LEU	2.5
1	C	417	GLU	2.5
1	C	890	ALA	2.5
1	B	662	MET	2.5
1	D	45	ILE	2.5
1	D	447	MET	2.5
1	D	48	SER	2.5
1	D	47	ALA	2.5
1	D	479	ALA	2.5
1	E	934	THR	2.5
1	F	38	ILE	2.5
1	E	926	TYR	2.5
1	A	767	ARG	2.5
1	F	107	VAL	2.5
1	E	323	ILE	2.5
1	C	399	VAL	2.5
1	F	830	GLN	2.5
1	D	982	PHE	2.5
1	A	975	ILE	2.5
1	F	716	VAL	2.5
1	A	705	GLU	2.5
1	E	102	ILE	2.5
1	A	134	SER	2.4
1	E	1011	MET	2.4
1	B	995	ALA	2.4
1	B	67	GLN	2.4
1	C	977	MET	2.4
1	E	357	LEU	2.4
1	E	867	ARG	2.4
1	F	350	LEU	2.4
1	D	68	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	834	GLY	2.4
1	D	1016	VAL	2.4
1	F	488	LEU	2.4
1	A	850	LYS	2.4
1	A	458	PHE	2.4
1	C	356	TYR	2.4
1	F	371	ALA	2.4
1	F	459	PHE	2.4
1	A	143	ILE	2.4
1	B	15	ILE	2.4
1	A	357	LEU	2.4
1	D	405	LEU	2.4
1	F	866	GLU	2.4
1	D	389	SER	2.4
1	F	1021	PHE	2.4
1	D	130	GLU	2.4
1	F	677	ALA	2.4
1	B	851	LEU	2.4
1	C	117	LEU	2.4
1	E	1007	VAL	2.3
1	B	404	LEU	2.3
1	C	700	ASN	2.3
1	E	798	MET	2.3
1	D	822	LEU	2.3
1	F	174	ASP	2.3
1	D	841	MET	2.3
1	A	300	LEU	2.3
1	A	337	ILE	2.3
1	D	578	LEU	2.3
1	E	353	LEU	2.3
1	B	715	SER	2.3
1	F	380	PHE	2.3
1	D	626	ILE	2.3
1	F	466	ILE	2.3
1	F	790	TYR	2.3
1	C	374	VAL	2.3
1	F	170	SER	2.3
1	C	980	LEU	2.3
1	E	145	THR	2.3
1	C	790	TYR	2.3
1	D	882	ILE	2.3
1	C	1016	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	890	ALA	2.3
1	E	806	SER	2.3
1	A	107	VAL	2.3
1	C	482	VAL	2.3
1	F	884	VAL	2.3
1	B	976	LEU	2.3
1	C	16	ALA	2.3
1	E	14	VAL	2.3
1	C	1045	THR	2.3
1	B	50	PRO	2.3
1	B	886	LEU	2.3
1	B	706	ALA	2.3
1	B	716	VAL	2.3
1	F	485	ALA	2.3
1	F	620	ALA	2.3
1	F	832	ALA	2.3
1	C	871	ASN	2.2
1	C	349	ILE	2.2
1	D	163	LYS	2.2
1	E	158	VAL	2.2
1	A	281	PHE	2.2
1	C	975	ILE	2.2
1	C	673	GLU	2.2
1	F	722	GLU	2.2
1	F	1011	MET	2.2
1	D	403	GLY	2.2
1	F	467	TYR	2.2
1	F	661	ALA	2.2
1	D	686	ASP	2.2
1	E	593	GLU	2.2
1	B	410	ILE	2.2
1	E	331	PRO	2.2
1	F	681	ASP	2.2
1	A	343	THR	2.2
1	A	45	ILE	2.2
1	B	46	SER	2.2
1	B	882	ILE	2.2
1	C	96	SER	2.2
1	E	659	LYS	2.2
1	B	618	ALA	2.2
1	D	878	ALA	2.2
1	A	27	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	575	MET	2.2
1	A	689	GLY	2.2
1	C	116	PRO	2.2
1	E	674	LEU	2.2
1	B	719	ASN	2.2
1	A	489	THR	2.2
1	B	978	THR	2.2
1	C	825	MET	2.2
1	D	78	MET	2.2
1	B	207	ILE	2.2
1	E	901	VAL	2.2
1	B	104	GLN	2.2
1	D	354	VAL	2.2
1	B	145	THR	2.2
1	E	344	LEU	2.1
1	F	868	LEU	2.1
1	A	130	GLU	2.1
1	A	327	TYR	2.1
1	E	976	LEU	2.1
1	B	108	GLN	2.1
1	D	662	MET	2.1
1	D	402	ILE	2.1
1	A	874	PRO	2.1
1	E	78	MET	2.1
1	D	442	LEU	2.1
1	D	5	PHE	2.1
1	A	72	ILE	2.1
1	F	390	ILE	2.1
1	F	498	LYS	2.1
1	F	801	PHE	2.1
1	E	439	GLN	2.1
1	A	386	PHE	2.1
1	B	396	PHE	2.1
1	B	407	ASP	2.1
1	D	33	ALA	2.1
1	F	679	GLY	2.1
1	D	12	ALA	2.1
1	A	127	VAL	2.1
1	B	982	PHE	2.1
1	C	867	ARG	2.1
1	B	45	ILE	2.1
1	D	879	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	393	LEU	2.1
1	A	641	GLU	2.1
1	D	127	VAL	2.1
1	E	412	VAL	2.1
1	B	125	GLN	2.0
1	C	470	PHE	2.0
1	D	317	PHE	2.0
1	F	575	MET	2.0
1	E	371	ALA	2.0
1	B	619	GLY	2.0
1	D	592	ASN	2.0
1	E	671	ILE	2.0
1	F	392	THR	2.0
1	F	503	GLY	2.0
1	B	11	PHE	2.0
1	F	825	MET	2.0
1	D	19	ILE	2.0
1	F	383	LEU	2.0
1	C	67	GLN	2.0
1	E	112	GLN	2.0
1	B	127	VAL	2.0
1	C	892	TYR	2.0
1	F	317	PHE	2.0
1	D	609	VAL	2.0
1	B	701	GLN	2.0

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

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

## 6.3 Carbohydrates ⓘ

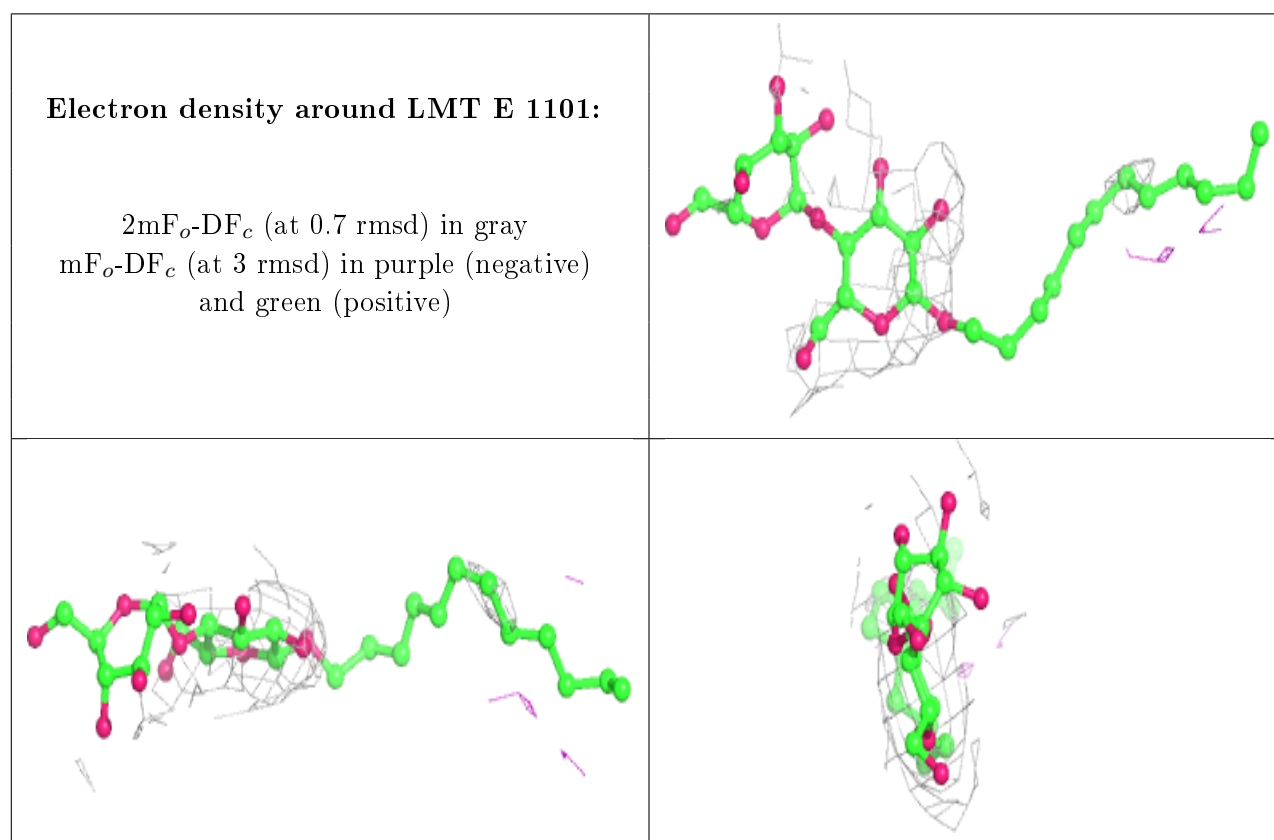
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

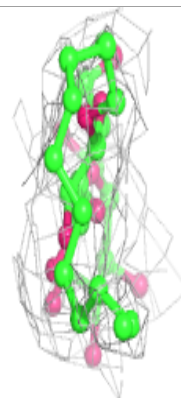
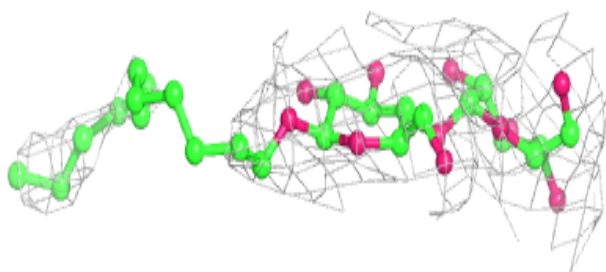
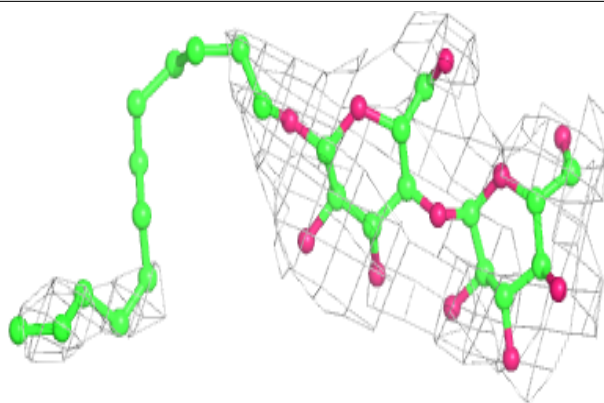
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LMT	E	1101	35/35	0.73	0.40	43,83,98,109	0
2	LMT	F	1101	35/35	0.81	0.37	19,65,82,87	0
2	LMT	B	1101	35/35	0.82	0.37	40,61,68,70	0
2	LMT	C	1101	35/35	0.84	0.33	29,44,62,65	0
2	LMT	D	1101	35/35	0.86	0.31	35,48,67,83	0
2	LMT	A	1101	35/35	0.88	0.32	40,56,74,75	0
3	NI	A	1102	1/1	0.97	0.08	31,31,31,31	0
3	NI	C	1102	1/1	0.99	0.12	33,33,33,33	0
3	NI	E	1102	1/1	0.99	0.08	64,64,64,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

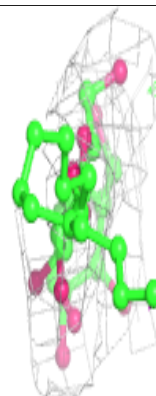
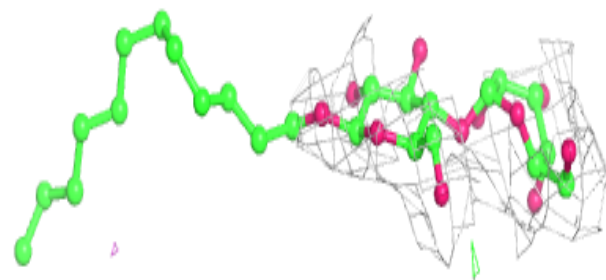
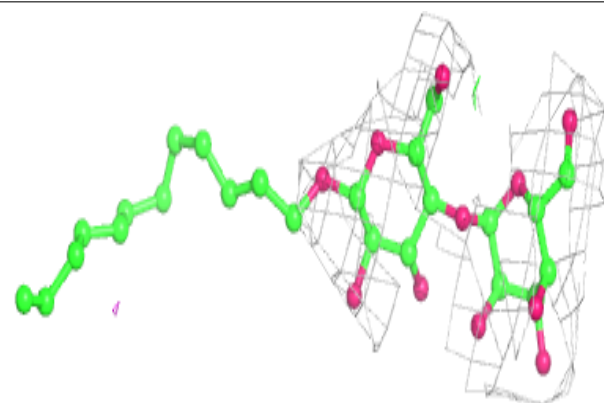


**Electron density around LMT F 1101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

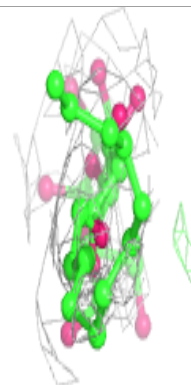
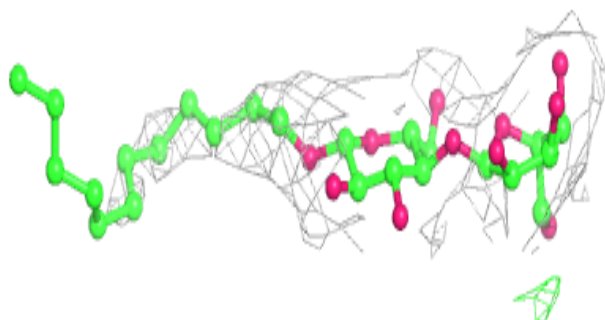
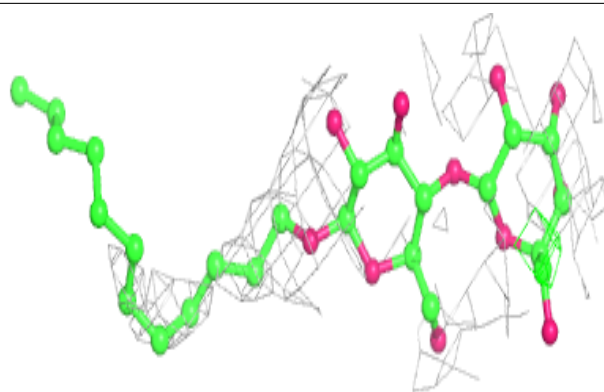
**Electron density around LMT B 1101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

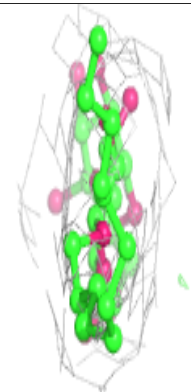
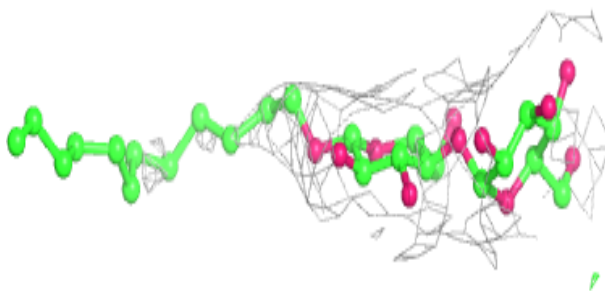
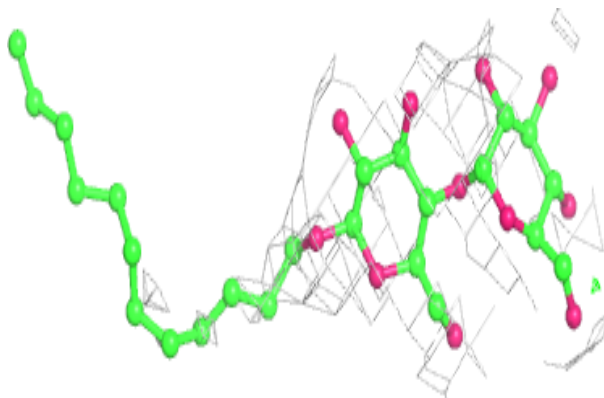


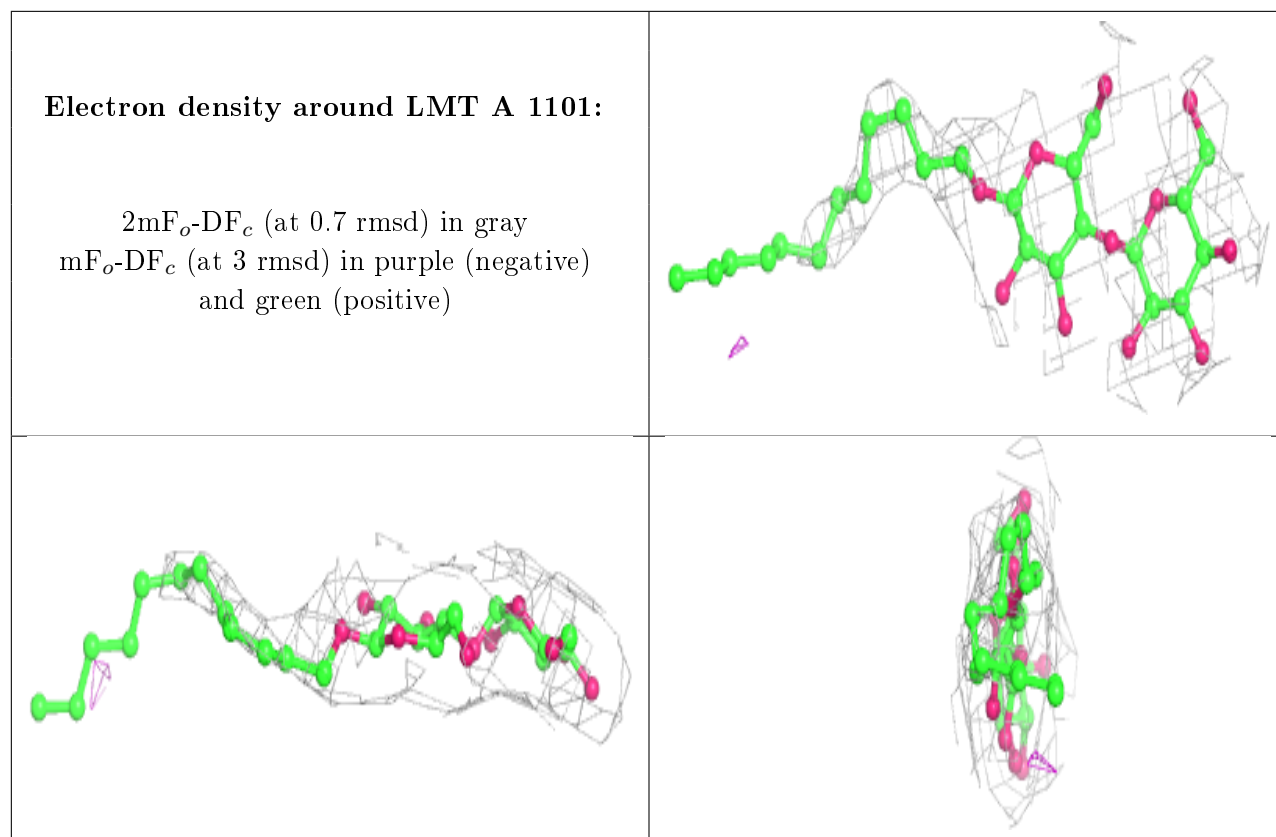
**Electron density around LMT C 1101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around LMT D 1101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.