



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:14 pm BST

PDB ID : 4ZJQ  
Title : Crystal structure of AcrB deletion mutant in complex with antibiotic in P21 space group  
Authors : Ababou, A.; Koronakis, V.  
Deposited on : 2015-04-29  
Resolution : 3.59 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

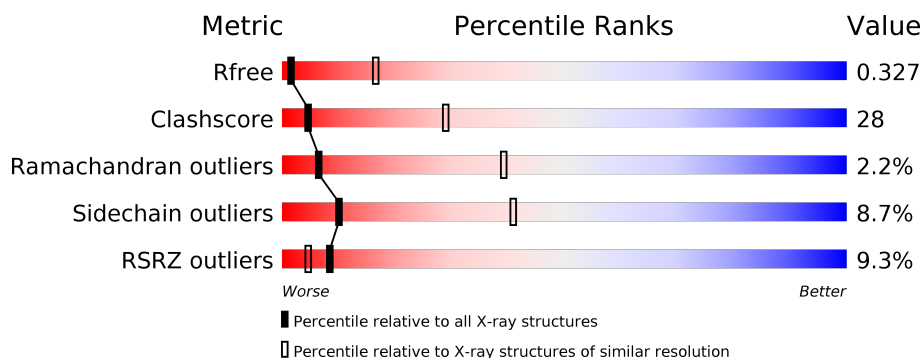
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.59 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	1044	<div> <div>7%</div> <div>48%</div> <div>47%</div> <div>• •</div> </div>
1	B	1044	<div> <div>7%</div> <div>48%</div> <div>46%</div> <div>6%</div> <div>•</div> </div>
1	C	1044	<div> <div>9%</div> <div>45%</div> <div>48%</div> <div>6%</div> <div>•</div> </div>
1	D	1044	<div> <div>7%</div> <div>48%</div> <div>45%</div> <div>6%</div> <div>•</div> </div>
1	E	1044	<div> <div>11%</div> <div>47%</div> <div>46%</div> <div>6%</div> <div>•</div> </div>
1	F	1044	<div> <div>13%</div> <div>43%</div> <div>49%</div> <div>6%</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	ERY	A	1101	-	-	-	X
2	ERY	D	1101	-	-	-	X
3	LMT	A	1102	-	-	-	X
3	LMT	B	2100	-	-	-	X
3	LMT	C	1101	-	-	-	X
3	LMT	D	1102	-	-	-	X
3	LMT	D	1103	-	-	-	X
3	LMT	F	2100	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 47697 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	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	B	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			
1	C	1036	Total	C	N	O	S	0	0	0
			7877	5063	1302	1469	43			
1	D	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	E	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			
1	F	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			

There are 36 discrepancies between the modelled and reference sequences:

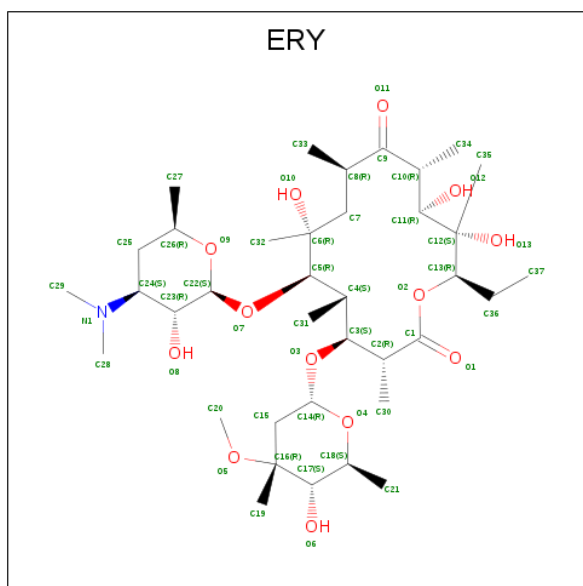
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	GLY	PHE	engineered mutation	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	PHE	deletion	UNP P31224
A	?	-	ALA	deletion	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	ARG	deletion	UNP P31224
B	?	GLY	PHE	engineered mutation	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	PHE	deletion	UNP P31224
B	?	-	ALA	deletion	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	ARG	deletion	UNP P31224
C	?	GLY	PHE	engineered mutation	UNP P31224
C	?	-	GLY	deletion	UNP P31224
C	?	-	PHE	deletion	UNP P31224
C	?	-	ALA	deletion	UNP P31224
C	?	-	GLY	deletion	UNP P31224

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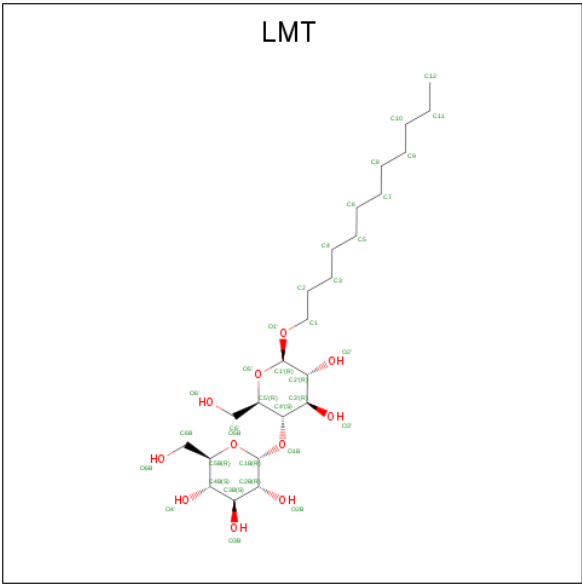
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P31224
D	?	GLY	PHE	engineered mutation	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	PHE	deletion	UNP P31224
D	?	-	ALA	deletion	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	ARG	deletion	UNP P31224
E	?	GLY	PHE	engineered mutation	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	PHE	deletion	UNP P31224
E	?	-	ALA	deletion	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	ARG	deletion	UNP P31224
F	?	GLY	PHE	engineered mutation	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	PHE	deletion	UNP P31224
F	?	-	ALA	deletion	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	ARG	deletion	UNP P31224

- Molecule 2 is ERYTHROMYCIN A (three-letter code: ERY) (formula:  $C_{37}H_{67}NO_{13}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			51	37	1	13		
2	D	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 3 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		
3	D	1	Total	C	O	0	0
			35	24	11		
3	D	1	Total	C	O	0	0
			35	24	11		
3	E	1	Total	C	O	0	0
			35	24	11		
3	F	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

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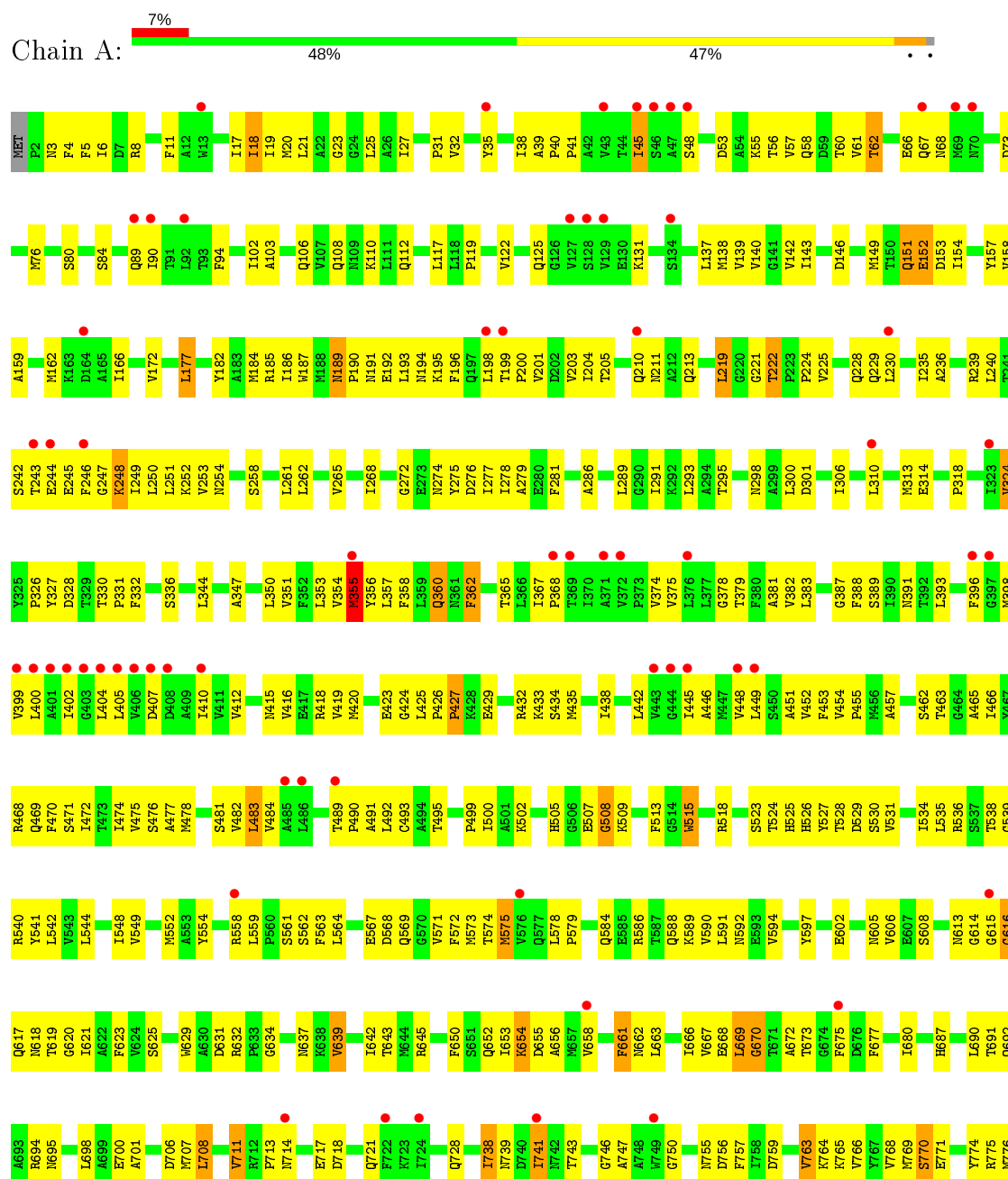
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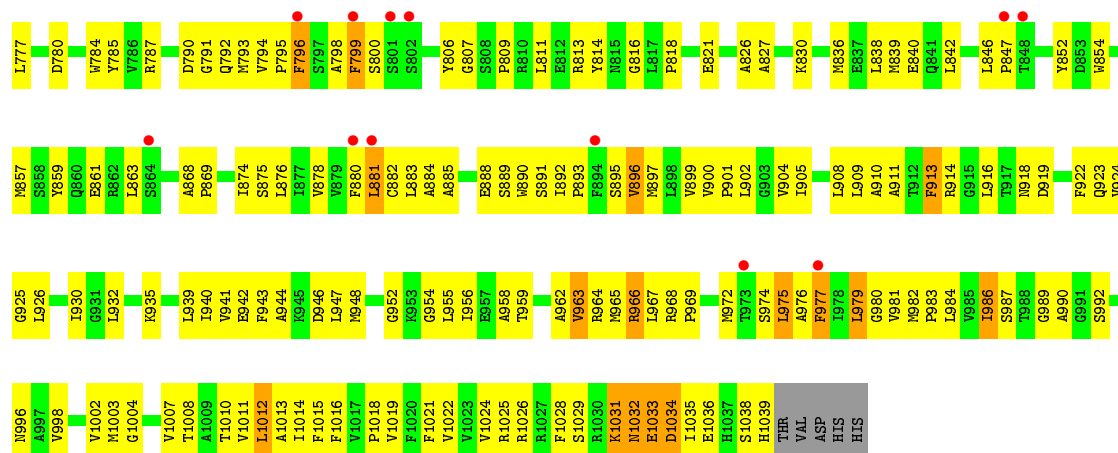
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Ni	0	0
			1	1		

### 3 Residue-property plots

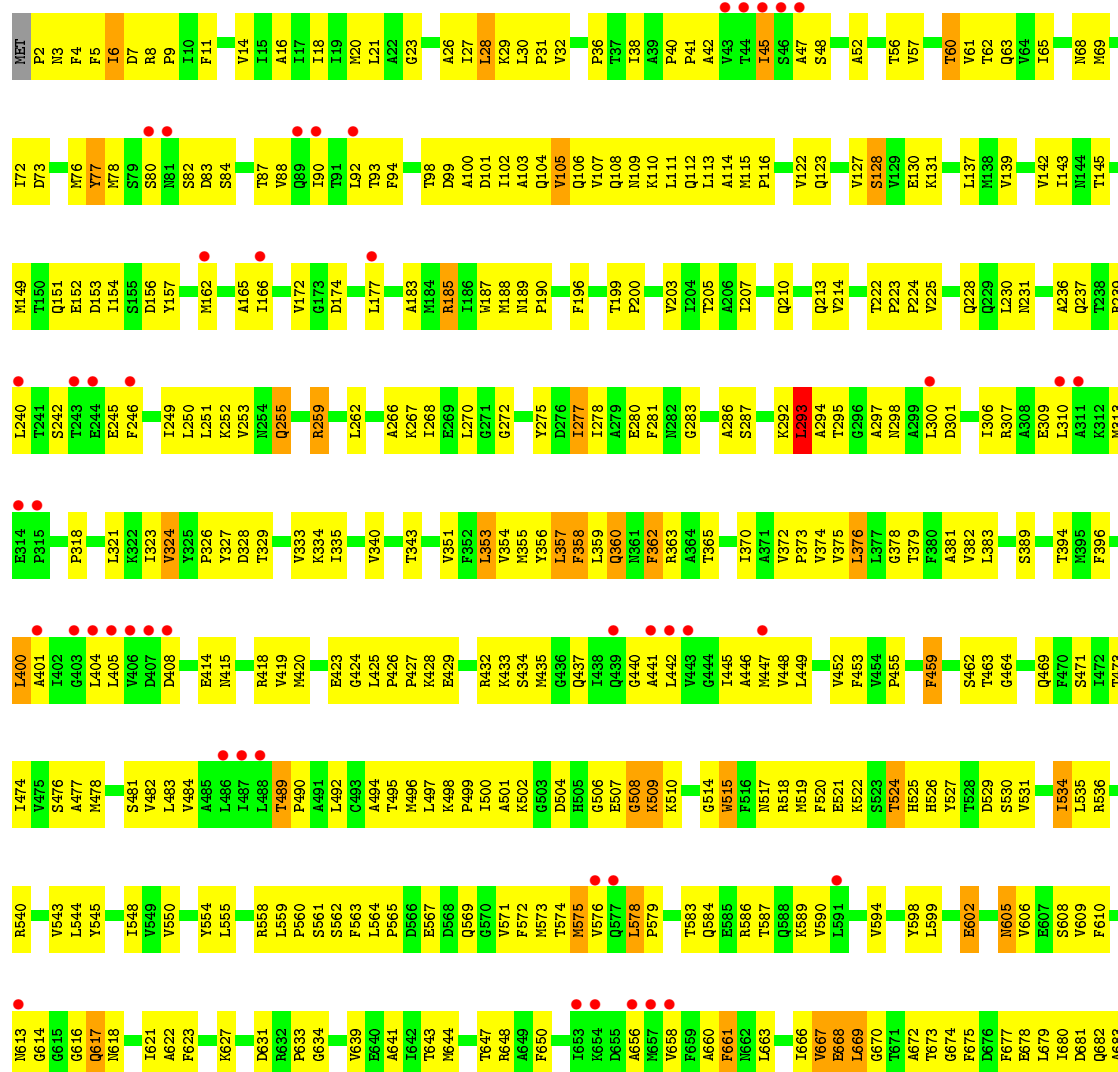
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

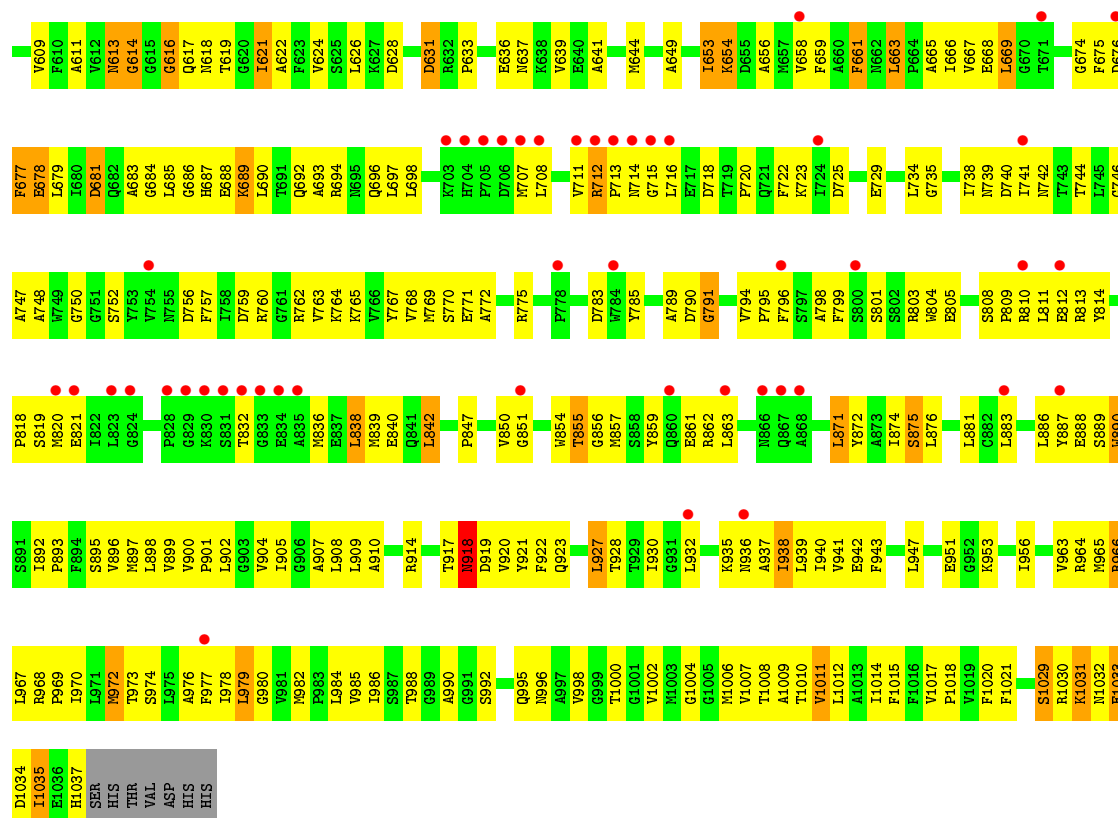




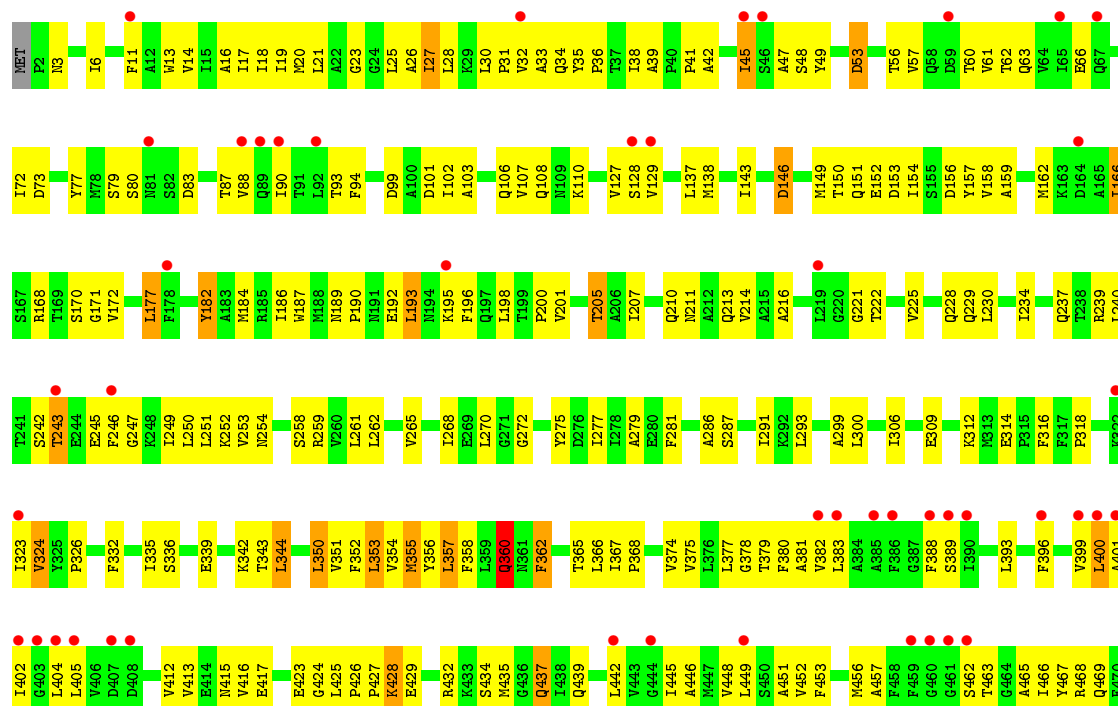
• Molecule 1: Multidrug efflux pump subunit AcrB

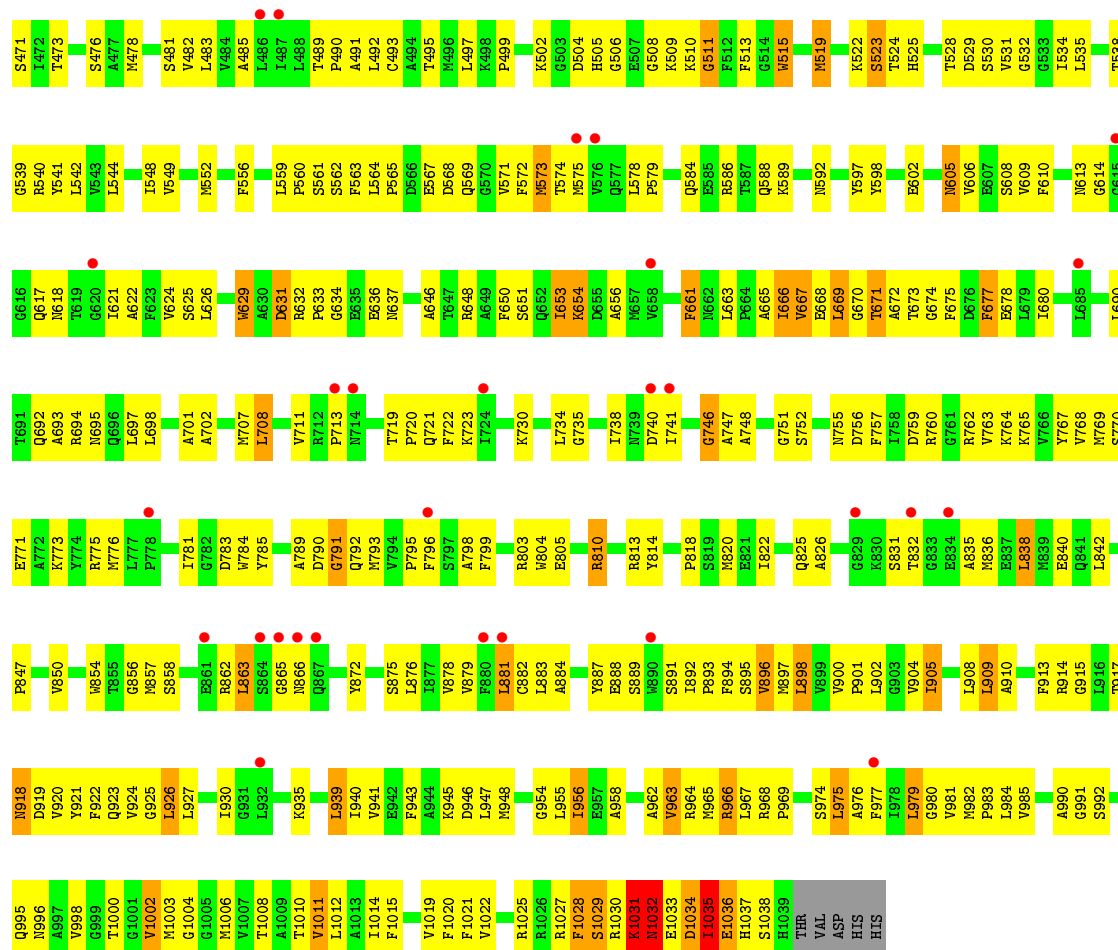




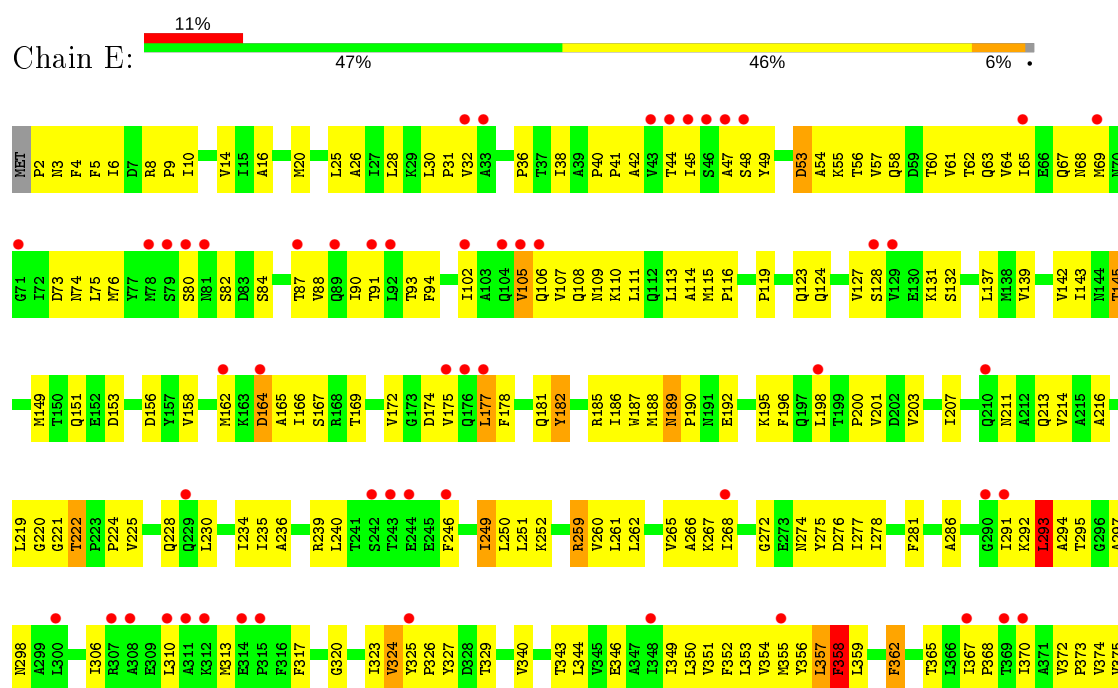


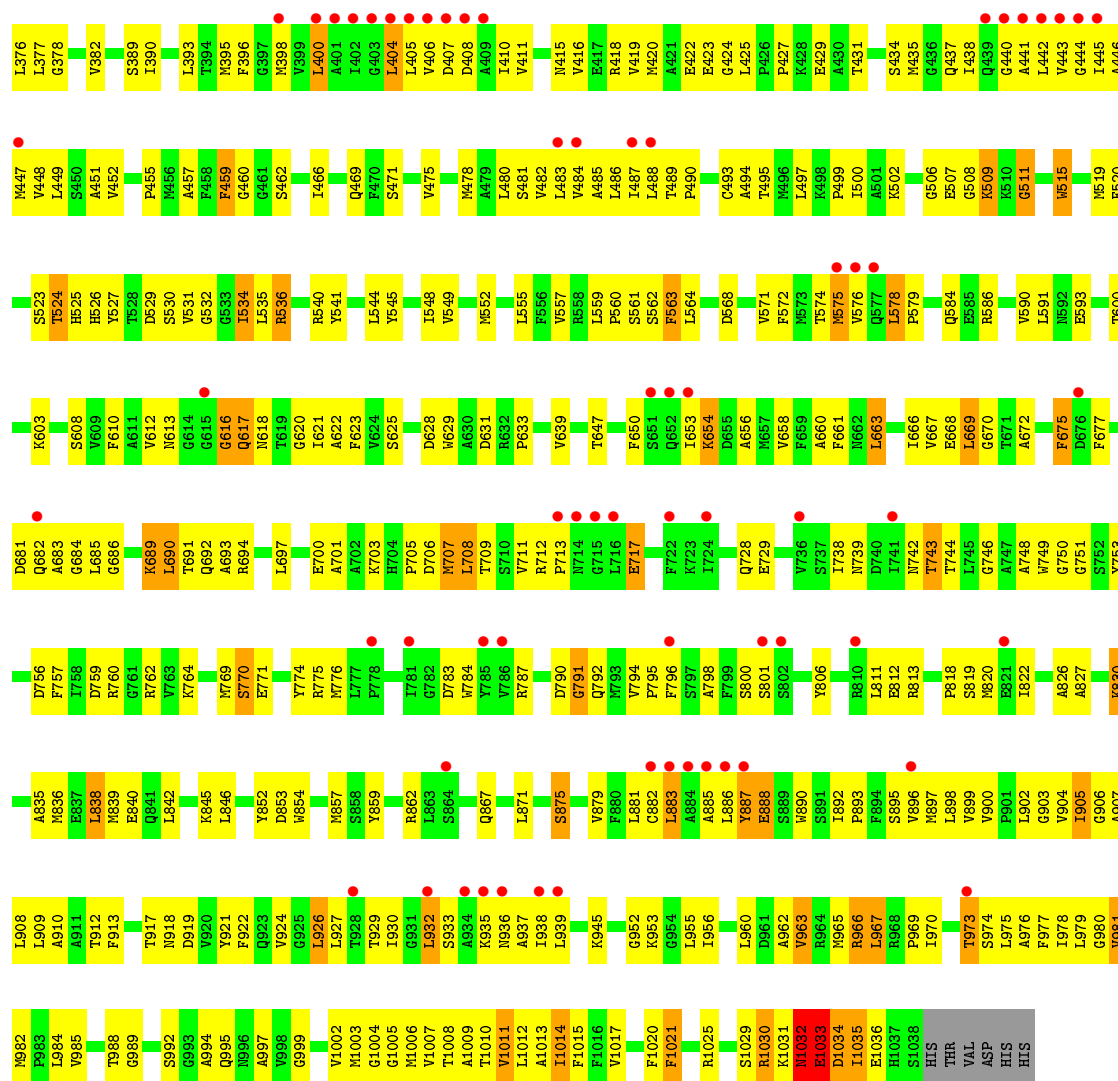
• Molecule 1: Multidrug efflux pump subunit AcrB



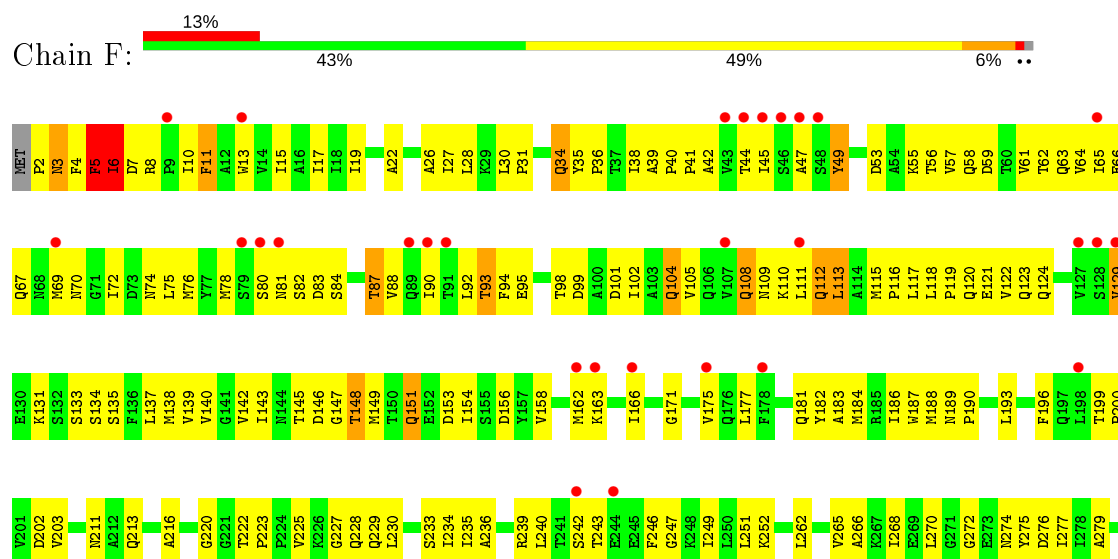


• Molecule 1: Multidrug efflux pump subunit AcrB





### Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.06Å 154.57Å 215.74Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	19.96 – 3.59 125.61 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.96-3.59) 96.5 (125.61-3.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, $R_{free}$	0.246 , 0.319 0.258 , 0.327	Depositor DCC
$R_{free}$ test set	5715 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	110.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 61.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.055 for -k,-h,-l 0.070 for k,h,-l 0.068 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	47697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	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 51.06 % 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 5.9200e-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, ERY

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	0.59	0/8043	0.85	10/10922 (0.1%)
1	B	0.59	0/8032	0.83	11/10907 (0.1%)
1	C	0.59	0/8026	0.87	7/10899 (0.1%)
1	D	0.56	1/8043 (0.0%)	0.81	9/10922 (0.1%)
1	E	0.57	1/8032 (0.0%)	0.82	10/10907 (0.1%)
1	F	0.56	0/8032	0.83	5/10907 (0.0%)
All	All	0.57	2/48208 (0.0%)	0.84	52/65464 (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	A	0	1
1	B	0	1
1	D	0	1
1	F	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	515	TRP	CB-CG	7.12	1.63	1.50
1	D	515	TRP	CB-CG	6.58	1.62	1.50

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	ASP	CB-CG-OD1	10.28	127.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	529	ASP	CB-CG-OD1	9.49	126.84	118.30
1	F	113	LEU	CA-CB-CG	9.17	136.39	115.30
1	A	529	ASP	CB-CG-OD1	8.95	126.36	118.30
1	E	529	ASP	CB-CG-OD1	7.96	125.46	118.30
1	B	357	LEU	CA-CB-CG	7.79	133.22	115.30
1	B	483	LEU	CA-CB-CG	7.70	133.02	115.30
1	E	357	LEU	CA-CB-CG	7.69	132.98	115.30
1	C	529	ASP	CB-CG-OD1	7.37	124.94	118.30
1	E	359	LEU	CA-CB-CG	7.35	132.21	115.30
1	E	883	LEU	CA-CB-CG	-7.35	98.39	115.30
1	C	92	LEU	CA-CB-CG	7.24	131.96	115.30
1	A	483	LEU	CA-CB-CG	6.98	131.35	115.30
1	B	497	LEU	CA-CB-CG	6.93	131.24	115.30
1	C	30	LEU	CA-CB-CG	6.58	130.43	115.30
1	B	883	LEU	CA-CB-CG	-6.48	100.39	115.30
1	A	1012	LEU	CA-CB-CG	6.43	130.08	115.30
1	C	405	LEU	CA-CB-CG	6.13	129.41	115.30
1	B	529	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	E	932	LEU	CA-CB-CG	-5.85	101.85	115.30
1	B	967	LEU	CA-CB-CG	5.78	128.60	115.30
1	D	350	LEU	CA-CB-CG	-5.70	102.19	115.30
1	F	863	LEU	CA-CB-CG	5.64	128.28	115.30
1	E	534	ILE	CG1-CB-CG2	-5.61	99.05	111.40
1	A	989	GLY	N-CA-C	-5.58	99.16	113.10
1	A	355	MET	CB-CG-SD	5.55	129.06	112.40
1	D	863	LEU	CA-CB-CG	5.52	127.99	115.30
1	D	400	LEU	CA-CB-CG	-5.51	102.63	115.30
1	F	967	LEU	CA-CB-CG	5.50	127.94	115.30
1	B	293	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	616	GLY	N-CA-C	-5.41	99.58	113.10
1	A	219	LEU	CA-CB-CG	5.39	127.70	115.30
1	D	193	LEU	CA-CB-CG	5.38	127.67	115.30
1	C	357	LEU	CA-CB-CG	5.37	127.65	115.30
1	D	669	LEU	CA-CB-CG	5.35	127.60	115.30
1	F	357	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	514	GLY	N-CA-C	5.29	126.33	113.10
1	A	117	LEU	CA-CB-CG	5.27	127.42	115.30
1	E	293	LEU	CA-CB-CG	5.26	127.39	115.30
1	C	425	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	B	359	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	967	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	515	TRP	CA-CB-CG	5.17	123.53	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	519	MET	CB-CG-SD	5.17	127.92	112.40
1	E	967	LEU	CA-CB-CG	5.16	127.16	115.30
1	D	1035	ILE	N-CA-C	5.14	124.89	111.00
1	E	669	LEU	N-CA-C	5.11	124.79	111.00
1	E	1032	ASN	C-N-CA	5.09	134.43	121.70
1	C	400	LEU	CA-CB-CG	5.07	126.95	115.30
1	F	75	LEU	CA-CB-CG	5.06	126.94	115.30
1	D	939	LEU	CA-CB-CG	-5.02	103.75	115.30
1	B	762	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	ASP	Peptide
1	B	1033	GLU	Peptide
1	D	1032	ASN	Peptide
1	F	1033	GLU	Peptide
1	F	1034	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	7893	0	8034	443	0
1	B	7883	0	8027	442	0
1	C	7877	0	8022	481	0
1	D	7893	0	8034	470	0
1	E	7883	0	8027	467	0
1	F	7883	0	8027	497	0
2	A	51	0	67	5	0
2	D	51	0	67	4	0
3	A	70	0	92	7	0
3	B	35	0	46	7	0
3	C	35	0	46	1	0
3	D	70	0	92	13	0
3	E	35	0	46	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	35	0	46	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	47697	0	48673	2723	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (2723) 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:F:34:GLN:HB2	1:F:333:VAL:HG22	1.45	0.98
1:A:225:VAL:H	1:B:776:MET:HE1	1.25	0.97
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.45	0.97
1:A:776:MET:HE1	1:C:225:VAL:H	1.29	0.96
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.44	0.96
1:C:893:PRO:HA	1:C:896:VAL:HG12	1.43	0.96
1:D:776:MET:HE1	1:F:225:VAL:H	1.30	0.96
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.47	0.93
1:C:887:TYR:O	1:C:889:SER:N	2.01	0.93
1:A:427:PRO:HD3	1:A:499:PRO:HB3	1.51	0.92
1:A:351:VAL:HG22	1:A:976:ALA:HB1	1.51	0.92
1:F:741:ILE:HG22	1:F:786:VAL:HG21	1.52	0.92
1:A:708:LEU:HD21	1:A:838:LEU:HD12	1.52	0.90
1:F:404:LEU:HG	1:F:449:LEU:HD13	1.52	0.90
1:B:356:TYR:O	1:B:358:PHE:N	2.05	0.90
1:C:196:PHE:O	1:C:252:LYS:NZ	2.06	0.89
1:A:874:ILE:HD13	1:C:25:LEU:HD21	1.54	0.89
1:A:445:ILE:HD13	1:A:935:LYS:HE3	1.54	0.89
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.55	0.88
1:C:343:THR:HG21	1:C:984:LEU:HD21	1.55	0.88
1:E:1032:ASN:N	1:E:1033:GLU:HB2	1.88	0.88
1:A:562:SER:HB2	1:A:919:ASP:HB3	1.54	0.87
1:C:356:TYR:HA	1:C:365:THR:HG21	1.55	0.87
1:B:896:VAL:HG21	1:B:938:ILE:HG13	1.55	0.87
1:C:914:ARG:NH2	1:C:985:VAL:O	2.08	0.87
1:F:932:LEU:HD13	1:F:1006:MET:HE2	1.56	0.87
1:F:262:LEU:HG	1:F:268:ILE:HD11	1.54	0.87
1:F:186:ILE:HG12	1:F:268:ILE:HG12	1.57	0.86
1:D:196:PHE:O	1:D:252:LYS:NZ	2.07	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:VAL:H	1:E:776:MET:HE1	1.37	0.86
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.56	0.86
1:C:360:GLN:OE1	1:C:517:ASN:ND2	2.09	0.86
1:E:530:SER:OG	3:E:1101:LMT:H1'	1.76	0.85
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.54	0.85
1:E:707:MET:HG2	1:E:838:LEU:HG	1.59	0.84
1:A:579:PRO:HD3	1:A:656:ALA:HB2	1.57	0.84
1:F:1034:ASP:HA	1:F:1035:ILE:HG12	1.59	0.83
1:A:350:LEU:HD22	1:A:979:LEU:HB3	1.58	0.83
1:A:108:GLN:NE2	1:B:109:ASN:O	2.12	0.83
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.58	0.82
1:D:1015:PHE:HE2	3:D:1102:LMT:H32	1.43	0.82
1:A:272:GLY:N	1:A:275:TYR:OH	2.12	0.82
1:B:196:PHE:O	1:B:252:LYS:NZ	2.11	0.82
1:B:189:ASN:HD22	1:B:267:LYS:HE2	1.44	0.82
1:E:351:VAL:HG22	1:E:976:ALA:HB1	1.60	0.82
1:C:156:ASP:OD1	1:C:760:ARG:NH2	2.13	0.82
1:C:59:ASP:OD2	1:C:59:ASP:N	2.09	0.82
1:C:351:VAL:HG22	1:C:976:ALA:HB1	1.60	0.81
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.60	0.81
1:A:632:ARG:NH1	1:A:637:ASN:O	2.14	0.81
1:C:939:LEU:HB3	1:C:966:ARG:HD2	1.62	0.80
1:D:669:LEU:HD12	1:D:670:GLY:H	1.43	0.80
1:C:918:ASN:HD21	1:C:923:GLN:HE21	1.27	0.80
1:C:380:PHE:HD2	1:C:383:LEU:HD12	1.43	0.80
1:C:428:LYS:HG2	1:C:494:ALA:HB1	1.63	0.80
1:D:23:GLY:HA2	1:D:381:ALA:HB2	1.62	0.80
1:D:6:ILE:HD12	1:D:432:ARG:HG2	1.63	0.80
1:A:584:GLN:HB2	1:A:617:GLN:HG2	1.64	0.79
1:E:404:LEU:HD21	1:E:449:LEU:HD22	1.63	0.79
1:F:83:ASP:HB2	1:F:87:THR:O	1.82	0.79
1:A:908:LEU:HD23	1:A:922:PHE:HZ	1.46	0.79
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.63	0.79
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.65	0.79
1:C:893:PRO:O	1:C:896:VAL:N	2.15	0.79
1:B:56:THR:O	1:B:60:THR:OG1	1.99	0.79
1:E:446:ALA:HB2	1:E:482:VAL:HG21	1.65	0.79
1:A:53:ASP:OD1	1:A:56:THR:OG1	2.00	0.79
1:B:415:ASN:OD1	1:B:418:ARG:NH1	2.14	0.78
1:E:272:GLY:N	1:E:275:TYR:OH	2.15	0.78
1:B:102:ILE:O	1:B:106:GLN:HG3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:398:MET:HG2	1:F:473:THR:HG21	1.65	0.78
1:F:698:LEU:HD11	1:F:713:PRO:HD3	1.64	0.78
1:A:941:VAL:HG13	1:A:1021:PHE:CD1	2.19	0.78
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.64	0.78
1:B:310:LEU:HD23	1:B:323:ILE:HG21	1.65	0.77
1:E:262:LEU:HG	1:E:268:ILE:HD11	1.64	0.77
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.66	0.77
1:E:896:VAL:HG21	1:E:938:ILE:HG13	1.66	0.77
1:B:156:ASP:OD1	1:B:760:ARG:NH2	2.18	0.77
1:B:966:ARG:O	1:B:970:ILE:HG12	1.85	0.77
1:C:659:PHE:CD2	1:C:712:ARG:HD2	2.20	0.77
1:D:108:GLN:NE2	1:E:109:ASN:O	2.17	0.77
1:F:893:PRO:O	1:F:896:VAL:N	2.18	0.77
1:F:896:VAL:HG23	1:F:937:ALA:HB3	1.67	0.77
1:D:519:MET:O	1:D:523:SER:OG	2.02	0.77
1:F:966:ARG:HB3	1:F:966:ARG:CZ	2.14	0.77
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.67	0.77
1:A:73:ASP:OD2	1:C:131:LYS:NZ	2.16	0.77
1:D:963:VAL:HA	1:D:966:ARG:HH22	1.50	0.76
1:E:73:ASP:H	1:E:106:GLN:HE22	1.32	0.76
1:E:974:SER:OG	1:E:1010:THR:HG21	1.84	0.76
1:C:984:LEU:O	1:C:996:ASN:ND2	2.18	0.76
1:A:400:LEU:HD21	1:A:925:GLY:HA2	1.66	0.76
1:C:396:PHE:CD1	1:C:998:VAL:HG21	2.20	0.76
1:C:892:ILE:HG23	1:C:941:VAL:HG11	1.68	0.76
1:D:253:VAL:HG12	1:D:259:ARG:HG2	1.66	0.76
1:D:1014:ILE:HG13	1:D:1015:PHE:HD1	1.51	0.76
1:E:102:ILE:O	1:E:106:GLN:HG3	1.85	0.76
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.66	0.76
1:E:448:VAL:HG13	1:E:879:VAL:HG22	1.67	0.76
1:E:356:TYR:O	1:E:358:PHE:N	2.17	0.76
1:C:356:TYR:O	1:C:358:PHE:N	2.19	0.76
1:F:5:PHE:O	1:F:7:ASP:N	2.19	0.76
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.67	0.75
1:C:3:ASN:N	1:C:3:ASN:OD1	2.17	0.75
1:C:414:GLU:HG2	1:C:968:ARG:HH11	1.51	0.75
1:E:1032:ASN:H	1:E:1033:GLU:HB2	1.49	0.75
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.68	0.75
1:D:424:GLY:HA3	1:D:502:LYS:HB3	1.67	0.75
1:D:908:LEU:HD23	1:D:922:PHE:HZ	1.52	0.75
1:E:156:ASP:OD1	1:E:760:ARG:NH2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:827:ALA:HB3	1:E:830:LYS:HD3	1.67	0.75
1:A:977:PHE:O	1:A:980:GLY:N	2.19	0.75
1:D:677:PHE:HB3	1:D:822:ILE:HB	1.68	0.75
1:E:694:ARG:HH11	1:E:820:MET:HE1	1.52	0.75
1:F:400:LEU:HB3	1:F:474:ILE:HD11	1.69	0.75
1:A:1032:ASN:HA	1:A:1035:ILE:HD11	1.69	0.75
1:C:356:TYR:C	1:C:358:PHE:H	1.90	0.75
1:D:60:THR:HG23	1:D:61:VAL:HG23	1.67	0.75
1:A:453:PHE:O	1:A:471:SER:OG	2.04	0.74
1:F:228:GLN:NE2	1:F:230:LEU:O	2.19	0.74
1:C:714:ASN:HB3	1:C:821:GLU:HB3	1.69	0.74
1:B:762:ARG:HG2	1:B:762:ARG:HH11	1.51	0.74
1:E:32:VAL:HG12	1:E:390:ILE:HB	1.67	0.74
1:E:62:THR:HG21	1:E:813:ARG:HD3	1.67	0.74
1:A:400:LEU:HD23	1:A:924:VAL:HG12	1.69	0.74
1:A:827:ALA:HB3	1:A:830:LYS:HD3	1.69	0.74
1:C:120:GLN:HA	1:C:123:GLN:HB2	1.68	0.74
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.69	0.74
1:A:382:VAL:HG11	1:A:476:SER:HB2	1.69	0.74
1:A:974:SER:OG	1:A:1010:THR:HG21	1.86	0.74
1:D:883:LEU:HD13	1:D:896:VAL:HG13	1.70	0.74
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.69	0.74
1:E:530:SER:OG	3:E:1101:LMT:O2'	2.04	0.74
1:D:400:LEU:HD23	1:D:924:VAL:HG12	1.70	0.73
1:E:228:GLN:NE2	1:E:230:LEU:O	2.21	0.73
1:D:977:PHE:O	1:D:980:GLY:N	2.22	0.73
1:E:1034:ASP:O	1:E:1036:GLU:N	2.20	0.73
1:E:396:PHE:O	1:E:400:LEU:HB2	1.88	0.73
1:A:694:ARG:NH2	1:A:717:GLU:OE1	2.21	0.73
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.69	0.73
1:E:356:TYR:C	1:E:358:PHE:H	1.92	0.73
1:A:984:LEU:O	1:A:996:ASN:ND2	2.22	0.73
1:F:356:TYR:O	1:F:358:PHE:N	2.22	0.73
1:B:762:ARG:HH12	1:C:117:LEU:HD13	1.53	0.73
1:D:770:SER:OG	1:D:771:GLU:O	2.06	0.73
1:C:507:GLU:HG2	1:C:518:ARG:HG3	1.71	0.72
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.71	0.72
1:C:449:LEU:HD21	1:C:932:LEU:HD23	1.71	0.72
1:D:735:GLY:O	1:D:789:ALA:N	2.23	0.72
1:D:456:MET:HG3	1:D:927:LEU:HD11	1.71	0.72
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:THR:HG23	1:E:61:VAL:HG23	1.69	0.72
1:E:694:ARG:HD2	1:E:713:PRO:HB3	1.69	0.72
1:C:239:ARG:HH12	1:C:756:ASP:H	1.37	0.72
1:D:355:MET:HB3	1:D:365:THR:OG1	1.90	0.72
1:F:99:ASP:HB3	1:F:102:ILE:HB	1.72	0.72
1:B:362:PHE:O	1:B:365:THR:HG22	1.90	0.72
1:C:158:VAL:HG22	1:C:162:MET:HE3	1.72	0.72
1:C:79:SER:HB3	1:C:814:TYR:HD1	1.54	0.72
1:A:728:GLN:HE22	1:A:738:ILE:HG21	1.54	0.72
1:C:426:PRO:HD2	1:C:429:GLU:HB3	1.70	0.72
1:D:453:PHE:O	1:D:471:SER:OG	2.07	0.71
1:A:491:ALA:O	1:A:495:THR:OG1	2.08	0.71
1:B:73:ASP:H	1:B:106:GLN:HE22	1.38	0.71
1:B:663:LEU:HD23	1:B:663:LEU:H	1.56	0.71
1:C:66:GLU:OE2	1:C:80:SER:OG	2.08	0.71
1:F:563:PHE:HB2	1:F:861:GLU:HG3	1.71	0.71
1:B:166:ILE:HD11	1:B:310:LEU:HD11	1.71	0.71
1:C:13:TRP:HH2	1:C:370:ILE:HD13	1.54	0.71
1:C:663:LEU:H	1:C:663:LEU:HD23	1.55	0.71
1:B:236:ALA:O	1:C:723:LYS:NZ	2.24	0.71
1:C:977:PHE:O	1:C:980:GLY:N	2.23	0.71
1:D:170:SER:HB2	1:E:75:LEU:H	1.55	0.71
1:B:680:ILE:HD11	1:B:814:TYR:HD2	1.54	0.71
1:B:404:LEU:HD23	1:B:478:MET:HG3	1.73	0.71
1:C:683:ALA:O	1:C:685:LEU:N	2.24	0.71
1:A:923:GLN:HG2	3:A:1103:LMT:H12	1.71	0.71
1:A:186:ILE:HB	1:A:768:VAL:HG22	1.70	0.71
1:B:26:ALA:O	1:B:30:LEU:HB2	1.91	0.71
1:B:700:GLU:HB3	1:B:842:LEU:HD22	1.72	0.71
1:E:44:THR:HG1	1:E:91:THR:HG1	1.35	0.71
1:C:889:SER:HB3	1:C:892:ILE:HG12	1.71	0.70
1:E:362:PHE:O	1:E:365:THR:HG22	1.91	0.70
1:E:593:GLU:OE1	1:E:654:LYS:NZ	2.23	0.70
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.73	0.70
1:B:555:LEU:HD11	1:B:909:LEU:HD12	1.72	0.70
1:D:272:GLY:N	1:D:275:TYR:OH	2.23	0.70
1:C:803:ARG:NH1	1:C:805:GLU:OE2	2.25	0.70
1:D:708:LEU:HD21	1:D:838:LEU:HD12	1.73	0.70
1:F:770:SER:OG	1:F:771:GLU:O	2.10	0.70
1:F:887:TYR:O	1:F:889:SER:N	2.24	0.70
1:C:669:LEU:HD13	1:C:856:GLY:HA2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:TYR:CZ	1:D:318:PRO:HD3	2.26	0.70
1:F:659:PHE:CD2	1:F:712:ARG:HD2	2.27	0.70
1:D:382:VAL:HG11	1:D:476:SER:HB2	1.74	0.70
1:B:452:VAL:HG23	1:B:453:PHE:CD2	2.27	0.70
1:B:448:VAL:HG13	1:B:879:VAL:HG22	1.74	0.70
1:D:80:SER:HB3	1:D:90:ILE:HG23	1.74	0.70
1:F:422:GLU:O	1:F:502:LYS:HG3	1.92	0.70
1:D:1014:ILE:HG13	1:D:1015:PHE:CD1	2.25	0.70
1:A:1014:ILE:HG13	1:A:1015:PHE:HD1	1.55	0.70
1:D:967:LEU:HD11	3:D:1102:LMT:H123	1.72	0.70
1:A:883:LEU:HD13	1:A:896:VAL:HG13	1.74	0.69
1:D:904:VAL:HG13	1:D:926:LEU:HD11	1.74	0.69
1:E:378:GLY:O	1:E:382:VAL:HG23	1.92	0.69
1:A:530:SER:CB	3:A:1102:LMT:H2O2	2.03	0.69
1:D:910:ALA:HB2	1:D:1004:GLY:HA3	1.74	0.69
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.75	0.69
1:F:348:ILE:HG13	1:F:402:ILE:HD13	1.74	0.69
1:C:453:PHE:HZ	1:C:928:THR:HG1	1.40	0.69
1:D:562:SER:HB2	1:D:919:ASP:HB3	1.74	0.69
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.27	0.69
1:B:356:TYR:C	1:B:358:PHE:H	1.96	0.69
1:E:706:ASP:O	1:E:830:LYS:NZ	2.24	0.69
1:A:230:LEU:HD21	1:B:804:TRP:HH2	1.57	0.69
1:C:380:PHE:CD2	1:C:383:LEU:HD12	2.27	0.69
1:E:691:THR:HG23	1:E:694:ARG:HH12	1.57	0.69
1:A:274:ASN:ND2	1:A:276:ASP:OD2	2.20	0.69
1:A:451:ALA:HB1	1:A:878:VAL:HG12	1.73	0.69
1:C:902:LEU:HD23	1:C:1012:LEU:HB3	1.73	0.69
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.27	0.69
1:D:39:ALA:HB2	1:D:668:GLU:HG3	1.73	0.69
1:A:1008:THR:O	1:A:1012:LEU:HB2	1.93	0.69
1:A:355:MET:HB3	1:A:365:THR:OG1	1.90	0.69
1:B:445:ILE:HG21	1:B:935:LYS:HD2	1.74	0.69
1:C:519:MET:O	1:C:523:SER:OG	2.08	0.69
1:E:562:SER:OG	1:E:563:PHE:N	2.24	0.69
1:A:277:ILE:HG12	1:A:614:GLY:HA3	1.75	0.69
1:C:902:LEU:HG	1:C:1012:LEU:HD23	1.74	0.69
1:E:442:LEU:O	1:E:445:ILE:HG13	1.93	0.69
1:F:196:PHE:O	1:F:252:LYS:NZ	2.24	0.69
1:F:382:VAL:HG11	1:F:476:SER:HB2	1.75	0.69
1:A:424:GLY:HA3	1:A:502:LYS:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:855:THR:HA	1:C:859:TYR:HB2	1.75	0.68
1:B:101:ASP:OD1	1:B:131:LYS:NZ	2.24	0.68
1:B:6:ILE:O	1:B:428:LYS:NZ	2.26	0.68
1:E:663:LEU:HD23	1:E:663:LEU:H	1.59	0.68
1:E:683:ALA:O	1:E:685:LEU:N	2.26	0.68
1:F:461:GLY:HA3	1:F:863:LEU:HD21	1.74	0.68
1:F:908:LEU:HD23	1:F:922:PHE:HZ	1.58	0.68
1:B:363:ARG:HD3	1:B:496:MET:O	1.92	0.68
1:C:104:GLN:OE1	1:C:108:GLN:NE2	2.27	0.68
1:F:108:GLN:HB2	1:F:129:VAL:HG21	1.75	0.68
1:F:452:VAL:O	1:F:455:PRO:HD2	1.93	0.68
1:E:770:SER:OG	1:E:771:GLU:O	2.11	0.68
1:E:41:PRO:HG2	1:E:94:PHE:HB2	1.76	0.68
1:C:918:ASN:ND2	1:C:923:GLN:HE21	1.90	0.68
1:D:609:VAL:HG22	1:D:624:VAL:HG13	1.75	0.68
1:D:617:GLN:NE2	1:F:220:GLY:O	2.25	0.68
1:A:770:SER:OG	1:A:771:GLU:O	2.10	0.68
1:B:41:PRO:HG2	1:B:94:PHE:HB2	1.76	0.68
1:A:25:LEU:HD21	1:B:874:ILE:HD11	1.76	0.68
1:F:42:ALA:HB2	1:F:93:THR:HG23	1.74	0.68
1:A:1014:ILE:HG13	1:A:1015:PHE:CD1	2.29	0.67
1:A:435:MET:HG3	1:A:490:PRO:HB3	1.75	0.67
2:D:1101:ERY:H151	2:D:1101:ERY:H302	1.75	0.67
1:D:568:ASP:OD1	1:D:632:ARG:NH1	2.17	0.67
1:D:914:ARG:NH1	1:D:1000:THR:OG1	2.26	0.67
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.76	0.67
1:D:1015:PHE:CE2	3:D:1102:LMT:H32	2.28	0.67
1:F:936:ASN:HD21	1:F:1010:THR:HG22	1.59	0.67
1:B:335:ILE:HG21	1:B:990:ALA:HB3	1.77	0.67
1:A:210:GLN:HE22	1:A:250:LEU:H	1.42	0.67
1:C:452:VAL:HG23	1:C:453:PHE:HD1	1.60	0.67
1:D:316:PHE:CD1	1:E:682:GLN:HG2	2.29	0.67
1:E:404:LEU:HD23	1:E:478:MET:HG3	1.76	0.67
1:B:272:GLY:N	1:B:275:TYR:OH	2.21	0.67
1:D:1030:ARG:O	1:D:1031:LYS:HE2	1.94	0.67
1:E:165:ALA:HB3	1:E:313:MET:CE	2.24	0.67
1:A:663:LEU:HD23	1:A:663:LEU:H	1.60	0.67
1:C:6:ILE:HG21	1:C:487:ILE:HG23	1.76	0.67
1:E:853:ASP:OD1	1:E:854:TRP:N	2.27	0.67
1:B:1014:ILE:HG13	1:B:1015:PHE:CD1	2.29	0.67
1:E:174:ASP:HB3	1:E:292:LYS:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ASN:O	1:A:6:ILE:HG12	1.94	0.67
1:C:738:ILE:O	1:C:741:ILE:HG13	1.95	0.67
1:D:535:LEU:HD21	1:D:1022:VAL:HG21	1.76	0.67
1:E:324:VAL:HG13	1:E:326:PRO:HD3	1.76	0.67
1:B:536:ARG:NH2	3:B:2100:LMT:O3B	2.28	0.67
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.77	0.67
1:E:375:VAL:HG11	1:E:405:LEU:HD22	1.75	0.67
1:F:700:GLU:HA	1:F:703:LYS:HE3	1.77	0.67
1:F:545:TYR:OH	1:F:898:LEU:O	2.06	0.67
3:B:2100:LMT:H5B	3:B:2100:LMT:H6E	1.77	0.66
1:D:400:LEU:HD11	1:D:1002:VAL:HG21	1.77	0.66
1:D:771:GLU:HG2	1:D:773:LYS:HG2	1.77	0.66
1:E:143:ILE:HG22	1:E:286:ALA:HB2	1.77	0.66
1:E:435:MET:SD	1:E:490:PRO:HB3	2.34	0.66
1:E:441:ALA:HA	1:E:886:LEU:HD21	1.76	0.66
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.77	0.66
1:A:31:PRO:HB2	1:A:389:SER:HB2	1.78	0.66
1:C:723:LYS:HG2	1:C:803:ARG:CZ	2.25	0.66
1:D:981:VAL:HG12	1:D:1003:MET:HE3	1.75	0.66
1:E:26:ALA:O	1:E:30:LEU:HB2	1.95	0.66
1:F:586:ARG:HA	1:F:589:LYS:HD2	1.77	0.66
1:B:770:SER:OG	1:B:771:GLU:O	2.13	0.66
1:C:614:GLY:HA2	1:C:616:GLY:N	2.10	0.66
1:C:940:ILE:HD13	1:C:963:VAL:HG22	1.76	0.66
1:E:977:PHE:O	1:E:980:GLY:N	2.28	0.66
1:A:17:ILE:HG22	1:B:881:LEU:HD21	1.77	0.66
1:B:378:GLY:O	1:B:382:VAL:HG23	1.95	0.66
1:C:735:GLY:O	1:C:789:ALA:N	2.28	0.66
1:D:897:MET:O	1:D:900:VAL:HG23	1.96	0.66
1:C:1014:ILE:HG13	1:C:1015:PHE:CD1	2.31	0.66
1:D:586:ARG:O	1:D:589:LYS:HB3	1.96	0.66
1:E:530:SER:CB	3:E:1101:LMT:H2O2	2.09	0.66
1:B:455:PRO:O	1:B:871:LEU:HD13	1.95	0.66
1:C:101:ASP:OD1	1:C:131:LYS:NZ	2.24	0.66
1:C:228:GLN:NE2	1:C:230:LEU:O	2.28	0.66
1:C:404:LEU:HB3	1:C:478:MET:SD	2.36	0.66
1:F:954:GLY:HA2	1:F:1035:ILE:HG13	1.78	0.66
1:A:281:PHE:HE1	1:A:608:SER:HB2	1.61	0.66
1:C:53:ASP:O	1:C:56:THR:HB	1.96	0.66
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.78	0.66
1:A:140:VAL:HB	1:A:289:LEU:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:THR:HB	1:A:826:ALA:HB3	1.77	0.66
1:D:293:LEU:HD11	1:D:299:ALA:HA	1.78	0.66
1:D:663:LEU:H	1:D:663:LEU:HD23	1.61	0.66
1:E:981:VAL:HG21	1:E:1002:VAL:HG11	1.76	0.66
1:C:414:GLU:HG2	1:C:968:ARG:NH1	2.10	0.65
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.78	0.65
1:D:730:LYS:O	1:D:734:LEU:HG	1.97	0.65
1:E:578:LEU:HD21	1:E:590:VAL:HG21	1.79	0.65
1:B:143:ILE:HG22	1:B:286:ALA:HB2	1.78	0.65
1:C:300:LEU:HD11	1:C:333:VAL:HG11	1.77	0.65
1:B:225:VAL:HG12	1:C:772:ALA:HB1	1.77	0.65
1:E:53:ASP:OD1	1:E:56:THR:OG1	2.11	0.65
1:B:100:ALA:HB1	1:B:131:LYS:HE3	1.79	0.65
1:B:14:VAL:HG22	1:C:881:LEU:HD13	1.79	0.65
1:B:166:ILE:HD11	1:B:310:LEU:CD1	2.26	0.65
1:B:562:SER:OG	1:B:563:PHE:N	2.26	0.65
1:C:836:MET:O	1:C:840:GLU:HG2	1.96	0.65
1:A:897:MET:O	1:A:900:VAL:HG23	1.97	0.65
1:B:883:LEU:HD13	1:B:896:VAL:HG11	1.76	0.65
1:C:372:VAL:HA	1:C:405:LEU:HD11	1.76	0.65
1:F:356:TYR:HA	1:F:365:THR:HG21	1.78	0.65
1:F:685:LEU:O	1:F:689:LYS:HB2	1.96	0.65
1:A:790:ASP:OD2	1:A:791:GLY:N	2.28	0.65
1:B:554:TYR:CZ	1:B:558:ARG:HG3	2.31	0.65
1:D:695:ASN:HA	1:D:698:LEU:HD12	1.78	0.65
1:D:836:MET:HE1	1:D:862:ARG:HB2	1.78	0.65
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.79	0.65
1:F:398:MET:HG2	1:F:473:THR:CG2	2.27	0.65
1:D:309:GLU:HA	1:D:312:LYS:HD2	1.79	0.65
1:E:691:THR:HG23	1:E:694:ARG:NH1	2.12	0.65
1:F:66:GLU:OE1	1:F:816:GLY:HA2	1.97	0.65
1:F:443:VAL:HG12	1:F:886:LEU:HD21	1.79	0.65
1:F:940:ILE:HA	1:F:966:ARG:NH1	2.12	0.65
1:A:18:ILE:HG13	1:B:881:LEU:HD23	1.79	0.65
1:F:940:ILE:HG12	1:F:966:ARG:HH22	1.62	0.65
1:A:112:GLN:HG3	1:B:112:GLN:OE1	1.96	0.64
1:D:992:SER:HA	1:D:995:GLN:HB2	1.79	0.64
1:E:14:VAL:HG22	1:F:881:LEU:HD13	1.80	0.64
1:E:219:LEU:HD13	1:F:778:PRO:HG3	1.77	0.64
1:A:1032:ASN:O	1:A:1033:GLU:HB2	1.97	0.64
1:B:508:GLY:HA2	1:B:518:ARG:HE	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:614:GLY:HA2	1:F:616:GLY:N	2.11	0.64
1:A:4:PHE:HB3	1:A:8:ARG:NH1	2.13	0.64
1:A:531:VAL:HG11	1:A:963:VAL:HG11	1.79	0.64
1:C:274:ASN:ND2	1:C:276:ASP:OD2	2.30	0.64
1:C:351:VAL:HG11	1:C:406:VAL:HG21	1.79	0.64
1:C:452:VAL:HG23	1:C:453:PHE:CD1	2.31	0.64
1:D:795:PRO:HG2	1:D:798:ALA:HB2	1.80	0.64
1:D:974:SER:OG	1:D:1010:THR:HG21	1.97	0.64
1:F:187:TRP:HB3	1:F:771:GLU:HA	1.80	0.64
1:C:1029:SER:OG	1:C:1030:ARG:N	2.30	0.64
1:F:578:LEU:HB2	1:F:618:ASN:O	1.98	0.64
1:B:165:ALA:HB3	1:B:313:MET:HE2	1.80	0.64
1:F:593:GLU:OE1	1:F:654:LYS:NZ	2.23	0.64
1:F:455:PRO:HB3	1:F:874:ILE:HG22	1.80	0.64
1:D:914:ARG:NH2	1:D:985:VAL:O	2.24	0.64
1:A:465:ALA:O	1:A:469:GLN:HG2	1.98	0.64
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.77	0.64
1:C:586:ARG:HA	1:C:589:LYS:HD2	1.80	0.64
1:C:78:MET:HG3	1:C:92:LEU:HD13	1.80	0.64
1:E:367:ILE:HB	1:E:368:PRO:HD3	1.80	0.64
1:F:587:THR:OG1	1:F:613:ASN:ND2	2.31	0.64
1:A:157:TYR:CZ	1:A:318:PRO:HD3	2.33	0.64
1:B:408:ASP:OD1	1:B:935:LYS:NZ	2.25	0.64
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.80	0.64
1:E:536:ARG:HG3	3:E:1101:LMT:O3B	1.96	0.64
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.78	0.63
1:B:709:THR:HG22	1:B:825:GLN:HG3	1.80	0.63
1:D:442:LEU:O	1:D:445:ILE:HG13	1.98	0.63
1:F:379:THR:HG23	1:F:476:SER:OG	1.98	0.63
1:D:18:ILE:HG13	1:E:881:LEU:HD23	1.78	0.63
1:F:380:PHE:HD2	1:F:383:LEU:HD12	1.63	0.63
1:F:343:THR:HG21	1:F:984:LEU:HD21	1.79	0.63
1:D:146:ASP:OD2	1:D:146:ASP:N	2.31	0.63
1:E:441:ALA:O	1:E:445:ILE:HG23	1.99	0.63
1:E:544:LEU:O	1:E:548:ILE:HG13	1.98	0.63
1:D:187:TRP:HH2	1:F:223:PRO:HD2	1.63	0.63
1:A:883:LEU:HB2	1:A:893:PRO:HB3	1.80	0.63
1:E:1030:ARG:H	1:E:1030:ARG:HH11	1.45	0.63
1:D:221:GLY:H	1:E:775:ARG:HH12	1.45	0.63
1:A:38:ILE:HG23	1:A:462:SER:HB2	1.81	0.63
1:B:340:VAL:HG22	1:B:396:PHE:HE1	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:VAL:HG23	1:B:82:SER:HB3	1.81	0.63
1:C:396:PHE:O	1:C:400:LEU:HB2	1.97	0.63
1:A:796:PHE:HD1	1:A:799:PHE:HE2	1.46	0.63
1:C:521:GLU:O	1:C:524:THR:HG23	1.99	0.63
1:C:890:TRP:CE3	1:C:890:TRP:HA	2.33	0.63
1:D:170:SER:OG	1:E:74:ASN:N	2.28	0.63
1:D:210:GLN:HE22	1:D:250:LEU:HB3	1.63	0.63
1:D:584:GLN:HB2	1:D:617:GLN:HG2	1.81	0.63
1:E:1008:THR:O	1:E:1012:LEU:HB2	1.99	0.63
1:D:31:PRO:O	1:D:389:SER:HB2	1.99	0.63
1:E:327:TYR:HB2	1:E:623:PHE:CZ	2.33	0.63
1:F:82:SER:HB2	1:F:811:LEU:HB2	1.80	0.63
1:A:669:LEU:HD22	1:A:670:GLY:H	1.63	0.63
1:A:66:GLU:OE1	1:A:816:GLY:HA2	1.99	0.63
1:D:678:GLU:HG2	1:D:814:TYR:CG	2.33	0.63
1:F:588:GLN:O	1:F:592:ASN:ND2	2.32	0.63
1:A:575:MET:HA	1:A:621:ILE:HG13	1.81	0.62
1:B:584:GLN:HB2	1:B:617:GLN:HG2	1.79	0.62
1:C:272:GLY:N	1:C:275:TYR:OH	2.26	0.62
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.80	0.62
1:F:348:ILE:HG12	1:F:372:VAL:HG11	1.80	0.62
1:A:400:LEU:HD11	1:A:1002:VAL:HG21	1.81	0.62
1:A:228:GLN:NE2	1:A:230:LEU:O	2.32	0.62
1:D:1029:SER:OG	1:D:1030:ARG:N	2.30	0.62
1:D:790:ASP:OD2	1:D:791:GLY:N	2.31	0.62
1:F:893:PRO:HA	1:F:896:VAL:HG12	1.79	0.62
1:B:1008:THR:O	1:B:1012:LEU:HB2	2.00	0.62
1:C:896:VAL:HG23	1:C:937:ALA:HB3	1.79	0.62
1:D:103:ALA:HA	1:D:106:GLN:HE21	1.64	0.62
1:A:243:THR:HG23	1:A:268:ILE:HG22	1.82	0.62
1:A:67:GLN:OE1	1:C:762:ARG:NH1	2.32	0.62
1:B:900:VAL:HG13	1:B:930:ILE:HG23	1.80	0.62
1:C:674:GLY:HA2	1:C:832:THR:HG23	1.80	0.62
1:E:351:VAL:HG21	1:E:406:VAL:HG11	1.80	0.62
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.80	0.62
1:A:244:GLU:HG2	1:A:248:LYS:HE2	1.81	0.62
1:C:386:PHE:CD2	1:C:472:ILE:HD11	2.34	0.62
1:F:404:LEU:HB3	1:F:478:MET:SD	2.39	0.62
1:F:939:LEU:HB3	1:F:966:ARG:NE	2.14	0.62
1:A:941:VAL:HG13	1:A:1021:PHE:HD1	1.65	0.62
1:A:795:PRO:HG2	1:A:798:ALA:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1014:ILE:HG13	1:F:1015:PHE:CD1	2.34	0.62
1:F:952:GLY:O	1:F:1036:GLU:HA	2.00	0.62
1:F:380:PHE:CD2	1:F:383:LEU:HD12	2.35	0.62
1:D:344:LEU:HD21	1:D:399:VAL:HA	1.80	0.62
1:D:457:ALA:O	1:D:468:ARG:NE	2.33	0.62
1:F:251:LEU:HD11	1:F:262:LEU:HA	1.81	0.62
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.80	0.62
1:B:507:GLU:O	1:B:509:LYS:N	2.33	0.62
1:C:616:GLY:HA3	1:C:618:ASN:N	2.15	0.62
1:C:939:LEU:HB3	1:C:966:ARG:CD	2.29	0.62
1:F:506:GLY:O	1:F:508:GLY:N	2.29	0.62
1:A:770:SER:HB3	1:A:775:ARG:HD3	1.81	0.62
1:A:785:TYR:HB3	1:A:793:MET:HB3	1.82	0.62
1:B:1014:ILE:HG13	1:B:1015:PHE:HD1	1.63	0.61
1:B:770:SER:HB3	1:B:775:ARG:HD3	1.81	0.61
1:C:693:ALA:O	1:C:696:GLN:HB3	2.00	0.61
1:A:84:SER:HB3	1:A:809:PRO:HA	1.82	0.61
1:B:36:PRO:HD2	1:B:38:ILE:HD11	1.81	0.61
1:B:691:THR:HG23	1:B:694:ARG:NH1	2.15	0.61
1:B:977:PHE:O	1:B:980:GLY:N	2.32	0.61
1:D:556:PHE:HD1	1:D:908:LEU:HD21	1.64	0.61
1:E:115:MET:O	1:E:123:GLN:NE2	2.33	0.61
1:F:120:GLN:HA	1:F:123:GLN:HB2	1.82	0.61
1:F:324:VAL:HG23	1:F:326:PRO:HD3	1.82	0.61
1:F:455:PRO:HG3	1:F:878:VAL:HG21	1.82	0.61
1:C:443:VAL:HG12	1:C:886:LEU:HD21	1.82	0.61
1:C:614:GLY:HA2	1:C:616:GLY:H	1.66	0.61
1:C:897:MET:O	1:C:900:VAL:HG23	2.00	0.61
1:F:356:TYR:C	1:F:358:PHE:H	2.04	0.61
1:F:892:ILE:HG23	1:F:941:VAL:HG11	1.81	0.61
1:A:80:SER:HB3	1:A:90:ILE:HG23	1.82	0.61
1:B:803:ARG:NH1	1:B:805:GLU:OE2	2.33	0.61
1:E:1015:PHE:HE2	3:E:1101:LMT:H11	1.65	0.61
1:E:187:TRP:HB3	1:E:771:GLU:HA	1.82	0.61
1:F:376:LEU:HD22	1:F:398:MET:HE3	1.81	0.61
1:B:647:THR:CG2	1:B:660:ALA:H	2.14	0.61
1:E:892:ILE:O	1:E:895:SER:OG	2.16	0.61
1:C:649:ALA:O	1:C:653:ILE:HG12	1.99	0.61
1:C:985:VAL:HG13	1:C:1000:THR:OG1	1.99	0.61
1:F:425:LEU:HD22	1:F:429:GLU:HG2	1.82	0.61
1:D:56:THR:O	1:D:60:THR:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:GLN:HG3	1:E:813:ARG:HD2	1.83	0.61
1:E:690:LEU:HD22	1:E:820:MET:SD	2.41	0.61
1:F:616:GLY:HA3	1:F:617:GLN:C	2.20	0.61
1:B:108:GLN:OE1	1:C:112:GLN:HB3	2.01	0.61
1:B:420:MET:HB3	1:B:500:ILE:HB	1.82	0.61
1:B:683:ALA:O	1:B:685:LEU:N	2.32	0.61
1:B:762:ARG:HG2	1:B:762:ARG:NH1	2.15	0.61
1:A:881:LEU:HD11	1:C:17:ILE:CG2	2.31	0.61
1:C:398:MET:HG2	1:C:473:THR:HG21	1.83	0.61
1:D:351:VAL:HG22	1:D:976:ALA:HB1	1.83	0.61
1:F:576:VAL:HG22	1:F:658:VAL:HG13	1.82	0.61
1:F:746:GLY:O	1:F:750:GLY:N	2.29	0.61
1:A:588:GLN:HE21	1:A:592:ASN:HD21	1.49	0.61
1:A:885:ALA:HB2	1:C:14:VAL:HG11	1.83	0.61
1:B:61:VAL:CG2	1:B:122:VAL:HG21	2.31	0.61
1:C:404:LEU:HD11	1:C:932:LEU:HD21	1.82	0.61
1:C:80:SER:HB3	1:C:90:ILE:HG23	1.81	0.61
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.82	0.61
1:D:182:TYR:HB2	1:D:764:LYS:NZ	2.16	0.61
1:F:163:LYS:HD2	1:F:177:LEU:HD23	1.81	0.61
1:B:262:LEU:HG	1:B:268:ILE:HD11	1.82	0.60
1:B:900:VAL:HB	1:B:901:PRO:HD3	1.83	0.60
1:C:72:ILE:HD12	1:C:75:LEU:HD22	1.83	0.60
1:C:871:LEU:HD22	1:C:927:LEU:HD11	1.83	0.60
1:C:935:LYS:HZ1	1:C:973:THR:HG21	1.65	0.60
1:D:186:ILE:HB	1:D:768:VAL:HG22	1.81	0.60
1:D:448:VAL:HG22	1:D:882:CYS:HB3	1.83	0.60
1:E:355:MET:SD	1:E:365:THR:HA	2.40	0.60
1:F:563:PHE:HD2	1:F:564:LEU:HB2	1.66	0.60
1:F:614:GLY:HA2	1:F:616:GLY:H	1.66	0.60
1:F:69:MET:HB3	1:F:72:ILE:HD11	1.81	0.60
1:B:1010:THR:O	1:B:1012:LEU:N	2.35	0.60
1:B:545:TYR:OH	1:B:898:LEU:O	2.16	0.60
1:C:465:ALA:HA	1:C:468:ARG:HH11	1.66	0.60
1:E:574:THR:HG23	1:E:622:ALA:HB3	1.82	0.60
1:B:404:LEU:HD21	1:B:449:LEU:HD22	1.82	0.60
1:B:574:THR:HG23	1:B:622:ALA:HB3	1.82	0.60
1:B:73:ASP:H	1:B:106:GLN:NE2	1.98	0.60
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.37	0.60
1:E:677:PHE:CZ	1:E:852:TYR:HB2	2.37	0.60
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:VAL:HA	1:C:118:LEU:CD2	2.31	0.60
1:D:770:SER:HB3	1:D:775:ARG:HD3	1.84	0.60
1:A:567:GLU:O	1:A:569:GLN:HG3	2.01	0.60
1:A:739:ASN:O	1:A:743:THR:HG23	2.00	0.60
1:A:939:LEU:HB3	1:A:966:ARG:HD2	1.82	0.60
1:B:674:GLY:HA2	1:B:825:GLN:HA	1.82	0.60
1:B:414:GLU:OE1	1:B:968:ARG:NH1	2.35	0.60
1:C:890:TRP:HA	1:C:890:TRP:HE3	1.66	0.60
1:E:73:ASP:H	1:E:106:GLN:NE2	1.98	0.60
1:F:902:LEU:HD23	1:F:1012:LEU:HB3	1.82	0.60
1:D:184:MET:HB2	1:D:757:PHE:CE2	2.37	0.60
1:E:56:THR:O	1:E:60:THR:HG22	2.00	0.60
1:F:683:ALA:O	1:F:685:LEU:N	2.35	0.60
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.83	0.60
1:C:137:LEU:HD22	1:C:293:LEU:HG	1.82	0.60
1:F:902:LEU:HG	1:F:1012:LEU:HD23	1.83	0.60
1:D:790:ASP:OD2	1:D:792:GLN:HG3	2.01	0.60
1:E:813:ARG:HH12	1:E:818:PRO:HG3	1.67	0.60
1:E:904:VAL:O	1:E:907:ALA:N	2.35	0.60
1:F:507:GLU:HG2	1:F:518:ARG:HG3	1.83	0.60
1:A:694:ARG:HD2	1:A:713:PRO:HB3	1.84	0.59
1:A:790:ASP:OD2	1:A:792:GLN:N	2.31	0.59
1:B:281:PHE:CE2	1:B:324:VAL:HG21	2.36	0.59
1:C:714:ASN:O	1:C:810:ARG:NH2	2.33	0.59
1:E:181:GLN:OE1	1:E:762:ARG:NH2	2.35	0.59
1:F:883:LEU:HD21	1:F:938:ILE:HD11	1.84	0.59
1:B:1032:ASN:HB3	1:B:1035:ILE:HG22	1.82	0.59
1:B:559:LEU:HG	1:B:560:PRO:HD2	1.83	0.59
1:C:239:ARG:NH1	1:C:756:ASP:H	1.99	0.59
1:C:586:ARG:O	1:C:589:LYS:HB2	2.02	0.59
1:C:69:MET:HG2	1:C:92:LEU:HD11	1.82	0.59
1:E:650:PHE:HA	1:E:654:LYS:HD3	1.83	0.59
1:F:563:PHE:CD2	1:F:564:LEU:HB2	2.37	0.59
1:F:277:ILE:HG12	1:F:614:GLY:O	2.02	0.59
1:A:941:VAL:HG22	1:A:1021:PHE:HB2	1.84	0.59
1:C:455:PRO:HG2	1:C:875:SER:HA	1.84	0.59
1:D:723:LYS:NZ	1:F:236:ALA:O	2.34	0.59
1:A:119:PRO:HB2	1:A:122:VAL:HB	1.83	0.59
1:F:445:ILE:HG23	1:F:935:LYS:HG3	1.83	0.59
1:F:693:ALA:O	1:F:696:GLN:HB3	2.02	0.59
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:VAL:HG13	1:B:902:LEU:HD22	1.84	0.59
1:C:616:GLY:HA3	1:C:617:GLN:C	2.23	0.59
1:E:251:LEU:HD11	1:E:265:VAL:HG21	1.84	0.59
1:F:1033:GLU:HG3	1:F:1034:ASP:HB2	1.83	0.59
1:F:421:ALA:O	1:F:503:GLY:N	2.32	0.59
1:D:343:THR:HG21	1:D:984:LEU:HD21	1.85	0.59
1:E:893:PRO:O	1:E:896:VAL:N	2.35	0.59
1:F:563:PHE:HE2	1:F:564:LEU:HD22	1.67	0.59
1:A:412:VAL:HG11	1:A:489:THR:HG22	1.84	0.59
1:A:908:LEU:HD23	1:A:922:PHE:CZ	2.33	0.59
1:B:327:TYR:HB2	1:B:623:PHE:CZ	2.38	0.59
1:B:610:PHE:HB3	1:B:623:PHE:HB3	1.85	0.59
1:C:1034:ASP:O	1:C:1035:ILE:HG12	2.02	0.59
1:C:404:LEU:HG	1:C:449:LEU:HD13	1.84	0.59
1:D:872:TYR:CE1	3:D:1103:LMT:H92	2.37	0.59
1:D:707:MET:HG2	1:D:838:LEU:HG	1.84	0.59
1:D:914:ARG:HG2	1:D:915:GLY:H	1.67	0.59
1:E:196:PHE:O	1:E:252:LYS:NZ	2.20	0.59
1:E:686:GLY:H	1:E:689:LYS:HE3	1.67	0.59
1:E:936:ASN:ND2	1:E:970:ILE:HG23	2.18	0.59
1:F:3:ASN:N	1:F:3:ASN:OD1	2.22	0.59
1:E:236:ALA:O	1:F:723:LYS:NZ	2.29	0.59
1:E:444:GLY:HA3	1:E:886:LEU:HD22	1.84	0.59
1:B:139:VAL:O	1:B:326:PRO:HD2	2.02	0.59
1:C:528:THR:HG21	1:C:964:ARG:HG3	1.85	0.59
1:A:426:PRO:HB2	1:A:429:GLU:OE2	2.03	0.59
1:B:62:THR:HG21	1:B:813:ARG:HD3	1.84	0.59
1:C:689:LYS:HE3	1:C:689:LYS:H	1.68	0.59
1:C:734:LEU:HD12	1:C:794:VAL:HG11	1.85	0.59
1:D:137:LEU:HD22	1:D:293:LEU:HG	1.84	0.59
1:D:426:PRO:HB3	1:D:428:LYS:NZ	2.18	0.59
1:D:400:LEU:HD21	1:D:925:GLY:HA2	1.83	0.59
1:E:899:VAL:HG21	1:E:937:ALA:HB2	1.85	0.59
1:F:563:PHE:HB2	1:F:861:GLU:CG	2.33	0.59
1:B:48:SER:HB3	1:B:87:THR:HG22	1.85	0.58
1:D:813:ARG:HH12	1:D:818:PRO:HG3	1.68	0.58
1:F:723:LYS:HG2	1:F:803:ARG:CZ	2.33	0.58
1:A:448:VAL:HG22	1:A:882:CYS:HB3	1.85	0.58
1:B:578:LEU:HB2	1:B:618:ASN:O	2.03	0.58
1:C:251:LEU:HD12	1:C:265:VAL:HG11	1.84	0.58
1:C:34:GLN:HG2	1:C:333:VAL:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1101:ERY:H2	2:D:1101:ERY:H352	1.85	0.58
1:D:198:LEU:HD11	1:D:252:LYS:HB2	1.85	0.58
1:E:1014:ILE:HG13	1:E:1015:PHE:HD1	1.68	0.58
1:E:164:ASP:N	1:E:164:ASP:OD1	2.36	0.58
1:A:1032:ASN:O	1:A:1032:ASN:ND2	2.33	0.58
1:B:442:LEU:O	1:B:445:ILE:HG13	2.03	0.58
1:B:383:LEU:HD21	1:B:473:THR:HA	1.84	0.58
1:B:647:THR:HG22	1:B:660:ALA:H	1.67	0.58
1:B:896:VAL:HG23	1:B:937:ALA:HB3	1.85	0.58
1:C:376:LEU:O	1:C:379:THR:N	2.36	0.58
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.85	0.58
1:A:757:PHE:CE1	1:A:759:ASP:HB2	2.38	0.58
1:B:905:ILE:O	1:B:909:LEU:HB2	2.03	0.58
1:C:182:TYR:HB2	1:C:764:LYS:NZ	2.18	0.58
1:F:574:THR:HG23	1:F:622:ALA:HB3	1.85	0.58
1:A:918:ASN:OD1	1:A:923:GLN:NE2	2.37	0.58
1:C:738:ILE:HD12	1:C:738:ILE:H	1.68	0.58
1:D:356:TYR:O	1:D:358:PHE:N	2.36	0.58
1:F:940:ILE:HD12	1:F:1017:VAL:HB	1.86	0.58
1:F:977:PHE:O	1:F:980:GLY:N	2.37	0.58
1:A:423:GLU:HB2	1:A:425:LEU:HD13	1.86	0.58
1:B:185:ARG:HH11	1:B:767:TYR:HB3	1.68	0.58
1:C:910:ALA:HB2	1:C:1004:GLY:HA3	1.85	0.58
1:E:900:VAL:O	1:E:904:VAL:HG23	2.03	0.58
1:A:396:PHE:CD2	1:A:998:VAL:HG21	2.38	0.58
1:B:535:LEU:HD22	1:B:1022:VAL:HG11	1.84	0.58
1:B:362:PHE:HA	1:B:365:THR:HG22	1.85	0.58
1:D:883:LEU:HB2	1:D:893:PRO:HB3	1.86	0.58
1:E:169:THR:HG21	1:E:306:ILE:HG13	1.85	0.58
1:E:213:GLN:HG2	1:E:239:ARG:HG3	1.85	0.58
1:E:214:VAL:HG11	1:F:742:ASN:HB3	1.85	0.58
1:A:151:GLN:HE21	1:A:152:GLU:HA	1.69	0.58
1:A:159:ALA:HB2	1:A:177:LEU:HD11	1.85	0.58
1:B:189:ASN:ND2	1:B:267:LYS:HE2	2.14	0.58
1:C:1014:ILE:HG13	1:C:1015:PHE:HD1	1.68	0.58
1:C:796:PHE:HA	1:C:799:PHE:CE2	2.38	0.58
1:D:210:GLN:HE22	1:D:250:LEU:H	1.50	0.58
1:D:568:ASP:O	1:D:629:TRP:HZ3	1.87	0.58
1:E:576:VAL:HG22	1:E:658:VAL:HG13	1.86	0.58
1:F:396:PHE:O	1:F:400:LEU:HB2	2.04	0.58
1:F:909:LEU:O	1:F:913:PHE:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TYR:CZ	1:A:564:LEU:HD23	2.38	0.58
1:A:578:LEU:HB2	1:A:618:ASN:O	2.04	0.58
1:B:363:ARG:HD2	1:B:498:LYS:HB2	1.86	0.58
1:B:62:THR:OG1	1:B:88:VAL:HG21	2.04	0.58
1:B:240:LEU:HB2	1:B:246:PHE:CE1	2.39	0.57
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.28	0.57
1:E:32:VAL:HG22	1:E:298:ASN:ND2	2.19	0.57
1:E:693:ALA:HB1	1:E:846:LEU:HD13	1.86	0.57
1:F:2:PRO:HD2	1:F:4:PHE:HD1	1.69	0.57
1:A:6:ILE:HD11	1:A:432:ARG:HE	1.68	0.57
1:A:198:LEU:HD23	1:A:787:ARG:HH21	1.68	0.57
1:C:415:ASN:ND2	1:C:438:ILE:HG21	2.19	0.57
1:D:262:LEU:HG	1:D:268:ILE:HD11	1.86	0.57
1:D:966:ARG:C	1:D:969:PRO:HD2	2.24	0.57
1:E:447:MET:HB3	1:E:882:CYS:SG	2.43	0.57
1:A:6:ILE:CD1	1:A:432:ARG:HE	2.16	0.57
1:B:573:MET:HB2	1:B:661:PHE:HE2	1.68	0.57
1:C:452:VAL:O	1:C:455:PRO:HD2	2.04	0.57
1:B:14:VAL:HG13	1:C:881:LEU:HD12	1.86	0.57
1:F:274:ASN:OD1	1:F:275:TYR:N	2.37	0.57
1:F:447:MET:HG2	1:F:886:LEU:HD22	1.84	0.57
1:F:65:ILE:HG21	1:F:90:ILE:HG13	1.86	0.57
1:A:62:THR:HG21	1:A:813:ARG:HD3	1.85	0.57
1:C:968:ARG:HG2	1:C:972:MET:HE2	1.86	0.57
1:E:31:PRO:HB2	1:E:389:SER:HB2	1.85	0.57
1:F:36:PRO:HD3	1:F:391:ASN:CG	2.25	0.57
1:A:457:ALA:O	1:A:468:ARG:NE	2.38	0.57
1:D:357:LEU:HD23	1:D:358:PHE:CD1	2.40	0.57
1:D:887:TYR:CD2	1:D:892:ILE:HG22	2.39	0.57
1:E:416:VAL:HG21	1:E:493:CYS:SG	2.44	0.57
1:B:376:LEU:O	1:B:379:THR:N	2.38	0.57
1:B:560:PRO:HG2	1:B:917:THR:HA	1.85	0.57
1:C:659:PHE:CE2	1:C:712:ARG:HB3	2.39	0.57
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.87	0.57
1:E:757:PHE:CE1	1:E:759:ASP:HB2	2.39	0.57
1:F:414:GLU:HG2	1:F:968:ARG:NH1	2.20	0.57
1:A:210:GLN:HE22	1:A:250:LEU:N	2.03	0.57
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.87	0.57
1:C:752:SER:O	1:C:767:TYR:HA	2.05	0.57
1:D:99:ASP:HB3	1:D:102:ILE:HB	1.85	0.57
1:D:72:ILE:HD13	1:D:107:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ILE:HG21	1:D:107:VAL:HG23	1.86	0.57
1:E:728:GLN:HE22	1:E:738:ILE:HG21	1.69	0.57
1:F:193:LEU:HD23	1:F:265:VAL:HB	1.86	0.57
1:A:146:ASP:OD2	1:A:146:ASP:N	2.29	0.57
1:A:56:THR:O	1:A:60:THR:HG22	2.03	0.57
1:B:83:ASP:HB2	1:B:87:THR:O	2.04	0.57
1:B:41:PRO:HD2	1:B:94:PHE:O	2.04	0.57
1:F:948:MET:HE1	1:F:955:LEU:HD12	1.87	0.57
1:A:196:PHE:O	1:A:252:LYS:NZ	2.25	0.57
1:C:583:THR:HA	1:C:617:GLN:OE1	2.04	0.57
1:C:681:ASP:HB3	1:C:818:PRO:O	2.03	0.57
1:A:355:MET:SD	1:A:410:ILE:HG12	2.45	0.57
1:A:470:PHE:CG	1:A:924:VAL:HG21	2.39	0.57
1:C:576:VAL:HG22	1:C:658:VAL:HG13	1.86	0.57
1:E:1014:ILE:HG13	1:E:1015:PHE:CD1	2.40	0.57
1:E:415:ASN:ND2	1:E:437:GLN:OE1	2.38	0.57
1:F:796:PHE:HA	1:F:799:PHE:CE2	2.39	0.57
1:A:895:SER:HB3	1:A:1024:VAL:HG21	1.87	0.56
1:B:741:ILE:HG22	1:B:796:PHE:HE1	1.70	0.56
1:C:677:PHE:HD2	1:C:678:GLU:N	2.03	0.56
1:C:918:ASN:C	1:C:918:ASN:HD22	2.08	0.56
1:D:1008:THR:O	1:D:1012:LEU:HB2	2.05	0.56
1:D:416:VAL:HG21	1:D:493:CYS:SG	2.45	0.56
1:E:137:LEU:HD12	1:E:329:THR:HG22	1.87	0.56
1:E:670:GLY:HA2	1:E:857:MET:SD	2.44	0.56
1:F:670:GLY:HA3	1:F:857:MET:HG2	1.87	0.56
1:D:943:PHE:O	1:D:947:LEU:HG	2.05	0.56
1:E:1015:PHE:CE2	3:E:1101:LMT:H32	2.40	0.56
1:F:757:PHE:CE1	1:F:759:ASP:HB2	2.39	0.56
1:D:465:ALA:O	1:D:469:GLN:HG2	2.05	0.56
1:D:540:ARG:HG3	1:D:541:TYR:CD1	2.40	0.56
1:E:48:SER:HB3	1:E:87:THR:HG22	1.86	0.56
1:F:482:VAL:O	1:F:486:LEU:HG	2.06	0.56
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.32	0.56
1:A:966:ARG:C	1:A:969:PRO:HD2	2.26	0.56
1:B:190:PRO:HB3	1:B:784:TRP:CH2	2.41	0.56
1:C:65:ILE:HG23	1:C:111:LEU:HD23	1.88	0.56
1:C:447:MET:O	1:C:451:ALA:HB2	2.04	0.56
1:C:277:ILE:HG12	1:C:614:GLY:O	2.06	0.56
1:E:108:GLN:HE22	1:F:112:GLN:HB3	1.70	0.56
1:E:408:ASP:OD1	1:E:935:LYS:NZ	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.39	0.56
1:B:650:PHE:HB3	1:B:658:VAL:HB	1.87	0.56
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.87	0.56
1:C:935:LYS:NZ	1:C:973:THR:HG21	2.20	0.56
1:D:368:PRO:HG3	1:D:413:VAL:HG21	1.87	0.56
1:D:926:LEU:O	1:D:930:ILE:HG13	2.06	0.56
1:E:650:PHE:HB3	1:E:658:VAL:HB	1.87	0.56
1:F:119:PRO:HB2	1:F:122:VAL:HB	1.88	0.56
1:A:839:MET:HE2	1:A:839:MET:HA	1.87	0.56
1:B:61:VAL:HG21	1:B:122:VAL:HG21	1.87	0.56
1:B:23:GLY:HA2	1:B:381:ALA:HB2	1.88	0.56
1:C:39:ALA:HB2	1:C:668:GLU:HG2	1.87	0.56
1:C:770:SER:OG	1:C:775:ARG:HG2	2.04	0.56
1:E:575:MET:HA	1:E:621:ILE:HG13	1.87	0.56
1:E:906:GLY:HA3	1:E:1008:THR:OG1	2.05	0.56
1:F:202:ASP:OD2	1:F:787:ARG:NH2	2.39	0.56
1:F:351:VAL:HG11	1:F:406:VAL:HG21	1.88	0.56
1:F:453:PHE:HZ	1:F:928:THR:HG1	1.53	0.56
1:F:956:ILE:H	1:F:956:ILE:HD12	1.71	0.56
1:D:23:GLY:HA3	1:D:377:LEU:O	2.06	0.56
1:A:362:PHE:O	1:A:365:THR:HG22	2.06	0.56
1:A:632:ARG:HB3	1:A:637:ASN:HB3	1.87	0.56
1:A:880:PHE:CE1	1:A:893:PRO:HB2	2.41	0.56
1:C:1032:ASN:N	1:C:1033:GLU:HB2	2.20	0.56
1:A:881:LEU:HD11	1:C:17:ILE:HG22	1.88	0.56
1:D:427:PRO:HD2	1:D:428:LYS:HZ3	1.71	0.56
1:F:13:TRP:HH2	1:F:370:ILE:HD13	1.70	0.56
1:B:898:LEU:HB3	1:B:1020:PHE:CZ	2.40	0.56
1:D:277:ILE:HA	1:D:613:ASN:O	2.05	0.56
1:E:156:ASP:OD2	1:E:764:LYS:NZ	2.38	0.56
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.88	0.56
1:E:751:GLY:HA2	1:E:769:MET:HG3	1.88	0.56
1:E:790:ASP:OD2	1:E:792:GLN:N	2.39	0.56
1:F:227:GLY:O	1:F:229:GLN:HG3	2.06	0.56
1:E:225:VAL:HG12	1:F:772:ALA:HB1	1.87	0.56
1:F:883:LEU:HD12	1:F:896:VAL:HG11	1.88	0.56
1:B:453:PHE:O	1:B:471:SER:OG	2.16	0.56
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.88	0.56
1:C:6:ILE:CG2	1:C:12:ALA:HB2	2.36	0.56
1:C:892:ILE:HG23	1:C:941:VAL:CG1	2.35	0.56
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:920:VAL:O	1:D:923:GLN:N	2.38	0.56
1:E:902:LEU:HG	1:E:1012:LEU:HD23	1.88	0.56
1:E:407:ASP:OD1	1:E:973:THR:OG1	2.20	0.56
1:E:424:GLY:HA3	1:E:502:LYS:HB2	1.88	0.56
1:E:905:ILE:O	1:E:909:LEU:HB2	2.06	0.56
1:F:675:PHE:CD2	1:F:854:TRP:HZ3	2.23	0.56
1:A:400:LEU:HD21	1:A:925:GLY:CA	2.35	0.56
1:A:586:ARG:O	1:A:589:LYS:HB3	2.06	0.56
1:B:796:PHE:HA	1:B:799:PHE:CE2	2.41	0.56
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.41	0.56
1:C:531:VAL:HG21	1:C:963:VAL:HG11	1.87	0.56
1:E:111:LEU:HD11	1:E:127:VAL:HB	1.88	0.56
1:D:17:ILE:HG22	1:E:881:LEU:HD21	1.88	0.56
1:A:591:LEU:HD11	1:A:620:GLY:HA3	1.86	0.55
1:B:1015:PHE:CE2	3:B:2100:LMT:H21	2.41	0.55
1:D:35:TYR:HB3	1:D:38:ILE:HD11	1.88	0.55
1:D:426:PRO:HD2	1:D:429:GLU:CG	2.37	0.55
1:A:32:VAL:HB	1:A:300:LEU:HD22	1.87	0.55
1:A:187:TRP:HB3	1:A:771:GLU:HA	1.88	0.55
1:B:3:ASN:O	1:B:6:ILE:HB	2.06	0.55
1:B:400:LEU:HG	1:B:924:VAL:HG12	1.88	0.55
1:B:400:LEU:HD11	1:B:925:GLY:HA2	1.87	0.55
1:D:27:ILE:HD11	1:D:380:PHE:CE1	2.40	0.55
1:E:555:LEU:HD11	1:E:909:LEU:HD12	1.88	0.55
1:F:540:ARG:HG3	1:F:541:TYR:CD1	2.41	0.55
1:F:662:ASN:O	1:F:673:THR:OG1	2.21	0.55
1:F:855:THR:HA	1:F:859:TYR:HB2	1.88	0.55
1:A:249:ILE:HD12	1:A:262:LEU:HD23	1.87	0.55
1:C:318:PRO:HG2	1:C:321:LEU:CB	2.37	0.55
1:E:985:VAL:HG22	1:E:999:GLY:HA3	1.88	0.55
1:F:371:ALA:O	1:F:375:VAL:HG23	2.06	0.55
1:A:982:MET:O	1:A:986:ILE:HG12	2.05	0.55
1:C:966:ARG:CZ	1:C:966:ARG:HB3	2.36	0.55
1:C:340:VAL:HG22	1:C:995:GLN:HE21	1.71	0.55
1:D:388:PHE:HE1	1:D:469:GLN:HE22	1.53	0.55
1:D:966:ARG:HB3	1:D:966:ARG:NH1	2.21	0.55
1:A:420:MET:HB3	1:A:500:ILE:HB	1.88	0.55
1:A:470:PHE:CD2	1:A:924:VAL:HG11	2.41	0.55
1:B:106:GLN:HA	1:B:109:ASN:ND2	2.22	0.55
1:B:899:VAL:HG21	1:B:937:ALA:CB	2.37	0.55
1:C:616:GLY:HA3	1:C:619:THR:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:GLN:NE2	1:D:332:PHE:HE2	2.04	0.55
1:E:239:ARG:HD3	1:E:756:ASP:O	2.07	0.55
1:E:559:LEU:HD21	1:E:917:THR:HA	1.88	0.55
1:E:701:ALA:HB3	1:E:711:VAL:HG11	1.88	0.55
1:E:796:PHE:O	1:E:800:SER:OG	2.19	0.55
1:F:616:GLY:HA3	1:F:618:ASN:N	2.21	0.55
1:A:172:VAL:HG22	1:A:306:ILE:HD11	1.88	0.55
1:A:425:LEU:HD23	1:A:429:GLU:HB2	1.88	0.55
1:A:427:PRO:CD	1:A:499:PRO:HB3	2.33	0.55
1:C:1031:LYS:HE3	1:C:1035:ILE:HD13	1.89	0.55
1:C:139:VAL:HB	1:C:327:TYR:HB3	1.87	0.55
1:C:240:LEU:HD11	1:C:249:ILE:HD11	1.88	0.55
1:C:785:TYR:CE2	1:C:795:PRO:HB3	2.41	0.55
1:D:31:PRO:HB2	1:D:389:SER:HB3	1.89	0.55
1:D:894:PHE:HA	1:D:897:MET:HE2	1.89	0.55
1:D:962:ALA:C	1:D:966:ARG:HH12	2.10	0.55
1:E:40:PRO:HD3	1:E:462:SER:OG	2.06	0.55
1:E:790:ASP:OD2	1:E:791:GLY:N	2.40	0.55
1:C:456:MET:HB3	1:C:871:LEU:HD21	1.89	0.55
1:C:53:ASP:OD1	1:C:56:THR:OG1	2.21	0.55
1:C:540:ARG:HG3	1:C:541:TYR:HD1	1.72	0.55
1:D:187:TRP:HB3	1:D:771:GLU:HA	1.89	0.55
1:D:908:LEU:HD23	1:D:922:PHE:CZ	2.37	0.55
1:F:187:TRP:HA	1:F:769:MET:O	2.06	0.55
1:F:836:MET:O	1:F:840:GLU:HG2	2.07	0.55
1:A:963:VAL:HG21	1:A:1018:PRO:HG3	1.89	0.55
1:D:396:PHE:CD1	1:D:998:VAL:HG21	2.42	0.55
1:E:425:LEU:HD22	1:E:429:GLU:HG2	1.89	0.55
1:E:700:GLU:HB3	1:E:842:LEU:HD22	1.88	0.55
1:E:900:VAL:HG13	1:E:930:ILE:HG23	1.88	0.55
1:F:463:THR:HG23	1:F:920:VAL:HG22	1.88	0.55
1:A:914:ARG:HH12	1:A:996:ASN:HB3	1.71	0.55
1:C:75:LEU:HD21	1:C:78:MET:HB2	1.89	0.55
1:E:116:PRO:HA	1:E:123:GLN:HE22	1.71	0.55
1:E:250:LEU:HD11	1:E:259:ARG:HB2	1.89	0.55
1:E:530:SER:OG	3:E:1101:LMT:C1'	2.54	0.55
1:F:1014:ILE:HG13	1:F:1015:PHE:HD1	1.71	0.55
1:F:753:TYR:OH	1:F:756:ASP:OD2	2.25	0.55
1:A:653:ILE:HG13	1:A:654:LYS:HE2	1.88	0.54
1:A:892:ILE:HA	1:A:1024:VAL:CG1	2.37	0.54
1:B:394:THR:O	1:B:473:THR:HG21	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:LEU:HB2	1:B:846:LEU:HD11	1.89	0.54
1:D:962:ALA:O	1:D:965:MET:HG2	2.07	0.54
1:E:3:ASN:HA	1:E:6:ILE:HD12	1.89	0.54
1:E:795:PRO:HG2	1:E:798:ALA:HB2	1.88	0.54
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.89	0.54
1:B:579:PRO:HD3	1:B:656:ALA:HB2	1.88	0.54
1:C:119:PRO:O	1:C:123:GLN:HG3	2.06	0.54
1:C:678:GLU:HG2	1:C:814:TYR:CD2	2.42	0.54
1:D:172:VAL:HG13	1:D:291:ILE:HG23	1.89	0.54
1:D:379:THR:HG23	1:D:476:SER:OG	2.08	0.54
1:E:291:ILE:HG21	1:E:306:ILE:HD11	1.88	0.54
1:D:762:ARG:NH1	1:E:67:GLN:HE21	2.05	0.54
1:E:748:ALA:O	1:E:770:SER:HB3	2.07	0.54
1:A:1031:LYS:HE2	1:A:1035:ILE:HG23	1.90	0.54
1:A:857:MET:HG2	2:A:1101:ERY:H202	1.88	0.54
1:A:562:SER:HB2	1:A:919:ASP:CB	2.31	0.54
1:A:701:ALA:HB3	1:A:711:VAL:HG11	1.89	0.54
1:B:910:ALA:HB2	1:B:1004:GLY:HA3	1.87	0.54
1:B:354:VAL:O	1:B:358:PHE:HB2	2.07	0.54
1:B:545:TYR:HE2	1:B:902:LEU:HD11	1.72	0.54
1:B:80:SER:HB3	1:B:90:ILE:HG23	1.88	0.54
1:C:34:GLN:CB	1:C:333:VAL:HG22	2.34	0.54
1:C:270:LEU:HD21	1:C:759:ASP:OD2	2.07	0.54
1:E:893:PRO:O	1:E:896:VAL:HG12	2.08	0.54
1:E:955:LEU:HD13	1:E:1025:ARG:HG2	1.89	0.54
1:E:966:ARG:O	1:E:970:ILE:HG12	2.07	0.54
1:F:171:GLY:O	1:F:293:LEU:HD23	2.08	0.54
1:F:914:ARG:NH2	1:F:985:VAL:O	2.40	0.54
1:A:187:TRP:HA	1:A:769:MET:O	2.06	0.54
1:C:1008:THR:O	1:C:1012:LEU:HB2	2.08	0.54
1:C:103:ALA:O	1:C:106:GLN:N	2.39	0.54
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.89	0.54
1:C:376:LEU:HD22	1:C:398:MET:HE3	1.90	0.54
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.90	0.54
1:E:281:PHE:CZ	1:E:324:VAL:HG21	2.42	0.54
1:A:902:LEU:HG	1:A:1012:LEU:HD23	1.89	0.54
1:A:38:ILE:HG12	1:A:466:ILE:HD11	1.90	0.54
1:A:796:PHE:HD1	1:A:799:PHE:CE2	2.26	0.54
1:B:250:LEU:HD11	1:B:259:ARG:HB2	1.89	0.54
1:C:409:ALA:O	1:C:413:VAL:HG23	2.07	0.54
1:C:757:PHE:CE1	1:C:759:ASP:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:889:SER:CB	1:C:892:ILE:HG12	2.38	0.54
1:D:941:VAL:HG13	1:D:1021:PHE:CD1	2.42	0.54
1:D:189:ASN:HB3	1:D:192:GLU:HB2	1.88	0.54
1:D:427:PRO:HD2	1:D:428:LYS:NZ	2.22	0.54
1:D:748:ALA:O	1:D:770:SER:HB3	2.08	0.54
1:D:891:SER:OG	1:D:1028:PHE:HB3	2.07	0.54
1:E:42:ALA:HB2	1:E:93:THR:HG23	1.90	0.54
1:F:78:MET:HG3	1:F:92:LEU:HD13	1.89	0.54
1:F:941:VAL:HG13	1:F:1021:PHE:CD1	2.43	0.54
3:B:2100:LMT:C5B	3:B:2100:LMT:H6E	2.38	0.54
1:B:327:TYR:HD1	1:B:623:PHE:CZ	2.25	0.54
1:C:520:PHE:O	1:C:524:THR:HG22	2.08	0.54
1:C:770:SER:HB3	1:C:775:ARG:HD3	1.89	0.54
1:D:221:GLY:N	1:E:775:ARG:HH12	2.06	0.54
1:F:584:GLN:HB2	1:F:617:GLN:HG2	1.89	0.54
1:F:938:ILE:O	1:F:942:GLU:HB3	2.08	0.54
1:B:548:ILE:HG23	1:B:905:ILE:HD13	1.89	0.54
1:C:453:PHE:HB3	1:C:471:SER:HA	1.90	0.54
1:E:317:PHE:HE2	1:E:323:ILE:HG12	1.73	0.54
1:C:723:LYS:HG2	1:C:803:ARG:NH2	2.22	0.54
1:E:572:PHE:HA	1:E:663:LEU:CD2	2.37	0.54
1:F:941:VAL:HG13	1:F:1021:PHE:CE1	2.42	0.54
1:F:49:TYR:HD1	1:F:57:VAL:HG12	1.71	0.54
1:F:770:SER:OG	1:F:775:ARG:HG2	2.08	0.54
1:A:251:LEU:HD12	1:A:265:VAL:HG11	1.88	0.54
1:C:382:VAL:HG11	1:C:476:SER:HB2	1.88	0.54
1:C:716:LEU:CD2	1:C:810:ARG:HE	2.20	0.54
1:D:1033:GLU:HB3	1:D:1035:ILE:HG12	1.90	0.54
1:E:108:GLN:NE2	1:F:112:GLN:HB3	2.23	0.54
1:E:139:VAL:O	1:E:326:PRO:HD2	2.08	0.54
1:E:584:GLN:HB2	1:E:617:GLN:HG2	1.88	0.54
1:E:686:GLY:O	1:E:689:LYS:N	2.40	0.54
1:F:871:LEU:HD22	1:F:927:LEU:HD11	1.89	0.54
1:F:528:THR:HG21	1:F:964:ARG:HG3	1.88	0.54
1:A:941:VAL:HG13	1:A:1021:PHE:CE1	2.43	0.54
1:A:108:GLN:NE2	1:B:109:ASN:HB2	2.23	0.54
1:A:388:PHE:CE1	1:A:472:ILE:HG21	2.43	0.54
1:E:175:VAL:HG23	1:F:70:ASN:ND2	2.23	0.54
1:F:892:ILE:HG23	1:F:941:VAL:CG1	2.38	0.54
1:C:770:SER:HG	1:C:775:ARG:HG2	1.72	0.53
1:D:677:PHE:HD2	1:D:678:GLU:N	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:836:MET:O	1:E:840:GLU:HG3	2.08	0.53
1:E:929:THR:O	1:E:933:SER:OG	2.23	0.53
1:F:527:TYR:HB2	3:F:2100:LMT:H82	1.90	0.53
1:A:707:MET:HB3	1:A:708:LEU:HD22	1.88	0.53
1:C:62:THR:HG21	1:C:813:ARG:HD3	1.90	0.53
1:D:905:ILE:O	1:D:909:LEU:HB2	2.08	0.53
1:E:166:ILE:O	1:E:169:THR:HB	2.07	0.53
1:F:6:ILE:C	1:F:8:ARG:H	2.12	0.53
1:F:908:LEU:HD23	1:F:922:PHE:CZ	2.41	0.53
1:C:747:ALA:O	1:C:769:MET:HA	2.08	0.53
1:D:3:ASN:HA	1:D:6:ILE:HD11	1.89	0.53
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.90	0.53
1:F:65:ILE:HG23	1:F:111:LEU:HD23	1.90	0.53
1:F:748:ALA:O	1:F:770:SER:HB3	2.07	0.53
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.43	0.53
1:B:521:GLU:O	1:B:524:THR:HG23	2.08	0.53
1:C:892:ILE:O	1:C:895:SER:OG	2.27	0.53
1:E:186:ILE:HD13	1:E:262:LEU:HD21	1.89	0.53
1:E:166:ILE:HD11	1:E:310:LEU:CD1	2.38	0.53
1:E:559:LEU:HD12	1:E:912:THR:OG1	2.09	0.53
1:F:587:THR:HG21	1:F:617:GLN:O	2.09	0.53
1:F:639:VAL:O	1:F:643:THR:HG23	2.07	0.53
1:A:796:PHE:HA	1:A:799:PHE:CE2	2.43	0.53
1:B:183:ALA:O	1:B:270:LEU:HD12	2.09	0.53
1:C:540:ARG:HG3	1:C:541:TYR:CD1	2.44	0.53
1:C:661:PHE:N	1:C:661:PHE:CD1	2.76	0.53
1:D:528:THR:HG21	1:D:964:ARG:HG3	1.89	0.53
1:D:757:PHE:CE1	1:D:759:ASP:HB2	2.42	0.53
1:E:978:ILE:O	1:E:982:MET:HB2	2.09	0.53
1:F:563:PHE:CE2	1:F:564:LEU:HD22	2.43	0.53
1:F:588:GLN:OE1	1:F:592:ASN:ND2	2.41	0.53
1:A:201:VAL:HA	1:A:204:ILE:HD12	1.90	0.53
1:A:650:PHE:HB3	1:A:658:VAL:HB	1.91	0.53
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.91	0.53
1:C:411:VAL:O	1:C:415:ASN:ND2	2.41	0.53
1:B:28:LEU:HD12	1:B:29:LYS:HD2	1.90	0.53
1:B:694:ARG:HH11	1:B:820:MET:HE1	1.72	0.53
1:D:1031:LYS:HG3	1:D:1033:GLU:CD	2.29	0.53
1:E:393:LEU:HD12	1:E:469:GLN:HG3	1.90	0.53
1:F:331:PRO:O	1:F:335:ILE:HG22	2.08	0.53
1:F:919:ASP:OD1	1:F:921:TYR:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.90	0.53
1:A:452:VAL:HA	1:A:875:SER:OG	2.09	0.53
1:B:415:ASN:ND2	1:B:434:SER:HB2	2.24	0.53
1:C:688:GLU:HB3	1:C:689:LYS:HE2	1.89	0.53
1:C:707:MET:SD	1:C:838:LEU:HB2	2.49	0.53
1:E:105:VAL:HG23	1:F:109:ASN:HD21	1.73	0.53
1:A:45:ILE:HD12	1:A:90:ILE:HB	1.91	0.53
1:A:982:MET:HB3	1:A:983:PRO:HD3	1.91	0.53
1:A:222:THR:HG23	1:B:275:TYR:HB2	1.91	0.53
1:B:908:LEU:HD23	1:B:922:PHE:HZ	1.73	0.53
1:C:350:LEU:HD23	1:C:979:LEU:HB3	1.90	0.53
1:C:661:PHE:N	1:C:661:PHE:HD1	2.06	0.53
1:D:150:THR:N	1:D:153:ASP:OD1	2.27	0.53
1:E:415:ASN:O	1:E:419:VAL:HG23	2.09	0.53
1:E:694:ARG:NH2	1:E:717:GLU:OE1	2.42	0.53
1:E:909:LEU:O	1:E:913:PHE:HB2	2.07	0.53
1:F:239:ARG:HD3	1:F:756:ASP:O	2.08	0.53
1:A:418:ARG:NH2	1:A:943:PHE:HE2	2.07	0.53
1:A:528:THR:HG21	1:A:964:ARG:HG3	1.90	0.53
1:B:1010:THR:C	1:B:1012:LEU:H	2.13	0.53
1:B:210:GLN:NE2	1:B:250:LEU:O	2.42	0.53
1:B:694:ARG:HD2	1:B:713:PRO:HB3	1.91	0.53
1:C:351:VAL:O	1:C:355:MET:HE2	2.09	0.53
1:D:240:LEU:HD12	1:D:246:PHE:CD2	2.44	0.53
1:D:32:VAL:HB	1:D:300:LEU:HD22	1.91	0.53
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.89	0.53
1:D:675:PHE:CD1	1:D:854:TRP:HZ3	2.27	0.53
1:E:16:ALA:HB2	1:E:488:LEU:HD13	1.91	0.53
1:E:246:PHE:O	1:E:249:ILE:HG23	2.08	0.53
1:F:567:GLU:O	1:F:569:GLN:HG3	2.09	0.53
1:F:610:PHE:HB3	1:F:623:PHE:HB2	1.90	0.53
1:F:955:LEU:HD21	1:F:1022:VAL:HA	1.91	0.53
1:A:721:GLN:OE1	1:A:807:GLY:HA3	2.09	0.52
1:B:893:PRO:O	1:B:896:VAL:HG12	2.08	0.52
1:C:450:SER:HB2	1:C:475:VAL:HA	1.90	0.52
1:C:720:PRO:HA	1:C:805:GLU:O	2.09	0.52
1:D:362:PHE:O	1:D:365:THR:HG22	2.08	0.52
1:E:612:VAL:N	1:E:621:ILE:O	2.27	0.52
1:F:401:ALA:O	1:F:404:LEU:N	2.42	0.52
1:F:880:PHE:C	1:F:880:PHE:CD2	2.83	0.52
1:F:905:ILE:O	1:F:909:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:939:LEU:HD12	1:F:970:ILE:HG12	1.91	0.52
1:A:242:SER:OG	1:A:245:GLU:HG3	2.08	0.52
1:A:53:ASP:O	1:A:56:THR:HB	2.09	0.52
1:B:678:GLU:HG2	1:B:814:TYR:CG	2.43	0.52
1:B:904:VAL:HG22	1:B:926:LEU:HD21	1.91	0.52
1:A:453:PHE:CE2	1:A:474:ILE:HD13	2.44	0.52
1:B:115:MET:O	1:B:123:GLN:NE2	2.42	0.52
1:E:563:PHE:O	1:E:564:LEU:HD12	2.09	0.52
1:F:146:ASP:OD2	1:F:320:GLY:HA3	2.10	0.52
1:F:492:LEU:HD13	1:F:496:MET:SD	2.49	0.52
1:F:721:GLN:OE1	1:F:807:GLY:HA3	2.08	0.52
1:F:5:PHE:C	1:F:7:ASP:H	2.09	0.52
1:F:670:GLY:CA	1:F:857:MET:HG2	2.39	0.52
1:F:932:LEU:HD11	1:F:977:PHE:CE2	2.45	0.52
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.92	0.52
1:A:882:CYS:O	1:A:885:ALA:HB3	2.09	0.52
1:B:704:HIS:HB2	1:B:708:LEU:HD12	1.91	0.52
1:A:225:VAL:N	1:B:776:MET:HE1	2.09	0.52
1:B:343:THR:OG1	1:B:984:LEU:HD21	2.10	0.52
1:D:207:ILE:O	1:D:211:ASN:HB3	2.09	0.52
1:D:228:GLN:NE2	1:D:230:LEU:O	2.38	0.52
1:E:36:PRO:HD2	1:E:38:ILE:HD11	1.92	0.52
1:E:927:LEU:HA	1:E:930:ILE:HD12	1.91	0.52
1:F:61:VAL:HA	1:F:118:LEU:CD2	2.39	0.52
1:D:723:LYS:HD2	1:F:235:ILE:O	2.09	0.52
1:F:565:PRO:HG2	1:F:567:GLU:OE2	2.09	0.52
1:B:575:MET:HE3	1:B:621:ILE:HD12	1.91	0.52
1:B:680:ILE:HD11	1:B:814:TYR:CD2	2.40	0.52
1:C:605:ASN:OD1	1:C:637:ASN:ND2	2.42	0.52
1:C:855:THR:CA	1:C:859:TYR:HB2	2.38	0.52
1:D:963:VAL:HA	1:D:966:ARG:NH2	2.23	0.52
1:F:509:LYS:HG2	1:F:513:PHE:HB2	1.92	0.52
1:A:310:LEU:O	1:A:314:GLU:HG3	2.09	0.52
1:A:568:ASP:CG	1:A:632:ARG:HH22	2.12	0.52
1:A:948:MET:SD	1:A:955:LEU:HA	2.50	0.52
1:C:465:ALA:HA	1:C:468:ARG:NH1	2.24	0.52
1:C:908:LEU:HD23	1:C:922:PHE:HZ	1.74	0.52
1:D:351:VAL:O	1:D:355:MET:HB2	2.10	0.52
1:E:530:SER:HG	3:E:1101:LMT:H1'	1.72	0.52
1:E:355:MET:HG2	1:E:365:THR:OG1	2.10	0.52
1:F:597:TYR:CD2	1:F:650:PHE:HZ	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:ALA:C	1:A:1015:PHE:H	2.12	0.52
1:B:578:LEU:HG	1:B:587:THR:OG1	2.09	0.52
1:B:741:ILE:HG22	1:B:796:PHE:CE1	2.44	0.52
1:C:966:ARG:NE	1:C:966:ARG:O	2.43	0.52
1:D:426:PRO:HB3	1:D:428:LYS:HZ3	1.74	0.52
1:D:584:GLN:N	1:D:617:GLN:HB3	2.24	0.52
1:E:106:GLN:HA	1:E:109:ASN:ND2	2.24	0.52
1:E:54:ALA:HB2	1:E:84:SER:HB3	1.90	0.52
1:F:939:LEU:HD22	1:F:966:ARG:HD2	1.92	0.52
1:A:453:PHE:CD2	1:A:474:ILE:HG21	2.45	0.52
1:B:327:TYR:HD1	1:B:623:PHE:CE1	2.27	0.52
1:B:690:LEU:HD22	1:B:820:MET:SD	2.50	0.52
1:C:524:THR:O	1:C:527:TYR:HB3	2.09	0.52
1:C:746:GLY:O	1:C:750:GLY:N	2.36	0.52
1:D:1031:LYS:HG3	1:D:1033:GLU:OE1	2.09	0.52
1:D:225:VAL:HG22	1:E:776:MET:HE2	1.92	0.52
1:D:360:GLN:NE2	1:D:513:PHE:O	2.43	0.52
1:E:813:ARG:NH1	1:E:818:PRO:HG3	2.25	0.52
1:E:343:THR:OG1	1:E:984:LEU:HD21	2.10	0.52
1:F:893:PRO:O	1:F:896:VAL:HG12	2.09	0.52
1:A:261:LEU:O	1:A:265:VAL:HG13	2.10	0.52
1:A:400:LEU:CD2	1:A:924:VAL:HG12	2.40	0.52
1:C:555:LEU:HD11	1:C:909:LEU:HD12	1.92	0.52
1:E:490:PRO:O	1:E:493:CYS:HB2	2.10	0.52
1:F:113:LEU:O	1:F:116:PRO:HD2	2.10	0.52
1:F:571:VAL:HG12	1:F:663:LEU:HD11	1.91	0.52
1:B:578:LEU:HD21	1:B:590:VAL:HG21	1.92	0.52
1:C:563:PHE:HB2	1:C:861:GLU:HB2	1.90	0.52
1:D:756:ASP:HB3	1:D:763:VAL:HG23	1.91	0.52
1:D:182:TYR:HB2	1:D:764:LYS:HZ3	1.72	0.52
1:D:396:PHE:HD1	1:D:921:TYR:CE2	2.28	0.52
1:E:372:VAL:HG23	1:E:373:PRO:CD	2.38	0.52
1:E:457:ALA:HB2	1:E:471:SER:OG	2.10	0.52
1:E:507:GLU:O	1:E:509:LYS:N	2.43	0.52
1:E:9:PRO:HG2	1:E:10:ILE:HD13	1.92	0.52
1:A:836:MET:O	1:A:840:GLU:HG3	2.09	0.51
1:B:68:ASN:CB	1:B:114:ALA:HB2	2.41	0.51
1:C:563:PHE:CE2	1:C:666:ILE:HD11	2.45	0.51
1:D:149:MET:HB2	1:D:153:ASP:HB2	1.90	0.51
1:E:826:ALA:HB2	1:E:835:ALA:HB2	1.91	0.51
1:E:883:LEU:HD13	1:E:896:VAL:HG11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:404:LEU:HD12	1:E:932:LEU:HD21	1.92	0.51
1:F:11:PHE:O	1:F:15:ILE:HG13	2.10	0.51
1:A:680:ILE:HD11	1:A:814:TYR:HD2	1.74	0.51
1:B:142:VAL:HG21	1:B:162:MET:HE3	1.91	0.51
1:C:146:ASP:O	1:C:148:THR:N	2.43	0.51
1:C:211:ASN:OD1	1:C:240:LEU:N	2.38	0.51
1:C:348:ILE:HG12	1:C:372:VAL:HG11	1.91	0.51
1:C:917:THR:O	1:C:919:ASP:N	2.43	0.51
1:F:616:GLY:HA3	1:F:619:THR:H	1.74	0.51
1:F:182:TYR:HD2	1:F:760:ARG:HH22	1.58	0.51
1:A:184:MET:HB3	1:A:766:VAL:HG13	1.92	0.51
1:A:539:GLY:O	1:A:542:LEU:HB2	2.10	0.51
1:B:639:VAL:O	1:B:643:THR:HG23	2.10	0.51
1:C:184:MET:HB2	1:C:757:PHE:CE2	2.45	0.51
1:C:992:SER:HA	1:C:995:GLN:HB2	1.91	0.51
1:E:1030:ARG:HD3	1:E:1030:ARG:N	2.26	0.51
1:F:451:ALA:O	1:F:878:VAL:HG11	2.11	0.51
1:F:561:SER:O	1:F:833:GLY:HA3	2.10	0.51
1:F:555:LEU:HD11	1:F:909:LEU:HD12	1.92	0.51
1:A:184:MET:HB2	1:A:757:PHE:CE2	2.45	0.51
1:B:1032:ASN:CB	1:B:1033:GLU:HB2	2.40	0.51
1:B:605:ASN:O	1:B:627:LYS:N	2.40	0.51
1:C:839:MET:HA	1:C:842:LEU:HD22	1.91	0.51
1:D:213:GLN:HG2	1:D:239:ARG:HG2	1.92	0.51
1:D:425:LEU:HD23	1:D:429:GLU:HB2	1.92	0.51
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.91	0.51
1:A:677:PHE:CZ	1:A:852:TYR:HB2	2.45	0.51
1:A:892:ILE:HG12	1:A:1025:ARG:HD3	1.93	0.51
1:B:872:TYR:HA	1:B:875:SER:HB3	1.93	0.51
1:D:900:VAL:HB	1:D:901:PRO:HD3	1.92	0.51
1:D:918:ASN:OD1	1:D:923:GLN:NE2	2.38	0.51
1:E:1031:LYS:HD3	1:E:1035:ILE:HG13	1.93	0.51
1:E:281:PHE:HB2	1:E:610:PHE:CD1	2.46	0.51
1:C:251:LEU:HD21	1:C:262:LEU:HB2	1.92	0.51
1:C:919:ASP:OD1	1:C:921:TYR:N	2.43	0.51
1:D:158:VAL:HG22	1:D:162:MET:HE3	1.92	0.51
1:D:393:LEU:HD13	1:D:466:ILE:HA	1.92	0.51
1:E:647:THR:HG22	1:E:660:ALA:H	1.75	0.51
1:F:638:LYS:HG2	1:F:640:GLU:H	1.76	0.51
1:F:694:ARG:HD3	1:F:820:MET:SD	2.50	0.51
1:F:95:GLU:O	1:F:98:THR:OG1	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASN:CG	1:A:240:LEU:HG	2.31	0.51
1:B:165:ALA:HB3	1:B:313:MET:CE	2.41	0.51
1:B:698:LEU:HD21	1:B:713:PRO:HD3	1.92	0.51
1:C:613:ASN:HD22	1:C:614:GLY:N	2.08	0.51
1:C:584:GLN:HB2	1:C:617:GLN:HG2	1.92	0.51
1:C:756:ASP:OD1	1:C:765:LYS:HA	2.11	0.51
1:C:461:GLY:HA3	1:C:863:LEU:HD21	1.92	0.51
1:D:243:THR:HG23	1:D:268:ILE:HG22	1.92	0.51
1:D:435:MET:SD	1:D:490:PRO:HB3	2.50	0.51
1:D:883:LEU:HD22	1:D:896:VAL:HG11	1.92	0.51
1:F:101:ASP:OD1	1:F:131:LYS:NZ	2.39	0.51
1:F:64:VAL:HG13	1:F:117:LEU:HB2	1.93	0.51
1:B:441:ALA:O	1:B:445:ILE:HG23	2.11	0.51
1:B:190:PRO:HG3	1:B:774:TYR:HB3	1.92	0.51
1:C:13:TRP:CZ2	1:C:492:LEU:HD21	2.45	0.51
1:C:588:GLN:O	1:C:592:ASN:ND2	2.43	0.51
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.46	0.51
1:D:251:LEU:HD11	1:D:262:LEU:HA	1.93	0.51
1:D:41:PRO:HG2	1:D:94:PHE:HB2	1.92	0.51
1:D:747:ALA:O	1:D:769:MET:HA	2.11	0.51
1:D:94:PHE:CE2	1:D:103:ALA:HB1	2.46	0.51
1:E:32:VAL:HG22	1:E:298:ASN:HD21	1.75	0.51
1:E:80:SER:HB3	1:E:90:ILE:HG23	1.93	0.51
1:A:691:THR:HG23	1:A:694:ARG:HH12	1.75	0.51
1:C:379:THR:HG23	1:C:476:SER:OG	2.10	0.51
1:C:872:TYR:OH	1:C:923:GLN:HG2	2.10	0.51
1:E:1010:THR:OG1	1:E:1011:VAL:N	2.44	0.51
1:E:356:TYR:C	1:E:358:PHE:N	2.60	0.51
1:E:375:VAL:HG13	1:E:480:LEU:HB3	1.92	0.51
1:E:897:MET:O	1:E:900:VAL:HG23	2.11	0.51
1:B:1015:PHE:HE2	3:B:2100:LMT:H21	1.75	0.51
1:B:372:VAL:O	1:B:375:VAL:N	2.44	0.51
1:C:663:LEU:CD2	1:C:663:LEU:H	2.24	0.51
1:C:939:LEU:HD12	1:C:970:ILE:HG12	1.91	0.51
1:D:33:ALA:HA	1:D:300:LEU:HD13	1.92	0.51
1:D:578:LEU:HB2	1:D:618:ASN:O	2.10	0.51
1:D:796:PHE:HA	1:D:799:PHE:CE2	2.46	0.51
1:A:388:PHE:CE2	1:A:472:ILE:HD13	2.46	0.50
1:A:35:TYR:OH	1:A:564:LEU:HD23	2.11	0.50
1:B:459:PHE:HB3	1:B:464:GLY:HA2	1.93	0.50
1:C:110:LYS:O	1:C:113:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:977:PHE:HD2	1:C:1006:MET:HG2	1.75	0.50
1:D:977:PHE:HD2	1:D:1006:MET:HG3	1.76	0.50
1:D:485:ALA:HA	1:D:489:THR:HB	1.92	0.50
1:E:310:LEU:HD23	1:E:323:ILE:HG21	1.92	0.50
1:E:459:PHE:CD2	1:E:871:LEU:HD12	2.46	0.50
1:E:610:PHE:HB3	1:E:623:PHE:HB3	1.92	0.50
1:B:31:PRO:HB2	1:B:389:SER:HB2	1.93	0.50
1:B:351:VAL:HG22	1:B:976:ALA:HB1	1.94	0.50
1:C:100:ALA:HB2	1:C:295:THR:HG21	1.93	0.50
1:C:35:TYR:HE1	1:C:665:ALA:HB1	1.76	0.50
1:D:210:GLN:NE2	1:D:250:LEU:HB3	2.27	0.50
1:D:540:ARG:HG3	1:D:541:TYR:HD1	1.75	0.50
1:E:200:PRO:HD2	1:E:744:THR:HG22	1.92	0.50
1:F:352:PHE:HA	1:F:355:MET:HE2	1.92	0.50
1:F:675:PHE:HB2	1:F:854:TRP:CZ3	2.46	0.50
1:A:31:PRO:HB2	1:A:389:SER:CB	2.40	0.50
1:B:1032:ASN:CA	1:B:1033:GLU:HB2	2.41	0.50
1:C:1032:ASN:HB3	1:C:1033:GLU:HA	1.94	0.50
1:C:465:ALA:O	1:C:468:ARG:HB3	2.11	0.50
1:C:83:ASP:HB2	1:C:87:THR:O	2.11	0.50
1:D:462:SER:O	1:D:466:ILE:HG12	2.11	0.50
1:D:982:MET:HB3	1:D:983:PRO:HD3	1.94	0.50
1:E:532:GLY:O	1:E:535:LEU:N	2.45	0.50
1:F:608:SER:OG	1:F:625:SER:HB3	2.11	0.50
1:F:770:SER:HB3	1:F:775:ARG:HD3	1.94	0.50
1:A:354:VAL:HG21	1:A:975:LEU:HB3	1.92	0.50
1:B:300:LEU:HD11	1:B:333:VAL:HG12	1.93	0.50
1:B:534:ILE:HG13	1:B:535:LEU:N	2.27	0.50
1:B:576:VAL:HG22	1:B:658:VAL:HG22	1.93	0.50
1:B:3:ASN:HA	1:B:6:ILE:HD13	1.94	0.50
1:B:952:GLY:O	1:B:1035:ILE:HG13	2.12	0.50
1:E:1021:PHE:O	1:E:1021:PHE:HD2	1.95	0.50
1:E:149:MET:HB2	1:E:153:ASP:CB	2.42	0.50
1:E:186:ILE:HG12	1:E:268:ILE:HG12	1.93	0.50
1:F:184:MET:HB2	1:F:757:PHE:CE2	2.47	0.50
1:F:409:ALA:O	1:F:413:VAL:HG23	2.12	0.50
1:F:900:VAL:HB	1:F:901:PRO:HD3	1.92	0.50
1:A:579:PRO:HD3	1:A:656:ALA:CB	2.34	0.50
1:A:884:ALA:N	1:A:893:PRO:HG3	2.26	0.50
1:C:905:ILE:O	1:C:909:LEU:HB2	2.12	0.50
1:E:415:ASN:HB3	1:E:434:SER:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:ASP:OD1	1:F:760:ARG:NH2	2.45	0.50
1:F:344:LEU:HD22	1:F:402:ILE:HD11	1.93	0.50
1:F:388:PHE:HD1	1:F:469:GLN:HE22	1.58	0.50
1:F:415:ASN:HB3	1:F:434:SER:HB2	1.92	0.50
1:F:187:TRP:HE3	1:F:770:SER:O	1.94	0.50
1:F:936:ASN:ND2	1:F:1010:THR:HG22	2.26	0.50
1:A:790:ASP:OD2	1:A:792:GLN:HG3	2.11	0.50
1:B:105:VAL:HG21	1:C:105:VAL:HG13	1.94	0.50
1:B:106:GLN:HA	1:B:109:ASN:HD21	1.77	0.50
1:B:294:ALA:HB3	1:B:297:ALA:HB2	1.94	0.50
1:B:796:PHE:CD1	1:B:799:PHE:HE2	2.30	0.50
1:C:942:GLU:HG3	1:C:943:PHE:N	2.26	0.50
1:D:509:LYS:HG2	1:D:510:LYS:HG3	1.93	0.50
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.46	0.50
1:D:836:MET:O	1:D:840:GLU:HG3	2.12	0.50
1:F:363:ARG:HE	1:F:498:LYS:HD2	1.76	0.50
1:A:602:GLU:OE2	1:A:645:ARG:NH1	2.45	0.50
1:B:759:ASP:OD1	1:B:760:ARG:HG3	2.11	0.50
1:C:358:PHE:O	1:C:359:LEU:HD23	2.12	0.50
1:D:485:ALA:O	1:D:490:PRO:HD3	2.10	0.50
1:F:572:PHE:HD1	1:F:661:PHE:O	1.94	0.50
1:A:324:VAL:HG12	1:A:326:PRO:HD3	1.94	0.50
1:A:891:SER:OG	1:A:1028:PHE:HB2	2.12	0.50
1:A:350:LEU:HD13	1:A:980:GLY:HA2	1.93	0.50
1:B:1010:THR:OG1	1:B:1011:VAL:N	2.45	0.50
1:B:424:GLY:HA3	1:B:502:LYS:HB2	1.93	0.50
1:B:897:MET:O	1:B:900:VAL:HG23	2.12	0.50
1:C:493:CYS:HA	1:C:497:LEU:HB2	1.93	0.50
1:D:940:ILE:HD13	1:D:963:VAL:HG23	1.93	0.50
1:E:520:PHE:O	1:E:524:THR:HG22	2.12	0.50
1:E:578:LEU:HB2	1:E:618:ASN:O	2.11	0.50
1:A:1033:GLU:H	1:A:1035:ILE:HG13	1.77	0.50
1:A:190:PRO:HG3	1:A:784:TRP:CH2	2.46	0.50
1:A:404:LEU:HD21	1:A:449:LEU:HD22	1.94	0.50
1:A:893:PRO:O	1:A:896:VAL:HG13	2.12	0.50
1:B:667:VAL:HB	1:B:668:GLU:OE2	2.12	0.50
1:C:34:GLN:CG	1:C:333:VAL:HG22	2.42	0.50
1:D:281:PHE:CE1	1:D:608:SER:HB2	2.46	0.50
1:D:785:TYR:HB3	1:D:793:MET:HB3	1.93	0.50
1:D:448:VAL:HG13	1:D:879:VAL:HG22	1.94	0.50
1:D:400:LEU:CD2	1:D:924:VAL:HG12	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:647:THR:HG23	1:E:660:ALA:HB3	1.93	0.50
1:F:139:VAL:O	1:F:326:PRO:HD2	2.12	0.50
1:F:2:PRO:O	1:F:5:PHE:HB3	2.12	0.50
1:A:445:ILE:CD1	1:A:935:LYS:HE3	2.36	0.49
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.94	0.49
1:C:156:ASP:OD2	1:C:764:LYS:NZ	2.38	0.49
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.93	0.49
1:E:440:GLY:O	1:E:886:LEU:HD11	2.12	0.49
1:F:121:GLU:O	1:F:124:GLN:HG2	2.12	0.49
1:F:573:MET:SD	1:F:623:PHE:HD1	2.34	0.49
1:F:239:ARG:NH1	1:F:756:ASP:H	2.10	0.49
1:F:896:VAL:HG23	1:F:937:ALA:CB	2.40	0.49
1:F:963:VAL:O	1:F:967:LEU:HB2	2.11	0.49
1:A:535:LEU:CD2	1:A:1022:VAL:HG21	2.41	0.49
1:B:340:VAL:HG22	1:B:396:PHE:CE1	2.45	0.49
1:B:899:VAL:HG21	1:B:937:ALA:HB2	1.93	0.49
1:D:1006:MET:O	1:D:1010:THR:HG23	2.12	0.49
1:D:210:GLN:NE2	1:D:250:LEU:H	2.08	0.49
1:D:277:ILE:HG12	1:D:614:GLY:HA3	1.92	0.49
1:D:672:ALA:O	1:D:832:THR:OG1	2.26	0.49
1:D:990:ALA:O	1:D:992:SER:N	2.45	0.49
1:E:485:ALA:HA	1:E:489:THR:OG1	2.11	0.49
1:E:190:PRO:HG3	1:E:774:TYR:HB3	1.93	0.49
1:A:959:THR:HG21	1:A:1022:VAL:HG22	1.93	0.49
1:B:564:LEU:CD1	1:B:666:ILE:HD12	2.42	0.49
1:B:573:MET:HB2	1:B:661:PHE:CE2	2.47	0.49
1:B:746:GLY:O	1:B:748:ALA:N	2.46	0.49
1:C:588:GLN:HG3	1:C:592:ASN:HD21	1.77	0.49
1:D:210:GLN:HE22	1:D:250:LEU:N	2.10	0.49
1:D:632:ARG:HD2	1:D:637:ASN:O	2.12	0.49
1:F:158:VAL:HG22	1:F:162:MET:HE3	1.94	0.49
1:F:602:GLU:HB3	1:F:606:VAL:HG23	1.94	0.49
1:A:900:VAL:O	1:A:904:VAL:HG23	2.12	0.49
1:B:447:MET:HB3	1:B:882:CYS:SG	2.52	0.49
1:B:922:PHE:O	1:B:926:LEU:HB2	2.12	0.49
1:D:945:LYS:NZ	1:D:1025:ARG:HH21	2.10	0.49
1:D:452:VAL:HG12	1:D:875:SER:OG	2.12	0.49
1:D:72:ILE:HG23	1:D:106:GLN:CB	2.41	0.49
1:D:948:MET:HE1	1:D:955:LEU:HA	1.94	0.49
1:E:189:ASN:HB3	1:E:192:GLU:HB2	1.95	0.49
1:E:445:ILE:HG21	1:E:935:LYS:HD2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:653:ILE:HG13	1:E:654:LYS:HD2	1.94	0.49
1:E:4:PHE:CE1	1:E:8:ARG:NE	2.80	0.49
1:E:927:LEU:HD23	1:E:930:ILE:HD12	1.94	0.49
1:A:475:VAL:O	1:A:478:MET:HB3	2.12	0.49
1:B:16:ALA:O	1:B:20:MET:HG3	2.12	0.49
1:C:13:TRP:HA	1:C:13:TRP:CE3	2.46	0.49
1:D:770:SER:OG	1:D:775:ARG:HG2	2.12	0.49
1:E:1032:ASN:H	1:E:1032:ASN:ND2	2.10	0.49
1:E:953:LYS:O	1:E:1035:ILE:HD13	2.13	0.49
1:E:211:ASN:CG	1:E:240:LEU:HG	2.33	0.49
1:E:145:THR:OG1	1:E:320:GLY:O	2.30	0.49
1:F:679:LEU:HD22	1:F:822:ILE:HD11	1.92	0.49
1:F:855:THR:CA	1:F:859:TYR:HB2	2.42	0.49
1:F:880:PHE:HB2	1:F:897:MET:SD	2.53	0.49
1:A:1025:ARG:NH1	1:A:1028:PHE:HB3	2.27	0.49
1:A:347:ALA:HA	1:A:350:LEU:HD12	1.94	0.49
1:A:954:GLY:HA2	1:A:1033:GLU:HA	1.93	0.49
1:A:955:LEU:HD23	1:A:1026:ARG:CZ	2.42	0.49
1:B:673:THR:HA	1:B:832:THR:OG1	2.12	0.49
1:B:706:ASP:O	1:B:830:LYS:HD3	2.12	0.49
1:B:790:ASP:OD2	1:B:791:GLY:N	2.45	0.49
1:C:250:LEU:HD13	1:C:259:ARG:HD2	1.92	0.49
3:D:1102:LMT:H31	3:D:1102:LMT:O2'	2.13	0.49
1:E:259:ARG:H	1:E:259:ARG:HD3	1.77	0.49
1:E:527:TYR:CZ	1:E:967:LEU:HD23	2.47	0.49
1:E:568:ASP:O	1:E:629:TRP:HZ3	1.95	0.49
1:F:1031:LYS:HD3	1:F:1031:LYS:O	2.12	0.49
1:F:3:ASN:HD22	1:F:435:MET:HG3	1.77	0.49
1:F:363:ARG:HH21	1:F:498:LYS:HD2	1.77	0.49
1:F:509:LYS:HE2	1:F:513:PHE:CD1	2.48	0.49
1:A:584:GLN:N	1:A:617:GLN:HB3	2.27	0.49
1:B:280:GLU:HG2	1:B:283:GLY:O	2.12	0.49
1:B:728:GLN:HE22	1:B:738:ILE:HG21	1.78	0.49
1:C:687:HIS:NE2	1:C:718:ASP:OD1	2.32	0.49
1:D:872:TYR:CD1	3:D:1103:LMT:H92	2.48	0.49
1:D:190:PRO:HG3	1:D:784:TRP:CZ2	2.48	0.49
1:E:354:VAL:O	1:E:358:PHE:HB2	2.12	0.49
1:A:910:ALA:HB2	1:A:1004:GLY:HA3	1.94	0.49
3:A:1102:LMT:H52	3:A:1102:LMT:H82	1.56	0.49
1:A:151:GLN:OE1	1:A:278:ILE:HG22	2.13	0.49
1:A:356:TYR:O	1:A:360:GLN:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:PRO:HG2	1:A:875:SER:HB2	1.94	0.49
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.48	0.49
1:C:453:PHE:HZ	1:C:928:THR:OG1	1.96	0.49
1:C:556:PHE:HD1	1:C:908:LEU:HD21	1.77	0.49
1:C:579:PRO:HD3	1:C:656:ALA:HB2	1.93	0.49
1:E:903:GLY:O	1:E:1005:GLY:HA2	2.12	0.49
1:E:1006:MET:O	1:E:1010:THR:HG23	2.13	0.49
1:E:169:THR:HG21	1:E:306:ILE:CG1	2.41	0.49
1:D:275:TYR:CD1	1:F:223:PRO:HD3	2.47	0.49
1:F:368:PRO:O	1:F:371:ALA:HB3	2.13	0.49
1:A:952:GLY:O	1:A:1036:GLU:N	2.44	0.49
1:A:131:LYS:HB2	1:A:295:THR:HB	1.95	0.49
1:A:251:LEU:HD21	1:A:262:LEU:HB2	1.95	0.49
1:C:27:ILE:HA	1:C:30:LEU:HD22	1.94	0.49
1:C:532:GLY:O	1:C:535:LEU:N	2.46	0.49
1:C:653:ILE:HG13	1:C:654:LYS:HE2	1.95	0.49
1:C:940:ILE:HA	1:C:966:ARG:NH1	2.27	0.49
1:D:362:PHE:N	1:D:362:PHE:CD1	2.80	0.49
1:D:567:GLU:O	1:D:569:GLN:HG3	2.13	0.49
1:E:246:PHE:O	1:E:262:LEU:HD23	2.12	0.49
1:D:187:TRP:HH2	1:F:223:PRO:CD	2.26	0.49
1:F:747:ALA:O	1:F:769:MET:HA	2.13	0.49
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.48	0.49
1:A:404:LEU:HD12	1:A:932:LEU:CD2	2.43	0.49
1:B:1032:ASN:OD1	1:B:1033:GLU:HB2	2.12	0.49
1:B:1035:ILE:HG13	1:B:1036:GLU:N	2.28	0.49
1:B:748:ALA:O	1:B:770:SER:HB3	2.13	0.49
1:C:230:LEU:HG	1:C:231:ASN:N	2.28	0.49
1:C:935:LYS:NZ	1:C:936:ASN:OD1	2.38	0.49
1:D:872:TYR:CD2	3:D:1103:LMT:H111	2.48	0.49
1:D:452:VAL:HG23	1:D:453:PHE:CD1	2.47	0.49
1:D:720:PRO:HA	1:D:805:GLU:O	2.13	0.49
1:E:978:ILE:HD13	1:E:1007:VAL:HG22	1.95	0.49
1:E:446:ALA:CB	1:E:482:VAL:HG21	2.38	0.49
1:E:187:TRP:HA	1:E:769:MET:O	2.13	0.49
1:A:158:VAL:HG22	1:A:162:MET:HE3	1.95	0.48
1:A:357:LEU:HD23	1:A:358:PHE:CD1	2.47	0.48
1:C:160:ALA:HB1	1:C:762:ARG:HD3	1.95	0.48
1:C:368:PRO:O	1:C:371:ALA:HB3	2.13	0.48
1:D:1033:GLU:OE1	1:D:1035:ILE:HG23	2.12	0.48
1:E:988:THR:HG22	1:E:989:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:MET:HG3	1:A:661:PHE:CE1	2.49	0.48
1:B:902:LEU:HG	1:B:1012:LEU:HD23	1.94	0.48
1:B:69:MET:CE	1:B:107:VAL:HG13	2.43	0.48
1:C:598:TYR:CE2	1:C:624:VAL:HG21	2.48	0.48
1:C:58:GLN:OE1	1:C:811:LEU:HB3	2.13	0.48
1:D:101:ASP:N	1:D:101:ASP:OD1	2.46	0.48
1:D:279:ALA:HB3	1:D:286:ALA:O	2.13	0.48
1:D:401:ALA:O	1:D:405:LEU:HG	2.13	0.48
1:D:437:GLN:O	1:D:437:GLN:NE2	2.46	0.48
1:D:574:THR:HG23	1:D:622:ALA:HB3	1.95	0.48
1:D:776:MET:HB3	1:F:228:GLN:OE1	2.13	0.48
1:D:948:MET:HE2	1:D:958:ALA:HB3	1.96	0.48
1:E:438:ILE:O	1:E:441:ALA:HB3	2.13	0.48
1:E:631:ASP:OD1	1:E:631:ASP:N	2.45	0.48
1:F:985:VAL:HG13	1:F:1000:THR:OG1	2.13	0.48
1:F:540:ARG:HG3	1:F:541:TYR:HD1	1.78	0.48
1:F:900:VAL:HG13	1:F:930:ILE:HG23	1.96	0.48
1:F:883:LEU:CD2	1:F:938:ILE:HD11	2.43	0.48
1:A:535:LEU:HD21	1:A:1022:VAL:HG21	1.96	0.48
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.48	0.48
1:A:794:VAL:HG12	1:A:798:ALA:HB3	1.95	0.48
1:A:784:TRP:HB2	1:A:796:PHE:CD2	2.48	0.48
1:A:926:LEU:O	1:A:930:ILE:HG13	2.13	0.48
1:C:227:GLY:O	1:C:229:GLN:HG3	2.12	0.48
1:C:876:LEU:HD21	1:C:930:ILE:HD13	1.95	0.48
1:D:211:ASN:O	1:D:755:ASN:ND2	2.44	0.48
1:D:984:LEU:O	1:D:996:ASN:ND2	2.40	0.48
1:E:977:PHE:CD2	1:E:1006:MET:HG3	2.49	0.48
1:F:455:PRO:HB3	1:F:874:ILE:CG2	2.42	0.48
1:F:63:GLN:HG2	1:F:67:GLN:OE1	2.13	0.48
1:A:948:MET:CE	1:A:958:ALA:HB3	2.42	0.48
1:C:185:ARG:HB3	1:C:187:TRP:NE1	2.27	0.48
1:C:900:VAL:O	1:C:904:VAL:HG23	2.14	0.48
1:D:1011:VAL:O	1:D:1012:LEU:HD12	2.14	0.48
1:D:151:GLN:CD	1:D:151:GLN:H	2.16	0.48
1:D:549:VAL:O	1:D:552:MET:HB3	2.14	0.48
1:E:201:VAL:HG22	1:E:743:THR:OG1	2.13	0.48
1:F:509:LYS:HE2	1:F:513:PHE:HB2	1.94	0.48
1:F:714:ASN:HB3	1:F:821:GLU:HB3	1.95	0.48
1:A:508:GLY:H	1:A:518:ARG:HG3	1.77	0.48
1:B:239:ARG:HD3	1:B:756:ASP:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.48	0.48
1:D:247:GLY:C	1:D:249:ILE:H	2.16	0.48
1:D:270:LEU:HD21	1:D:759:ASP:OD1	2.14	0.48
1:D:673:THR:HB	1:D:826:ALA:H	1.78	0.48
1:D:674:GLY:HA2	1:D:825:GLN:HG2	1.96	0.48
1:D:981:VAL:HG21	1:D:1002:VAL:HG11	1.95	0.48
1:E:910:ALA:HB2	1:E:1004:GLY:HA3	1.96	0.48
1:E:883:LEU:HD13	1:E:896:VAL:CG1	2.43	0.48
1:F:560:PRO:O	1:F:917:THR:OG1	2.20	0.48
1:F:668:GLU:H	1:F:668:GLU:CD	2.15	0.48
1:A:530:SER:CB	3:A:1102:LMT:O2'	2.56	0.48
1:A:360:GLN:OE1	1:A:513:PHE:HB3	2.14	0.48
1:A:738:ILE:HA	1:A:741:ILE:HG13	1.95	0.48
1:B:1017:VAL:N	1:B:1018:PRO:HD2	2.28	0.48
1:B:188:MET:HA	1:B:266:ALA:CB	2.43	0.48
1:B:231:ASN:OD1	1:C:617:GLN:NE2	2.47	0.48
1:B:573:MET:SD	1:B:623:PHE:HD1	2.36	0.48
1:D:343:THR:HG22	1:D:344:LEU:HD23	1.95	0.48
1:D:400:LEU:HA	1:D:400:LEU:HD12	1.46	0.48
1:E:102:ILE:O	1:E:105:VAL:HG12	2.13	0.48
1:E:992:SER:HA	1:E:995:GLN:HB2	1.95	0.48
1:F:251:LEU:HD21	1:F:262:LEU:HB2	1.95	0.48
1:F:318:PRO:HG2	1:F:321:LEU:HG	1.95	0.48
1:F:579:PRO:HD3	1:F:656:ALA:HB2	1.95	0.48
1:F:939:LEU:HB3	1:F:966:ARG:CD	2.44	0.48
1:F:974:SER:OG	1:F:1010:THR:HG21	2.13	0.48
1:B:936:ASN:ND2	1:B:970:ILE:HG23	2.29	0.48
1:D:884:ALA:HA	1:D:889:SER:O	2.14	0.48
1:E:281:PHE:CE1	1:E:608:SER:HB2	2.49	0.48
1:F:183:ALA:O	1:F:270:LEU:HD12	2.13	0.48
1:F:521:GLU:O	1:F:524:THR:HG23	2.13	0.48
1:E:225:VAL:HG13	1:F:776:MET:SD	2.54	0.48
1:F:80:SER:OG	1:F:90:ILE:HG23	2.13	0.48
1:A:393:LEU:HD22	1:A:470:PHE:CE1	2.49	0.48
1:A:187:TRP:HE3	1:A:770:SER:O	1.97	0.48
1:B:281:PHE:HE1	1:B:608:SER:HB2	1.79	0.48
1:B:154:ILE:HG22	1:B:287:SER:HB3	1.96	0.48
1:B:770:SER:HG	1:B:775:ARG:HG2	1.78	0.48
1:C:200:PRO:HB2	1:C:744:THR:HG22	1.96	0.48
1:C:422:GLU:O	1:C:502:LYS:HG3	2.14	0.48
1:C:559:LEU:HG	1:C:560:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:LEU:HD21	1:D:262:LEU:HB2	1.96	0.48
1:D:344:LEU:HD21	1:D:399:VAL:HG22	1.96	0.48
1:F:463:THR:HG22	1:F:467:TYR:CZ	2.48	0.48
1:F:459:PHE:CE1	1:F:871:LEU:HG	2.49	0.48
1:F:939:LEU:O	1:F:966:ARG:NH1	2.47	0.48
1:A:184:MET:HG2	1:A:246:PHE:CE2	2.49	0.48
1:A:549:VAL:O	1:A:552:MET:HB3	2.13	0.48
1:A:673:THR:HG21	1:A:830:LYS:O	2.14	0.48
1:B:36:PRO:O	1:B:38:ILE:HG13	2.14	0.48
1:D:110:LYS:HD3	1:D:110:LYS:HA	1.58	0.48
1:D:25:LEU:HA	1:D:28:LEU:HD12	1.95	0.48
1:E:564:LEU:CD1	1:E:666:ILE:HD12	2.43	0.48
1:F:1006:MET:O	1:F:1009:ALA:HB3	2.14	0.48
1:F:149:MET:HG3	1:F:154:ILE:HG13	1.96	0.48
1:F:642:ILE:HA	1:F:645:ARG:NH1	2.29	0.48
1:A:186:ILE:HG12	1:A:268:ILE:HG12	1.96	0.48
1:A:757:PHE:HE1	1:A:759:ASP:HB2	1.78	0.48
1:A:125:GLN:OE1	1:A:765:LYS:HE3	2.13	0.48
1:C:966:ARG:NH1	1:C:966:ARG:HB3	2.28	0.48
1:D:17:ILE:CG2	1:E:881:LEU:HD21	2.44	0.48
1:F:455:PRO:HG2	1:F:875:SER:HA	1.96	0.48
1:F:951:GLU:O	1:F:953:LYS:N	2.47	0.48
1:A:859:TYR:O	1:A:863:LEU:HG	2.14	0.47
1:B:1021:PHE:O	1:B:1025:ARG:HB2	2.13	0.47
1:B:116:PRO:HA	1:B:123:GLN:HE22	1.78	0.47
1:B:423:GLU:OE1	1:B:433:LYS:HE3	2.14	0.47
1:B:534:ILE:HD11	1:B:1019:VAL:HG21	1.96	0.47
1:C:372:VAL:HB	1:C:373:PRO:CD	2.44	0.47
1:C:575:MET:HA	1:C:621:ILE:HG13	1.96	0.47
1:C:795:PRO:HG2	1:C:798:ALA:HB2	1.96	0.47
1:D:895:SER:HA	1:D:1020:PHE:HB3	1.96	0.47
1:D:213:GLN:HA	1:D:237:GLN:O	2.14	0.47
1:D:532:GLY:HA2	1:D:535:LEU:HB2	1.96	0.47
1:E:367:ILE:HD11	1:E:497:LEU:HD13	1.96	0.47
1:F:1020:PHE:O	1:F:1024:VAL:HG23	2.14	0.47
1:F:274:ASN:OD1	1:F:276:ASP:N	2.42	0.47
1:F:725:ASP:OD1	1:F:803:ARG:NH2	2.43	0.47
1:A:140:VAL:N	1:A:289:LEU:O	2.45	0.47
1:A:330:THR:HB	1:A:331:PRO:HD3	1.95	0.47
1:A:344:LEU:HD11	1:A:398:MET:CB	2.44	0.47
1:A:527:TYR:O	1:A:531:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:THR:HG21	1:C:984:LEU:CD2	2.34	0.47
1:C:715:GLY:HA2	1:C:810:ARG:NH2	2.29	0.47
1:D:826:ALA:HB2	1:D:835:ALA:HB2	1.95	0.47
1:D:927:LEU:HA	1:D:930:ILE:HD12	1.95	0.47
1:E:451:ALA:O	1:E:875:SER:OG	2.25	0.47
1:E:515:TRP:O	1:E:519:MET:HG3	2.13	0.47
1:E:746:GLY:O	1:E:750:GLY:N	2.43	0.47
1:E:677:PHE:CE1	1:E:852:TYR:HB2	2.49	0.47
1:F:402:ILE:O	1:F:406:VAL:HG22	2.14	0.47
1:F:45:ILE:HD12	1:F:90:ILE:HB	1.96	0.47
1:F:472:ILE:HG23	1:F:473:THR:N	2.29	0.47
1:F:504:ASP:C	1:F:506:GLY:N	2.67	0.47
1:F:555:LEU:HB3	1:F:908:LEU:HB3	1.95	0.47
1:F:737:SER:O	1:F:740:ASP:HB2	2.14	0.47
1:A:17:ILE:CG2	1:B:881:LEU:HD21	2.43	0.47
1:C:1010:THR:OG1	1:C:1011:VAL:N	2.46	0.47
1:C:565:PRO:HG2	1:C:567:GLU:OE2	2.14	0.47
1:D:530:SER:OG	3:D:1102:LMT:H1'	2.14	0.47
1:D:522:LYS:O	1:D:525:HIS:HB3	2.15	0.47
1:D:73:ASP:OD2	1:F:131:LYS:NZ	2.38	0.47
1:D:41:PRO:HD2	1:D:94:PHE:O	2.14	0.47
1:E:310:LEU:HG	1:E:323:ILE:HG13	1.96	0.47
1:F:137:LEU:HD11	1:F:303:ALA:HB2	1.96	0.47
1:F:242:SER:O	1:F:246:PHE:HD1	1.96	0.47
1:F:369:THR:O	1:F:373:PRO:HD2	2.14	0.47
1:F:3:ASN:HD21	1:F:439:GLN:HG3	1.80	0.47
1:A:902:LEU:HD21	1:A:1016:PHE:HB2	1.96	0.47
1:B:515:TRP:O	1:B:519:MET:HG3	2.14	0.47
1:B:631:ASP:C	1:B:633:PRO:HD3	2.34	0.47
1:C:171:GLY:O	1:C:293:LEU:HD23	2.14	0.47
1:C:146:ASP:OD2	1:C:320:GLY:HA3	2.15	0.47
1:D:1028:PHE:O	1:D:1029:SER:HB2	2.15	0.47
1:D:216:ALA:HB1	1:D:234:ILE:HG22	1.96	0.47
1:E:675:PHE:CE2	1:E:839:MET:HG3	2.48	0.47
1:E:932:LEU:HD23	1:E:932:LEU:HA	1.51	0.47
1:A:153:ASP:OD2	1:A:182:TYR:OH	2.32	0.47
1:A:210:GLN:NE2	1:A:250:LEU:H	2.09	0.47
1:A:379:THR:OG1	1:A:477:ALA:HA	2.14	0.47
1:B:32:VAL:HG22	1:B:298:ASN:ND2	2.30	0.47
1:B:555:LEU:HB3	1:B:908:LEU:HB3	1.95	0.47
1:D:941:VAL:HG13	1:D:1021:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:670:GLY:HA2	1:D:857:MET:HE3	1.96	0.47
1:E:5:PHE:CE1	1:E:487:ILE:HG12	2.50	0.47
1:F:311:ALA:O	1:F:314:GLU:HB2	2.14	0.47
1:F:564:LEU:HD23	1:F:665:ALA:HB3	1.95	0.47
1:F:685:LEU:HD22	1:F:689:LYS:NZ	2.30	0.47
1:A:1015:PHE:HE2	3:A:1102:LMT:H21	1.79	0.47
1:A:900:VAL:HB	1:A:901:PRO:HD3	1.97	0.47
1:B:469:GLN:O	1:B:473:THR:OG1	2.29	0.47
1:B:956:ILE:H	1:B:956:ILE:HG13	1.49	0.47
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.50	0.47
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.96	0.47
1:D:1027:ARG:O	1:D:1028:PHE:HB2	2.15	0.47
1:D:353:LEU:HD22	1:D:353:LEU:HA	1.70	0.47
1:E:250:LEU:HD13	1:E:261:LEU:HD23	1.96	0.47
1:E:352:PHE:CE1	1:E:365:THR:HG23	2.50	0.47
1:F:382:VAL:HG11	1:F:476:SER:CB	2.44	0.47
1:F:935:LYS:NZ	1:F:973:THR:HG21	2.30	0.47
1:A:563:PHE:C	1:A:564:LEU:HD12	2.34	0.47
1:A:763:VAL:HG12	1:B:63:GLN:OE1	2.15	0.47
1:B:137:LEU:HD12	1:B:329:THR:HG22	1.96	0.47
1:C:918:ASN:O	1:C:918:ASN:ND2	2.41	0.47
1:D:352:PHE:HD2	1:D:353:LEU:HD23	1.80	0.47
1:D:356:TYR:O	1:D:360:GLN:N	2.42	0.47
1:E:346:GLU:O	1:E:349:ILE:N	2.48	0.47
1:F:110:LYS:O	1:F:113:LEU:HB2	2.15	0.47
1:F:190:PRO:HB3	1:F:784:TRP:CH2	2.50	0.47
1:F:704:HIS:CE1	1:F:842:LEU:HD11	2.50	0.47
1:A:449:LEU:O	1:A:453:PHE:HD1	1.97	0.47
1:A:962:ALA:O	1:A:965:MET:HG2	2.15	0.47
1:B:520:PHE:O	1:B:524:THR:HG22	2.14	0.47
1:A:221:GLY:HA3	1:B:775:ARG:HH12	1.79	0.47
1:C:587:THR:HG21	1:C:618:ASN:HA	1.96	0.47
1:C:722:PHE:HD1	1:C:804:TRP:CD2	2.33	0.47
1:C:739:ASN:O	1:C:742:ASN:HB2	2.14	0.47
1:D:21:LEU:HA	1:D:21:LEU:HD13	1.74	0.47
1:D:166:ILE:HD13	1:D:309:GLU:HG2	1.97	0.47
1:D:673:THR:HA	1:D:832:THR:OG1	2.14	0.47
1:D:697:LEU:HD23	1:D:822:ILE:HD13	1.97	0.47
1:D:884:ALA:N	1:D:893:PRO:HG3	2.30	0.47
1:E:142:VAL:HG21	1:E:162:MET:HE3	1.96	0.47
1:E:343:THR:HG22	1:E:344:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:THR:OG1	1:E:91:THR:OG1	2.13	0.47
1:F:151:GLN:NE2	1:F:279:ALA:O	2.47	0.47
1:F:696:GLN:HG2	1:F:846:LEU:HD22	1.96	0.47
1:F:876:LEU:HD21	1:F:930:ILE:HD13	1.96	0.47
1:F:910:ALA:HB2	1:F:1004:GLY:HA3	1.96	0.47
1:A:966:ARG:HB3	1:A:966:ARG:HH11	1.80	0.47
1:B:701:ALA:HB3	1:B:711:VAL:HG11	1.96	0.47
1:B:897:MET:O	1:B:899:VAL:N	2.47	0.47
1:B:904:VAL:O	1:B:906:GLY:N	2.48	0.47
1:C:293:LEU:HD11	1:C:299:ALA:HA	1.96	0.47
1:C:527:TYR:O	1:C:531:VAL:HG23	2.15	0.47
1:C:54:ALA:HB3	1:C:808:SER:O	2.15	0.47
1:D:445:ILE:HD13	1:D:935:LYS:HE3	1.96	0.47
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.80	0.47
1:E:355:MET:CE	1:E:368:PRO:HG2	2.44	0.47
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.96	0.47
1:F:355:MET:SD	1:F:368:PRO:HB2	2.55	0.47
1:F:759:ASP:OD1	1:F:760:ARG:HG3	2.14	0.47
1:F:756:ASP:OD1	1:F:765:LYS:HA	2.15	0.47
1:F:899:VAL:HA	1:F:902:LEU:HD13	1.97	0.47
1:A:544:LEU:O	1:A:548:ILE:HG13	2.14	0.47
1:A:211:ASN:O	1:A:755:ASN:ND2	2.45	0.47
1:C:1010:THR:O	1:C:1012:LEU:N	2.48	0.47
1:C:121:GLU:O	1:C:124:GLN:HG2	2.15	0.47
1:C:261:LEU:O	1:C:265:VAL:HG13	2.15	0.47
1:D:579:PRO:HD3	1:D:656:ALA:HB2	1.96	0.47
1:D:785:TYR:CB	1:D:793:MET:HB3	2.45	0.47
1:D:893:PRO:O	1:D:896:VAL:HG13	2.15	0.47
1:E:220:GLY:HA3	1:E:230:LEU:O	2.15	0.47
1:E:47:ALA:HB2	1:E:127:VAL:HG13	1.97	0.47
1:F:146:ASP:OD2	1:F:146:ASP:N	2.40	0.47
1:F:45:ILE:HG21	1:F:111:LEU:HG	1.96	0.47
1:F:876:LEU:CD2	1:F:930:ILE:HG21	2.45	0.47
1:A:438:ILE:O	1:A:442:LEU:HG	2.15	0.47
1:A:695:ASN:HA	1:A:698:LEU:HD12	1.97	0.47
1:B:151:GLN:OE1	1:B:278:ILE:HA	2.16	0.47
1:B:396:PHE:O	1:B:400:LEU:HB2	2.14	0.47
1:B:408:ASP:OD2	1:B:481:SER:OG	2.22	0.47
1:B:594:VAL:HG22	1:B:650:PHE:CZ	2.50	0.47
1:B:631:ASP:N	1:B:631:ASP:OD1	2.48	0.47
1:B:663:LEU:CD2	1:B:663:LEU:H	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ASN:HB2	1:C:258:SER:OG	2.15	0.47
1:D:72:ILE:HG23	1:D:106:GLN:HB2	1.97	0.47
1:E:697:LEU:HD23	1:E:822:ILE:HD13	1.97	0.47
1:F:1030:ARG:C	1:F:1032:ASN:H	2.18	0.47
1:F:669:LEU:HD23	1:F:669:LEU:HA	1.72	0.47
1:F:746:GLY:O	1:F:748:ALA:N	2.48	0.47
1:A:1013:ALA:C	1:A:1015:PHE:N	2.68	0.46
1:B:545:TYR:CE2	1:B:1020:PHE:HZ	2.32	0.46
1:B:401:ALA:O	1:B:405:LEU:HG	2.15	0.46
1:B:36:PRO:HG3	1:B:469:GLN:HG3	1.98	0.46
1:B:986:ILE:O	1:B:986:ILE:HG22	2.15	0.46
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.97	0.46
1:C:318:PRO:HG2	1:C:321:LEU:HG	1.97	0.46
1:C:239:ARG:HD3	1:C:756:ASP:O	2.15	0.46
1:A:888:GLU:CD	1:C:8:ARG:HB3	2.36	0.46
1:D:544:LEU:O	1:D:548:ILE:HG13	2.15	0.46
1:D:701:ALA:HB3	1:D:711:VAL:HG11	1.97	0.46
1:D:694:ARG:HD2	1:D:713:PRO:HB3	1.97	0.46
1:D:45:ILE:HD12	1:D:90:ILE:HB	1.96	0.46
1:E:350:LEU:HD13	1:E:980:GLY:HA2	1.97	0.46
1:E:326:PRO:O	1:E:623:PHE:HE2	1.98	0.46
1:E:908:LEU:HD23	1:E:922:PHE:HZ	1.81	0.46
1:D:881:LEU:HD11	1:F:17:ILE:CG2	2.45	0.46
1:F:58:GLN:HA	1:F:62:THR:HB	1.96	0.46
1:F:723:LYS:HB3	1:F:803:ARG:HG3	1.98	0.46
1:F:955:LEU:O	1:F:958:ALA:N	2.48	0.46
1:A:222:THR:HA	1:A:224:PRO:HD3	1.97	0.46
1:A:541:TYR:N	1:A:541:TYR:CD1	2.80	0.46
1:A:796:PHE:O	1:A:800:SER:OG	2.13	0.46
1:B:157:TYR:CZ	1:B:318:PRO:HD3	2.51	0.46
1:C:378:GLY:O	1:C:382:VAL:HG23	2.15	0.46
1:C:486:LEU:O	1:C:490:PRO:HG2	2.15	0.46
1:D:383:LEU:HB3	1:D:388:PHE:HB2	1.98	0.46
1:D:451:ALA:HB1	1:D:878:VAL:HG12	1.98	0.46
1:D:892:ILE:HG12	1:D:1025:ARG:CD	2.46	0.46
1:E:200:PRO:O	1:E:203:VAL:N	2.48	0.46
1:E:151:GLN:NE2	1:E:277:ILE:O	2.48	0.46
1:E:899:VAL:HG21	1:E:937:ALA:CB	2.45	0.46
1:F:15:ILE:O	1:F:19:ILE:HG13	2.15	0.46
1:F:240:LEU:HD12	1:F:246:PHE:CD2	2.50	0.46
1:A:239:ARG:NH1	1:A:756:ASP:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:ARG:HH12	1:A:818:PRO:HG3	1.79	0.46
1:B:326:PRO:O	1:B:623:PHE:HE2	1.98	0.46
1:B:435:MET:HG3	1:B:490:PRO:HB3	1.97	0.46
1:C:246:PHE:HA	1:C:249:ILE:HG12	1.97	0.46
1:D:588:GLN:HB2	1:D:613:ASN:HD22	1.80	0.46
1:E:143:ILE:HG22	1:E:286:ALA:CB	2.45	0.46
1:E:251:LEU:HD12	1:E:265:VAL:HG11	1.98	0.46
1:D:225:VAL:N	1:E:776:MET:HE1	2.19	0.46
1:F:135:SER:HB3	1:F:668:GLU:HB3	1.97	0.46
1:F:284:GLN:HG3	1:F:285:PRO:HD2	1.98	0.46
1:F:375:VAL:HB	1:F:405:LEU:HD22	1.97	0.46
1:A:470:PHE:CD1	1:A:924:VAL:HG21	2.49	0.46
1:B:156:ASP:OD2	1:B:764:LYS:NZ	2.39	0.46
1:B:712:ARG:CD	1:B:823:LEU:HB2	2.46	0.46
1:B:889:SER:HB3	1:B:892:ILE:HB	1.96	0.46
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.96	0.46
1:D:955:LEU:HD21	1:D:1022:VAL:HG13	1.98	0.46
1:D:423:GLU:HB2	1:D:425:LEU:HD13	1.97	0.46
1:D:415:ASN:OD1	1:D:434:SER:HB2	2.15	0.46
1:D:412:VAL:HG11	1:D:489:THR:HG22	1.97	0.46
1:E:355:MET:CE	1:E:410:ILE:HG12	2.45	0.46
1:E:76:MET:HG2	1:E:859:TYR:OH	2.14	0.46
1:F:104:GLN:HG3	1:F:105:VAL:N	2.24	0.46
1:F:367:ILE:HG21	1:F:489:THR:HG23	1.97	0.46
1:F:940:ILE:HA	1:F:966:ARG:HH12	1.79	0.46
2:A:1101:ERY:H321	2:A:1101:ERY:H8	1.74	0.46
1:A:423:GLU:OE2	1:A:433:LYS:HE2	2.16	0.46
1:A:770:SER:OG	1:A:775:ARG:HG2	2.15	0.46
1:B:685:LEU:HD11	1:B:849:GLY:HA3	1.98	0.46
1:D:240:LEU:HD12	1:D:246:PHE:CE2	2.50	0.46
1:D:457:ALA:HA	1:D:468:ARG:HA	1.97	0.46
1:E:434:SER:O	1:E:437:GLN:HB2	2.15	0.46
1:E:416:VAL:HG11	1:E:497:LEU:HD23	1.97	0.46
1:F:211:ASN:CG	1:F:240:LEU:HG	2.36	0.46
1:F:375:VAL:HG21	1:F:405:LEU:HD13	1.97	0.46
1:F:450:SER:HB3	1:F:478:MET:HB2	1.98	0.46
1:F:358:PHE:CD1	1:F:972:MET:HG2	2.51	0.46
1:A:142:VAL:HG21	1:A:158:VAL:HG22	1.98	0.46
1:A:190:PRO:HD3	1:A:774:TYR:CD1	2.51	0.46
1:A:449:LEU:HB3	1:A:478:MET:SD	2.56	0.46
1:B:7:ASP:CG	1:B:432:ARG:HH21	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:ALA:O	1:B:915:GLY:N	2.48	0.46
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.97	0.46
1:C:562:SER:HB2	1:C:919:ASP:HB3	1.97	0.46
1:D:563:PHE:CE1	3:D:1103:LMT:H5B	2.50	0.46
1:D:149:MET:HG3	1:D:154:ILE:HG13	1.97	0.46
1:D:810:ARG:HG3	1:D:810:ARG:O	2.14	0.46
1:E:187:TRP:HE3	1:E:770:SER:O	1.97	0.46
1:E:274:ASN:ND2	1:E:276:ASP:OD2	2.30	0.46
1:F:300:LEU:HD11	1:F:333:VAL:HG11	1.98	0.46
1:F:531:VAL:HG21	1:F:963:VAL:HG11	1.98	0.46
1:F:891:SER:HB3	1:F:1028:PHE:CD2	2.50	0.46
1:A:407:ASP:OD2	1:A:935:LYS:HG2	2.15	0.46
1:B:440:GLY:O	1:B:886:LEU:HD11	2.16	0.46
1:B:382:VAL:HG11	1:B:476:SER:OG	2.16	0.46
1:B:679:LEU:HA	1:B:679:LEU:HD12	1.80	0.46
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.46	0.46
1:C:748:ALA:O	1:C:770:SER:HB3	2.15	0.46
1:E:926:LEU:O	1:E:930:ILE:HG13	2.15	0.46
1:D:187:TRP:CH2	1:F:223:PRO:HD2	2.48	0.46
1:F:364:ALA:HA	1:F:367:ILE:HD12	1.98	0.46
1:F:465:ALA:HA	1:F:468:ARG:NH1	2.31	0.46
1:F:940:ILE:HG12	1:F:966:ARG:NH2	2.29	0.46
1:A:110:LYS:HA	1:A:110:LYS:HD3	1.58	0.46
1:A:20:MET:SD	1:A:374:VAL:HG22	2.55	0.46
1:A:462:SER:O	1:A:466:ILE:HG12	2.15	0.46
1:A:615:GLY:N	1:A:616:GLY:HA2	2.31	0.46
1:A:667:VAL:HG12	1:A:668:GLU:OE1	2.16	0.46
1:B:149:MET:HB2	1:B:153:ASP:HB2	1.97	0.46
1:B:530:SER:O	1:B:534:ILE:HG23	2.16	0.46
1:B:563:PHE:O	1:B:564:LEU:HD12	2.15	0.46
1:B:277:ILE:HA	1:B:613:ASN:O	2.16	0.46
1:C:344:LEU:HA	1:C:399:VAL:HG22	1.97	0.46
1:C:790:ASP:OD2	1:C:791:GLY:N	2.49	0.46
1:D:1032:ASN:HB3	1:D:1033:GLU:H	1.44	0.46
1:D:149:MET:HB2	1:D:153:ASP:CB	2.45	0.46
1:D:365:THR:O	1:D:368:PRO:HD2	2.16	0.46
1:D:597:TYR:CD2	1:D:650:PHE:CZ	3.04	0.46
1:D:831:SER:OG	1:D:832:THR:N	2.47	0.46
1:E:57:VAL:HG23	1:E:82:SER:HB3	1.98	0.46
1:F:635:GLU:O	1:F:638:LYS:HB3	2.16	0.46
1:A:968:ARG:O	1:A:972:MET:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LEU:HD13	1:B:294:ALA:O	2.15	0.46
1:B:906:GLY:O	1:B:910:ALA:N	2.49	0.46
1:B:941:VAL:HG13	1:B:1021:PHE:CE1	2.51	0.46
1:C:142:VAL:HG21	1:C:158:VAL:HG22	1.98	0.46
1:C:571:VAL:N	1:C:626:LEU:HD12	2.30	0.46
1:C:631:ASP:C	1:C:633:PRO:HD3	2.36	0.46
1:C:182:TYR:HD2	1:C:760:ARG:HH22	1.64	0.46
1:C:899:VAL:HG21	1:C:937:ALA:HB2	1.98	0.46
1:C:972:MET:HB2	1:C:972:MET:HE2	1.91	0.46
1:F:211:ASN:OD1	1:F:240:LEU:N	2.45	0.46
1:F:659:PHE:HE2	1:F:712:ARG:HB3	1.80	0.46
1:A:102:ILE:HG21	1:C:101:ASP:HB3	1.98	0.46
1:A:391:ASN:OD1	1:A:393:LEU:N	2.48	0.46
1:A:505:HIS:O	1:A:507:GLU:N	2.49	0.46
1:A:554:TYR:CZ	1:A:558:ARG:HG3	2.51	0.46
1:B:941:VAL:HG13	1:B:1021:PHE:CD1	2.51	0.46
1:B:242:SER:HB2	1:B:245:GLU:HG3	1.98	0.46
1:B:509:LYS:HD3	1:B:510:LYS:HE2	1.97	0.46
1:B:522:LYS:O	1:B:525:HIS:HB3	2.16	0.46
1:B:404:LEU:HD12	1:B:932:LEU:HD21	1.97	0.46
1:C:685:LEU:O	1:C:689:LYS:NZ	2.38	0.46
1:D:449:LEU:HB3	1:D:478:MET:SD	2.56	0.46
1:D:636:GLU:N	1:D:636:GLU:OE1	2.42	0.46
1:E:906:GLY:HA2	1:E:1008:THR:HG21	1.97	0.46
1:E:545:TYR:HE2	1:E:902:LEU:HD11	1.81	0.46
1:E:350:LEU:CD1	1:E:980:GLY:HA2	2.46	0.46
1:F:272:GLY:N	1:F:275:TYR:OH	2.28	0.46
1:F:378:GLY:O	1:F:382:VAL:HG23	2.16	0.46
1:B:4:PHE:CE1	1:B:8:ARG:NE	2.84	0.45
1:B:594:VAL:HG22	1:B:650:PHE:CE2	2.52	0.45
1:C:908:LEU:HD23	1:C:922:PHE:CZ	2.50	0.45
1:C:956:ILE:H	1:C:956:ILE:HD12	1.81	0.45
1:D:16:ALA:O	1:D:20:MET:HG3	2.17	0.45
1:D:667:VAL:O	1:D:668:GLU:HG2	2.16	0.45
1:D:763:VAL:HG12	1:E:63:GLN:OE1	2.15	0.45
1:D:963:VAL:CA	1:D:966:ARG:HH22	2.25	0.45
1:E:1010:THR:O	1:E:1012:LEU:N	2.50	0.45
1:E:188:MET:HE3	1:E:784:TRP:HZ3	1.81	0.45
1:E:531:VAL:HG11	1:E:963:VAL:HG11	1.98	0.45
1:D:275:TYR:HB2	1:F:222:THR:HB	1.99	0.45
1:F:677:PHE:O	1:F:821:GLU:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:CD2	1:A:481:SER:HB3	2.37	0.45
1:A:759:ASP:HB3	1:A:764:LYS:HE3	1.99	0.45
1:B:111:LEU:HD11	1:B:127:VAL:HB	1.98	0.45
1:B:527:TYR:O	1:B:531:VAL:HG23	2.16	0.45
1:B:78:MET:HG3	1:B:92:LEU:HG	1.97	0.45
1:C:871:LEU:O	1:C:875:SER:HB2	2.17	0.45
1:C:900:VAL:HB	1:C:901:PRO:HD3	1.98	0.45
1:C:920:VAL:HG12	1:C:921:TYR:N	2.31	0.45
1:C:920:VAL:O	1:C:923:GLN:HB2	2.16	0.45
1:D:309:GLU:O	1:D:312:LYS:HB2	2.17	0.45
1:E:158:VAL:HG22	1:E:162:MET:HE3	1.97	0.45
1:E:58:GLN:OE1	1:E:811:LEU:HD13	2.16	0.45
1:D:881:LEU:HD11	1:F:17:ILE:HG22	1.97	0.45
1:F:216:ALA:HB1	1:F:234:ILE:HG22	1.97	0.45
1:F:531:VAL:O	1:F:534:ILE:HG13	2.16	0.45
1:A:200:PRO:O	1:A:203:VAL:N	2.48	0.45
1:A:707:MET:O	1:A:827:ALA:N	2.49	0.45
1:A:981:VAL:HG11	1:A:1003:MET:HB2	1.98	0.45
1:B:932:LEU:HD23	1:B:932:LEU:HA	1.76	0.45
1:C:667:VAL:HB	1:C:668:GLU:OE2	2.16	0.45
1:D:1010:THR:OG1	1:D:1011:VAL:N	2.49	0.45
1:D:30:LEU:HD12	1:D:30:LEU:HA	1.83	0.45
1:D:79:SER:HA	1:D:813:ARG:O	2.15	0.45
1:E:2:PRO:O	1:E:6:ILE:HG13	2.16	0.45
1:E:327:TYR:HD1	1:E:623:PHE:CE1	2.33	0.45
1:F:653:ILE:O	1:F:654:LYS:HE2	2.16	0.45
1:A:1033:GLU:O	1:A:1034:ASP:HB2	2.15	0.45
1:A:448:VAL:O	1:A:451:ALA:HB3	2.17	0.45
1:A:457:ALA:HB1	1:A:468:ARG:HG3	1.97	0.45
1:A:53:ASP:O	1:A:57:VAL:HG23	2.16	0.45
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.19	0.45
1:B:104:GLN:HG3	1:B:131:LYS:HG3	1.98	0.45
1:B:525:HIS:O	1:B:526:HIS:C	2.53	0.45
1:B:187:TRP:HA	1:B:769:MET:O	2.16	0.45
1:C:45:ILE:HD12	1:C:90:ILE:HB	1.98	0.45
1:D:261:LEU:O	1:D:265:VAL:HG13	2.16	0.45
1:D:491:ALA:O	1:D:495:THR:OG1	2.26	0.45
1:E:291:ILE:HD13	1:E:306:ILE:HD13	1.96	0.45
1:E:370:ILE:O	1:E:374:VAL:HG23	2.16	0.45
1:E:530:SER:OG	3:E:1101:LMT:C2'	2.64	0.45
1:F:400:LEU:HD12	1:F:400:LEU:HA	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:ASN:ND2	1:F:435:MET:HG3	2.31	0.45
1:F:527:TYR:CD1	3:F:2100:LMT:H71	2.51	0.45
1:E:235:ILE:N	1:F:722:PHE:O	2.45	0.45
1:A:889:SER:HB3	1:A:892:ILE:HB	1.97	0.45
1:B:300:LEU:HD11	1:B:333:VAL:CG1	2.46	0.45
1:B:372:VAL:HG12	1:B:405:LEU:HB3	1.99	0.45
1:B:501:ALA:O	1:B:504:ASP:HB2	2.17	0.45
1:B:675:PHE:CD1	1:B:854:TRP:HZ3	2.34	0.45
1:C:310:LEU:O	1:C:314:GLU:HG3	2.17	0.45
1:E:524:THR:O	1:E:527:TYR:HB3	2.17	0.45
1:E:896:VAL:HG21	1:E:938:ILE:CG1	2.42	0.45
1:F:142:VAL:HG12	1:F:321:LEU:HD22	1.99	0.45
1:F:216:ALA:HB1	1:F:234:ILE:CG2	2.46	0.45
1:F:826:ALA:HB3	1:F:830:LYS:HG3	1.97	0.45
1:A:795:PRO:O	1:A:798:ALA:HB3	2.16	0.45
1:A:944:ALA:HB2	1:A:959:THR:HA	1.99	0.45
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.80	0.45
1:B:572:PHE:CE1	1:B:643:THR:HG22	2.51	0.45
1:C:525:HIS:O	1:C:526:HIS:C	2.53	0.45
1:D:383:LEU:HD11	1:D:473:THR:HG23	1.97	0.45
1:D:573:MET:HG3	1:D:661:PHE:CE1	2.52	0.45
1:E:1030:ARG:HG2	1:E:1030:ARG:O	2.17	0.45
1:E:449:LEU:HA	1:E:449:LEU:HD23	1.86	0.45
1:E:527:TYR:CE2	1:E:967:LEU:HD23	2.52	0.45
1:E:966:ARG:C	1:E:969:PRO:HD2	2.37	0.45
1:E:9:PRO:HB3	1:E:495:THR:HG21	1.99	0.45
1:F:154:ILE:HG22	1:F:287:SER:HB3	1.99	0.45
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.98	0.45
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.74	0.45
1:A:639:VAL:HG11	1:A:662:ASN:HB2	1.99	0.45
1:A:675:PHE:CD1	1:A:854:TRP:HZ3	2.35	0.45
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.98	0.45
1:B:738:ILE:HA	1:B:741:ILE:HG13	1.99	0.45
1:C:1010:THR:C	1:C:1012:LEU:H	2.20	0.45
1:C:595:THR:HG23	1:C:609:VAL:HB	1.99	0.45
1:C:677:PHE:CD2	1:C:678:GLU:N	2.85	0.45
1:C:187:TRP:HA	1:C:769:MET:O	2.17	0.45
1:C:463:THR:HG23	1:C:920:VAL:HG22	1.98	0.45
1:D:190:PRO:HG3	1:D:784:TRP:CH2	2.52	0.45
1:D:693:ALA:HB1	1:D:850:VAL:HG11	1.97	0.45
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1013:ALA:C	1:B:1015:PHE:H	2.19	0.45
1:B:47:ALA:HB2	1:B:127:VAL:HA	1.98	0.45
1:C:714:ASN:N	1:C:821:GLU:O	2.50	0.45
1:C:847:PRO:HG2	1:C:850:VAL:HG21	1.97	0.45
1:D:214:VAL:HG23	1:D:237:GLN:HB3	1.99	0.45
1:D:375:VAL:HG21	1:D:481:SER:HA	1.99	0.45
1:D:456:MET:HE3	1:D:456:MET:HB3	1.74	0.45
1:D:350:LEU:HD22	1:D:979:LEU:HB3	1.99	0.45
1:E:198:LEU:HD23	1:E:787:ARG:HH21	1.82	0.45
1:E:562:SER:HB3	1:E:919:ASP:HB3	1.97	0.45
1:F:293:LEU:HD22	1:F:297:ALA:HB3	1.99	0.45
1:F:69:MET:CB	1:F:72:ILE:HD11	2.46	0.45
1:F:769:MET:HG2	1:F:770:SER:N	2.31	0.45
1:A:796:PHE:HA	1:A:799:PHE:HE2	1.80	0.45
1:B:1035:ILE:HG13	1:B:1036:GLU:H	1.81	0.45
1:C:694:ARG:HD3	1:C:820:MET:SD	2.57	0.45
1:D:254:ASN:ND2	1:D:258:SER:OG	2.44	0.45
1:D:339:GLU:OE1	1:D:342:LYS:HD3	2.17	0.45
1:D:424:GLY:CA	1:D:502:LYS:HB3	2.43	0.45
1:D:584:GLN:H	1:D:617:GLN:HB3	1.82	0.45
1:D:680:ILE:HD11	1:D:814:TYR:HD2	1.82	0.45
1:E:1013:ALA:C	1:E:1015:PHE:H	2.20	0.45
1:E:770:SER:HB3	1:E:775:ARG:HD3	1.98	0.45
1:E:883:LEU:HA	1:E:883:LEU:HD23	1.64	0.45
1:E:905:ILE:HG13	1:E:905:ILE:O	2.16	0.45
1:F:166:ILE:HG22	1:F:175:VAL:HG21	1.99	0.45
1:F:368:PRO:O	1:F:406:VAL:HG12	2.16	0.45
1:F:368:PRO:HB3	1:F:409:ALA:HB3	1.99	0.45
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.99	0.45
1:A:383:LEU:O	1:A:387:GLY:N	2.51	0.45
1:A:525:HIS:O	1:A:528:THR:N	2.49	0.45
1:A:687:HIS:HE2	1:A:718:ASP:CG	2.20	0.45
1:A:776:MET:HE1	1:C:225:VAL:N	2.13	0.45
1:B:139:VAL:HB	1:B:327:TYR:HB3	1.97	0.45
1:B:669:LEU:CD2	1:B:670:GLY:H	2.30	0.45
1:B:920:VAL:O	1:B:923:GLN:N	2.48	0.45
1:C:531:VAL:O	1:C:534:ILE:HG13	2.17	0.45
1:D:356:TYR:C	1:D:358:PHE:H	2.20	0.45
1:D:378:GLY:O	1:D:382:VAL:HG23	2.16	0.45
1:E:675:PHE:C	1:E:675:PHE:CD1	2.90	0.45
1:F:200:PRO:HB2	1:F:744:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:456:MET:HE3	1:F:467:TYR:O	2.16	0.45
1:F:39:ALA:HB2	1:F:668:GLU:HG2	1.98	0.45
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.98	0.44
1:A:239:ARG:HH12	1:A:756:ASP:HB2	1.82	0.44
1:A:939:LEU:O	1:A:942:GLU:HB3	2.17	0.44
1:A:943:PHE:O	1:A:947:LEU:HG	2.17	0.44
1:A:966:ARG:HB3	1:A:966:ARG:NH1	2.32	0.44
1:B:841:GLN:O	1:B:844:SER:OG	2.33	0.44
1:B:883:LEU:HD21	1:B:938:ILE:HD11	1.99	0.44
1:C:185:ARG:HB3	1:C:187:TRP:HE1	1.82	0.44
1:C:584:GLN:HE21	1:C:584:GLN:HB2	1.56	0.44
1:C:677:PHE:O	1:C:821:GLU:HA	2.17	0.44
1:D:26:ALA:O	1:D:30:LEU:HB2	2.17	0.44
1:E:281:PHE:HB2	1:E:610:PHE:CE1	2.52	0.44
1:E:739:ASN:O	1:E:742:ASN:HB2	2.17	0.44
1:F:188:MET:HA	1:F:266:ALA:CB	2.47	0.44
1:A:367:ILE:HG12	1:A:492:LEU:HB3	1.99	0.44
1:A:559:LEU:HD11	1:A:911:ALA:HB3	1.98	0.44
1:B:52:ALA:HB1	1:B:56:THR:HB	2.00	0.44
1:B:559:LEU:CG	1:B:560:PRO:HD2	2.46	0.44
1:B:185:ARG:NH1	1:B:767:TYR:HB3	2.31	0.44
1:B:770:SER:OG	1:B:775:ARG:HG2	2.17	0.44
1:C:574:THR:HG23	1:C:622:ALA:HB3	1.99	0.44
1:D:923:GLN:NE2	3:D:1103:LMT:H32	2.32	0.44
1:D:539:GLY:O	1:D:542:LEU:HB2	2.17	0.44
1:D:588:GLN:NE2	1:D:592:ASN:OD1	2.50	0.44
1:D:677:PHE:CD2	1:D:678:GLU:N	2.85	0.44
1:D:781:ILE:HD13	1:D:781:ILE:HA	1.81	0.44
1:D:83:ASP:HB2	1:D:87:THR:O	2.17	0.44
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.97	0.44
1:E:6:ILE:HD13	1:E:431:THR:HG22	1.99	0.44
1:E:466:ILE:HD13	1:E:564:LEU:HD11	1.98	0.44
1:E:64:VAL:O	1:E:68:ASN:ND2	2.50	0.44
1:D:14:VAL:HG11	1:E:885:ALA:HB2	1.99	0.44
1:F:200:PRO:O	1:F:203:VAL:N	2.50	0.44
1:F:350:LEU:O	1:F:353:LEU:N	2.49	0.44
1:F:555:LEU:HD23	1:F:555:LEU:HA	1.67	0.44
1:F:239:ARG:HH12	1:F:756:ASP:H	1.65	0.44
1:A:457:ALA:HB2	1:A:471:SER:OG	2.16	0.44
1:A:746:GLY:O	1:A:750:GLY:N	2.43	0.44
1:A:771:GLU:HB3	1:A:774:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:SER:OG	3:B:2100:LMT:H1'	2.17	0.44
1:B:710:SER:O	1:B:712:ARG:HG3	2.17	0.44
1:C:186:ILE:O	1:C:768:VAL:HG23	2.17	0.44
1:C:450:SER:CB	1:C:475:VAL:HA	2.47	0.44
1:C:631:ASP:N	1:C:631:ASP:OD1	2.49	0.44
1:C:636:GLU:N	1:C:636:GLU:OE2	2.47	0.44
1:C:974:SER:OG	1:C:1010:THR:HG21	2.17	0.44
1:D:210:GLN:HE22	1:D:250:LEU:CB	2.28	0.44
1:D:945:LYS:NZ	1:D:1025:ARG:NH2	2.65	0.44
1:E:771:GLU:HB3	1:E:774:TYR:CD1	2.52	0.44
1:F:1034:ASP:H	1:F:1035:ILE:HG23	1.83	0.44
1:F:393:LEU:HD22	1:F:466:ILE:HG23	1.98	0.44
1:F:199:THR:HG22	1:F:785:TYR:O	2.18	0.44
1:F:926:LEU:O	1:F:929:THR:HB	2.18	0.44
1:F:943:PHE:HD2	1:F:965:MET:HE3	1.81	0.44
1:A:955:LEU:HD21	1:A:1022:VAL:HG13	1.98	0.44
1:A:1025:ARG:HA	1:A:1025:ARG:HD2	1.78	0.44
1:B:1030:ARG:NH1	1:B:1031:LYS:HB2	2.32	0.44
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.39	0.44
1:B:559:LEU:HD22	1:B:918:ASN:HB2	1.99	0.44
1:B:441:ALA:HA	1:B:886:LEU:HD21	1.99	0.44
1:C:253:VAL:HG22	1:C:259:ARG:HG2	1.98	0.44
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.99	0.44
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.99	0.44
1:D:532:GLY:O	1:D:535:LEU:N	2.51	0.44
1:E:1010:THR:C	1:E:1012:LEU:H	2.21	0.44
1:E:190:PRO:HB3	1:E:784:TRP:CE3	2.52	0.44
1:E:68:ASN:CB	1:E:114:ALA:HB2	2.46	0.44
1:E:6:ILE:HG23	1:E:494:ALA:HB2	2.00	0.44
1:F:353:LEU:HA	1:F:353:LEU:HD22	1.71	0.44
1:F:504:ASP:C	1:F:506:GLY:H	2.18	0.44
1:F:889:SER:CB	1:F:892:ILE:HG12	2.46	0.44
1:B:102:ILE:O	1:B:105:VAL:HG12	2.18	0.44
1:B:842:LEU:O	1:B:845:LYS:HB2	2.18	0.44
1:C:102:ILE:HD13	1:C:102:ILE:HA	1.76	0.44
1:C:184:MET:HE3	1:C:184:MET:HA	2.00	0.44
1:C:2:PRO:O	1:C:5:PHE:HB3	2.18	0.44
1:C:456:MET:CB	1:C:871:LEU:HD21	2.46	0.44
1:C:65:ILE:HG21	1:C:90:ILE:HD12	1.98	0.44
1:C:967:LEU:O	1:C:970:ILE:HB	2.17	0.44
1:D:1034:ASP:HA	1:D:1035:ILE:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:PHE:O	1:D:336:SER:HB3	2.18	0.44
1:E:182:TYR:HB2	1:E:764:LYS:NZ	2.32	0.44
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.47	0.44
1:F:418:ARG:HB3	1:F:418:ARG:NH1	2.32	0.44
1:F:860:GLN:O	1:F:863:LEU:HB3	2.17	0.44
1:B:895:SER:HA	1:B:1020:PHE:HB3	2.00	0.44
1:B:644:MET:HE2	1:B:648:ARG:HB2	1.99	0.44
1:C:421:ALA:O	1:C:503:GLY:N	2.35	0.44
1:D:1015:PHE:HZ	3:D:1102:LMT:H52	1.82	0.44
1:D:189:ASN:HA	1:D:190:PRO:HD3	1.72	0.44
1:D:667:VAL:HB	1:D:668:GLU:CD	2.38	0.44
1:D:756:ASP:OD1	1:D:765:LYS:HA	2.18	0.44
1:D:156:ASP:OD1	1:D:760:ARG:NH2	2.50	0.44
1:E:20:MET:HA	1:E:377:LEU:HD13	1.99	0.44
1:E:549:VAL:O	1:E:552:MET:HB3	2.18	0.44
1:F:78:MET:HG3	1:F:92:LEU:CD1	2.46	0.44
1:F:438:ILE:HG22	1:F:943:PHE:CZ	2.53	0.44
1:A:344:LEU:HD11	1:A:398:MET:HB2	2.00	0.44
1:B:199:THR:O	1:B:203:VAL:HG23	2.18	0.44
1:B:40:PRO:HD3	1:B:462:SER:OG	2.17	0.44
1:B:573:MET:CB	1:B:661:PHE:HE2	2.31	0.44
1:A:888:GLU:OE2	1:C:11:PHE:HB2	2.18	0.44
1:C:331:PRO:O	1:C:335:ILE:HG22	2.17	0.44
1:C:932:LEU:HD13	1:C:1006:MET:CE	2.48	0.44
1:D:902:LEU:HD23	1:D:1012:LEU:HB3	2.00	0.44
1:D:424:GLY:HA3	1:D:502:LYS:CB	2.42	0.44
1:D:435:MET:O	1:D:439:GLN:HB2	2.18	0.44
1:D:605:ASN:O	1:D:626:LEU:HD23	2.18	0.44
1:D:702:ALA:HB2	1:D:711:VAL:HG21	1.98	0.44
1:D:721:GLN:HG2	1:F:233:SER:HB2	2.00	0.44
1:D:966:ARG:HB3	1:D:966:ARG:HH11	1.83	0.44
1:E:376:LEU:HD22	1:E:398:MET:HE3	1.99	0.44
1:E:579:PRO:HD3	1:E:656:ALA:HB2	2.00	0.44
1:F:11:PHE:CE2	1:F:15:ILE:HD11	2.53	0.44
1:F:246:PHE:O	1:F:262:LEU:HD23	2.17	0.44
1:F:434:SER:O	1:F:438:ILE:HG12	2.17	0.44
1:F:572:PHE:HA	1:F:663:LEU:HD21	2.00	0.44
1:F:666:ILE:HB	1:F:857:MET:SD	2.58	0.44
1:A:211:ASN:OD1	1:A:240:LEU:HG	2.18	0.44
1:A:277:ILE:HA	1:A:613:ASN:O	2.17	0.44
1:A:701:ALA:CB	1:A:711:VAL:HG11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:TYR:CE1	1:A:795:PRO:HB3	2.53	0.44
1:B:544:LEU:O	1:B:548:ILE:HG13	2.18	0.44
1:B:599:LEU:HD23	1:B:599:LEU:HA	1.73	0.44
1:C:182:TYR:HB2	1:C:764:LYS:HZ3	1.82	0.44
1:C:356:TYR:C	1:C:358:PHE:N	2.59	0.44
1:C:590:VAL:O	1:C:593:GLU:HB2	2.18	0.44
1:E:216:ALA:HB1	1:E:234:ILE:HG22	1.99	0.44
1:F:889:SER:HB3	1:F:892:ILE:HG12	2.00	0.44
1:B:116:PRO:HA	1:B:123:GLN:NE2	2.33	0.44
1:B:143:ILE:O	1:B:321:LEU:HA	2.18	0.44
1:B:811:LEU:HA	1:B:811:LEU:HD23	1.85	0.44
1:B:930:ILE:H	1:B:930:ILE:HG13	1.69	0.44
1:C:456:MET:HE3	1:C:467:TYR:O	2.17	0.44
1:C:455:PRO:HB3	1:C:874:ILE:HG22	2.00	0.44
1:C:883:LEU:CD2	1:C:938:ILE:HD11	2.48	0.44
1:D:270:LEU:HA	1:D:270:LEU:HD12	1.77	0.44
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.82	0.44
1:E:842:LEU:O	1:E:845:LYS:HB2	2.18	0.44
1:E:887:TYR:O	1:E:888:GLU:HB2	2.17	0.44
1:F:420:MET:HB3	1:F:500:ILE:HB	2.00	0.44
1:F:773:LYS:HE2	1:F:774:TYR:CE2	2.52	0.44
1:F:825:GLN:HB3	1:F:830:LYS:NZ	2.32	0.44
1:A:191:ASN:O	1:A:194:ASN:N	2.51	0.43
1:B:379:THR:OG1	1:B:477:ALA:HA	2.18	0.43
1:B:985:VAL:HG22	1:B:999:GLY:HA3	2.00	0.43
1:D:242:SER:OG	1:D:245:GLU:HG3	2.18	0.43
1:D:631:ASP:C	1:D:633:PRO:HD3	2.38	0.43
1:D:201:VAL:HG21	1:D:740:ASP:OD2	2.18	0.43
1:E:1013:ALA:O	1:E:1015:PHE:N	2.51	0.43
1:E:203:VAL:O	1:E:207:ILE:HG13	2.18	0.43
1:E:443:VAL:O	1:E:446:ALA:HB3	2.18	0.43
1:E:600:THR:O	1:E:603:LYS:HB2	2.18	0.43
1:E:584:GLN:N	1:E:617:GLN:HB3	2.33	0.43
1:F:35:TYR:CG	1:F:38:ILE:HD12	2.52	0.43
1:F:532:GLY:O	1:F:535:LEU:N	2.51	0.43
1:F:812:GLU:O	1:F:818:PRO:HA	2.18	0.43
1:A:219:LEU:HD13	1:B:778:PRO:HG3	1.99	0.43
1:A:327:TYR:OH	1:A:663:LEU:HD13	2.18	0.43
1:B:255:GLN:H	1:B:255:GLN:HG3	1.43	0.43
1:B:400:LEU:HA	1:B:400:LEU:HD13	1.86	0.43
1:B:425:LEU:HD11	1:B:433:LYS:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:ALA:O	1:B:644:MET:HB3	2.18	0.43
1:C:247:GLY:C	1:C:249:ILE:H	2.21	0.43
1:C:39:ALA:HB2	1:C:668:GLU:CG	2.48	0.43
1:D:102:ILE:O	1:D:106:GLN:HG3	2.18	0.43
1:D:690:LEU:HD22	1:D:820:MET:SD	2.58	0.43
1:D:968:ARG:HB3	1:D:969:PRO:HD3	2.00	0.43
1:D:350:LEU:HD13	1:D:979:LEU:C	2.39	0.43
1:E:531:VAL:O	1:E:534:ILE:HG13	2.18	0.43
1:A:631:ASP:N	1:A:631:ASP:OD1	2.51	0.43
1:B:69:MET:HE1	1:B:107:VAL:HG13	2.00	0.43
1:B:414:GLU:OE1	1:B:968:ARG:HD3	2.17	0.43
1:B:691:THR:HG23	1:B:694:ARG:HH12	1.84	0.43
1:B:701:ALA:HB2	1:B:839:MET:HE3	2.01	0.43
1:C:579:PRO:HD3	1:C:656:ALA:CB	2.49	0.43
1:C:725:ASP:HB3	1:C:801:SER:HB3	2.00	0.43
1:C:893:PRO:HA	1:C:896:VAL:CG1	2.31	0.43
1:E:584:GLN:N	1:E:617:GLN:OE1	2.33	0.43
1:F:143:ILE:HG22	1:F:286:ALA:HB2	2.00	0.43
1:F:367:ILE:CG2	1:F:489:THR:HG23	2.49	0.43
1:F:597:TYR:CD2	1:F:650:PHE:CZ	3.06	0.43
1:A:137:LEU:HD22	1:A:293:LEU:HG	1.99	0.43
1:A:654:LYS:HD3	1:A:654:LYS:HA	1.80	0.43
1:A:58:GLN:HG3	1:A:813:ARG:HD2	1.99	0.43
1:A:897:MET:O	1:A:899:VAL:N	2.51	0.43
1:B:172:VAL:HG22	1:B:306:ILE:HD11	1.99	0.43
1:A:235:ILE:HD11	1:B:721:GLN:HB2	2.00	0.43
1:C:974:SER:O	1:C:978:ILE:HG13	2.18	0.43
1:D:159:ALA:HB2	1:D:177:LEU:HD11	2.01	0.43
1:E:422:GLU:HB3	1:E:423:GLU:HG3	2.00	0.43
1:E:922:PHE:O	1:E:926:LEU:HB2	2.18	0.43
1:E:883:LEU:HD21	1:E:938:ILE:HD11	1.99	0.43
1:E:952:GLY:O	1:E:1035:ILE:HB	2.18	0.43
1:F:1008:THR:O	1:F:1012:LEU:HB2	2.18	0.43
1:F:535:LEU:HD21	1:F:1022:VAL:HG21	2.01	0.43
1:F:34:GLN:HB2	1:F:333:VAL:CG2	2.33	0.43
1:F:456:MET:HB3	1:F:871:LEU:HD21	1.99	0.43
1:A:416:VAL:HG21	1:A:493:CYS:SG	2.58	0.43
1:A:190:PRO:HG3	1:A:784:TRP:CZ2	2.54	0.43
1:B:573:MET:O	1:B:661:PHE:HD2	2.01	0.43
1:B:65:ILE:O	1:B:69:MET:HG2	2.17	0.43
1:B:945:LYS:HZ2	1:B:1025:ARG:NH2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASP:OD1	1:C:222:THR:HG21	2.18	0.43
1:C:493:CYS:SG	1:C:497:LEU:HD22	2.58	0.43
1:C:564:LEU:HD12	1:C:564:LEU:HA	1.83	0.43
1:C:602:GLU:HG3	1:C:605:ASN:HD22	1.84	0.43
1:C:641:ALA:O	1:C:644:MET:HB3	2.18	0.43
1:C:901:PRO:O	1:C:905:ILE:HG22	2.19	0.43
1:C:936:ASN:ND2	1:C:1010:THR:HG22	2.33	0.43
1:D:62:THR:OG1	1:D:88:VAL:HG21	2.18	0.43
1:D:45:ILE:HD12	1:D:90:ILE:HD12	2.00	0.43
1:E:415:ASN:OD1	1:E:418:ARG:NH1	2.52	0.43
1:E:757:PHE:HE1	1:E:759:ASP:HB2	1.79	0.43
1:F:328:ASP:O	1:F:331:PRO:HD2	2.19	0.43
1:F:525:HIS:O	1:F:528:THR:N	2.51	0.43
1:F:631:ASP:C	1:F:633:PRO:HD3	2.38	0.43
1:A:926:LEU:HD22	3:A:1103:LMT:C4	2.48	0.43
1:A:700:GLU:HB3	1:A:842:LEU:HD22	1.99	0.43
1:A:948:MET:HE2	1:A:958:ALA:HB3	2.00	0.43
1:B:151:GLN:HG2	1:B:152:GLU:N	2.33	0.43
1:B:602:GLU:HB3	1:B:606:VAL:HG23	1.99	0.43
1:B:707:MET:CE	1:B:834:GLU:HB3	2.49	0.43
1:C:38:ILE:HG23	1:C:462:SER:HB2	2.00	0.43
1:C:659:PHE:HE2	1:C:712:ARG:HB3	1.83	0.43
1:C:83:ASP:HA	1:C:809:PRO:O	2.19	0.43
1:D:356:TYR:C	1:D:358:PHE:N	2.72	0.43
1:D:559:LEU:HG	1:D:560:PRO:HD2	1.99	0.43
1:D:572:PHE:CE2	1:D:624:VAL:HB	2.54	0.43
1:D:898:LEU:HB3	1:D:1020:PHE:CE2	2.54	0.43
1:D:939:LEU:HD23	1:D:939:LEU:HA	1.67	0.43
1:E:106:GLN:HA	1:E:109:ASN:HD21	1.83	0.43
1:E:483:LEU:O	1:E:487:ILE:N	2.49	0.43
1:D:229:GLN:HG2	1:E:586:ARG:HE	1.84	0.43
1:F:898:LEU:HD13	1:F:1020:PHE:CD2	2.54	0.43
1:F:1017:VAL:O	1:F:1020:PHE:HB2	2.18	0.43
1:F:171:GLY:HA3	1:F:302:THR:HG23	2.01	0.43
1:F:30:LEU:HA	1:F:31:PRO:HD3	1.92	0.43
1:F:506:GLY:C	1:F:508:GLY:H	2.18	0.43
1:F:666:ILE:CG2	1:F:669:LEU:HB2	2.49	0.43
1:F:935:LYS:HZ3	1:F:973:THR:HG21	1.82	0.43
1:A:152:GLU:HG2	1:A:152:GLU:H	1.29	0.43
1:A:881:LEU:HD12	1:C:18:ILE:HG13	2.00	0.43
1:A:939:LEU:HD23	1:A:939:LEU:HA	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:VAL:O	1:B:207:ILE:HG13	2.19	0.43
1:C:370:ILE:O	1:C:374:VAL:HG23	2.18	0.43
1:C:990:ALA:O	1:C:992:SER:N	2.51	0.43
1:D:490:PRO:O	1:D:493:CYS:HB2	2.19	0.43
1:D:509:LYS:O	1:D:511:GLY:N	2.50	0.43
1:F:240:LEU:HD12	1:F:246:PHE:CG	2.54	0.43
1:F:649:ALA:O	1:F:653:ILE:HG12	2.19	0.43
1:A:236:ALA:O	1:B:723:LYS:NZ	2.43	0.43
1:A:429:GLU:H	1:A:429:GLU:CD	2.22	0.43
1:A:534:ILE:CD1	1:A:1019:VAL:HG22	2.49	0.43
1:B:200:PRO:O	1:B:203:VAL:N	2.52	0.43
1:B:419:VAL:HG21	1:B:434:SER:HB3	2.00	0.43
1:B:576:VAL:HG22	1:B:658:VAL:HG13	2.00	0.43
1:B:418:ARG:HD2	1:B:965:MET:HB2	1.99	0.43
1:C:182:TYR:HB2	1:C:764:LYS:HZ2	1.83	0.43
1:D:1025:ARG:HA	1:D:1025:ARG:HD2	1.86	0.43
1:D:45:ILE:HA	1:D:128:SER:O	2.19	0.43
1:D:314:GLU:OE1	1:D:323:ILE:HD12	2.19	0.43
1:D:362:PHE:O	1:D:366:LEU:HG	2.18	0.43
1:D:20:MET:HG2	1:D:374:VAL:HA	2.00	0.43
1:D:568:ASP:O	1:D:629:TRP:CZ3	2.70	0.43
1:D:648:ARG:O	1:D:651:SER:OG	2.32	0.43
1:E:647:THR:CG2	1:E:660:ALA:H	2.32	0.43
1:E:701:ALA:CB	1:E:711:VAL:HG11	2.47	0.43
1:F:408:ASP:OD2	1:F:445:ILE:HD12	2.19	0.43
1:F:393:LEU:HD13	1:F:466:ILE:HA	2.00	0.43
1:F:602:GLU:HB3	1:F:606:VAL:CG2	2.48	0.43
1:F:704:HIS:HE1	1:F:842:LEU:HD11	1.83	0.43
1:A:1007:VAL:HG12	1:A:1008:THR:N	2.33	0.43
1:A:375:VAL:HG22	1:A:484:VAL:HG21	2.01	0.43
1:A:531:VAL:HG12	1:A:535:LEU:HD12	1.99	0.43
1:A:527:TYR:OH	1:A:963:VAL:HG22	2.19	0.43
1:A:399:VAL:HG11	1:A:984:LEU:HD11	2.00	0.43
1:B:300:LEU:HD23	1:B:334:LYS:HG2	2.00	0.43
1:B:492:LEU:O	1:B:496:MET:HG2	2.18	0.43
1:B:598:TYR:HB2	1:B:609:VAL:HG21	2.01	0.43
1:B:694:ARG:NH2	1:B:717:GLU:OE1	2.52	0.43
1:C:213:GLN:HE22	1:C:238:THR:HG23	1.84	0.43
1:C:358:PHE:HD2	1:C:972:MET:SD	2.41	0.43
1:C:371:ALA:O	1:C:375:VAL:HG23	2.18	0.43
1:C:759:ASP:OD1	1:C:760:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:812:GLU:HB2	1:C:819:SER:O	2.18	0.43
2:D:1101:ERY:H312	2:D:1101:ERY:H303	2.00	0.43
1:D:207:ILE:CD1	1:D:768:VAL:HG21	2.49	0.43
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.56	0.43
1:F:146:ASP:O	1:F:148:THR:N	2.51	0.43
1:F:435:MET:SD	1:F:490:PRO:HG3	2.59	0.43
1:F:897:MET:O	1:F:900:VAL:HG23	2.18	0.43
1:F:438:ILE:HG22	1:F:943:PHE:HZ	1.83	0.43
1:A:251:LEU:HD11	1:A:265:VAL:HG21	2.00	0.43
1:B:540:ARG:O	1:B:543:VAL:HB	2.19	0.43
1:B:701:ALA:CB	1:B:711:VAL:HG11	2.49	0.43
1:C:200:PRO:O	1:C:203:VAL:N	2.52	0.43
1:C:393:LEU:O	1:C:396:PHE:HB2	2.19	0.43
1:D:350:LEU:HD13	1:D:979:LEU:HB3	1.99	0.43
1:D:597:TYR:OH	1:D:646:ALA:HA	2.19	0.43
1:D:66:GLU:OE2	1:D:80:SER:OG	2.24	0.43
1:E:400:LEU:HG	1:E:924:VAL:HG12	2.01	0.43
1:E:591:LEU:HD11	1:E:620:GLY:HA3	2.00	0.43
1:E:738:ILE:HD12	1:E:738:ILE:H	1.83	0.43
1:E:945:LYS:HZ2	1:E:1025:ARG:NH2	2.16	0.43
1:E:982:MET:HA	1:E:1003:MET:HE3	2.01	0.43
1:F:153:ASP:O	1:F:156:ASP:HB3	2.18	0.43
1:D:63:GLN:HE21	1:F:763:VAL:HG12	1.84	0.43
1:A:210:GLN:NE2	1:A:250:LEU:O	2.52	0.42
1:A:21:LEU:HD13	1:A:21:LEU:HA	1.70	0.42
1:A:162:MET:HG2	1:A:313:MET:SD	2.59	0.42
1:B:730:LYS:O	1:B:734:LEU:HG	2.19	0.42
1:C:898:LEU:HB3	1:C:1020:PHE:CE2	2.54	0.42
1:C:362:PHE:CE2	1:C:366:LEU:HD21	2.53	0.42
1:D:72:ILE:HD13	1:D:107:VAL:HA	2.01	0.42
1:D:171:GLY:O	1:D:293:LEU:HD23	2.19	0.42
1:D:694:ARG:NH1	1:D:820:MET:SD	2.91	0.42
1:D:531:VAL:HG21	1:D:963:VAL:HG11	2.00	0.42
1:E:221:GLY:HA3	1:F:775:ARG:HH12	1.83	0.42
1:E:973:THR:HG22	1:E:974:SER:N	2.34	0.42
1:E:994:ALA:O	1:E:997:ALA:N	2.52	0.42
1:F:274:ASN:ND2	1:F:276:ASP:OD2	2.52	0.42
1:F:361:ASN:O	1:F:364:ALA:N	2.52	0.42
1:F:631:ASP:OD1	1:F:631:ASP:N	2.51	0.42
1:F:639:VAL:HG11	1:F:662:ASN:OD1	2.19	0.42
1:A:955:LEU:O	1:A:959:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LEU:HD21	1:B:262:LEU:HB2	2.00	0.42
1:B:517:ASN:O	1:B:521:GLU:HB2	2.19	0.42
1:B:72:ILE:HG23	1:B:106:GLN:HB3	2.00	0.42
1:B:5:PHE:C	1:B:8:ARG:H	2.22	0.42
1:E:139:VAL:HG13	1:E:178:PHE:CE1	2.54	0.42
1:F:452:VAL:HG13	1:F:879:VAL:HG23	2.02	0.42
1:A:279:ALA:HB3	1:A:286:ALA:O	2.19	0.42
1:A:355:MET:HB3	1:A:365:THR:HG1	1.82	0.42
1:B:45:ILE:HA	1:B:128:SER:O	2.19	0.42
1:B:210:GLN:HE22	1:B:250:LEU:N	2.18	0.42
1:B:353:LEU:HD22	1:B:353:LEU:HA	1.78	0.42
1:B:356:TYR:C	1:B:358:PHE:N	2.63	0.42
1:B:62:THR:O	1:B:65:ILE:N	2.52	0.42
1:B:714:ASN:HB2	1:B:823:LEU:HG	2.01	0.42
1:B:738:ILE:HA	1:B:741:ILE:CD1	2.49	0.42
1:C:1006:MET:O	1:C:1009:ALA:HB3	2.19	0.42
1:C:104:GLN:HG3	1:C:105:VAL:N	2.33	0.42
1:C:27:ILE:HD13	1:C:27:ILE:HG21	1.85	0.42
1:C:354:VAL:O	1:C:358:PHE:HB2	2.20	0.42
1:B:228:GLN:O	1:C:583:THR:HG21	2.19	0.42
1:C:6:ILE:HG22	1:C:6:ILE:O	2.19	0.42
1:D:669:LEU:CD1	1:D:670:GLY:H	2.24	0.42
1:D:752:SER:O	1:D:767:TYR:HA	2.20	0.42
1:E:222:THR:HA	1:E:224:PRO:HD3	2.00	0.42
1:E:975:LEU:O	1:E:979:LEU:HG	2.19	0.42
1:A:254:ASN:HB2	1:A:258:SER:HG	1.84	0.42
1:A:400:LEU:HA	1:A:400:LEU:HD12	1.76	0.42
1:A:569:GLN:NE2	1:A:663:LEU:HG	2.34	0.42
1:A:777:LEU:O	1:A:780:ASP:N	2.44	0.42
1:B:21:LEU:HD23	1:B:21:LEU:HA	1.76	0.42
1:B:694:ARG:HH11	1:B:820:MET:CE	2.33	0.42
1:B:708:LEU:HD11	1:B:838:LEU:HD12	2.00	0.42
1:C:124:GLN:HG3	1:C:125:GLN:N	2.30	0.42
1:C:226:LYS:NZ	1:C:226:LYS:HB3	2.34	0.42
1:C:172:VAL:HG13	1:C:291:ILE:HG23	2.01	0.42
1:C:36:PRO:O	1:C:38:ILE:HG13	2.20	0.42
1:C:572:PHE:CE2	1:C:624:VAL:HB	2.53	0.42
1:C:708:LEU:HD13	1:C:838:LEU:HD12	2.01	0.42
1:C:675:PHE:HB2	1:C:854:TRP:CZ3	2.55	0.42
1:D:1035:ILE:HB	1:D:1036:GLU:H	1.43	0.42
1:D:53:ASP:O	1:D:56:THR:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:ASN:OD1	1:D:637:ASN:ND2	2.52	0.42
1:D:671:THR:OG1	1:D:674:GLY:HA3	2.20	0.42
1:E:293:LEU:HD11	1:E:297:ALA:O	2.19	0.42
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.84	0.42
1:E:482:VAL:O	1:E:486:LEU:HG	2.19	0.42
1:E:525:HIS:O	1:E:526:HIS:C	2.57	0.42
1:E:540:ARG:HB2	1:E:541:TYR:HD1	1.84	0.42
1:F:19:ILE:O	1:F:22:ALA:HB3	2.19	0.42
1:F:636:GLU:OE2	1:F:636:GLU:N	2.52	0.42
1:F:638:LYS:HE2	1:F:640:GLU:HG3	2.00	0.42
1:F:796:PHE:CD1	1:F:799:PHE:HE2	2.36	0.42
1:F:939:LEU:HB3	1:F:966:ARG:HD2	2.01	0.42
1:A:963:VAL:CG2	1:A:1018:PRO:HG3	2.49	0.42
1:A:139:VAL:HB	1:A:327:TYR:HB3	2.00	0.42
1:B:228:GLN:NE2	1:B:230:LEU:O	2.49	0.42
1:B:251:LEU:HD11	1:B:262:LEU:HA	2.02	0.42
1:B:932:LEU:O	1:B:933:SER:C	2.58	0.42
1:C:187:TRP:HE3	1:C:770:SER:O	2.03	0.42
1:C:893:PRO:O	1:C:895:SER:N	2.52	0.42
1:D:143:ILE:HG22	1:D:286:ALA:CB	2.49	0.42
1:D:182:TYR:HA	1:D:182:TYR:HD1	1.69	0.42
1:D:504:ASP:C	1:D:506:GLY:H	2.22	0.42
1:D:889:SER:HB2	1:D:892:ILE:HD12	2.00	0.42
1:E:977:PHE:HD2	1:E:1006:MET:HG3	1.85	0.42
1:E:527:TYR:OH	1:E:1014:ILE:HB	2.20	0.42
1:E:196:PHE:HB3	1:E:252:LYS:HE2	2.01	0.42
1:E:53:ASP:OD2	1:E:55:LYS:N	2.50	0.42
1:E:576:VAL:HB	1:E:620:GLY:O	2.20	0.42
1:D:168:ARG:HB3	1:E:75:LEU:HD22	2.02	0.42
1:F:140:VAL:HG11	1:F:310:LEU:HD21	2.01	0.42
1:F:376:LEU:O	1:F:379:THR:N	2.51	0.42
1:A:151:GLN:HE21	1:A:152:GLU:CA	2.30	0.42
1:A:244:GLU:CG	1:A:248:LYS:HE2	2.47	0.42
1:A:61:VAL:HG21	1:A:122:VAL:HG21	2.01	0.42
1:C:188:MET:HA	1:C:266:ALA:HB2	2.00	0.42
1:C:693:ALA:HB1	1:C:850:VAL:HG11	2.00	0.42
1:B:214:VAL:HG11	1:C:742:ASN:HB3	2.02	0.42
1:D:923:GLN:HG2	3:D:1103:LMT:H52	2.01	0.42
1:D:13:TRP:CE2	1:D:492:LEU:HD21	2.55	0.42
1:E:681:ASP:HB3	1:E:818:PRO:O	2.20	0.42
1:E:748:ALA:HB3	1:E:749:TRP:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:836:MET:HG2	1:E:854:TRP:CH2	2.55	0.42
1:F:27:ILE:HG23	1:F:380:PHE:HB3	2.02	0.42
1:F:610:PHE:O	1:F:623:PHE:N	2.43	0.42
1:A:94:PHE:CZ	1:A:103:ALA:HB1	2.55	0.42
1:A:39:ALA:HA	1:A:40:PRO:HD2	1.68	0.42
1:A:770:SER:HB2	1:A:784:TRP:CH2	2.55	0.42
1:B:370:ILE:O	1:B:374:VAL:HG23	2.20	0.42
1:A:229:GLN:HE21	1:B:586:ARG:HD3	1.83	0.42
1:B:559:LEU:HD12	1:B:912:THR:OG1	2.19	0.42
1:C:108:GLN:HB3	1:C:129:VAL:HG11	2.01	0.42
1:C:698:LEU:CD1	1:C:713:PRO:HD3	2.49	0.42
1:C:201:VAL:HG21	1:C:740:ASP:OD1	2.19	0.42
2:D:1101:ERY:H4	2:D:1101:ERY:H71	1.41	0.42
1:D:417:GLU:OE1	1:D:497:LEU:HD11	2.20	0.42
1:E:267:LYS:HD3	1:E:771:GLU:OE2	2.20	0.42
1:E:293:LEU:HD13	1:E:294:ALA:O	2.20	0.42
1:E:654:LYS:HB3	1:E:654:LYS:HE3	1.78	0.42
1:E:812:GLU:HB2	1:E:819:SER:O	2.19	0.42
1:F:509:LYS:HB3	1:F:514:GLY:HA3	2.02	0.42
1:F:736:VAL:HG11	1:F:786:VAL:HB	2.02	0.42
1:A:68:ASN:O	1:A:110:LYS:HB3	2.19	0.42
1:A:298:ASN:HB3	1:A:301:ASP:HB2	2.02	0.42
1:A:57:VAL:HA	1:A:60:THR:HG22	2.01	0.42
1:A:905:ILE:HG13	1:A:905:ILE:O	2.19	0.42
1:B:185:ARG:NH1	1:B:767:TYR:HD1	2.18	0.42
1:B:564:LEU:HD11	1:B:666:ILE:HD12	2.00	0.42
1:B:674:GLY:H	1:B:832:THR:HG23	1.85	0.42
1:B:796:PHE:O	1:B:800:SER:OG	2.31	0.42
1:C:311:ALA:O	1:C:315:PRO:HD3	2.19	0.42
1:C:707:MET:HG3	1:C:838:LEU:HG	2.02	0.42
1:C:836:MET:HG2	1:C:854:TRP:CH2	2.55	0.42
1:D:354:VAL:HG21	1:D:975:LEU:HB3	2.00	0.42
1:D:813:ARG:NH2	1:D:818:PRO:HD3	2.34	0.42
1:E:249:ILE:O	1:E:262:LEU:N	2.48	0.42
1:E:390:ILE:HG23	1:E:395:MET:SD	2.59	0.42
1:E:520:PHE:O	1:E:523:SER:OG	2.38	0.42
1:F:11:PHE:HD2	1:F:11:PHE:O	2.01	0.42
1:F:13:TRP:NE1	1:F:492:LEU:HD21	2.34	0.42
1:F:543:VAL:O	1:F:546:LEU:HB2	2.20	0.42
1:F:669:LEU:HD22	1:F:856:GLY:HA2	2.02	0.42
1:A:1035:ILE:HG22	1:A:1036:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:O	1:A:355:MET:HB2	2.20	0.42
1:A:738:ILE:H	1:A:738:ILE:HD12	1.84	0.42
1:B:294:ALA:HB3	1:B:297:ALA:CB	2.49	0.42
1:B:453:PHE:CD1	1:B:474:ILE:HG22	2.55	0.42
1:C:211:ASN:CG	1:C:240:LEU:HG	2.39	0.42
1:C:152:GLU:HG2	1:C:275:TYR:HE2	1.84	0.42
1:C:654:LYS:HD3	1:C:654:LYS:HA	1.60	0.42
1:C:876:LEU:HD23	1:C:876:LEU:HA	1.70	0.42
1:C:941:VAL:HG13	1:C:1021:PHE:CD1	2.54	0.42
1:D:251:LEU:CD1	1:D:265:VAL:HG21	2.50	0.42
1:D:448:VAL:O	1:D:451:ALA:HB3	2.20	0.42
1:D:610:PHE:O	1:D:622:ALA:HA	2.19	0.42
1:D:574:THR:CG2	1:D:622:ALA:HB3	2.49	0.42
1:D:654:LYS:HD3	1:D:654:LYS:HA	1.70	0.42
1:D:795:PRO:O	1:D:798:ALA:HB3	2.20	0.42
1:E:3:ASN:HA	1:E:6:ILE:CD1	2.50	0.42
1:E:455:PRO:O	1:E:871:LEU:HD13	2.20	0.42
1:E:917:THR:O	1:E:919:ASP:N	2.52	0.42
1:F:138:MET:HE1	1:F:325:TYR:HD2	1.84	0.42
1:F:486:LEU:O	1:F:490:PRO:HG2	2.19	0.42
1:F:769:MET:HG2	1:F:770:SER:H	1.85	0.42
1:A:1021:PHE:CZ	1:A:1025:ARG:HG3	2.55	0.42
1:A:138:MET:HE2	1:A:328:ASP:OD1	2.19	0.42
1:A:525:HIS:O	1:A:526:HIS:C	2.58	0.42
1:A:821:GLU:OE1	2:A:1101:ERY:H24	2.20	0.42
1:B:130:GLU:HG2	1:C:113:LEU:HD21	2.02	0.42
1:B:281:PHE:HB2	1:B:610:PHE:CD1	2.55	0.42
1:B:484:VAL:O	1:B:489:THR:HG23	2.19	0.42
1:B:675:PHE:CE1	1:B:677:PHE:HB2	2.54	0.42
1:B:831:SER:OG	1:B:834:GLU:HG3	2.20	0.42
1:B:98:THR:HG22	1:B:99:ASP:N	2.35	0.42
1:C:935:LYS:O	1:C:938:ILE:HB	2.19	0.42
1:D:1002:VAL:HG12	1:D:1003:MET:N	2.35	0.42
1:E:30:LEU:HA	1:E:30:LEU:HD12	1.93	0.42
1:E:310:LEU:HD23	1:E:325:TYR:OH	2.20	0.42
1:E:559:LEU:HG	1:E:560:PRO:HD2	2.02	0.42
1:F:1010:THR:O	1:F:1012:LEU:N	2.53	0.42
1:F:447:MET:O	1:F:451:ALA:HB2	2.20	0.42
1:F:452:VAL:HG23	1:F:453:PHE:CD1	2.55	0.42
1:F:590:VAL:O	1:F:593:GLU:HB2	2.19	0.42
1:F:708:LEU:HD13	1:F:838:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:757:PHE:HE1	1:F:759:ASP:HB2	1.85	0.42
1:A:378:GLY:O	1:A:381:ALA:HB3	2.19	0.41
1:A:454:VAL:O	1:A:457:ALA:HB3	2.20	0.41
1:A:642:ILE:HA	1:A:645:ARG:NH1	2.35	0.41
1:A:80:SER:HA	1:A:89:GLN:O	2.20	0.41
1:B:277:ILE:HG22	1:B:614:GLY:HA3	2.00	0.41
1:B:373:PRO:O	1:B:376:LEU:HB2	2.19	0.41
1:C:156:ASP:OD2	1:C:182:TYR:HB2	2.19	0.41
1:C:143:ILE:O	1:C:321:LEU:HD22	2.20	0.41
1:C:55:LYS:HE2	1:C:55:LYS:HB3	1.91	0.41
1:D:723:LYS:HG2	1:D:803:ARG:CZ	2.50	0.41
1:D:746:GLY:O	1:D:748:ALA:N	2.53	0.41
1:E:110:LYS:HD3	1:E:110:LYS:HA	1.53	0.41
1:E:188:MET:HE2	1:E:188:MET:HB2	1.84	0.41
1:E:250:LEU:HD12	1:E:260:VAL:O	2.19	0.41
1:E:124:GLN:NE2	1:E:753:TYR:HD2	2.18	0.41
1:F:344:LEU:HD11	1:F:376:LEU:HD13	2.01	0.41
1:F:453:PHE:CE2	1:F:474:ILE:HD12	2.55	0.41
1:F:509:LYS:CG	1:F:513:PHE:HB2	2.50	0.41
1:A:185:ARG:HB3	1:A:187:TRP:NE1	2.35	0.41
1:A:425:LEU:HB3	1:A:429:GLU:HG3	2.01	0.41
1:A:574:THR:HG21	1:A:594:VAL:HG11	2.01	0.41
1:A:940:ILE:HG12	1:A:966:ARG:NH2	2.35	0.41
1:B:1031:LYS:HA	1:B:1032:ASN:HA	1.76	0.41
1:B:524:THR:O	1:B:527:TYR:HB3	2.19	0.41
1:C:415:ASN:OD1	1:C:418:ARG:NH2	2.51	0.41
1:C:536:ARG:NH1	3:C:1101:LMT:O4'	2.53	0.41
1:C:5:PHE:C	1:C:7:ASP:H	2.22	0.41
1:D:977:PHE:CD2	1:D:1006:MET:HG3	2.54	0.41
1:D:31:PRO:HB2	1:D:389:SER:CB	2.50	0.41
1:D:324:VAL:HG12	1:D:326:PRO:HD3	2.01	0.41
1:D:434:SER:O	1:D:437:GLN:N	2.53	0.41
1:E:36:PRO:O	1:E:38:ILE:HG13	2.19	0.41
1:E:65:ILE:O	1:E:69:MET:HG2	2.19	0.41
1:E:75:LEU:HG	1:E:76:MET:N	2.35	0.41
1:F:812:GLU:HB2	1:F:819:SER:O	2.19	0.41
1:B:115:MET:HB2	1:B:116:PRO:HD3	2.02	0.41
1:B:188:MET:CE	1:B:200:PRO:HG3	2.50	0.41
1:B:298:ASN:HB3	1:B:301:ASP:HB2	2.02	0.41
1:B:76:MET:HB3	1:B:77:TYR:HD2	1.85	0.41
1:B:736:VAL:HG11	1:B:786:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910:ALA:O	1:B:914:ARG:HB2	2.20	0.41
1:B:945:LYS:NZ	1:B:1025:ARG:NH2	2.68	0.41
1:B:9:PRO:HB3	1:B:495:THR:OG1	2.21	0.41
1:C:1017:VAL:N	1:C:1018:PRO:HD2	2.36	0.41
1:C:360:GLN:HE21	1:C:360:GLN:HB3	1.66	0.41
1:C:567:GLU:O	1:C:569:GLN:HG3	2.20	0.41
1:C:69:MET:O	1:C:72:ILE:HD11	2.19	0.41
1:C:966:ARG:O	1:C:969:PRO:HG2	2.21	0.41
1:E:68:ASN:HB3	1:E:114:ALA:HB2	2.01	0.41
1:F:966:ARG:O	1:F:970:ILE:HG13	2.21	0.41
1:A:149:MET:HG3	1:A:154:ILE:HG13	2.01	0.41
1:A:419:VAL:HG13	1:A:423:GLU:CD	2.40	0.41
1:A:61:VAL:CG2	1:A:122:VAL:HG21	2.51	0.41
1:A:914:ARG:HD3	1:A:916:LEU:HD23	2.01	0.41
1:B:190:PRO:HB3	1:B:784:TRP:CZ3	2.55	0.41
1:B:42:ALA:HB2	1:B:93:THR:HG23	2.01	0.41
1:C:3:ASN:ND2	1:C:435:MET:HG3	2.34	0.41
1:C:5:PHE:CD2	1:C:5:PHE:C	2.93	0.41
1:C:716:LEU:HD23	1:C:810:ARG:HE	1.84	0.41
1:D:1034:ASP:HA	1:D:1035:ILE:O	2.19	0.41
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.50	0.41
1:E:694:ARG:NH1	1:E:820:MET:HE1	2.27	0.41
1:E:939:LEU:HA	1:E:939:LEU:HD23	1.76	0.41
1:F:133:SER:HB2	1:F:292:LYS:HD3	2.02	0.41
1:F:143:ILE:HG22	1:F:286:ALA:CB	2.50	0.41
1:F:417:GLU:OE2	1:F:497:LEU:HD11	2.21	0.41
1:F:40:PRO:HA	1:F:41:PRO:HD3	1.94	0.41
1:D:888:GLU:OE1	1:F:8:ARG:HB3	2.20	0.41
1:A:536:ARG:NH1	3:A:1102:LMT:O4'	2.53	0.41
1:A:5:PHE:HE2	1:A:11:PHE:CD1	2.39	0.41
1:A:955:LEU:HD23	1:A:1026:ARG:NH2	2.35	0.41
1:A:990:ALA:O	1:A:992:SER:N	2.54	0.41
1:B:882:CYS:O	1:B:885:ALA:HB3	2.21	0.41
1:C:110:LYS:HA	1:C:110:LYS:HD3	1.61	0.41
1:C:398:MET:HG2	1:C:473:THR:CG2	2.49	0.41
1:C:978:ILE:O	1:C:982:MET:HB2	2.20	0.41
1:D:36:PRO:O	1:D:38:ILE:HG13	2.20	0.41
1:D:405:LEU:HD23	1:D:481:SER:HB3	2.02	0.41
1:D:631:ASP:OD1	1:D:631:ASP:N	2.53	0.41
1:D:653:ILE:HG13	1:D:654:LYS:HE2	2.02	0.41
1:D:35:TYR:HE1	1:D:665:ALA:HB1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:784:TRP:HB2	1:D:796:PHE:CD2	2.56	0.41
1:E:158:VAL:CG1	1:E:177:LEU:HD21	2.51	0.41
1:E:564:LEU:HD13	1:E:666:ILE:HD12	2.01	0.41
1:E:751:GLY:CA	1:E:769:MET:HG3	2.50	0.41
1:E:794:VAL:HG12	1:E:798:ALA:HB3	2.02	0.41
1:E:677:PHE:HB3	1:E:822:ILE:HB	2.03	0.41
1:E:890:TRP:O	1:E:893:PRO:HD2	2.20	0.41
1:E:904:VAL:O	1:E:906:GLY:N	2.53	0.41
1:E:919:ASP:OD1	1:E:921:TYR:N	2.53	0.41
1:F:438:ILE:O	1:F:441:ALA:HB3	2.21	0.41
1:F:569:GLN:HA	1:F:629:TRP:HH2	1.86	0.41
1:F:632:ARG:HA	1:F:637:ASN:HD22	1.84	0.41
1:A:420:MET:HE3	1:A:500:ILE:HD12	2.03	0.41
1:A:58:GLN:OE1	1:A:811:LEU:HD13	2.21	0.41
1:A:618:ASN:OD1	1:A:619:THR:HG23	2.21	0.41
1:B:586:ARG:O	1:B:589:LYS:HB3	2.21	0.41
1:B:757:PHE:CE1	1:B:759:ASP:HB2	2.56	0.41
1:D:534:ILE:HD11	1:D:1019:VAL:HG22	2.03	0.41
1:D:210:GLN:HE22	1:D:250:LEU:CA	2.34	0.41
1:D:467:TYR:CE2	1:D:920:VAL:HG22	2.56	0.41
1:D:72:ILE:HG23	1:D:106:GLN:HB3	2.02	0.41
1:E:32:VAL:H	1:E:298:ASN:ND2	2.18	0.41
1:E:956:ILE:O	1:E:960:LEU:HB2	2.20	0.41
1:F:84:SER:HB3	1:F:809:PRO:HA	2.02	0.41
1:A:139:VAL:O	1:A:139:VAL:HG12	2.20	0.41
1:A:573:MET:HE3	1:A:623:PHE:HE1	1.86	0.41
1:B:982:MET:HA	1:B:1003:MET:HE3	2.02	0.41
1:B:222:THR:HA	1:B:224:PRO:HD3	2.02	0.41
1:B:213:GLN:HA	1:B:237:GLN:O	2.21	0.41
1:B:647:THR:HG23	1:B:660:ALA:HB3	2.02	0.41
1:B:712:ARG:HD2	1:B:823:LEU:HB2	2.03	0.41
1:B:985:VAL:HG22	1:B:999:GLY:CA	2.51	0.41
1:B:99:ASP:HB3	1:B:102:ILE:HB	2.02	0.41
1:C:27:ILE:HA	1:C:30:LEU:HB2	2.02	0.41
1:C:375:VAL:HA	1:C:480:LEU:HD13	2.03	0.41
1:C:914:ARG:HD2	1:C:1000:THR:HG21	2.01	0.41
1:C:940:ILE:HG12	1:C:966:ARG:NH2	2.35	0.41
1:D:137:LEU:HG	1:D:138:MET:HG2	2.02	0.41
1:D:201:VAL:O	1:D:205:THR:OG1	2.34	0.41
1:D:47:ALA:HB2	1:D:127:VAL:HG13	2.03	0.41
1:D:563:PHE:CD2	1:D:666:ILE:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:836:MET:HE1	1:D:862:ARG:CB	2.48	0.41
1:D:948:MET:CE	1:D:955:LEU:HA	2.50	0.41
1:E:1015:PHE:HE2	3:E:1101:LMT:C1	2.33	0.41
1:E:113:LEU:HA	1:E:113:LEU:HD23	1.92	0.41
1:E:143:ILE:HG21	1:E:281:PHE:CD2	2.56	0.41
1:E:452:VAL:HA	1:E:875:SER:OG	2.21	0.41
1:F:181:GLN:HG2	1:F:182:TYR:N	2.35	0.41
1:F:669:LEU:HD13	1:F:856:GLY:C	2.40	0.41
1:F:738:ILE:H	1:F:738:ILE:HD12	1.85	0.41
1:A:955:LEU:HB2	1:A:1032:ASN:O	2.20	0.41
1:A:154:ILE:O	1:A:157:TYR:N	2.54	0.41
1:A:602:GLU:HB3	1:A:606:VAL:HG23	2.03	0.41
1:A:868:ALA:N	1:A:869:PRO:HD2	2.36	0.41
1:B:188:MET:HE1	1:B:200:PRO:HG3	2.03	0.41
3:B:2100:LMT:O5B	3:B:2100:LMT:H6E	2.21	0.41
1:B:916:LEU:HA	1:B:916:LEU:HD13	1.83	0.41
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.86	0.41
1:D:941:VAL:HG22	1:D:1021:PHE:HB2	2.02	0.41
1:D:335:ILE:O	1:D:339:GLU:HG2	2.20	0.41
1:D:722:PHE:HD1	1:D:804:TRP:CE2	2.39	0.41
1:D:865:GLY:O	1:D:866:ASN:HB2	2.21	0.41
1:D:559:LEU:HD22	1:D:918:ASN:HB2	2.03	0.41
1:D:954:GLY:HA2	1:D:1033:GLU:O	2.21	0.41
1:E:211:ASN:OD1	1:E:239:ARG:HA	2.20	0.41
1:E:240:LEU:HB2	1:E:246:PHE:CZ	2.56	0.41
1:E:557:VAL:C	1:E:559:LEU:H	2.24	0.41
1:F:914:ARG:HD2	1:F:1000:THR:HG21	2.03	0.41
1:F:382:VAL:O	1:F:386:PHE:HD2	2.03	0.41
1:F:811:LEU:HA	1:F:811:LEU:HD23	1.83	0.41
1:F:548:ILE:O	1:F:905:ILE:HD13	2.21	0.41
1:A:398:MET:O	1:A:402:ILE:HG13	2.21	0.41
1:A:714:ASN:N	1:A:821:GLU:O	2.51	0.41
1:A:846:LEU:HB3	1:A:847:PRO:HD2	2.02	0.41
1:A:980:GLY:O	1:A:983:PRO:HD2	2.20	0.41
1:B:426:PRO:HD2	1:B:429:GLU:HB3	2.02	0.41
1:B:883:LEU:HD23	1:B:883:LEU:HA	1.60	0.41
1:C:358:PHE:CD2	1:C:972:MET:SD	3.14	0.41
1:C:599:LEU:HA	1:C:599:LEU:HD23	1.90	0.41
1:C:602:GLU:HG3	1:C:605:ASN:ND2	2.36	0.41
1:D:17:ILE:HG23	1:D:21:LEU:HD23	2.02	0.41
1:D:360:GLN:HE21	1:D:360:GLN:HB3	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1032:ASN:OD1	1:E:1033:GLU:HA	2.21	0.41
1:E:460:GLY:N	1:E:867:GLN:OE1	2.44	0.41
1:F:974:SER:CB	1:F:1010:THR:HG21	2.50	0.41
1:F:1017:VAL:N	1:F:1018:PRO:HD2	2.35	0.41
1:F:13:TRP:HE1	1:F:492:LEU:HD21	1.86	0.41
1:F:572:PHE:CE1	1:F:643:THR:HG22	2.56	0.41
1:F:716:LEU:HA	1:F:716:LEU:HD13	1.93	0.41
1:A:191:ASN:O	1:A:193:LEU:N	2.54	0.41
1:A:247:GLY:C	1:A:249:ILE:H	2.24	0.41
1:A:332:PHE:O	1:A:336:SER:HB3	2.21	0.41
1:B:534:ILE:HD11	1:B:1019:VAL:CG2	2.50	0.41
1:B:616:GLY:O	1:B:618:ASN:N	2.54	0.41
1:B:771:GLU:O	1:B:775:ARG:HG2	2.21	0.41
1:B:790:ASP:OD2	1:B:792:GLN:N	2.53	0.41
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.99	0.41
1:D:222:THR:OG1	1:E:275:TYR:O	2.39	0.41
1:D:602:GLU:HB3	1:D:606:VAL:HG23	2.03	0.41
1:D:722:PHE:CD1	1:D:804:TRP:CE2	3.09	0.41
1:D:956:ILE:H	1:D:956:ILE:HG13	1.47	0.41
1:E:185:ARG:HH12	1:E:769:MET:HE3	1.86	0.41
1:E:886:LEU:HA	1:E:886:LEU:HD12	1.80	0.41
1:E:935:LYS:O	1:E:936:ASN:C	2.59	0.41
1:F:548:ILE:HD13	1:F:1012:LEU:HD21	2.03	0.41
1:F:408:ASP:O	1:F:412:VAL:HG23	2.20	0.41
1:F:770:SER:HG	1:F:775:ARG:HG2	1.85	0.41
1:F:967:LEU:O	1:F:970:ILE:HB	2.21	0.41
1:A:668:GLU:HA	2:A:1101:ERY:H213	2.02	0.41
1:A:687:HIS:O	1:A:691:THR:OG1	2.20	0.41
1:A:909:LEU:O	1:A:913:PHE:HB2	2.21	0.41
1:B:1019:VAL:HG23	1:B:1019:VAL:H	1.56	0.41
1:B:572:PHE:HD1	1:B:661:PHE:O	2.03	0.41
1:B:2:PRO:O	1:B:6:ILE:HD12	2.21	0.41
1:B:842:LEU:HA	1:B:842:LEU:HD23	1.85	0.41
1:C:1007:VAL:HG12	1:C:1008:THR:N	2.34	0.41
1:C:216:ALA:HB1	1:C:234:ILE:HG22	2.03	0.41
1:C:26:ALA:HB1	1:C:384:ALA:CB	2.51	0.41
1:C:361:ASN:O	1:C:364:ALA:N	2.51	0.41
1:C:79:SER:HB3	1:C:814:TYR:CD1	2.44	0.41
1:C:872:TYR:O	1:C:876:LEU:HG	2.20	0.41
1:C:947:LEU:HD11	1:C:965:MET:HE1	2.03	0.41
1:D:189:ASN:O	1:D:193:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:854:TRP:HE3	1:D:858:SER:HG	1.67	0.41
1:E:190:PRO:HB2	1:E:783:ASP:O	2.20	0.41
1:E:188:MET:HA	1:E:266:ALA:CB	2.51	0.41
1:E:616:GLY:O	1:E:618:ASN:N	2.54	0.41
1:E:694:ARG:HD3	1:E:820:MET:HE2	2.03	0.41
1:F:39:ALA:HB2	1:F:668:GLU:CG	2.51	0.41
1:F:414:GLU:HG2	1:F:968:ARG:HH11	1.85	0.41
1:F:723:LYS:HG2	1:F:803:ARG:NH1	2.36	0.41
1:F:927:LEU:HD22	1:F:930:ILE:HD12	2.04	0.41
1:F:407:ASP:HB2	1:F:973:THR:OG1	2.21	0.41
1:B:567:GLU:O	1:B:569:GLN:HG3	2.21	0.40
1:C:434:SER:O	1:C:437:GLN:N	2.51	0.40
1:C:587:THR:HG21	1:C:617:GLN:O	2.22	0.40
1:C:951:GLU:O	1:C:953:LYS:N	2.54	0.40
1:D:182:TYR:O	1:D:764:LYS:HB3	2.21	0.40
1:D:446:ALA:HB2	1:D:482:VAL:HG21	2.03	0.40
1:D:511:GLY:HA2	1:D:515:TRP:NE1	2.36	0.40
1:D:917:THR:O	1:D:919:ASP:N	2.54	0.40
1:D:920:VAL:HG12	1:D:921:TYR:N	2.36	0.40
1:E:240:LEU:HD12	1:E:246:PHE:CD2	2.56	0.40
1:E:405:LEU:HD23	1:E:481:SER:HB3	2.03	0.40
1:F:402:ILE:HG21	1:F:402:ILE:HD13	1.88	0.40
1:A:396:PHE:O	1:A:400:LEU:HB2	2.22	0.40
1:A:939:LEU:CB	1:A:966:ARG:HD2	2.50	0.40
1:B:174:ASP:HB3	1:B:292:LYS:HB2	2.04	0.40
1:B:555:LEU:HD23	1:B:555:LEU:HA	1.73	0.40
1:B:951:GLU:O	1:B:953:LYS:N	2.54	0.40
1:C:152:GLU:HG2	1:C:275:TYR:CE2	2.56	0.40
1:C:591:LEU:HB3	1:C:611:ALA:HB1	2.03	0.40
1:C:697:LEU:HD21	1:C:839:MET:HE3	2.02	0.40
1:D:42:ALA:HB2	1:D:93:THR:HG22	2.03	0.40
1:D:393:LEU:HD11	1:D:466:ILE:HD12	2.03	0.40
1:E:445:ILE:HG22	1:E:938:ILE:HG21	2.02	0.40
1:E:574:THR:CG2	1:E:622:ALA:HB3	2.50	0.40
1:E:705:PRO:HA	1:E:708:LEU:O	2.21	0.40
1:E:770:SER:OG	1:E:775:ARG:HG2	2.22	0.40
1:F:1010:THR:C	1:F:1012:LEU:H	2.25	0.40
1:F:1013:ALA:C	1:F:1015:PHE:H	2.24	0.40
1:F:162:MET:HG2	1:F:313:MET:SD	2.62	0.40
1:F:738:ILE:O	1:F:741:ILE:HG13	2.21	0.40
1:F:902:LEU:HD21	1:F:1016:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:977:PHE:O	1:F:978:ILE:C	2.60	0.40
1:A:184:MET:HG2	1:A:246:PHE:CD2	2.56	0.40
1:A:572:PHE:CE1	1:A:643:THR:HG22	2.56	0.40
1:B:84:SER:HB3	1:B:809:PRO:HA	2.03	0.40
1:C:568:ASP:OD1	1:C:639:VAL:HG23	2.21	0.40
1:C:666:ILE:HB	1:C:857:MET:SD	2.61	0.40
1:C:675:PHE:CD2	1:C:854:TRP:HZ3	2.40	0.40
1:C:907:ALA:O	1:C:910:ALA:HB3	2.20	0.40
1:C:974:SER:CB	1:C:1010:THR:HG21	2.51	0.40
1:D:1010:THR:O	1:D:1012:LEU:N	2.55	0.40
1:D:751:GLY:HA2	1:D:769:MET:HG3	2.04	0.40
1:D:842:LEU:HA	1:D:842:LEU:HD23	1.99	0.40
1:E:903:GLY:HA2	1:E:1009:ALA:HB2	2.04	0.40
1:E:1017:VAL:O	1:E:1020:PHE:HB2	2.21	0.40
1:E:251:LEU:CD1	1:E:265:VAL:HG21	2.50	0.40
1:E:420:MET:HB3	1:E:500:ILE:HB	2.03	0.40
1:E:557:VAL:O	1:E:559:LEU:N	2.54	0.40
1:E:631:ASP:C	1:E:633:PRO:HD3	2.41	0.40
1:E:887:TYR:CD2	1:E:892:ILE:HG22	2.57	0.40
1:E:962:ALA:O	1:E:965:MET:N	2.54	0.40
1:F:247:GLY:C	1:F:249:ILE:H	2.24	0.40
1:A:955:LEU:H	1:A:1033:GLU:HA	1.85	0.40
2:A:1101:ERY:H26	2:A:1101:ERY:O6	2.20	0.40
1:A:19:ILE:HD13	1:A:19:ILE:HG21	1.80	0.40
1:A:455:PRO:HG2	1:A:875:SER:CB	2.51	0.40
1:A:597:TYR:CD2	1:A:650:PHE:CZ	3.10	0.40
1:B:309:GLU:O	1:B:313:MET:HG3	2.22	0.40
1:B:434:SER:O	1:B:437:GLN:HB2	2.21	0.40
1:B:677:PHE:CZ	1:B:852:TYR:HB2	2.57	0.40
1:C:368:PRO:O	1:C:406:VAL:HG12	2.21	0.40
1:C:445:ILE:HG23	1:C:935:LYS:HG3	2.03	0.40
1:D:249:ILE:HD12	1:D:262:LEU:HD23	2.02	0.40
1:D:412:VAL:O	1:D:416:VAL:HG23	2.22	0.40
1:D:53:ASP:O	1:D:57:VAL:HG23	2.21	0.40
1:D:77:TYR:OH	1:D:856:GLY:HA2	2.21	0.40
1:E:69:MET:HE1	1:E:107:VAL:HG13	2.03	0.40
1:E:407:ASP:O	1:E:411:VAL:HG23	2.21	0.40
1:E:527:TYR:O	1:E:531:VAL:HG23	2.22	0.40
1:E:882:CYS:O	1:E:885:ALA:HB3	2.21	0.40
1:F:188:MET:HA	1:F:266:ALA:HB2	2.02	0.40
1:F:35:TYR:CD1	1:F:38:ILE:HD12	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:VAL:HG22	1:F:396:PHE:HE2	1.86	0.40
1:F:790:ASP:OD2	1:F:791:GLY:N	2.53	0.40
1:A:563:PHE:O	1:A:564:LEU:HD12	2.21	0.40
1:A:747:ALA:O	1:A:769:MET:HA	2.21	0.40
1:A:890:TRP:CZ2	1:C:10:ILE:HG23	2.56	0.40
1:A:948:MET:HG2	1:A:1035:ILE:HD12	2.02	0.40
1:B:1036:GLU:O	1:B:1037:HIS:ND1	2.54	0.40
1:B:681:ASP:HB2	1:B:690:LEU:HG	2.04	0.40
1:B:899:VAL:HA	1:B:902:LEU:HD13	2.04	0.40
1:C:1017:VAL:O	1:C:1020:PHE:HB2	2.21	0.40
1:C:3:ASN:HB3	1:C:490:PRO:HG2	2.03	0.40
1:C:434:SER:O	1:C:438:ILE:HG12	2.22	0.40
1:C:57:VAL:HG23	1:C:82:SER:HB3	2.03	0.40
1:C:679:LEU:HD12	1:C:851:GLY:O	2.21	0.40
1:C:686:GLY:HA3	1:C:689:LYS:NZ	2.36	0.40
1:C:883:LEU:HD23	1:C:883:LEU:HA	1.76	0.40
1:C:883:LEU:CD1	1:C:938:ILE:HD11	2.52	0.40
1:C:939:LEU:CD1	1:C:970:ILE:HG12	2.51	0.40
3:D:1102:LMT:H31	3:D:1102:LMT:H2O2	1.85	0.40
1:D:108:GLN:OE1	1:D:129:VAL:HB	2.21	0.40
1:D:193:LEU:HD13	1:D:200:PRO:HD3	2.03	0.40
1:D:19:ILE:HD13	1:D:19:ILE:HG21	1.89	0.40
1:D:20:MET:HB3	1:D:377:LEU:HD13	2.03	0.40
1:E:419:VAL:HG21	1:E:434:SER:HB3	2.04	0.40
1:E:471:SER:O	1:E:475:VAL:HG23	2.20	0.40
1:E:9:PRO:HB3	1:E:495:THR:CG2	2.51	0.40
1:F:26:ALA:HB1	1:F:384:ALA:CB	2.52	0.40
1:F:375:VAL:HA	1:F:480:LEU:HD13	2.04	0.40
1:F:53:ASP:O	1:F:56:THR:OG1	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1036/1044 (99%)	902 (87%)	117 (11%)	17 (2%)	9	46
1	B	1035/1044 (99%)	896 (87%)	117 (11%)	22 (2%)	7	40
1	C	1034/1044 (99%)	896 (87%)	119 (12%)	19 (2%)	8	43
1	D	1036/1044 (99%)	894 (86%)	116 (11%)	26 (2%)	5	36
1	E	1035/1044 (99%)	894 (86%)	116 (11%)	25 (2%)	6	37
1	F	1035/1044 (99%)	891 (86%)	118 (11%)	26 (2%)	5	36
All	All	6211/6264 (99%)	5373 (86%)	703 (11%)	135 (2%)	6	39

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	987	SER
1	A	1033	GLU
1	B	357	LEU
1	B	508	GLY
1	B	672	ALA
1	B	888	GLU
1	B	1029	SER
1	B	1033	GLU
1	C	357	LEU
1	C	509	LYS
1	C	888	GLU
1	C	1035	ILE
1	D	357	LEU
1	D	508	GLY
1	D	1028	PHE
1	D	1029	SER
1	D	1032	ASN
1	D	1035	ILE
1	D	1037	HIS
1	E	357	LEU
1	E	888	GLU
1	E	1029	SER
1	E	1033	GLU
1	E	1035	ILE
1	F	6	ILE
1	F	134	SER
1	F	357	LEU
1	F	509	LYS
1	F	684	GLY
1	F	888	GLU

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Mol	Chain	Res	Type
1	F	1034	ASP
1	F	1036	GLU
1	A	360	GLN
1	A	508	GLY
1	A	509	LYS
1	A	670	GLY
1	A	1038	SER
1	B	509	LYS
1	C	147	GLY
1	C	684	GLY
1	C	1031	LYS
1	C	1033	GLU
1	D	511	GLY
1	D	1031	LYS
1	E	508	GLY
1	E	509	LYS
1	E	669	LEU
1	E	672	ALA
1	E	684	GLY
1	F	147	GLY
1	F	675	PHE
1	F	918	ASN
1	A	986	ILE
1	A	1029	SER
1	B	360	GLN
1	B	684	GLY
1	B	905	ILE
1	B	918	ASN
1	C	360	GLN
1	C	614	GLY
1	C	1029	SER
1	D	918	ASN
1	D	1034	ASP
1	D	1038	SER
1	E	358	PHE
1	E	616	GLY
1	F	299	ALA
1	F	507	GLU
1	F	1035	ILE
1	A	62	THR
1	A	248	LYS
1	B	617	GLN

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Mol	Chain	Res	Type
1	B	898	LEU
1	B	1031	LYS
1	C	6	ILE
1	C	918	ASN
1	D	360	GLN
1	D	671	THR
1	D	898	LEU
1	E	506	GLY
1	E	617	GLN
1	E	918	ASN
1	E	1034	ASP
1	F	148	THR
1	F	616	GLY
1	F	1031	LYS
1	A	672	ALA
1	A	1011	VAL
1	B	376	LEU
1	B	1011	VAL
1	C	148	THR
1	C	248	LYS
1	D	505	HIS
1	D	634	GLY
1	D	1036	GLU
1	E	132	SER
1	E	511	GLY
1	E	887	TYR
1	E	898	LEU
1	F	360	GLN
1	F	633	PRO
1	F	1037	HIS
1	C	616	GLY
1	D	847	PRO
1	D	863	LEU
1	F	5	PHE
1	A	634	GLY
1	C	1011	VAL
1	D	1011	VAL
1	F	1011	VAL
1	C	653	ILE
1	D	791	GLY
1	A	427	PRO
1	B	1014	ILE

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Mol	Chain	Res	Type
1	C	791	GLY
1	D	991	GLY
1	E	639	VAL
1	E	905	ILE
1	E	1011	VAL
1	E	1014	ILE
1	A	639	VAL
1	B	506	GLY
1	B	565	PRO
1	D	565	PRO
1	D	653	ILE
1	D	746	GLY
1	E	791	GLY
1	F	412	VAL
1	F	614	GLY
1	F	905	ILE
1	A	666	ILE
1	B	634	GLY
1	B	791	GLY
1	B	847	PRO
1	F	791	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	846/852 (99%)	782 (92%)	64 (8%)	13	45
1	B	845/852 (99%)	772 (91%)	73 (9%)	10	41
1	C	844/852 (99%)	766 (91%)	78 (9%)	9	39
1	D	846/852 (99%)	779 (92%)	67 (8%)	12	44
1	E	845/852 (99%)	775 (92%)	70 (8%)	11	42
1	F	845/852 (99%)	758 (90%)	87 (10%)	7	34
All	All	5071/5112 (99%)	4632 (91%)	439 (9%)	10	41

All (439) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	27	ILE
1	A	45	ILE
1	A	48	SER
1	A	76	MET
1	A	151	GLN
1	A	152	GLU
1	A	166	ILE
1	A	177	LEU
1	A	189	ASN
1	A	195	LYS
1	A	199	THR
1	A	205	THR
1	A	222	THR
1	A	253	VAL
1	A	324	VAL
1	A	353	LEU
1	A	355	MET
1	A	362	PHE
1	A	463	THR
1	A	483	LEU
1	A	515	TRP
1	A	523	SER
1	A	524	THR
1	A	538	THR
1	A	540	ARG
1	A	561	SER
1	A	571	VAL
1	A	575	MET
1	A	605	ASN
1	A	625	SER
1	A	629	TRP
1	A	652	GLN
1	A	654	LYS
1	A	655	ASP
1	A	661	PHE
1	A	669	LEU
1	A	690	LEU
1	A	692	GLN
1	A	706	ASP
1	A	708	LEU
1	A	711	VAL

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Mol	Chain	Res	Type
1	A	738	ILE
1	A	741	ILE
1	A	763	VAL
1	A	770	SER
1	A	796	PHE
1	A	799	PHE
1	A	806	TYR
1	A	861	GLU
1	A	876	LEU
1	A	881	LEU
1	A	896	VAL
1	A	913	PHE
1	A	946	ASP
1	A	956	ILE
1	A	963	VAL
1	A	966	ARG
1	A	975	LEU
1	A	977	PHE
1	A	979	LEU
1	A	1031	LYS
1	A	1032	ASN
1	A	1039	HIS
1	B	6	ILE
1	B	11	PHE
1	B	18	ILE
1	B	27	ILE
1	B	28	LEU
1	B	45	ILE
1	B	60	THR
1	B	77	TYR
1	B	105	VAL
1	B	128	SER
1	B	145	THR
1	B	177	LEU
1	B	185	ARG
1	B	205	THR
1	B	249	ILE
1	B	253	VAL
1	B	255	GLN
1	B	259	ARG
1	B	277	ILE
1	B	293	LEU

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Mol	Chain	Res	Type
1	B	295	THR
1	B	324	VAL
1	B	353	LEU
1	B	355	MET
1	B	358	PHE
1	B	360	GLN
1	B	362	PHE
1	B	400	LEU
1	B	459	PHE
1	B	463	THR
1	B	489	THR
1	B	515	TRP
1	B	524	THR
1	B	534	ILE
1	B	550	VAL
1	B	561	SER
1	B	571	VAL
1	B	575	MET
1	B	578	LEU
1	B	583	THR
1	B	602	GLU
1	B	605	ASN
1	B	661	PHE
1	B	667	VAL
1	B	668	GLU
1	B	669	LEU
1	B	682	GLN
1	B	689	LYS
1	B	690	LEU
1	B	708	LEU
1	B	709	THR
1	B	712	ARG
1	B	717	GLU
1	B	729	GLU
1	B	738	ILE
1	B	741	ILE
1	B	762	ARG
1	B	770	SER
1	B	799	PHE
1	B	806	TYR
1	B	830	LYS
1	B	838	LEU

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Mol	Chain	Res	Type
1	B	905	ILE
1	B	909	LEU
1	B	926	LEU
1	B	953	LYS
1	B	956	ILE
1	B	963	VAL
1	B	966	ARG
1	B	977	PHE
1	B	979	LEU
1	B	981	VAL
1	B	988	THR
1	C	3	ASN
1	C	5	PHE
1	C	7	ASP
1	C	13	TRP
1	C	28	LEU
1	C	48	SER
1	C	49	TYR
1	C	59	ASP
1	C	68	ASN
1	C	69	MET
1	C	76	MET
1	C	82	SER
1	C	87	THR
1	C	102	ILE
1	C	104	GLN
1	C	112	GLN
1	C	121	GLU
1	C	145	THR
1	C	153	ASP
1	C	177	LEU
1	C	182	TYR
1	C	195	LYS
1	C	199	THR
1	C	222	THR
1	C	293	LEU
1	C	353	LEU
1	C	358	PHE
1	C	360	GLN
1	C	362	PHE
1	C	363	ARG
1	C	439	GLN

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Mol	Chain	Res	Type
1	C	447	MET
1	C	462	SER
1	C	482	VAL
1	C	510	LYS
1	C	523	SER
1	C	524	THR
1	C	538	THR
1	C	561	SER
1	C	571	VAL
1	C	613	ASN
1	C	621	ILE
1	C	628	ASP
1	C	631	ASP
1	C	654	LYS
1	C	661	PHE
1	C	663	LEU
1	C	669	LEU
1	C	676	ASP
1	C	677	PHE
1	C	678	GLU
1	C	681	ASP
1	C	689	LYS
1	C	690	LEU
1	C	692	GLN
1	C	711	VAL
1	C	712	ARG
1	C	729	GLU
1	C	763	VAL
1	C	771	GLU
1	C	783	ASP
1	C	838	LEU
1	C	842	LEU
1	C	855	THR
1	C	862	ARG
1	C	871	LEU
1	C	875	SER
1	C	890	TRP
1	C	918	ASN
1	C	927	LEU
1	C	938	ILE
1	C	966	ARG
1	C	972	MET

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Mol	Chain	Res	Type
1	C	979	LEU
1	C	986	ILE
1	C	988	THR
1	C	1002	VAL
1	C	1037	HIS
1	D	11	PHE
1	D	27	ILE
1	D	45	ILE
1	D	48	SER
1	D	49	TYR
1	D	53	ASP
1	D	146	ASP
1	D	152	GLU
1	D	166	ILE
1	D	177	LEU
1	D	182	TYR
1	D	195	LYS
1	D	205	THR
1	D	243	THR
1	D	324	VAL
1	D	344	LEU
1	D	353	LEU
1	D	355	MET
1	D	360	GLN
1	D	362	PHE
1	D	404	LEU
1	D	428	LYS
1	D	437	GLN
1	D	463	THR
1	D	483	LEU
1	D	523	SER
1	D	524	THR
1	D	538	THR
1	D	561	SER
1	D	564	LEU
1	D	571	VAL
1	D	573	MET
1	D	575	MET
1	D	605	ASN
1	D	621	ILE
1	D	625	SER
1	D	629	TRP

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Mol	Chain	Res	Type
1	D	631	ASP
1	D	654	LYS
1	D	661	PHE
1	D	666	ILE
1	D	667	VAL
1	D	677	PHE
1	D	692	GLN
1	D	708	LEU
1	D	719	THR
1	D	738	ILE
1	D	741	ILE
1	D	783	ASP
1	D	810	ARG
1	D	838	LEU
1	D	876	LEU
1	D	881	LEU
1	D	896	VAL
1	D	905	ILE
1	D	909	LEU
1	D	913	PHE
1	D	926	LEU
1	D	946	ASP
1	D	956	ILE
1	D	963	VAL
1	D	966	ARG
1	D	975	LEU
1	D	979	LEU
1	D	1002	VAL
1	D	1031	LYS
1	D	1032	ASN
1	E	25	LEU
1	E	28	LEU
1	E	45	ILE
1	E	49	TYR
1	E	53	ASP
1	E	88	VAL
1	E	105	VAL
1	E	119	PRO
1	E	128	SER
1	E	131	LYS
1	E	145	THR
1	E	164	ASP

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Mol	Chain	Res	Type
1	E	177	LEU
1	E	182	TYR
1	E	189	ASN
1	E	195	LYS
1	E	222	THR
1	E	249	ILE
1	E	259	ARG
1	E	293	LEU
1	E	295	THR
1	E	324	VAL
1	E	353	LEU
1	E	358	PHE
1	E	362	PHE
1	E	400	LEU
1	E	404	LEU
1	E	459	PHE
1	E	524	THR
1	E	536	ARG
1	E	561	SER
1	E	563	PHE
1	E	571	VAL
1	E	575	MET
1	E	578	LEU
1	E	625	SER
1	E	628	ASP
1	E	654	LYS
1	E	661	PHE
1	E	663	LEU
1	E	667	VAL
1	E	668	GLU
1	E	675	PHE
1	E	689	LYS
1	E	690	LEU
1	E	692	GLN
1	E	703	LYS
1	E	707	MET
1	E	708	LEU
1	E	709	THR
1	E	712	ARG
1	E	717	GLU
1	E	729	GLU
1	E	743	THR

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Mol	Chain	Res	Type
1	E	770	SER
1	E	801	SER
1	E	806	TYR
1	E	830	LYS
1	E	838	LEU
1	E	862	ARG
1	E	875	SER
1	E	926	LEU
1	E	963	VAL
1	E	966	ARG
1	E	973	THR
1	E	981	VAL
1	E	1021	PHE
1	E	1030	ARG
1	E	1032	ASN
1	E	1033	GLU
1	F	3	ASN
1	F	5	PHE
1	F	6	ILE
1	F	10	ILE
1	F	11	PHE
1	F	28	LEU
1	F	34	GLN
1	F	44	THR
1	F	49	TYR
1	F	55	LYS
1	F	59	ASP
1	F	76	MET
1	F	81	ASN
1	F	87	THR
1	F	93	THR
1	F	104	GLN
1	F	108	GLN
1	F	112	GLN
1	F	115	MET
1	F	129	VAL
1	F	145	THR
1	F	151	GLN
1	F	189	ASN
1	F	243	THR
1	F	293	LEU
1	F	321	LEU

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Mol	Chain	Res	Type
1	F	353	LEU
1	F	358	PHE
1	F	415	ASN
1	F	448	VAL
1	F	463	THR
1	F	482	VAL
1	F	510	LYS
1	F	515	TRP
1	F	523	SER
1	F	524	THR
1	F	538	THR
1	F	550	VAL
1	F	564	LEU
1	F	571	VAL
1	F	573	MET
1	F	578	LEU
1	F	602	GLU
1	F	605	ASN
1	F	628	ASP
1	F	631	ASP
1	F	644	MET
1	F	652	GLN
1	F	654	LYS
1	F	661	PHE
1	F	663	LEU
1	F	668	GLU
1	F	669	LEU
1	F	681	ASP
1	F	690	LEU
1	F	692	GLN
1	F	698	LEU
1	F	712	ARG
1	F	738	ILE
1	F	770	SER
1	F	771	GLU
1	F	783	ASP
1	F	785	TYR
1	F	801	SER
1	F	806	TYR
1	F	838	LEU
1	F	842	LEU
1	F	862	ARG

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Mol	Chain	Res	Type
1	F	871	LEU
1	F	875	SER
1	F	880	PHE
1	F	881	LEU
1	F	890	TRP
1	F	905	ILE
1	F	913	PHE
1	F	916	LEU
1	F	927	LEU
1	F	938	ILE
1	F	953	LYS
1	F	966	ARG
1	F	979	LEU
1	F	986	ILE
1	F	988	THR
1	F	1028	PHE
1	F	1031	LYS
1	F	1035	ILE
1	F	1037	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	210	GLN
1	A	229	GLN
1	A	592	ASN
1	A	728	GLN
1	B	106	GLN
1	B	123	GLN
1	B	189	ASN
1	C	81	ASN
1	C	104	GLN
1	C	108	GLN
1	C	274	ASN
1	C	584	GLN
1	C	588	GLN
1	C	592	ASN
1	C	613	ASN
1	C	728	GLN
1	C	918	ASN
1	C	996	ASN

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Mol	Chain	Res	Type
1	D	58	GLN
1	D	63	GLN
1	D	112	GLN
1	D	210	GLN
1	D	229	GLN
1	D	437	GLN
1	D	469	GLN
1	D	588	GLN
1	D	592	ASN
1	D	613	ASN
1	D	825	GLN
1	E	67	GLN
1	E	106	GLN
1	E	123	GLN
1	E	161	ASN
1	E	298	ASN
1	E	732	GLN
1	F	70	ASN
1	F	109	ASN
1	F	181	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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$
3	LMT	D	1103	-	36,36,36	1.92	8 (22%)	47,47,47	1.31	7 (14%)
2	ERY	D	1101	-	53,53,53	1.28	2 (3%)	82,82,82	2.03	27 (32%)
3	LMT	A	1103	-	36,36,36	1.89	10 (27%)	47,47,47	1.58	9 (19%)
3	LMT	F	2100	-	36,36,36	1.74	8 (22%)	47,47,47	1.11	4 (8%)
3	LMT	A	1102	-	36,36,36	1.76	9 (25%)	47,47,47	1.14	4 (8%)
3	LMT	B	2100	-	36,36,36	1.73	9 (25%)	47,47,47	1.93	14 (29%)
3	LMT	D	1102	-	36,36,36	1.81	9 (25%)	47,47,47	1.41	7 (14%)
3	LMT	E	1101	-	36,36,36	1.89	11 (30%)	47,47,47	1.63	8 (17%)
3	LMT	C	1101	-	36,36,36	1.79	8 (22%)	47,47,47	1.43	6 (12%)
2	ERY	A	1101	-	53,53,53	1.14	2 (3%)	82,82,82	1.86	18 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	D	1103	-	-	14/21/61/61	0/2/2/2
2	ERY	D	1101	-	-	48/72/107/107	0/3/3/3
3	LMT	A	1103	-	-	14/21/61/61	0/2/2/2
3	LMT	F	2100	-	-	12/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	13/21/61/61	0/2/2/2
3	LMT	B	2100	-	-	11/21/61/61	0/2/2/2
3	LMT	D	1102	-	-	11/21/61/61	0/2/2/2
3	LMT	E	1101	-	-	11/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
2	ERY	A	1101	-	-	33/72/107/107	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	ERY	O2-C1	5.43	1.47	1.34
2	A	1101	ERY	O2-C1	5.17	1.46	1.34
3	A	1103	LMT	O5'-C5'	4.58	1.55	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1103	LMT	O5'-C5'	4.51	1.55	1.44
3	D	1102	LMT	O3B-C3B	4.36	1.53	1.43
3	E	1101	LMT	O5B-C1B	4.30	1.52	1.41
3	E	1101	LMT	O1'-C1'	4.22	1.47	1.40
3	D	1103	LMT	O5B-C1B	4.17	1.52	1.41
3	D	1103	LMT	O1'-C1'	3.97	1.47	1.40
3	D	1103	LMT	O3B-C3B	3.94	1.52	1.43
3	B	2100	LMT	O5B-C1B	3.92	1.51	1.41
3	F	2100	LMT	O5'-C5'	3.91	1.53	1.44
3	A	1102	LMT	O5B-C1B	3.78	1.51	1.41
3	E	1101	LMT	O5'-C5'	3.73	1.53	1.44
3	A	1103	LMT	O1'-C1'	3.73	1.46	1.40
3	C	1101	LMT	O5'-C5'	3.69	1.53	1.44
3	A	1102	LMT	O5'-C5'	3.63	1.53	1.44
3	A	1103	LMT	O3B-C3B	3.61	1.51	1.43
3	C	1101	LMT	O3B-C3B	3.59	1.51	1.43
3	D	1102	LMT	O1'-C1'	3.57	1.46	1.40
3	D	1103	LMT	O5'-C1'	3.53	1.50	1.41
3	B	2100	LMT	C6'-C5'	-3.50	1.40	1.51
3	D	1102	LMT	C6'-C5'	-3.49	1.40	1.51
3	A	1102	LMT	O1'-C1'	3.46	1.46	1.40
3	F	2100	LMT	O5'-C1'	3.42	1.50	1.41
3	C	1101	LMT	C6'-C5'	-3.38	1.40	1.51
3	C	1101	LMT	O1'-C1'	3.37	1.46	1.40
3	A	1103	LMT	O5B-C1B	3.31	1.50	1.41
3	A	1103	LMT	O5'-C1'	3.31	1.50	1.41
3	A	1102	LMT	C6'-C5'	-3.30	1.40	1.51
3	F	2100	LMT	C6'-C5'	-3.27	1.40	1.51
3	D	1102	LMT	O5'-C5'	3.27	1.52	1.44
3	A	1103	LMT	C6'-C5'	-3.25	1.41	1.51
3	F	2100	LMT	O5B-C1B	3.22	1.50	1.41
3	F	2100	LMT	O3B-C3B	3.19	1.50	1.43
3	B	2100	LMT	O1'-C1'	3.19	1.45	1.40
3	E	1101	LMT	C6'-C5'	-3.18	1.41	1.51
3	F	2100	LMT	O1'-C1'	3.15	1.45	1.40
3	C	1101	LMT	O5'-C1'	3.14	1.49	1.41
3	D	1103	LMT	C6'-C5'	-3.06	1.41	1.51
3	D	1103	LMT	O2'-C2'	3.04	1.50	1.43
3	B	2100	LMT	O5'-C5'	2.99	1.51	1.44
3	B	2100	LMT	O2'-C2'	2.93	1.49	1.43
3	D	1102	LMT	C3'-C2'	-2.93	1.44	1.52
3	E	1101	LMT	O5'-C1'	2.91	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1102	LMT	O5'-C1'	2.89	1.49	1.41
3	A	1102	LMT	O5'-C1'	2.72	1.48	1.41
3	E	1101	LMT	C3B-C2B	-2.69	1.45	1.52
3	C	1101	LMT	O5B-C1B	2.67	1.48	1.41
3	A	1102	LMT	C3'-C2'	-2.67	1.45	1.52
3	A	1102	LMT	O3B-C3B	2.67	1.49	1.43
3	E	1101	LMT	O2'-C2'	2.63	1.49	1.43
3	F	2100	LMT	O2'-C2'	2.63	1.49	1.43
3	C	1101	LMT	O2'-C2'	2.58	1.49	1.43
3	B	2100	LMT	O3B-C3B	2.58	1.49	1.43
3	A	1102	LMT	O2'-C2'	2.56	1.49	1.43
3	A	1102	LMT	C3B-C2B	-2.51	1.45	1.52
3	D	1103	LMT	O3'-C3'	2.47	1.48	1.43
3	D	1102	LMT	O2'-C2'	2.45	1.48	1.43
3	B	2100	LMT	O3'-C3'	2.44	1.48	1.43
2	D	1101	ERY	O11-C9	2.44	1.25	1.21
3	D	1102	LMT	O5B-C1B	2.41	1.48	1.41
3	F	2100	LMT	C3'-C2'	-2.39	1.46	1.52
3	A	1103	LMT	O2'-C2'	2.32	1.48	1.43
3	B	2100	LMT	O5'-C1'	2.30	1.47	1.41
3	C	1101	LMT	C3'-C2'	-2.28	1.46	1.52
3	E	1101	LMT	O5B-C5B	2.23	1.49	1.44
3	A	1103	LMT	C3'-C2'	-2.19	1.46	1.52
2	A	1101	ERY	C25-C26	2.16	1.55	1.51
3	D	1102	LMT	O1B-C1B	-2.15	1.35	1.41
3	A	1103	LMT	O2B-C2B	2.14	1.48	1.43
3	B	2100	LMT	C3'-C2'	-2.10	1.47	1.52
3	E	1101	LMT	C3'-C2'	-2.08	1.47	1.52
3	A	1103	LMT	O3'-C3'	2.07	1.47	1.43
3	E	1101	LMT	C4B-C3B	-2.02	1.47	1.52
3	E	1101	LMT	C5-C4	2.01	1.62	1.51

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	LMT	O5B-C5B-C4B	5.53	119.73	109.69
3	E	1101	LMT	C1B-C2B-C3B	-5.51	98.53	110.00
2	D	1101	ERY	C20-O5-C16	5.24	128.48	117.55
3	C	1101	LMT	C4B-C3B-C2B	5.07	119.67	110.82
2	A	1101	ERY	C20-O5-C16	4.72	127.40	117.55
2	D	1101	ERY	C12-C11-C10	4.65	122.25	116.43
3	B	2100	LMT	O5B-C5B-C4B	4.59	118.03	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2100	LMT	C4B-C3B-C2B	4.57	118.81	110.82
3	C	1101	LMT	C1B-C2B-C3B	4.54	119.44	110.00
3	D	1102	LMT	C4B-C3B-C2B	4.50	118.68	110.82
2	D	1101	ERY	O2-C13-C36	4.46	115.88	107.40
2	A	1101	ERY	O2-C13-C12	4.45	114.55	107.29
2	D	1101	ERY	O2-C1-C2	4.39	121.19	111.56
3	B	2100	LMT	C1B-C2B-C3B	4.12	118.57	110.00
2	D	1101	ERY	O2-C1-O1	-4.11	116.27	123.94
3	B	2100	LMT	O3B-C3B-C4B	-4.05	100.98	110.35
2	A	1101	ERY	O12-C11-C10	4.04	116.75	110.71
3	E	1101	LMT	C1B-O5B-C5B	3.94	121.43	113.69
2	D	1101	ERY	O4-C18-C21	3.89	115.09	106.70
2	A	1101	ERY	C29-N1-C24	3.88	124.77	113.11
2	A	1101	ERY	O7-C5-C6	3.86	111.15	106.39
2	A	1101	ERY	C26-C25-C24	3.85	117.20	110.46
2	A	1101	ERY	C22-C23-C24	3.76	115.34	109.19
3	A	1103	LMT	C3B-C4B-C5B	3.66	116.76	110.24
3	B	2100	LMT	C3B-C4B-C5B	3.54	116.55	110.24
3	F	2100	LMT	O5B-C5B-C4B	3.50	116.04	109.69
2	A	1101	ERY	C15-C16-C17	3.47	113.88	107.67
3	E	1101	LMT	O1'-C1'-C2'	3.45	113.68	108.30
2	A	1101	ERY	C25-C24-C23	3.42	114.89	109.97
3	E	1101	LMT	O5B-C5B-C4B	3.32	115.73	109.69
3	D	1102	LMT	C3B-C4B-C5B	3.30	116.12	110.24
3	A	1103	LMT	O1B-C1B-C2B	3.29	116.63	108.10
2	D	1101	ERY	O12-C11-C10	3.29	115.63	110.71
3	D	1103	LMT	C1B-C2B-C3B	3.27	116.80	110.00
2	A	1101	ERY	C35-C12-C13	3.23	115.86	111.31
2	D	1101	ERY	C29-N1-C24	3.20	122.74	113.11
3	D	1102	LMT	C1B-C2B-C3B	3.18	116.62	110.00
2	D	1101	ERY	C22-O7-C5	3.16	121.74	116.25
2	A	1101	ERY	O12-C11-C12	-3.07	100.95	106.68
2	A	1101	ERY	O9-C26-C25	3.06	113.83	109.14
2	D	1101	ERY	O7-C22-C23	3.06	116.03	108.10
2	A	1101	ERY	O4-C18-C21	3.04	113.26	106.70
2	D	1101	ERY	O11-C9-C8	-3.03	115.65	121.26
3	B	2100	LMT	O5B-C1B-C2B	2.95	116.59	110.35
2	D	1101	ERY	O12-C11-C12	-2.95	101.18	106.68
2	D	1101	ERY	O8-C23-C22	2.93	117.17	110.05
3	B	2100	LMT	C1B-O5B-C5B	2.93	119.44	113.69
3	B	2100	LMT	C6B-C5B-C4B	-2.92	106.15	113.00
3	E	1101	LMT	O1B-C1B-C2B	-2.91	100.55	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2100	LMT	C1B-O1B-C4'	-2.90	110.78	117.96
3	D	1103	LMT	O1B-C4'-C3'	2.90	115.00	107.28
2	D	1101	ERY	C25-C24-N1	-2.88	107.54	115.67
2	A	1101	ERY	C19-C16-C15	-2.81	105.47	110.49
3	B	2100	LMT	O5'-C1'-O1'	-2.81	103.32	109.97
3	A	1103	LMT	C1'-O5'-C5'	2.78	119.15	113.69
2	D	1101	ERY	C34-C10-C11	-2.77	110.94	114.38
3	C	1101	LMT	O1'-C1'-C2'	-2.76	103.99	108.30
2	A	1101	ERY	O10-C6-C5	-2.75	102.38	107.59
2	D	1101	ERY	C35-C12-C13	2.70	115.11	111.31
3	D	1103	LMT	O5B-C5B-C6B	2.64	113.00	106.44
3	E	1101	LMT	C1'-C2'-C3'	2.64	115.50	110.00
2	A	1101	ERY	O6-C17-C18	-2.59	104.84	109.39
3	D	1102	LMT	C1'-O5'-C5'	2.56	118.71	113.69
2	D	1101	ERY	C3-C2-C1	2.55	115.23	110.01
3	C	1101	LMT	C1B-O1B-C4'	-2.51	111.76	117.96
3	A	1103	LMT	O2B-C2B-C1B	2.46	116.02	110.05
2	A	1101	ERY	C33-C8-C7	-2.46	105.29	109.81
2	D	1101	ERY	C30-C2-C3	2.45	118.47	112.92
2	D	1101	ERY	O3-C3-C4	2.44	111.16	108.22
2	D	1101	ERY	C29-N1-C28	2.43	117.55	110.38
3	A	1103	LMT	O1'-C1'-C2'	2.43	112.09	108.30
3	D	1102	LMT	C1B-O5B-C5B	-2.42	108.94	113.69
3	A	1102	LMT	O3'-C3'-C2'	-2.41	104.77	110.35
3	B	2100	LMT	O2B-C2B-C1B	-2.40	104.22	110.05
3	A	1103	LMT	O5'-C5'-C4'	2.38	114.76	109.75
3	A	1103	LMT	O5B-C1B-C2B	-2.36	105.35	110.35
2	D	1101	ERY	C11-C10-C9	2.33	113.35	109.57
3	A	1102	LMT	C1'-O5'-C5'	2.32	118.25	113.69
3	A	1102	LMT	O5B-C5B-C4B	2.31	113.88	109.69
3	C	1101	LMT	O3B-C3B-C4B	-2.31	105.02	110.35
2	D	1101	ERY	C19-C16-C15	-2.27	106.44	110.49
3	A	1103	LMT	C1B-O1B-C4'	-2.25	112.40	117.96
3	D	1103	LMT	O5B-C5B-C4B	2.25	113.77	109.69
3	B	2100	LMT	O1B-C1B-C2B	-2.24	102.29	108.10
3	E	1101	LMT	C2'-C3'-C4'	2.23	114.78	109.68
3	D	1102	LMT	O4'-C4B-C3B	-2.22	105.22	110.35
2	D	1101	ERY	C3-C4-C5	2.21	115.94	111.19
3	D	1103	LMT	C4B-C3B-C2B	2.20	114.67	110.82
3	B	2100	LMT	C3'-C4'-C5'	2.18	115.92	110.93
3	D	1103	LMT	C1'-C2'-C3'	2.17	114.51	110.00
3	B	2100	LMT	O3B-C3B-C2B	-2.15	105.38	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1102	LMT	O5B-C1B-C2B	2.13	114.86	110.35
3	E	1101	LMT	O5'-C5'-C6'	2.12	111.71	106.44
2	D	1101	ERY	C34-C10-C9	2.10	111.72	108.08
3	A	1102	LMT	C2'-C3'-C4'	2.09	114.46	109.68
2	D	1101	ERY	O6-C17-C18	-2.08	105.75	109.39
3	B	2100	LMT	C1-O1'-C1'	2.06	117.26	113.84
3	C	1101	LMT	O3B-C3B-C2B	-2.05	105.61	110.35
2	D	1101	ERY	C16-C15-C14	-2.05	111.52	115.07
3	D	1103	LMT	C1'-O5'-C5'	2.04	117.69	113.69
3	F	2100	LMT	C6B-C5B-C4B	-2.04	108.23	113.00
2	A	1101	ERY	C30-C2-C3	2.03	117.51	112.92
2	D	1101	ERY	O11-C9-C10	2.02	123.47	120.60
3	F	2100	LMT	C3B-C4B-C5B	2.02	113.83	110.24

There are no chirality outliers.

All (179) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1103	LMT	C2'-C1'-O1'-C1
3	D	1103	LMT	O5'-C1'-O1'-C1
2	D	1101	ERY	C9-C10-C11-C12
2	D	1101	ERY	C10-C11-C12-C13
2	D	1101	ERY	C10-C11-C12-C35
2	D	1101	ERY	C10-C11-C12-O13
2	D	1101	ERY	O12-C11-C12-C13
2	D	1101	ERY	O12-C11-C12-C35
2	D	1101	ERY	O12-C11-C12-O13
2	D	1101	ERY	C2-C1-O2-C13
2	D	1101	ERY	O1-C1-O2-C13
2	D	1101	ERY	C4-C5-C6-C7
2	D	1101	ERY	C4-C5-C6-C32
2	D	1101	ERY	C4-C5-C6-O10
2	D	1101	ERY	O7-C5-C6-C7
2	D	1101	ERY	O7-C5-C6-C32
2	D	1101	ERY	O7-C5-C6-O10
2	D	1101	ERY	C5-C6-C7-C8
2	D	1101	ERY	C32-C6-C7-C8
2	D	1101	ERY	C7-C8-C9-C10
2	D	1101	ERY	C7-C8-C9-O11
2	D	1101	ERY	C15-C14-O3-C3
2	D	1101	ERY	O4-C14-O3-C3
2	D	1101	ERY	C15-C16-O5-C20

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Mol	Chain	Res	Type	Atoms
2	D	1101	ERY	C19-C16-O5-C20
3	A	1103	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	C2-C1-O1'-C1'
3	A	1102	LMT	C2'-C1'-O1'-C1
3	B	2100	LMT	C2-C1-O1'-C1'
3	D	1102	LMT	C2-C1-O1'-C1'
2	A	1101	ERY	C11-C12-C13-O2
2	A	1101	ERY	C11-C12-C13-C36
2	A	1101	ERY	C35-C12-C13-O2
2	A	1101	ERY	C35-C12-C13-C36
2	A	1101	ERY	O13-C12-C13-O2
2	A	1101	ERY	O13-C12-C13-C36
2	A	1101	ERY	C12-C13-O2-C1
2	A	1101	ERY	O2-C13-C36-C37
2	A	1101	ERY	C2-C1-O2-C13
2	A	1101	ERY	O2-C1-C2-C3
2	A	1101	ERY	C4-C5-C6-C7
2	A	1101	ERY	C4-C5-C6-O10
2	A	1101	ERY	O7-C5-C6-C7
2	A	1101	ERY	O7-C5-C6-C32
2	A	1101	ERY	O7-C5-C6-O10
2	A	1101	ERY	C15-C14-O3-C3
2	A	1101	ERY	O4-C14-O3-C3
2	A	1101	ERY	C17-C16-O5-C20
2	D	1101	ERY	O9-C22-O7-C5
3	F	2100	LMT	C3-C4-C5-C6
3	D	1103	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	C4B-C5B-C6B-O6B
3	C	1101	LMT	O5B-C5B-C6B-O6B
2	A	1101	ERY	O1-C1-O2-C13
3	A	1103	LMT	C5-C6-C7-C8
3	E	1101	LMT	O5B-C5B-C6B-O6B
3	C	1101	LMT	C1-C2-C3-C4
3	A	1102	LMT	O5B-C5B-C6B-O6B
3	D	1102	LMT	O5B-C5B-C6B-O6B
2	A	1101	ERY	O3-C3-C4-C31
2	A	1101	ERY	C2-C3-C4-C31
2	A	1101	ERY	O3-C3-C4-C5
2	A	1101	ERY	C2-C3-C4-C5
3	B	2100	LMT	C4B-C5B-C6B-O6B
3	A	1102	LMT	O5'-C1'-O1'-C1
3	F	2100	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
3	A	1103	LMT	C4B-C5B-C6B-O6B
3	B	2100	LMT	C4-C5-C6-C7
3	E	1101	LMT	O5'-C5'-C6'-O6'
3	A	1102	LMT	C5-C6-C7-C8
3	D	1102	LMT	C4B-C5B-C6B-O6B
3	C	1101	LMT	C4B-C5B-C6B-O6B
2	D	1101	ERY	C36-C13-O2-C1
3	A	1103	LMT	O5'-C5'-C6'-O6'
3	C	1101	LMT	C4'-C5'-C6'-O6'
3	E	1101	LMT	C4B-C5B-C6B-O6B
3	B	2100	LMT	O5B-C1B-O1B-C4'
2	A	1101	ERY	O1-C1-C2-C3
3	F	2100	LMT	O5'-C5'-C6'-O6'
3	D	1103	LMT	C4B-C5B-C6B-O6B
3	E	1101	LMT	O1'-C1-C2-C3
3	A	1102	LMT	C4'-C5'-C6'-O6'
2	D	1101	ERY	C25-C24-N1-C28
2	D	1101	ERY	C25-C24-N1-C29
3	B	2100	LMT	O5B-C5B-C6B-O6B
3	E	1101	LMT	C4'-C5'-C6'-O6'
3	D	1103	LMT	C3-C4-C5-C6
3	D	1102	LMT	C11-C10-C9-C8
3	C	1101	LMT	C6-C7-C8-C9
3	E	1101	LMT	C11-C10-C9-C8
3	C	1101	LMT	O5'-C5'-C6'-O6'
3	C	1101	LMT	C2'-C1'-O1'-C1
3	F	2100	LMT	C6-C7-C8-C9
3	A	1103	LMT	C3-C4-C5-C6
3	C	1101	LMT	C3-C4-C5-C6
3	C	1101	LMT	C11-C10-C9-C8
3	C	1101	LMT	O1'-C1-C2-C3
3	F	2100	LMT	O1'-C1-C2-C3
3	F	2100	LMT	C11-C10-C9-C8
2	D	1101	ERY	C23-C24-N1-C28
2	D	1101	ERY	C23-C24-N1-C29
3	C	1101	LMT	O5'-C1'-O1'-C1
3	D	1103	LMT	C2-C3-C4-C5
3	B	2100	LMT	C5-C6-C7-C8
3	D	1102	LMT	C7-C8-C9-C10
3	D	1103	LMT	C1-C2-C3-C4
3	A	1103	LMT	C1-C2-C3-C4
3	A	1102	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	F	2100	LMT	C5-C6-C7-C8
3	A	1103	LMT	C9-C10-C11-C12
3	A	1103	LMT	C7-C8-C9-C10
3	B	2100	LMT	C11-C10-C9-C8
3	A	1103	LMT	C2'-C1'-O1'-C1
3	F	2100	LMT	C7-C8-C9-C10
3	B	2100	LMT	C3-C4-C5-C6
2	D	1101	ERY	C35-C12-C13-O2
2	D	1101	ERY	C35-C12-C13-C36
3	B	2100	LMT	C7-C8-C9-C10
2	D	1101	ERY	C11-C12-C13-O2
3	D	1102	LMT	C4-C5-C6-C7
3	A	1103	LMT	C2-C3-C4-C5
3	D	1102	LMT	C2-C3-C4-C5
3	A	1102	LMT	C9-C10-C11-C12
2	D	1101	ERY	O10-C6-C7-C8
2	A	1101	ERY	C32-C6-C7-C8
3	B	2100	LMT	C6-C7-C8-C9
3	D	1103	LMT	C4'-C5'-C6'-O6'
3	D	1103	LMT	O1'-C1-C2-C3
3	D	1102	LMT	C6-C7-C8-C9
2	D	1101	ERY	C6-C7-C8-C33
2	A	1101	ERY	C4-C5-C6-C32
3	C	1101	LMT	C2-C1-O1'-C1'
3	A	1103	LMT	C4'-C5'-C6'-O6'
3	A	1102	LMT	O5'-C5'-C6'-O6'
3	D	1103	LMT	C7-C8-C9-C10
3	F	2100	LMT	C9-C10-C11-C12
3	A	1102	LMT	C1-C2-C3-C4
3	E	1101	LMT	C6-C7-C8-C9
2	D	1101	ERY	O2-C13-C36-C37
2	D	1101	ERY	C17-C16-O5-C20
3	D	1103	LMT	C4-C5-C6-C7
2	D	1101	ERY	C12-C13-C36-C37
2	A	1101	ERY	C12-C13-C36-C37
3	A	1103	LMT	C6-C7-C8-C9
2	D	1101	ERY	C6-C7-C8-C9
2	A	1101	ERY	C36-C13-O2-C1
2	D	1101	ERY	C34-C10-C11-C12
3	A	1102	LMT	C3-C4-C5-C6
3	D	1103	LMT	O5'-C5'-C6'-O6'
3	A	1103	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
3	A	1102	LMT	C2-C3-C4-C5
2	D	1101	ERY	C1-C2-C3-O3
2	A	1101	ERY	C15-C16-O5-C20
3	E	1101	LMT	C2B-C1B-O1B-C4'
2	A	1101	ERY	C6-C7-C8-C33
2	D	1101	ERY	C34-C10-C9-O11
3	D	1103	LMT	C3'-C4'-O1B-C1B
3	F	2100	LMT	C2'-C1'-O1'-C1
3	D	1102	LMT	C2'-C1'-O1'-C1
3	D	1102	LMT	O5'-C1'-O1'-C1
3	D	1103	LMT	C5'-C4'-O1B-C1B
3	E	1101	LMT	C9-C10-C11-C12
3	D	1102	LMT	C9-C10-C11-C12
2	D	1101	ERY	C30-C2-C3-C4
3	F	2100	LMT	O5B-C5B-C6B-O6B
2	A	1101	ERY	O1-C1-C2-C30
2	D	1101	ERY	C2-C3-O3-C14
2	D	1101	ERY	C9-C10-C11-O12
3	E	1101	LMT	O5B-C1B-O1B-C4'
2	D	1101	ERY	O13-C12-C13-C36
2	A	1101	ERY	C6-C7-C8-C9
3	B	2100	LMT	C2B-C1B-O1B-C4'
2	D	1101	ERY	C1-C2-C3-C4
2	D	1101	ERY	C33-C8-C9-C10
2	D	1101	ERY	C11-C10-C9-O11
3	A	1102	LMT	C2-C1-O1'-C1'
3	E	1101	LMT	C2-C1-O1'-C1'
3	F	2100	LMT	O5'-C1'-O1'-C1
2	A	1101	ERY	O2-C1-C2-C30

There are no ring outliers.

10 monomers are involved in 49 short contacts:

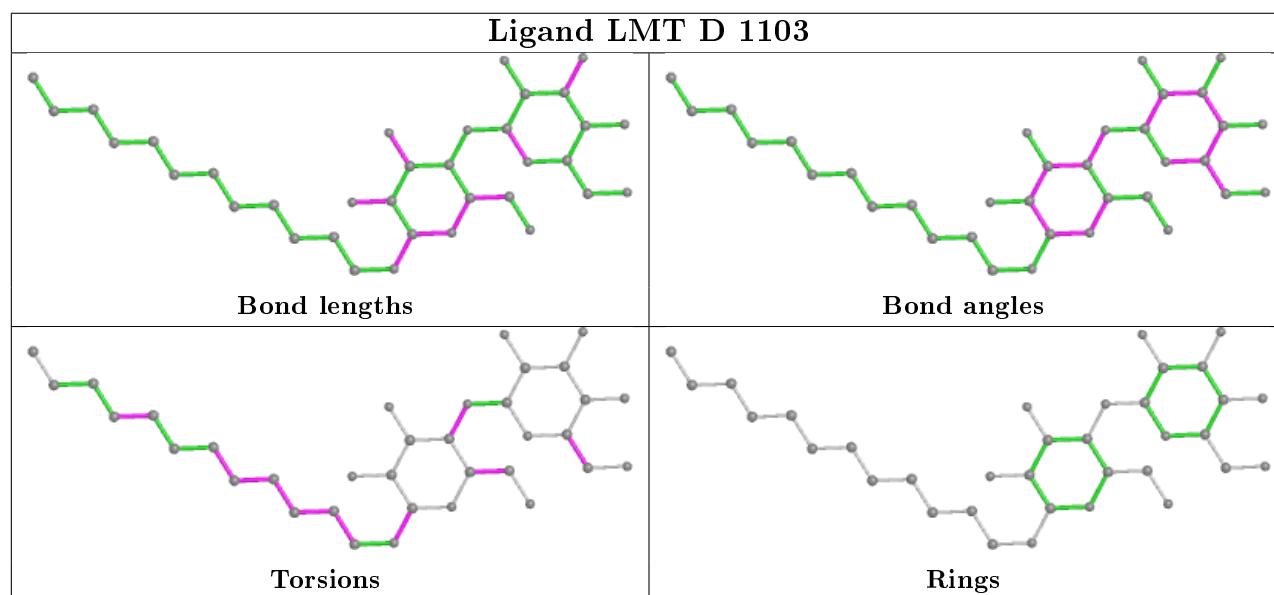
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1103	LMT	6	0
2	D	1101	ERY	4	0
3	A	1103	LMT	2	0
3	F	2100	LMT	2	0
3	A	1102	LMT	5	0
3	B	2100	LMT	7	0
3	D	1102	LMT	7	0
3	E	1101	LMT	10	0

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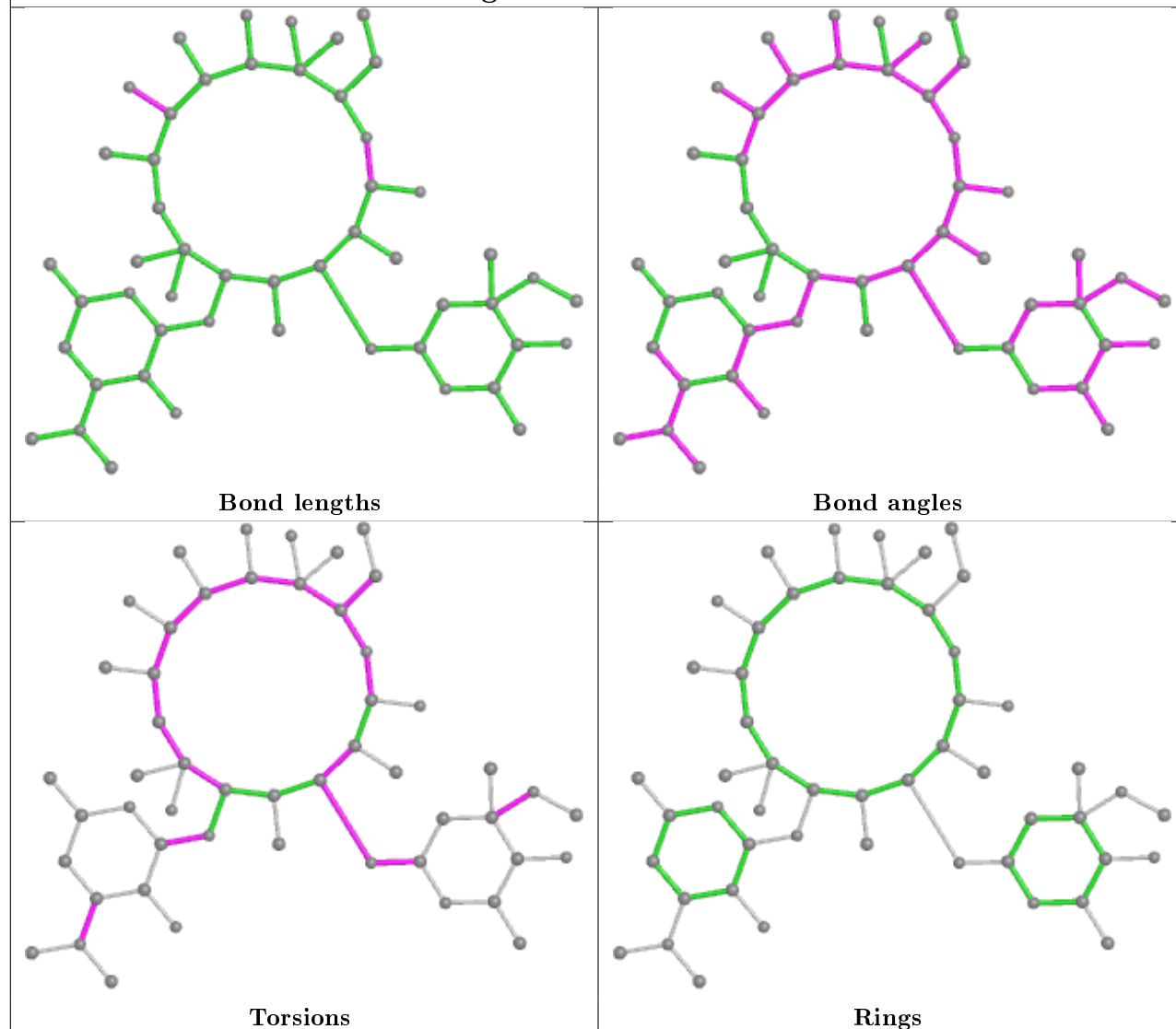
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1101	LMT	1	0
2	A	1101	ERY	5	0

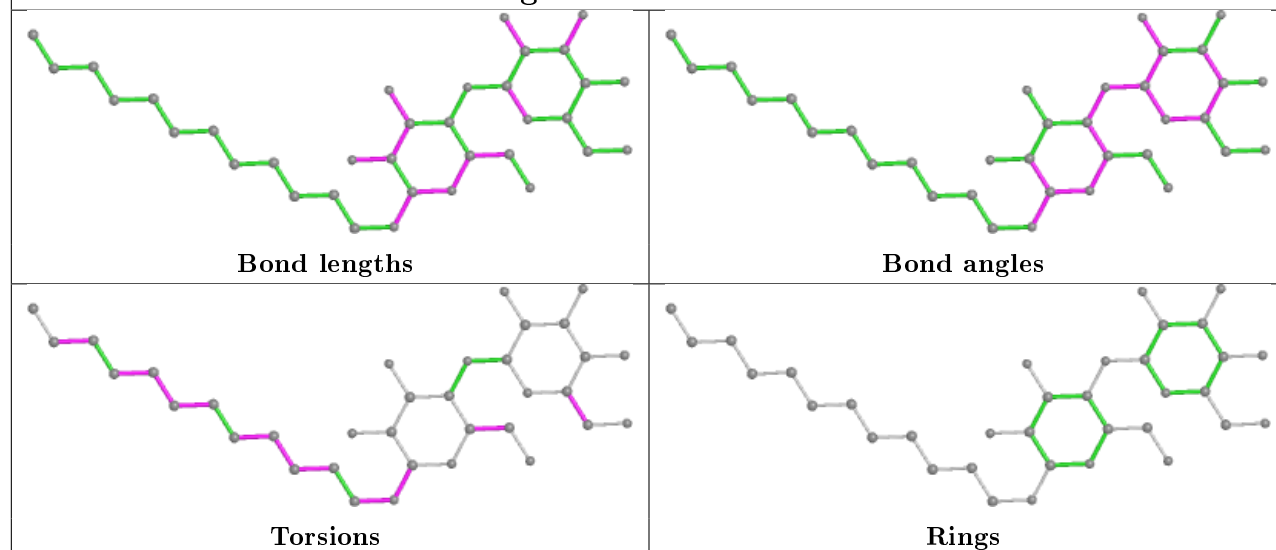
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

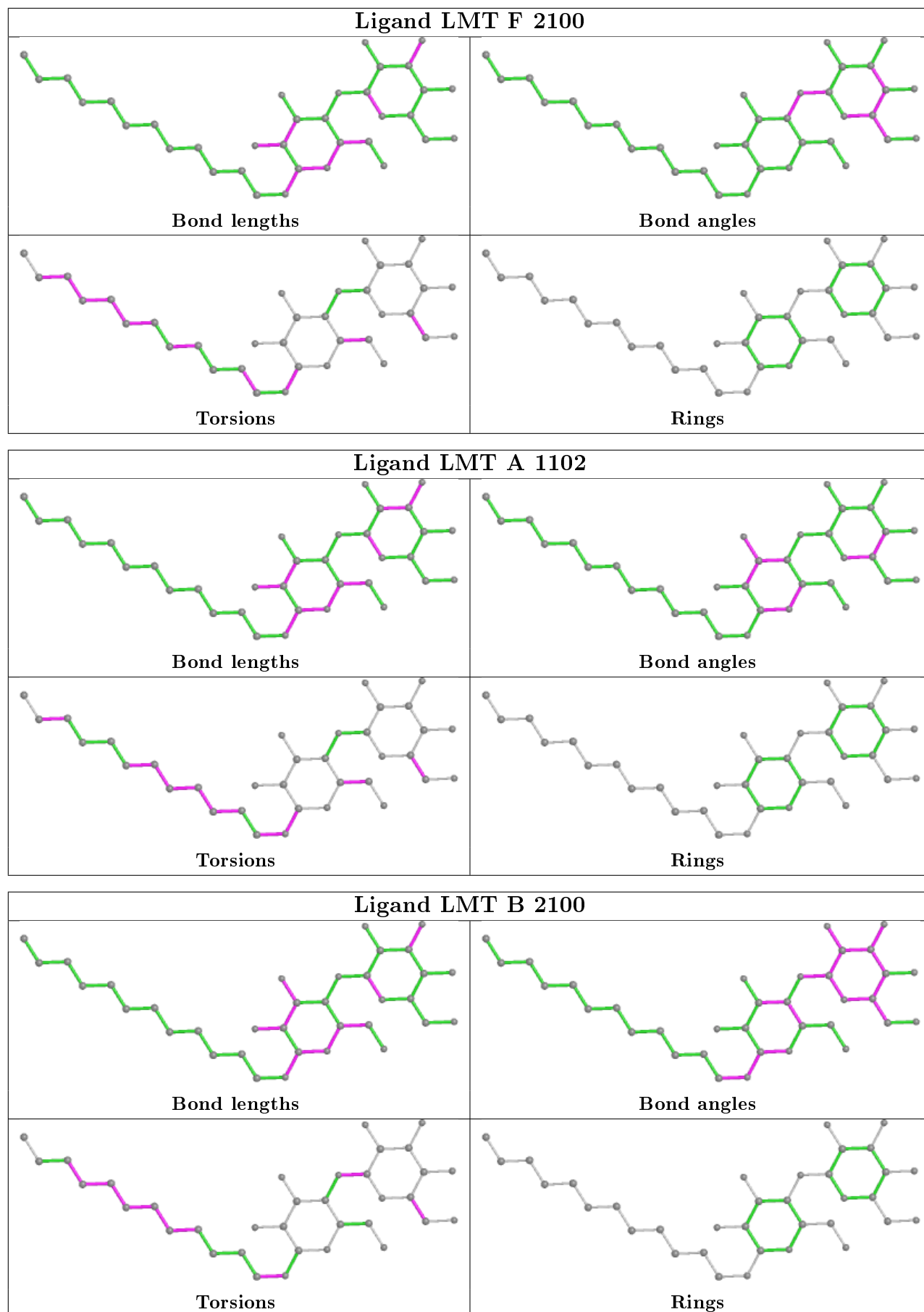


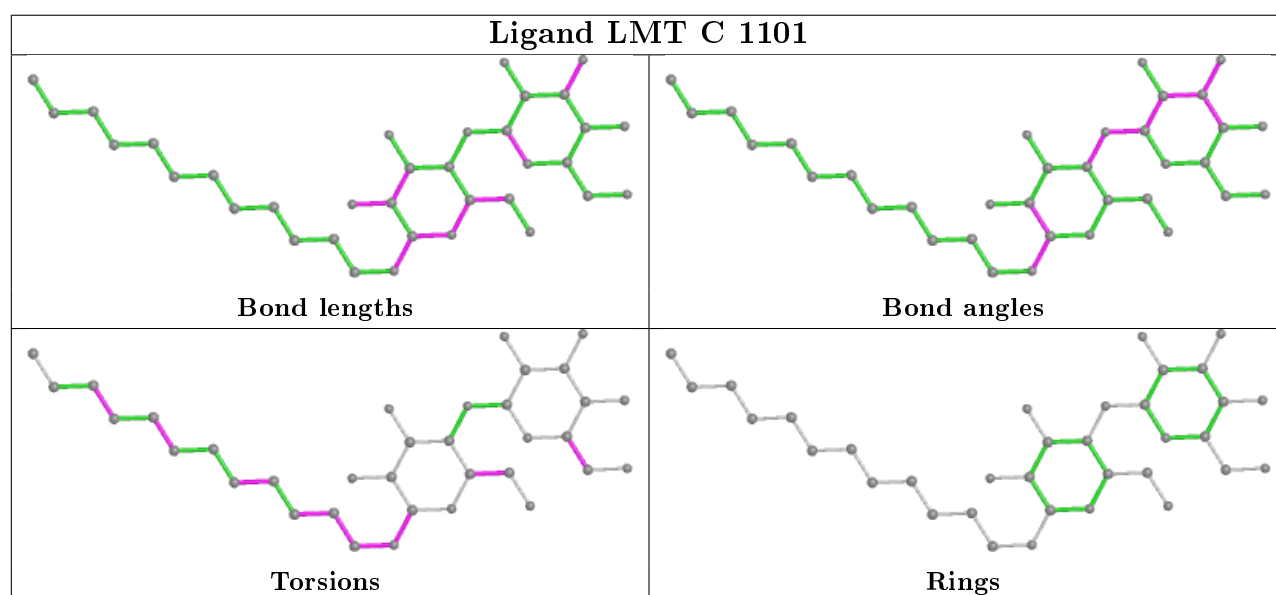
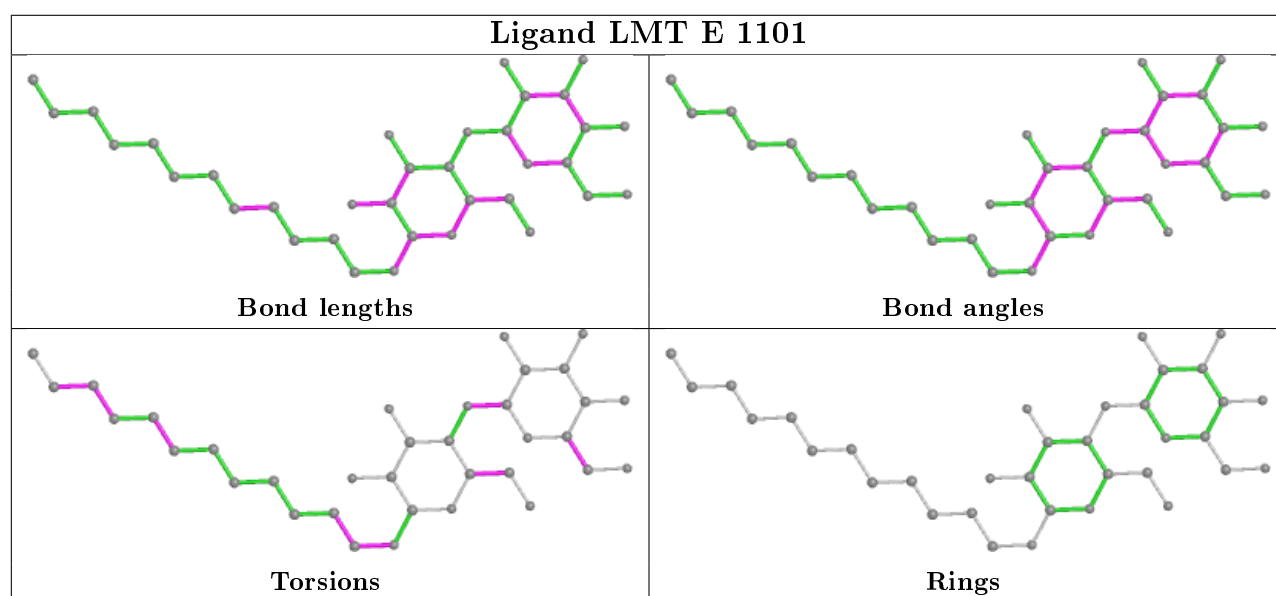
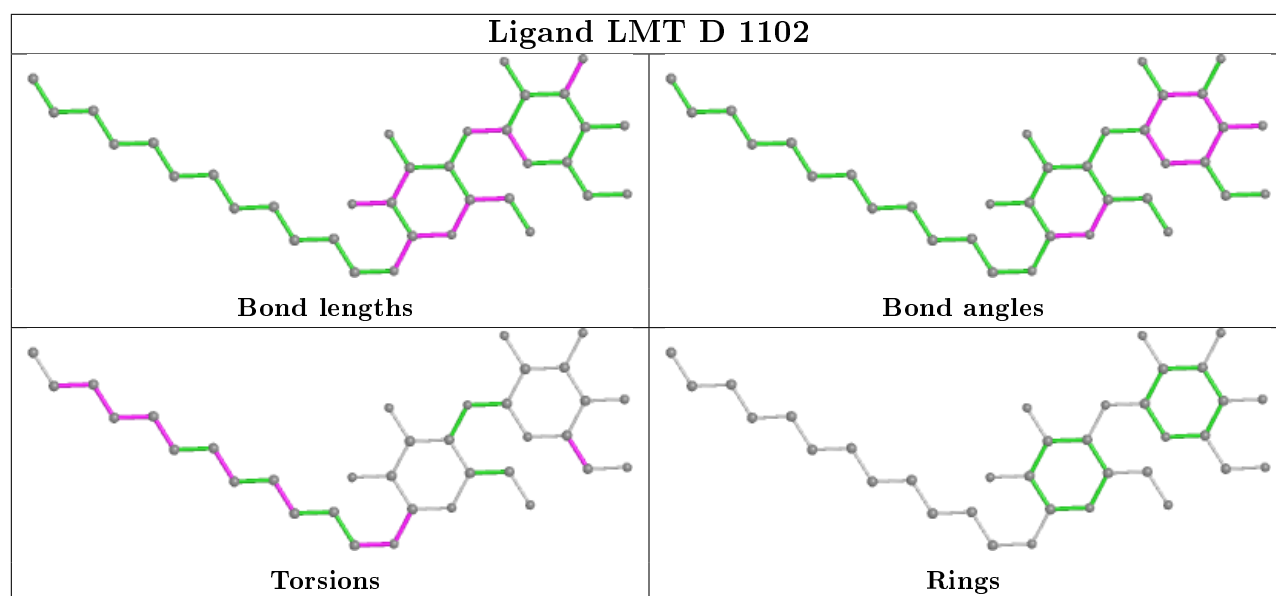
## Ligand ERY D 1101

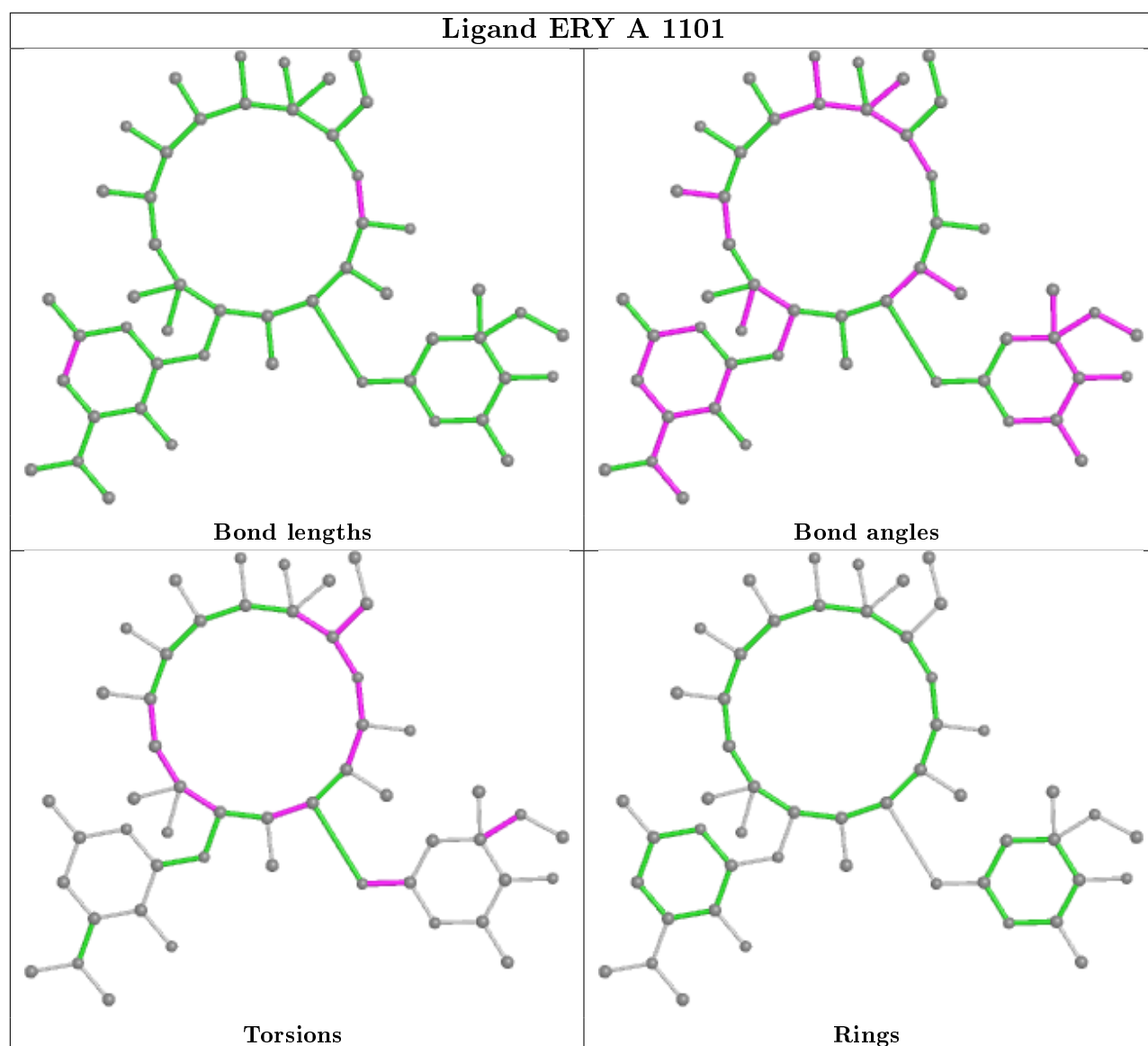


## Ligand LMT A 1103









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1038/1044 (99%)	0.17	76 (7%)	15 9	36, 75, 109, 154	0
1	B	1037/1044 (99%)	0.13	75 (7%)	15 9	31, 73, 111, 151	0
1	C	1036/1044 (99%)	0.33	99 (9%)	8 4	35, 76, 112, 139	0
1	D	1038/1044 (99%)	0.15	74 (7%)	16 9	34, 84, 123, 154	0
1	E	1037/1044 (99%)	0.32	119 (11%)	4 3	46, 87, 118, 148	0
1	F	1037/1044 (99%)	0.47	136 (13%)	3 2	41, 85, 119, 143	0
All	All	6223/6264 (99%)	0.26	579 (9%)	8 4	31, 81, 116, 154	0

All (579) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	714	ASN	10.9
1	C	714	ASN	10.3
1	C	715	GLY	9.4
1	E	314	GLU	9.1
1	A	404	LEU	9.0
1	D	864	SER	8.8
1	A	407	ASP	8.8
1	F	402	ILE	8.6
1	F	403	GLY	8.5
1	A	403	GLY	8.5
1	F	48	SER	8.4
1	F	406	VAL	8.1
1	F	405	LEU	8.0
1	F	449	LEU	8.0
1	E	407	ASP	7.8
1	F	445	ILE	7.4
1	D	865	GLY	7.2
1	E	315	PRO	7.2
1	C	79	SER	7.1

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Mol	Chain	Res	Type	RSRZ
1	F	47	ALA	6.9
1	A	400	LEU	6.9
1	E	404	LEU	6.8
1	E	405	LEU	6.7
1	E	408	ASP	6.7
1	F	474	ILE	6.6
1	F	442	LEU	6.5
1	E	291	ILE	6.5
1	A	401	ALA	6.5
1	C	403	GLY	6.5
1	C	402	ILE	6.5
1	C	398	MET	6.4
1	A	402	ILE	6.4
1	F	707	MET	6.4
1	C	449	LEU	6.2
1	F	715	GLY	6.2
1	D	404	LEU	6.2
1	D	866	ASN	6.1
1	E	310	LEU	6.1
1	C	810	ARG	6.0
1	C	473	THR	6.0
1	A	405	LEU	6.0
1	C	48	SER	5.9
1	F	80	SER	5.8
1	C	831	SER	5.8
1	E	311	ALA	5.8
1	F	404	LEU	5.8
1	F	830	LYS	5.7
1	F	398	MET	5.7
1	E	406	VAL	5.6
1	F	481	SER	5.6
1	F	107	VAL	5.6
1	C	405	LEU	5.6
1	E	488	LEU	5.5
1	D	386	PHE	5.5
1	E	403	GLY	5.5
1	D	400	LEU	5.5
1	C	401	ALA	5.4
1	E	401	ALA	5.4
1	A	445	ILE	5.4
1	C	577	GLN	5.4
1	D	460	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	F	821	GLU	5.3
1	C	707	MET	5.2
1	C	445	ILE	5.2
1	C	821	GLU	5.1
1	C	33	ALA	5.1
1	C	706	ASP	5.1
1	F	706	ASP	5.1
1	F	446	ALA	5.1
1	F	407	ASP	5.1
1	F	831	SER	5.1
1	C	830	LYS	5.0
1	E	714	ASN	5.0
1	A	134	SER	5.0
1	F	448	VAL	5.0
1	E	307	ARG	4.9
1	D	383	LEU	4.9
1	B	404	LEU	4.9
1	C	390	ILE	4.9
1	D	403	GLY	4.9
1	F	444	GLY	4.9
1	F	810	ARG	4.9
1	F	708	LEU	4.8
1	F	46	SER	4.8
1	E	46	SER	4.8
1	C	80	SER	4.8
1	C	832	THR	4.8
1	E	78	MET	4.8
1	F	478	MET	4.7
1	D	486	LEU	4.7
1	B	315	PRO	4.7
1	F	473	THR	4.6
1	A	406	VAL	4.6
1	A	449	LEU	4.6
1	F	701	ALA	4.6
1	E	653	ILE	4.6
1	F	883	LEU	4.5
1	E	676	ASP	4.5
1	F	400	LEU	4.5
1	E	33	ALA	4.5
1	F	401	ALA	4.5
1	C	127	VAL	4.5
1	C	829	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	385	ALA	4.4
1	C	389	SER	4.4
1	C	406	VAL	4.4
1	E	864	SER	4.4
1	F	81	ASN	4.4
1	E	308	ALA	4.4
1	E	443	VAL	4.3
1	F	399	VAL	4.3
1	C	69	MET	4.3
1	A	128	SER	4.3
1	F	501	ALA	4.3
1	E	801	SER	4.2
1	A	408	ASP	4.2
1	C	81	ASN	4.2
1	F	860	GLN	4.2
1	E	92	LEU	4.2
1	F	128	SER	4.2
1	B	864	SER	4.2
1	E	928	THR	4.2
1	C	575	MET	4.1
1	C	576	VAL	4.1
1	F	867	GLN	4.1
1	F	653	ILE	4.1
1	D	67	GLN	4.1
1	D	401	ALA	4.1
1	F	69	MET	4.1
1	E	652	GLN	4.0
1	B	405	LEU	4.0
1	B	890	TRP	4.0
1	F	801	SER	4.0
1	C	658	VAL	4.0
1	B	801	SER	4.0
1	E	885	ALA	4.0
1	E	736	VAL	4.0
1	E	402	ILE	4.0
1	C	399	VAL	4.0
1	F	741	ILE	4.0
1	D	834	GLU	4.0
1	C	404	LEU	3.9
1	C	448	VAL	3.9
1	F	111	LEU	3.9
1	E	400	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	128	SER	3.9
1	D	724	ILE	3.9
1	C	834	GLU	3.9
1	F	44	THR	3.9
1	A	615	GLY	3.9
1	C	866	ASN	3.9
1	C	724	ILE	3.8
1	A	198	LEU	3.8
1	E	576	VAL	3.8
1	B	403	GLY	3.8
1	A	369	THR	3.8
1	C	446	ALA	3.8
1	F	716	LEU	3.8
1	B	658	VAL	3.8
1	F	502	LYS	3.8
1	B	89	GLN	3.8
1	A	92	LEU	3.7
1	B	830	LYS	3.7
1	B	314	GLU	3.7
1	E	80	SER	3.7
1	C	395	MET	3.7
1	E	441	ALA	3.7
1	A	368	PRO	3.7
1	C	388	PHE	3.7
1	E	883	LEU	3.7
1	F	704	HIS	3.7
1	E	724	ILE	3.7
1	F	443	VAL	3.7
1	D	459	PHE	3.6
1	D	11	PHE	3.6
1	B	162	MET	3.6
1	C	708	LEU	3.6
1	E	938	ILE	3.6
1	A	47	ALA	3.6
1	C	833	GLY	3.6
1	B	977	PHE	3.6
1	F	89	GLN	3.6
1	C	243	THR	3.6
1	F	79	SER	3.6
1	C	474	ILE	3.6
1	A	486	LEU	3.6
1	B	44	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	886	LEU	3.6
1	E	198	LEU	3.6
1	E	577	GLN	3.6
1	D	89	GLN	3.5
1	F	834	GLU	3.5
1	E	398	MET	3.5
1	F	936	ASN	3.5
1	D	405	LEU	3.5
1	C	676	ASP	3.5
1	F	441	ALA	3.5
1	F	932	LEU	3.5
1	F	863	LEU	3.5
1	A	444	GLY	3.5
1	B	407	ASP	3.5
1	C	867	GLN	3.5
1	A	796	PHE	3.5
1	F	778	PRO	3.4
1	E	300	LEU	3.4
1	F	726	ILE	3.4
1	F	198	LEU	3.4
1	F	864	SER	3.4
1	A	714	ASN	3.4
1	B	613	ASN	3.4
1	B	408	ASP	3.4
1	F	671	THR	3.4
1	A	802	SER	3.4
1	E	243	THR	3.4
1	F	724	ILE	3.4
1	C	716	LEU	3.3
1	C	164	ASP	3.3
1	B	46	SER	3.3
1	F	703	LYS	3.3
1	C	14	VAL	3.3
1	A	864	SER	3.3
1	F	175	VAL	3.3
1	B	406	VAL	3.3
1	F	977	PHE	3.3
1	F	43	VAL	3.2
1	B	486	LEU	3.2
1	E	32	VAL	3.2
1	F	65	ILE	3.2
1	E	162	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	484	VAL	3.2
1	C	68	ASN	3.2
1	B	246	PHE	3.2
1	C	400	LEU	3.2
1	F	577	GLN	3.2
1	A	399	VAL	3.2
1	D	246	PHE	3.2
1	E	177	LEU	3.2
1	E	164	ASP	3.2
1	F	13	TRP	3.2
1	F	163	LYS	3.2
1	D	796	PHE	3.2
1	A	847	PRO	3.1
1	A	372	VAL	3.1
1	E	290	GLY	3.1
1	F	879	VAL	3.1
1	A	164	ASP	3.1
1	F	654	LYS	3.1
1	A	355	MET	3.1
1	F	372	VAL	3.1
1	F	408	ASP	3.1
1	D	402	ILE	3.1
1	F	935	LYS	3.1
1	D	576	VAL	3.1
1	C	883	LEU	3.1
1	E	442	LEU	3.1
1	E	129	VAL	3.0
1	E	439	GLN	3.0
1	F	730	LYS	3.0
1	E	81	ASN	3.0
1	E	369	THR	3.0
1	D	46	SER	3.0
1	F	823	LEU	3.0
1	A	894	PHE	3.0
1	C	444	GLY	3.0
1	E	939	LEU	3.0
1	D	129	VAL	3.0
1	B	487	ILE	3.0
1	E	47	ALA	3.0
1	E	741	ILE	3.0
1	F	463	THR	3.0
1	F	658	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	881	LEU	3.0
1	F	178	PHE	2.9
1	A	246	PHE	2.9
1	B	931	GLY	2.9
1	B	934	ALA	2.9
1	F	890	TRP	2.9
1	B	177	LEU	2.9
1	E	65	ILE	2.9
1	F	576	VAL	2.9
1	D	45	ILE	2.9
1	A	410	ILE	2.9
1	E	932	LEU	2.9
1	B	243	THR	2.9
1	D	32	VAL	2.9
1	C	396	PHE	2.9
1	A	658	VAL	2.9
1	F	832	THR	2.9
1	A	485	ALA	2.9
1	E	575	MET	2.9
1	A	67	GLN	2.9
1	A	848	THR	2.9
1	C	823	LEU	2.9
1	B	577	GLN	2.9
1	F	709	THR	2.8
1	D	407	ASP	2.8
1	E	715	GLY	2.8
1	D	322	LYS	2.8
1	C	671	THR	2.8
1	A	35	TYR	2.8
1	D	741	ILE	2.8
1	A	90	ILE	2.8
1	C	828	PRO	2.8
1	F	796	PHE	2.8
1	B	710	SER	2.8
1	D	90	ILE	2.8
1	B	45	ILE	2.8
1	D	487	ILE	2.8
1	C	860	GLN	2.8
1	D	128	SER	2.8
1	F	410	ILE	2.8
1	A	43	VAL	2.8
1	F	488	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	933	SER	2.8
1	B	81	ASN	2.8
1	E	367	ILE	2.8
1	C	481	SER	2.8
1	B	736	VAL	2.8
1	F	825	GLN	2.8
1	C	310	LEU	2.8
1	F	652	GLN	2.8
1	C	835	ALA	2.8
1	B	973	THR	2.8
1	E	409	ALA	2.8
1	C	713	PRO	2.7
1	B	310	LEU	2.7
1	D	88	VAL	2.7
1	F	482	VAL	2.7
1	E	45	ILE	2.7
1	D	243	THR	2.7
1	D	713	PRO	2.7
1	D	164	ASP	2.7
1	C	778	PRO	2.7
1	D	832	THR	2.7
1	E	887	TYR	2.7
1	A	13	TRP	2.7
1	E	440	GLY	2.7
1	A	89	GLN	2.7
1	B	656	ALA	2.7
1	C	704	HIS	2.7
1	A	396	PHE	2.7
1	E	105	VAL	2.7
1	F	90	ILE	2.7
1	C	442	LEU	2.7
1	D	714	ASN	2.7
1	D	442	LEU	2.7
1	E	483	LEU	2.7
1	F	802	SER	2.7
1	C	820	MET	2.7
1	A	397	GLY	2.7
1	E	487	ILE	2.7
1	F	824	GLY	2.7
1	C	13	TRP	2.7
1	B	439	GLN	2.7
1	F	835	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	977	PHE	2.7
1	E	246	PHE	2.7
1	C	129	VAL	2.6
1	D	59	ASP	2.6
1	A	448	VAL	2.6
1	D	861	GLU	2.6
1	D	575	MET	2.6
1	D	390	ILE	2.6
1	B	799	PHE	2.6
1	D	867	GLN	2.6
1	A	46	SER	2.6
1	E	89	GLN	2.6
1	B	443	VAL	2.6
1	E	444	GLY	2.6
1	C	166	ILE	2.6
1	C	741	ILE	2.6
1	D	778	PRO	2.6
1	B	80	SER	2.6
1	B	488	LEU	2.6
1	C	65	ILE	2.6
1	E	934	ALA	2.6
1	F	928	THR	2.6
1	B	311	ALA	2.6
1	C	754	VAL	2.6
1	C	868	ALA	2.6
1	E	884	ALA	2.6
1	B	47	ALA	2.6
1	D	461	GLY	2.6
1	F	710	SER	2.6
1	A	69	MET	2.5
1	B	894	PHE	2.5
1	F	45	ILE	2.5
1	A	443	VAL	2.5
1	C	91	THR	2.5
1	E	973	THR	2.5
1	E	175	VAL	2.5
1	A	376	LEU	2.5
1	D	382	VAL	2.5
1	B	730	LYS	2.5
1	E	69	MET	2.5
1	A	48	SER	2.5
1	A	724	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	777	LEU	2.5
1	D	81	ASN	2.5
1	B	591	LEU	2.5
1	E	778	PRO	2.5
1	C	117	LEU	2.5
1	E	242	SER	2.5
1	C	887	TYR	2.5
1	A	70	ASN	2.5
1	C	863	LEU	2.5
1	E	370	ILE	2.5
1	C	784	TRP	2.5
1	D	890	TRP	2.5
1	A	880	PHE	2.5
1	F	9	PRO	2.5
1	E	445	ILE	2.5
1	F	798	ALA	2.5
1	E	781	ILE	2.4
1	F	477	ALA	2.4
1	E	43	VAL	2.4
1	B	576	VAL	2.4
1	B	831	SER	2.4
1	E	802	SER	2.4
1	F	242	SER	2.4
1	A	244	GLU	2.4
1	D	219	LEU	2.4
1	B	300	LEU	2.4
1	E	896	VAL	2.4
1	F	244	GLU	2.4
1	A	323	ILE	2.4
1	F	826	ALA	2.4
1	B	240	LEU	2.4
1	C	712	ARG	2.4
1	F	127	VAL	2.4
1	E	176	GLN	2.4
1	E	882	CYS	2.4
1	A	722	PHE	2.4
1	E	44	THR	2.4
1	B	401	ALA	2.4
1	F	876	LEU	2.4
1	E	244	GLU	2.4
1	D	408	ASP	2.4
1	B	865	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	243	THR	2.4
1	A	881	LEU	2.4
1	F	736	VAL	2.4
1	F	742	ASN	2.4
1	C	219	LEU	2.4
1	E	722	PHE	2.4
1	C	800	SER	2.4
1	F	713	PRO	2.4
1	F	91	THR	2.4
1	E	713	PRO	2.3
1	F	485	ALA	2.3
1	B	90	ILE	2.3
1	D	178	PHE	2.3
1	E	651	SER	2.3
1	A	741	ILE	2.3
1	B	932	LEU	2.3
1	C	932	LEU	2.3
1	B	796	PHE	2.3
1	C	322	LYS	2.3
1	E	312	LYS	2.3
1	E	104	GLN	2.3
1	D	92	LEU	2.3
1	C	703	LYS	2.3
1	C	711	VAL	2.3
1	C	851	GLY	2.3
1	F	396	PHE	2.3
1	E	810	ARG	2.3
1	B	244	GLU	2.3
1	E	716	LEU	2.3
1	B	441	ALA	2.3
1	B	657	MET	2.3
1	D	620	GLY	2.3
1	F	702	ALA	2.3
1	D	399	VAL	2.3
1	E	210	GLN	2.3
1	A	675	PHE	2.3
1	E	786	VAL	2.3
1	B	43	VAL	2.3
1	F	129	VAL	2.3
1	B	778	PRO	2.3
1	C	936	ASN	2.3
1	C	323	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	166	ILE	2.3
1	E	796	PHE	2.3
1	E	348	ILE	2.2
1	E	447	MET	2.2
1	B	834	GLU	2.2
1	F	734	LEU	2.2
1	A	371	ALA	2.2
1	C	371	ALA	2.2
1	B	737	SER	2.2
1	E	615	GLY	2.2
1	B	447	MET	2.2
1	C	9	PRO	2.2
1	D	462	SER	2.2
1	C	111	LEU	2.2
1	A	973	THR	2.2
1	E	935	LYS	2.2
1	C	824	GLY	2.2
1	E	682	GLN	2.2
1	F	804	TRP	2.2
1	E	821	GLU	2.2
1	B	728	GLN	2.2
1	B	166	ILE	2.2
1	F	376	LEU	2.2
1	F	887	TYR	2.2
1	A	199	THR	2.2
1	C	796	PHE	2.2
1	A	558	ARG	2.2
1	B	92	LEU	2.2
1	E	91	THR	2.2
1	D	880	PHE	2.2
1	A	129	VAL	2.1
1	E	48	SER	2.1
1	F	786	VAL	2.1
1	E	102	ILE	2.1
1	F	675	PHE	2.1
1	F	615	GLY	2.1
1	B	836	MET	2.1
1	A	749	TRP	2.1
1	B	724	ILE	2.1
1	B	935	LYS	2.1
1	C	478	MET	2.1
1	C	705	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	785	TYR	2.1
1	B	654	LYS	2.1
1	B	714	ASN	2.1
1	D	389	SER	2.1
1	C	32	VAL	2.1
1	E	355	MET	2.1
1	F	705	PRO	2.1
1	D	396	PHE	2.1
1	D	195	LYS	2.1
1	F	866	ASN	2.1
1	D	323	ILE	2.1
1	D	615	GLY	2.1
1	E	229	GLN	2.1
1	E	484	VAL	2.1
1	B	726	ILE	2.1
1	E	936	ASN	2.1
1	A	489	THR	2.1
1	D	740	ASP	2.1
1	F	744	THR	2.1
1	A	127	VAL	2.1
1	D	977	PHE	2.1
1	B	777	LEU	2.1
1	A	801	SER	2.1
1	B	442	LEU	2.1
1	D	449	LEU	2.1
1	A	977	PHE	2.1
1	E	268	ILE	2.1
1	E	325	TYR	2.1
1	D	829	GLY	2.1
1	F	558	ARG	2.1
1	E	106	GLN	2.1
1	D	388	PHE	2.1
1	F	462	SER	2.0
1	B	938	ILE	2.0
1	A	230	LEU	2.0
1	B	866	ASN	2.0
1	D	685	LEU	2.0
1	E	79	SER	2.0
1	F	162	MET	2.0
1	A	576	VAL	2.0
1	D	932	LEU	2.0
1	F	452	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	799	PHE	2.0
1	F	676	ASP	2.0
1	A	210	GLN	2.0
1	B	653	ILE	2.0
1	F	613	ASN	2.0
1	C	812	GLU	2.0
1	E	71	GLY	2.0
1	D	65	ILE	2.0
1	D	658	VAL	2.0
1	F	797	SER	2.0
1	A	45	ILE	2.0
1	E	87	THR	2.0
1	A	310	LEU	2.0
1	D	444	GLY	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.

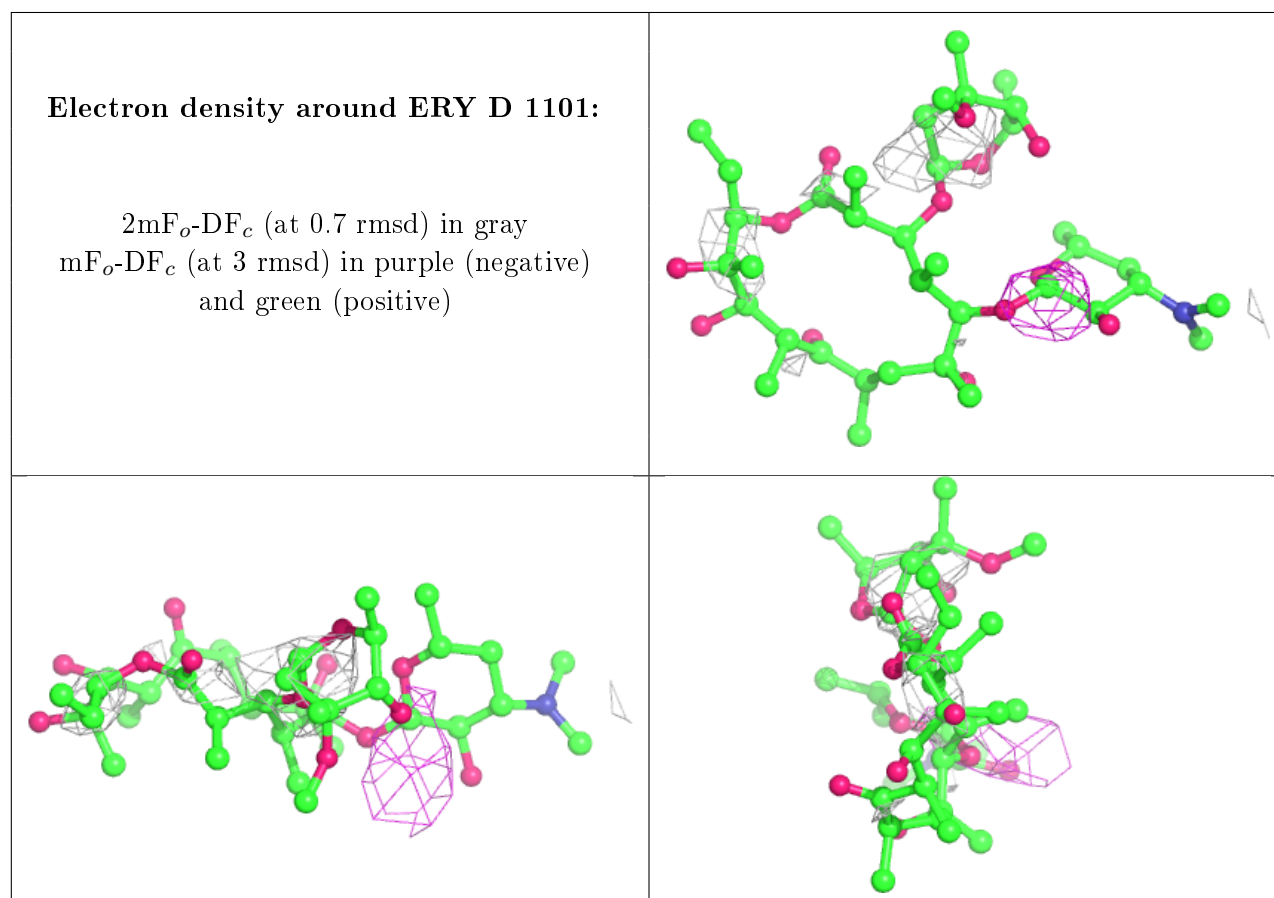
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ERY	D	1101	51/51	0.68	1.24	62,93,101,108	51
3	LMT	D	1103	35/35	0.73	0.41	77,92,105,106	0
3	LMT	D	1102	35/35	0.76	0.43	38,74,82,84	0
3	LMT	F	2100	35/35	0.77	0.51	49,75,87,96	0
2	ERY	A	1101	51/51	0.77	1.26	81,93,101,104	51
3	LMT	A	1102	35/35	0.79	0.41	49,70,79,82	0
3	LMT	C	1101	35/35	0.79	0.41	62,75,83,87	0
3	LMT	B	2100	35/35	0.79	0.48	34,66,78,87	0
3	LMT	E	1101	35/35	0.80	0.45	63,72,86,108	0

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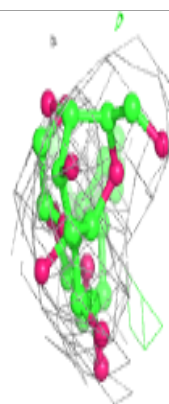
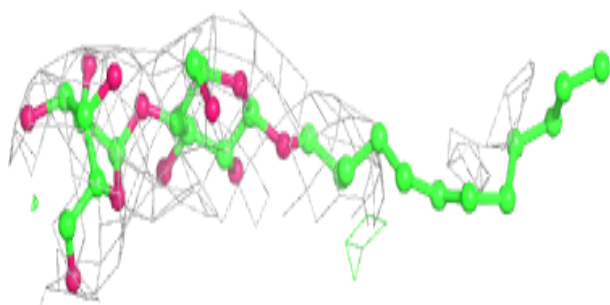
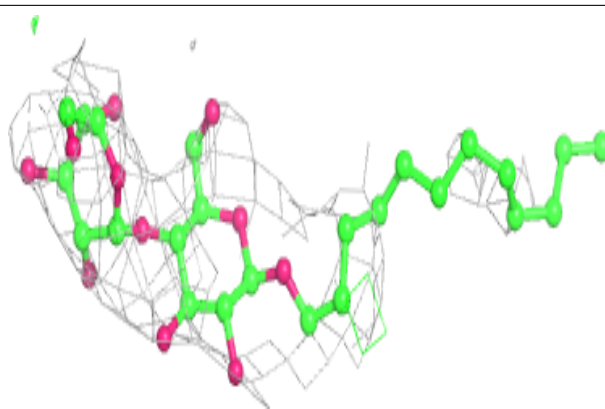
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LMT	A	1103	35/35	0.85	0.80	65,90,106,109	0
4	NI	C	1102	1/1	0.99	0.21	77,77,77,77	0
4	NI	A	1104	1/1	0.99	0.21	67,67,67,67	0
4	NI	E	1102	1/1	0.99	0.21	73,73,73,73	0

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.

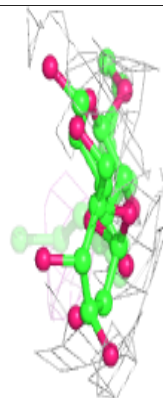
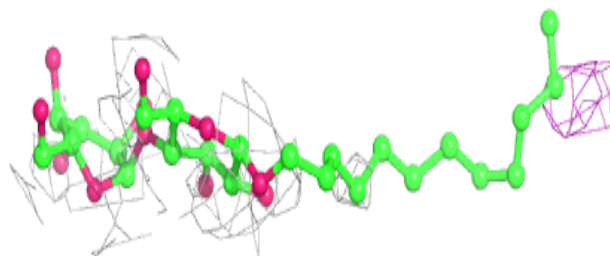
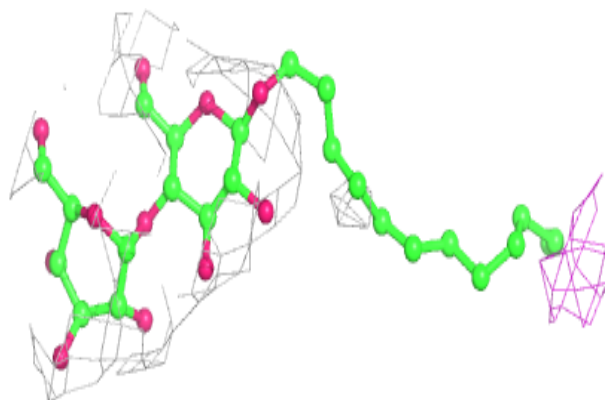


**Electron density around LMT D 1103:**

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

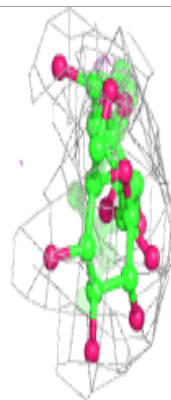
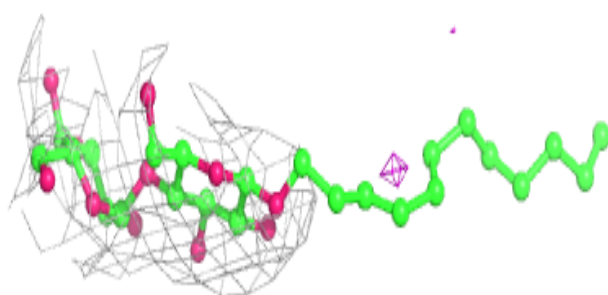
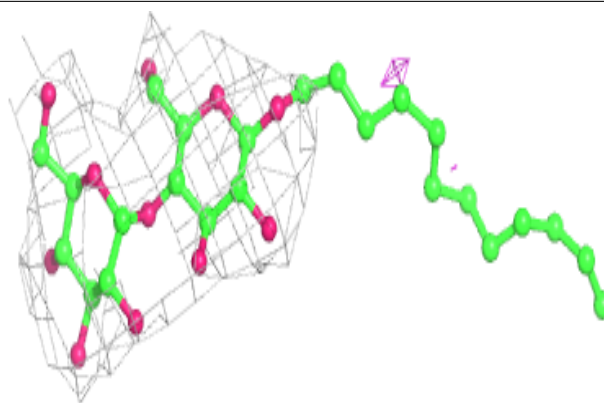
**Electron density around LMT D 1102:**

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

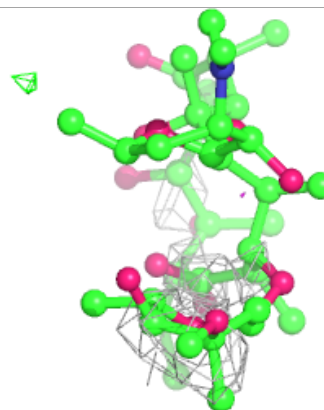
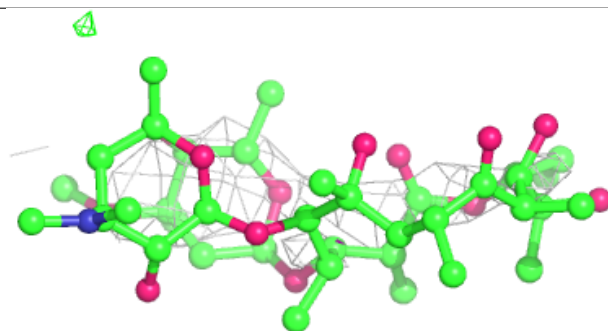
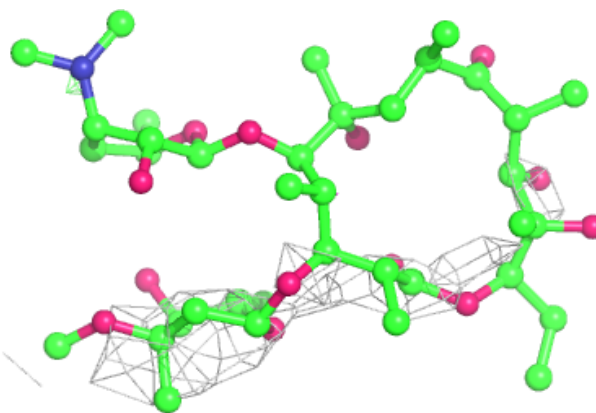


**Electron density around LMT F 2100:**

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

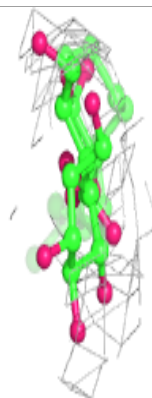
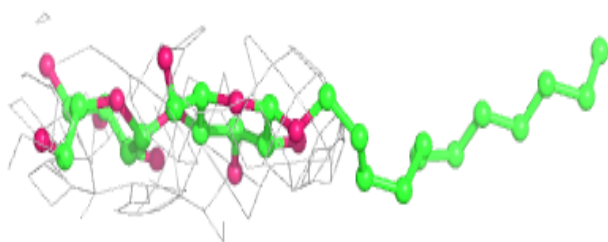
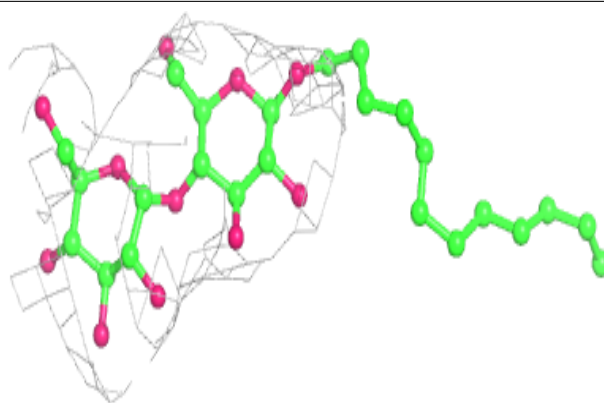
**Electron density around ERY A 1101:**

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

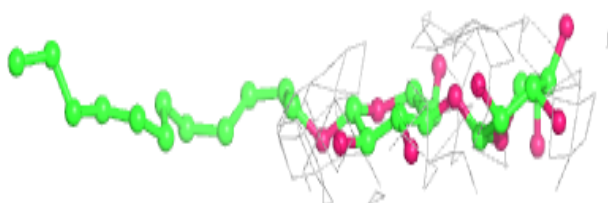
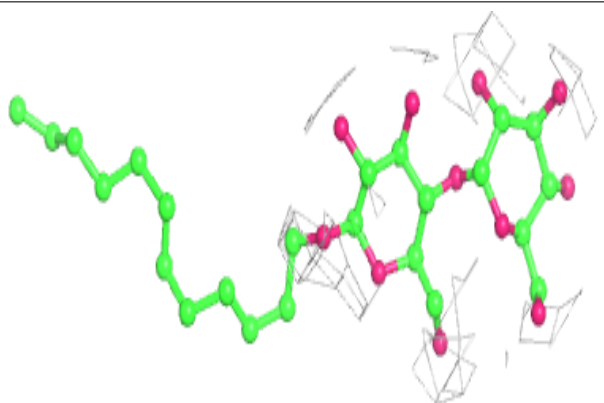


**Electron density around LMT A 1102:**

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

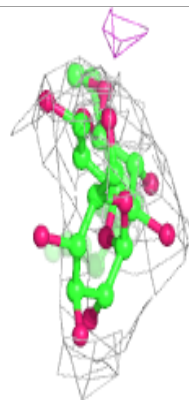
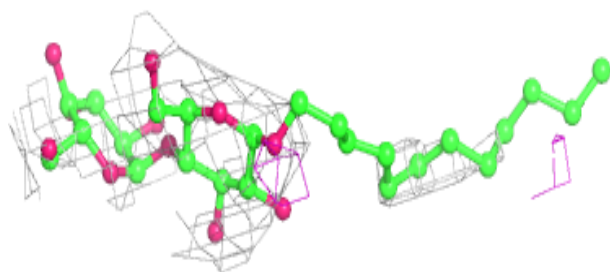
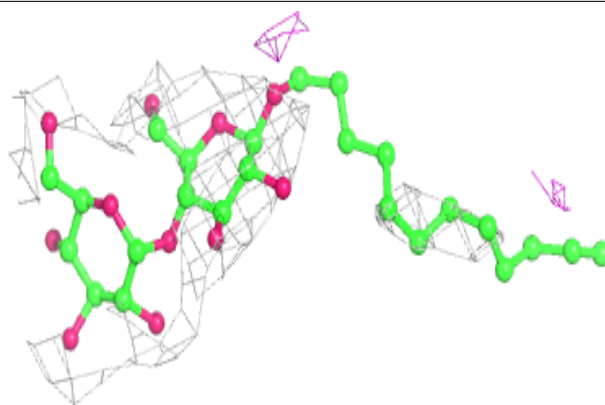
**Electron density around LMT C 1101:**

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

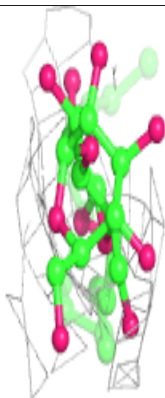
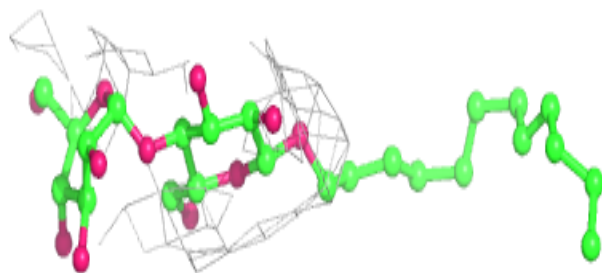
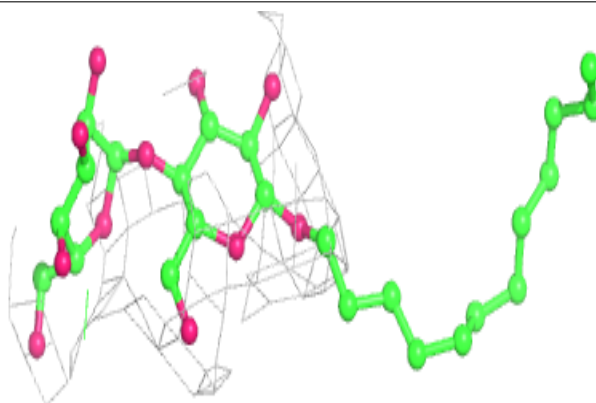


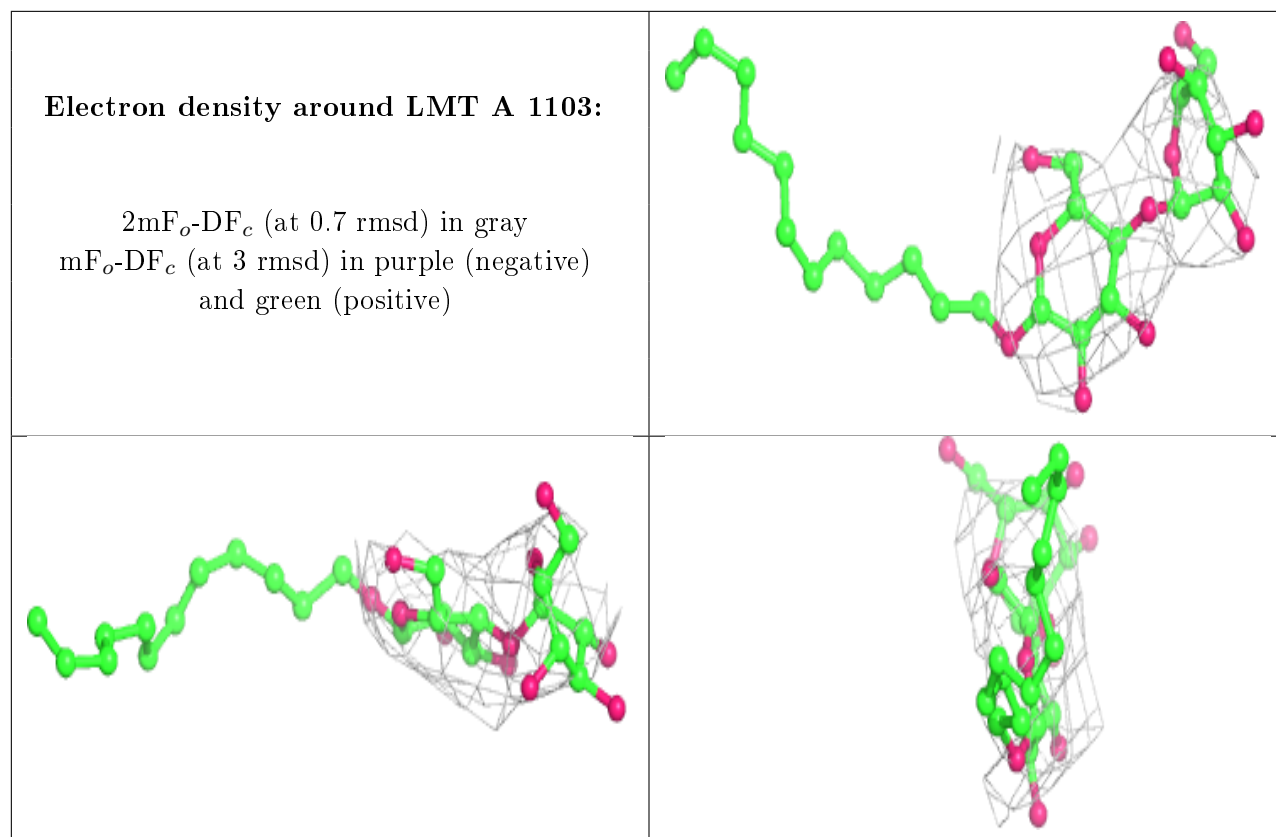
**Electron density around LMT B 2100:**

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

**Electron density around LMT E 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.