



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:58 pm BST

PDB ID : 4ZJO
Title : Crystal structure of AcrB triple mutant in complex with antibiotic in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-29
Resolution : 3.60 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (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

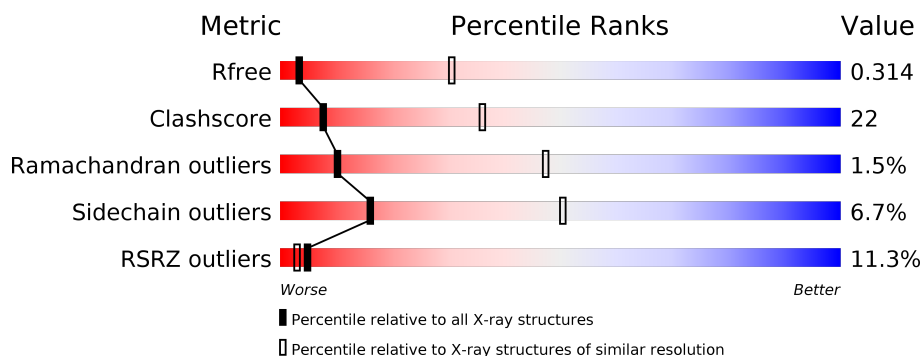
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1049	<div> <div>9%</div> <div>53%</div> <div>41%</div> <div>• •</div> </div>
1	B	1049	<div> <div>7%</div> <div>56%</div> <div>39%</div> <div>• •</div> </div>
1	C	1049	<div> <div>12%</div> <div>52%</div> <div>42%</div> <div>5% •</div> </div>
1	D	1049	<div> <div>12%</div> <div>55%</div> <div>39%</div> <div>5% •</div> </div>
1	E	1049	<div> <div>14%</div> <div>54%</div> <div>41%</div> <div>• •</div> </div>
1	F	1049	<div> <div>14%</div> <div>54%</div> <div>41%</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	B	1101	X	-	-	-
3	LMT	D	1103	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 47876 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	B	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	C	1044	Total	C	N	O	S	0	0	0
			7924	5090	1312	1479	43			
1	D	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	F	1046	Total	C	N	O	S	0	0	0
			7939	5099	1314	1483	43			

There are 18 discrepancies between the modelled and reference sequences:

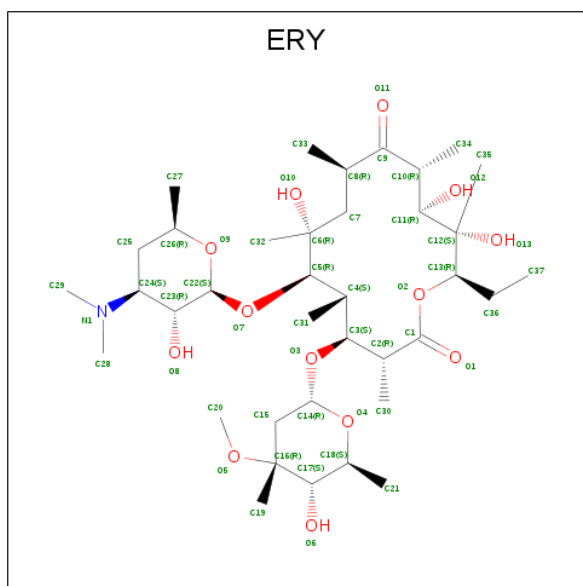
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	ALA	PHE	engineered mutation	UNP P31224
A	617	ALA	PHE	engineered mutation	UNP P31224
A	620	ALA	ARG	engineered mutation	UNP P31224
B	615	ALA	PHE	engineered mutation	UNP P31224
B	617	ALA	PHE	engineered mutation	UNP P31224
B	620	ALA	ARG	engineered mutation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

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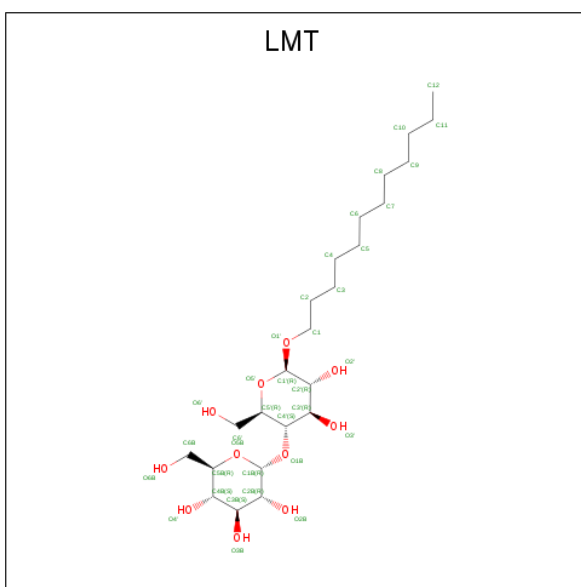
Chain	Residue	Modelled	Actual	Comment	Reference
F	620	ALA	ARG	engineered mutation	UNP P31224

- Molecule 2 is 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-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

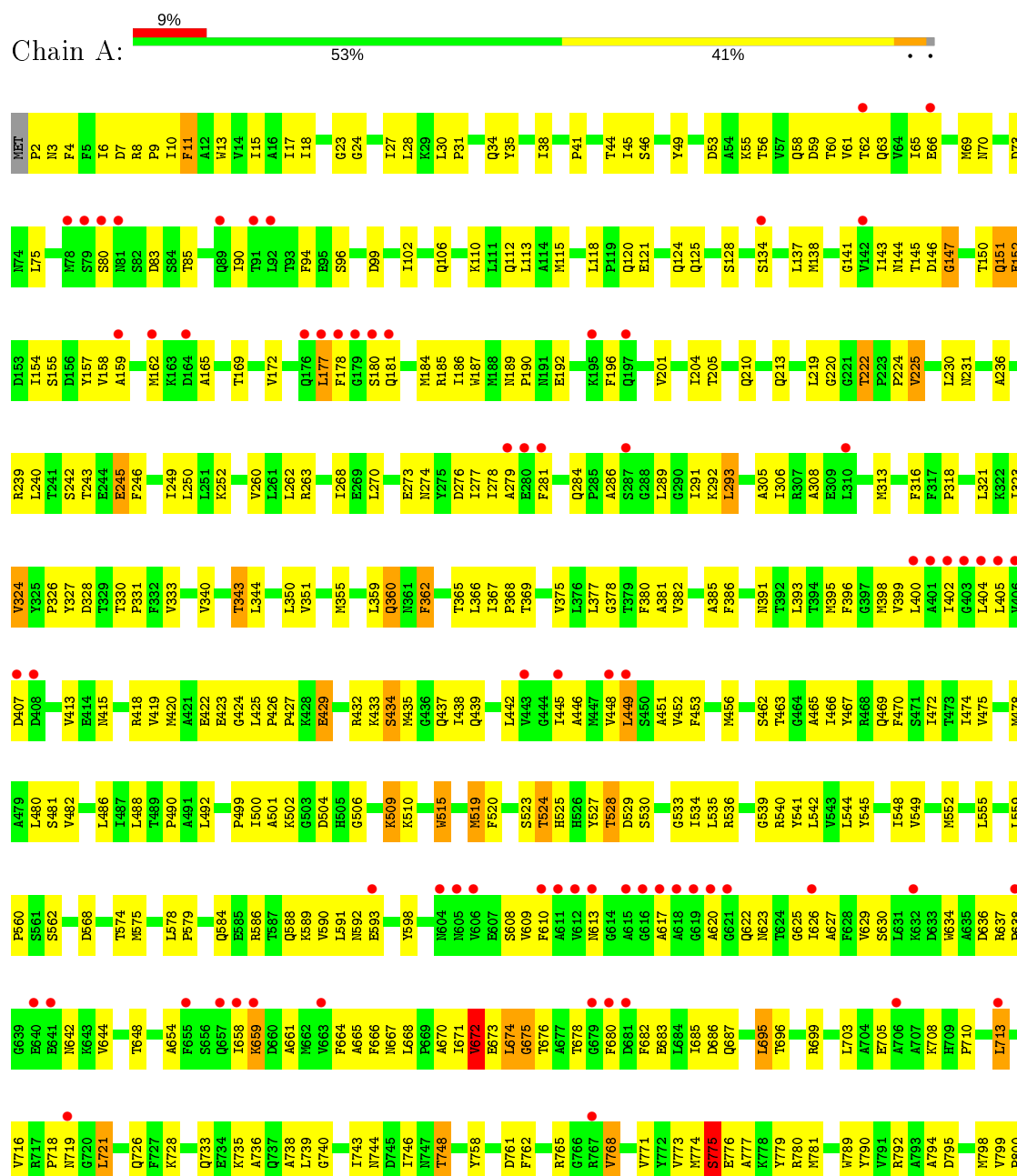
- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

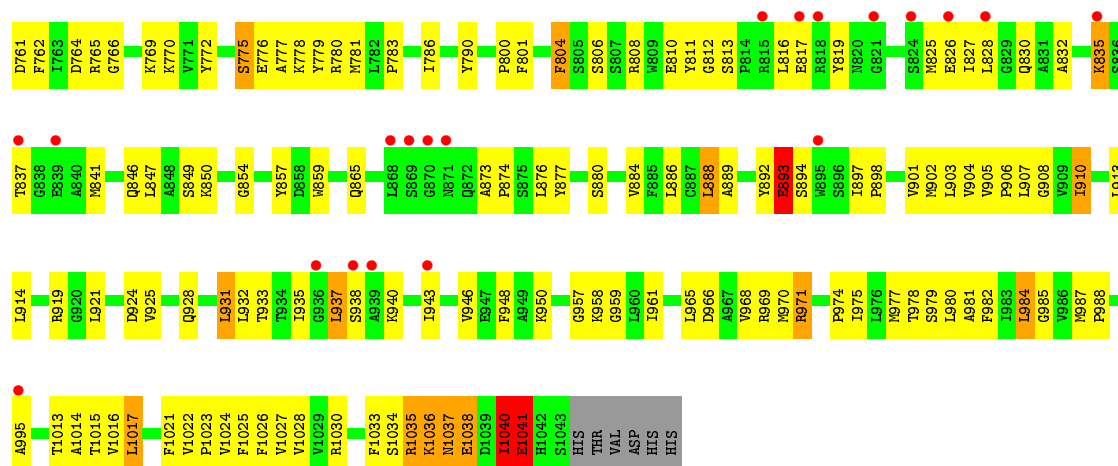
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

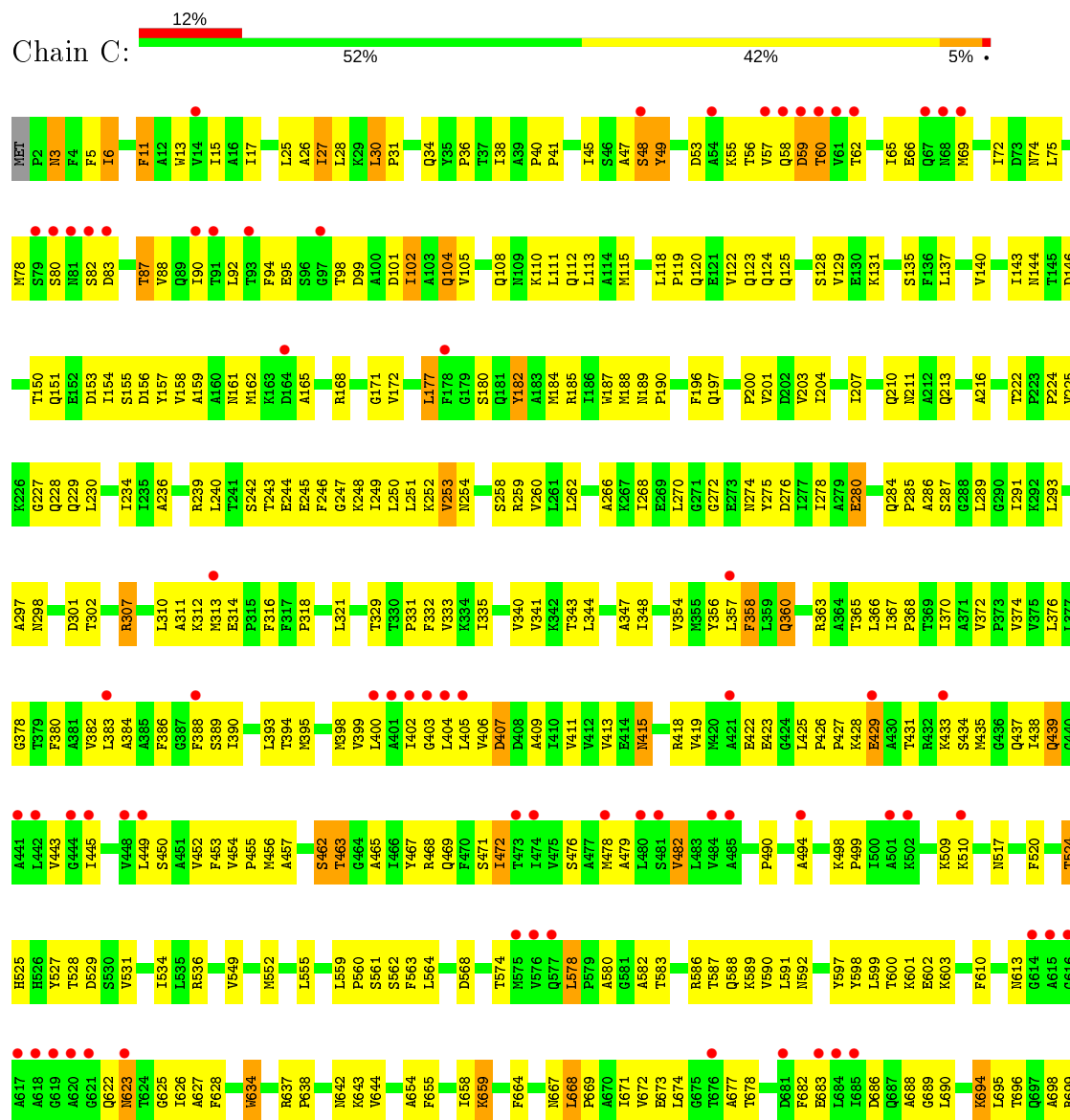
- Molecule 1: Multidrug efflux pump subunit AcrB

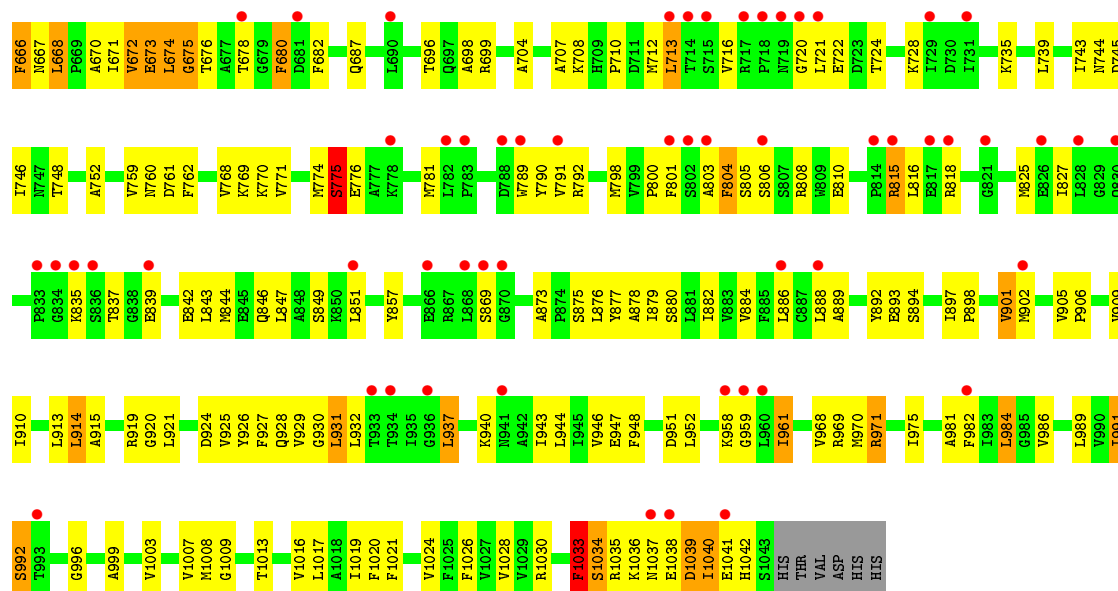




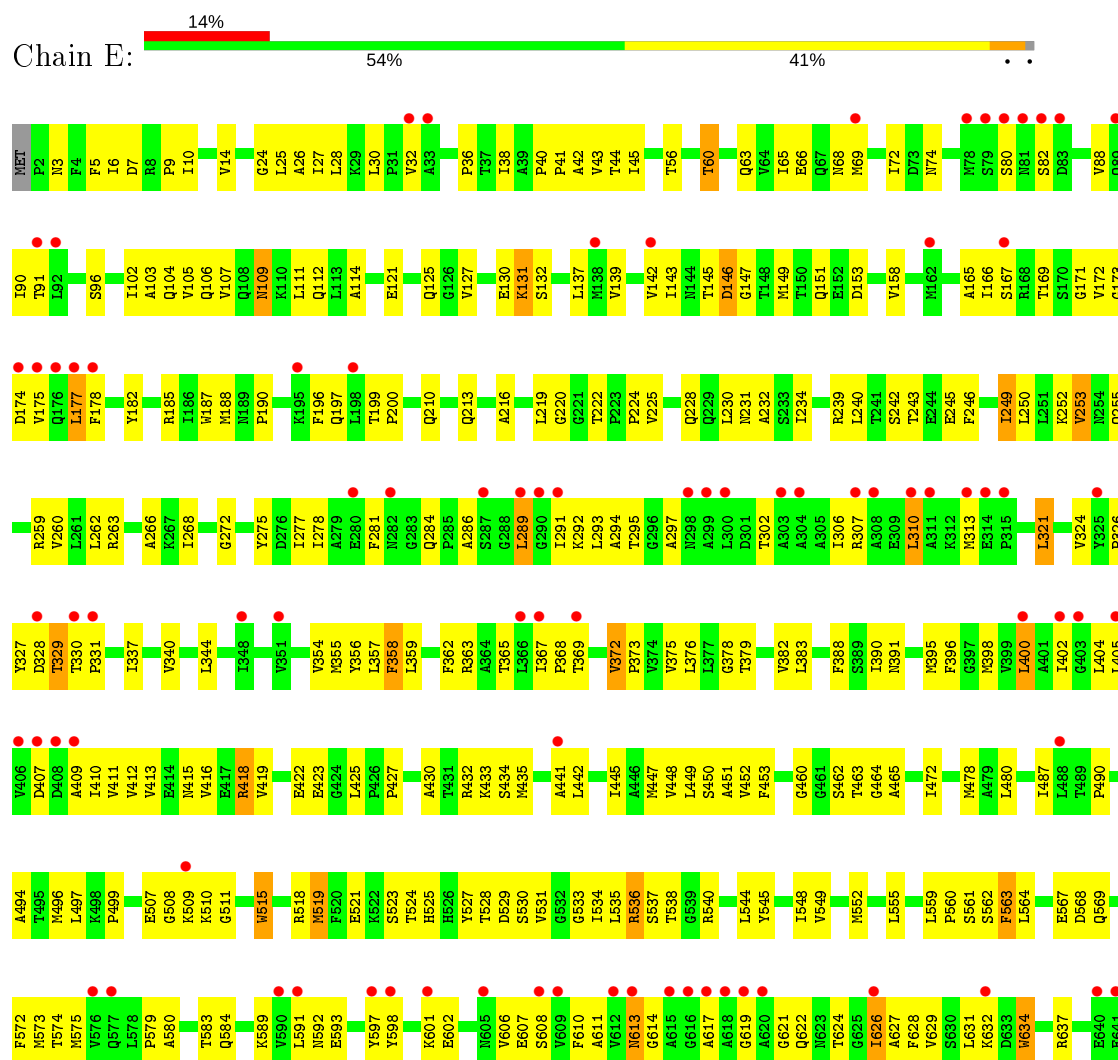


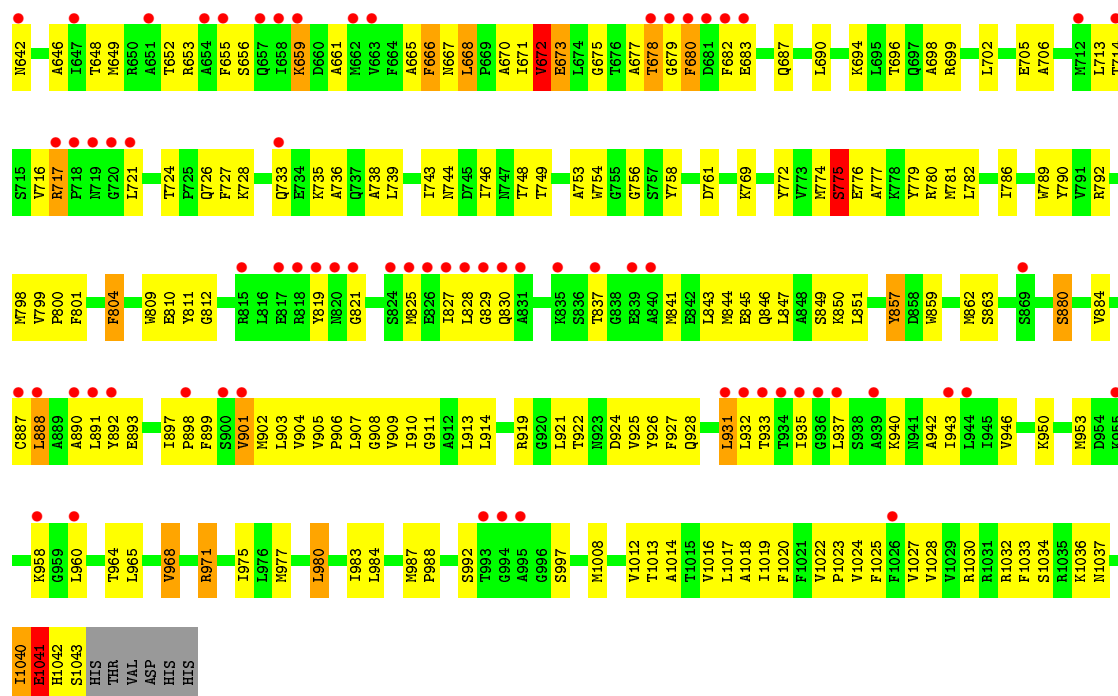
• Molecule 1: Multidrug efflux pump subunit AcrB





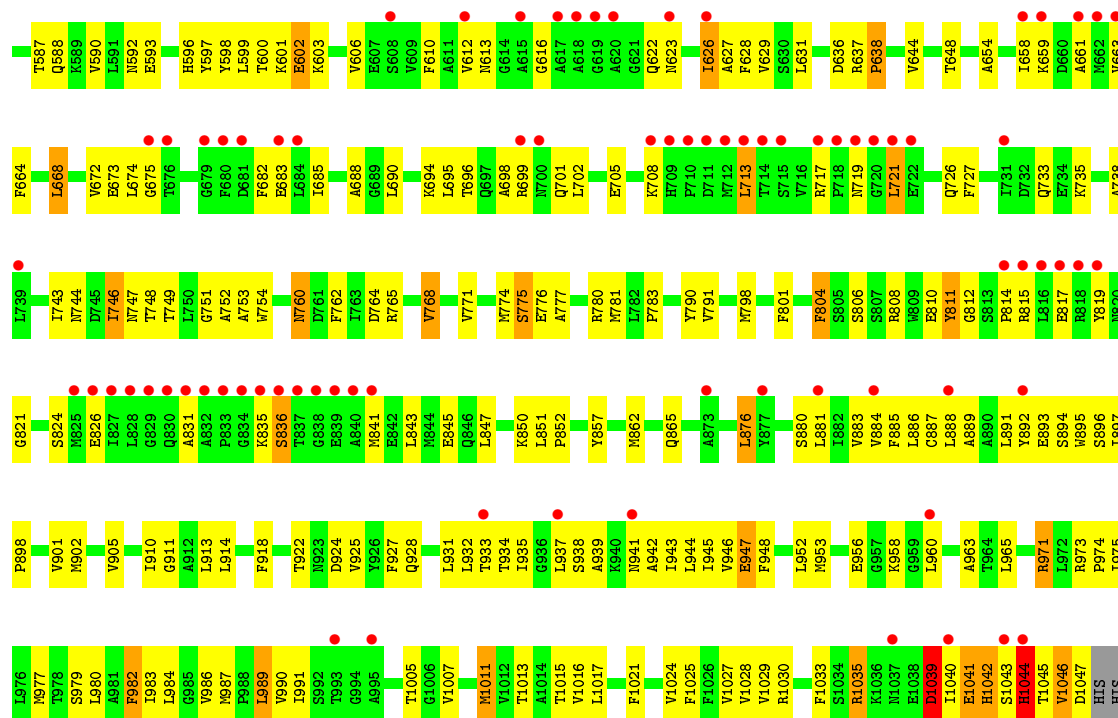
- Molecule 1: Multidrug efflux pump subunit AcrB





- Molecule 1: Multidrug efflux pump subunit AcrB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.18Å 156.77Å 218.17Å 90.00° 93.09° 90.00°	Depositor
Resolution (Å)	19.96 – 3.60 108.93 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.96-3.60) 97.1 (108.93-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.238 , 0.307 0.248 , 0.314	Depositor DCC
R_{free} test set	5867 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	101.0	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	47876	wwPDB-VP
Average B, all atoms (Å ²)	88.0	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 41.84 % 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 2.2263e-04.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1/8056 (0.0%)	0.81	5/10940 (0.0%)
1	B	0.59	0/8056	0.81	9/10940 (0.1%)
1	C	0.58	1/8074 (0.0%)	0.84	11/10965 (0.1%)
1	D	0.55	1/8056 (0.0%)	0.80	9/10940 (0.1%)
1	E	0.56	1/8056 (0.0%)	0.80	7/10940 (0.1%)
1	F	0.57	0/8089	0.83	6/10986 (0.1%)
All	All	0.57	4/48387 (0.0%)	0.82	47/65711 (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	2
1	C	0	1
1	D	0	1
1	F	0	2
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	TRP	CB-CG	7.98	1.64	1.50
1	E	515	TRP	CB-CG	7.12	1.63	1.50
1	D	515	TRP	CB-CG	6.65	1.62	1.50
1	C	895	TRP	CB-CG	-5.62	1.40	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	529	ASP	CB-CG-OD1	11.89	129.00	118.30
1	B	529	ASP	CB-CG-OD1	11.82	128.94	118.30
1	C	529	ASP	CB-CG-OD1	9.63	126.97	118.30
1	B	293	LEU	CA-CB-CG	8.59	135.06	115.30
1	A	529	ASP	CB-CG-OD1	8.09	125.58	118.30
1	F	529	ASP	CB-CG-OD2	-7.38	111.65	118.30
1	E	529	ASP	CB-CG-OD1	7.24	124.81	118.30
1	C	944	LEU	CA-CB-CG	7.22	131.90	115.30
1	C	30	LEU	CA-CB-CG	7.11	131.64	115.30
1	A	675	GLY	N-CA-C	6.98	130.56	113.10
1	D	529	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	449	LEU	CA-CB-CG	6.78	130.90	115.30
1	D	377	LEU	CB-CG-CD2	-6.70	99.60	111.00
1	B	937	LEU	CA-CB-CG	-6.66	99.99	115.30
1	B	1017	LEU	CA-CB-CG	6.63	130.56	115.30
1	C	1041	GLU	N-CA-C	-6.36	93.83	111.00
1	D	483	LEU	CA-CB-CG	6.30	129.80	115.30
1	C	937	LEU	CA-CB-CG	-6.24	100.94	115.30
1	E	359	LEU	CA-CB-CG	6.13	129.41	115.30
1	D	1033	PHE	N-CA-C	-6.13	94.45	111.00
1	C	400	LEU	CA-CB-CG	6.08	129.29	115.30
1	B	350	LEU	CA-CB-CG	-6.06	101.36	115.30
1	B	359	LEU	CA-CB-CG	5.84	128.72	115.30
1	E	1041	GLU	C-N-CA	5.80	136.21	121.70
1	D	519	MET	CB-CG-SD	5.70	129.51	112.40
1	B	529	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	E	289	LEU	CA-CB-CG	-5.62	102.38	115.30
1	B	888	LEU	CA-CB-CG	-5.60	102.43	115.30
1	C	713	LEU	CA-CB-CG	5.58	128.13	115.30
1	F	847	LEU	CA-CB-CG	5.57	128.12	115.30
1	E	519	MET	CB-CG-SD	5.56	129.09	112.40
1	A	519	MET	CB-CG-SD	5.56	129.09	112.40
1	B	893	GLU	N-CA-C	-5.44	96.32	111.00
1	F	989	LEU	CA-CB-CG	5.40	127.71	115.30
1	E	293	LEU	CA-CB-CG	5.32	127.54	115.30
1	D	511	GLY	N-CA-C	5.31	126.38	113.10
1	E	888	LEU	CA-CB-CG	-5.31	103.09	115.30
1	F	92	LEU	CA-CB-CG	5.28	127.45	115.30
1	D	937	LEU	CA-CB-CG	-5.26	103.20	115.30
1	D	675	GLY	N-CA-C	5.21	126.14	113.10
1	C	529	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	F	357	LEU	CA-CB-CG	5.19	127.23	115.30
1	C	702	LEU	CA-CB-CG	5.13	127.10	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1041	GLU	C-N-CA	5.11	134.46	121.70
1	A	972	LEU	CA-CB-CG	5.10	127.03	115.30
1	D	720	GLY	N-CA-C	-5.09	100.38	113.10
1	C	1041	GLU	CA-C-N	5.02	128.24	117.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1033	PHE	Peptide
1	B	1036	LYS	Peptide
1	B	1040	ILE	Peptide
1	C	1036	LYS	Peptide
1	D	1033	PHE	Peptide
1	F	1039	ASP	Peptide
1	F	1041	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7907	0	8050	386	0
1	B	7907	0	8050	338	0
1	C	7924	0	8064	394	1
1	D	7907	0	8050	344	1
1	E	7907	0	8050	345	0
1	F	7939	0	8077	376	0
2	A	51	0	67	10	0
2	D	51	0	67	5	0
3	A	70	0	92	5	0
3	B	35	0	46	5	0
3	C	35	0	46	1	0
3	D	70	0	92	9	0
3	E	35	0	46	3	0
3	F	35	0	46	5	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
All	All	47876	0	48843	2113	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (2113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:SER:OG	3:A:1102:LMT:O2'	1.59	1.15
1:A:427:PRO:HD3	1:A:499:PRO:HB3	1.41	1.03
1:C:831:ALA:HB3	1:C:835:LYS:HG3	1.42	0.98
1:E:340:VAL:HG21	1:E:395:MET:HB3	1.46	0.98
1:A:144:ASN:O	1:A:284:GLN:NE2	2.01	0.94
1:D:196:PHE:O	1:D:252:LYS:NZ	2.01	0.94
1:C:808:ARG:NH1	1:C:810:GLU:OE2	2.00	0.93
1:A:971:ARG:HG2	1:A:974:PRO:HG2	1.50	0.93
1:A:781:MET:HE1	1:C:225:VAL:H	1.33	0.93
1:D:618:ALA:O	1:D:815:ARG:NH2	2.01	0.93
1:F:1040:ILE:HA	1:F:1041:GLU:HB2	1.48	0.92
1:D:225:VAL:H	1:E:781:MET:HE1	1.35	0.92
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.50	0.92
1:E:196:PHE:O	1:E:252:LYS:NZ	2.02	0.92
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.52	0.91
1:D:564:LEU:HB2	1:D:671:ILE:HD11	1.51	0.91
1:C:894:SER:HB3	1:C:897:ILE:HG12	1.53	0.90
1:B:350:LEU:HD13	1:B:984:LEU:HB3	1.53	0.89
1:F:298:ASN:ND2	1:F:301:ASP:OD2	2.05	0.89
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.55	0.88
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.55	0.88
1:F:831:ALA:HB3	1:F:835:LYS:HG3	1.53	0.88
1:F:363:ARG:HH21	1:F:498:LYS:HD2	1.36	0.87
1:E:593:GLU:OE1	1:E:659:LYS:NZ	2.06	0.87
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.08	0.87
1:D:144:ASN:O	1:D:284:GLN:NE2	2.08	0.86
1:F:941:ASN:HD21	1:F:1015:THR:HG22	1.40	0.86
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.08	0.86
1:C:40:PRO:HD2	1:C:674:LEU:HD21	1.55	0.85
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.59	0.85
1:B:196:PHE:O	1:B:252:LYS:NZ	2.10	0.84
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:TRP:O	1:A:519:MET:HG3	1.79	0.83
1:C:1039:ASP:HB3	1:C:1040:ILE:HA	1.59	0.83
1:B:668:LEU:HD23	1:B:668:LEU:H	1.42	0.82
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.60	0.82
1:C:578:LEU:HG	1:C:587:THR:HG22	1.60	0.82
1:E:3:ASN:HA	1:E:6:ILE:HD12	1.62	0.82
1:B:3:ASN:HA	1:B:6:ILE:HD12	1.60	0.81
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.62	0.81
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.60	0.81
1:B:101:ASP:OD1	1:B:131:LYS:NZ	2.12	0.81
1:A:134:SER:OG	2:A:1101:ERY:H323	1.80	0.81
1:D:228:GLN:NE2	1:D:230:LEU:O	2.14	0.80
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.11	0.80
1:F:383:LEU:HD23	1:F:472:ILE:HD13	1.63	0.80
1:C:210:GLN:HE22	1:C:250:LEU:HB3	1.45	0.80
1:E:415:ASN:OD1	1:E:418:ARG:NH1	2.13	0.80
1:A:579:PRO:HD3	1:A:661:ALA:HB2	1.64	0.80
1:B:383:LEU:HD21	1:B:473:THR:HA	1.64	0.80
1:A:931:LEU:HD13	3:A:1103:LMT:H42	1.62	0.79
1:A:562:SER:HB2	1:A:924:ASP:HB3	1.64	0.79
1:B:56:THR:O	1:B:60:THR:OG1	2.00	0.79
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.63	0.79
1:F:892:TYR:O	1:F:894:SER:N	2.14	0.78
1:D:236:ALA:O	1:E:728:LYS:NZ	2.17	0.78
1:D:213:GLN:HG2	1:D:239:ARG:HG2	1.65	0.78
1:A:879:ILE:HD13	1:C:25:LEU:HD21	1.63	0.78
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.66	0.78
1:D:244:GLU:HG2	1:D:248:LYS:HE2	1.64	0.78
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.66	0.78
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.47	0.78
1:A:696:THR:HG23	1:A:699:ARG:HH12	1.47	0.78
1:E:451:ALA:O	1:E:880:SER:OG	2.01	0.78
1:F:509:LYS:HB3	1:F:514:GLY:HA3	1.64	0.78
1:C:222:THR:HA	1:C:224:PRO:HD3	1.67	0.77
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.67	0.77
1:E:680:PHE:HD1	1:E:859:TRP:HZ3	1.31	0.77
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.65	0.77
1:C:428:LYS:HG2	1:C:494:ALA:HB1	1.67	0.77
1:D:225:VAL:HG12	1:E:777:ALA:HB1	1.66	0.77
1:D:137:LEU:HD22	1:D:293:LEU:HG	1.67	0.77
1:A:225:VAL:H	1:B:781:MET:HE1	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:GLY:O	1:B:510:LYS:N	2.15	0.76
1:D:800:PRO:HG2	1:D:803:ALA:HB2	1.66	0.76
1:A:637:ARG:NH1	1:A:642:ASN:O	2.18	0.76
1:A:186:ILE:HB	1:A:773:VAL:HG22	1.65	0.76
1:C:274:ASN:ND2	1:C:276:ASP:OD2	2.19	0.76
1:F:462:SER:HB3	1:F:865:GLN:HG2	1.67	0.76
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.66	0.75
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.68	0.75
1:D:562:SER:HB2	1:D:924:ASP:HB3	1.68	0.75
1:A:225:VAL:HG12	1:B:777:ALA:HB1	1.68	0.75
1:E:222:THR:HA	1:E:224:PRO:HD3	1.67	0.75
1:B:775:SER:OG	1:B:776:GLU:O	2.05	0.74
1:C:945:ILE:HA	1:C:971:ARG:HH12	1.53	0.74
1:E:7:ASP:OD1	1:E:432:ARG:NH2	2.19	0.74
1:F:683:GLU:HG2	1:F:819:TYR:CD2	2.22	0.74
1:B:511:GLY:HA2	1:B:515:TRP:HE1	1.53	0.74
1:F:610:PHE:HB3	1:F:628:PHE:HB2	1.69	0.74
1:A:34:GLN:HB2	1:A:333:VAL:HG22	1.70	0.74
1:C:418:ARG:O	1:C:422:GLU:HB2	1.88	0.74
1:D:405:LEU:HD22	1:D:481:SER:HB3	1.69	0.74
1:D:901:VAL:HG21	1:D:943:ILE:HG13	1.68	0.74
1:E:733:GLN:HE22	1:E:743:ILE:HG21	1.53	0.74
1:B:901:VAL:HG21	1:B:943:ILE:HG13	1.69	0.74
1:D:986:VAL:HG12	1:D:1008:MET:HE3	1.69	0.74
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.69	0.74
1:F:195:LYS:HZ1	1:F:196:PHE:HE1	1.32	0.74
1:A:196:PHE:O	1:A:252:LYS:NZ	2.21	0.74
1:C:445:ILE:HG12	1:C:940:LYS:HG3	1.70	0.74
1:D:781:MET:HE1	1:F:225:VAL:H	1.52	0.74
1:B:415:ASN:HD22	1:B:434:SER:HB2	1.53	0.73
1:D:919:ARG:HG2	1:D:920:GLY:H	1.52	0.73
1:A:545:TYR:OH	1:A:903:LEU:O	2.04	0.73
1:D:146:ASP:OD2	1:D:146:ASP:N	2.21	0.73
1:A:38:ILE:HG23	1:A:462:SER:HB2	1.70	0.73
1:B:530:SER:OG	3:B:1101:LMT:O2'	2.06	0.73
1:E:678:THR:HA	1:E:837:THR:OG1	1.89	0.73
1:D:699:ARG:NH1	1:D:825:MET:SD	2.61	0.73
1:C:3:ASN:N	1:C:3:ASN:OD1	2.13	0.73
1:B:846:GLN:O	1:B:849:SER:OG	2.07	0.73
1:D:222:THR:HA	1:D:224:PRO:HD3	1.70	0.73
1:B:363:ARG:HD3	1:B:496:MET:O	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLY:N	1:B:275:TYR:OH	2.22	0.72
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.69	0.72
1:C:562:SER:HB2	1:C:924:ASP:HB3	1.70	0.72
1:D:362:PHE:O	1:D:366:LEU:HG	1.90	0.72
1:E:919:ARG:HB3	1:E:921:LEU:HD23	1.70	0.72
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.71	0.72
1:F:253:VAL:HG13	1:F:259:ARG:HG2	1.71	0.72
1:F:901:VAL:HG23	1:F:942:ALA:HB3	1.70	0.72
1:C:944:LEU:HB3	1:C:971:ARG:CZ	2.20	0.72
1:E:698:ALA:HB1	1:E:851:LEU:HD13	1.71	0.72
1:C:520:PHE:O	1:C:524:THR:HG22	1.90	0.71
1:C:971:ARG:HB3	1:C:971:ARG:CZ	2.18	0.71
1:F:530:SER:HG	3:F:1101:LMT:H2O2	1.37	0.71
1:B:808:ARG:NH1	1:B:810:GLU:OE2	2.23	0.71
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.71	0.71
1:E:682:PHE:CZ	1:E:857:TYR:HB2	2.26	0.71
1:C:944:LEU:HB3	1:C:971:ARG:NE	2.05	0.71
1:E:250:LEU:HD21	1:E:253:VAL:HG22	1.73	0.71
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.72	0.71
1:E:562:SER:OG	1:E:563:PHE:N	2.21	0.71
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.73	0.71
1:D:9:PRO:HG2	1:D:10:ILE:HD12	1.71	0.71
1:A:928:GLN:HG2	3:A:1103:LMT:H21	1.73	0.71
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.73	0.71
1:C:582:ALA:HA	1:C:586:ARG:NH2	2.06	0.70
1:E:262:LEU:HG	1:E:268:ILE:HD11	1.73	0.70
1:E:668:LEU:H	1:E:668:LEU:HD23	1.55	0.70
1:E:448:VAL:HG13	1:E:884:VAL:HG22	1.73	0.70
1:B:383:LEU:HD11	1:B:473:THR:HG23	1.71	0.70
1:C:144:ASN:O	1:C:284:GLN:NE2	2.23	0.70
1:A:424:GLY:HA3	1:A:502:LYS:HB3	1.72	0.70
1:D:134:SER:HB2	2:D:1101:ERY:O10	1.90	0.70
1:A:70:ASN:O	1:A:110:LYS:NZ	2.25	0.70
1:A:274:ASN:ND2	1:A:276:ASP:OD2	2.25	0.70
1:E:441:ALA:O	1:E:445:ILE:HG23	1.91	0.70
1:C:775:SER:OG	1:C:776:GLU:O	2.10	0.70
1:D:580:ALA:HB1	1:D:724:THR:HG22	1.74	0.70
1:F:808:ARG:NH1	1:F:810:GLU:OE2	2.25	0.69
1:A:644:VAL:HG11	1:A:667:ASN:HB2	1.74	0.69
1:F:943:ILE:O	1:F:947:GLU:HB3	1.91	0.69
1:C:366:LEU:O	1:C:370:ILE:HG13	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:846:GLN:O	1:D:849:SER:OG	2.08	0.69
1:E:652:THR:HG23	1:E:665:ALA:HB3	1.74	0.69
1:C:242:SER:HB2	1:C:245:GLU:HG3	1.72	0.69
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.28	0.69
1:B:69:MET:HE1	1:B:107:VAL:HG13	1.75	0.69
1:B:236:ALA:O	1:C:728:LYS:NZ	2.19	0.69
1:B:452:VAL:HG23	1:B:453:PHE:CD2	2.27	0.69
1:C:453:PHE:O	1:C:471:SER:OG	2.11	0.69
1:D:262:LEU:HG	1:D:268:ILE:HD11	1.75	0.69
1:D:886:LEU:HD13	1:F:18:ILE:HG13	1.74	0.69
1:C:159:ALA:HB2	1:C:177:LEU:HD11	1.75	0.69
1:F:32:VAL:HG22	1:F:390:ILE:HB	1.74	0.69
1:B:24:GLY:O	1:B:27:ILE:HG22	1.93	0.68
1:C:171:GLY:HA3	1:C:302:THR:OG1	1.92	0.68
1:D:139:VAL:HB	1:D:327:TYR:HB3	1.74	0.68
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.74	0.68
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.74	0.68
1:B:238:THR:OG1	1:C:728:LYS:NZ	2.26	0.68
1:B:668:LEU:CD2	1:B:668:LEU:H	2.07	0.68
1:E:174:ASP:HB3	1:E:292:LYS:HB2	1.76	0.68
1:F:418:ARG:O	1:F:422:GLU:HB2	1.94	0.68
1:F:45:ILE:HD12	1:F:90:ILE:HB	1.75	0.68
1:A:687:GLN:HG2	1:C:316:PHE:CD1	2.29	0.68
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.76	0.68
1:D:536:ARG:NH1	3:D:1102:LMT:O3B	2.27	0.68
1:A:986:VAL:HG21	1:A:1007:VAL:HG11	1.76	0.68
1:C:702:LEU:HD12	1:C:851:LEU:HD11	1.76	0.68
1:D:586:ARG:O	1:D:589:LYS:HB3	1.94	0.68
1:B:7:ASP:OD2	1:B:432:ARG:NH2	2.25	0.67
1:C:318:PRO:HG2	1:C:321:LEU:HB2	1.75	0.67
1:C:356:TYR:C	1:C:358:PHE:H	1.96	0.67
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.74	0.67
1:F:719:ASN:HB3	1:F:826:GLU:HB3	1.76	0.67
1:A:775:SER:OG	1:A:776:GLU:O	2.11	0.67
1:D:26:ALA:O	1:D:30:LEU:HB2	1.94	0.67
1:E:143:ILE:HG22	1:E:286:ALA:HB2	1.77	0.67
1:F:250:LEU:HD11	1:F:259:ARG:HB3	1.74	0.67
1:E:213:GLN:HG2	1:E:239:ARG:HG3	1.77	0.67
1:D:668:LEU:H	1:D:668:LEU:HD23	1.59	0.67
1:F:753:ALA:O	1:F:775:SER:HB3	1.93	0.67
1:F:81:ASN:OD1	1:F:815:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.76	0.67
1:E:327:TYR:HD1	1:E:628:PHE:HZ	1.43	0.67
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.75	0.67
1:A:419:VAL:HG11	1:A:433:LYS:HG2	1.77	0.67
1:A:343:THR:HG21	1:A:989:LEU:HD21	1.76	0.67
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.30	0.67
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.77	0.67
1:D:164:ASP:HB3	1:D:168:ARG:HH21	1.60	0.67
1:D:198:LEU:HD23	1:D:792:ARG:HH21	1.60	0.67
1:F:876:LEU:HD22	1:F:932:LEU:HD11	1.75	0.67
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.75	0.66
1:A:73:ASP:OD2	1:C:131:LYS:NZ	2.27	0.66
1:E:242:SER:HB2	1:E:245:GLU:HG3	1.77	0.66
1:F:910:ILE:O	1:F:914:LEU:HB2	1.94	0.66
1:A:699:ARG:HD2	1:A:718:PRO:HB3	1.77	0.66
1:A:243:THR:HG23	1:A:268:ILE:HG22	1.77	0.66
1:F:99:ASP:HB3	1:F:102:ILE:HB	1.76	0.66
1:B:696:THR:HG23	1:B:699:ARG:NH1	2.11	0.66
1:E:971:ARG:O	1:E:975:ILE:HG12	1.96	0.66
1:D:60:THR:HG23	1:D:61:VAL:HG23	1.76	0.66
1:C:83:ASP:HB2	1:C:87:THR:O	1.95	0.66
1:D:108:GLN:NE2	1:E:109:ASN:HB2	2.11	0.66
1:D:355:MET:HB3	1:D:365:THR:OG1	1.96	0.65
1:E:104:GLN:HB2	1:E:131:LYS:HE3	1.78	0.65
1:A:733:GLN:HE22	1:A:743:ILE:HG21	1.61	0.65
1:A:888:LEU:HD13	1:A:901:VAL:HG13	1.78	0.65
1:A:222:THR:HG23	1:B:275:TYR:HB2	1.79	0.65
1:B:434:SER:HA	1:B:437:GLN:HB2	1.77	0.65
1:B:597:TYR:HE1	1:B:601:LYS:HD2	1.59	0.65
1:E:508:GLY:O	1:E:510:LYS:N	2.30	0.65
1:B:82:SER:HA	1:B:88:VAL:HG22	1.78	0.65
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.31	0.65
1:D:38:ILE:HG23	1:D:462:SER:HB2	1.78	0.65
1:E:239:ARG:HH12	1:E:761:ASP:HB2	1.61	0.65
1:A:588:GLN:NE2	1:A:592:ASN:OD1	2.28	0.65
1:A:857:TYR:HE2	1:C:312:LYS:HZ1	1.44	0.65
1:C:465:ALA:HA	1:C:468:ARG:HH11	1.61	0.65
1:F:941:ASN:ND2	1:F:1015:THR:HG22	2.11	0.65
1:F:937:LEU:HD11	1:F:982:PHE:HE2	1.61	0.65
1:C:654:ALA:O	1:C:658:ILE:HG12	1.96	0.65
1:E:580:ALA:HB1	1:E:724:THR:HG22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:578:LEU:HG	1:F:587:THR:HG22	1.77	0.65
1:A:80:SER:HB3	1:A:90:ILE:HG12	1.77	0.65
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.79	0.65
1:E:775:SER:OG	1:E:776:GLU:O	2.15	0.65
1:F:196:PHE:O	1:F:252:LYS:NZ	2.28	0.65
1:C:455:PRO:HG3	1:C:883:VAL:HG21	1.78	0.65
1:C:945:ILE:HG13	1:C:971:ARG:HH22	1.61	0.65
1:F:262:LEU:HG	1:F:268:ILE:HD11	1.78	0.65
1:F:211:ASN:HD22	1:F:760:ASN:HD21	1.44	0.65
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.78	0.65
1:D:680:PHE:HE1	1:D:844:MET:HG3	1.62	0.65
1:F:443:VAL:O	1:F:447:MET:HB3	1.96	0.65
1:B:362:PHE:O	1:B:365:THR:HG22	1.96	0.65
1:B:832:ALA:HB3	1:B:835:LYS:HB2	1.79	0.65
1:D:360:GLN:NE2	1:D:513:PHE:HB3	2.11	0.65
1:C:82:SER:HB2	1:C:816:LEU:HB2	1.78	0.64
1:F:137:LEU:HD11	1:F:303:ALA:HB2	1.79	0.64
1:B:919:ARG:HB3	1:B:921:LEU:HD23	1.79	0.64
1:C:1019:ILE:HG13	1:C:1020:PHE:CD1	2.33	0.64
1:F:455:PRO:HG3	1:F:883:VAL:HG21	1.78	0.64
1:A:222:THR:HA	1:A:224:PRO:HD3	1.79	0.64
1:A:740:GLY:O	1:A:794:ALA:N	2.29	0.64
1:B:696:THR:HG23	1:B:699:ARG:HH12	1.61	0.64
1:C:196:PHE:O	1:C:252:LYS:NZ	2.27	0.64
1:C:56:THR:O	1:C:60:THR:OG1	2.12	0.64
1:C:713:LEU:HD11	1:C:843:LEU:HD12	1.79	0.64
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.78	0.64
1:E:6:ILE:HG23	1:E:494:ALA:HB2	1.80	0.64
1:F:1041:GLU:HB3	1:F:1042:HIS:HB3	1.79	0.64
1:A:948:PHE:O	1:A:952:LEU:HG	1.98	0.64
1:F:937:LEU:HD13	1:F:1011:MET:HG2	1.79	0.64
1:D:243:THR:HG23	1:D:268:ILE:HG22	1.79	0.64
1:F:600:THR:O	1:F:603:LYS:HG3	1.98	0.64
1:F:690:LEU:O	1:F:694:LYS:HB2	1.97	0.64
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.80	0.64
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.77	0.64
1:B:185:ARG:HG2	1:B:187:TRP:CZ2	2.32	0.64
1:D:735:LYS:O	1:D:739:LEU:HG	1.97	0.64
1:D:971:ARG:HH21	1:D:975:ILE:HD11	1.63	0.64
1:A:141:GLY:HA3	1:A:324:VAL:HG12	1.79	0.64
1:C:360:GLN:OE1	1:C:517:ASN:ND2	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:ALA:HB3	1:E:313:MET:CE	2.26	0.64
1:E:442:LEU:O	1:E:445:ILE:HG13	1.97	0.64
1:A:913:LEU:HD23	1:A:927:PHE:HZ	1.63	0.64
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.80	0.63
1:A:427:PRO:CD	1:A:499:PRO:HB3	2.22	0.63
1:A:544:LEU:O	1:A:548:ILE:HG13	1.98	0.63
1:B:143:ILE:HG22	1:B:286:ALA:HB2	1.78	0.63
1:B:597:TYR:CE1	1:B:601:LYS:HD2	2.33	0.63
1:B:703:LEU:HD21	1:B:718:PRO:HD3	1.78	0.63
1:C:66:GLU:OE1	1:C:821:GLY:HA2	1.98	0.63
1:C:897:ILE:O	1:C:901:VAL:HG12	1.98	0.63
1:F:597:TYR:HE1	1:F:601:LYS:HD2	1.62	0.63
1:F:57:VAL:HG23	1:F:82:SER:HB3	1.80	0.63
1:A:134:SER:HG	2:A:1101:ERY:H323	1.60	0.63
1:B:26:ALA:O	1:B:30:LEU:HB2	1.98	0.63
1:B:545:TYR:CE2	1:B:1025:PHE:HZ	2.16	0.63
2:A:1101:ERY:O10	2:A:1101:ERY:O1	2.16	0.63
1:A:112:GLN:HG3	1:B:112:GLN:OE1	1.98	0.63
1:C:597:TYR:HE1	1:C:601:LYS:HD2	1.63	0.63
1:E:240:LEU:HB2	1:E:246:PHE:CE1	2.33	0.63
1:F:188:MET:HA	1:F:266:ALA:HB2	1.78	0.63
1:F:463:THR:HG23	1:F:925:VAL:HG22	1.81	0.63
1:B:910:ILE:O	1:B:914:LEU:HB2	1.98	0.63
1:D:637:ARG:HB3	1:D:642:ASN:HB3	1.78	0.63
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.79	0.63
1:A:520:PHE:O	1:A:524:THR:HG22	1.99	0.63
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.80	0.63
1:E:508:GLY:HA2	1:E:518:ARG:HH21	1.63	0.63
1:A:400:LEU:HD23	1:A:929:VAL:HG12	1.80	0.63
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.81	0.63
1:D:1013:THR:O	1:D:1017:LEU:HB2	1.99	0.63
1:D:775:SER:OG	1:D:776:GLU:O	2.16	0.63
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.80	0.63
1:C:588:GLN:NE2	1:C:592:ASN:OD1	2.32	0.63
1:D:682:PHE:HB3	1:D:827:ILE:HB	1.80	0.63
1:E:228:GLN:NE2	1:E:230:LEU:O	2.30	0.63
1:E:801:PHE:HD1	1:E:804:PHE:HE2	1.44	0.63
1:B:14:VAL:HG13	1:C:886:LEU:HD12	1.81	0.63
1:C:30:LEU:HD23	1:C:390:ILE:HD11	1.80	0.63
1:D:108:GLN:O	1:D:112:GLN:HG2	1.98	0.63
1:D:637:ARG:NH1	1:D:642:ASN:O	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:682:PHE:HB3	1:E:827:ILE:HB	1.80	0.62
1:F:195:LYS:HB3	1:F:196:PHE:HD1	1.64	0.62
1:F:27:ILE:HA	1:F:30:LEU:HD22	1.80	0.62
1:F:382:VAL:HG21	1:F:476:SER:HB2	1.80	0.62
1:F:6:ILE:CG2	1:F:12:ALA:HB2	2.28	0.62
1:C:372:VAL:HG22	1:C:405:LEU:HD11	1.81	0.62
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.79	0.62
1:B:544:LEU:O	1:B:548:ILE:HG13	1.99	0.62
1:B:783:PRO:O	1:B:786:ILE:HG12	1.99	0.62
1:C:800:PRO:HG2	1:C:803:ALA:HB2	1.82	0.62
1:F:455:PRO:HG2	1:F:880:SER:HA	1.82	0.62
1:F:66:GLU:OE1	1:F:821:GLY:HA2	1.99	0.62
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.81	0.62
1:B:637:ARG:HB3	1:B:642:ASN:HB3	1.81	0.62
1:C:841:MET:O	1:C:845:GLU:HG2	2.00	0.62
1:D:680:PHE:CE1	1:D:844:MET:HG3	2.35	0.62
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.22	0.62
1:B:455:PRO:HG2	1:B:880:SER:OG	1.98	0.62
1:C:228:GLN:NE2	1:C:230:LEU:O	2.33	0.62
1:C:688:ALA:O	1:C:690:LEU:N	2.32	0.62
1:D:278:ILE:HG13	1:D:613:ASN:HB3	1.81	0.62
1:E:655:PHE:HA	1:E:659:LYS:HD3	1.81	0.62
1:A:45:ILE:HD12	1:A:90:ILE:HB	1.81	0.62
1:C:801:PHE:HA	1:C:804:PHE:CE2	2.34	0.62
1:E:294:ALA:HB3	1:E:297:ALA:HB2	1.82	0.62
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.33	0.62
1:A:219:LEU:HD13	1:B:783:PRO:HG3	1.82	0.62
1:F:947:GLU:HG3	1:F:948:PHE:CD1	2.35	0.62
1:A:1035:ARG:HG2	1:A:1036:LYS:H	1.65	0.61
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.82	0.61
1:A:705:GLU:HB3	1:A:847:LEU:HD22	1.81	0.61
1:A:919:ARG:NH2	1:A:990:VAL:O	2.29	0.61
1:B:654:ALA:O	1:B:658:ILE:HG12	2.00	0.61
1:F:343:THR:HG21	1:F:989:LEU:HD23	1.82	0.61
1:F:952:LEU:O	1:F:956:GLU:HB2	1.99	0.61
1:A:53:ASP:OD1	1:A:56:THR:OG1	2.15	0.61
1:B:240:LEU:HB2	1:B:246:PHE:CE1	2.35	0.61
1:D:582:ALA:HA	1:D:586:ARG:NH2	2.15	0.61
1:B:637:ARG:HA	1:B:642:ASN:HD22	1.65	0.61
1:D:201:VAL:HA	1:D:204:ILE:HD12	1.80	0.61
1:E:534:ILE:HG22	3:E:1101:LMT:H5'	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.83	0.61
1:C:404:LEU:HB3	1:C:478:MET:SD	2.40	0.61
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.01	0.61
1:F:947:GLU:HG3	1:F:948:PHE:HD1	1.63	0.61
1:D:141:GLY:HA3	1:D:324:VAL:HG12	1.82	0.61
1:A:240:LEU:HB2	1:A:246:PHE:HE1	1.66	0.61
1:B:753:ALA:O	1:B:775:SER:HB3	1.99	0.61
1:B:658:ILE:O	1:B:659:LYS:HD2	2.01	0.61
1:D:888:LEU:HD13	1:D:901:VAL:HG13	1.82	0.61
1:E:519:MET:O	1:E:523:SER:OG	2.14	0.61
1:F:448:VAL:HG21	1:F:939:ALA:HB1	1.83	0.61
1:F:452:VAL:O	1:F:455:PRO:HD2	2.00	0.61
1:A:672:VAL:O	1:A:674:LEU:N	2.33	0.61
1:B:262:LEU:HG	1:B:268:ILE:HD11	1.81	0.61
1:C:3:ASN:O	1:C:6:ILE:N	2.33	0.61
1:D:251:LEU:HD11	1:D:262:LEU:HA	1.83	0.61
1:E:272:GLY:N	1:E:275:TYR:OH	2.29	0.61
1:A:35:TYR:HB3	1:A:38:ILE:HD11	1.83	0.61
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.83	0.61
1:A:777:ALA:HB1	1:C:225:VAL:HG12	1.83	0.61
1:C:905:VAL:HG13	1:C:935:ILE:HG12	1.83	0.61
1:D:1034:SER:O	1:D:1034:SER:OG	2.13	0.61
1:A:150:THR:OG1	1:A:152:GLU:HG2	2.01	0.60
1:A:549:VAL:O	1:A:552:MET:HB3	2.01	0.60
1:B:174:ASP:HB3	1:B:292:LYS:HB2	1.82	0.60
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.83	0.60
1:E:187:TRP:HE3	1:E:775:SER:O	1.85	0.60
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.31	0.60
1:F:482:VAL:O	1:F:486:LEU:HG	2.00	0.60
1:B:9:PRO:HB3	1:B:495:THR:HG21	1.84	0.60
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.83	0.60
1:C:27:ILE:HA	1:C:30:LEU:HD22	1.83	0.60
1:C:574:THR:HG21	1:C:598:TYR:HE2	1.66	0.60
1:D:281:PHE:CE1	1:D:608:SER:HB2	2.36	0.60
1:D:190:PRO:HG3	1:D:789:TRP:CZ2	2.36	0.60
1:D:991:ILE:HG22	1:D:992:SER:H	1.66	0.60
1:F:363:ARG:HE	1:F:498:LYS:HB2	1.65	0.60
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.83	0.60
1:E:682:PHE:CD2	1:E:827:ILE:HD12	2.37	0.60
1:F:382:VAL:HG11	1:F:476:SER:HB3	1.84	0.60
1:F:685:ILE:HD11	1:F:819:TYR:HD2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ALA:O	1:A:658:ILE:HG12	2.01	0.60
1:B:441:ALA:O	1:B:445:ILE:HG23	2.02	0.60
1:E:32:VAL:HG12	1:E:390:ILE:HB	1.81	0.60
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.84	0.60
1:C:952:LEU:O	1:C:956:GLU:HB2	2.01	0.60
1:E:950:LYS:HA	1:E:953:MET:HE3	1.82	0.60
1:A:1026:PHE:CZ	1:A:1030:ARG:HG3	2.37	0.60
1:A:744:ASN:O	1:A:748:THR:HG23	2.01	0.60
1:C:135:SER:HB3	1:C:673:GLU:HA	1.82	0.60
1:C:155:SER:HB3	1:C:180:SER:H	1.67	0.60
1:F:696:THR:HG23	1:F:699:ARG:HH12	1.67	0.60
1:C:698:ALA:O	1:C:701:GLN:HB3	2.02	0.60
1:E:9:PRO:HG2	1:E:10:ILE:HD12	1.83	0.60
1:F:83:ASP:HB2	1:F:87:THR:O	2.01	0.60
1:C:574:THR:HG23	1:C:627:ALA:HB3	1.84	0.60
1:C:945:ILE:HA	1:C:971:ARG:NH1	2.16	0.60
1:D:574:THR:HG23	1:D:627:ALA:HB3	1.84	0.60
1:D:658:ILE:HG13	1:D:659:LYS:HE2	1.84	0.60
1:E:26:ALA:O	1:E:30:LEU:HB2	2.01	0.60
1:E:901:VAL:HG23	1:E:942:ALA:HB3	1.82	0.60
1:A:960:LEU:HD21	1:A:1027:VAL:HG13	1.84	0.60
1:A:144:ASN:ND2	1:A:146:ASP:OD2	2.35	0.60
1:C:982:PHE:HD2	1:C:1011:MET:HG2	1.66	0.60
1:C:228:GLN:NE2	1:C:230:LEU:H	2.00	0.60
1:F:151:GLN:HE22	1:F:278:ILE:HA	1.66	0.60
1:F:764:ASP:OD1	1:F:765:ARG:HG3	2.02	0.60
1:A:1018:ALA:O	1:A:1022:VAL:HG23	2.02	0.59
1:A:185:ARG:HB3	1:A:187:TRP:NE1	2.17	0.59
1:B:195:LYS:HB3	1:B:196:PHE:HD1	1.67	0.59
1:B:139:VAL:O	1:B:326:PRO:HD2	2.01	0.59
1:D:32:VAL:HB	1:D:300:LEU:HD22	1.84	0.59
1:D:35:TYR:HB3	1:D:38:ILE:HD11	1.84	0.59
1:B:1037:ASN:N	1:B:1038:GLU:HB3	2.17	0.59
1:C:65:ILE:HG23	1:C:111:LEU:HD23	1.83	0.59
1:C:244:GLU:HG2	1:C:248:LYS:HE3	1.84	0.59
1:D:540:ARG:NH2	3:D:1102:LMT:O6B	2.35	0.59
1:D:544:LEU:HA	1:D:547:ILE:HD12	1.84	0.59
1:D:790:TYR:HB3	1:D:798:MET:HB3	1.85	0.59
1:D:925:VAL:O	1:D:928:GLN:N	2.35	0.59
1:A:901:VAL:HG21	1:A:943:ILE:HG13	1.83	0.59
1:E:613:ASN:HD22	1:E:614:GLY:N	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:HD12	1:C:101:ASP:HB3	1.83	0.59
1:A:781:MET:HE1	1:C:225:VAL:N	2.11	0.59
1:B:733:GLN:HE22	1:B:743:ILE:HG21	1.67	0.59
1:C:465:ALA:HA	1:C:468:ARG:NH1	2.18	0.59
1:C:744:ASN:O	1:C:748:THR:HG23	2.02	0.59
1:D:578:LEU:HD21	1:D:590:VAL:HG21	1.84	0.59
1:F:284:GLN:HG3	1:F:285:PRO:HD2	1.85	0.59
1:F:356:TYR:HA	1:F:365:THR:HG21	1.84	0.59
1:A:736:ALA:HB1	1:A:746:ILE:HD11	1.84	0.59
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.38	0.59
1:E:1016:VAL:HG13	3:E:1101:LMT:H112	1.84	0.59
1:F:885:PHE:HD2	1:F:886:LEU:HD22	1.66	0.59
1:A:758:TYR:OH	1:A:761:ASP:OD1	2.16	0.59
1:D:166:ILE:HD11	1:D:310:LEU:HD13	1.85	0.59
1:D:781:MET:HB3	1:F:228:GLN:NE2	2.17	0.59
1:D:971:ARG:CZ	1:D:971:ARG:HB3	2.32	0.59
1:B:344:LEU:HD13	1:B:376:LEU:HD13	1.84	0.59
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.38	0.59
1:E:56:THR:O	1:E:60:THR:OG1	2.18	0.59
1:F:144:ASN:OD1	1:F:148:THR:HA	2.02	0.59
1:A:593:GLU:OE2	1:A:659:LYS:NZ	2.35	0.59
1:D:375:VAL:HG21	1:D:481:SER:HA	1.85	0.59
1:C:586:ARG:O	1:C:589:LYS:HB2	2.03	0.59
1:D:159:ALA:HB2	1:D:177:LEU:HD11	1.85	0.59
1:F:979:SER:CB	1:F:1015:THR:HG21	2.33	0.59
1:F:344:LEU:O	1:F:348:ILE:HG13	2.02	0.59
1:A:38:ILE:CG2	1:A:462:SER:HB2	2.33	0.58
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.84	0.58
1:D:519:MET:O	1:D:523:SER:OG	2.18	0.58
1:F:324:VAL:HG23	1:F:326:PRO:HD3	1.84	0.58
1:C:943:ILE:O	1:C:947:GLU:HB3	2.03	0.58
1:E:1032:ARG:HA	1:E:1032:ARG:NE	2.17	0.58
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.84	0.58
1:E:327:TYR:HD1	1:E:628:PHE:CZ	2.21	0.58
1:A:375:VAL:HG21	1:A:481:SER:HA	1.83	0.58
1:A:900:SER:HB3	1:A:1029:VAL:HG21	1.85	0.58
1:E:531:VAL:O	1:E:534:ILE:HG13	2.03	0.58
1:A:1016:VAL:HG13	3:A:1102:LMT:H112	1.85	0.58
1:B:1033:PHE:CD1	1:B:1034:SER:HB3	2.38	0.58
1:B:501:ALA:O	1:B:504:ASP:HB2	2.04	0.58
1:C:272:GLY:N	1:C:275:TYR:OH	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ASN:HA	1:D:320:GLY:O	2.03	0.58
1:D:36:PRO:O	1:D:38:ILE:HG13	2.04	0.58
1:E:911:GLY:HA3	1:E:1013:THR:OG1	2.03	0.58
1:A:112:GLN:OE1	1:A:115:MET:HG3	2.03	0.58
1:B:562:SER:HB3	1:B:924:ASP:HB3	1.85	0.58
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.85	0.58
1:C:568:ASP:O	1:C:634:TRP:HH2	1.87	0.58
1:C:682:PHE:HE2	1:C:702:LEU:HD11	1.69	0.58
1:E:705:GLU:HB3	1:E:847:LEU:HD22	1.83	0.58
1:A:210:GLN:HE22	1:A:250:LEU:HB3	1.68	0.58
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.86	0.58
1:A:869:SER:OG	1:A:870:GLY:N	2.35	0.58
1:B:979:SER:OG	1:B:1015:THR:HG21	2.03	0.58
1:C:203:VAL:O	1:C:207:ILE:HG13	2.03	0.58
1:D:102:ILE:HD12	1:F:101:ASP:HB3	1.86	0.58
1:D:38:ILE:CG2	1:D:462:SER:HB2	2.34	0.58
1:A:186:ILE:HD11	1:A:246:PHE:HD2	1.69	0.58
1:A:18:ILE:HG13	1:B:886:LEU:HD23	1.85	0.58
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.85	0.58
1:D:563:PHE:HD2	1:D:671:ILE:HD13	1.69	0.58
1:D:698:ALA:HB1	1:D:851:LEU:HD13	1.86	0.58
1:F:379:THR:HG23	1:F:476:SER:OG	2.04	0.58
1:F:973:ARG:HG2	1:F:977:MET:HE2	1.85	0.58
1:A:878:ALA:O	1:A:882:ILE:HG12	2.03	0.58
1:B:442:LEU:O	1:B:445:ILE:HG13	2.04	0.58
1:B:99:ASP:HB3	1:B:102:ILE:HB	1.86	0.58
1:C:332:PHE:HD1	1:C:634:TRP:CZ2	2.22	0.58
1:D:101:ASP:OD1	1:D:131:LYS:HE2	2.03	0.58
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.85	0.57
1:A:575:MET:CG	1:A:664:PHE:HB2	2.33	0.57
1:E:888:LEU:HD21	1:E:943:ILE:HD11	1.85	0.57
1:B:163:LYS:HD2	1:B:177:LEU:HG	1.85	0.57
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.86	0.57
1:C:683:GLU:HB3	1:C:858:ASP:HB3	1.86	0.57
1:C:740:GLY:O	1:C:794:ALA:N	2.36	0.57
1:D:170:SER:OG	1:E:74:ASN:N	2.34	0.57
1:D:434:SER:O	1:D:438:ILE:HG12	2.04	0.57
1:E:1032:ARG:HE	1:E:1032:ARG:HA	1.68	0.57
1:F:242:SER:HB2	1:F:245:GLU:HG3	1.86	0.57
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.39	0.57
1:B:47:ALA:HB2	1:B:127:VAL:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:VAL:HG22	1:C:259:ARG:HG2	1.86	0.57
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.84	0.57
1:C:746:ILE:HG13	1:C:747:ASN:N	2.19	0.57
1:C:730:ASP:OD2	1:C:808:ARG:NH2	2.36	0.57
1:C:947:GLU:HG3	1:C:948:PHE:N	2.19	0.57
1:D:351:VAL:HG22	1:D:981:ALA:HB1	1.85	0.57
1:F:352:PHE:HA	1:F:355:MET:HE2	1.86	0.57
1:F:562:SER:HB2	1:F:924:ASP:HB3	1.86	0.57
1:D:672:VAL:HB	1:D:673:GLU:CD	2.25	0.57
1:E:574:THR:HG23	1:E:627:ALA:HB3	1.85	0.57
1:B:404:LEU:HD21	1:B:449:LEU:HD22	1.85	0.57
1:E:1013:THR:O	1:E:1017:LEU:HB2	2.04	0.57
1:E:24:GLY:O	1:E:27:ILE:HG22	2.03	0.57
1:F:894:SER:HG	1:F:896:SER:HG	1.51	0.57
1:A:728:LYS:NZ	1:C:236:ALA:O	2.30	0.57
1:C:388:PHE:CE2	1:C:472:ILE:HG21	2.39	0.57
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.40	0.57
1:D:790:TYR:HD1	1:D:800:PRO:HA	1.69	0.57
1:D:910:ILE:O	1:D:914:LEU:HB2	2.05	0.57
1:E:173:GLY:O	1:F:70:ASN:ND2	2.35	0.57
2:A:1101:ERY:H352	2:A:1101:ERY:H71	1.87	0.57
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.70	0.57
1:A:960:LEU:O	1:A:964:THR:HG23	2.05	0.57
1:A:146:ASP:OD2	1:A:146:ASP:N	2.37	0.57
1:A:368:PRO:HG3	1:A:413:VAL:HG21	1.87	0.57
1:C:47:ALA:HB3	1:C:88:VAL:HG13	1.86	0.57
1:C:587:THR:HG21	1:C:622:GLN:O	2.05	0.57
1:D:878:ALA:O	1:D:882:ILE:HG12	2.03	0.57
1:E:355:MET:HE3	1:E:410:ILE:HG12	1.87	0.57
1:F:140:VAL:HG23	1:F:291:ILE:HD13	1.87	0.57
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.40	0.57
1:B:907:LEU:HG	1:B:1017:LEU:HD23	1.87	0.57
1:C:66:GLU:OE2	1:C:80:SER:OG	2.14	0.57
1:D:3:ASN:O	1:D:6:ILE:N	2.37	0.57
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.70	0.57
1:F:361:ASN:HD21	1:F:498:LYS:HD3	1.70	0.57
1:F:775:SER:OG	1:F:776:GLU:O	2.20	0.57
1:F:746:ILE:HG22	1:F:791:VAL:HG21	1.87	0.57
1:D:744:ASN:O	1:D:748:THR:HG23	2.05	0.56
1:E:355:MET:CE	1:E:410:ILE:HG12	2.34	0.56
1:E:210:GLN:HG2	1:F:733:GLN:NE2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:TYR:HB3	1:D:57:VAL:HG22	1.86	0.56
1:E:158:VAL:HG11	1:E:177:LEU:HD21	1.85	0.56
1:A:187:TRP:HE3	1:A:775:SER:O	1.88	0.56
1:E:1041:GLU:HB3	1:E:1042:HIS:HB2	1.86	0.56
1:A:355:MET:HE1	1:A:368:PRO:HG2	1.87	0.56
1:B:188:MET:HA	1:B:266:ALA:HB2	1.87	0.56
1:B:535:LEU:HD22	1:B:1027:VAL:HG11	1.87	0.56
1:D:253:VAL:HG12	1:D:259:ARG:HG2	1.87	0.56
1:F:1039:ASP:HB3	1:F:1040:ILE:HA	1.86	0.56
1:D:113:LEU:HD11	1:F:128:SER:HB3	1.87	0.56
1:F:434:SER:O	1:F:438:ILE:HG12	2.05	0.56
1:B:764:ASP:OD1	1:B:765:ARG:HG3	2.05	0.56
1:D:157:TYR:CZ	1:D:318:PRO:HD3	2.41	0.56
1:D:544:LEU:O	1:D:548:ILE:HG13	2.05	0.56
1:E:460:GLY:O	1:E:463:THR:OG1	2.23	0.56
1:E:683:GLU:HG2	1:E:819:TYR:CD2	2.40	0.56
1:F:574:THR:HG23	1:F:627:ALA:HB3	1.87	0.56
1:F:925:VAL:O	1:F:928:GLN:N	2.38	0.56
1:A:482:VAL:O	1:A:486:LEU:HG	2.06	0.56
1:A:888:LEU:HD13	1:A:901:VAL:CG1	2.36	0.56
1:B:183:ALA:O	1:B:270:LEU:HD12	2.05	0.56
1:B:971:ARG:HB3	1:B:971:ARG:CZ	2.34	0.56
1:C:752:ALA:O	1:C:774:MET:HA	2.06	0.56
1:E:908:GLY:HA2	1:E:1014:ALA:HB2	1.87	0.56
1:F:698:ALA:O	1:F:701:GLN:HB3	2.06	0.56
1:A:637:ARG:HB3	1:A:642:ASN:HB3	1.88	0.56
1:C:3:ASN:HA	1:C:6:ILE:HB	1.88	0.56
1:D:393:LEU:HB3	1:D:470:PHE:CE1	2.41	0.56
1:E:545:TYR:CE2	1:E:1025:PHE:HZ	2.22	0.56
1:E:606:VAL:HA	1:E:631:LEU:HD23	1.88	0.56
1:F:53:ASP:OD1	1:F:56:THR:OG1	2.18	0.56
1:D:211:ASN:O	1:D:760:ASN:ND2	2.39	0.56
1:E:324:VAL:HG13	1:E:326:PRO:HD3	1.86	0.56
1:F:654:ALA:O	1:F:658:ILE:HG12	2.05	0.56
1:A:1040:ILE:HG23	1:A:1041:GLU:H	1.70	0.56
1:A:719:ASN:HB2	1:A:828:LEU:HG	1.88	0.56
1:E:537:SER:OG	1:E:540:ARG:NH2	2.39	0.56
1:E:607:GLU:HA	1:E:632:LYS:HE2	1.87	0.56
1:E:680:PHE:CD1	1:E:859:TRP:HZ3	2.17	0.56
1:E:559:LEU:HD21	1:E:922:THR:HA	1.87	0.56
1:F:1016:VAL:HG13	3:F:1101:LMT:H112	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:PRO:O	1:F:5:PHE:HB3	2.06	0.56
1:F:817:GLU:HB2	1:F:824:SER:O	2.06	0.56
1:A:897:ILE:HA	1:A:1029:VAL:HG11	1.86	0.56
1:A:462:SER:O	1:A:466:ILE:HG12	2.06	0.56
1:C:979:SER:HA	1:C:1011:MET:HE3	1.88	0.56
1:D:435:MET:O	1:D:439:GLN:HB2	2.06	0.56
1:E:1018:ALA:O	1:E:1022:VAL:HG23	2.06	0.56
1:E:445:ILE:HD12	1:E:449:LEU:HD12	1.88	0.56
1:D:235:ILE:O	1:E:728:LYS:HD2	2.06	0.56
1:D:959:GLY:HA2	1:D:1039:ASP:HA	1.87	0.56
1:D:948:PHE:O	1:D:952:LEU:HG	2.05	0.56
1:E:690:LEU:HD22	1:E:694:LYS:HG2	1.87	0.56
1:F:599:LEU:O	1:F:603:LYS:HG2	2.06	0.56
1:B:146:ASP:HB2	1:B:148:THR:OG1	2.06	0.55
1:B:652:THR:CG2	1:B:665:ALA:H	2.20	0.55
1:C:453:PHE:HB3	1:C:471:SER:HA	1.87	0.55
1:A:519:MET:O	1:A:523:SER:OG	2.21	0.55
1:B:616:GLY:HA2	1:B:626:ILE:HD13	1.89	0.55
1:B:847:LEU:O	1:B:850:LYS:HB2	2.05	0.55
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.88	0.55
1:A:423:GLU:HB2	1:A:425:LEU:HD12	1.89	0.55
1:B:1013:THR:O	1:B:1017:LEU:HB2	2.06	0.55
1:D:913:LEU:HD23	1:D:927:PHE:HZ	1.71	0.55
1:F:74:ASN:O	1:F:94:PHE:HD2	1.90	0.55
1:A:617:ALA:HA	2:A:1101:ERY:H353	1.88	0.55
1:B:172:VAL:HG13	1:B:291:ILE:HG23	1.87	0.55
1:B:685:ILE:HD11	1:B:819:TYR:CD2	2.41	0.55
1:C:860:THR:HA	1:C:864:TYR:HB2	1.87	0.55
1:D:293:LEU:HD22	1:D:297:ALA:HB3	1.89	0.55
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.87	0.55
1:A:846:GLN:O	1:A:849:SER:OG	2.19	0.55
1:C:110:LYS:O	1:C:113:LEU:HB2	2.06	0.55
1:C:600:THR:O	1:C:603:LYS:HG3	2.06	0.55
1:E:1019:ILE:HG13	1:E:1020:PHE:CD1	2.41	0.55
1:E:281:PHE:HD1	1:E:610:PHE:HD1	1.55	0.55
1:E:354:VAL:HG22	1:E:980:LEU:HD23	1.89	0.55
1:E:450:SER:HB3	1:E:478:MET:HE1	1.87	0.55
1:E:591:LEU:HD13	1:E:611:ALA:HB1	1.88	0.55
1:A:946:VAL:HG13	1:A:1026:PHE:CD1	2.42	0.55
1:B:119:PRO:HG2	1:B:122:VAL:HB	1.89	0.55
1:B:555:LEU:HB3	1:B:913:LEU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:583:THR:OG1	1:D:586:ARG:HG3	2.06	0.55
1:E:1019:ILE:HG13	1:E:1020:PHE:HD1	1.71	0.55
1:E:281:PHE:CE1	1:E:608:SER:HB2	2.42	0.55
1:A:155:SER:HB3	1:A:180:SER:H	1.71	0.55
1:A:584:GLN:HB2	1:A:622:GLN:HG2	1.87	0.55
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.41	0.55
1:C:65:ILE:HD11	1:C:118:LEU:HD11	1.89	0.55
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.87	0.55
1:F:219:LEU:O	1:F:231:ASN:ND2	2.38	0.55
1:A:1033:PHE:HD2	1:A:1034:SER:N	2.04	0.55
1:A:976:LEU:O	1:A:980:LEU:HB2	2.06	0.55
1:C:1034:SER:OG	1:C:1038:GLU:O	2.22	0.55
1:C:278:ILE:HG13	1:C:613:ASN:HB3	1.88	0.55
1:C:671:ILE:HG21	1:C:674:LEU:HD12	1.88	0.55
1:E:337:ILE:HA	1:E:395:MET:HE2	1.89	0.55
1:E:909:VAL:HA	1:E:931:LEU:HD21	1.89	0.55
1:F:947:GLU:HG3	1:F:948:PHE:N	2.21	0.55
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.88	0.55
1:B:726:GLN:CD	1:B:812:GLY:HA3	2.27	0.55
1:B:744:ASN:O	1:B:748:THR:HG23	2.06	0.55
1:C:36:PRO:O	1:C:38:ILE:HG13	2.07	0.55
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.89	0.55
1:C:463:THR:HG23	1:C:925:VAL:HG22	1.89	0.55
1:C:971:ARG:NH2	1:C:975:ILE:HD11	2.22	0.55
1:D:400:LEU:HD11	1:D:1007:VAL:HG21	1.89	0.55
1:E:199:THR:HG21	1:E:792:ARG:H	1.72	0.55
1:E:388:PHE:CE2	1:E:472:ILE:HG21	2.42	0.55
1:F:144:ASN:O	1:F:284:GLN:NE2	2.40	0.55
1:B:985:GLY:O	1:B:988:PRO:HD2	2.07	0.55
1:C:941:ASN:ND2	1:C:1015:THR:HG22	2.22	0.55
1:D:175:VAL:HG11	1:D:289:LEU:HD22	1.89	0.55
1:E:252:LYS:HE3	1:E:260:VAL:HG21	1.89	0.55
1:E:544:LEU:O	1:E:548:ILE:HG13	2.07	0.55
1:F:644:VAL:O	1:F:648:THR:HG23	2.06	0.55
1:F:197:GLN:HA	1:F:798:MET:SD	2.47	0.55
1:B:448:VAL:HG13	1:B:884:VAL:HG22	1.89	0.54
1:C:735:LYS:O	1:C:739:LEU:HG	2.06	0.54
1:C:743:ILE:HD12	1:C:743:ILE:H	1.73	0.54
1:D:393:LEU:HD22	1:D:470:PHE:HE1	1.72	0.54
1:E:702:LEU:HD11	1:E:847:LEU:HB3	1.88	0.54
1:F:705:GLU:HA	1:F:708:LYS:NZ	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HG	1:A:231:ASN:N	2.21	0.54
1:B:235:ILE:O	1:C:728:LYS:HD2	2.07	0.54
1:D:45:ILE:HA	1:D:128:SER:O	2.06	0.54
1:F:590:VAL:O	1:F:593:GLU:HB2	2.07	0.54
1:B:743:ILE:HA	1:B:746:ILE:HD12	1.89	0.54
1:D:583:THR:HG21	1:F:229:GLN:HA	1.88	0.54
1:D:888:LEU:HD22	1:D:901:VAL:HG11	1.89	0.54
1:E:396:PHE:HD1	1:E:926:TYR:HE2	1.55	0.54
1:F:1021:PHE:HB3	1:F:1025:PHE:CE1	2.43	0.54
1:F:559:LEU:HD23	1:F:560:PRO:CD	2.37	0.54
1:E:82:SER:HA	1:E:88:VAL:HG22	1.88	0.54
1:F:358:PHE:CD2	1:F:977:MET:HG3	2.41	0.54
1:D:687:GLN:HG2	1:F:316:PHE:CD1	2.42	0.54
1:D:969:ARG:NH1	1:D:970:MET:HB3	2.23	0.54
1:C:307:ARG:NH2	1:C:314:GLU:OE2	2.38	0.54
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.89	0.54
1:F:166:ILE:HG22	1:F:175:VAL:HG21	1.90	0.54
1:F:905:VAL:HG13	1:F:935:ILE:HG12	1.90	0.54
1:B:531:VAL:O	1:B:534:ILE:HG13	2.08	0.54
1:C:200:PRO:HB2	1:C:749:THR:HG22	1.89	0.54
1:C:671:ILE:HD13	1:C:674:LEU:HD12	1.90	0.54
1:D:420:MET:HB3	1:D:500:ILE:HB	1.90	0.54
1:A:6:ILE:HD11	1:A:432:ARG:HE	1.73	0.54
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.89	0.54
1:A:685:ILE:HD11	1:A:819:TYR:HD2	1.72	0.54
1:B:492:LEU:O	1:B:496:MET:HG2	2.08	0.54
1:D:137:LEU:HD23	1:D:291:ILE:HG22	1.89	0.54
1:F:121:GLU:O	1:F:124:GLN:HG2	2.08	0.54
1:B:610:PHE:HB3	1:B:628:PHE:HB3	1.90	0.54
1:F:159:ALA:HB2	1:F:177:LEU:HD11	1.88	0.54
1:F:841:MET:O	1:F:845:GLU:HG2	2.08	0.54
1:B:892:TYR:O	1:B:893:GLU:HB2	2.08	0.54
1:C:356:TYR:HA	1:C:365:THR:HG21	1.89	0.54
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.89	0.54
1:E:391:ASN:O	1:E:395:MET:HG2	2.07	0.54
1:E:680:PHE:HB2	1:E:863:SER:OG	2.07	0.54
1:E:776:GLU:HB3	1:E:779:TYR:CD1	2.43	0.54
1:F:775:SER:OG	1:F:780:ARG:HG2	2.08	0.54
1:A:159:ALA:HB2	1:A:177:LEU:HD11	1.89	0.53
1:A:685:ILE:HD11	1:A:819:TYR:CD2	2.43	0.53
1:B:932:LEU:HD23	1:B:935:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:TYR:O	1:C:358:PHE:N	2.41	0.53
1:E:375:VAL:O	1:E:379:THR:OG1	2.22	0.53
1:F:187:TRP:HE3	1:F:775:SER:O	1.91	0.53
1:F:188:MET:HA	1:F:266:ALA:CB	2.37	0.53
1:F:559:LEU:HD23	1:F:560:PRO:HD2	1.89	0.53
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.90	0.53
1:A:913:LEU:HD23	1:A:927:PHE:CZ	2.44	0.53
1:B:187:TRP:HE3	1:B:775:SER:O	1.91	0.53
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.08	0.53
1:E:680:PHE:HE2	1:E:829:GLY:HA3	1.73	0.53
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.91	0.53
1:C:356:TYR:C	1:C:358:PHE:N	2.62	0.53
1:C:456:MET:HB3	1:C:876:LEU:HD21	1.89	0.53
1:C:58:GLN:HA	1:C:62:THR:HB	1.88	0.53
1:C:913:LEU:HD23	1:C:927:PHE:HZ	1.72	0.53
1:C:75:LEU:HD11	1:C:92:LEU:HD12	1.90	0.53
1:D:61:VAL:HG21	1:D:122:VAL:HG21	1.89	0.53
1:E:447:MET:HB3	1:E:887:CYS:SG	2.48	0.53
1:F:113:LEU:O	1:F:116:PRO:HD2	2.07	0.53
1:F:272:GLY:N	1:F:275:TYR:OH	2.34	0.53
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.08	0.53
1:A:801:PHE:HA	1:A:804:PHE:CE2	2.44	0.53
1:B:327:TYR:HB2	1:B:628:PHE:HE2	1.74	0.53
1:C:591:LEU:HD11	1:C:625:GLY:HA3	1.89	0.53
1:C:644:VAL:HG11	1:C:667:ASN:HB2	1.91	0.53
1:D:587:THR:OG1	1:D:622:GLN:O	2.19	0.53
1:D:676:THR:O	3:D:1103:LMT:O6B	2.14	0.53
1:E:327:TYR:CD1	1:E:628:PHE:HZ	2.24	0.53
1:F:913:LEU:HD23	1:F:927:PHE:HZ	1.73	0.53
1:A:41:PRO:HD3	1:A:96:SER:HA	1.91	0.53
1:B:485:ALA:O	1:B:490:PRO:HD3	2.08	0.53
1:B:5:PHE:CE1	1:B:487:ILE:HG12	2.44	0.53
1:D:156:ASP:OD2	1:D:769:LYS:NZ	2.32	0.53
1:D:155:SER:HB3	1:D:180:SER:H	1.73	0.53
1:D:366:LEU:HA	1:D:369:THR:HB	1.91	0.53
1:E:102:ILE:O	1:E:106:GLN:HG3	2.09	0.53
1:E:549:VAL:O	1:E:552:MET:HB3	2.08	0.53
1:F:195:LYS:NZ	1:F:196:PHE:HE1	2.06	0.53
1:A:418:ARG:NH2	1:A:948:PHE:HE2	2.06	0.53
1:B:166:ILE:HD11	1:B:310:LEU:CD1	2.39	0.53
1:C:293:LEU:HD11	1:C:297:ALA:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:VAL:HG22	1:D:390:ILE:HB	1.89	0.53
1:D:712:MET:SD	1:D:835:LYS:HE2	2.49	0.53
1:E:743:ILE:H	1:E:743:ILE:HD12	1.74	0.53
1:B:23:GLY:HA2	1:B:381:ALA:HB2	1.90	0.53
1:E:589:LYS:O	1:E:592:ASN:HB2	2.08	0.53
1:E:225:VAL:HG12	1:F:777:ALA:HB1	1.91	0.53
1:F:979:SER:OG	1:F:1015:THR:HG21	2.08	0.53
1:C:960:LEU:O	1:C:964:THR:HG23	2.08	0.53
1:D:99:ASP:HB3	1:D:102:ILE:HB	1.91	0.53
1:E:407:ASP:O	1:E:411:VAL:HG23	2.08	0.53
1:F:184:MET:HB2	1:F:762:PHE:CE2	2.44	0.53
1:F:453:PHE:HZ	1:F:933:THR:HG1	1.56	0.53
1:B:682:PHE:HB3	1:B:827:ILE:HB	1.91	0.53
1:E:213:GLN:HE21	1:E:239:ARG:HG3	1.72	0.53
1:E:38:ILE:HG22	1:E:462:SER:HB3	1.91	0.53
1:F:960:LEU:HD21	1:F:1027:VAL:HA	1.91	0.53
1:A:971:ARG:C	1:A:974:PRO:HD2	2.29	0.53
1:D:274:ASN:ND2	1:D:276:ASP:OD2	2.38	0.53
1:F:727:PHE:CE1	1:F:783:PRO:HB3	2.43	0.53
1:A:533:GLY:O	1:A:536:ARG:HB2	2.08	0.52
1:C:53:ASP:OD1	1:C:56:THR:OG1	2.08	0.52
1:C:686:ASP:HB3	1:C:823:PRO:HB2	1.91	0.52
1:D:696:THR:HA	1:D:699:ARG:NH1	2.25	0.52
1:E:568:ASP:O	1:E:634:TRP:HZ3	1.92	0.52
1:F:188:MET:HB3	1:F:193:LEU:HD11	1.92	0.52
1:F:456:MET:HB3	1:F:876:LEU:HD21	1.90	0.52
1:F:616:GLY:HA2	1:F:626:ILE:HD12	1.89	0.52
1:F:414:GLU:HG2	1:F:973:ARG:NH1	2.24	0.52
1:A:648:THR:HB	1:A:665:ALA:O	2.09	0.52
1:A:937:LEU:O	1:A:940:LYS:HB3	2.08	0.52
1:C:841:MET:HG2	1:C:859:TRP:CH2	2.44	0.52
1:D:272:GLY:N	1:D:275:TYR:OH	2.40	0.52
1:D:400:LEU:HD23	1:D:929:VAL:HG12	1.90	0.52
1:E:910:ILE:O	1:E:914:LEU:HB2	2.09	0.52
3:F:1101:LMT:H3O2	3:F:1101:LMT:H2O1	1.56	0.52
1:A:857:TYR:HE2	1:C:312:LYS:NZ	2.08	0.52
1:C:427:PRO:HD3	1:C:499:PRO:HB3	1.91	0.52
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.44	0.52
1:D:728:LYS:HG2	1:D:808:ARG:CZ	2.39	0.52
1:F:576:VAL:HG22	1:F:663:VAL:HG13	1.91	0.52
1:F:587:THR:OG1	1:F:613:ASN:ND2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ALA:HA	1:C:314:GLU:CD	2.30	0.52
1:E:441:ALA:HA	1:E:891:LEU:HD21	1.90	0.52
1:F:463:THR:HG22	1:F:467:TYR:CZ	2.44	0.52
1:B:950:LYS:HZ1	1:B:1030:ARG:CZ	2.22	0.52
1:B:165:ALA:HB3	1:B:313:MET:CE	2.40	0.52
1:B:778:LYS:HG3	1:B:779:TYR:CE1	2.45	0.52
1:B:971:ARG:O	1:B:975:ILE:HG12	2.10	0.52
1:C:699:ARG:HD3	1:C:825:MET:SD	2.48	0.52
1:D:545:TYR:HB2	1:D:1021:PHE:CE2	2.44	0.52
1:D:47:ALA:HB2	1:D:127:VAL:HG13	1.91	0.52
1:E:968:VAL:HG21	1:E:1023:PRO:HG3	1.91	0.52
1:E:521:GLU:HA	1:E:524:THR:HG22	1.91	0.52
1:F:588:GLN:NE2	1:F:592:ASN:OD1	2.43	0.52
1:F:937:LEU:HD11	1:F:982:PHE:CE2	2.45	0.52
1:F:343:THR:HG21	1:F:989:LEU:CD2	2.39	0.52
1:A:318:PRO:HD2	1:A:321:LEU:HG	1.91	0.52
1:B:9:PRO:HG2	1:B:10:ILE:HD12	1.92	0.52
1:B:344:LEU:O	1:B:348:ILE:HG13	2.08	0.52
1:E:375:VAL:HG13	1:E:480:LEU:HB3	1.91	0.52
1:F:1040:ILE:CA	1:F:1041:GLU:HB2	2.31	0.52
1:F:412:VAL:O	1:F:416:VAL:HG23	2.10	0.52
1:F:568:ASP:OD1	1:F:637:ARG:NH1	2.41	0.52
1:F:77:TYR:HB2	1:F:819:TYR:CE1	2.45	0.52
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.44	0.52
1:A:901:VAL:HG21	1:A:943:ILE:CG1	2.40	0.52
1:D:184:MET:HB3	1:D:771:VAL:HG13	1.92	0.52
1:E:165:ALA:HB3	1:E:313:MET:HE3	1.91	0.52
1:B:544:LEU:HD23	1:B:1021:PHE:CZ	2.45	0.52
1:B:185:ARG:HD2	1:B:772:TYR:HB2	1.92	0.52
1:C:1036:LYS:O	1:C:1037:ASN:ND2	2.39	0.52
1:C:382:VAL:HG21	1:C:476:SER:HB2	1.91	0.52
1:C:531:VAL:O	1:C:534:ILE:HG13	2.09	0.52
1:C:610:PHE:O	1:C:627:ALA:HA	2.10	0.52
1:C:5:PHE:CD2	1:C:6:ILE:HG12	2.45	0.52
1:B:228:GLN:OE1	1:C:781:MET:HB3	2.09	0.52
1:C:354:VAL:HG23	1:C:984:LEU:HD12	1.90	0.52
1:D:146:ASP:HB2	1:D:148:THR:HG23	1.91	0.52
1:D:728:LYS:HB2	1:D:810:GLU:CD	2.31	0.52
1:E:185:ARG:HB3	1:E:187:TRP:NE1	2.25	0.52
1:E:375:VAL:HG13	1:E:480:LEU:CB	2.40	0.52
1:E:534:ILE:CD1	1:E:1024:VAL:HG22	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:564:LEU:HD13	1:E:671:ILE:HD12	1.92	0.52
1:F:13:TRP:CH2	1:F:370:ILE:HD13	2.45	0.52
1:F:183:ALA:O	1:F:270:LEU:HD12	2.10	0.52
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.45	0.52
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.92	0.52
1:A:743:ILE:HD12	1:A:743:ILE:H	1.75	0.52
1:A:910:ILE:O	1:A:914:LEU:HB2	2.10	0.52
1:B:418:ARG:HD3	1:B:970:MET:HB2	1.91	0.52
1:B:363:ARG:HD2	1:B:498:LYS:HG3	1.92	0.52
1:E:579:PRO:HD3	1:E:661:ALA:HB2	1.92	0.52
1:D:768:VAL:HG12	1:E:63:GLN:OE1	2.09	0.52
1:F:982:PHE:HD2	1:F:1011:MET:HG2	1.74	0.52
1:A:391:ASN:O	1:A:395:MET:HG2	2.10	0.51
1:A:897:ILE:HD11	1:A:1030:ARG:HD3	1.92	0.51
1:B:185:ARG:HH11	1:B:772:TYR:HB3	1.76	0.51
1:C:453:PHE:HD2	1:C:456:MET:CE	2.23	0.51
1:C:743:ILE:HA	1:C:746:ILE:HG23	1.92	0.51
1:F:64:VAL:HG12	1:F:114:ALA:HB1	1.91	0.51
1:F:143:ILE:O	1:F:321:LEU:HD22	2.10	0.51
1:F:447:MET:SD	1:F:887:CYS:HB3	2.50	0.51
1:F:549:VAL:O	1:F:552:MET:HB3	2.10	0.51
1:A:953:MET:HE2	1:A:963:ALA:HB3	1.92	0.51
1:C:153:ASP:OD2	1:C:182:TYR:OH	2.28	0.51
1:B:766:GLY:O	1:C:59:ASP:HB2	2.10	0.51
1:D:672:VAL:HB	1:D:673:GLU:OE2	2.10	0.51
1:A:775:SER:HB3	1:A:780:ARG:HD3	1.92	0.51
1:B:602:GLU:HB3	1:B:606:VAL:HG23	1.92	0.51
1:D:242:SER:OG	1:D:245:GLU:HG2	2.10	0.51
1:E:363:ARG:HD3	1:E:496:MET:O	2.11	0.51
1:E:423:GLU:OE1	1:E:433:LYS:HE3	2.11	0.51
1:E:653:ARG:O	1:E:656:SER:OG	2.25	0.51
1:F:34:GLN:HB2	1:F:333:VAL:CG2	2.38	0.51
1:F:453:PHE:O	1:F:471:SER:OG	2.19	0.51
1:A:574:THR:HG21	1:A:598:TYR:CE2	2.46	0.51
1:A:575:MET:HG3	1:A:664:PHE:HB2	1.92	0.51
1:B:418:ARG:HB3	1:B:418:ARG:CZ	2.40	0.51
1:B:431:THR:HG21	1:B:494:ALA:HB2	1.92	0.51
1:C:925:VAL:O	1:C:928:GLN:N	2.43	0.51
1:D:408:ASP:OD2	1:D:940:LYS:NZ	2.40	0.51
1:D:400:LEU:HD21	1:D:930:GLY:HA2	1.93	0.51
1:E:166:ILE:O	1:E:169:THR:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:562:SER:HB3	1:E:924:ASP:HB3	1.91	0.51
1:A:85:THR:HG21	1:A:620:ALA:HB3	1.92	0.51
1:A:9:PRO:HG2	1:A:10:ILE:HD12	1.93	0.51
1:B:946:VAL:HG13	1:B:1026:PHE:CD1	2.45	0.51
1:B:242:SER:HB2	1:B:245:GLU:HG3	1.93	0.51
1:C:945:ILE:CG1	1:C:971:ARG:HH22	2.24	0.51
1:D:194:ASN:CG	1:D:790:TYR:HD2	2.14	0.51
1:D:400:LEU:CD2	1:D:929:VAL:HG12	2.40	0.51
1:F:530:SER:OG	3:F:1101:LMT:O2'	2.12	0.51
1:F:534:ILE:HG22	3:F:1101:LMT:H5'	1.92	0.51
1:F:702:LEU:HD12	1:F:851:LEU:HD11	1.93	0.51
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.93	0.51
1:B:58:GLN:HA	1:B:62:THR:HB	1.92	0.51
1:C:669:PRO:HD3	1:C:677:ALA:O	2.11	0.51
1:C:751:GLY:O	1:C:754:TRP:N	2.44	0.51
1:C:971:ARG:HG2	1:C:974:PRO:HG3	1.93	0.51
1:D:219:LEU:O	1:D:231:ASN:ND2	2.43	0.51
1:E:754:TRP:CZ2	1:E:786:ILE:HD13	2.46	0.51
1:E:960:LEU:HD21	1:E:1027:VAL:HA	1.93	0.51
1:F:3:ASN:HD22	1:F:435:MET:HG3	1.75	0.51
1:D:699:ARG:NH2	1:D:722:GLU:OE1	2.44	0.51
1:F:801:PHE:CD1	1:F:804:PHE:HE2	2.29	0.51
1:F:560:PRO:HB2	1:F:836:SER:OG	2.11	0.51
1:A:377:LEU:O	1:A:380:PHE:HB2	2.10	0.51
1:A:426:PRO:HB2	1:A:429:GLU:OE2	2.11	0.51
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.92	0.51
1:D:946:VAL:HG13	1:D:1026:PHE:CD1	2.46	0.51
1:F:378:GLY:O	1:F:382:VAL:HG23	2.10	0.51
1:F:948:PHE:CE1	1:F:971:ARG:HD3	2.45	0.51
1:A:404:LEU:HD21	1:A:449:LEU:HD22	1.92	0.51
1:B:423:GLU:O	1:B:502:LYS:HD2	2.10	0.51
1:B:758:TYR:HE1	1:B:770:LYS:HG2	1.76	0.51
1:C:382:VAL:HG11	1:C:476:SER:HB3	1.93	0.51
1:D:634:TRP:CD1	1:D:634:TRP:N	2.74	0.51
1:E:291:ILE:HG21	1:E:306:ILE:HD11	1.92	0.51
1:E:340:VAL:O	1:E:344:LEU:HG	2.11	0.51
1:E:80:SER:HB3	1:E:90:ILE:HG12	1.92	0.51
1:F:254:ASN:HB2	1:F:258:SER:O	2.10	0.51
1:F:598:TYR:CE2	1:F:629:VAL:HG21	2.46	0.51
1:F:898:PRO:O	1:F:902:MET:HG2	2.11	0.51
1:A:1036:LYS:HA	1:A:1038:GLU:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLY:HA3	1:A:230:LEU:O	2.11	0.50
1:A:683:GLU:HG2	1:A:819:TYR:CD2	2.46	0.50
1:C:380:PHE:HA	1:C:383:LEU:HD12	1.93	0.50
1:D:520:PHE:O	1:D:524:THR:HG22	2.10	0.50
1:D:533:GLY:O	1:D:536:ARG:HB2	2.10	0.50
1:F:356:TYR:C	1:F:358:PHE:H	2.14	0.50
1:F:504:ASP:C	1:F:506:GLY:H	2.13	0.50
1:B:270:LEU:HD11	1:B:762:PHE:HZ	1.76	0.50
1:B:419:VAL:HG21	1:B:434:SER:HB3	1.93	0.50
1:C:1040:ILE:O	1:C:1041:GLU:HG3	2.11	0.50
1:D:350:LEU:HD13	1:D:984:LEU:HB3	1.93	0.50
1:E:1041:GLU:HB3	1:E:1042:HIS:CB	2.41	0.50
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.93	0.50
1:D:1040:ILE:HG12	1:D:1041:GLU:H	1.75	0.50
1:D:728:LYS:HB2	1:D:810:GLU:OE1	2.10	0.50
1:F:140:VAL:HG11	1:F:310:LEU:HD21	1.93	0.50
1:D:150:THR:OG1	1:D:152:GLU:HG2	2.11	0.50
1:D:888:LEU:HB2	1:D:898:PRO:HB3	1.93	0.50
1:F:222:THR:HA	1:F:224:PRO:HD3	1.93	0.50
1:F:971:ARG:HB3	1:F:971:ARG:NH1	2.26	0.50
1:A:1033:PHE:CD2	1:A:1034:SER:N	2.80	0.50
1:A:330:THR:HB	1:A:331:PRO:HD3	1.93	0.50
1:A:420:MET:HB3	1:A:500:ILE:HB	1.92	0.50
1:B:950:LYS:HZ1	1:B:1030:ARG:NH2	2.09	0.50
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.46	0.50
1:A:316:PHE:CG	1:B:687:GLN:HG2	2.46	0.50
1:C:298:ASN:ND2	1:C:301:ASP:OD2	2.41	0.50
1:F:58:GLN:HA	1:F:62:THR:HB	1.93	0.50
1:A:17:ILE:HG22	1:B:886:LEU:HD21	1.93	0.50
1:A:857:TYR:H	1:A:857:TYR:HD2	1.59	0.50
1:C:1043:SER:HB2	1:C:1044:HIS:HB3	1.93	0.50
1:E:36:PRO:HD3	1:E:391:ASN:OD1	2.11	0.50
1:E:72:ILE:HD13	1:E:107:VAL:HG22	1.94	0.50
1:E:897:ILE:N	1:E:898:PRO:HD2	2.26	0.50
1:F:559:LEU:HD21	1:F:922:THR:HA	1.93	0.50
1:B:583:THR:HG22	1:B:585:GLU:H	1.76	0.50
1:C:1043:SER:CB	1:C:1044:HIS:HB3	2.41	0.50
1:D:368:PRO:HG3	1:D:413:VAL:HG21	1.92	0.50
1:D:393:LEU:HD11	1:D:466:ILE:HD12	1.94	0.50
1:F:743:ILE:HD12	1:F:743:ILE:H	1.75	0.50
1:C:757:SER:O	1:C:772:TYR:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:876:LEU:HD22	1:C:932:LEU:HD11	1.94	0.50
1:D:108:GLN:OE1	1:D:129:VAL:HB	2.12	0.50
1:D:457:ALA:HA	1:D:468:ARG:HA	1.93	0.50
1:E:362:PHE:O	1:E:365:THR:HG22	2.11	0.50
1:E:412:VAL:O	1:E:416:VAL:HG23	2.12	0.50
1:F:801:PHE:HA	1:F:804:PHE:CE2	2.47	0.50
1:B:149:MET:HB2	1:B:153:ASP:HB2	1.94	0.50
1:C:284:GLN:HG3	1:C:285:PRO:HD2	1.94	0.50
1:C:479:ALA:O	1:C:482:VAL:HG23	2.11	0.50
1:C:574:THR:HG21	1:C:598:TYR:CE2	2.45	0.50
1:D:419:VAL:HG11	1:D:433:LYS:HG2	1.94	0.50
1:E:507:GLU:HG2	1:E:518:ARG:HA	1.94	0.50
1:E:525:HIS:HA	1:E:528:THR:HG22	1.93	0.50
1:E:530:SER:OG	3:E:1101:LMT:O2'	2.12	0.50
1:B:682:PHE:CD2	1:B:827:ILE:HD12	2.47	0.49
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.92	0.49
1:C:465:ALA:O	1:C:469:GLN:HG2	2.12	0.49
1:D:58:GLN:HA	1:D:62:THR:HB	1.93	0.49
1:E:225:VAL:HG13	1:F:781:MET:SD	2.51	0.49
1:E:355:MET:SD	1:E:368:PRO:HG2	2.51	0.49
1:E:841:MET:O	1:E:845:GLU:HG3	2.12	0.49
1:F:531:VAL:O	1:F:534:ILE:HG13	2.12	0.49
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.94	0.49
1:A:728:LYS:HB2	1:A:810:GLU:OE1	2.13	0.49
1:B:151:GLN:OE1	1:B:278:ILE:HA	2.12	0.49
1:A:17:ILE:CG2	1:B:886:LEU:HD21	2.43	0.49
1:E:102:ILE:O	1:E:105:VAL:HG12	2.12	0.49
1:E:219:LEU:HD12	1:E:232:ALA:HB3	1.94	0.49
1:E:404:LEU:HD21	1:E:449:LEU:HD22	1.94	0.49
1:F:61:VAL:HA	1:F:118:LEU:CD2	2.42	0.49
1:F:187:TRP:HA	1:F:774:MET:O	2.12	0.49
1:B:903:LEU:HB3	1:B:1025:PHE:CZ	2.47	0.49
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.95	0.49
1:D:375:VAL:HB	1:D:405:LEU:HD13	1.95	0.49
1:D:928:GLN:HE22	3:D:1103:LMT:H12	1.77	0.49
1:E:415:ASN:O	1:E:419:VAL:HG23	2.12	0.49
1:F:380:PHE:O	1:F:383:LEU:HB2	2.12	0.49
1:F:636:ASP:C	1:F:638:PRO:HD3	2.33	0.49
1:B:3:ASN:HD21	1:B:432:ARG:HD3	1.75	0.49
1:B:435:MET:HG3	1:B:490:PRO:HB3	1.94	0.49
1:B:424:GLY:HA3	1:B:502:LYS:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:GLN:HA	1:C:123:GLN:HB2	1.94	0.49
1:C:407:ASP:O	1:C:411:VAL:HG23	2.12	0.49
1:D:743:ILE:HG23	1:D:746:ILE:HD12	1.94	0.49
1:E:713:LEU:HD11	1:E:843:LEU:HD12	1.93	0.49
1:A:165:ALA:HB3	1:A:313:MET:HE1	1.95	0.49
1:A:252:LYS:HE3	1:A:260:VAL:HG21	1.93	0.49
1:A:776:GLU:HB3	1:A:779:TYR:CD1	2.47	0.49
1:A:682:PHE:HB3	1:A:827:ILE:HB	1.94	0.49
1:C:242:SER:CB	1:C:245:GLU:HG3	2.41	0.49
1:C:568:ASP:O	1:C:634:TRP:CH2	2.66	0.49
1:C:764:ASP:OD1	1:C:765:ARG:HG3	2.12	0.49
1:D:239:ARG:HD2	1:D:761:ASP:O	2.12	0.49
1:A:35:TYR:HE1	1:A:670:ALA:HB1	1.76	0.49
1:A:435:MET:HG3	1:A:490:PRO:HB3	1.95	0.49
1:A:671:ILE:HG22	1:A:674:LEU:HB3	1.93	0.49
1:C:242:SER:HB2	1:C:245:GLU:H	1.77	0.49
1:C:434:SER:O	1:C:438:ILE:HG12	2.13	0.49
1:C:455:PRO:HG2	1:C:880:SER:HA	1.94	0.49
1:C:948:PHE:O	1:C:952:LEU:HG	2.12	0.49
1:D:598:TYR:HB3	1:D:606:VAL:HG11	1.93	0.49
1:D:752:ALA:O	1:D:774:MET:HA	2.12	0.49
1:E:137:LEU:HD12	1:E:329:THR:HG22	1.94	0.49
1:E:575:MET:HE3	1:E:617:ALA:HB3	1.94	0.49
1:E:736:ALA:HB1	1:E:746:ILE:HD11	1.94	0.49
1:F:990:VAL:HG13	1:F:1005:THR:OG1	2.13	0.49
1:F:571:VAL:N	1:F:631:LEU:HD12	2.27	0.49
1:C:897:ILE:HD12	1:C:946:VAL:CG1	2.43	0.49
1:E:121:GLU:O	1:E:125:GLN:HB2	2.13	0.49
1:A:1037:ASN:HA	1:A:1038:GLU:HB2	1.94	0.49
1:A:676:THR:H	1:A:862:MET:HE3	1.78	0.49
1:C:108:GLN:HB3	1:C:129:VAL:HG11	1.94	0.49
1:D:225:VAL:HG13	1:E:781:MET:SD	2.53	0.49
1:E:234:ILE:HD11	1:F:754:TRP:CE3	2.47	0.49
1:F:33:ALA:O	1:F:391:ASN:HA	2.13	0.49
1:F:11:PHE:O	1:F:15:ILE:HG13	2.13	0.49
1:F:15:ILE:O	1:F:19:ILE:HG13	2.13	0.49
1:F:897:ILE:O	1:F:901:VAL:HG12	2.12	0.49
1:A:137:LEU:HD22	1:A:293:LEU:HG	1.94	0.49
1:A:6:ILE:HG22	1:A:490:PRO:HB2	1.94	0.49
1:A:680:PHE:HD1	1:A:859:TRP:HZ3	1.60	0.49
1:B:946:VAL:HG13	1:B:1026:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:GLY:O	1:C:382:VAL:HG23	2.12	0.49
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.94	0.49
1:D:164:ASP:HB3	1:D:168:ARG:NH2	2.25	0.49
1:F:49:TYR:HD1	1:F:57:VAL:HG12	1.78	0.49
1:F:563:PHE:CD2	1:F:564:LEU:HB2	2.48	0.49
1:F:971:ARG:C	1:F:974:PRO:HD2	2.33	0.49
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.48	0.48
1:B:455:PRO:O	1:B:876:LEU:HD13	2.13	0.48
1:C:150:THR:O	1:C:154:ILE:HG13	2.13	0.48
1:C:254:ASN:HB2	1:C:258:SER:O	2.13	0.48
1:D:583:THR:HA	1:D:622:GLN:OE1	2.12	0.48
1:A:246:PHE:HA	1:A:249:ILE:HG13	1.95	0.48
1:A:350:LEU:HD13	1:A:984:LEU:O	2.13	0.48
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.95	0.48
1:A:979:SER:OG	1:A:1015:THR:HG21	2.13	0.48
1:B:1024:VAL:O	1:B:1028:VAL:HG23	2.13	0.48
1:C:832:ALA:O	1:C:835:LYS:HB2	2.13	0.48
1:B:10:ILE:HB	1:C:893:GLU:OE1	2.13	0.48
1:D:986:VAL:HG21	1:D:1007:VAL:HG11	1.94	0.48
1:E:1016:VAL:HG12	1:E:1016:VAL:O	2.13	0.48
1:A:404:LEU:HD12	1:A:937:LEU:CD2	2.42	0.48
1:B:58:GLN:O	1:B:63:GLN:HG3	2.13	0.48
1:B:790:TYR:HD1	1:B:800:PRO:HA	1.78	0.48
1:C:211:ASN:OD1	1:C:240:LEU:N	2.42	0.48
1:C:910:ILE:O	1:C:914:LEU:HB2	2.12	0.48
1:E:567:GLU:HG3	1:E:670:ALA:HB2	1.94	0.48
1:A:420:MET:HB2	1:A:500:ILE:HD12	1.96	0.48
1:A:281:PHE:CZ	1:A:608:SER:HB2	2.48	0.48
1:A:792:ARG:HB2	1:A:798:MET:SD	2.53	0.48
1:B:678:THR:HA	1:B:837:THR:OG1	2.13	0.48
1:B:695:LEU:HD22	1:B:825:MET:SD	2.53	0.48
1:C:913:LEU:HD23	1:C:927:PHE:CZ	2.47	0.48
1:D:197:GLN:HA	1:D:798:MET:SD	2.53	0.48
1:D:391:ASN:O	1:D:395:MET:HG2	2.13	0.48
1:F:58:GLN:O	1:F:62:THR:HB	2.14	0.48
1:D:893:GLU:OE1	1:F:8:ARG:HB3	2.13	0.48
1:A:636:ASP:O	1:A:638:PRO:HD3	2.13	0.48
1:A:187:TRP:HA	1:A:774:MET:O	2.13	0.48
1:B:352:PHE:C	1:B:352:PHE:CD2	2.87	0.48
1:B:416:VAL:HG21	1:B:493:CYS:SG	2.54	0.48
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1019:ILE:HG13	1:D:1020:PHE:CD1	2.48	0.48
1:E:987:MET:HA	1:E:1008:MET:HE3	1.95	0.48
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.95	0.48
1:A:378:GLY:O	1:A:381:ALA:HB3	2.14	0.48
1:B:211:ASN:ND2	1:B:760:ASN:HD22	2.11	0.48
1:B:765:ARG:HH21	1:B:769:LYS:HZ1	1.61	0.48
1:B:762:PHE:HE2	1:B:770:LYS:O	1.97	0.48
1:B:7:ASP:O	1:B:8:ARG:HG3	2.13	0.48
1:B:801:PHE:HA	1:B:804:PHE:CE2	2.48	0.48
1:D:946:VAL:HG13	1:D:1026:PHE:CE1	2.48	0.48
1:D:94:PHE:CZ	1:D:103:ALA:HB1	2.48	0.48
1:D:422:GLU:HB3	1:D:423:GLU:HG3	1.95	0.48
1:E:696:THR:HG23	1:E:699:ARG:NH1	2.24	0.48
1:E:753:ALA:O	1:E:775:SER:HB3	2.13	0.48
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.95	0.48
1:A:382:VAL:O	1:A:386:PHE:HD1	1.97	0.48
1:B:27:ILE:HD13	1:B:380:PHE:CD1	2.48	0.48
1:D:27:ILE:HD11	1:D:380:PHE:CD1	2.49	0.48
1:E:545:TYR:OH	1:E:903:LEU:O	2.26	0.48
1:F:746:ILE:HG22	1:F:791:VAL:HG11	1.95	0.48
1:A:591:LEU:HD11	1:A:625:GLY:HA3	1.96	0.48
1:A:568:ASP:CG	1:A:637:ARG:HH22	2.17	0.48
1:A:919:ARG:HG2	1:A:920:GLY:H	1.79	0.48
1:B:644:VAL:O	1:B:648:THR:HG23	2.13	0.48
1:D:801:PHE:HA	1:D:804:PHE:CE2	2.49	0.48
1:E:682:PHE:HZ	1:E:857:TYR:HB2	1.73	0.48
1:E:690:LEU:HD13	1:E:694:LYS:HB3	1.96	0.48
1:F:366:LEU:O	1:F:370:ILE:HG13	2.13	0.48
1:F:412:VAL:HG23	1:F:442:LEU:HD21	1.96	0.48
1:A:888:LEU:HD22	1:A:901:VAL:HG11	1.95	0.48
1:B:291:ILE:HG21	1:B:306:ILE:CD1	2.43	0.48
1:C:201:VAL:HG22	1:C:748:THR:OG1	2.13	0.48
1:D:449:LEU:HB3	1:D:478:MET:SD	2.54	0.48
1:D:55:LYS:NZ	1:F:238:THR:HG23	2.29	0.48
1:E:281:PHE:CZ	1:E:324:VAL:HG21	2.49	0.48
1:F:744:ASN:O	1:F:748:THR:HG23	2.13	0.48
1:F:983:ILE:O	1:F:987:MET:HB2	2.14	0.48
1:A:610:PHE:O	1:A:627:ALA:HA	2.13	0.48
1:B:139:VAL:HB	1:B:327:TYR:HB3	1.96	0.48
1:B:588:GLN:HB2	1:B:613:ASN:HD22	1.78	0.48
1:C:751:GLY:O	1:C:753:ALA:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:726:GLN:CD	1:E:812:GLY:HA3	2.34	0.48
1:E:44:THR:HG1	1:E:91:THR:HG1	1.60	0.48
1:F:1025:PHE:O	1:F:1029:VAL:HG23	2.13	0.48
1:F:409:ALA:O	1:F:413:VAL:HG23	2.13	0.48
1:F:548:ILE:O	1:F:910:ILE:HD13	2.13	0.48
1:A:686:ASP:HB2	1:A:695:LEU:HD12	1.96	0.47
1:A:726:GLN:OE1	1:A:812:GLY:HA3	2.13	0.47
1:A:953:MET:HE1	1:A:960:LEU:HD12	1.96	0.47
1:B:898:PRO:O	1:B:902:MET:HG3	2.13	0.47
1:C:228:GLN:HE21	1:C:230:LEU:H	1.62	0.47
1:D:913:LEU:HD23	1:D:927:PHE:CZ	2.48	0.47
1:E:733:GLN:NE2	1:E:743:ILE:HG21	2.26	0.47
1:F:456:MET:HB2	1:F:876:LEU:HD11	1.95	0.47
1:F:446:ALA:HA	1:F:478:MET:HE2	1.95	0.47
1:A:442:LEU:O	1:A:445:ILE:HG13	2.13	0.47
1:B:1040:ILE:HG23	1:B:1041:GLU:N	2.29	0.47
1:B:146:ASP:OD2	1:B:146:ASP:N	2.46	0.47
1:B:412:VAL:O	1:B:416:VAL:HG23	2.14	0.47
1:C:456:MET:HE3	1:C:467:TYR:O	2.14	0.47
1:C:58:GLN:OE1	1:C:816:LEU:HB3	2.14	0.47
1:D:316:PHE:CG	1:E:687:GLN:HG2	2.49	0.47
1:F:150:THR:N	1:F:153:ASP:OD1	2.42	0.47
1:F:201:VAL:HA	1:F:204:ILE:HD12	1.96	0.47
1:F:251:LEU:HD11	1:F:262:LEU:HA	1.96	0.47
1:F:453:PHE:CE1	1:F:474:ILE:HG21	2.49	0.47
1:F:525:HIS:HA	1:F:528:THR:HG22	1.95	0.47
1:A:905:VAL:O	1:A:909:VAL:HG23	2.14	0.47
1:C:388:PHE:HE2	1:C:472:ILE:HG13	1.78	0.47
1:B:971:ARG:NH1	1:B:971:ARG:HB3	2.29	0.47
1:C:78:MET:HG3	1:C:92:LEU:HD13	1.96	0.47
1:D:781:MET:HB3	1:F:228:GLN:HE22	1.78	0.47
1:E:38:ILE:HG23	1:E:465:ALA:HB3	1.94	0.47
1:E:756:GLY:CA	1:E:774:MET:HG3	2.45	0.47
1:F:520:PHE:O	1:F:524:THR:HG22	2.13	0.47
1:F:610:PHE:O	1:F:628:PHE:N	2.32	0.47
1:F:6:ILE:HG21	1:F:12:ALA:HB2	1.94	0.47
1:A:279:ALA:HB3	1:A:286:ALA:O	2.14	0.47
1:A:448:VAL:O	1:A:451:ALA:HB3	2.15	0.47
1:A:509:LYS:HG2	1:A:510:LYS:HG3	1.95	0.47
1:B:974:PRO:HA	1:B:977:MET:CE	2.44	0.47
1:C:244:GLU:CG	1:C:248:LYS:HE3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:VAL:HG11	1:C:395:MET:CB	2.42	0.47
1:D:53:ASP:OD1	1:D:56:THR:OG1	2.25	0.47
1:F:447:MET:HG3	1:F:448:VAL:N	2.30	0.47
1:F:559:LEU:CD2	1:F:922:THR:HA	2.45	0.47
1:F:187:TRP:HB3	1:F:776:GLU:HG2	1.96	0.47
1:F:5:PHE:CZ	1:F:8:ARG:HD2	2.49	0.47
1:F:971:ARG:HG2	1:F:974:PRO:HG3	1.96	0.47
1:A:465:ALA:O	1:A:469:GLN:HG2	2.14	0.47
1:B:344:LEU:HD23	1:B:402:ILE:HD11	1.96	0.47
1:B:409:ALA:O	1:B:413:VAL:HG23	2.15	0.47
1:B:415:ASN:O	1:B:419:VAL:HG23	2.15	0.47
1:C:1042:HIS:O	1:C:1043:SER:HB3	2.13	0.47
1:C:137:LEU:O	1:C:329:THR:HG23	2.14	0.47
1:C:197:GLN:HA	1:C:798:MET:SD	2.54	0.47
1:D:462:SER:O	1:D:466:ILE:HG12	2.15	0.47
1:E:913:LEU:HD23	1:E:927:PHE:HZ	1.79	0.47
1:F:352:PHE:HA	1:F:355:MET:CE	2.45	0.47
1:F:509:LYS:HG2	1:F:513:PHE:HB2	1.96	0.47
1:A:527:TYR:CD2	1:A:972:LEU:HG	2.49	0.47
1:A:574:THR:CG2	1:A:627:ALA:HB3	2.44	0.47
1:A:44:THR:HA	1:A:90:ILE:O	2.15	0.47
1:B:145:THR:O	1:B:284:GLN:NE2	2.46	0.47
1:C:55:LYS:HE2	1:C:55:LYS:HB3	1.70	0.47
1:D:183:ALA:HB2	1:D:273:GLU:HG3	1.97	0.47
1:D:34:GLN:OE1	1:D:670:ALA:HB1	2.15	0.47
1:D:30:LEU:HD11	1:D:384:ALA:HA	1.97	0.47
1:D:388:PHE:HE1	1:D:469:GLN:HE22	1.61	0.47
1:D:790:TYR:HE1	1:D:800:PRO:HB3	1.79	0.47
1:E:197:GLN:HA	1:E:798:MET:SD	2.55	0.47
1:A:134:SER:OG	2:A:1101:ERY:C32	2.56	0.47
1:A:418:ARG:O	1:A:422:GLU:HB2	2.14	0.47
1:A:739:LEU:HD12	1:A:799:VAL:HG11	1.97	0.47
1:B:555:LEU:HD23	1:B:555:LEU:HA	1.56	0.47
1:B:82:SER:HB2	1:B:816:LEU:HB2	1.95	0.47
1:C:108:GLN:O	1:C:112:GLN:HB2	2.14	0.47
1:C:370:ILE:O	1:C:374:VAL:HG23	2.15	0.47
1:C:376:LEU:HD22	1:C:398:MET:HE3	1.96	0.47
1:C:568:ASP:HB2	1:C:643:LYS:HG3	1.96	0.47
1:E:960:LEU:O	1:E:964:THR:HG23	2.15	0.47
1:E:992:SER:O	1:E:997:SER:HB2	2.14	0.47
1:F:185:ARG:HB3	1:F:187:TRP:NE1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:365:THR:O	1:F:368:PRO:HD2	2.14	0.47
1:F:597:TYR:CE1	1:F:601:LYS:HD2	2.46	0.47
3:A:1102:LMT:O5B	3:A:1102:LMT:H6E	2.15	0.47
1:A:190:PRO:HD3	1:A:779:TYR:CD1	2.50	0.47
1:A:535:LEU:HD22	1:A:1027:VAL:HG21	1.95	0.47
1:A:658:ILE:HG13	1:A:659:LYS:HE2	1.96	0.47
1:B:463:THR:HG22	1:B:563:PHE:HE2	1.80	0.47
1:C:404:LEU:HG	1:C:449:LEU:HD13	1.96	0.47
1:C:971:ARG:HB3	1:C:971:ARG:NH1	2.30	0.47
1:C:944:LEU:HB3	1:C:971:ARG:NH2	2.29	0.47
2:D:1101:ERY:H251	2:D:1101:ERY:H283	1.67	0.47
1:E:430:ALA:O	1:E:433:LYS:HB3	2.14	0.47
1:F:1035:ARG:HD3	1:F:1035:ARG:HA	1.74	0.47
1:F:362:PHE:O	1:F:366:LEU:HG	2.14	0.47
1:F:751:GLY:O	1:F:753:ALA:N	2.48	0.47
1:B:1016:VAL:HG13	3:B:1101:LMT:H102	1.96	0.47
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.55	0.47
1:B:222:THR:HA	1:B:224:PRO:HD3	1.96	0.47
1:C:187:TRP:HE3	1:C:775:SER:O	1.98	0.47
1:A:781:MET:SD	1:C:225:VAL:HG13	2.55	0.47
1:D:246:PHE:O	1:D:262:LEU:HD23	2.15	0.47
1:E:575:MET:HA	1:E:626:ILE:HG13	1.97	0.47
1:F:752:ALA:O	1:F:774:MET:HA	2.15	0.47
1:F:5:PHE:CE1	1:F:8:ARG:HD2	2.49	0.47
1:A:181:GLN:HB3	1:A:273:GLU:OE1	2.15	0.47
1:A:929:VAL:O	1:A:932:LEU:HB2	2.15	0.47
1:B:801:PHE:CD1	1:B:804:PHE:HE2	2.33	0.47
1:C:140:VAL:HG23	1:C:291:ILE:HD13	1.97	0.47
1:C:452:VAL:O	1:C:455:PRO:HD2	2.15	0.47
1:E:602:GLU:HB3	1:E:606:VAL:HG23	1.97	0.47
1:E:909:VAL:HG13	1:E:931:LEU:HD11	1.96	0.47
1:F:1024:VAL:O	1:F:1028:VAL:HG23	2.15	0.47
1:F:986:VAL:HG21	1:F:1007:VAL:HG11	1.96	0.47
1:A:540:ARG:HB2	1:A:541:TYR:CD1	2.49	0.46
1:B:169:THR:HG21	1:B:306:ILE:HG13	1.97	0.46
1:B:937:LEU:HD23	1:B:937:LEU:HA	1.49	0.46
1:C:49:TYR:HD1	1:C:57:VAL:HG12	1.81	0.46
1:D:417:GLU:OE1	1:D:497:LEU:HD11	2.15	0.46
1:D:573:MET:HG2	1:D:628:PHE:HD1	1.80	0.46
1:D:555:LEU:HD13	1:D:913:LEU:HB2	1.97	0.46
1:E:142:VAL:HG12	1:E:321:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:VAL:HA	1:E:390:ILE:O	2.15	0.46
1:E:330:THR:HB	1:E:331:PRO:HD3	1.97	0.46
1:F:881:LEU:HD21	1:F:905:VAL:HG11	1.98	0.46
1:A:154:ILE:O	1:A:157:TYR:N	2.49	0.46
1:A:328:ASP:O	1:A:331:PRO:HD2	2.15	0.46
1:A:453:PHE:CE2	1:A:474:ILE:HG21	2.50	0.46
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.97	0.46
1:A:4:PHE:O	1:A:8:ARG:HD2	2.15	0.46
1:B:277:ILE:HA	1:B:613:ASN:O	2.15	0.46
1:B:817:GLU:OE1	1:B:826:GLU:HB2	2.15	0.46
1:C:112:GLN:O	1:C:115:MET:HB2	2.15	0.46
1:C:182:TYR:O	1:C:769:LYS:HD3	2.14	0.46
1:C:426:PRO:HD2	1:C:429:GLU:CB	2.46	0.46
1:C:668:LEU:H	1:C:668:LEU:HG	1.46	0.46
1:D:182:TYR:HB2	1:D:769:LYS:NZ	2.30	0.46
1:D:971:ARG:NH1	1:D:971:ARG:HB3	2.29	0.46
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.80	0.46
1:D:225:VAL:N	1:E:781:MET:HE1	2.17	0.46
1:E:801:PHE:HA	1:E:804:PHE:CE2	2.50	0.46
1:F:664:PHE:HD2	1:F:717:ARG:CD	2.28	0.46
1:A:236:ALA:O	1:B:728:LYS:NZ	2.46	0.46
1:A:434:SER:O	1:A:438:ILE:HG12	2.15	0.46
1:B:652:THR:HG22	1:B:665:ALA:H	1.80	0.46
1:D:961:ILE:HG13	1:D:961:ILE:H	1.12	0.46
1:A:151:GLN:HG3	1:A:152:GLU:N	2.30	0.46
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.30	0.46
1:B:36:PRO:O	1:B:38:ILE:HG13	2.15	0.46
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.98	0.46
1:C:672:VAL:HG23	1:C:673:GLU:OE2	2.15	0.46
1:D:931:LEU:HD13	3:D:1103:LMT:H81	1.98	0.46
1:E:40:PRO:HA	1:E:41:PRO:HD3	1.68	0.46
1:E:675:GLY:HA3	1:E:862:MET:SD	2.56	0.46
1:F:760:ASN:O	1:F:771:VAL:HB	2.14	0.46
1:A:112:GLN:HG3	1:B:112:GLN:CD	2.36	0.46
1:A:423:GLU:OE2	1:A:433:LYS:HE2	2.15	0.46
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.97	0.46
1:B:511:GLY:O	1:B:515:TRP:NE1	2.49	0.46
1:C:907:LEU:HG	1:C:1017:LEU:HD23	1.97	0.46
1:C:1040:ILE:HG12	1:C:1041:GLU:N	2.26	0.46
1:C:119:PRO:O	1:C:123:GLN:HG3	2.15	0.46
2:D:1101:ERY:H272	2:D:1101:ERY:H292	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:TYR:HB2	1:E:769:LYS:HZ2	1.81	0.46
1:D:781:MET:HE1	1:F:225:VAL:HG13	1.96	0.46
1:F:27:ILE:HA	1:F:30:LEU:CD2	2.46	0.46
1:F:664:PHE:HE2	1:F:717:ARG:HB3	1.80	0.46
1:F:452:VAL:HG13	1:F:884:VAL:CG2	2.46	0.46
1:A:1040:ILE:HG23	1:A:1041:GLU:N	2.30	0.46
1:A:721:LEU:HA	1:A:721:LEU:HD12	1.81	0.46
1:A:736:ALA:HB2	1:A:804:PHE:HB2	1.98	0.46
1:E:172:VAL:HG22	1:E:306:ILE:HD11	1.98	0.46
1:F:311:ALA:HA	1:F:314:GLU:HG3	1.98	0.46
1:F:524:THR:O	1:F:528:THR:HG22	2.16	0.46
1:A:83:ASP:HB3	1:A:85:THR:H	1.80	0.46
1:B:143:ILE:HG21	1:B:281:PHE:CD2	2.51	0.46
1:B:203:VAL:HG12	1:B:207:ILE:HD11	1.97	0.46
1:C:341:VAL:O	1:C:344:LEU:HB3	2.16	0.46
1:D:1024:VAL:O	1:D:1028:VAL:HG23	2.16	0.46
1:D:673:GLU:HB2	2:D:1101:ERY:H213	1.97	0.46
1:D:416:VAL:HG21	1:D:493:CYS:SG	2.56	0.46
1:E:10:ILE:HG12	1:F:895:TRP:HB2	1.98	0.46
1:E:744:ASN:O	1:E:748:THR:HG23	2.16	0.46
1:E:904:VAL:O	1:E:907:LEU:HB2	2.16	0.46
1:A:359:LEU:C	1:A:360:GLN:HG2	2.34	0.46
1:A:545:TYR:CE2	1:A:1025:PHE:HZ	2.34	0.46
1:B:188:MET:HA	1:B:266:ALA:CB	2.46	0.46
1:C:222:THR:HA	1:C:224:PRO:CD	2.43	0.46
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.46	0.46
1:C:434:SER:O	1:C:437:GLN:HB2	2.15	0.46
1:C:457:ALA:HB2	1:C:471:SER:OG	2.15	0.46
1:C:894:SER:HG	1:C:896:SER:HG	1.62	0.46
1:C:898:PRO:HA	1:C:901:VAL:HG12	1.97	0.46
3:D:1103:LMT:H112	3:D:1103:LMT:H82	1.79	0.46
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.98	0.46
1:D:453:PHE:CE2	1:D:932:LEU:HB3	2.51	0.46
1:D:971:ARG:NH2	1:D:975:ILE:HD11	2.31	0.46
1:E:634:TRP:N	1:E:634:TRP:CD1	2.79	0.46
1:E:652:THR:CG2	1:E:665:ALA:H	2.28	0.46
1:B:1033:PHE:CE1	1:B:1034:SER:HB3	2.51	0.46
1:B:344:LEU:HD11	1:B:398:MET:CE	2.46	0.46
1:C:398:MET:O	1:C:402:ILE:HG13	2.16	0.46
1:D:573:MET:HB2	1:D:666:PHE:HE1	1.81	0.46
1:E:289:LEU:HD23	1:E:289:LEU:HA	1.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:904:VAL:HG21	1:E:942:ALA:HB2	1.98	0.46
1:F:578:LEU:HB3	1:F:579:PRO:HD2	1.98	0.46
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.51	0.46
1:B:1026:PHE:O	1:B:1030:ARG:HB2	2.16	0.46
1:B:195:LYS:HB3	1:B:196:PHE:CD1	2.51	0.46
1:B:576:VAL:HG22	1:B:663:VAL:HG22	1.98	0.46
1:B:683:GLU:HG2	1:B:819:TYR:CG	2.51	0.46
1:C:187:TRP:HA	1:C:774:MET:O	2.16	0.46
1:D:897:ILE:HG12	1:D:1030:ARG:HD3	1.97	0.46
1:D:568:ASP:O	1:D:634:TRP:HZ3	1.98	0.46
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.98	0.46
1:D:919:ARG:HD3	1:D:921:LEU:HD23	1.98	0.46
1:F:572:PHE:CE1	1:F:648:THR:HG22	2.51	0.46
1:A:429:GLU:H	1:A:429:GLU:CD	2.18	0.45
1:B:405:LEU:HD22	1:B:481:SER:HB3	1.96	0.45
1:C:310:LEU:O	1:C:314:GLU:HG3	2.16	0.45
1:C:969:ARG:HH11	1:C:970:MET:HB3	1.81	0.45
1:D:610:PHE:O	1:D:627:ALA:HA	2.16	0.45
1:D:573:MET:HG2	1:D:628:PHE:CD1	2.51	0.45
1:E:356:TYR:C	1:E:358:PHE:H	2.19	0.45
1:E:418:ARG:O	1:E:422:GLU:HB2	2.15	0.45
1:E:425:LEU:HD12	1:E:430:ALA:HA	1.98	0.45
1:E:847:LEU:O	1:E:850:LYS:HB2	2.16	0.45
1:F:281:PHE:CE1	1:F:324:VAL:HG21	2.51	0.45
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.97	0.45
1:F:894:SER:HB3	1:F:897:ILE:HG12	1.98	0.45
1:F:953:MET:HE2	1:F:963:ALA:HB3	1.98	0.45
1:A:467:TYR:HE1	1:A:925:VAL:HG22	1.81	0.45
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.67	0.45
1:A:2:PRO:O	1:A:6:ILE:HG23	2.16	0.45
1:A:857:TYR:N	1:A:857:TYR:CD2	2.85	0.45
1:B:270:LEU:HA	1:B:270:LEU:HD12	1.78	0.45
1:B:520:PHE:O	1:B:524:THR:HG22	2.16	0.45
1:C:11:PHE:O	1:C:11:PHE:HD2	1.99	0.45
1:C:246:PHE:O	1:C:262:LEU:HD23	2.15	0.45
1:D:415:ASN:HB3	1:D:434:SER:HB2	1.98	0.45
1:D:442:LEU:HA	1:D:442:LEU:HD23	1.67	0.45
1:D:485:ALA:O	1:D:490:PRO:HD3	2.16	0.45
1:E:728:LYS:HB2	1:E:810:GLU:OE1	2.15	0.45
1:F:195:LYS:HB3	1:F:196:PHE:CD1	2.48	0.45
1:A:452:VAL:HA	1:A:880:SER:OG	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:TYR:H	1:A:926:TYR:HD1	1.64	0.45
1:A:404:LEU:HD12	1:A:937:LEU:HD21	1.98	0.45
1:A:985:GLY:O	1:A:988:PRO:HD2	2.17	0.45
1:C:165:ALA:HB3	1:C:313:MET:CE	2.46	0.45
1:C:382:VAL:O	1:C:386:PHE:HD2	1.99	0.45
1:C:658:ILE:O	1:C:658:ILE:HG13	2.17	0.45
1:C:563:PHE:HB2	1:C:866:GLU:HB2	1.97	0.45
1:D:225:VAL:HG22	1:E:781:MET:HE2	1.97	0.45
1:D:919:ARG:HG2	1:D:920:GLY:N	2.26	0.45
1:E:358:PHE:CD1	1:E:977:MET:HG2	2.51	0.45
1:F:504:ASP:C	1:F:506:GLY:N	2.70	0.45
1:A:172:VAL:CG2	1:A:306:ILE:HD11	2.46	0.45
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.51	0.45
1:B:294:ALA:HB3	1:B:297:ALA:HB2	1.97	0.45
1:B:957:GLY:O	1:B:1041:GLU:HA	2.16	0.45
1:D:310:LEU:O	1:D:314:GLU:HG3	2.17	0.45
1:E:105:VAL:HB	1:F:105:VAL:HG13	1.99	0.45
1:E:398:MET:HB3	1:E:398:MET:HE3	1.87	0.45
1:E:515:TRP:O	1:E:519:MET:HG3	2.16	0.45
1:F:3:ASN:N	1:F:3:ASN:OD1	2.49	0.45
1:F:459:PHE:CE1	1:F:876:LEU:HG	2.51	0.45
1:F:701:GLN:HE22	1:F:852:PRO:HD3	1.81	0.45
1:A:145:THR:C	1:A:147:GLY:H	2.20	0.45
1:A:574:THR:OG1	1:A:664:PHE:O	2.24	0.45
1:A:801:PHE:CD1	1:A:804:PHE:HE2	2.35	0.45
1:A:965:LEU:HD23	1:A:965:LEU:HA	1.64	0.45
1:C:280:GLU:HG3	1:C:285:PRO:HA	1.98	0.45
1:C:686:ASP:OD1	1:C:690:LEU:HB2	2.17	0.45
1:D:542:LEU:O	1:D:546:LEU:HG	2.16	0.45
1:D:654:ALA:O	1:D:658:ILE:HG12	2.17	0.45
1:D:947:GLU:O	1:D:951:ASP:HB2	2.17	0.45
1:D:999:ALA:O	1:D:1003:VAL:HG23	2.16	0.45
1:E:66:GLU:OE1	1:E:821:GLY:HA2	2.17	0.45
1:F:84:SER:HB3	1:F:814:PRO:HA	1.98	0.45
1:A:242:SER:OG	1:A:245:GLU:HG2	2.16	0.45
1:D:375:VAL:HG11	1:D:405:LEU:HD22	1.98	0.45
1:D:876:LEU:HD23	1:D:879:ILE:HD12	1.98	0.45
1:D:996:GLY:O	1:D:999:ALA:N	2.49	0.45
1:D:112:GLN:NE2	1:E:112:GLN:HB3	2.32	0.45
1:E:14:VAL:HG13	1:F:886:LEU:HD12	1.98	0.45
1:F:510:LYS:O	1:F:512:PHE:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1101:ERY:H8	2:A:1101:ERY:H321	1.64	0.45
1:A:584:GLN:N	1:A:622:GLN:HB3	2.31	0.45
1:A:775:SER:OG	1:A:780:ARG:HG2	2.16	0.45
1:B:255:GLN:HG3	1:B:255:GLN:H	1.29	0.45
1:B:888:LEU:HA	1:B:888:LEU:HD23	1.75	0.45
1:C:443:VAL:HG12	1:C:891:LEU:CD2	2.46	0.45
1:C:987:MET:O	1:C:991:ILE:HG22	2.17	0.45
1:D:932:LEU:HD23	1:D:932:LEU:HA	1.75	0.45
1:D:991:ILE:HG22	1:D:992:SER:N	2.29	0.45
1:E:533:GLY:O	1:E:536:ARG:HB2	2.17	0.45
1:E:619:GLY:O	1:E:624:THR:HG21	2.17	0.45
1:E:758:TYR:HB2	1:E:772:TYR:CE1	2.51	0.45
1:A:889:ALA:HA	1:A:894:SER:O	2.17	0.45
1:B:729:ILE:HG22	1:B:731:ILE:HD13	1.99	0.45
1:C:240:LEU:HD11	1:C:249:ILE:HD11	1.98	0.45
1:C:789:TRP:O	1:C:801:PHE:HD2	1.98	0.45
1:C:682:PHE:CZ	1:C:857:TYR:HB2	2.52	0.45
1:C:941:ASN:HD21	1:C:1015:THR:HG22	1.81	0.45
1:D:240:LEU:HD22	1:D:245:GLU:OE1	2.17	0.45
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.98	0.45
1:D:889:ALA:HA	1:D:894:SER:O	2.17	0.45
1:E:983:ILE:HD13	1:E:1012:VAL:HG22	1.99	0.45
1:E:230:LEU:HG	1:E:231:ASN:N	2.31	0.45
1:E:899:PHE:HD2	1:E:902:MET:HE2	1.82	0.45
1:F:664:PHE:HD2	1:F:717:ARG:HD3	1.82	0.45
1:E:219:LEU:HD11	1:F:727:PHE:CD1	2.51	0.45
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.46	0.45
1:A:703:LEU:HD21	1:A:718:PRO:HD3	1.99	0.45
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.82	0.45
1:D:925:VAL:HG12	1:D:926:TYR:N	2.30	0.45
1:F:363:ARG:NH2	1:F:498:LYS:HD2	2.18	0.45
1:F:659:LYS:HD3	1:F:659:LYS:HA	1.84	0.45
1:B:143:ILE:O	1:B:321:LEU:HA	2.16	0.45
1:B:356:TYR:C	1:B:358:PHE:H	2.21	0.45
1:C:844:MET:HA	1:C:847:LEU:HD22	1.98	0.45
1:D:875:SER:O	1:D:879:ILE:HG13	2.17	0.45
1:E:1024:VAL:O	1:E:1028:VAL:HG23	2.17	0.45
1:E:166:ILE:HD11	1:E:310:LEU:CD1	2.48	0.45
1:E:344:LEU:HD23	1:E:402:ILE:HD11	1.99	0.45
1:E:448:VAL:HA	1:E:451:ALA:HB3	1.99	0.45
1:F:314:GLU:HB2	1:F:315:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:578:LEU:CG	1:F:587:THR:HG22	2.47	0.45
1:F:664:PHE:CD2	1:F:717:ARG:HD3	2.52	0.45
1:A:350:LEU:HA	1:A:350:LEU:HD23	1.76	0.44
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.66	0.44
1:B:699:ARG:HE	1:B:703:LEU:HD11	1.82	0.44
1:B:931:LEU:HD23	1:B:931:LEU:HA	1.73	0.44
1:C:527:TYR:OH	1:C:1019:ILE:O	2.24	0.44
1:C:11:PHE:O	1:C:15:ILE:HG13	2.17	0.44
1:C:227:GLY:O	1:C:229:GLN:HG3	2.17	0.44
1:D:406:VAL:O	1:D:410:ILE:HG13	2.16	0.44
1:D:58:GLN:O	1:D:63:GLN:HG3	2.17	0.44
1:D:343:THR:HG21	1:D:989:LEU:HD21	1.99	0.44
1:F:901:VAL:HG23	1:F:942:ALA:CB	2.43	0.44
1:A:1038:GLU:HA	1:A:1039:ASP:HB3	1.99	0.44
1:A:500:ILE:HG22	1:A:501:ALA:O	2.17	0.44
1:C:926:TYR:HD2	1:C:1003:VAL:HG22	1.82	0.44
1:C:216:ALA:HB1	1:C:234:ILE:HG22	1.99	0.44
1:D:759:VAL:HG12	1:D:760:ASN:HB2	1.99	0.44
1:D:839:GLU:O	1:D:842:GLU:HB3	2.17	0.44
1:D:316:PHE:CD1	1:E:687:GLN:HG2	2.52	0.44
1:E:680:PHE:CZ	1:E:844:MET:HG3	2.52	0.44
1:A:541:TYR:N	1:A:541:TYR:CD1	2.85	0.44
1:B:324:VAL:HG13	1:B:326:PRO:HD3	2.00	0.44
1:B:534:ILE:HG22	3:B:1101:LMT:H5'	1.99	0.44
1:B:685:ILE:HD11	1:B:819:TYR:HD2	1.80	0.44
1:B:950:LYS:NZ	1:B:1030:ARG:NH2	2.64	0.44
1:C:185:ARG:HB3	1:C:187:TRP:NE1	2.32	0.44
1:C:394:THR:O	1:C:398:MET:HG3	2.18	0.44
1:C:425:LEU:HD23	1:C:425:LEU:HA	1.80	0.44
1:F:375:VAL:HG13	1:F:480:LEU:HB2	2.00	0.44
1:F:69:MET:HA	1:F:72:ILE:HD11	1.99	0.44
1:A:609:VAL:HG13	1:A:629:VAL:HG22	1.99	0.44
1:A:7:ASP:O	1:A:8:ARG:HG3	2.17	0.44
1:A:80:SER:CB	1:A:90:ILE:HG12	2.46	0.44
1:B:461:GLY:HA2	1:B:865:GLN:HE21	1.82	0.44
1:C:1016:VAL:HG12	1:C:1016:VAL:O	2.18	0.44
1:C:858:ASP:OD2	1:C:859:TRP:N	2.51	0.44
1:D:67:GLN:NE2	1:F:768:VAL:HG13	2.31	0.44
1:D:678:THR:HA	1:D:837:THR:OG1	2.18	0.44
1:F:743:ILE:O	1:F:746:ILE:HG13	2.18	0.44
1:A:426:PRO:O	1:A:429:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LEU:HD12	1:A:544:LEU:HA	1.83	0.44
1:A:623:ASN:N	1:A:623:ASN:OD1	2.48	0.44
1:B:281:PHE:HZ	1:B:324:VAL:HG21	1.80	0.44
1:B:418:ARG:HD2	1:B:422:GLU:OE1	2.17	0.44
1:B:605:ASN:HD22	1:B:647:ILE:HD11	1.83	0.44
1:B:741:VAL:HG21	1:B:804:PHE:CE1	2.53	0.44
1:D:568:ASP:OD1	1:D:637:ARG:NH1	2.42	0.44
1:D:579:PRO:HD3	1:D:661:ALA:HB2	1.98	0.44
1:E:378:GLY:O	1:E:382:VAL:HG23	2.17	0.44
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.74	0.44
1:B:652:THR:HG23	1:B:665:ALA:HB3	1.99	0.44
1:B:690:LEU:HD11	1:B:854:GLY:HA3	2.00	0.44
1:C:31:PRO:HB2	1:C:389:SER:CB	2.47	0.44
1:C:403:GLY:O	1:C:406:VAL:HG22	2.17	0.44
1:E:404:LEU:HD12	1:E:937:LEU:HD21	2.00	0.44
1:E:375:VAL:HG11	1:E:405:LEU:HD22	1.98	0.44
1:E:573:MET:HG3	1:E:666:PHE:HE1	1.81	0.44
1:E:706:ALA:HB1	1:E:716:VAL:HG11	2.00	0.44
1:A:1038:GLU:HA	1:A:1039:ASP:CB	2.47	0.44
2:A:1101:ERY:H18	2:A:1101:ERY:H5	1.99	0.44
1:A:960:LEU:H	1:A:1039:ASP:HA	1.82	0.44
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.99	0.44
1:C:549:VAL:O	1:C:552:MET:HB3	2.18	0.44
1:D:463:THR:HG22	1:D:563:PHE:CE1	2.53	0.44
1:D:502:LYS:H	1:D:502:LYS:HG2	1.47	0.44
1:E:111:LEU:HD11	1:E:127:VAL:HB	1.99	0.44
1:E:845:GLU:HG3	1:E:859:TRP:HZ2	1.82	0.44
1:E:903:LEU:O	1:E:906:PRO:HD2	2.18	0.44
1:F:1039:ASP:OD2	1:F:1041:GLU:HG3	2.18	0.44
1:B:559:LEU:HG	1:B:560:PRO:HD2	2.00	0.44
1:B:904:VAL:HG13	1:B:907:LEU:HD22	2.00	0.44
1:B:959:GLY:HA2	1:B:1040:ILE:HG22	1.98	0.44
1:C:443:VAL:HG12	1:C:891:LEU:HD21	2.00	0.44
1:C:587:THR:OG1	1:C:613:ASN:ND2	2.50	0.44
1:C:582:ALA:HB3	1:C:623:ASN:HB3	1.99	0.44
1:D:153:ASP:OD2	1:D:182:TYR:OH	2.35	0.44
1:E:637:ARG:HB3	1:E:642:ASN:HB3	2.00	0.44
1:E:727:PHE:HD1	1:E:809:TRP:CE2	2.36	0.44
1:F:279:ALA:HB2	1:F:612:VAL:HG22	2.00	0.44
1:F:944:LEU:HD13	1:F:975:ILE:HG12	2.00	0.44
1:A:3:ASN:O	1:A:4:PHE:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:MET:CE	1:B:200:PRO:HG3	2.48	0.44
1:E:555:LEU:HB3	1:E:913:LEU:HB3	2.00	0.44
1:E:846:GLN:O	1:E:849:SER:OG	2.35	0.44
1:F:664:PHE:CE2	1:F:717:ARG:HB3	2.53	0.44
1:A:201:VAL:HA	1:A:204:ILE:HD12	2.00	0.43
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.81	0.43
1:B:228:GLN:O	1:C:583:THR:HG21	2.17	0.43
1:C:983:ILE:HD13	1:C:1012:VAL:HG22	2.00	0.43
1:D:549:VAL:O	1:D:552:MET:HB3	2.18	0.43
1:E:932:LEU:HA	1:E:932:LEU:HD23	1.77	0.43
1:F:688:ALA:HB3	1:F:690:LEU:HG	1.99	0.43
1:F:751:GLY:O	1:F:754:TRP:N	2.51	0.43
1:A:1034:SER:OG	1:A:1035:ARG:N	2.51	0.43
1:A:937:LEU:HA	1:A:937:LEU:HD23	1.85	0.43
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.98	0.43
1:B:335:ILE:HG21	1:B:995:ALA:HB3	2.00	0.43
1:B:969:ARG:NH1	1:B:970:MET:HB3	2.32	0.43
1:C:728:LYS:HG2	1:C:808:ARG:CZ	2.49	0.43
1:C:190:PRO:HB3	1:C:789:TRP:CZ3	2.53	0.43
1:C:865:GLN:O	1:C:868:LEU:HB3	2.18	0.43
1:D:428:LYS:HG2	1:D:428:LYS:H	1.24	0.43
1:D:201:VAL:HG21	1:D:745:ASP:OD2	2.18	0.43
1:D:781:MET:HE1	1:F:225:VAL:N	2.27	0.43
1:E:190:PRO:HG3	1:E:779:TYR:HB3	2.00	0.43
1:E:43:VAL:HG11	1:E:104:GLN:HG3	2.00	0.43
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.56	0.43
1:F:143:ILE:HG22	1:F:286:ALA:HB2	2.01	0.43
1:F:404:LEU:HG	1:F:449:LEU:HD13	2.01	0.43
1:F:572:PHE:CD1	1:F:648:THR:HG22	2.53	0.43
1:A:844:MET:HE1	1:A:847:LEU:HD12	2.00	0.43
1:B:572:PHE:CD1	1:B:648:THR:HG22	2.53	0.43
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.46	0.43
1:D:894:SER:HB3	1:D:897:ILE:HB	2.00	0.43
1:E:42:ALA:HB3	1:E:132:SER:HB3	2.00	0.43
1:E:167:SER:CB	1:E:175:VAL:HG21	2.46	0.43
1:E:743:ILE:HA	1:E:746:ILE:HD12	2.00	0.43
1:E:931:LEU:O	1:E:935:ILE:HG13	2.18	0.43
1:D:622:GLN:NE2	1:F:220:GLY:O	2.49	0.43
1:A:1038:GLU:HB3	1:A:1039:ASP:C	2.38	0.43
1:A:762:PHE:O	1:A:768:VAL:HA	2.17	0.43
1:B:426:PRO:HG2	1:B:429:GLU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ASP:OD2	1:C:182:TYR:HB2	2.18	0.43
1:C:409:ALA:O	1:C:413:VAL:HG23	2.18	0.43
1:C:775:SER:HB2	1:C:789:TRP:CH2	2.53	0.43
1:C:940:LYS:NZ	1:C:978:THR:HG21	2.33	0.43
1:D:210:GLN:OE1	1:D:250:LEU:HB3	2.18	0.43
1:D:492:LEU:HA	1:D:492:LEU:HD23	1.65	0.43
1:E:901:VAL:HG21	1:E:943:ILE:HG13	2.00	0.43
1:E:987:MET:HB3	1:E:988:PRO:HD3	1.99	0.43
1:A:270:LEU:HA	1:A:270:LEU:HD12	1.73	0.43
1:B:61:VAL:HG22	1:B:118:LEU:HD22	2.00	0.43
1:B:583:THR:HG22	1:B:584:GLN:N	2.33	0.43
1:B:873:ALA:N	1:B:874:PRO:HD2	2.32	0.43
1:C:72:ILE:HD12	1:C:75:LEU:HD22	1.99	0.43
1:C:869:SER:HG	1:C:928:GLN:HE22	1.64	0.43
1:C:953:MET:HE3	1:C:953:MET:HB2	1.88	0.43
1:D:247:GLY:C	1:D:249:ILE:H	2.22	0.43
1:D:563:PHE:CD2	1:D:671:ILE:HD13	2.52	0.43
1:E:983:ILE:HG23	1:E:1008:MET:HE2	1.99	0.43
1:E:1041:GLU:OE1	1:E:1042:HIS:HB2	2.18	0.43
1:E:188:MET:HA	1:E:266:ALA:HB2	2.00	0.43
1:E:508:GLY:HA2	1:E:518:ARG:NH2	2.32	0.43
1:E:597:TYR:CE1	1:E:601:LYS:HD2	2.53	0.43
1:E:887:CYS:O	1:E:890:ALA:HB3	2.19	0.43
1:F:457:ALA:HB2	1:F:471:SER:OG	2.18	0.43
1:F:587:THR:HG21	1:F:622:GLN:O	2.18	0.43
1:F:623:ASN:OD1	1:F:623:ASN:N	2.49	0.43
1:F:65:ILE:CG2	1:F:90:ILE:HD12	2.49	0.43
1:F:80:SER:CB	1:F:90:ILE:HG12	2.49	0.43
1:A:185:ARG:HB3	1:A:187:TRP:HE1	1.82	0.43
1:A:169:THR:HG21	1:A:306:ILE:HG13	2.01	0.43
1:A:350:LEU:HD22	1:A:984:LEU:HD13	2.00	0.43
1:B:684:LEU:HD12	1:B:684:LEU:HA	1.84	0.43
1:B:711:ASP:OD2	1:F:850:LYS:NZ	2.40	0.43
1:B:948:PHE:CE2	1:B:971:ARG:HD2	2.54	0.43
1:C:201:VAL:HA	1:C:204:ILE:HD12	2.00	0.43
1:C:664:PHE:CD2	1:C:717:ARG:HD2	2.54	0.43
1:D:1016:VAL:HG12	1:D:1016:VAL:O	2.19	0.43
1:D:625:GLY:O	1:D:626:ILE:HD12	2.18	0.43
1:D:76:MET:HB2	1:D:93:THR:O	2.18	0.43
1:D:404:LEU:HD12	1:D:937:LEU:HD21	1.99	0.43
1:E:568:ASP:O	1:E:634:TRP:CZ3	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:509:LYS:HB3	1:F:514:GLY:CA	2.42	0.43
1:A:46:SER:HB2	1:A:128:SER:OG	2.18	0.43
1:A:184:MET:HG2	1:A:246:PHE:CE2	2.54	0.43
1:A:728:LYS:HB2	1:A:810:GLU:CD	2.39	0.43
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.64	0.43
1:B:978:THR:O	1:B:981:ALA:N	2.52	0.43
1:A:102:ILE:CD1	1:C:101:ASP:HB3	2.47	0.43
1:C:124:GLN:HG3	1:C:125:GLN:N	2.34	0.43
1:C:897:ILE:HD12	1:C:946:VAL:HG11	2.01	0.43
1:D:388:PHE:CE2	1:D:472:ILE:HG21	2.54	0.43
1:D:79:SER:HA	1:D:818:ARG:O	2.19	0.43
1:E:902:MET:O	1:E:905:VAL:HG23	2.19	0.43
1:E:950:LYS:NZ	1:E:1030:ARG:HE	2.17	0.43
1:F:146:ASP:OD2	1:F:147:GLY:N	2.52	0.43
1:F:746:ILE:HG13	1:F:747:ASN:N	2.33	0.43
1:A:393:LEU:HD11	1:A:466:ILE:HD12	2.01	0.43
1:A:685:ILE:HD12	1:A:858:ASP:HB2	2.01	0.43
1:A:961:ILE:HG13	1:A:961:ILE:H	1.20	0.43
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.54	0.43
1:B:61:VAL:HG21	1:B:122:VAL:HG21	2.00	0.43
1:B:249:ILE:HG12	1:B:262:LEU:HB2	2.01	0.43
1:B:187:TRP:HB3	1:B:776:GLU:HA	2.01	0.43
1:B:925:VAL:O	1:B:928:GLN:N	2.52	0.43
1:C:247:GLY:C	1:C:249:ILE:H	2.22	0.43
1:C:344:LEU:HA	1:C:399:VAL:HG22	2.01	0.43
1:D:556:PHE:HZ	3:D:1103:LMT:H52	1.84	0.43
1:D:465:ALA:O	1:D:469:GLN:HG2	2.18	0.43
1:E:200:PRO:HB2	1:E:749:THR:HG22	2.01	0.43
1:E:965:LEU:HD23	1:E:965:LEU:HA	1.80	0.43
1:F:248:LYS:HA	1:F:261:LEU:HD13	2.00	0.43
1:F:3:ASN:C	1:F:5:PHE:N	2.71	0.43
1:F:610:PHE:N	1:F:628:PHE:O	2.46	0.43
1:A:442:LEU:HA	1:A:442:LEU:HD23	1.77	0.43
1:B:568:ASP:OD1	1:B:644:VAL:HG23	2.19	0.43
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.99	0.43
1:B:987:MET:HB3	1:B:988:PRO:HD3	2.01	0.43
1:C:435:MET:O	1:C:439:GLN:HB2	2.19	0.43
1:C:462:SER:HB3	1:C:865:GLN:HG2	2.00	0.43
1:D:108:GLN:HE21	1:E:109:ASN:HB2	1.81	0.43
1:D:344:LEU:HD22	1:D:402:ILE:CD1	2.43	0.43
1:D:182:TYR:HB2	1:D:769:LYS:HZ3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:VAL:HG13	1:E:130:GLU:O	2.18	0.43
1:E:409:ALA:O	1:E:413:VAL:HG23	2.19	0.43
1:E:950:LYS:HZ1	1:E:1030:ARG:NH2	2.17	0.43
1:A:362:PHE:O	1:A:365:THR:HG22	2.19	0.43
1:A:396:PHE:CD1	1:A:926:TYR:HE2	2.37	0.43
1:A:699:ARG:HE	1:A:718:PRO:HG3	1.84	0.43
1:A:857:TYR:N	1:A:857:TYR:HD2	2.16	0.43
1:C:568:ASP:OD1	1:C:637:ARG:NH1	2.49	0.43
1:D:362:PHE:O	1:D:365:THR:HG22	2.18	0.43
1:E:327:TYR:CD1	1:E:628:PHE:CZ	3.04	0.43
1:E:68:ASN:CB	1:E:114:ALA:HB2	2.49	0.43
1:E:739:LEU:HD12	1:E:799:VAL:HG11	2.00	0.43
1:E:781:MET:HB2	1:E:782:LEU:HG	2.01	0.43
1:F:401:ALA:O	1:F:404:LEU:N	2.52	0.43
1:F:735:LYS:O	1:F:738:ALA:HB3	2.19	0.43
1:A:366:LEU:HA	1:A:369:THR:HB	2.01	0.42
1:A:85:THR:HG21	1:A:620:ALA:CB	2.48	0.42
1:B:101:ASP:N	1:B:131:LYS:HZ3	2.17	0.42
1:C:331:PRO:O	1:C:335:ILE:HG22	2.19	0.42
1:C:57:VAL:HG23	1:C:82:SER:HB3	2.00	0.42
1:D:203:VAL:O	1:D:207:ILE:HG13	2.20	0.42
1:D:239:ARG:NH1	1:D:761:ASP:O	2.52	0.42
1:D:324:VAL:HG13	1:D:326:PRO:HD3	2.00	0.42
1:D:559:LEU:HA	1:D:560:PRO:HD2	1.66	0.42
1:D:909:VAL:HG22	1:D:931:LEU:HD21	2.01	0.42
1:E:391:ASN:C	1:E:395:MET:HG2	2.39	0.42
1:E:400:LEU:HA	1:E:400:LEU:HD13	1.63	0.42
1:F:151:GLN:HE22	1:F:278:ILE:HG22	1.84	0.42
2:A:1101:ERY:C1	2:A:1101:ERY:HO10	2.32	0.42
1:A:382:VAL:O	1:A:385:ALA:HB3	2.19	0.42
1:A:549:VAL:HG13	1:A:552:MET:HE2	2.01	0.42
1:A:56:THR:O	1:A:60:THR:HG22	2.19	0.42
1:B:1035:ARG:O	1:B:1037:ASN:HB2	2.19	0.42
1:B:1040:ILE:HG12	1:B:1041:GLU:H	1.83	0.42
1:B:378:GLY:O	1:B:382:VAL:HG23	2.19	0.42
1:B:616:GLY:CA	1:B:626:ILE:HD13	2.48	0.42
1:C:157:TYR:O	1:C:161:ASN:HB2	2.18	0.42
1:C:674:LEU:HA	1:C:674:LEU:HD23	1.75	0.42
1:D:5:PHE:CE1	1:D:487:ILE:HG12	2.54	0.42
1:D:605:ASN:HD22	1:D:647:ILE:HD11	1.84	0.42
1:D:876:LEU:HA	1:D:876:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:VAL:HG11	1:E:497:LEU:HD23	2.01	0.42
1:F:446:ALA:HA	1:F:478:MET:CE	2.49	0.42
1:A:240:LEU:HD12	1:A:246:PHE:CE1	2.54	0.42
1:A:246:PHE:O	1:A:262:LEU:HB3	2.20	0.42
1:A:586:ARG:O	1:A:589:LYS:HB3	2.19	0.42
1:B:368:PRO:HG3	1:B:413:VAL:HG21	2.01	0.42
1:B:717:ARG:HD2	1:B:828:LEU:HB2	2.01	0.42
1:B:790:TYR:HE1	1:B:800:PRO:HB3	1.84	0.42
1:B:931:LEU:O	1:B:935:ILE:HG13	2.20	0.42
1:B:974:PRO:HA	1:B:977:MET:HE3	2.02	0.42
1:B:414:GLU:HG3	1:B:977:MET:HE1	2.01	0.42
1:C:423:GLU:OE1	1:C:433:LYS:HE2	2.19	0.42
1:D:360:GLN:HE21	1:D:360:GLN:HB3	1.39	0.42
1:D:544:LEU:O	1:D:547:ILE:HB	2.19	0.42
1:E:30:LEU:HA	1:E:30:LEU:HD12	1.77	0.42
1:F:979:SER:HB3	1:F:1015:THR:HG21	1.99	0.42
1:F:177:LEU:HD23	1:F:177:LEU:HA	1.74	0.42
1:F:913:LEU:HD23	1:F:927:PHE:CZ	2.54	0.42
1:A:1017:LEU:O	1:A:1021:PHE:HD1	2.02	0.42
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.85	0.42
1:A:75:LEU:HD21	1:C:168:ARG:HD3	2.02	0.42
1:B:1036:LYS:O	1:B:1038:GLU:HA	2.20	0.42
1:B:310:LEU:HD23	1:B:323:ILE:HG21	2.01	0.42
1:B:574:THR:HG21	1:B:598:TYR:HE2	1.84	0.42
1:C:343:THR:HG21	1:C:989:LEU:HD23	2.01	0.42
1:C:450:SER:O	1:C:454:VAL:HG23	2.20	0.42
1:C:599:LEU:O	1:C:603:LYS:HG2	2.20	0.42
1:D:293:LEU:HD11	1:D:299:ALA:HA	2.02	0.42
1:E:145:THR:O	1:E:284:GLN:NE2	2.53	0.42
1:E:210:GLN:HG2	1:F:733:GLN:HE21	1.84	0.42
1:E:572:PHE:CE1	1:E:648:THR:HG22	2.55	0.42
1:E:735:LYS:O	1:E:738:ALA:HB3	2.19	0.42
1:F:375:VAL:HA	1:F:480:LEU:HD13	2.01	0.42
1:F:135:SER:HB3	1:F:673:GLU:HB3	2.01	0.42
1:F:889:ALA:HB2	1:F:898:PRO:HG2	2.01	0.42
1:B:1030:ARG:HH11	1:B:1030:ARG:HD2	1.70	0.42
1:B:428:LYS:HG2	1:B:494:ALA:HB1	2.01	0.42
1:B:903:LEU:HD13	1:B:1025:PHE:CD2	2.54	0.42
1:B:919:ARG:NH2	1:B:921:LEU:HD21	2.35	0.42
1:C:189:ASN:OD1	1:C:190:PRO:HD2	2.19	0.42
1:C:703:LEU:CD1	1:C:718:PRO:HD3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:VAL:HG12	1:C:777:ALA:HB1	2.01	0.42
1:C:860:THR:CA	1:C:864:TYR:HB2	2.50	0.42
1:C:80:SER:HB3	1:C:90:ILE:HG23	2.02	0.42
1:C:932:LEU:O	1:C:933:THR:C	2.57	0.42
2:D:1101:ERY:H4	2:D:1101:ERY:H71	1.79	0.42
1:E:572:PHE:CD1	1:E:648:THR:HG22	2.54	0.42
1:E:679:GLY:HA2	1:E:830:GLN:HA	2.00	0.42
1:F:1040:ILE:HG22	1:F:1044:HIS:HB2	2.00	0.42
1:F:450:SER:O	1:F:454:VAL:HG23	2.19	0.42
1:F:726:GLN:NE2	1:F:812:GLY:HA3	2.35	0.42
1:A:65:ILE:O	1:A:69:MET:HG2	2.20	0.42
1:B:261:LEU:HD12	1:B:263:ARG:NH2	2.35	0.42
1:B:435:MET:O	1:B:439:GLN:HG3	2.19	0.42
1:C:524:THR:O	1:C:528:THR:HG22	2.19	0.42
1:C:694:LYS:HE3	1:C:694:LYS:H	1.85	0.42
1:C:3:ASN:C	1:C:6:ILE:H	2.23	0.42
1:C:714:THR:OG1	1:C:832:ALA:HA	2.20	0.42
1:C:888:LEU:HA	1:C:888:LEU:HD23	1.80	0.42
1:D:110:LYS:HA	1:D:110:LYS:HD3	1.76	0.42
1:E:950:LYS:NZ	1:E:1030:ARG:HH21	2.18	0.42
1:F:45:ILE:O	1:F:89:GLN:HA	2.20	0.42
1:F:658:ILE:HG13	1:F:658:ILE:O	2.19	0.42
1:F:721:LEU:HA	1:F:721:LEU:HD12	1.83	0.42
1:F:851:LEU:HB3	1:F:852:PRO:HD2	2.02	0.42
1:B:157:TYR:CZ	1:B:318:PRO:HD3	2.55	0.42
1:B:905:VAL:HB	1:B:906:PRO:HD3	2.02	0.42
1:C:415:ASN:O	1:C:419:VAL:HG23	2.19	0.42
1:C:559:LEU:HA	1:C:560:PRO:HD2	1.70	0.42
1:D:377:LEU:O	1:D:380:PHE:HB2	2.19	0.42
1:D:525:HIS:NE2	1:D:529:ASP:OD2	2.53	0.42
1:D:598:TYR:CE2	1:D:629:VAL:HG21	2.55	0.42
1:D:582:ALA:HB3	1:D:623:ASN:HB3	2.01	0.42
1:E:445:ILE:HG21	1:E:940:LYS:HD2	2.01	0.42
1:F:227:GLY:O	1:F:229:GLN:HG3	2.19	0.42
1:F:382:VAL:HG11	1:F:476:SER:CB	2.49	0.42
1:F:898:PRO:HA	1:F:901:VAL:HG12	2.01	0.42
1:F:965:LEU:HA	1:F:965:LEU:HD23	1.79	0.42
1:A:138:MET:HE2	1:A:138:MET:HB3	1.72	0.42
1:A:59:ASP:HB3	1:C:763:ILE:CD1	2.48	0.42
1:A:842:GLU:HG2	1:A:846:GLN:OE1	2.20	0.42
1:B:540:ARG:HH22	3:B:1101:LMT:H6'1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:ALA:HA	1:B:894:SER:O	2.20	0.42
1:C:1033:PHE:O	1:C:1035:ARG:N	2.51	0.42
1:C:34:GLN:HB2	1:C:333:VAL:CG2	2.49	0.42
1:D:279:ALA:HB3	1:D:286:ALA:O	2.19	0.42
1:D:534:ILE:HD11	1:D:1024:VAL:HG22	2.01	0.42
1:D:644:VAL:HG11	1:D:667:ASN:HB2	2.02	0.42
1:D:82:SER:HB2	1:D:816:LEU:HB2	2.00	0.42
1:E:1041:GLU:HB3	1:E:1042:HIS:CA	2.50	0.42
1:E:383:LEU:HD23	1:E:383:LEU:HA	1.83	0.42
1:E:65:ILE:O	1:E:69:MET:HG2	2.19	0.42
1:E:925:VAL:O	1:E:928:GLN:N	2.53	0.42
1:F:361:ASN:ND2	1:F:498:LYS:HD3	2.34	0.42
1:F:602:GLU:HB3	1:F:606:VAL:HG23	2.01	0.42
1:F:675:GLY:HA3	1:F:862:MET:HG2	2.01	0.42
1:A:178:PHE:HA	1:A:277:ILE:HG21	2.01	0.42
1:A:324:VAL:HG13	1:A:326:PRO:HD3	2.01	0.42
1:A:426:PRO:HD2	1:A:429:GLU:HG3	2.01	0.42
1:A:790:TYR:HB3	1:A:798:MET:HB3	2.00	0.42
1:B:7:ASP:C	1:B:8:ARG:HG3	2.40	0.42
1:C:453:PHE:HD2	1:C:456:MET:HE2	1.84	0.42
1:C:95:GLU:O	1:C:98:THR:OG1	2.24	0.42
1:D:576:VAL:HG21	1:D:591:LEU:HD23	2.02	0.42
1:D:38:ILE:HG22	1:D:674:LEU:HD13	2.02	0.42
1:D:991:ILE:CG2	1:D:992:SER:H	2.28	0.42
1:E:277:ILE:H	1:E:277:ILE:HG13	1.56	0.42
1:E:583:THR:HG22	1:E:584:GLN:N	2.35	0.42
1:E:672:VAL:H	1:E:672:VAL:HG22	1.54	0.42
1:E:190:PRO:HB3	1:E:789:TRP:CD2	2.55	0.42
1:E:527:TYR:OH	1:E:968:VAL:HG22	2.20	0.42
1:F:398:MET:HE3	1:F:398:MET:HB3	1.73	0.42
1:F:571:VAL:HG12	1:F:668:LEU:HD11	2.01	0.42
1:F:948:PHE:CD1	1:F:971:ARG:HD3	2.54	0.42
1:A:1036:LYS:C	1:A:1038:GLU:HG2	2.41	0.42
1:A:121:GLU:O	1:A:125:GLN:HB2	2.20	0.42
1:A:355:MET:CE	1:A:368:PRO:HG2	2.49	0.42
1:A:475:VAL:O	1:A:478:MET:HB3	2.20	0.42
1:A:58:GLN:HA	1:A:62:THR:HB	2.01	0.42
1:A:971:ARG:O	1:A:975:ILE:HG12	2.20	0.42
1:B:345:VAL:HA	1:B:348:ILE:HD12	2.01	0.42
1:B:735:LYS:O	1:B:739:LEU:HG	2.20	0.42
1:B:950:LYS:HE2	1:B:950:LYS:HB2	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:961:ILE:O	1:B:965:LEU:HG	2.20	0.42
1:C:26:ALA:HB1	1:C:384:ALA:HB2	2.02	0.42
1:C:45:ILE:HD11	1:C:69:MET:HE3	2.02	0.42
1:C:559:LEU:HD23	1:C:560:PRO:CD	2.50	0.42
1:D:902:MET:O	1:D:905:VAL:HG23	2.20	0.42
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.49	0.42
1:E:376:LEU:HA	1:E:376:LEU:HD23	1.91	0.42
1:E:584:GLN:HB2	1:E:622:GLN:HG2	2.01	0.42
1:F:911:GLY:HA2	1:F:1013:THR:HG21	2.02	0.42
1:F:11:PHE:HD2	1:F:11:PHE:O	2.02	0.42
1:F:344:LEU:HD22	1:F:402:ILE:HD11	2.01	0.42
1:F:344:LEU:HD13	1:F:402:ILE:HD11	2.01	0.42
1:F:668:LEU:H	1:F:668:LEU:HG	1.26	0.42
1:F:945:ILE:HA	1:F:971:ARG:HH22	1.85	0.42
1:A:1040:ILE:O	1:A:1041:GLU:HG3	2.19	0.41
1:A:120:GLN:O	1:A:124:GLN:HG2	2.20	0.41
1:A:11:PHE:CE1	1:A:15:ILE:HD11	2.55	0.41
1:A:622:GLN:HE21	1:C:222:THR:CG2	2.33	0.41
1:A:775:SER:OG	1:A:776:GLU:N	2.53	0.41
1:A:921:LEU:HA	1:A:921:LEU:HD13	1.86	0.41
1:A:951:ASP:O	1:A:955:LYS:HB2	2.19	0.41
1:A:407:ASP:OD1	1:A:978:THR:HG21	2.19	0.41
1:A:990:VAL:HG22	1:A:1004:GLY:HA3	2.01	0.41
1:B:401:ALA:O	1:B:405:LEU:HG	2.20	0.41
1:B:692:HIS:NE2	1:B:813:SER:HB2	2.35	0.41
1:C:158:VAL:HG22	1:C:162:MET:CE	2.50	0.41
1:C:13:TRP:O	1:C:17:ILE:HG13	2.19	0.41
1:C:188:MET:HA	1:C:266:ALA:CB	2.49	0.41
1:C:363:ARG:HH21	1:C:498:LYS:HD2	1.85	0.41
1:D:442:LEU:O	1:D:445:ILE:HG13	2.20	0.41
1:D:515:TRP:O	1:D:519:MET:HG3	2.19	0.41
1:D:573:MET:HB2	1:D:666:PHE:CE1	2.55	0.41
1:E:555:LEU:HA	1:E:555:LEU:HD23	1.66	0.41
1:E:572:PHE:HA	1:E:668:LEU:CD2	2.50	0.41
1:E:758:TYR:HB2	1:E:772:TYR:HE1	1.84	0.41
1:E:937:LEU:HA	1:E:937:LEU:HD23	1.56	0.41
1:F:452:VAL:HG13	1:F:884:VAL:HG23	2.02	0.41
1:F:811:TYR:HD1	1:F:811:TYR:HA	1.72	0.41
1:F:682:PHE:CZ	1:F:857:TYR:HB2	2.55	0.41
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.51	0.41
1:B:510:LYS:HA	1:B:510:LYS:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1036:LYS:HE2	1:D:1036:LYS:HB2	1.59	0.41
1:D:659:LYS:HD3	1:D:659:LYS:HA	1.38	0.41
1:E:104:GLN:CB	1:E:131:LYS:HE3	2.48	0.41
1:E:453:PHE:HZ	1:E:933:THR:HA	1.85	0.41
1:E:5:PHE:CE1	1:E:487:ILE:HG12	2.56	0.41
1:F:465:ALA:HA	1:F:468:ARG:HH11	1.85	0.41
1:B:17:ILE:HD13	1:B:17:ILE:HG21	1.80	0.41
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.85	0.41
1:B:239:ARG:NH1	1:B:761:ASP:HB2	2.35	0.41
1:C:48:SER:O	1:C:122:VAL:HA	2.20	0.41
1:C:31:PRO:HB2	1:C:389:SER:HB3	2.00	0.41
1:D:616:GLY:HA2	1:D:626:ILE:HD13	2.02	0.41
1:D:791:VAL:HG21	1:D:804:PHE:HZ	1.86	0.41
1:E:355:MET:HB2	1:E:355:MET:HE3	1.90	0.41
1:E:354:VAL:O	1:E:358:PHE:HB2	2.21	0.41
1:F:153:ASP:OD2	1:F:182:TYR:OH	2.37	0.41
1:F:55:LYS:HB3	1:F:55:LYS:HE2	1.77	0.41
1:F:211:ASN:ND2	1:F:760:ASN:HD21	2.15	0.41
1:F:932:LEU:O	1:F:933:THR:C	2.59	0.41
1:F:953:MET:HE1	1:F:960:LEU:HD12	2.02	0.41
1:A:435:MET:O	1:A:439:GLN:HB2	2.20	0.41
1:A:451:ALA:HB1	1:A:883:VAL:HG12	2.02	0.41
1:B:317:PHE:CE2	1:B:323:ILE:HD13	2.55	0.41
1:B:894:SER:HB2	1:B:897:ILE:HD12	2.01	0.41
1:B:966:ASP:O	1:B:969:ARG:HB3	2.21	0.41
1:C:40:PRO:HB2	1:C:94:PHE:O	2.20	0.41
1:C:696:THR:HG23	1:C:699:ARG:HH12	1.85	0.41
1:D:273:GLU:OE2	1:D:770:LYS:HD2	2.20	0.41
1:E:535:LEU:HA	1:E:535:LEU:HD23	1.85	0.41
1:E:717:ARG:HE	1:E:828:LEU:HD12	1.84	0.41
1:A:1033:PHE:HD2	1:A:1034:SER:H	1.66	0.41
1:A:225:VAL:HG13	1:B:781:MET:SD	2.60	0.41
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.86	0.41
1:B:400:LEU:HD12	1:B:933:THR:HG21	2.02	0.41
1:B:647:ILE:HG12	1:B:650:ARG:NH1	2.35	0.41
1:B:877:TYR:HA	1:B:877:TYR:HD2	1.73	0.41
1:C:393:LEU:CD1	1:C:469:GLN:HG3	2.46	0.41
1:C:563:PHE:CD2	1:C:564:LEU:HB2	2.55	0.41
1:D:142:VAL:HG21	1:D:158:VAL:HG22	2.02	0.41
1:D:280:GLU:HG2	1:D:285:PRO:HA	2.02	0.41
1:D:154:ILE:HG22	1:D:287:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:PRO:HG2	1:D:3:ASN:H	1.85	0.41
1:D:847:LEU:HD23	1:D:847:LEU:HA	1.83	0.41
1:D:892:TYR:OH	1:D:946:VAL:HB	2.20	0.41
1:D:396:PHE:HE1	1:D:999:ALA:HB1	1.85	0.41
1:E:621:GLY:O	1:E:624:THR:HG22	2.21	0.41
1:F:196:PHE:CD2	1:F:260:VAL:HG13	2.55	0.41
1:F:95:GLU:O	1:F:98:THR:OG1	2.29	0.41
1:A:158:VAL:HG22	1:A:162:MET:CE	2.50	0.41
1:A:225:VAL:HG22	1:B:781:MET:HE2	2.02	0.41
1:A:467:TYR:CE1	1:A:925:VAL:HG22	2.56	0.41
1:A:527:TYR:CE2	1:A:968:VAL:HG13	2.56	0.41
1:B:228:GLN:HE21	1:B:230:LEU:H	1.68	0.41
1:B:398:MET:HE3	1:B:398:MET:HB3	1.64	0.41
1:B:506:GLY:C	1:B:508:GLY:H	2.22	0.41
1:B:542:LEU:HA	1:B:542:LEU:HD23	1.85	0.41
1:C:34:GLN:HB2	1:C:333:VAL:HG13	2.01	0.41
1:C:597:TYR:CD2	1:C:655:PHE:HZ	2.38	0.41
1:C:623:ASN:N	1:C:623:ASN:OD1	2.43	0.41
1:C:678:THR:O	1:C:830:GLN:HG2	2.21	0.41
1:C:731:ILE:HG21	1:C:746:ILE:HD13	2.03	0.41
1:C:156:ASP:CG	1:C:769:LYS:HZ3	2.22	0.41
1:D:873:ALA:HB2	3:D:1103:LMT:H21	2.03	0.41
1:D:255:GLN:H	1:D:255:GLN:CD	2.24	0.41
1:D:361:ASN:HB3	1:D:364:ALA:HB3	2.03	0.41
1:D:393:LEU:HD12	1:D:469:GLN:HG3	2.02	0.41
1:D:801:PHE:O	1:D:805:SER:OG	2.34	0.41
1:E:220:GLY:HA3	1:E:230:LEU:O	2.20	0.41
1:E:559:LEU:HD23	1:E:560:PRO:CD	2.50	0.41
1:E:888:LEU:HA	1:E:888:LEU:HD23	1.74	0.41
1:F:250:LEU:CD1	1:F:259:ARG:HB3	2.46	0.41
1:F:344:LEU:HA	1:F:399:VAL:HG22	2.02	0.41
1:F:559:LEU:HA	1:F:560:PRO:HD2	1.56	0.41
1:A:141:GLY:O	1:A:323:ILE:HG23	2.20	0.41
1:A:24:GLY:O	1:A:27:ILE:HB	2.21	0.41
1:A:504:ASP:C	1:A:506:GLY:H	2.24	0.41
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.78	0.41
1:B:775:SER:OG	1:B:780:ARG:HG2	2.20	0.41
1:D:1034:SER:O	1:D:1035:ARG:HB2	2.21	0.41
1:D:94:PHE:CE2	1:D:103:ALA:HB1	2.56	0.41
1:E:942:ALA:O	1:E:946:VAL:HG23	2.21	0.41
1:F:533:GLY:O	1:F:536:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:OE1	1:A:821:GLY:HA2	2.21	0.41
1:A:925:VAL:HG12	1:A:926:TYR:N	2.35	0.41
1:B:950:LYS:NZ	1:B:1030:ARG:HH21	2.18	0.41
1:B:188:MET:HB3	1:B:193:LEU:HD11	2.03	0.41
1:C:270:LEU:HD11	1:C:762:PHE:HZ	1.86	0.41
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.89	0.41
1:C:465:ALA:O	1:C:468:ARG:HB3	2.20	0.41
1:D:18:ILE:HG21	1:D:18:ILE:HD13	1.83	0.41
1:E:139:VAL:O	1:E:326:PRO:HD2	2.21	0.41
1:E:369:THR:O	1:E:373:PRO:CD	2.69	0.41
1:E:448:VAL:O	1:E:452:VAL:HG13	2.20	0.41
1:E:598:TYR:CE2	1:E:629:VAL:HG21	2.56	0.41
1:F:1039:ASP:HB3	1:F:1041:GLU:HB2	2.03	0.41
1:F:1045:THR:O	1:F:1046:VAL:HB	2.21	0.41
1:D:687:GLN:HG2	1:F:316:PHE:CE1	2.56	0.41
1:F:23:GLY:HA3	1:F:377:LEU:HB3	2.02	0.41
1:A:292:LYS:NZ	2:A:1101:ERY:O11	2.53	0.41
1:A:246:PHE:O	1:A:262:LEU:HD23	2.21	0.41
1:A:488:LEU:HD12	1:A:488:LEU:HA	1.76	0.41
1:A:555:LEU:HA	1:A:555:LEU:HD23	1.60	0.41
1:A:659:LYS:HD3	1:A:659:LYS:HA	1.51	0.41
1:B:194:ASN:CG	1:B:790:TYR:HD2	2.24	0.41
1:B:211:ASN:OD1	1:B:239:ARG:HA	2.21	0.41
1:B:562:SER:OG	1:B:563:PHE:N	2.53	0.41
1:C:154:ILE:HG22	1:C:287:SER:HB3	2.03	0.41
1:C:431:THR:HG21	1:C:490:PRO:O	2.21	0.41
1:C:610:PHE:HB3	1:C:628:PHE:HB2	2.02	0.41
1:D:143:ILE:HG22	1:D:286:ALA:CB	2.51	0.41
1:D:140:VAL:HB	1:D:289:LEU:HB2	2.02	0.41
1:D:708:LYS:C	1:D:710:PRO:HD3	2.42	0.41
1:E:699:ARG:HD3	1:E:825:MET:HE2	2.03	0.41
1:E:790:TYR:CE1	1:E:800:PRO:HB3	2.56	0.41
1:E:932:LEU:HD23	1:E:935:ILE:HD12	2.02	0.41
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.55	0.41
1:F:578:LEU:HD22	1:F:661:ALA:HB3	2.03	0.41
1:A:278:ILE:CG1	1:A:613:ASN:HB3	2.47	0.41
1:A:735:LYS:O	1:A:738:ALA:HB3	2.20	0.41
1:C:406:VAL:O	1:C:407:ASP:C	2.59	0.41
1:C:578:LEU:CG	1:C:587:THR:HG22	2.42	0.41
1:C:682:PHE:CE1	1:C:857:TYR:HB2	2.55	0.41
1:D:166:ILE:HA	1:D:166:ILE:HD13	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:743:ILE:HD12	1:D:743:ILE:H	1.86	0.41
1:E:435:MET:SD	1:E:490:PRO:HB3	2.61	0.41
1:E:646:ALA:O	1:E:649:MET:HB3	2.21	0.41
1:E:717:ARG:NE	1:E:828:LEU:HD12	2.36	0.41
1:F:199:THR:HG22	1:F:790:TYR:O	2.21	0.41
1:F:452:VAL:C	1:F:455:PRO:HD2	2.41	0.41
1:F:469:GLN:O	1:F:472:ILE:HG22	2.21	0.41
1:A:1041:GLU:HB3	1:A:1042:HIS:H	1.68	0.41
1:A:305:ALA:O	1:A:308:ALA:HB3	2.20	0.41
1:A:344:LEU:HD11	1:A:398:MET:CB	2.51	0.41
1:A:708:LYS:C	1:A:710:PRO:HD3	2.42	0.41
1:A:944:LEU:HB3	1:A:971:ARG:CZ	2.51	0.41
1:A:99:ASP:HB3	1:A:102:ILE:HB	2.03	0.41
1:B:213:GLN:HE22	1:B:238:THR:HG23	1.85	0.41
1:B:394:THR:O	1:B:473:THR:HG21	2.20	0.41
1:B:457:ALA:HB2	1:B:471:SER:OG	2.19	0.41
1:B:919:ARG:HH21	1:B:921:LEU:HD21	1.86	0.41
1:C:926:TYR:CD2	1:C:1003:VAL:HG22	2.55	0.41
1:C:380:PHE:CD2	1:C:383:LEU:HD12	2.56	0.41
1:C:937:LEU:HD23	1:C:937:LEU:HA	1.64	0.41
1:C:940:LYS:O	1:C:943:ILE:HB	2.21	0.41
1:C:987:MET:HB3	1:C:988:PRO:HD3	2.03	0.41
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.56	0.41
1:D:944:LEU:HA	1:D:944:LEU:HD23	1.65	0.41
1:E:775:SER:OG	1:E:780:ARG:HG2	2.21	0.41
1:F:199:THR:HB	1:F:749:THR:HG21	2.03	0.41
1:F:5:PHE:O	1:F:7:ASP:N	2.49	0.41
1:A:186:ILE:HB	1:A:773:VAL:CG2	2.44	0.40
1:A:448:VAL:HG22	1:A:887:CYS:HB3	2.02	0.40
1:A:367:ILE:HG12	1:A:492:LEU:HB3	2.04	0.40
1:A:525:HIS:HA	1:A:528:THR:HG22	2.03	0.40
1:A:539:GLY:O	1:A:542:LEU:HB2	2.21	0.40
1:A:910:ILE:HG13	1:A:910:ILE:O	2.20	0.40
1:B:362:PHE:HA	1:B:365:THR:HG22	2.03	0.40
1:B:679:GLY:HA2	1:B:830:GLN:HA	2.02	0.40
1:B:841:MET:HG2	1:B:859:TRP:CH2	2.57	0.40
1:B:932:LEU:HD23	1:B:932:LEU:HA	1.78	0.40
1:C:882:ILE:O	1:C:886:LEU:HD23	2.21	0.40
1:D:915:ALA:HB2	1:D:1009:GLY:HA3	2.03	0.40
1:D:510:LYS:O	1:D:512:PHE:N	2.54	0.40
1:E:171:GLY:HA3	1:E:302:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:ARG:O	1:E:367:ILE:HG13	2.20	0.40
1:E:911:GLY:HA2	1:E:1013:THR:HG21	2.03	0.40
1:E:396:PHE:HD1	1:E:926:TYR:CE2	2.34	0.40
1:F:443:VAL:HG12	1:F:891:LEU:HD21	2.03	0.40
1:F:420:MET:HB3	1:F:500:ILE:HB	2.02	0.40
1:F:713:LEU:HD21	1:F:843:LEU:HD12	2.03	0.40
1:F:79:SER:O	1:F:91:THR:HB	2.21	0.40
1:A:1016:VAL:HG12	1:A:1016:VAL:O	2.21	0.40
1:A:534:ILE:CD1	1:A:1024:VAL:HG22	2.52	0.40
1:B:1016:VAL:HG13	3:B:1101:LMT:C10	2.51	0.40
1:B:418:ARG:O	1:B:422:GLU:HB2	2.21	0.40
1:B:542:LEU:O	1:B:546:LEU:HG	2.22	0.40
1:B:719:ASN:HB2	1:B:828:LEU:HG	2.03	0.40
1:B:948:PHE:CZ	1:B:971:ARG:HD2	2.55	0.40
1:C:930:GLY:HA2	1:C:1007:VAL:HG23	2.02	0.40
1:C:143:ILE:O	1:C:321:LEU:HD22	2.21	0.40
1:C:182:TYR:HA	1:C:182:TYR:HD1	1.65	0.40
1:C:775:SER:OG	1:C:780:ARG:HG2	2.22	0.40
1:D:452:VAL:HA	1:D:880:SER:OG	2.22	0.40
1:E:448:VAL:HG13	1:E:884:VAL:CG2	2.47	0.40
1:F:544:LEU:HD23	1:F:1021:PHE:CZ	2.57	0.40
1:F:356:TYR:C	1:F:358:PHE:N	2.74	0.40
1:F:892:TYR:C	1:F:894:SER:H	2.14	0.40
1:A:375:VAL:HG13	1:A:480:LEU:CB	2.51	0.40
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.82	0.40
1:B:938:SER:OG	1:B:1014:ALA:HB1	2.20	0.40
1:B:354:VAL:O	1:B:358:PHE:HB2	2.21	0.40
1:B:419:VAL:HG12	1:B:425:LEU:HD12	2.02	0.40
1:B:540:ARG:O	1:B:543:VAL:HB	2.22	0.40
1:B:736:ALA:HB1	1:B:741:VAL:HG23	2.03	0.40
1:C:102:ILE:HG23	1:C:102:ILE:HD12	1.84	0.40
1:C:536:ARG:NH2	3:C:1101:LMT:O3B	2.55	0.40
1:C:120:GLN:O	1:C:123:GLN:HB2	2.22	0.40
1:C:509:LYS:HD2	1:C:509:LYS:HA	1.79	0.40
1:C:555:LEU:HA	1:C:555:LEU:HD23	1.79	0.40
1:D:61:VAL:CG2	1:D:122:VAL:HG21	2.51	0.40
1:D:507:GLU:O	1:D:508:GLY:O	2.38	0.40
1:D:574:THR:HG21	1:D:598:TYR:CE2	2.56	0.40
1:D:877:TYR:CE1	3:D:1103:LMT:H91	2.57	0.40
1:E:103:ALA:HA	1:E:106:GLN:OE1	2.21	0.40
1:E:775:SER:HB3	1:E:780:ARG:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:415:ASN:ND2	1:F:434:SER:HB2	2.36	0.40
1:F:63:GLN:O	1:F:67:GLN:HG3	2.22	0.40
1:F:888:LEU:HD21	1:F:943:ILE:HD11	2.02	0.40
1:A:13:TRP:O	1:A:17:ILE:HG13	2.21	0.40
1:A:30:LEU:HA	1:A:31:PRO:HD3	1.86	0.40
1:A:351:VAL:O	1:A:355:MET:HG2	2.21	0.40
1:A:402:ILE:HG21	1:A:402:ILE:HD13	1.81	0.40
1:B:736:ALA:HB1	1:B:746:ILE:HD11	2.03	0.40
1:C:1041:GLU:HB3	1:C:1042:HIS:CA	2.52	0.40
1:C:104:GLN:HG3	1:C:105:VAL:N	2.35	0.40
1:C:388:PHE:HE2	1:C:472:ILE:CG1	2.34	0.40
1:C:659:LYS:HA	1:C:659:LYS:HD3	1.27	0.40
1:A:63:GLN:OE1	1:C:768:VAL:HG12	2.21	0.40
1:C:953:MET:HE1	1:C:960:LEU:HD12	2.03	0.40
1:C:979:SER:HA	1:C:1011:MET:CE	2.51	0.40
1:D:573:MET:O	1:D:666:PHE:HD1	2.05	0.40
1:D:704:ALA:O	1:D:707:ALA:HB3	2.22	0.40
1:E:907:LEU:HG	1:E:1017:LEU:HD23	2.03	0.40
1:F:1021:PHE:HD2	1:F:1025:PHE:CZ	2.39	0.40
1:F:1041:GLU:HB3	1:F:1042:HIS:CB	2.50	0.40
1:F:535:LEU:HA	1:F:535:LEU:HD23	1.63	0.40
1:F:931:LEU:O	1:F:934:THR:HB	2.21	0.40
1:B:196:PHE:CD1	1:B:196:PHE:N	2.90	0.40
1:B:278:ILE:HG13	1:B:613:ASN:HB3	2.04	0.40
1:B:743:ILE:HA	1:B:746:ILE:CD1	2.50	0.40
1:C:196:PHE:CD2	1:C:260:VAL:HG13	2.56	0.40
1:B:233:SER:HB2	1:C:726:GLN:HG2	2.02	0.40
1:D:448:VAL:HG13	1:D:884:VAL:HG22	2.03	0.40
1:D:888:LEU:CD1	1:D:901:VAL:HG13	2.48	0.40
1:E:463:THR:OG1	1:E:464:GLY:N	2.54	0.40
1:F:13:TRP:HH2	1:F:370:ILE:HD13	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:HIS:NE2	1:D:525:HIS:NE2[1_556]	2.02	0.18

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	1040/1049 (99%)	951 (91%)	75 (7%)	14 (1%)	12	50
1	B	1040/1049 (99%)	957 (92%)	70 (7%)	13 (1%)	12	50
1	C	1042/1049 (99%)	954 (92%)	72 (7%)	16 (2%)	10	47
1	D	1040/1049 (99%)	946 (91%)	79 (8%)	15 (1%)	11	48
1	E	1040/1049 (99%)	960 (92%)	63 (6%)	17 (2%)	9	46
1	F	1044/1049 (100%)	945 (90%)	83 (8%)	16 (2%)	10	47
All	All	6246/6294 (99%)	5713 (92%)	442 (7%)	91 (2%)	10	47

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	LYS
1	A	673	GLU
1	A	675	GLY
1	A	991	ILE
1	A	1040	ILE
1	B	509	LYS
1	B	677	ALA
1	B	893	GLU
1	B	1038	GLU
1	B	1040	ILE
1	C	1035	ARG
1	C	1036	LYS
1	C	1043	SER
1	D	508	GLY
1	D	511	GLY
1	D	673	GLU
1	D	675	GLY
1	D	992	SER
1	D	1034	SER
1	D	1040	ILE

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Mol	Chain	Res	Type
1	E	509	LYS
1	E	672	VAL
1	E	677	ALA
1	F	511	GLY
1	F	893	GLU
1	A	147	GLY
1	A	869	SER
1	B	672	VAL
1	B	673	GLU
1	B	1037	ASN
1	B	1041	GLU
1	C	146	ASP
1	C	360	GLN
1	C	689	GLY
1	C	1041	GLU
1	D	509	LYS
1	D	991	ILE
1	D	1037	ASN
1	D	1039	ASP
1	E	893	GLU
1	E	1034	SER
1	E	1037	ASN
1	F	146	ASP
1	F	1033	PHE
1	F	1042	HIS
1	F	1046	VAL
1	B	263	ARG
1	B	507	GLU
1	C	893	GLU
1	C	1037	ASN
1	E	147	GLY
1	E	673	GLU
1	E	1033	PHE
1	F	360	GLN
1	F	836	SER
1	A	992	SER
1	A	1038	GLU
1	C	357	LEU
1	C	407	ASP
1	C	1042	HIS
1	D	869	SER
1	D	1042	HIS

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Mol	Chain	Res	Type
1	E	775	SER
1	E	1041	GLU
1	F	147	GLY
1	A	775	SER
1	C	775	SER
1	D	775	SER
1	E	263	ARG
1	E	892	TYR
1	F	357	LEU
1	F	507	GLU
1	F	509	LYS
1	F	1044	HIS
1	A	263	ARG
1	A	765	ARG
1	C	765	ARG
1	D	1038	GLU
1	E	146	ASP
1	E	357	LEU
1	E	511	GLY
1	E	1040	ILE
1	F	1039	ASP
1	C	6	ILE
1	F	638	PRO
1	A	672	VAL
1	B	638	PRO
1	A	910	ILE
1	B	910	ILE
1	C	638	PRO
1	F	6	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	845/852 (99%)	786 (93%)	59 (7%)	15	48
1	B	845/852 (99%)	788 (93%)	57 (7%)	16	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	847/852 (99%)	787 (93%)	60 (7%)	14	48
1	D	845/852 (99%)	795 (94%)	50 (6%)	19	55
1	E	845/852 (99%)	788 (93%)	57 (7%)	16	50
1	F	849/852 (100%)	791 (93%)	58 (7%)	16	50
All	All	5076/5112 (99%)	4735 (93%)	341 (7%)	16	50

All (341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	28	LEU
1	A	49	TYR
1	A	151	GLN
1	A	152	GLU
1	A	177	LEU
1	A	205	THR
1	A	222	THR
1	A	225	VAL
1	A	245	GLU
1	A	293	LEU
1	A	324	VAL
1	A	327	TYR
1	A	343	THR
1	A	360	GLN
1	A	362	PHE
1	A	415	ASN
1	A	429	GLU
1	A	434	SER
1	A	437	GLN
1	A	456	MET
1	A	463	THR
1	A	472	ILE
1	A	524	THR
1	A	528	THR
1	A	626	ILE
1	A	630	SER
1	A	634	TRP
1	A	659	LYS
1	A	666	PHE
1	A	668	LEU
1	A	672	VAL

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Mol	Chain	Res	Type
1	A	674	LEU
1	A	678	THR
1	A	695	LEU
1	A	713	LEU
1	A	716	VAL
1	A	721	LEU
1	A	748	THR
1	A	768	VAL
1	A	775	SER
1	A	795	ASP
1	A	804	PHE
1	A	806	SER
1	A	811	TYR
1	A	857	TYR
1	A	901	VAL
1	A	922	THR
1	A	931	LEU
1	A	951	ASP
1	A	958	LYS
1	A	961	ILE
1	A	964	THR
1	A	968	VAL
1	A	971	ARG
1	A	980	LEU
1	A	984	LEU
1	A	1033	PHE
1	A	1035	ARG
1	B	11	PHE
1	B	21	LEU
1	B	28	LEU
1	B	49	TYR
1	B	60	THR
1	B	96	SER
1	B	105	VAL
1	B	109	ASN
1	B	128	SER
1	B	146	ASP
1	B	182	TYR
1	B	185	ARG
1	B	249	ILE
1	B	253	VAL
1	B	255	GLN

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Mol	Chain	Res	Type
1	B	259	ARG
1	B	267	LYS
1	B	277	ILE
1	B	293	LEU
1	B	295	THR
1	B	310	LEU
1	B	321	LEU
1	B	329	THR
1	B	343	THR
1	B	352	PHE
1	B	355	MET
1	B	358	PHE
1	B	372	VAL
1	B	400	LEU
1	B	418	ARG
1	B	429	GLU
1	B	538	THR
1	B	561	SER
1	B	571	VAL
1	B	602	GLU
1	B	626	ILE
1	B	628	PHE
1	B	634	TRP
1	B	668	LEU
1	B	672	VAL
1	B	714	THR
1	B	717	ARG
1	B	721	LEU
1	B	775	SER
1	B	804	PHE
1	B	806	SER
1	B	811	TYR
1	B	835	LYS
1	B	931	LEU
1	B	958	LYS
1	B	968	VAL
1	B	971	ARG
1	B	980	LEU
1	B	982	PHE
1	B	984	LEU
1	B	1035	ARG
1	B	1041	GLU

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Mol	Chain	Res	Type
1	C	3	ASN
1	C	11	PHE
1	C	27	ILE
1	C	28	LEU
1	C	48	SER
1	C	49	TYR
1	C	59	ASP
1	C	60	THR
1	C	87	THR
1	C	102	ILE
1	C	104	GLN
1	C	151	GLN
1	C	177	LEU
1	C	182	TYR
1	C	243	THR
1	C	253	VAL
1	C	280	GLU
1	C	307	ARG
1	C	358	PHE
1	C	415	ASN
1	C	429	GLU
1	C	439	GLN
1	C	462	SER
1	C	463	THR
1	C	472	ILE
1	C	482	VAL
1	C	510	LYS
1	C	524	THR
1	C	561	SER
1	C	578	LEU
1	C	602	GLU
1	C	623	ASN
1	C	626	ILE
1	C	634	TRP
1	C	659	LYS
1	C	668	LEU
1	C	694	LYS
1	C	695	LEU
1	C	713	LEU
1	C	721	LEU
1	C	746	ILE
1	C	775	SER

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Mol	Chain	Res	Type
1	C	795	ASP
1	C	804	PHE
1	C	837	THR
1	C	847	LEU
1	C	865	GLN
1	C	876	LEU
1	C	938	SER
1	C	947	GLU
1	C	958	LYS
1	C	971	ARG
1	C	980	LEU
1	C	984	LEU
1	C	991	ILE
1	C	993	THR
1	C	1033	PHE
1	C	1035	ARG
1	C	1037	ASN
1	C	1040	ILE
1	D	28	LEU
1	D	45	ILE
1	D	49	TYR
1	D	146	ASP
1	D	151	GLN
1	D	152	GLU
1	D	177	LEU
1	D	222	THR
1	D	243	THR
1	D	245	GLU
1	D	310	LEU
1	D	324	VAL
1	D	343	THR
1	D	355	MET
1	D	360	GLN
1	D	362	PHE
1	D	428	LYS
1	D	472	ILE
1	D	524	THR
1	D	561	SER
1	D	564	LEU
1	D	571	VAL
1	D	602	GLU
1	D	626	ILE

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Mol	Chain	Res	Type
1	D	630	SER
1	D	634	TRP
1	D	659	LYS
1	D	666	PHE
1	D	668	LEU
1	D	672	VAL
1	D	674	LEU
1	D	680	PHE
1	D	713	LEU
1	D	716	VAL
1	D	721	LEU
1	D	775	SER
1	D	804	PHE
1	D	806	SER
1	D	815	ARG
1	D	857	TYR
1	D	901	VAL
1	D	914	LEU
1	D	931	LEU
1	D	958	LYS
1	D	961	ILE
1	D	968	VAL
1	D	971	ARG
1	D	982	PHE
1	D	984	LEU
1	D	1033	PHE
1	E	25	LEU
1	E	28	LEU
1	E	45	ILE
1	E	60	THR
1	E	96	SER
1	E	109	ASN
1	E	131	LYS
1	E	146	ASP
1	E	151	GLN
1	E	177	LEU
1	E	243	THR
1	E	249	ILE
1	E	253	VAL
1	E	255	GLN
1	E	259	ARG
1	E	295	THR

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Mol	Chain	Res	Type
1	E	310	LEU
1	E	321	LEU
1	E	329	THR
1	E	358	PHE
1	E	372	VAL
1	E	400	LEU
1	E	418	ARG
1	E	536	ARG
1	E	538	THR
1	E	561	SER
1	E	563	PHE
1	E	569	GLN
1	E	613	ASN
1	E	626	ILE
1	E	634	TRP
1	E	659	LYS
1	E	666	PHE
1	E	667	ASN
1	E	668	LEU
1	E	672	VAL
1	E	673	GLU
1	E	678	THR
1	E	680	PHE
1	E	714	THR
1	E	717	ARG
1	E	721	LEU
1	E	775	SER
1	E	804	PHE
1	E	811	TYR
1	E	857	TYR
1	E	880	SER
1	E	901	VAL
1	E	931	LEU
1	E	958	LYS
1	E	968	VAL
1	E	971	ARG
1	E	980	LEU
1	E	984	LEU
1	E	1036	LYS
1	E	1040	ILE
1	E	1043	SER
1	F	3	ASN

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Mol	Chain	Res	Type
1	F	11	PHE
1	F	28	LEU
1	F	48	SER
1	F	49	TYR
1	F	59	ASP
1	F	60	THR
1	F	87	THR
1	F	104	GLN
1	F	112	GLN
1	F	129	VAL
1	F	177	LEU
1	F	253	VAL
1	F	293	LEU
1	F	307	ARG
1	F	362	PHE
1	F	400	LEU
1	F	429	GLU
1	F	447	MET
1	F	448	VAL
1	F	462	SER
1	F	482	VAL
1	F	510	LYS
1	F	524	THR
1	F	571	VAL
1	F	578	LEU
1	F	596	HIS
1	F	602	GLU
1	F	626	ILE
1	F	668	LEU
1	F	672	VAL
1	F	674	LEU
1	F	695	LEU
1	F	713	LEU
1	F	721	LEU
1	F	746	ILE
1	F	760	ASN
1	F	768	VAL
1	F	775	SER
1	F	804	PHE
1	F	806	SER
1	F	811	TYR
1	F	876	LEU

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Mol	Chain	Res	Type
1	F	918	PHE
1	F	938	SER
1	F	947	GLU
1	F	958	LYS
1	F	971	ARG
1	F	980	LEU
1	F	982	PHE
1	F	984	LEU
1	F	991	ILE
1	F	1011	MET
1	F	1030	ARG
1	F	1035	ARG
1	F	1043	SER
1	F	1044	HIS
1	F	1047	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	151	GLN
1	B	213	GLN
1	B	737	GLN
1	B	760	ASN
1	C	67	GLN
1	C	104	GLN
1	C	274	ASN
1	D	123	GLN
1	D	360	GLN
1	D	1001	ASN
1	E	81	ASN
1	E	213	GLN
1	E	604	ASN
1	E	613	ASN
1	F	151	GLN
1	F	228	GLN
1	F	760	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	F	1101	-	36,36,36	1.81	8 (22%)	47,47,47	1.36	8 (17%)
3	LMT	D	1102	-	36,36,36	1.85	10 (27%)	47,47,47	1.00	3 (6%)
3	LMT	B	1101	-	36,36,36	1.86	9 (25%)	47,47,47	1.87	11 (23%)
3	LMT	A	1102	-	36,36,36	1.78	9 (25%)	47,47,47	1.14	5 (10%)
3	LMT	C	1101	-	36,36,36	1.76	9 (25%)	47,47,47	1.50	8 (17%)
3	LMT	E	1101	-	36,36,36	1.85	9 (25%)	47,47,47	1.31	6 (12%)
3	LMT	D	1103	-	36,36,36	1.77	8 (22%)	47,47,47	1.54	9 (19%)
2	ERY	D	1101	-	53,53,53	1.38	5 (9%)	82,82,82	2.00	23 (28%)
2	ERY	A	1101	-	53,53,53	1.27	5 (9%)	82,82,82	2.01	24 (29%)
3	LMT	A	1103	-	36,36,36	1.91	8 (22%)	47,47,47	1.46	8 (17%)

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	F	1101	-	-	9/21/61/61	0/2/2/2
3	LMT	D	1102	-	-	15/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	B	1101	-	1/1/10/10	11/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	8/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	10/21/61/61	0/2/2/2
3	LMT	E	1101	-	-	10/21/61/61	0/2/2/2
3	LMT	D	1103	-	-	11/21/61/61	0/2/2/2
2	ERY	D	1101	-	-	13/72/107/107	0/3/3/3
2	ERY	A	1101	-	-	38/72/107/107	0/3/3/3
3	LMT	A	1103	-	-	13/21/61/61	0/2/2/2

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ERY	O2-C1	5.38	1.46	1.34
2	D	1101	ERY	O2-C1	5.26	1.46	1.34
3	A	1103	LMT	O5'-C5'	5.12	1.56	1.44
3	D	1103	LMT	O5B-C1B	4.25	1.52	1.41
3	B	1101	LMT	O1'-C1'	4.25	1.47	1.40
3	E	1101	LMT	O1'-C1'	4.24	1.47	1.40
3	D	1102	LMT	O1'-C1'	4.20	1.47	1.40
3	A	1102	LMT	O5'-C5'	4.16	1.54	1.44
3	F	1101	LMT	O5'-C5'	4.01	1.54	1.44
3	F	1101	LMT	O1'-C1'	3.94	1.46	1.40
3	E	1101	LMT	O5'-C5'	3.87	1.53	1.44
3	D	1103	LMT	O5'-C5'	3.86	1.53	1.44
3	C	1101	LMT	O5'-C5'	3.86	1.53	1.44
3	A	1103	LMT	O5B-C1B	3.85	1.51	1.41
3	C	1101	LMT	O1'-C1'	3.80	1.46	1.40
3	B	1101	LMT	O5'-C5'	3.74	1.53	1.44
3	D	1102	LMT	O5B-C1B	3.67	1.51	1.41
3	A	1103	LMT	O5'-C1'	3.65	1.51	1.41
3	B	1101	LMT	O5B-C1B	3.65	1.51	1.41
3	F	1101	LMT	O5'-C1'	3.64	1.51	1.41
3	D	1103	LMT	O1'-C1'	3.61	1.46	1.40
3	A	1102	LMT	O5B-C1B	3.58	1.51	1.41
3	A	1103	LMT	O3B-C3B	3.55	1.51	1.43
3	B	1101	LMT	O5'-C1'	3.49	1.50	1.41
3	A	1103	LMT	O1'-C1'	3.48	1.46	1.40
3	D	1102	LMT	C6'-C5'	-3.39	1.40	1.51
3	E	1101	LMT	O5'-C1'	3.39	1.50	1.41
3	C	1101	LMT	O5'-C1'	3.37	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	LMT	O1'-C1'	3.37	1.45	1.40
3	C	1101	LMT	O5B-C1B	3.35	1.50	1.41
3	B	1101	LMT	O3B-C3B	3.34	1.50	1.43
3	D	1102	LMT	O3B-C3B	3.34	1.50	1.43
3	D	1102	LMT	O5'-C5'	3.33	1.52	1.44
3	F	1101	LMT	C6'-C5'	-3.26	1.40	1.51
3	D	1102	LMT	O5'-C1'	3.25	1.50	1.41
3	E	1101	LMT	O5B-C1B	3.23	1.50	1.41
3	E	1101	LMT	C3'-C2'	-3.20	1.44	1.52
3	D	1103	LMT	C6'-C5'	-3.18	1.41	1.51
3	D	1103	LMT	O5'-C1'	3.18	1.49	1.41
3	A	1103	LMT	C6'-C5'	-3.09	1.41	1.51
3	A	1102	LMT	O3B-C3B	3.07	1.50	1.43
3	C	1101	LMT	C6'-C5'	-3.03	1.41	1.51
3	A	1102	LMT	C6'-C5'	-2.98	1.41	1.51
3	E	1101	LMT	O3B-C3B	2.97	1.50	1.43
3	F	1101	LMT	O5B-C1B	2.97	1.49	1.41
3	D	1103	LMT	O3B-C3B	2.95	1.49	1.43
3	A	1102	LMT	O5'-C1'	2.94	1.49	1.41
3	E	1101	LMT	C6'-C5'	-2.86	1.42	1.51
3	B	1101	LMT	C6'-C5'	-2.84	1.42	1.51
3	F	1101	LMT	O3B-C3B	2.78	1.49	1.43
3	B	1101	LMT	O3'-C3'	2.64	1.49	1.43
3	C	1101	LMT	O2'-C2'	2.53	1.48	1.43
3	D	1102	LMT	O2'-C2'	2.51	1.48	1.43
3	C	1101	LMT	C3B-C2B	-2.49	1.46	1.52
3	F	1101	LMT	C3'-C2'	-2.46	1.46	1.52
3	B	1101	LMT	O2'-C2'	2.46	1.48	1.43
3	A	1103	LMT	O3'-C3'	2.43	1.48	1.43
2	D	1101	ERY	C25-C26	2.43	1.56	1.51
3	E	1101	LMT	C3B-C2B	-2.41	1.46	1.52
3	A	1103	LMT	O2'-C2'	2.40	1.48	1.43
3	A	1102	LMT	O2'-C2'	2.39	1.48	1.43
3	D	1103	LMT	O3'-C3'	2.39	1.48	1.43
3	D	1103	LMT	O2'-C2'	2.38	1.48	1.43
2	D	1101	ERY	O11-C9	2.37	1.25	1.21
3	D	1102	LMT	C3B-C2B	-2.34	1.46	1.52
3	D	1102	LMT	O3'-C3'	2.34	1.48	1.43
3	F	1101	LMT	O2'-C2'	2.32	1.48	1.43
2	A	1101	ERY	C25-C26	2.32	1.56	1.51
3	C	1101	LMT	O3'-C3'	2.27	1.48	1.43
3	B	1101	LMT	C5-C4	2.26	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1101	LMT	C3'-C2'	-2.22	1.46	1.52
3	E	1101	LMT	C5-C4	2.21	1.64	1.51
3	A	1102	LMT	C3'-C2'	-2.19	1.46	1.52
3	D	1102	LMT	C3'-C2'	-2.18	1.46	1.52
2	A	1101	ERY	O6-C17	2.12	1.47	1.42
2	A	1101	ERY	O11-C9	2.12	1.25	1.21
2	D	1101	ERY	O9-C22	2.11	1.47	1.41
3	A	1102	LMT	C5-C4	2.06	1.63	1.51
2	D	1101	ERY	C22-C23	2.05	1.58	1.52
2	A	1101	ERY	O3-C14	2.01	1.46	1.41

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	ERY	O7-C5-C6	5.93	113.71	106.39
2	D	1101	ERY	C20-O5-C16	5.43	128.89	117.55
3	B	1101	LMT	O5'-C5'-C6'	5.41	119.89	106.44
2	A	1101	ERY	C20-O5-C16	5.30	128.60	117.55
2	D	1101	ERY	O12-C11-C10	5.28	118.61	110.71
2	A	1101	ERY	O2-C1-O1	-4.89	114.81	123.94
2	A	1101	ERY	O7-C5-C6	4.68	112.16	106.39
3	B	1101	LMT	O1'-C1'-C2'	4.56	115.43	108.30
2	A	1101	ERY	O12-C11-C10	4.51	117.46	110.71
2	D	1101	ERY	C15-C16-C17	4.39	115.53	107.67
3	D	1103	LMT	C1'-O5'-C5'	-4.29	105.26	113.69
3	B	1101	LMT	O5'-C5'-C4'	-4.18	100.94	109.75
2	D	1101	ERY	C29-N1-C24	4.09	125.41	113.11
2	A	1101	ERY	C29-N1-C24	4.02	125.18	113.11
2	A	1101	ERY	C15-C16-C17	3.99	114.81	107.67
2	A	1101	ERY	C13-O2-C1	-3.91	111.23	118.18
3	C	1101	LMT	C3B-C4B-C5B	3.90	117.20	110.24
3	B	1101	LMT	C4B-C3B-C2B	3.84	117.53	110.82
3	A	1103	LMT	C3B-C4B-C5B	3.83	117.07	110.24
2	D	1101	ERY	C25-C24-N1	-3.79	104.97	115.67
3	A	1103	LMT	C1B-O1B-C4'	-3.75	108.69	117.96
2	A	1101	ERY	O2-C1-C2	3.68	119.63	111.56
3	B	1101	LMT	C1B-O1B-C4'	-3.59	109.08	117.96
3	E	1101	LMT	O5'-C5'-C6'	3.55	115.26	106.44
2	A	1101	ERY	O3-C3-C4	3.54	112.48	108.22
3	B	1101	LMT	C1'-O5'-C5'	-3.49	106.83	113.69
2	A	1101	ERY	O2-C13-C36	3.44	113.95	107.40
3	F	1101	LMT	C1B-C2B-C3B	3.39	117.06	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	ERY	O9-C26-C25	3.37	114.29	109.14
2	A	1101	ERY	C19-C16-C15	-3.32	104.57	110.49
3	A	1103	LMT	O5B-C5B-C4B	3.31	115.70	109.69
3	D	1103	LMT	C1'-C2'-C3'	3.23	116.72	110.00
3	D	1103	LMT	O5'-C5'-C4'	-3.17	103.07	109.75
2	A	1101	ERY	O7-C5-C4	-3.16	106.81	111.54
3	C	1101	LMT	O1'-C1'-C2'	3.16	113.23	108.30
3	C	1101	LMT	O5B-C5B-C4B	3.16	115.43	109.69
3	A	1102	LMT	C1B-C2B-C3B	3.16	116.57	110.00
3	E	1101	LMT	O5B-C5B-C4B	3.14	115.39	109.69
3	E	1101	LMT	C3B-C4B-C5B	3.13	115.82	110.24
2	A	1101	ERY	O7-C22-C23	3.06	116.02	108.10
3	F	1101	LMT	C4B-C3B-C2B	2.99	116.05	110.82
3	C	1101	LMT	O2B-C2B-C1B	-2.95	102.88	110.05
3	D	1103	LMT	C3'-C4'-C5'	-2.90	104.27	110.93
2	A	1101	ERY	C33-C8-C7	-2.90	104.47	109.81
3	C	1101	LMT	C1B-O5B-C5B	2.87	119.33	113.69
3	F	1101	LMT	O5B-C5B-C4B	2.86	114.89	109.69
3	B	1101	LMT	O5B-C5B-C4B	2.86	114.89	109.69
2	D	1101	ERY	O4-C18-C21	2.85	112.86	106.70
2	D	1101	ERY	O13-C12-C11	2.82	114.58	108.90
3	D	1102	LMT	O1'-C1'-C2'	2.78	112.64	108.30
2	D	1101	ERY	C22-O9-C26	2.74	117.24	112.91
2	D	1101	ERY	C19-C16-C15	-2.72	105.64	110.49
3	A	1103	LMT	C1'-O5'-C5'	2.71	119.02	113.69
3	F	1101	LMT	O4'-C4B-C3B	-2.70	104.10	110.35
3	D	1103	LMT	O5B-C5B-C4B	2.68	114.57	109.69
2	A	1101	ERY	O10-C6-C32	-2.68	102.30	108.47
3	D	1103	LMT	O1'-C1'-C2'	2.67	112.47	108.30
3	F	1101	LMT	O4'-C4B-C5B	2.64	115.84	109.30
3	E	1101	LMT	O1'-C1'-C2'	2.63	112.40	108.30
3	E	1101	LMT	C1B-O1B-C4'	-2.62	111.48	117.96
3	A	1102	LMT	C1B-O1B-C4'	-2.60	111.53	117.96
2	D	1101	ERY	C31-C4-C3	-2.59	106.76	111.40
3	C	1101	LMT	O1B-C4'-C3'	2.58	114.15	107.28
3	F	1101	LMT	O2B-C2B-C1B	-2.58	103.79	110.05
3	B	1101	LMT	O5B-C1B-C2B	2.55	115.76	110.35
3	C	1101	LMT	C1B-O1B-C4'	-2.55	111.66	117.96
3	F	1101	LMT	C1-O1'-C1'	2.52	118.03	113.84
3	C	1101	LMT	O5'-C5'-C6'	2.52	112.70	106.44
2	D	1101	ERY	C26-C25-C24	2.50	114.83	110.46
2	D	1101	ERY	O3-C3-C4	-2.50	105.21	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1103	LMT	O5B-C5B-C6B	2.46	112.55	106.44
3	A	1103	LMT	C4B-C3B-C2B	2.45	115.11	110.82
3	A	1102	LMT	O1B-C1B-C2B	2.45	114.44	108.10
3	A	1103	LMT	O5'-C5'-C4'	2.44	114.90	109.75
2	A	1101	ERY	C33-C8-C9	2.43	115.28	109.44
2	D	1101	ERY	C33-C8-C7	-2.39	105.42	109.81
3	A	1102	LMT	C2'-C3'-C4'	2.38	115.11	109.68
3	B	1101	LMT	O2B-C2B-C3B	2.37	115.82	110.35
2	A	1101	ERY	O4-C18-C21	2.36	111.80	106.70
3	D	1103	LMT	O5'-C5'-C6'	2.36	112.30	106.44
3	E	1101	LMT	C1-O1'-C1'	2.35	117.74	113.84
2	D	1101	ERY	C7-C6-C5	2.30	114.97	110.48
2	D	1101	ERY	O13-C12-C13	-2.28	103.61	107.28
2	D	1101	ERY	O10-C6-C5	-2.27	103.28	107.59
2	A	1101	ERY	C22-O7-C5	2.23	120.13	116.25
2	D	1101	ERY	C33-C8-C9	2.20	114.73	109.44
3	A	1102	LMT	C1'-C2'-C3'	2.20	114.58	110.00
2	D	1101	ERY	C3-C4-C5	-2.17	106.52	111.19
3	B	1101	LMT	C3B-C4B-C5B	2.16	114.10	110.24
3	A	1103	LMT	C2'-C3'-C4'	-2.16	104.75	109.68
3	A	1103	LMT	O3'-C3'-C2'	2.15	115.33	110.35
3	F	1101	LMT	O5'-C5'-C6'	2.15	111.78	106.44
2	D	1101	ERY	C36-C13-C12	-2.15	111.12	115.20
3	B	1101	LMT	O1'-C1-C2	2.15	117.09	109.56
2	A	1101	ERY	C30-C2-C3	2.15	117.78	112.92
2	A	1101	ERY	C35-C12-C13	2.14	114.32	111.31
3	D	1103	LMT	O1B-C4'-C3'	2.13	112.95	107.28
2	D	1101	ERY	C6-C5-C4	-2.13	111.03	114.05
2	A	1101	ERY	O1-C1-C2	-2.10	118.45	124.08
3	D	1102	LMT	O5B-C1B-C2B	2.10	114.80	110.35
2	D	1101	ERY	O7-C22-C23	2.07	113.47	108.10
2	A	1101	ERY	O2-C13-C12	2.07	110.66	107.29
2	A	1101	ERY	C7-C6-C5	2.04	114.47	110.48
2	A	1101	ERY	C35-C12-C11	-2.02	109.51	113.05
3	D	1102	LMT	O2B-C2B-C3B	-2.01	105.71	110.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1101	LMT	C3B

All (138) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1102	LMT	C2-C1-O1'-C1'
3	B	1101	LMT	C2'-C1'-O1'-C1
3	B	1101	LMT	O5'-C1'-O1'-C1
3	C	1101	LMT	C2-C1-O1'-C1'
3	E	1101	LMT	C2'-C1'-O1'-C1
3	E	1101	LMT	C2-C1-O1'-C1'
3	D	1103	LMT	O5'-C1'-O1'-C1
3	D	1103	LMT	C2-C1-O1'-C1'
2	D	1101	ERY	C6-C7-C8-C33
2	D	1101	ERY	C23-C24-N1-C29
2	D	1101	ERY	C25-C24-N1-C29
2	A	1101	ERY	C9-C10-C11-C12
2	A	1101	ERY	C9-C10-C11-O12
2	A	1101	ERY	C34-C10-C11-C12
2	A	1101	ERY	C34-C10-C11-O12
2	A	1101	ERY	C10-C11-C12-C13
2	A	1101	ERY	C10-C11-C12-C35
2	A	1101	ERY	C10-C11-C12-O13
2	A	1101	ERY	O12-C11-C12-C13
2	A	1101	ERY	O12-C11-C12-C35
2	A	1101	ERY	O12-C11-C12-O13
2	A	1101	ERY	C11-C12-C13-O2
2	A	1101	ERY	C35-C12-C13-C36
2	A	1101	ERY	O13-C12-C13-O2
2	A	1101	ERY	O2-C13-C36-C37
2	A	1101	ERY	C2-C1-O2-C13
2	A	1101	ERY	C32-C6-C7-C8
2	A	1101	ERY	C23-C24-N1-C29
2	A	1101	ERY	C25-C24-N1-C28
3	A	1103	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	O5'-C5'-C6'-O6'
3	C	1101	LMT	O5B-C5B-C6B-O6B
3	E	1101	LMT	O5'-C5'-C6'-O6'
3	D	1103	LMT	C4B-C5B-C6B-O6B
3	F	1101	LMT	O5'-C5'-C6'-O6'
3	A	1103	LMT	C4'-C5'-C6'-O6'
3	B	1101	LMT	O5B-C5B-C6B-O6B
3	C	1101	LMT	C4B-C5B-C6B-O6B
3	D	1103	LMT	C4-C5-C6-C7
3	A	1103	LMT	O5B-C5B-C6B-O6B
3	E	1101	LMT	C4'-C5'-C6'-O6'
3	D	1102	LMT	O5B-C5B-C6B-O6B
3	F	1101	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
3	D	1103	LMT	O5B-C5B-C6B-O6B
2	A	1101	ERY	C2-C3-C4-C31
3	D	1102	LMT	C4'-C5'-C6'-O6'
2	A	1101	ERY	O4-C14-O3-C3
3	A	1102	LMT	C4'-C5'-C6'-O6'
3	B	1101	LMT	O5'-C5'-C6'-O6'
3	A	1103	LMT	C4B-C5B-C6B-O6B
3	D	1102	LMT	O5'-C5'-C6'-O6'
3	B	1101	LMT	C4B-C5B-C6B-O6B
3	B	1101	LMT	C4'-C5'-C6'-O6'
2	A	1101	ERY	O2-C1-C2-C3
3	D	1102	LMT	C4B-C5B-C6B-O6B
3	A	1102	LMT	O5'-C5'-C6'-O6'
2	A	1101	ERY	C2-C3-C4-C5
3	E	1101	LMT	O5'-C1'-O1'-C1
3	D	1103	LMT	C4'-C5'-C6'-O6'
2	A	1101	ERY	C25-C24-N1-C29
3	D	1102	LMT	C3-C4-C5-C6
3	D	1102	LMT	C11-C10-C9-C8
3	D	1102	LMT	C2'-C1'-O1'-C1
3	A	1102	LMT	C2'-C1'-O1'-C1
3	C	1101	LMT	C2'-C1'-O1'-C1
3	C	1101	LMT	C3-C4-C5-C6
3	A	1103	LMT	C5-C6-C7-C8
2	A	1101	ERY	O3-C3-C4-C5
3	B	1101	LMT	C2-C3-C4-C5
2	A	1101	ERY	C23-C24-N1-C28
3	A	1102	LMT	O5'-C1'-O1'-C1
3	C	1101	LMT	O5'-C1'-O1'-C1
2	D	1101	ERY	C2-C1-O2-C13
3	A	1102	LMT	C3-C4-C5-C6
3	C	1101	LMT	C6-C7-C8-C9
3	E	1101	LMT	C5-C6-C7-C8
3	E	1101	LMT	C11-C10-C9-C8
3	A	1103	LMT	C7-C8-C9-C10
3	B	1101	LMT	O1'-C1-C2-C3
3	D	1103	LMT	O5'-C5'-C6'-O6'
3	D	1102	LMT	C4-C5-C6-C7
2	A	1101	ERY	C19-C16-O5-C20
3	C	1101	LMT	C1-C2-C3-C4
3	E	1101	LMT	C1-C2-C3-C4
3	D	1102	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	D	1103	LMT	C1-C2-C3-C4
3	A	1103	LMT	C4-C5-C6-C7
3	F	1101	LMT	C1-C2-C3-C4
3	E	1101	LMT	O1'-C1-C2-C3
2	A	1101	ERY	O3-C3-C4-C31
3	A	1103	LMT	O5B-C1B-O1B-C4'
3	A	1103	LMT	C9-C10-C11-C12
3	D	1103	LMT	C7-C8-C9-C10
3	A	1102	LMT	C6-C7-C8-C9
3	F	1101	LMT	C6-C7-C8-C9
3	D	1102	LMT	O5'-C1'-O1'-C1
2	A	1101	ERY	C11-C12-C13-C36
3	B	1101	LMT	C4-C5-C6-C7
2	A	1101	ERY	O10-C6-C7-C8
2	D	1101	ERY	O7-C5-C6-C7
3	D	1103	LMT	C11-C10-C9-C8
2	D	1101	ERY	C4-C5-C6-O10
3	A	1103	LMT	C1-C2-C3-C4
3	D	1102	LMT	C6-C7-C8-C9
3	C	1101	LMT	C7-C8-C9-C10
3	F	1101	LMT	C2-C1-O1'-C1'
2	A	1101	ERY	C4-C5-O7-C22
2	A	1101	ERY	C6-C5-O7-C22
2	D	1101	ERY	C15-C16-O5-C20
2	D	1101	ERY	C19-C16-O5-C20
2	A	1101	ERY	C15-C16-O5-C20
3	A	1102	LMT	C7-C8-C9-C10
3	A	1103	LMT	C6-C7-C8-C9
3	D	1102	LMT	O1'-C1-C2-C3
3	C	1101	LMT	O1'-C1-C2-C3
2	D	1101	ERY	O2-C13-C36-C37
2	D	1101	ERY	C17-C16-O5-C20
2	A	1101	ERY	O1-C1-C2-C3
3	F	1101	LMT	O5B-C5B-C6B-O6B
3	D	1102	LMT	C7-C8-C9-C10
3	B	1101	LMT	C6-C7-C8-C9
2	A	1101	ERY	O1-C1-C2-C30
3	E	1101	LMT	C9-C10-C11-C12
3	F	1101	LMT	C5-C6-C7-C8
2	A	1101	ERY	C6-C7-C8-C33
2	D	1101	ERY	C12-C13-C36-C37
2	A	1101	ERY	C12-C13-C36-C37

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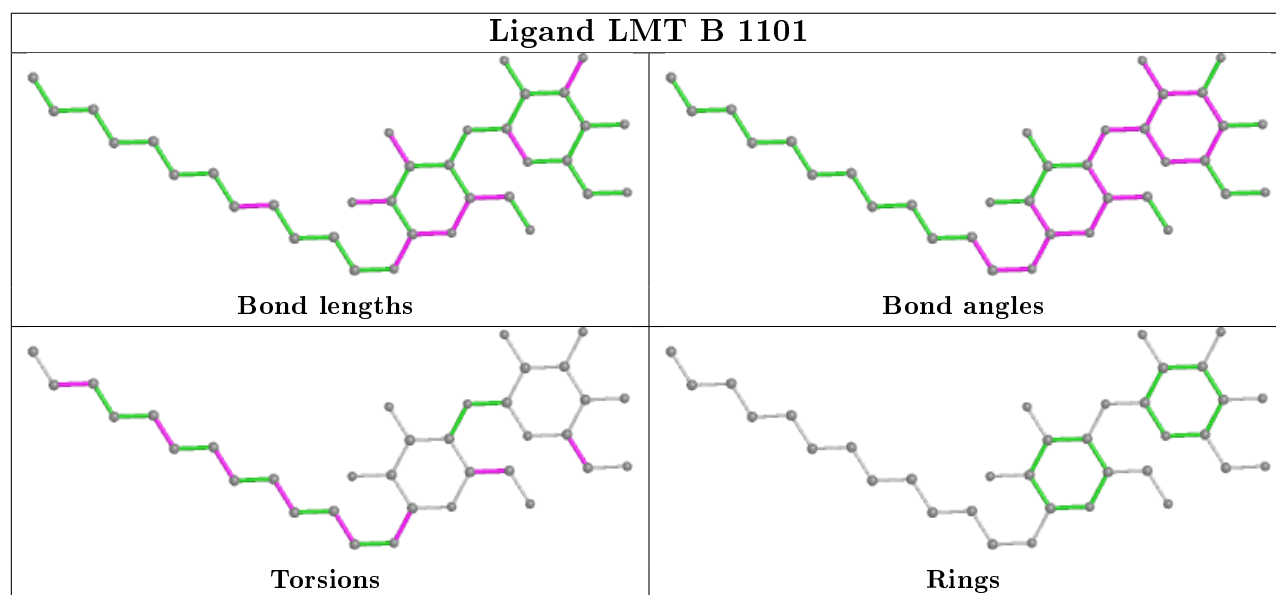
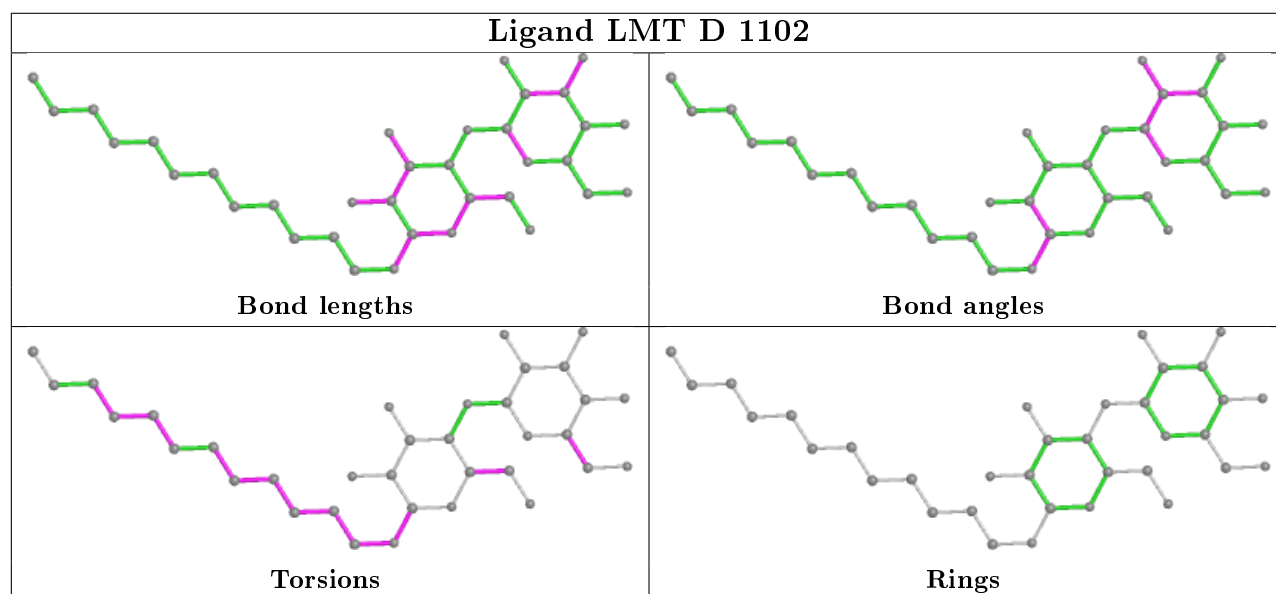
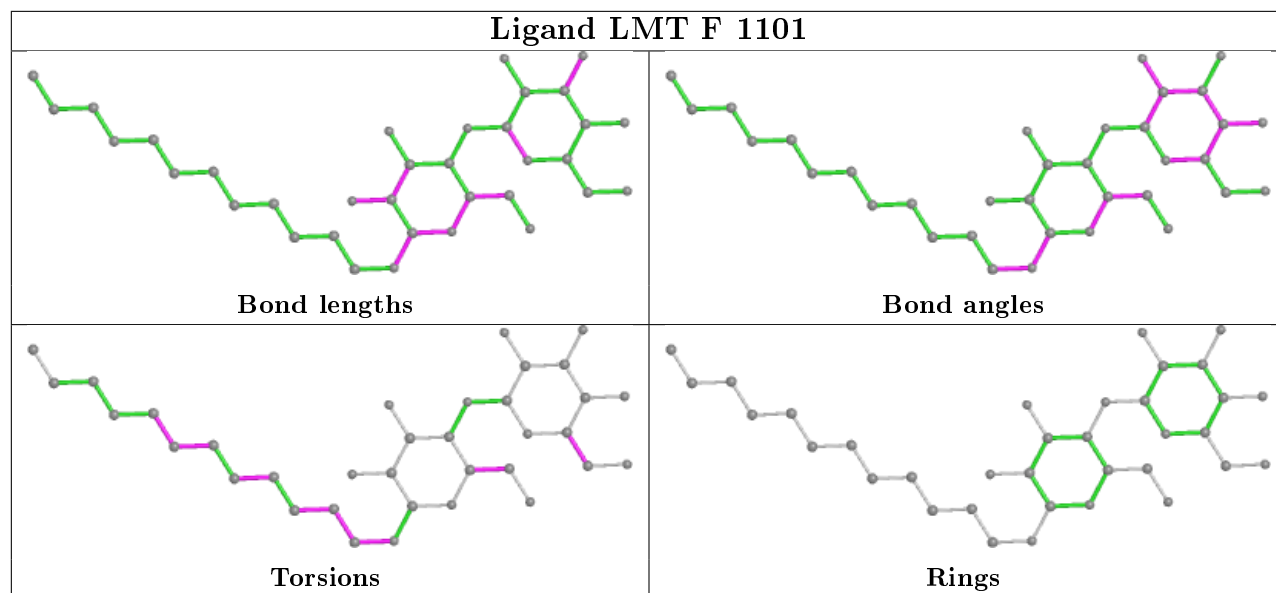
Mol	Chain	Res	Type	Atoms
3	A	1102	LMT	O1'-C1-C2-C3
2	A	1101	ERY	O1-C1-O2-C13
3	F	1101	LMT	O1'-C1-C2-C3
2	A	1101	ERY	C17-C16-O5-C20
3	A	1103	LMT	C2B-C1B-O1B-C4'
3	D	1102	LMT	C2-C3-C4-C5
3	F	1101	LMT	C3-C4-C5-C6
3	D	1103	LMT	C2-C3-C4-C5
2	D	1101	ERY	C6-C7-C8-C9
2	D	1101	ERY	C15-C14-O3-C3
3	B	1101	LMT	C9-C10-C11-C12

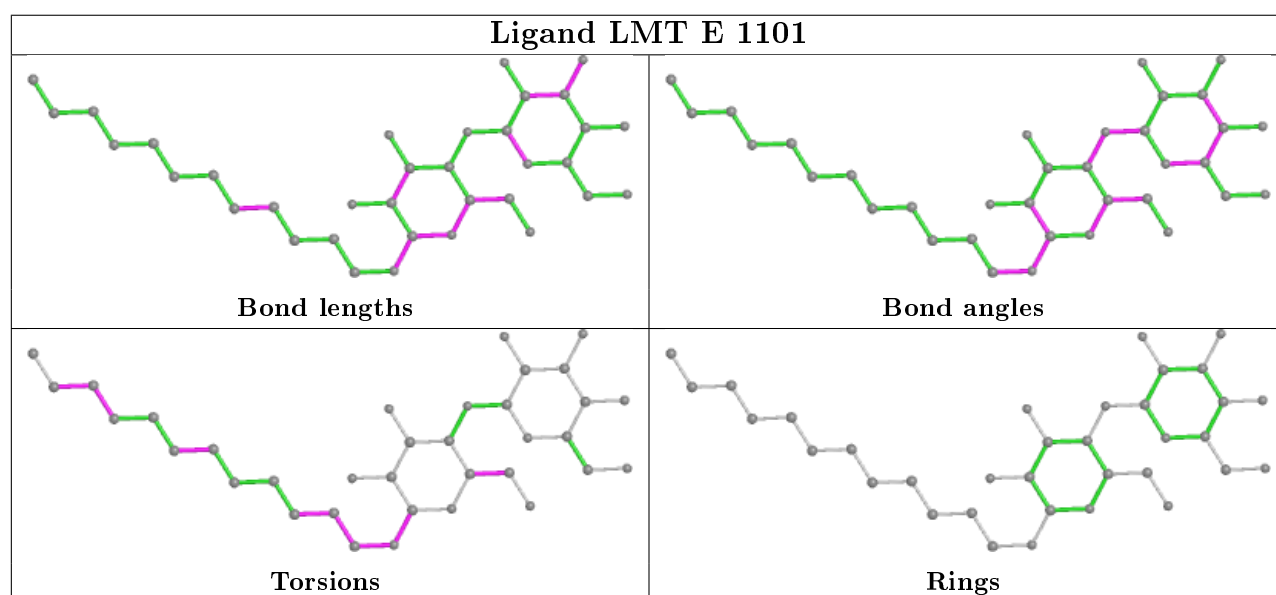
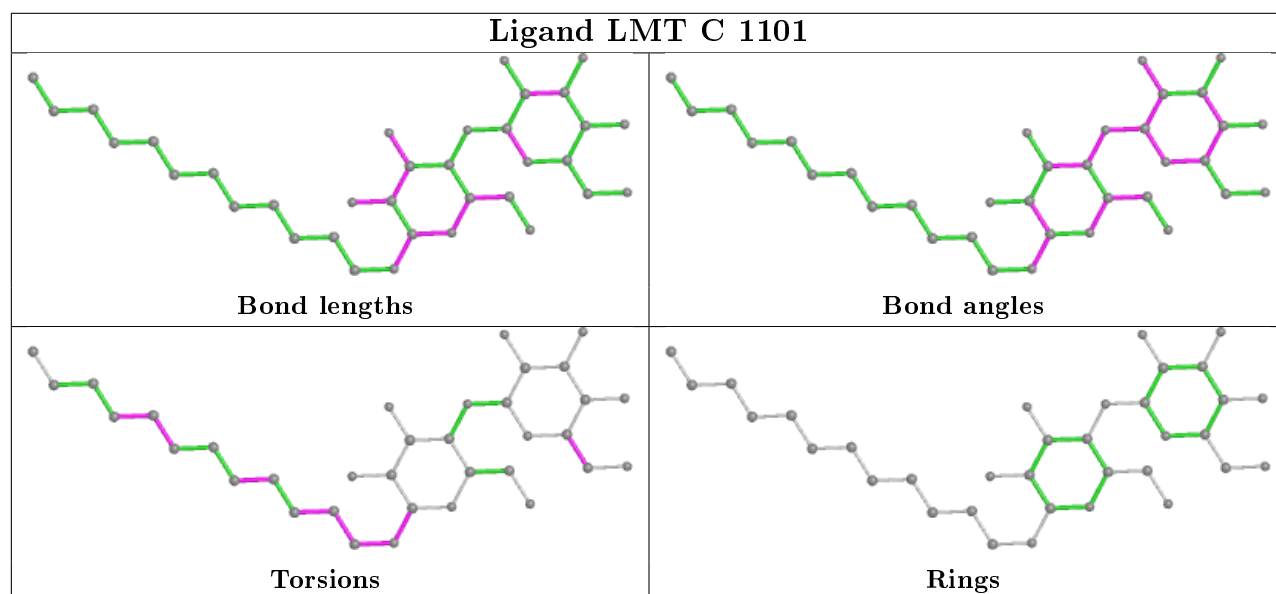
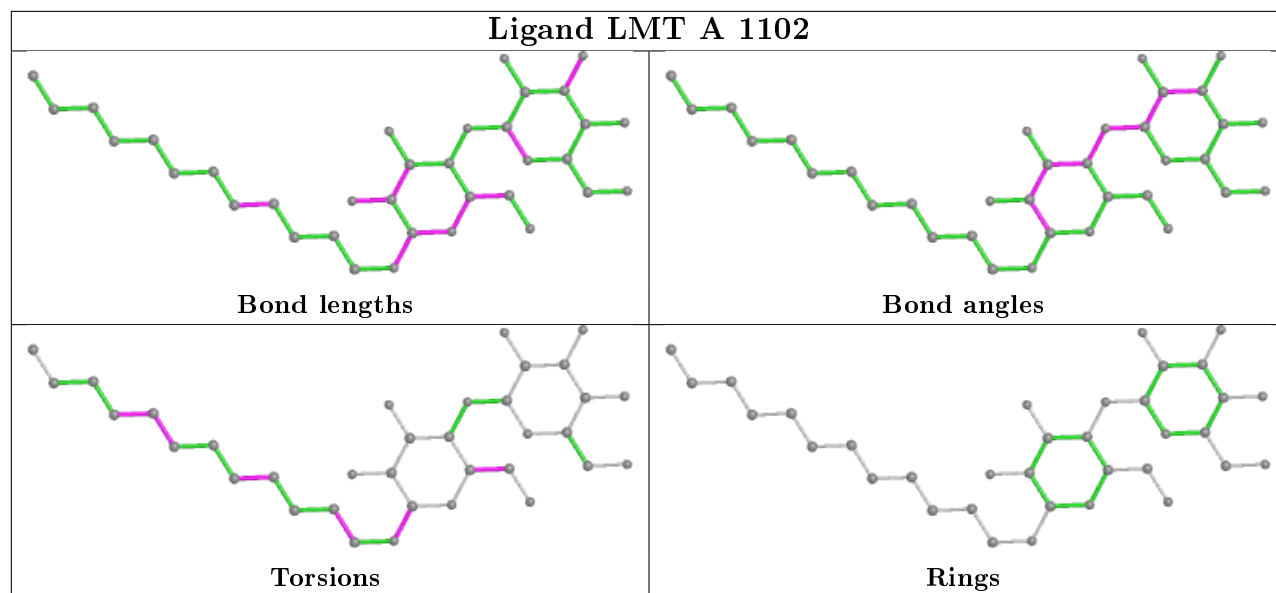
There are no ring outliers.

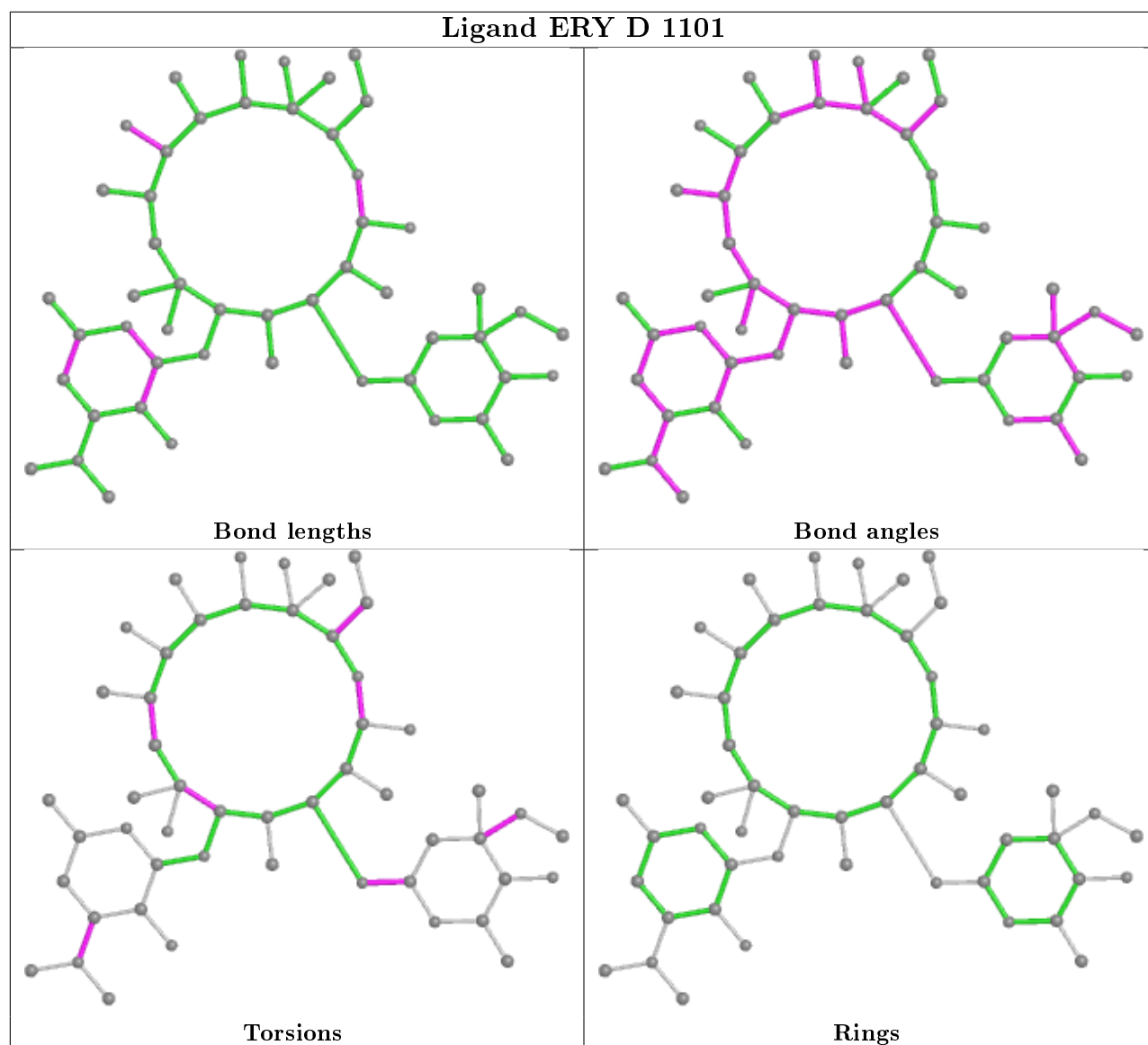
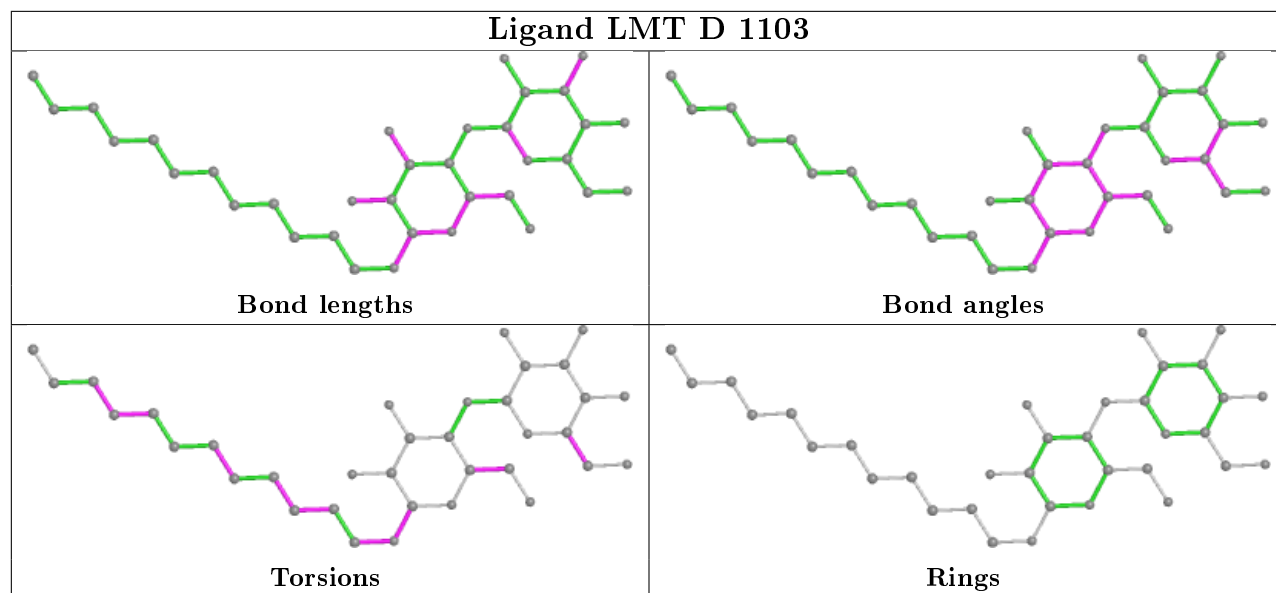
10 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1101	LMT	5	0
3	D	1102	LMT	2	0
3	B	1101	LMT	5	0
3	A	1102	LMT	3	0
3	C	1101	LMT	1	0
3	E	1101	LMT	3	0
3	D	1103	LMT	7	0
2	D	1101	ERY	5	0
2	A	1101	ERY	10	0
3	A	1103	LMT	2	0

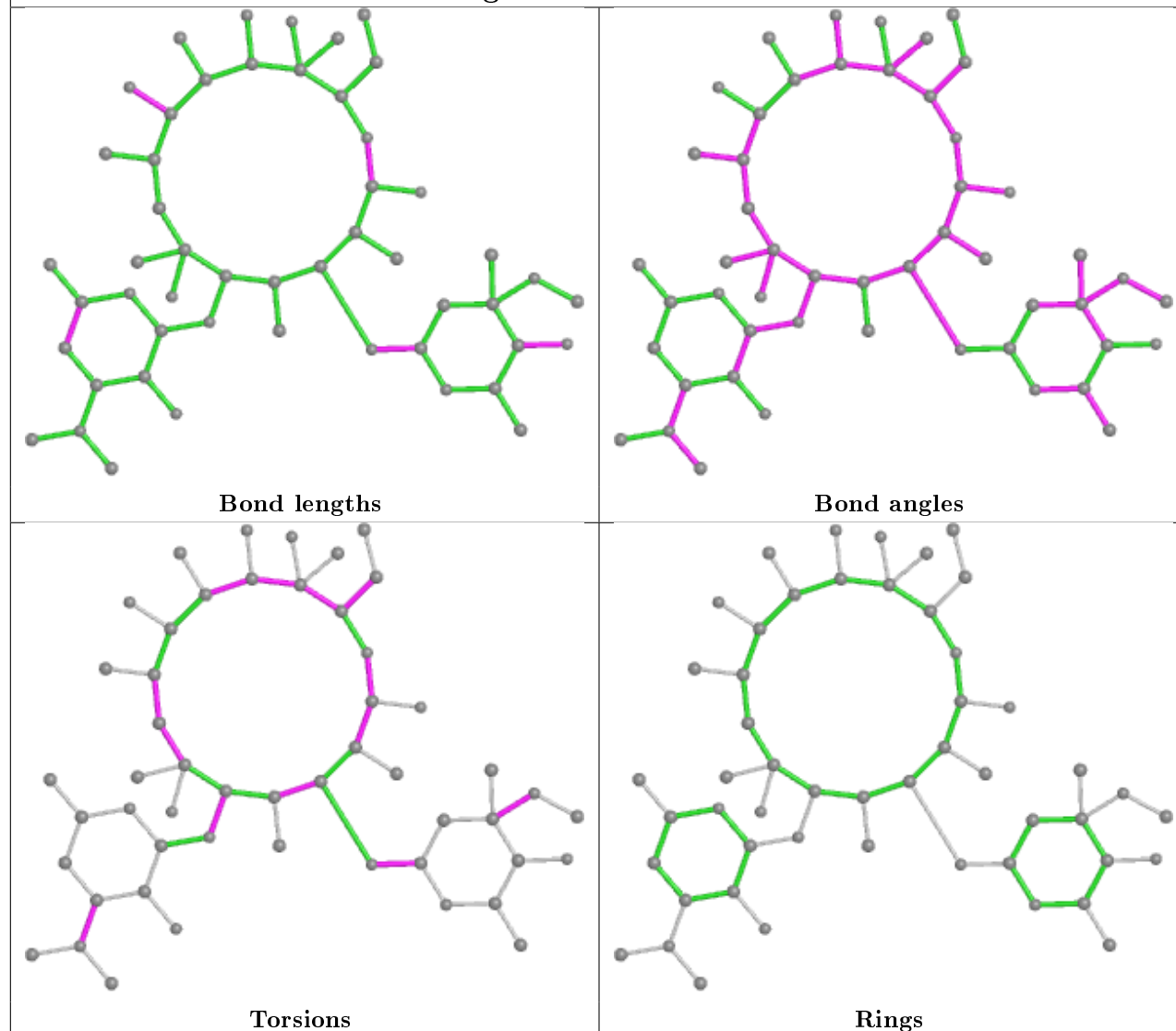
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



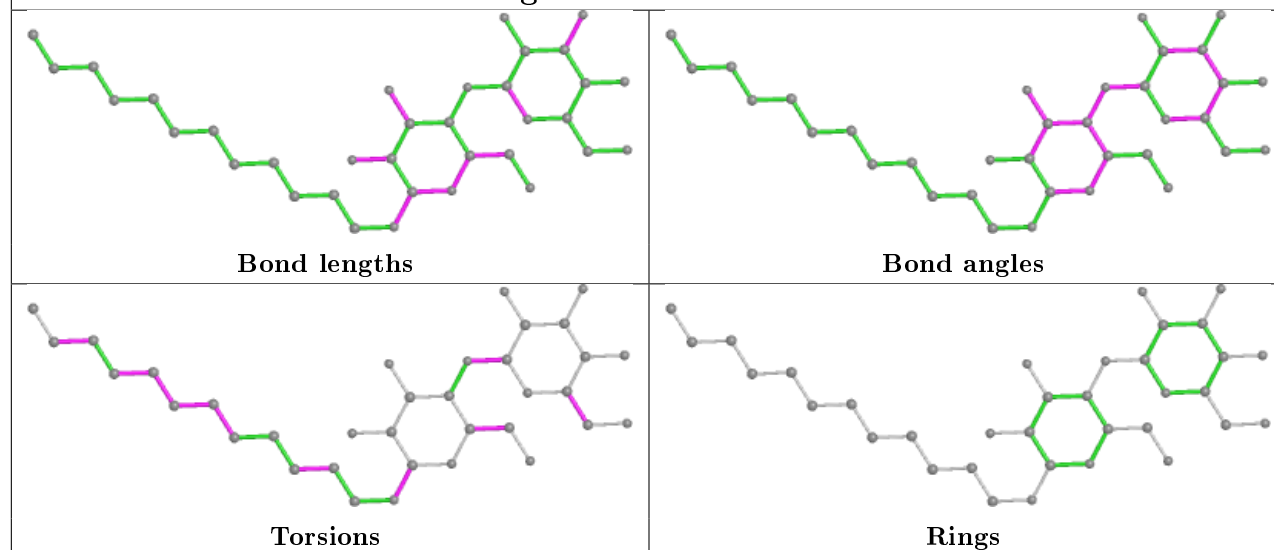




Ligand ERY A 1101



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, 95th 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 ²)	Q<0.9
1	A	1042/1049 (99%)	0.39	98 (9%)	8 4	49, 83, 120, 150	0
1	B	1042/1049 (99%)	0.29	73 (7%)	16 9	45, 81, 117, 154	0
1	C	1044/1049 (99%)	0.59	122 (11%)	4 3	40, 83, 120, 176	0
1	D	1042/1049 (99%)	0.54	122 (11%)	4 3	43, 94, 130, 161	0
1	E	1042/1049 (99%)	0.56	151 (14%)	2 1	57, 94, 125, 151	0
1	F	1046/1049 (99%)	0.67	144 (13%)	2 2	44, 89, 124, 158	0
All	All	6258/6294 (99%)	0.51	710 (11%)	5 3	40, 87, 124, 176	0

All (710) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	719	ASN	14.3
1	C	720	GLY	14.3
1	F	80	SER	11.7
1	F	720	GLY	11.1
1	C	618	ALA	10.0
1	B	869	SER	9.9
1	D	619	GLY	9.9
1	C	80	SER	9.3
1	C	619	GLY	9.2
1	F	835	LYS	9.2
1	C	83	ASP	9.1
1	D	720	GLY	9.1
1	C	719	ASN	8.8
1	F	82	SER	8.4
1	E	618	ALA	8.2
1	F	618	ALA	8.1
1	F	79	SER	8.1
1	F	83	ASP	8.0
1	F	826	GLU	7.8

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Mol	Chain	Res	Type	RSRZ
1	D	719	ASN	7.8
1	F	837	THR	7.8
1	D	869	SER	7.5
1	C	81	ASN	7.4
1	E	681	ASP	7.3
1	F	619	GLY	7.3
1	C	617	ALA	7.0
1	F	836	SER	7.0
1	C	79	SER	6.9
1	E	619	GLY	6.9
1	F	712	MET	6.8
1	C	82	SER	6.7
1	E	658	ILE	6.7
1	B	618	ALA	6.6
1	B	619	GLY	6.6
1	C	836	SER	6.6
1	D	618	ALA	6.5
1	E	80	SER	6.4
1	F	81	ASN	6.3
1	F	711	ASP	6.2
1	D	615	ALA	6.1
1	C	721	LEU	6.1
1	D	620	ALA	6.0
1	B	719	ASN	6.0
1	E	657	GLN	6.0
1	A	449	LEU	6.0
1	E	719	ASN	6.0
1	D	401	ALA	5.9
1	A	619	GLY	5.9
1	F	713	LEU	5.8
1	B	617	ALA	5.8
1	A	620	ALA	5.8
1	F	815	ARG	5.8
1	C	815	ARG	5.7
1	F	681	ASP	5.7
1	F	829	GLY	5.6
1	B	80	SER	5.6
1	B	817	GLU	5.6
1	F	58	GLN	5.6
1	D	616	GLY	5.6
1	F	817	GLU	5.6
1	D	460	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	E	291	ILE	5.6
1	C	816	LEU	5.5
1	A	658	ILE	5.5
1	E	655	PHE	5.5
1	E	615	ALA	5.5
1	E	678	THR	5.5
1	F	718	PRO	5.4
1	D	178	PHE	5.4
1	C	835	LYS	5.4
1	E	617	ALA	5.4
1	F	828	LEU	5.4
1	D	621	GLY	5.4
1	E	830	GLN	5.3
1	A	605	ASN	5.3
1	C	837	THR	5.3
1	F	60	THR	5.3
1	B	620	ALA	5.2
1	E	290	GLY	5.2
1	F	617	ALA	5.2
1	C	616	GLY	5.2
1	E	720	GLY	5.2
1	C	712	MET	5.2
1	D	826	GLU	5.1
1	C	817	GLU	5.1
1	F	831	ALA	5.1
1	C	826	GLU	5.0
1	C	403	GLY	5.0
1	F	839	GLU	5.0
1	B	79	SER	5.0
1	F	577	GLN	5.0
1	F	676	THR	4.9
1	F	888	LEU	4.9
1	F	402	ILE	4.9
1	F	620	ALA	4.9
1	E	310	LEU	4.9
1	E	78	MET	4.9
1	C	449	LEU	4.8
1	F	834	GLY	4.8
1	F	721	LEU	4.8
1	A	617	ALA	4.7
1	F	69	MET	4.7
1	F	840	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	617	ALA	4.7
1	F	1037	ASN	4.7
1	F	449	LEU	4.7
1	F	662	MET	4.7
1	E	826	GLU	4.7
1	E	81	ASN	4.7
1	F	717	ARG	4.6
1	E	79	SER	4.6
1	E	307	ARG	4.6
1	D	81	ASN	4.6
1	E	943	ILE	4.6
1	A	1039	ASP	4.6
1	E	659	LYS	4.5
1	F	832	ALA	4.5
1	D	461	GLY	4.5
1	C	494	ALA	4.5
1	A	615	ALA	4.5
1	D	80	SER	4.5
1	A	618	ALA	4.4
1	B	678	THR	4.4
1	D	681	ASP	4.4
1	B	720	GLY	4.4
1	D	721	LEU	4.4
1	E	620	ALA	4.4
1	E	616	GLY	4.4
1	D	83	ASP	4.4
1	B	616	GLY	4.4
1	C	615	ALA	4.3
1	F	62	THR	4.3
1	B	577	GLN	4.3
1	C	620	ALA	4.3
1	A	445	ILE	4.3
1	F	500	ILE	4.3
1	C	445	ILE	4.2
1	F	481	SER	4.2
1	B	818	ARG	4.2
1	B	870	GLY	4.2
1	C	818	ARG	4.2
1	B	81	ASN	4.2
1	A	179	GLY	4.2
1	A	616	GLY	4.2
1	C	681	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	59	ASP	4.2
1	B	895	TRP	4.2
1	E	314	GLU	4.1
1	D	815	ARG	4.1
1	C	834	GLY	4.1
1	C	614	GLY	4.1
1	A	92	LEU	4.1
1	C	1011	MET	4.1
1	B	78	MET	4.1
1	F	501	ALA	4.0
1	E	869	SER	4.0
1	F	68	ASN	4.0
1	D	817	GLU	4.0
1	E	818	ARG	4.0
1	E	933	THR	4.0
1	A	78	MET	4.0
1	A	164	ASP	4.0
1	D	79	SER	4.0
1	A	79	SER	4.0
1	D	78	MET	4.0
1	A	719	ASN	4.0
1	E	315	PRO	4.0
1	A	900	SER	4.0
1	B	662	MET	4.0
1	F	57	VAL	3.9
1	E	888	LEU	3.9
1	E	900	SER	3.9
1	E	605	ASN	3.9
1	B	229	GLN	3.9
1	C	62	THR	3.9
1	A	178	PHE	3.9
1	B	615	ALA	3.9
1	C	833	PRO	3.9
1	E	682	PHE	3.9
1	E	819	TYR	3.8
1	F	400	LEU	3.8
1	E	177	LEU	3.8
1	E	993	THR	3.8
1	E	817	GLU	3.8
1	B	400	LEU	3.8
1	C	481	SER	3.8
1	D	1041	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	282	ASN	3.8
1	A	1037	ASN	3.8
1	D	663	VAL	3.8
1	F	941	ASN	3.8
1	B	826	GLU	3.8
1	E	300	LEU	3.8
1	A	960	LEU	3.7
1	F	680	PHE	3.7
1	D	404	LEU	3.7
1	C	684	LEU	3.7
1	C	404	LEU	3.7
1	D	462	SER	3.7
1	E	407	ASP	3.7
1	E	308	ALA	3.7
1	F	70	ASN	3.7
1	F	282	ASN	3.7
1	B	715	SER	3.7
1	A	959	GLY	3.7
1	D	834	GLY	3.7
1	A	1040	ILE	3.7
1	E	406	VAL	3.7
1	B	718	PRO	3.6
1	D	718	PRO	3.6
1	F	404	LEU	3.6
1	A	400	LEU	3.6
1	E	441	ALA	3.6
1	E	718	PRO	3.6
1	A	659	LYS	3.6
1	F	833	PRO	3.6
1	E	33	ALA	3.6
1	A	402	ILE	3.6
1	A	610	PHE	3.6
1	A	401	ALA	3.6
1	C	91	THR	3.6
1	F	830	GLN	3.6
1	B	837	THR	3.5
1	F	442	LEU	3.5
1	C	68	ASN	3.5
1	E	712	MET	3.5
1	C	442	LEU	3.5
1	A	663	VAL	3.5
1	D	400	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	611	ALA	3.5
1	E	82	SER	3.5
1	D	423	GLU	3.5
1	A	655	PHE	3.5
1	D	678	THR	3.5
1	D	389	SER	3.5
1	C	683	GLU	3.5
1	C	444	GLY	3.4
1	F	708	LYS	3.4
1	C	711	ASP	3.4
1	C	802	SER	3.4
1	A	681	ASP	3.4
1	F	406	VAL	3.4
1	C	838	GLY	3.4
1	E	827	ILE	3.4
1	F	66	GLU	3.4
1	F	576	VAL	3.4
1	D	866	GLU	3.4
1	A	181	GLN	3.4
1	E	328	ASP	3.4
1	E	831	ALA	3.4
1	E	839	GLU	3.4
1	F	65	ILE	3.4
1	B	681	ASP	3.4
1	D	614	GLY	3.4
1	F	13	TRP	3.3
1	F	816	LEU	3.3
1	E	299	ALA	3.3
1	B	488	LEU	3.3
1	F	818	ARG	3.3
1	A	641	GLU	3.3
1	D	82	SER	3.3
1	D	933	THR	3.3
1	C	825	MET	3.3
1	D	886	LEU	3.3
1	B	67	GLN	3.3
1	B	943	ILE	3.3
1	D	958	LYS	3.3
1	D	407	ASP	3.3
1	E	835	LYS	3.3
1	F	504	ASP	3.3
1	A	612	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	402	ILE	3.3
1	E	932	LEU	3.2
1	E	679	GLY	3.2
1	C	421	ALA	3.2
1	F	1043	SER	3.2
1	E	403	GLY	3.2
1	F	933	THR	3.2
1	C	400	LEU	3.2
1	A	80	SER	3.2
1	E	32	VAL	3.2
1	E	663	VAL	3.2
1	F	827	ILE	3.2
1	A	606	VAL	3.2
1	C	936	GLY	3.2
1	F	659	LYS	3.2
1	B	815	ARG	3.2
1	F	91	THR	3.2
1	F	699	ARG	3.2
1	D	828	LEU	3.2
1	B	403	GLY	3.2
1	E	488	LEU	3.2
1	C	441	ALA	3.2
1	C	888	LEU	3.2
1	E	944	LEU	3.2
1	F	675	GLY	3.2
1	E	576	VAL	3.2
1	A	403	GLY	3.1
1	F	405	LEU	3.1
1	F	825	MET	3.1
1	C	48	SER	3.1
1	F	503	GLY	3.1
1	A	640	GLU	3.1
1	D	32	VAL	3.1
1	E	642	ASN	3.1
1	A	964	THR	3.1
1	D	322	LYS	3.1
1	C	1044	HIS	3.1
1	A	404	LEU	3.1
1	C	501	ALA	3.1
1	F	502	LYS	3.1
1	E	175	VAL	3.1
1	E	287	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	404	LEU	3.1
1	C	676	THR	3.1
1	F	626	ILE	3.1
1	D	870	GLY	3.1
1	E	891	LEU	3.1
1	D	836	SER	3.1
1	E	936	GLY	3.1
1	C	935	ILE	3.1
1	D	288	GLY	3.1
1	C	621	GLY	3.1
1	E	815	ARG	3.1
1	F	612	VAL	3.1
1	E	640	GLU	3.1
1	E	612	VAL	3.1
1	F	661	ALA	3.1
1	D	839	GLU	3.1
1	C	577	GLN	3.0
1	A	632	LYS	3.0
1	E	683	GLU	3.0
1	D	445	ILE	3.0
1	E	609	VAL	3.0
1	C	937	LEU	3.0
1	E	92	LEU	3.0
1	A	958	LYS	3.0
1	C	448	VAL	3.0
1	F	474	ILE	3.0
1	D	194	ASN	3.0
1	B	63	GLN	3.0
1	C	783	PRO	3.0
1	E	892	TYR	3.0
1	A	657	GLN	3.0
1	D	715	SER	3.0
1	F	877	TYR	3.0
1	F	78	MET	3.0
1	F	722	GLU	3.0
1	D	11	PHE	3.0
1	C	575	MET	2.9
1	D	713	LEU	2.9
1	C	388	PHE	2.9
1	C	718	PRO	2.9
1	C	943	ILE	2.9
1	E	820	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	826	GLU	2.9
1	B	871	ASN	2.9
1	D	818	ARG	2.9
1	E	994	GLY	2.9
1	D	179	GLY	2.9
1	B	91	THR	2.9
1	E	601	LYS	2.9
1	C	713	LEU	2.9
1	A	91	THR	2.9
1	F	67	GLN	2.9
1	C	69	MET	2.9
1	F	407	ASP	2.9
1	D	803	ALA	2.9
1	E	303	ALA	2.9
1	D	323	ILE	2.8
1	D	402	ILE	2.8
1	A	830	GLN	2.8
1	A	835	LYS	2.8
1	F	615	ALA	2.8
1	A	949	ALA	2.8
1	D	960	LEU	2.8
1	D	624	THR	2.8
1	E	405	LEU	2.8
1	C	401	ALA	2.8
1	A	817	GLU	2.8
1	D	1037	ASN	2.8
1	D	287	SER	2.8
1	D	830	GLN	2.8
1	D	851	LEU	2.8
1	B	576	VAL	2.8
1	E	613	ASN	2.8
1	A	961	ILE	2.8
1	E	840	ALA	2.8
1	C	784	ASP	2.8
1	A	613	ASN	2.8
1	C	822	LEU	2.8
1	E	142	VAL	2.8
1	F	993	THR	2.8
1	C	856	GLY	2.8
1	C	57	VAL	2.8
1	F	731	ILE	2.8
1	A	142	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	83	ASP	2.7
1	E	821	GLY	2.7
1	F	937	LEU	2.7
1	F	658	ILE	2.7
1	C	405	LEU	2.7
1	D	888	LEU	2.7
1	D	788	ASP	2.7
1	F	246	PHE	2.7
1	F	663	VAL	2.7
1	B	868	LEU	2.7
1	F	88	VAL	2.7
1	C	14	VAL	2.7
1	B	714	THR	2.7
1	C	1037	ASN	2.7
1	D	789	TRP	2.7
1	A	134	SER	2.7
1	A	767	ARG	2.7
1	C	982	PHE	2.7
1	E	931	LEU	2.7
1	F	575	MET	2.7
1	C	60	THR	2.7
1	E	837	THR	2.7
1	A	195	LYS	2.7
1	B	939	ALA	2.7
1	E	825	MET	2.6
1	C	474	ILE	2.6
1	F	608	SER	2.6
1	D	801	PHE	2.6
1	E	680	PHE	2.6
1	B	683	GLU	2.6
1	F	683	GLU	2.6
1	D	487	ILE	2.6
1	D	173	GLY	2.6
1	D	868	LEU	2.6
1	A	621	GLY	2.6
1	B	828	LEU	2.6
1	D	486	LEU	2.6
1	F	398	MET	2.6
1	E	91	THR	2.6
1	F	714	THR	2.6
1	E	654	ALA	2.6
1	A	81	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	162	MET	2.6
1	E	509	LYS	2.6
1	F	92	LEU	2.6
1	E	890	ALA	2.5
1	B	835	LYS	2.5
1	B	635	ALA	2.5
1	A	162	MET	2.5
1	B	661	ALA	2.5
1	C	58	GLN	2.5
1	F	995	ALA	2.5
1	E	178	PHE	2.5
1	D	325	TYR	2.5
1	F	12	ALA	2.5
1	D	717	ARG	2.5
1	A	942	ALA	2.5
1	C	54	ALA	2.5
1	F	178	PHE	2.5
1	A	902	MET	2.5
1	C	97	GLY	2.5
1	E	330	THR	2.5
1	C	814	PRO	2.5
1	B	638	PRO	2.5
1	A	679	GLY	2.5
1	D	140	VAL	2.5
1	F	445	ILE	2.5
1	B	995	ALA	2.5
1	E	995	ALA	2.5
1	C	313	MET	2.5
1	A	406	VAL	2.5
1	B	178	PHE	2.5
1	C	473	THR	2.5
1	C	933	THR	2.5
1	D	459	PHE	2.5
1	D	610	PHE	2.5
1	C	478	MET	2.4
1	F	401	ALA	2.4
1	F	838	GLY	2.4
1	A	281	PHE	2.4
1	C	839	GLU	2.4
1	E	400	LEU	2.4
1	B	821	GLY	2.4
1	F	64	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	576	VAL	2.4
1	E	662	MET	2.4
1	E	717	ARG	2.4
1	F	884	VAL	2.4
1	C	828	LEU	2.4
1	B	663	VAL	2.4
1	A	176	GLN	2.4
1	E	367	ILE	2.4
1	E	313	MET	2.4
1	C	178	PHE	2.4
1	E	577	GLN	2.4
1	F	403	GLY	2.4
1	C	934	THR	2.4
1	D	62	THR	2.4
1	D	87	THR	2.4
1	D	806	SER	2.4
1	A	962	GLU	2.4
1	D	628	PHE	2.4
1	A	405	LEU	2.4
1	C	788	ASP	2.4
1	C	941	ASN	2.4
1	D	959	GLY	2.4
1	E	402	ILE	2.4
1	E	887	CYS	2.4
1	E	282	ASN	2.4
1	C	865	GLN	2.4
1	F	709	HIS	2.4
1	F	873	ALA	2.4
1	E	733	GLN	2.4
1	D	66	GLU	2.4
1	C	717	ARG	2.4
1	F	7	ASP	2.4
1	F	892	TYR	2.4
1	C	576	VAL	2.4
1	F	960	LEU	2.4
1	B	66	GLU	2.4
1	E	641	GLU	2.4
1	E	714	THR	2.4
1	C	871	ASN	2.3
1	E	598	TYR	2.3
1	F	453	PHE	2.3
1	D	141	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	83	ASP	2.3
1	B	406	VAL	2.3
1	B	721	LEU	2.3
1	E	69	MET	2.3
1	F	89	GLN	2.3
1	A	713	LEU	2.3
1	A	408	ASP	2.3
1	C	502	LYS	2.3
1	D	31	PRO	2.3
1	A	443	VAL	2.3
1	F	739	LEU	2.3
1	D	575	MET	2.3
1	E	408	ASP	2.3
1	C	685	ILE	2.3
1	C	782	LEU	2.3
1	F	61	VAL	2.3
1	D	731	ILE	2.3
1	F	448	VAL	2.3
1	F	814	PRO	2.3
1	A	407	ASP	2.3
1	B	230	LEU	2.3
1	D	993	THR	2.3
1	E	632	LYS	2.3
1	A	177	LEU	2.3
1	C	1045	THR	2.3
1	D	802	SER	2.3
1	E	935	ILE	2.3
1	F	117	LEU	2.3
1	D	714	THR	2.3
1	C	485	ALA	2.3
1	C	803	ALA	2.3
1	F	679	GLY	2.3
1	D	661	ALA	2.3
1	D	835	LYS	2.3
1	F	441	ALA	2.3
1	E	176	GLN	2.3
1	C	940	LYS	2.3
1	E	409	ALA	2.3
1	C	59	ASP	2.3
1	C	164	ASP	2.3
1	B	366	LEU	2.2
1	D	33	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	778	LYS	2.2
1	E	960	LEU	2.2
1	A	680	PHE	2.2
1	D	936	GLY	2.2
1	B	717	ARG	2.2
1	D	164	ASP	2.2
1	E	138	MET	2.2
1	E	348	ILE	2.2
1	D	623	ASN	2.2
1	B	936	GLY	2.2
1	D	403	GLY	2.2
1	D	729	ILE	2.2
1	D	791	VAL	2.2
1	F	881	LEU	2.2
1	A	66	GLU	2.2
1	A	953	MET	2.2
1	B	92	LEU	2.2
1	B	575	MET	2.2
1	E	331	PRO	2.2
1	A	180	SER	2.2
1	A	803	ALA	2.2
1	D	447	MET	2.2
1	E	828	LEU	2.2
1	F	819	TYR	2.2
1	A	280	GLU	2.2
1	E	829	GLY	2.2
1	A	899	PHE	2.2
1	F	176	GLN	2.2
1	D	195	LYS	2.2
1	D	783	PRO	2.2
1	F	516	PHE	2.2
1	D	782	LEU	2.2
1	F	484	VAL	2.2
1	A	197	GLN	2.2
1	E	597	TYR	2.2
1	D	577	GLN	2.2
1	C	429	GLU	2.2
1	E	198	LEU	2.2
1	E	590	VAL	2.2
1	C	67	GLN	2.2
1	F	684	LEU	2.2
1	B	177	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	480	LEU	2.2
1	C	623	ASN	2.2
1	E	167	SER	2.2
1	E	937	LEU	2.2
1	D	90	ILE	2.2
1	F	1044	HIS	2.2
1	D	67	GLN	2.2
1	A	939	ALA	2.2
1	A	287	SER	2.2
1	E	824	SER	2.2
1	B	839	GLU	2.2
1	F	710	PRO	2.1
1	E	651	ALA	2.1
1	A	448	VAL	2.1
1	E	298	ASN	2.1
1	F	14	VAL	2.1
1	F	1040	ILE	2.1
1	A	159	ALA	2.1
1	C	357	LEU	2.1
1	F	230	LEU	2.1
1	D	821	GLY	2.1
1	D	833	PRO	2.1
1	E	898	PRO	2.1
1	B	59	ASP	2.1
1	E	901	VAL	2.1
1	E	955	LYS	2.1
1	E	311	ALA	2.1
1	B	626	ILE	2.1
1	E	289	LEU	2.1
1	F	841	MET	2.1
1	A	62	THR	2.1
1	A	604	ASN	2.1
1	A	89	GLN	2.1
1	C	383	LEU	2.1
1	D	902	MET	2.1
1	A	626	ILE	2.1
1	D	626	ILE	2.1
1	E	174	ASP	2.1
1	E	325	TYR	2.1
1	B	938	SER	2.1
1	E	195	LYS	2.1
1	E	626	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	934	THR	2.1
1	A	593	GLU	2.1
1	C	90	ILE	2.1
1	C	824	SER	2.1
1	E	369	THR	2.1
1	A	706	ALA	2.1
1	A	946	VAL	2.1
1	D	612	VAL	2.1
1	A	310	LEU	2.1
1	B	716	VAL	2.1
1	A	885	PHE	2.1
1	B	623	ASN	2.1
1	E	647	ILE	2.1
1	F	335	ILE	2.1
1	B	824	SER	2.1
1	D	814	PRO	2.1
1	E	608	SER	2.1
1	E	721	LEU	2.1
1	E	366	LEU	2.1
1	C	995	ALA	2.0
1	C	61	VAL	2.0
1	F	700	ASN	2.0
1	B	179	GLY	2.0
1	E	280	GLU	2.0
1	E	958	LYS	2.0
1	F	444	GLY	2.0
1	B	402	ILE	2.0
1	A	638	PRO	2.0
1	F	356	TYR	2.0
1	D	934	THR	2.0
1	E	351	VAL	2.0
1	D	29	LYS	2.0
1	A	279	ALA	2.0
1	A	886	LEU	2.0
1	E	591	LEU	2.0
1	F	107	VAL	2.0
1	C	93	THR	2.0
1	C	801	PHE	2.0
1	F	177	LEU	2.0
1	D	63	GLN	2.0
1	E	89	GLN	2.0
1	A	995	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	941	ASN	2.0
1	F	623	ASN	2.0
1	A	952	LEU	2.0
1	B	287	SER	2.0
1	C	433	LYS	2.0
1	C	958	LYS	2.0
1	D	982	PHE	2.0
1	D	1038	GLU	2.0
1	E	304	ALA	2.0
1	E	939	ALA	2.0
1	C	484	VAL	2.0
1	C	510	LYS	2.0
1	C	1016	VAL	2.0
1	D	433	LYS	2.0
1	B	621	GLY	2.0
1	F	339	GLU	2.0
1	D	690	LEU	2.0
1	E	1026	PHE	2.0
1	F	715	SER	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, 95th 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.

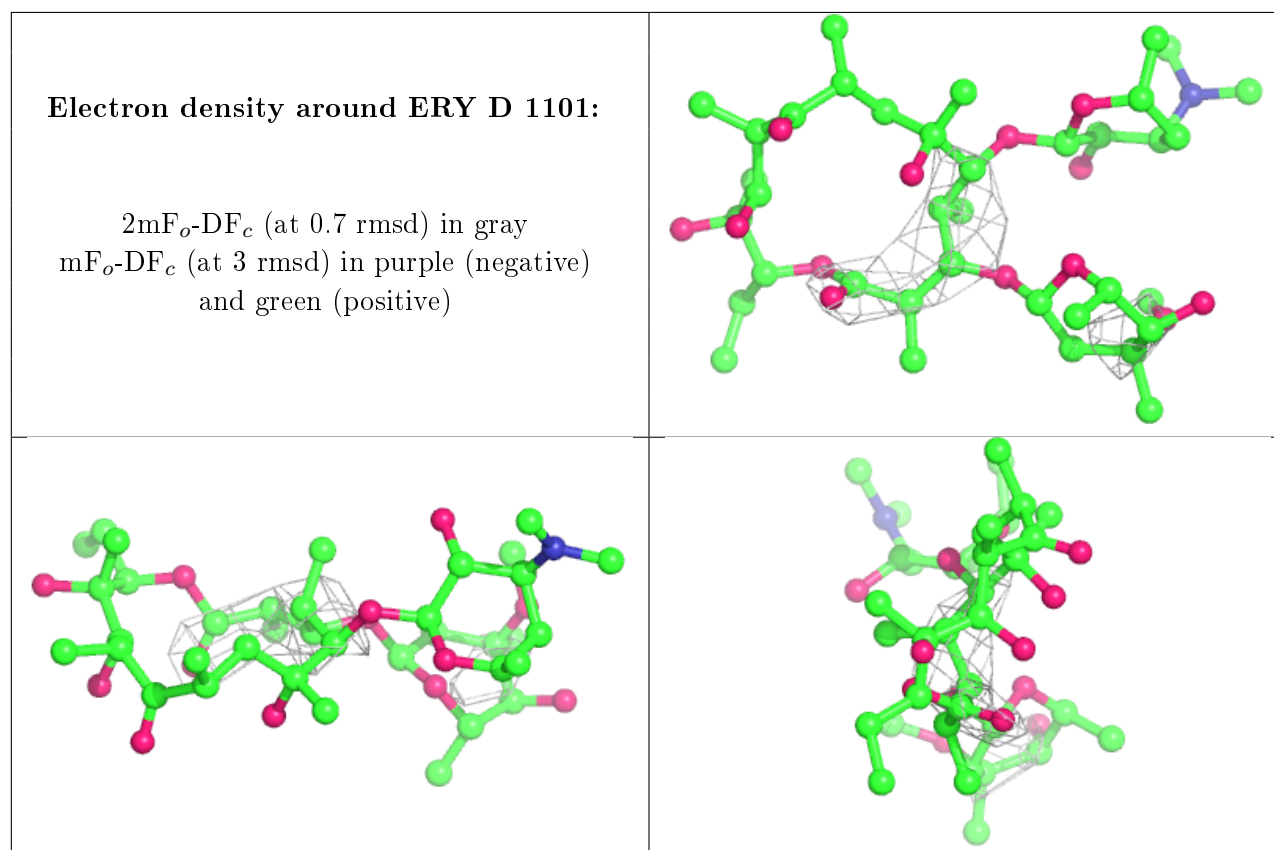
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ERY	D	1101	51/51	0.68	1.10	73,92,103,104	51
3	LMT	D	1103	35/35	0.77	0.42	79,94,108,110	0
2	ERY	A	1101	51/51	0.80	1.12	75,87,97,106	51
3	LMT	C	1101	35/35	0.81	0.45	55,72,93,98	0

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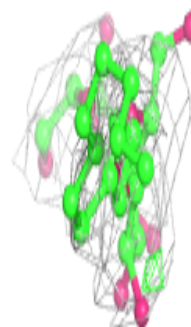
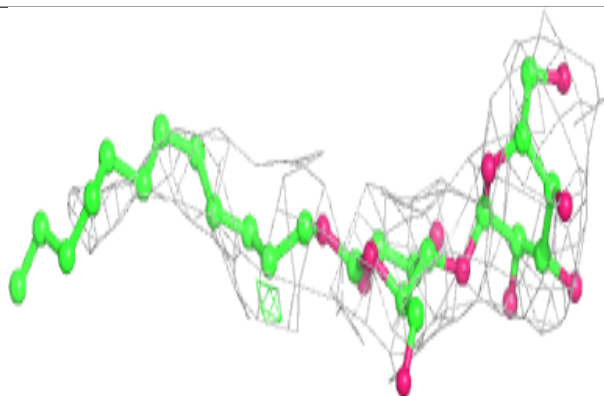
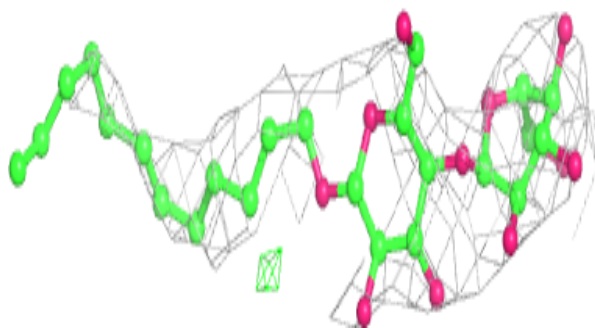
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	LMT	E	1101	35/35	0.83	0.53	57,76,88,116	0
3	LMT	D	1102	35/35	0.83	0.38	55,79,93,93	0
3	LMT	B	1101	35/35	0.84	0.57	49,76,101,110	0
3	LMT	A	1103	35/35	0.84	1.07	58,93,104,107	0
3	LMT	F	1101	35/35	0.85	0.65	49,77,91,99	0
3	LMT	A	1102	35/35	0.90	0.56	26,76,84,88	0
4	NI	E	1102	1/1	0.98	0.13	94,94,94,94	0
4	NI	C	1102	1/1	0.99	0.12	62,62,62,62	0
4	NI	A	1104	1/1	0.99	0.15	54,54,54,54	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.

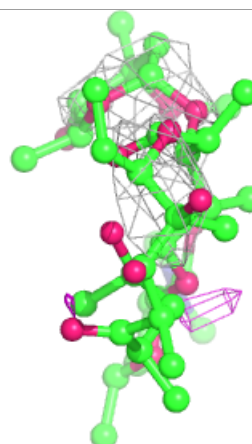
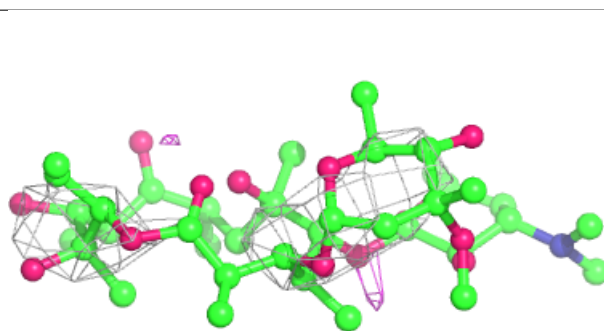
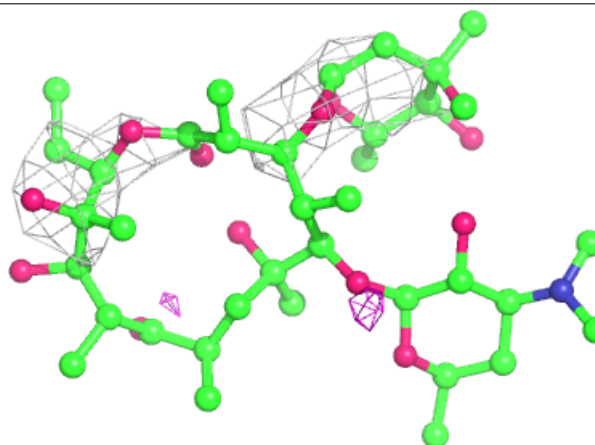


Electron density around LMT D 1103:

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

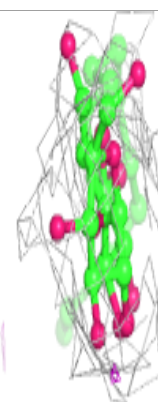
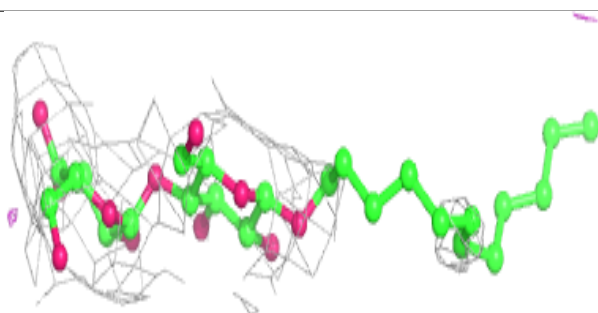
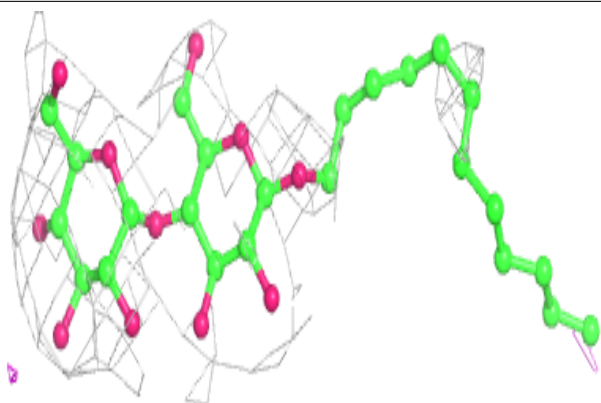
**Electron density around ERY A 1101:**

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

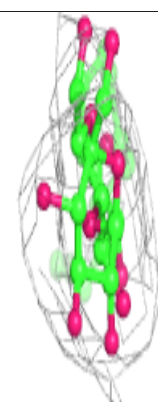
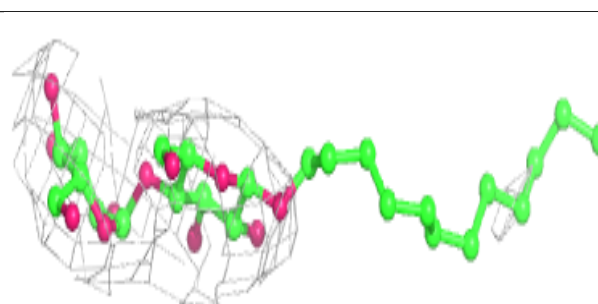
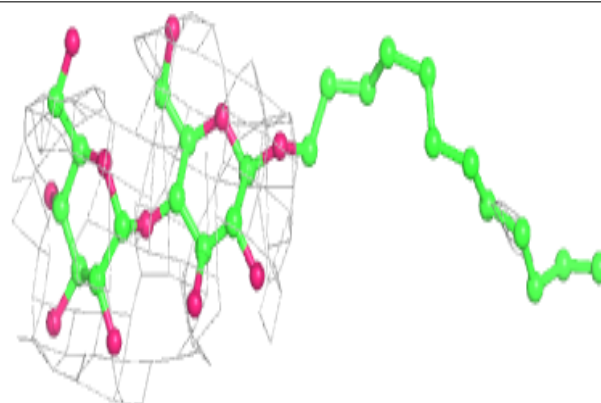


Electron density around LMT C 1101:

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

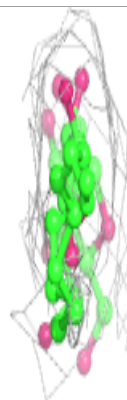
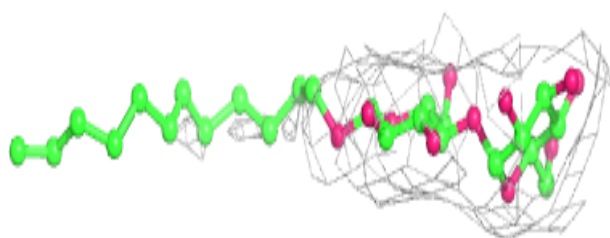
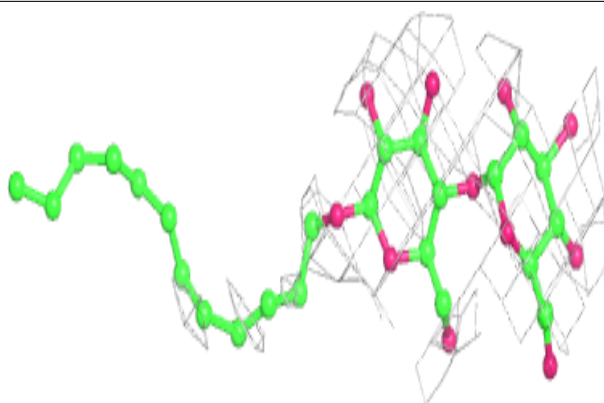
**Electron density around LMT E 1101:**

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

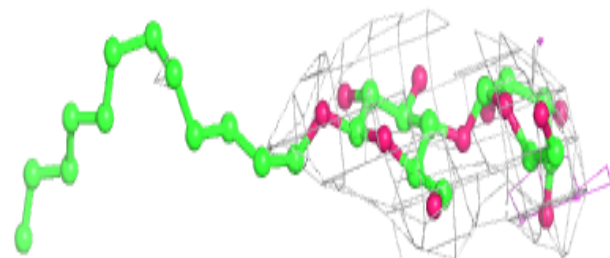
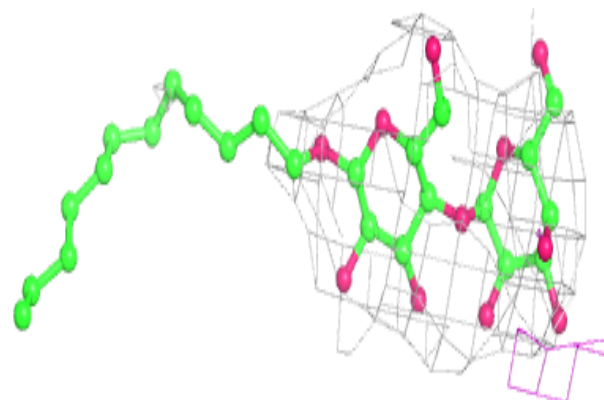


Electron density around LMT D 1102:

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

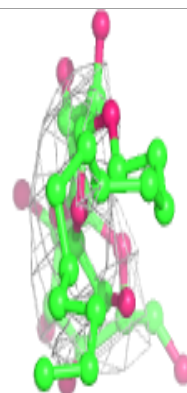
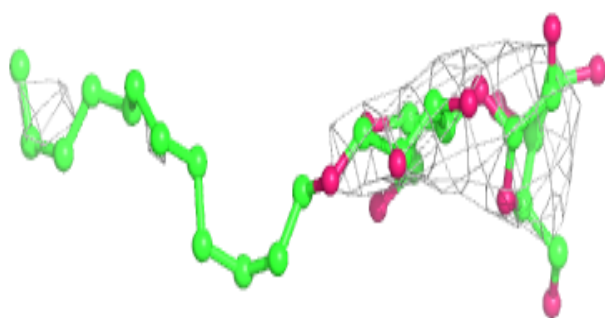
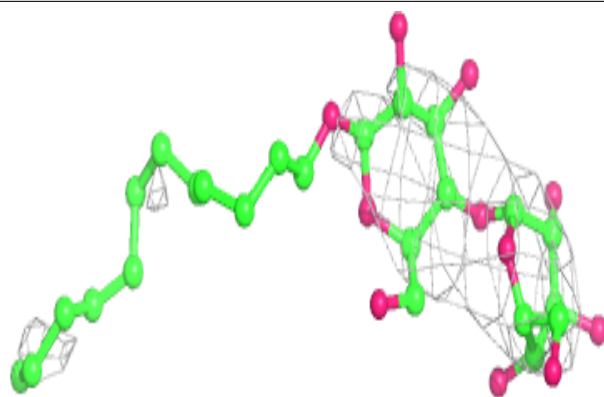
**Electron density around LMT B 1101:**

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

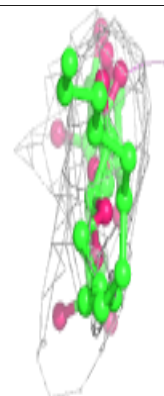
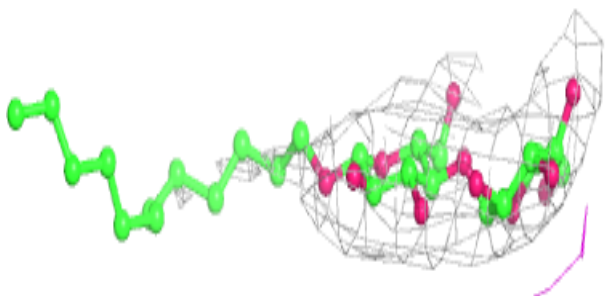
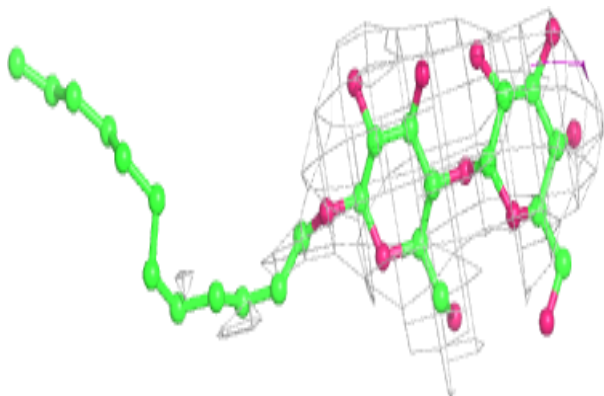


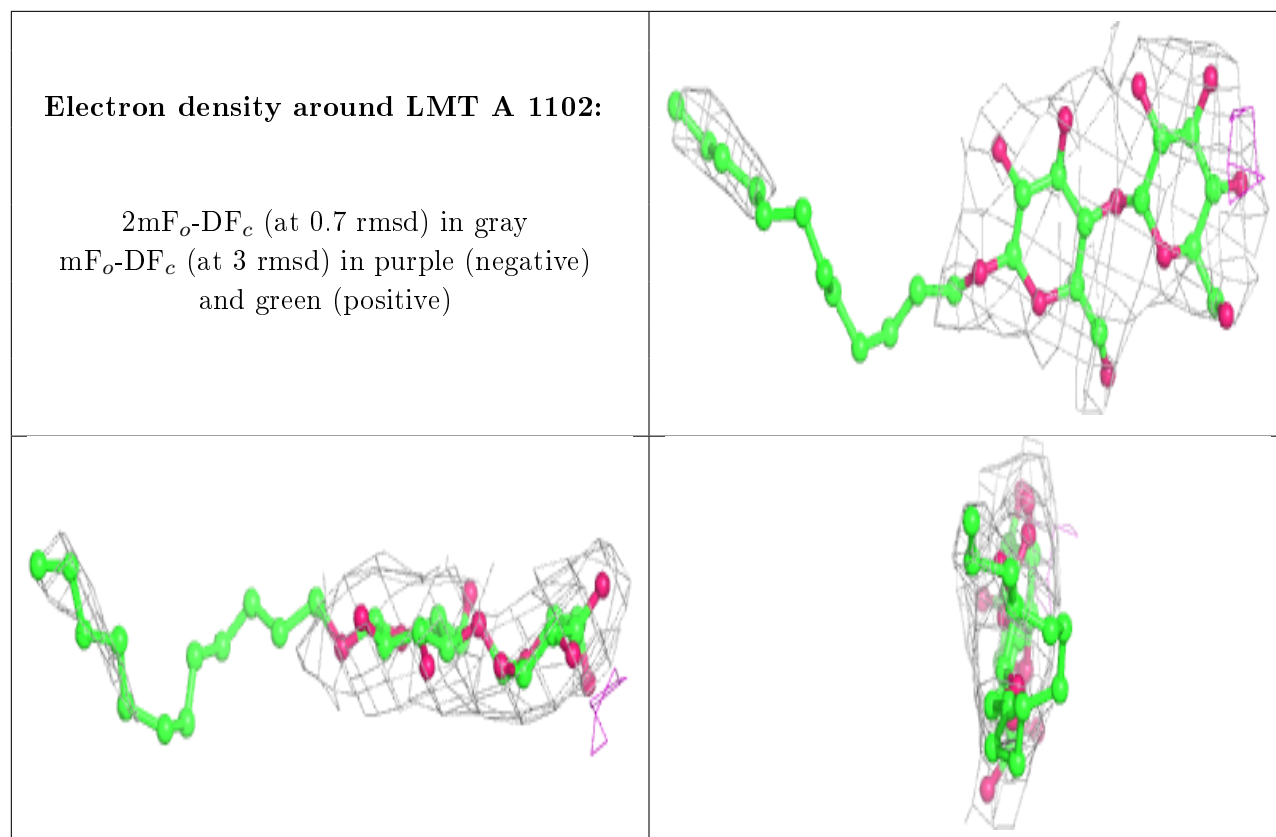
Electron density around LMT A 1103:

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

**Electron density around LMT F 1101:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.