



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 12:13 pm GMT

PDB ID : 4ZJL  
Title : Crystal structure of AcrB in complex with antibiotic in P21 space group  
Authors : Ababou, A.; Koronakis, V.  
Deposited on : 2015-04-29  
Resolution : 3.47 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

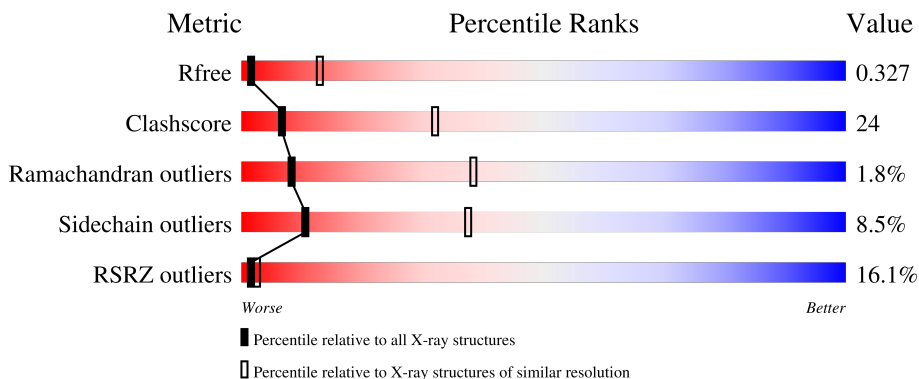
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.47 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	1049	
1	B	1049	
1	C	1049	
1	D	1049	
1	E	1049	

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Mol	Chain	Length	Quality of chain
1	F	1049	<p>20% 50% 43% 6% ..</p>

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	D	1101	-	-	-	X
3	LMT	A	1103	-	-	-	X
3	LMT	D	1103	-	-	-	X

## 2 Entry composition [i](#)

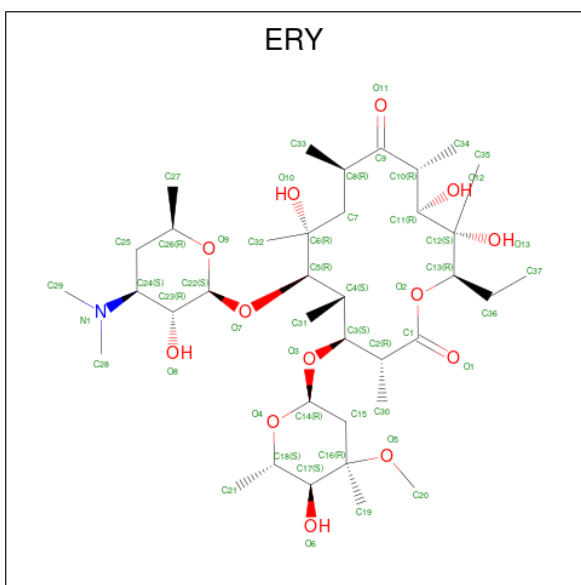
There are 4 unique types of molecules in this entry. The entry contains 47962 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

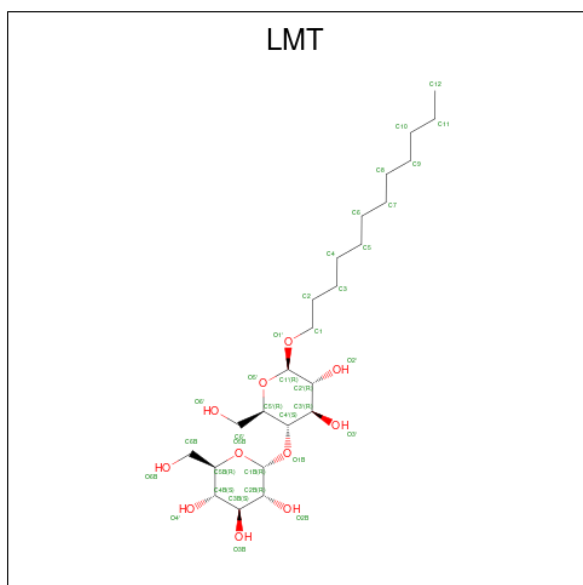
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1044	Total 7942	C 5105	N 1315	O 1479	S 43	0	0	0
1	B	1042	Total 7925	C 5095	N 1311	O 1476	S 43	0	0	0
1	C	1042	Total 7925	C 5095	N 1311	O 1476	S 43	0	0	0
1	D	1042	Total 7925	C 5095	N 1311	O 1476	S 43	0	0	0
1	E	1042	Total 7925	C 5095	N 1311	O 1476	S 43	0	0	0
1	F	1043	Total 7935	C 5101	N 1314	O 1477	S 43	0	0	0

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



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

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



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

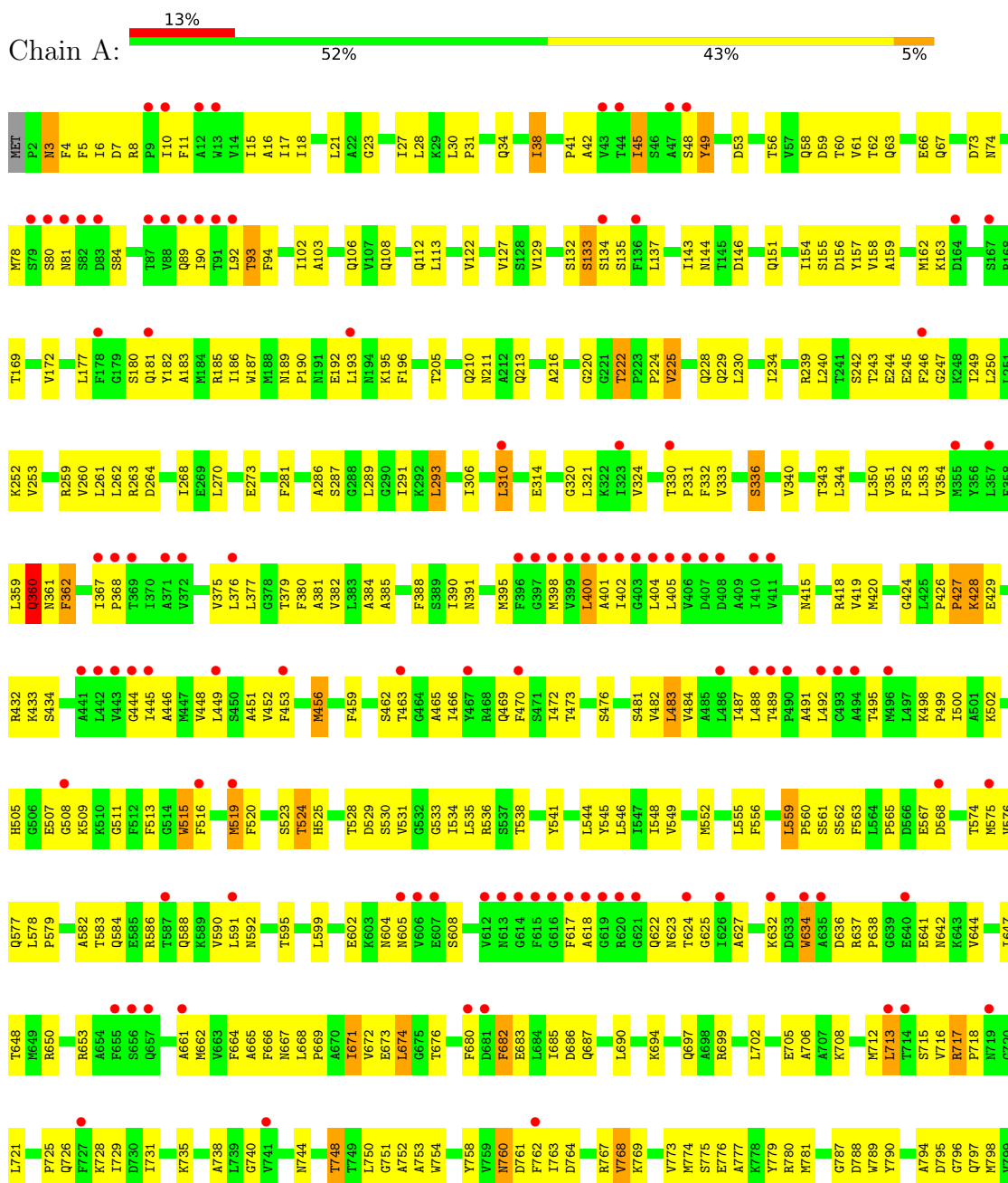
- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

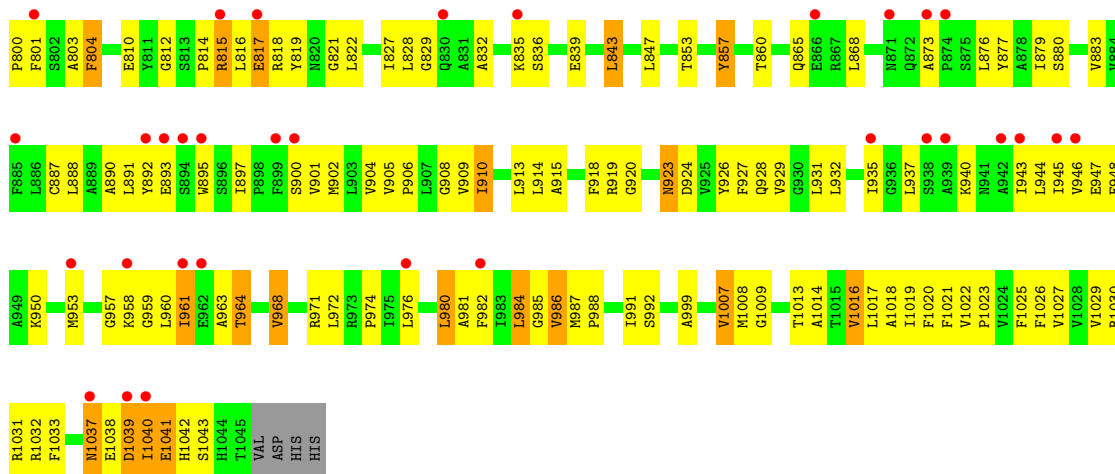
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	1	Total 1	Ni 1	0	0
4	C	1	Total 1	Ni 1	0	0
4	E	1	Total 1	Ni 1	0	0

### 3 Residue-property plots i

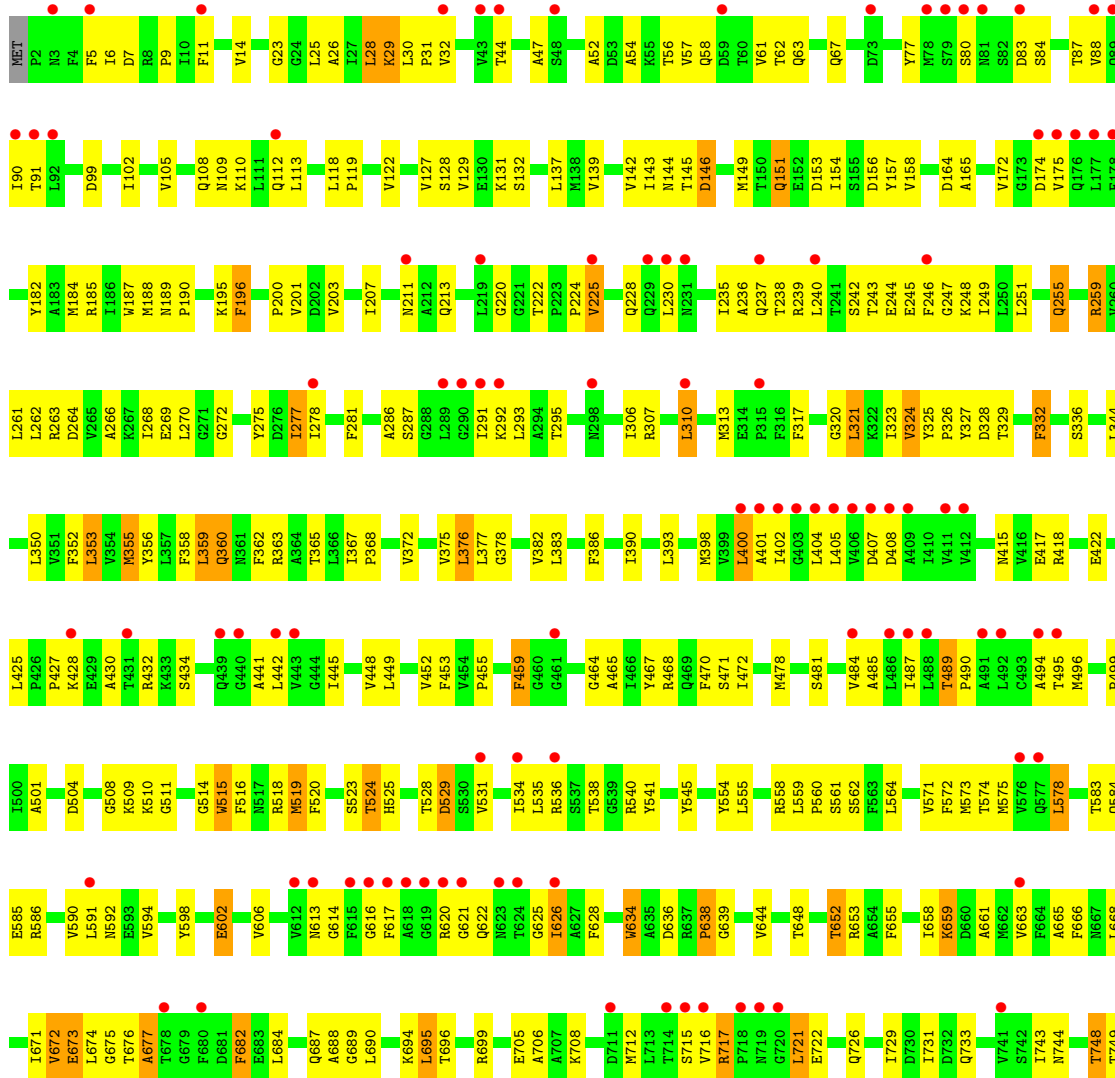
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Multidrug efflux pump subunit AcrB

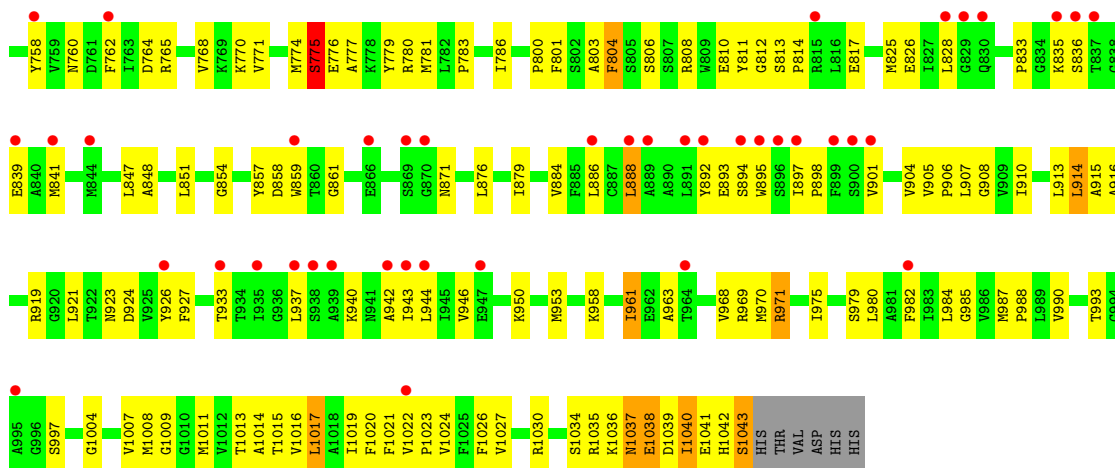




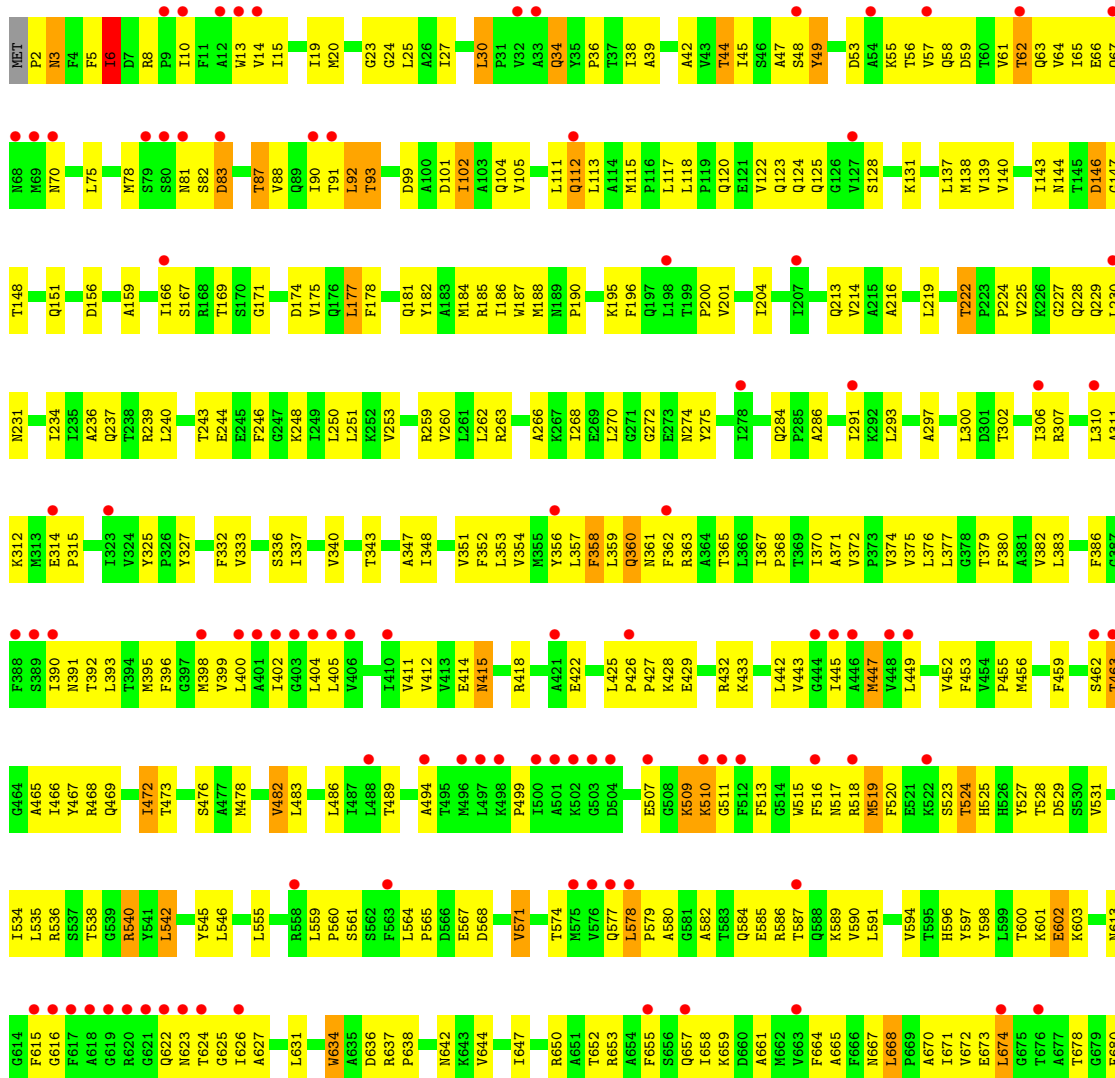
• Molecule 1: Multidrug efflux pump subunit AcrB





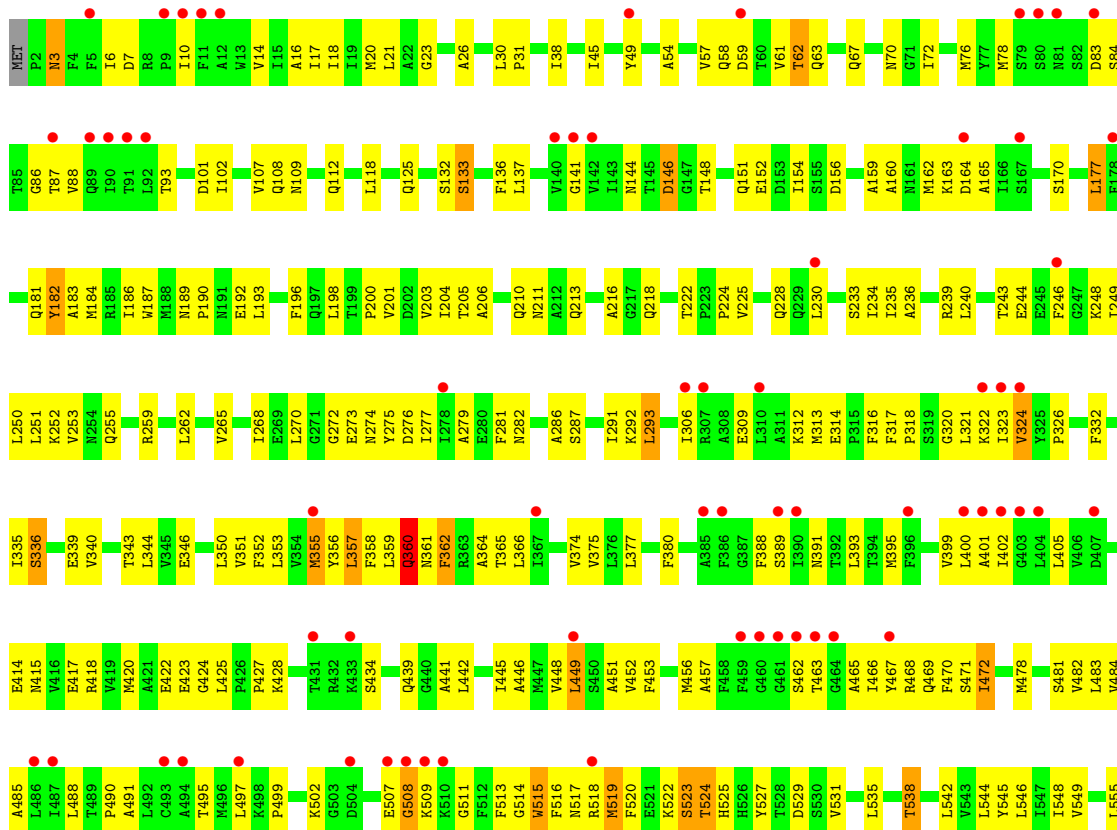


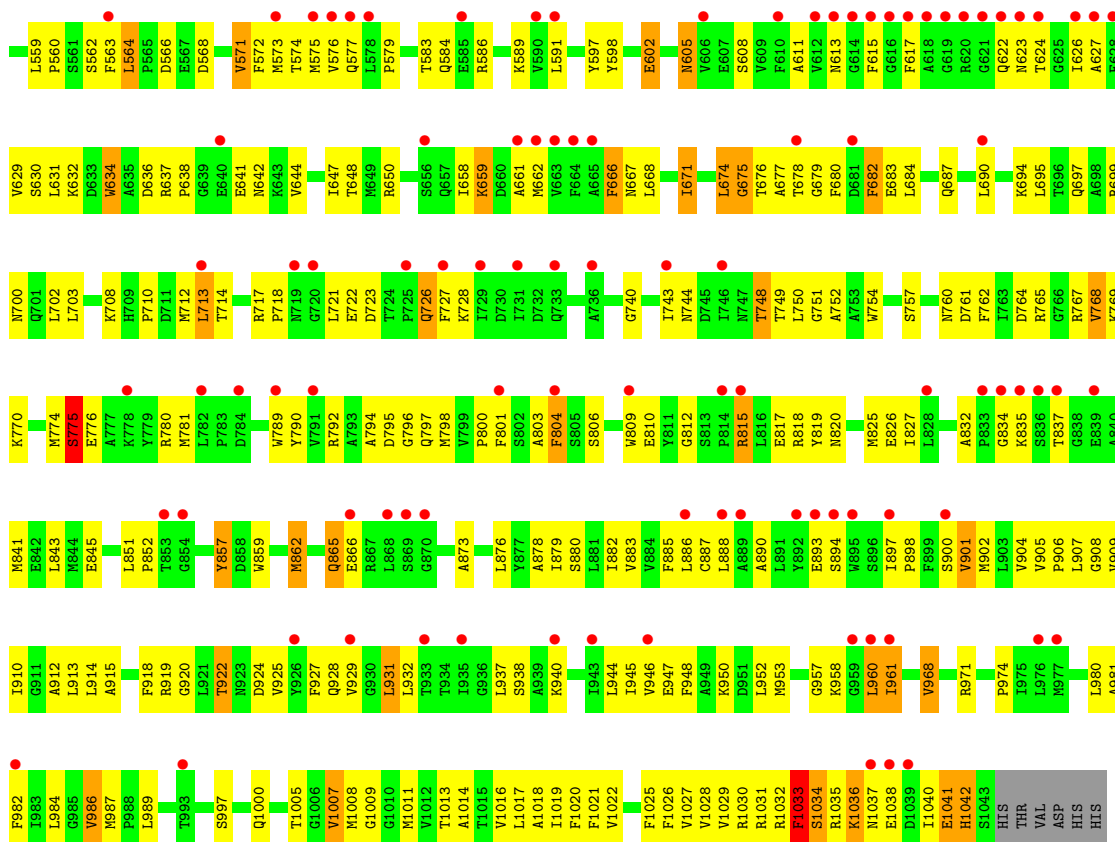
• Molecule 1: Multidrug efflux pump subunit AcrB



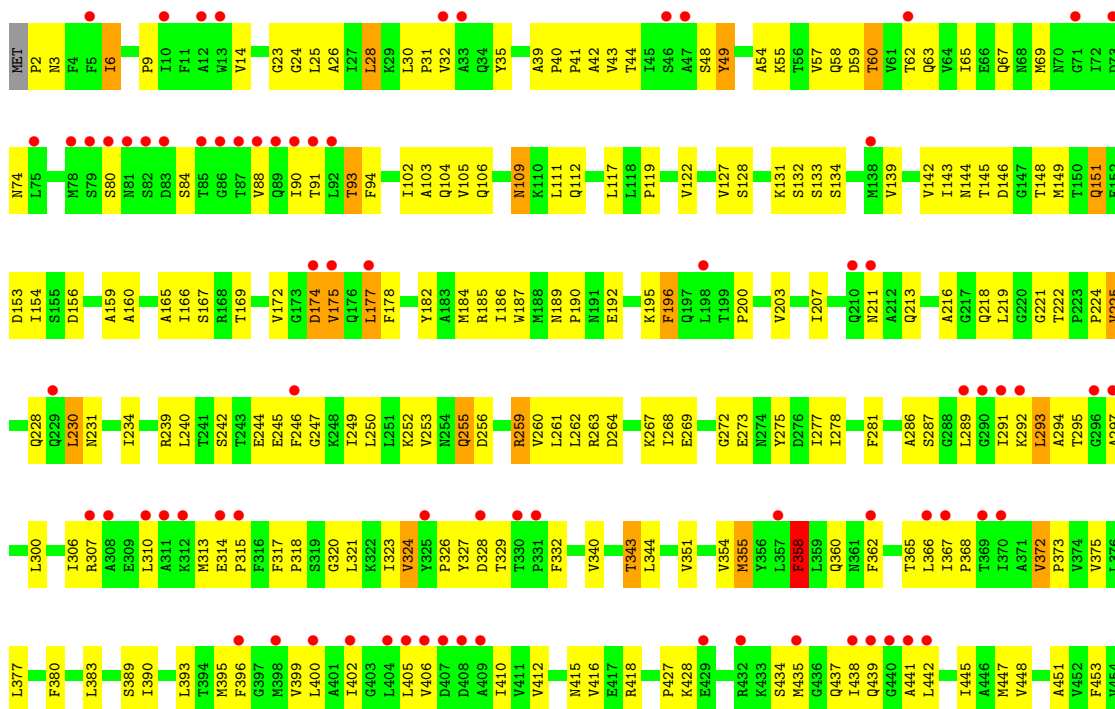


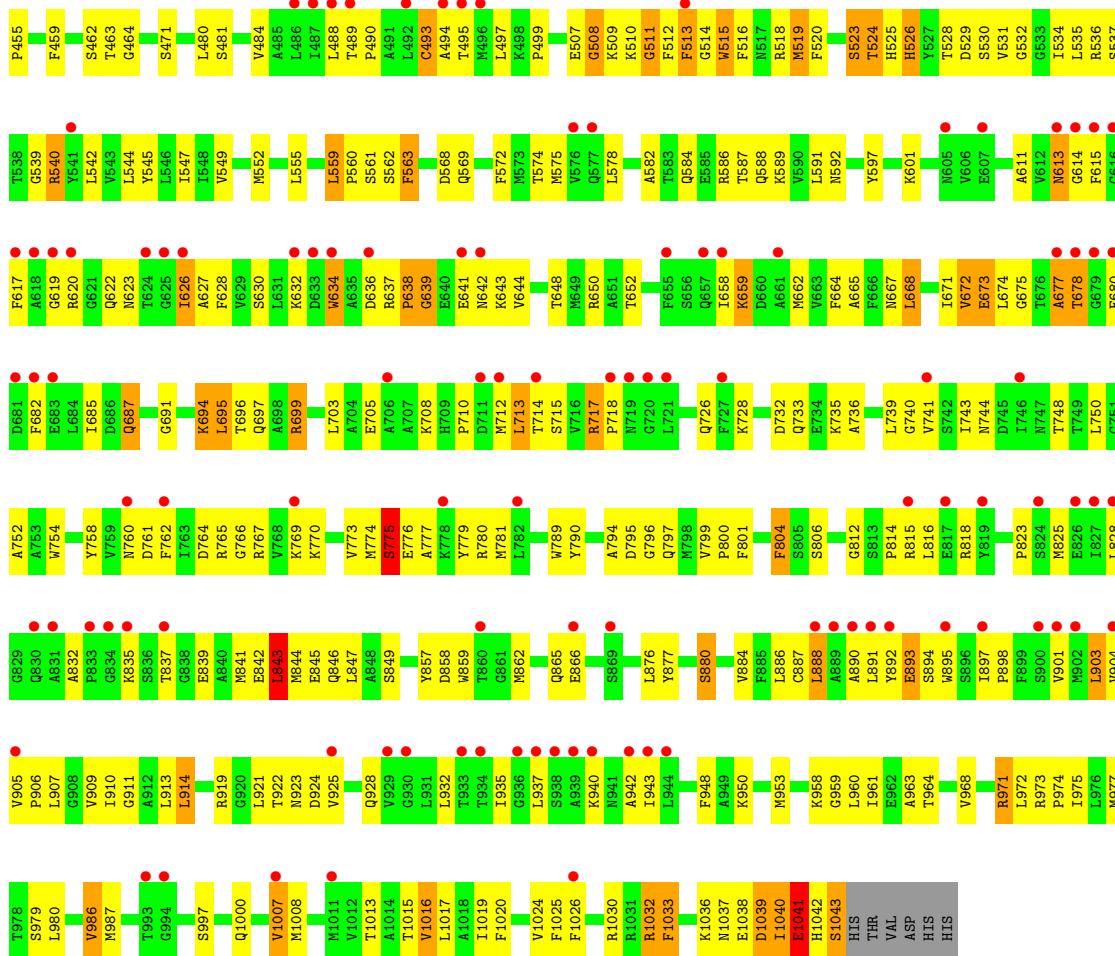
• Molecule 1: Multidrug efflux pump subunit AcrB



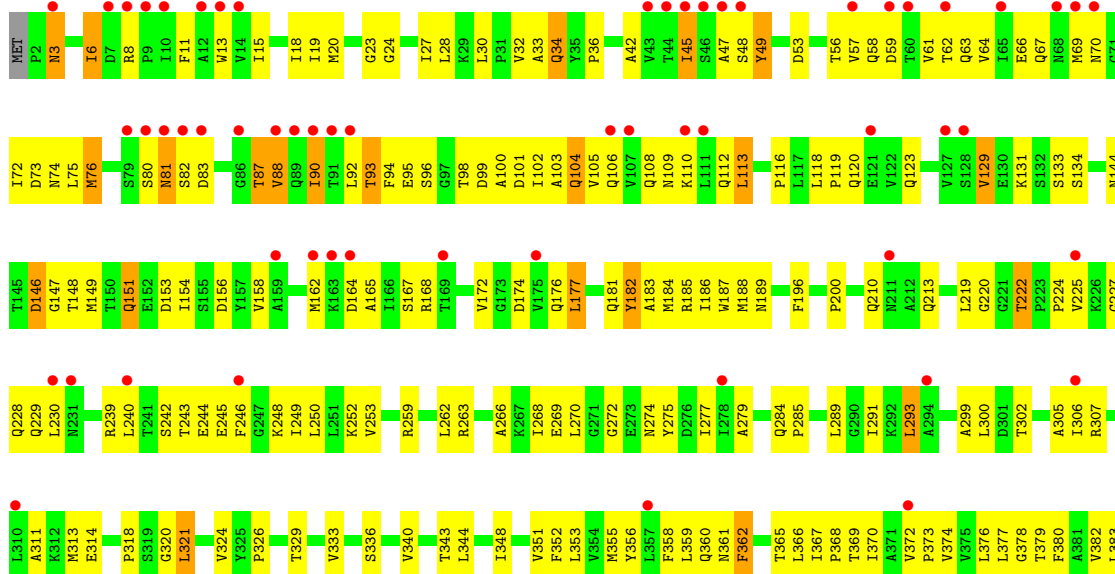


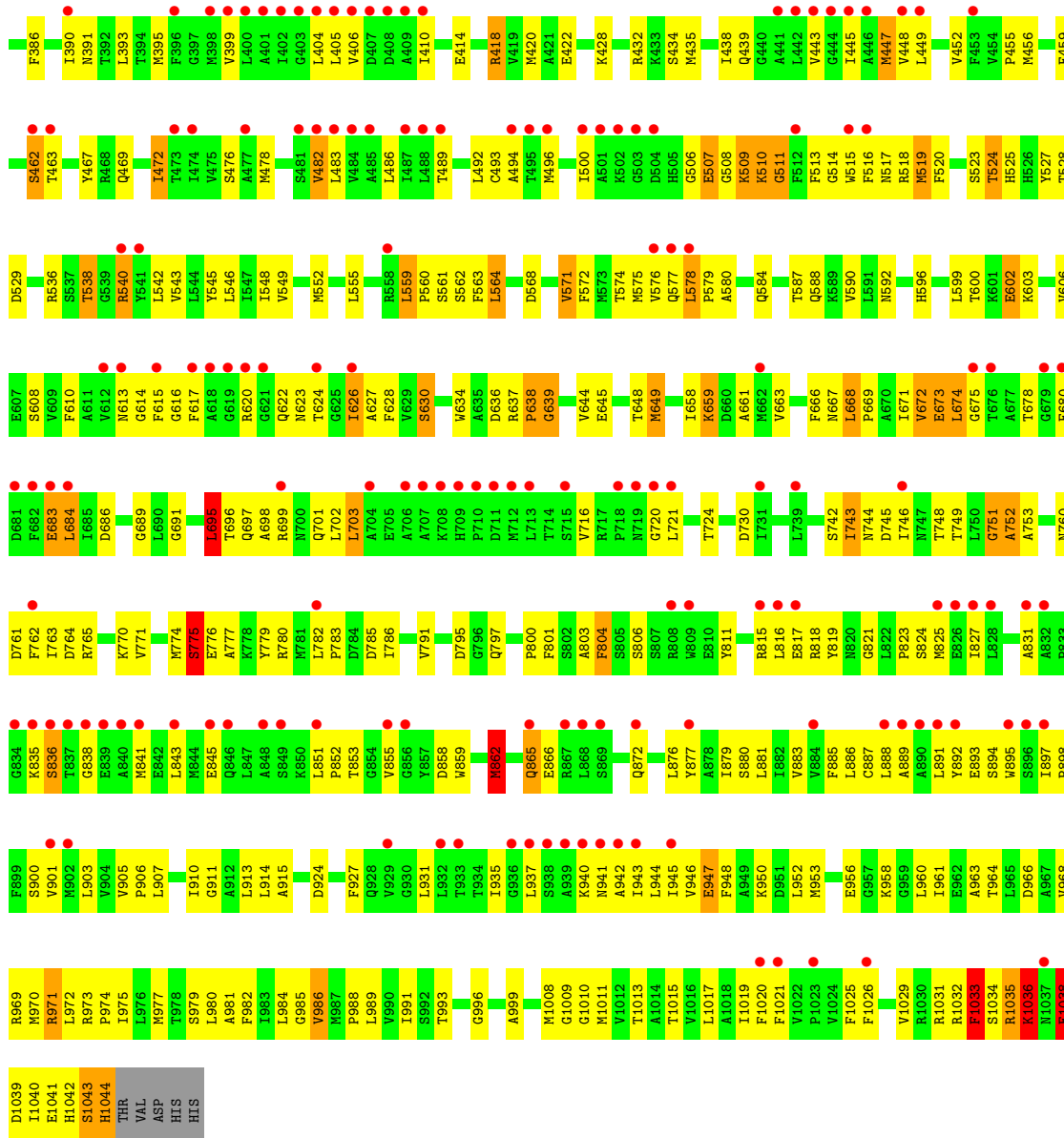
• Molecule 1: Multidrug efflux pump subunit AcrB





• Molecule 1: Multidrug efflux pump subunit AcrB





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.95Å 155.66Å 217.01Å 90.00° 92.67° 90.00°	Depositor
Resolution (Å)	19.97 – 3.47 108.39 – 3.47	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.97-3.47) 92.9 (108.39-3.47)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.49Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.251 , 0.321 0.258 , 0.327	Depositor DCC
$R_{free}$ test set	6376 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	91.0	Xtrriage
Anisotropy	0.300	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.056 for -k,-h,-l 0.066 for k,h,-l 0.060 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	47962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.53 % 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 1.5068e-04.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, ERY, NI

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	1/8094 (0.0%)	0.83	6/10990 (0.1%)
1	B	0.59	1/8076 (0.0%)	0.83	7/10965 (0.1%)
1	C	0.59	0/8076	0.85	8/10965 (0.1%)
1	D	0.55	1/8076 (0.0%)	0.81	3/10965 (0.0%)
1	E	0.57	2/8076 (0.0%)	0.83	7/10965 (0.1%)
1	F	0.57	0/8087	0.86	7/10980 (0.1%)
All	All	0.58	5/48485 (0.0%)	0.84	38/65830 (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	E	0	1
1	F	0	2
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	515	TRP	CB-CG	7.95	1.64	1.50
1	A	515	TRP	CB-CG	7.35	1.63	1.50
1	E	493	CYS	CB-SG	-7.17	1.70	1.82
1	E	515	TRP	CB-CG	6.61	1.62	1.50
1	B	515	TRP	CB-CG	5.40	1.59	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	529	ASP	CB-CG-OD1	12.19	129.28	118.30
1	C	540	ARG	NE-CZ-NH2	9.67	125.14	120.30
1	B	529	ASP	CB-CG-OD1	9.03	126.42	118.30
1	D	529	ASP	CB-CG-OD1	8.46	125.91	118.30
1	E	529	ASP	CB-CG-OD1	7.85	125.36	118.30
1	F	529	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	C	92	LEU	CA-CB-CG	6.82	130.99	115.30
1	B	888	LEU	CA-CB-CG	-6.55	100.23	115.30
1	B	359	LEU	CA-CB-CG	6.47	130.19	115.30
1	B	293	LEU	CA-CB-CG	6.22	129.62	115.30
1	E	293	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	1017	LEU	CA-CB-CG	6.12	129.38	115.30
1	C	540	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	A	449	LEU	CA-CB-CG	6.09	129.31	115.30
1	C	30	LEU	CA-CB-CG	6.06	129.23	115.30
1	F	972	LEU	CA-CB-CG	6.01	129.13	115.30
1	F	684	LEU	CA-CB-CG	5.99	129.09	115.30
1	C	515	TRP	CA-CB-CG	5.72	124.58	113.70
1	A	456	MET	CB-CG-SD	-5.68	95.35	112.40
1	C	616	GLY	N-CA-C	-5.63	99.03	113.10
1	B	1037	ASN	C-N-CA	5.62	135.75	121.70
1	D	449	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	972	LEU	CA-CB-CG	5.61	128.20	115.30
1	E	972	LEU	CA-CB-CG	5.49	127.92	115.30
1	C	83	ASP	N-CA-C	5.49	125.81	111.00
1	C	529	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	376	LEU	CA-CB-CG	-5.28	103.15	115.30
1	E	843	LEU	CA-CB-CG	5.24	127.34	115.30
1	E	117	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	357	LEU	CA-CB-CG	5.16	127.17	115.30
1	E	914	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	888	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	F	695	LEU	CA-CB-CG	5.14	127.13	115.30
1	F	113	LEU	CA-CB-CG	5.13	127.11	115.30
1	F	1036	LYS	N-CA-C	5.10	124.77	111.00
1	A	38	ILE	CG1-CB-CG2	-5.10	100.18	111.40
1	E	888	LEU	CA-CB-CG	-5.06	103.65	115.30
1	A	529	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	1039	ASP	Peptide
1	B	1039	ASP	Peptide
1	B	132	SER	Peptide
1	C	834	GLY	Peptide
1	D	1033	PHE	Peptide
1	E	1039	ASP	Peptide
1	F	1036	LYS	Peptide
1	F	1041	GLU	Peptide

## 5.2 Too-close contacts [i](#)

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	7942	0	8080	420	0
1	B	7925	0	8066	330	0
1	C	7925	0	8066	424	0
1	D	7925	0	8066	414	0
1	E	7925	0	8066	394	0
1	F	7935	0	8073	390	0
2	A	51	0	67	6	0
2	D	51	0	67	12	0
3	A	70	0	92	14	0
3	B	35	0	46	5	0
3	C	35	0	46	2	0
3	D	70	0	92	6	0
3	E	35	0	46	5	0
3	F	35	0	46	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	47962	0	48919	2279	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (2279) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:VAL:H	1:E:781:MET:HE1	1.13	1.09
1:A:225:VAL:H	1:B:781:MET:HE1	1.15	1.06
1:F:941:ASN:HD21	1:F:1015:THR:HG22	1.18	1.04
1:D:210:GLN:HE22	1:D:250:LEU:HB3	1.27	0.99
1:E:691:GLY:H	1:E:694:LYS:HE3	1.27	0.98
1:A:781:MET:HE1	1:C:225:VAL:H	1.28	0.96
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.48	0.96
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.49	0.94
1:A:134:SER:OG	2:A:1101:ERY:H323	1.67	0.93
1:D:228:GLN:NE2	1:D:230:LEU:O	2.01	0.93
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.51	0.91
1:D:415:ASN:HD22	1:D:434:SER:HB2	1.34	0.91
1:B:775:SER:OG	1:B:776:GLU:O	1.88	0.91
1:D:225:VAL:HG12	1:E:777:ALA:HB1	1.50	0.90
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.53	0.89
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.54	0.88
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.56	0.87
1:B:901:VAL:HG21	1:B:943:ILE:HG13	1.57	0.87
1:A:644:VAL:HG11	1:A:667:ASN:HB2	1.54	0.87
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.56	0.87
1:C:894:SER:HB3	1:C:897:ILE:HG12	1.57	0.87
1:F:559:LEU:HD23	1:F:560:PRO:HD2	1.55	0.87
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.56	0.86
1:C:892:TYR:O	1:C:894:SER:N	2.07	0.86
1:F:937:LEU:HD13	1:F:1011:MET:HE2	1.56	0.86
1:A:424:GLY:HA3	1:A:502:LYS:HB3	1.58	0.86
1:E:516:PHE:HA	1:E:519:MET:HG3	1.57	0.86
1:B:696:THR:HG23	1:B:699:ARG:HH12	1.38	0.86
1:A:38:ILE:HD11	1:A:466:ILE:HD11	1.57	0.86
1:A:877:TYR:OH	1:A:928:GLN:NE2	2.09	0.85
1:B:350:LEU:HD13	1:B:984:LEU:HB3	1.58	0.85
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	1.58	0.85
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.59	0.85
1:B:525:HIS:CD2	1:B:529:ASP:OD2	2.31	0.84
1:F:3:ASN:HD22	1:F:435:MET:HG3	1.42	0.84
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.11	0.83
1:C:428:LYS:HG2	1:C:494:ALA:HB1	1.60	0.83
1:D:38:ILE:HG23	1:D:462:SER:HB2	1.60	0.83
1:F:356:TYR:HA	1:F:365:THR:HG21	1.60	0.83
1:C:740:GLY:O	1:C:794:ALA:N	2.12	0.83
1:F:901:VAL:HG23	1:F:942:ALA:HB3	1.58	0.83
1:C:465:ALA:HA	1:C:468:ARG:HH12	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:THR:HA	1:E:224:PRO:HD3	1.61	0.82
1:A:935:ILE:HD12	3:A:1103:LMT:H72	1.62	0.82
1:B:971:ARG:O	1:B:975:ILE:HG12	1.78	0.82
1:C:356:TYR:HA	1:C:365:THR:HG21	1.60	0.82
1:D:445:ILE:HD13	1:D:940:LYS:HE3	1.60	0.82
1:A:971:ARG:HG2	1:A:974:PRO:HG2	1.61	0.82
1:A:832:ALA:HB3	1:A:835:LYS:HD3	1.60	0.81
1:A:530:SER:HG	3:A:1102:LMT:H2O2	1.02	0.81
1:B:525:HIS:NE2	1:B:529:ASP:OD2	2.12	0.81
1:C:579:PRO:HD3	1:C:661:ALA:HB2	1.63	0.81
1:D:187:TRP:HB3	1:D:776:GLU:HA	1.63	0.81
1:A:137:LEU:HD22	1:A:293:LEU:HG	1.60	0.81
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.63	0.81
1:E:559:LEU:HD22	1:E:560:PRO:HD2	1.63	0.81
1:E:225:VAL:HG12	1:F:777:ALA:HB1	1.63	0.80
1:D:1034:SER:OG	1:D:1035:ARG:N	2.14	0.80
1:C:3:ASN:N	1:C:3:ASN:OD1	2.14	0.80
1:A:562:SER:HB2	1:A:924:ASP:HB3	1.63	0.80
1:D:244:GLU:HG2	1:D:248:LYS:HE2	1.63	0.80
1:A:445:ILE:HD13	1:A:940:LYS:HE3	1.63	0.80
1:C:240:LEU:HB2	1:C:246:PHE:HE1	1.47	0.80
1:A:690:LEU:HB3	1:A:694:LYS:HD3	1.64	0.79
1:D:181:GLN:OE1	1:D:767:ARG:NH2	2.15	0.79
1:D:740:GLY:O	1:D:794:ALA:N	2.14	0.79
1:E:530:SER:OG	3:E:1101:LMT:O2'	1.66	0.79
1:A:67:GLN:OE1	1:C:767:ARG:NH1	2.15	0.79
1:D:700:ASN:HA	1:D:703:LEU:HD12	1.63	0.79
1:A:427:PRO:HD3	1:A:499:PRO:HB3	1.65	0.79
1:D:690:LEU:HB3	1:D:694:LYS:HD3	1.65	0.79
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.65	0.79
1:E:415:ASN:ND2	1:E:437:GLN:OE1	2.16	0.78
1:D:137:LEU:HD22	1:D:293:LEU:HG	1.65	0.78
1:A:181:GLN:OE1	1:A:767:ARG:NH2	2.16	0.78
1:B:516:PHE:HA	1:B:519:MET:HG3	1.65	0.78
1:E:959:GLY:HA2	1:E:1040:ILE:HB	1.65	0.78
1:A:222:THR:HA	1:A:224:PRO:HD3	1.64	0.77
1:B:508:GLY:O	1:B:510:LYS:N	2.16	0.77
1:A:1037:ASN:HA	1:A:1038:GLU:HB2	1.63	0.77
1:E:979:SER:OG	1:E:1015:THR:HG21	1.84	0.77
1:D:507:GLU:O	1:D:509:LYS:N	2.17	0.77
1:B:151:GLN:HE22	1:B:278:ILE:HA	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:PHE:HA	1:F:355:MET:HE2	1.67	0.77
1:D:196:PHE:O	1:D:252:LYS:NZ	2.18	0.77
1:A:579:PRO:HD3	1:A:661:ALA:HB2	1.66	0.77
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.66	0.77
1:C:664:PHE:HD2	1:C:717:ARG:HD2	1.50	0.77
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.67	0.77
1:E:832:ALA:HB3	1:E:835:LYS:HD3	1.67	0.77
1:D:775:SER:OG	1:D:776:GLU:O	2.02	0.76
1:B:14:VAL:HG22	1:C:886:LEU:HD12	1.64	0.76
1:B:228:GLN:NE2	1:C:781:MET:SD	2.59	0.76
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.17	0.76
1:E:196:PHE:O	1:E:252:LYS:NZ	2.17	0.76
1:C:971:ARG:HB3	1:C:971:ARG:CZ	2.15	0.76
1:B:668:LEU:HD23	1:B:668:LEU:H	1.50	0.76
1:E:971:ARG:O	1:E:975:ILE:HG12	1.85	0.76
1:A:901:VAL:HG21	1:A:943:ILE:HG13	1.68	0.76
1:E:652:THR:HG23	1:E:665:ALA:HB3	1.67	0.75
1:C:34:GLN:HE21	1:C:333:VAL:HG22	1.50	0.75
1:D:453:PHE:O	1:D:471:SER:OG	2.04	0.75
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.68	0.75
1:A:1039:ASP:HA	1:A:1040:ILE:HB	1.68	0.75
1:C:944:LEU:HB3	1:C:971:ARG:NE	2.01	0.75
1:D:448:VAL:HG22	1:D:887:CYS:HB3	1.67	0.75
1:C:382:VAL:HG21	1:C:476:SER:HB2	1.69	0.75
1:C:228:GLN:NE2	1:C:230:LEU:O	2.19	0.74
1:F:775:SER:OG	1:F:776:GLU:O	2.04	0.74
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.69	0.74
1:A:758:TYR:OH	1:A:761:ASP:OD1	2.05	0.74
1:E:340:VAL:HG21	1:E:395:MET:HB3	1.69	0.74
1:D:491:ALA:O	1:D:495:THR:OG1	2.04	0.74
1:B:228:GLN:HE22	1:C:781:MET:HB3	1.52	0.74
1:A:350:LEU:HD22	1:A:984:LEU:HB3	1.69	0.74
1:A:986:VAL:HG21	1:A:1007:VAL:HG11	1.69	0.74
1:C:307:ARG:NH2	1:C:314:GLU:OE2	2.21	0.74
1:D:586:ARG:O	1:D:589:LYS:HB3	1.88	0.74
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.71	0.73
1:B:26:ALA:O	1:B:30:LEU:HB2	1.89	0.73
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.23	0.73
1:E:588:GLN:O	1:E:592:ASN:ND2	2.22	0.73
1:A:360:GLN:NE2	1:A:513:PHE:HB3	2.03	0.73
1:B:1035:ARG:HG3	1:B:1036:LYS:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:PHE:HA	1:D:519:MET:SD	2.29	0.73
1:E:775:SER:OG	1:E:776:GLU:O	2.06	0.73
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.17	0.73
1:B:1037:ASN:HA	1:B:1038:GLU:HB2	1.71	0.72
1:D:579:PRO:HD3	1:D:661:ALA:HB2	1.70	0.72
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.71	0.72
1:C:699:ARG:NH1	1:C:825:MET:SD	2.62	0.72
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.71	0.72
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.70	0.72
1:F:58:GLN:OE1	1:F:818:ARG:NH1	2.23	0.72
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.72	0.72
1:B:7:ASP:OD2	1:B:432:ARG:NH2	2.22	0.72
1:D:236:ALA:O	1:E:728:LYS:NZ	2.19	0.72
1:B:187:TRP:NE1	1:B:269:GLU:OE2	2.23	0.71
1:F:156:ASP:OD1	1:F:765:ARG:NH2	2.23	0.71
1:B:6:ILE:O	1:B:428:LYS:NZ	2.23	0.71
1:B:696:THR:HG23	1:B:699:ARG:NH1	2.04	0.71
1:B:1036:LYS:HA	1:B:1038:GLU:HG2	1.72	0.71
1:D:343:THR:HG21	1:D:989:LEU:HD21	1.71	0.71
1:E:428:LYS:HG2	1:E:494:ALA:HB1	1.72	0.71
1:F:83:ASP:HB2	1:F:87:THR:O	1.89	0.71
1:A:225:VAL:N	1:B:781:MET:HE1	2.00	0.71
1:B:415:ASN:HD22	1:B:434:SER:HB2	1.56	0.71
1:D:156:ASP:OD2	1:D:769:LYS:NZ	2.23	0.71
1:F:892:TYR:O	1:F:894:SER:N	2.24	0.71
1:A:637:ARG:NH1	1:A:642:ASN:O	2.23	0.71
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.73	0.71
1:D:781:MET:HE1	1:F:225:VAL:HG13	1.73	0.71
1:A:740:GLY:O	1:A:794:ALA:N	2.22	0.71
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.72	0.70
1:D:888:LEU:HD13	1:D:901:VAL:HG13	1.70	0.70
1:E:42:ALA:HB2	1:E:93:THR:HG23	1.73	0.70
1:F:667:ASN:O	1:F:678:THR:OG1	2.07	0.70
1:C:53:ASP:OD1	1:C:56:THR:OG1	2.08	0.70
1:A:210:GLN:NE2	1:A:250:LEU:O	2.24	0.70
1:B:236:ALA:O	1:C:728:LYS:NZ	2.16	0.70
1:B:262:LEU:HG	1:B:268:ILE:HD11	1.71	0.70
1:B:508:GLY:HA2	1:B:518:ARG:HH21	1.55	0.70
1:C:941:ASN:ND2	1:C:1015:THR:HG22	2.07	0.70
1:A:225:VAL:HG12	1:B:777:ALA:HB1	1.73	0.70
1:B:901:VAL:HG23	1:B:942:ALA:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:GLU:HG2	1:C:518:ARG:HG3	1.73	0.70
1:D:699:ARG:NH1	1:D:825:MET:SD	2.64	0.70
1:D:317:PHE:CD2	1:D:321:LEU:HD12	2.26	0.70
1:D:583:THR:HG21	1:F:229:GLN:HA	1.74	0.70
1:F:525:HIS:HA	1:F:528:THR:HG22	1.74	0.70
1:A:451:ALA:HB1	1:A:883:VAL:HG12	1.72	0.70
1:A:452:VAL:HG11	3:A:1103:LMT:H111	1.74	0.70
1:F:452:VAL:O	1:F:455:PRO:HD2	1.91	0.70
1:E:448:VAL:HG13	1:E:884:VAL:HG22	1.74	0.69
1:E:562:SER:HB3	1:E:924:ASP:HB3	1.74	0.69
1:B:452:VAL:HG23	1:B:453:PHE:CD2	2.27	0.69
1:F:262:LEU:HG	1:F:268:ILE:HD11	1.74	0.69
1:B:404:LEU:HD23	1:B:478:MET:HG3	1.73	0.69
1:A:605:ASN:HD22	1:A:647:ILE:HD11	1.56	0.69
1:A:775:SER:OG	1:A:776:GLU:O	2.10	0.69
1:A:945:ILE:HG13	1:A:971:ARG:HH22	1.56	0.69
1:D:519:MET:O	1:D:523:SER:OG	2.10	0.69
1:F:153:ASP:OD2	1:F:182:TYR:OH	2.09	0.69
1:F:746:ILE:HG22	1:F:791:VAL:HG21	1.75	0.69
1:F:941:ASN:ND2	1:F:1015:THR:HG22	2.01	0.69
1:C:568:ASP:OD1	1:C:637:ARG:NH1	2.20	0.69
1:D:18:ILE:HG13	1:E:886:LEU:HD23	1.75	0.69
1:D:326:PRO:O	1:D:630:SER:OG	2.11	0.69
1:A:879:ILE:HD13	1:C:25:LEU:HD21	1.74	0.69
1:D:781:MET:HE1	1:F:225:VAL:H	1.57	0.69
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.73	0.69
1:A:426:PRO:HB2	1:A:429:GLU:OE2	1.93	0.69
1:A:637:ARG:HB3	1:A:642:ASN:HB3	1.74	0.69
1:C:580:ALA:HB1	1:C:724:THR:HG23	1.74	0.69
1:D:1037:ASN:HA	1:D:1038:GLU:HB2	1.75	0.69
1:B:531:VAL:O	1:B:534:ILE:HG13	1.93	0.69
1:D:355:MET:HB3	1:D:365:THR:OG1	1.92	0.69
1:C:519:MET:O	1:C:523:SER:OG	2.06	0.68
1:D:535:LEU:HD21	1:D:1027:VAL:HG21	1.75	0.68
1:C:520:PHE:O	1:C:524:THR:HG22	1.92	0.68
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.74	0.68
1:D:109:ASN:HD21	1:F:129:VAL:HG23	1.58	0.68
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.28	0.68
1:C:831:ALA:HB3	1:C:835:LYS:HG3	1.74	0.68
1:B:156:ASP:OD1	1:B:765:ARG:NH2	2.27	0.68
1:D:971:ARG:HG2	1:D:974:PRO:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:762:PHE:CE1	1:F:764:ASP:HB2	2.29	0.68
1:C:841:MET:O	1:C:845:GLU:HG2	1.94	0.68
1:E:986:VAL:HG21	1:E:1007:VAL:HG11	1.74	0.68
1:A:957:GLY:O	1:A:1042:HIS:N	2.27	0.68
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.75	0.68
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.75	0.68
1:D:442:LEU:O	1:D:445:ILE:HG13	1.94	0.68
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.76	0.67
1:F:222:THR:HA	1:F:224:PRO:HD3	1.75	0.67
1:A:80:SER:HB3	1:A:90:ILE:HG12	1.76	0.67
1:D:350:LEU:HD13	1:D:984:LEU:HB3	1.77	0.67
1:E:242:SER:HB2	1:E:245:GLU:H	1.58	0.67
1:F:577:GLN:HG3	1:F:624:THR:HG22	1.76	0.67
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.77	0.67
1:D:516:PHE:O	1:D:519:MET:HG2	1.94	0.67
1:E:159:ALA:O	1:E:767:ARG:NH2	2.28	0.67
1:F:937:LEU:HD11	1:F:982:PHE:CE2	2.30	0.67
1:B:559:LEU:HD23	1:B:560:PRO:HD2	1.76	0.67
1:C:682:PHE:CE1	1:C:857:TYR:HB2	2.29	0.67
1:E:680:PHE:CZ	1:E:844:MET:HG3	2.29	0.67
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.77	0.67
1:E:262:LEU:HG	1:E:268:ILE:HD11	1.76	0.67
1:B:146:ASP:OD2	1:B:146:ASP:N	2.23	0.67
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.77	0.67
1:A:332:PHE:O	1:A:336:SER:HB3	1.94	0.67
1:B:139:VAL:HB	1:B:327:TYR:HB3	1.76	0.67
1:C:775:SER:OG	1:C:776:GLU:O	2.12	0.67
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.77	0.67
1:E:441:ALA:O	1:E:445:ILE:HG23	1.95	0.67
1:F:404:LEU:HG	1:F:449:LEU:HD13	1.77	0.67
1:F:885:PHE:HD2	1:F:886:LEU:HD22	1.60	0.67
1:C:907:LEU:HG	1:C:1017:LEU:HD23	1.76	0.66
1:A:931:LEU:HB3	3:A:1103:LMT:H51	1.77	0.66
1:A:971:ARG:CZ	1:A:971:ARG:HB3	2.24	0.66
1:B:448:VAL:HG13	1:B:884:VAL:HG22	1.77	0.66
1:D:213:GLN:HG2	1:D:239:ARG:HG2	1.75	0.66
1:D:800:PRO:HG2	1:D:803:ALA:HB2	1.77	0.66
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.76	0.66
1:A:932:LEU:HA	3:A:1103:LMT:H71	1.78	0.66
1:A:465:ALA:O	1:A:469:GLN:HG2	1.96	0.66
1:C:578:LEU:HG	1:C:587:THR:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:705:GLU:HB3	1:E:847:LEU:HD22	1.78	0.66
1:F:894:SER:HB3	1:F:897:ILE:HG12	1.77	0.66
1:C:404:LEU:HG	1:C:449:LEU:HD13	1.77	0.66
1:E:986:VAL:HG11	1:E:1007:VAL:HG12	1.77	0.66
1:D:902:MET:O	1:D:905:VAL:HG23	1.96	0.66
1:E:901:VAL:HG21	1:E:943:ILE:HG13	1.77	0.66
1:F:966:ASP:OD1	1:F:969:ARG:NH1	2.29	0.66
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.75	0.66
1:D:415:ASN:HD22	1:D:434:SER:CB	2.07	0.66
1:D:1035:ARG:HH22	1:D:1036:LYS:HE3	1.61	0.66
1:F:610:PHE:HB3	1:F:628:PHE:HB2	1.78	0.66
1:B:555:LEU:HB3	1:B:913:LEU:HB3	1.78	0.66
1:B:971:ARG:HB3	1:B:971:ARG:CZ	2.24	0.66
1:C:668:LEU:HD23	1:C:668:LEU:H	1.61	0.65
1:C:120:GLN:HA	1:C:123:GLN:HB2	1.79	0.65
1:F:324:VAL:HG23	1:F:326:PRO:HD3	1.76	0.65
1:F:817:GLU:OE2	1:F:825:MET:HA	1.96	0.65
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.78	0.65
1:B:688:ALA:O	1:B:690:LEU:N	2.29	0.65
1:E:574:THR:HG23	1:E:627:ALA:HB3	1.79	0.65
1:E:801:PHE:HA	1:E:804:PHE:CE2	2.31	0.65
1:F:562:SER:HB2	1:F:924:ASP:HB3	1.77	0.65
1:A:781:MET:HE3	1:C:228:GLN:HB2	1.78	0.65
1:D:465:ALA:O	1:D:469:GLN:HG2	1.97	0.65
1:E:324:VAL:HG13	1:E:326:PRO:HD3	1.79	0.65
1:E:696:THR:HG23	1:E:699:ARG:NH1	2.12	0.65
1:C:940:LYS:NZ	1:C:978:THR:HG21	2.11	0.65
1:C:1038:GLU:HA	1:C:1039:ASP:HB2	1.77	0.65
1:E:588:GLN:HE21	1:E:592:ASN:HD21	1.44	0.65
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.78	0.65
2:D:1101:ERY:H18	2:D:1101:ERY:H5	1.77	0.65
1:B:352:PHE:HD2	1:B:353:LEU:HD23	1.61	0.65
1:F:831:ALA:HB3	1:F:835:LYS:HG3	1.78	0.65
1:F:943:ILE:O	1:F:947:GLU:HB3	1.96	0.65
1:B:540:ARG:NH2	3:B:1101:LMT:O6B	2.30	0.65
1:F:434:SER:O	1:F:438:ILE:HG12	1.97	0.65
1:F:587:THR:OG1	1:F:613:ASN:ND2	2.26	0.65
1:D:211:ASN:O	1:D:760:ASN:ND2	2.30	0.65
1:D:418:ARG:O	1:D:422:GLU:HB2	1.97	0.64
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.79	0.64
1:A:155:SER:HB3	1:A:180:SER:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:LEU:O	1:C:361:ASN:N	2.31	0.64
1:F:482:VAL:O	1:F:486:LEU:HG	1.97	0.64
1:A:491:ALA:O	1:A:495:THR:OG1	2.13	0.64
1:A:563:PHE:HE2	1:A:671:ILE:HD13	1.62	0.64
1:E:508:GLY:O	1:E:510:LYS:N	2.30	0.64
1:F:695:LEU:HD22	1:F:855:VAL:HG22	1.79	0.64
1:E:907:LEU:HG	1:E:1017:LEU:HD23	1.78	0.64
1:A:6:ILE:HD11	1:A:432:ARG:HE	1.63	0.64
1:A:18:ILE:HG13	1:B:886:LEU:HD23	1.80	0.64
1:B:578:LEU:HD21	1:B:590:VAL:HG21	1.80	0.64
1:D:790:TYR:HB3	1:D:798:MET:HB3	1.79	0.64
1:E:14:VAL:HG22	1:F:886:LEU:HD12	1.79	0.64
1:A:565:PRO:HG2	1:A:567:GLU:OE2	1.98	0.64
1:F:399:VAL:HG11	1:F:989:LEU:HD21	1.80	0.64
1:D:470:PHE:CD2	1:D:929:VAL:HG11	2.33	0.64
1:A:507:GLU:O	1:A:509:LYS:N	2.30	0.64
1:B:445:ILE:HG21	1:B:940:LYS:HD2	1.79	0.64
1:A:516:PHE:HA	1:A:519:MET:HG3	1.78	0.63
1:C:482:VAL:O	1:C:486:LEU:HG	1.97	0.63
1:A:728:LYS:NZ	1:C:236:ALA:O	2.16	0.63
1:B:1037:ASN:HA	1:B:1038:GLU:CB	2.29	0.63
1:D:418:ARG:NH2	1:D:948:PHE:HE2	1.95	0.63
1:B:536:ARG:NH1	3:B:1101:LMT:O3B	2.31	0.63
1:B:146:ASP:OD2	1:B:320:GLY:HA3	1.98	0.63
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.29	0.63
1:C:272:GLY:N	1:C:275:TYR:OH	2.26	0.63
1:C:356:TYR:C	1:C:358:PHE:H	2.01	0.63
1:D:146:ASP:OD2	1:D:146:ASP:N	2.19	0.63
1:D:222:THR:OG1	1:E:275:TYR:O	2.16	0.63
1:E:80:SER:HB3	1:E:90:ILE:HG12	1.80	0.63
1:D:253:VAL:HG12	1:D:259:ARG:HG2	1.79	0.63
1:D:360:GLN:OE1	1:D:513:PHE:HB3	1.98	0.63
1:E:49:TYR:HE1	1:E:60:THR:HG21	1.62	0.63
1:C:597:TYR:HE1	1:C:601:LYS:HD2	1.64	0.63
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.63	0.63
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.79	0.63
1:A:588:GLN:NE2	1:A:592:ASN:OD1	2.31	0.63
1:C:634:TRP:N	1:C:634:TRP:CD1	2.63	0.62
1:F:120:GLN:HA	1:F:123:GLN:HB2	1.79	0.62
1:A:928:GLN:OE1	3:A:1103:LMT:O6'	2.10	0.62
1:B:658:ILE:O	1:B:659:LYS:HD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:726:GLN:NE2	1:D:812:GLY:HA3	2.14	0.62
1:E:139:VAL:O	1:E:326:PRO:HD2	1.99	0.62
1:E:415:ASN:CG	1:E:418:ARG:HH12	2.02	0.62
1:E:559:LEU:HD11	1:E:922:THR:HA	1.82	0.62
1:F:456:MET:HA	1:F:876:LEU:HD21	1.80	0.62
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.63	0.62
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.81	0.62
1:B:87:THR:HG21	1:B:620:ARG:HH12	1.65	0.62
1:D:183:ALA:HB2	1:D:273:GLU:HG3	1.81	0.62
1:E:153:ASP:OD2	1:E:182:TYR:OH	2.18	0.62
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.34	0.62
1:F:636:ASP:O	1:F:638:PRO:HD3	1.99	0.62
1:A:359:LEU:O	1:A:361:ASN:N	2.33	0.62
1:B:1013:THR:O	1:B:1017:LEU:HB2	1.98	0.62
1:C:352:PHE:HD2	1:C:353:LEU:HD23	1.63	0.62
1:B:362:PHE:HA	1:B:365:THR:HG22	1.81	0.62
1:B:717:ARG:HD2	1:B:828:LEU:HB2	1.81	0.62
1:C:907:LEU:HD23	1:C:1017:LEU:HB3	1.81	0.62
1:D:617:PHE:HD2	2:D:1101:ERY:H361	1.63	0.62
1:B:764:ASP:OD1	1:B:765:ARG:HG3	2.00	0.62
1:E:272:GLY:N	1:E:275:TYR:OH	2.25	0.62
1:E:568:ASP:O	1:E:634:TRP:HZ3	1.83	0.62
1:E:634:TRP:N	1:E:634:TRP:CD1	2.68	0.62
1:E:919:ARG:HB3	1:E:921:LEU:HD23	1.80	0.62
1:D:225:VAL:N	1:E:781:MET:HE1	1.99	0.62
1:B:1034:SER:OG	1:B:1035:ARG:N	2.28	0.61
1:E:534:ILE:HG22	3:E:1101:LMT:H5 <sup>7</sup>	1.81	0.61
1:D:318:PRO:HD2	1:D:321:LEU:HG	1.81	0.61
2:D:1101:ERY:H323	2:D:1101:ERY:H211	1.82	0.61
1:A:744:ASN:O	1:A:748:THR:HG23	2.00	0.61
1:C:185:ARG:HB3	1:C:187:TRP:NE1	2.15	0.61
1:D:945:ILE:HG13	1:D:971:ARG:HH22	1.65	0.61
1:E:43:VAL:HG22	1:E:131:LYS:HG3	1.80	0.61
1:F:753:ALA:O	1:F:775:SER:HB3	1.99	0.61
1:A:350:LEU:HD13	1:A:984:LEU:O	1.99	0.61
1:C:452:VAL:O	1:C:455:PRO:HD2	2.00	0.61
1:D:712:MET:SD	1:D:835:LYS:HE2	2.40	0.61
1:E:259:ARG:H	1:E:259:ARG:HD3	1.65	0.61
1:C:201:VAL:HG23	1:C:749:THR:HG23	1.82	0.61
1:A:45:ILE:HG23	1:A:129:VAL:HG22	1.83	0.61
1:E:435:MET:SD	1:E:490:PRO:HB3	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:PHE:HD2	1:F:353:LEU:HD23	1.64	0.61
1:A:452:VAL:HA	1:A:880:SER:OG	2.00	0.61
1:E:174:ASP:HB3	1:E:292:LYS:HB2	1.83	0.61
1:E:572:PHE:HA	1:E:668:LEU:HD21	1.83	0.61
1:F:600:THR:O	1:F:603:LYS:HG3	2.01	0.61
1:A:211:ASN:OD1	1:A:240:LEU:HG	2.01	0.61
1:E:219:LEU:HD13	1:F:783:PRO:HG3	1.82	0.61
1:B:327:TYR:HB2	1:B:628:PHE:CZ	2.35	0.61
1:E:327:TYR:HB2	1:E:628:PHE:CZ	2.36	0.61
1:C:137:LEU:HD22	1:C:293:LEU:HD23	1.82	0.60
1:A:108:GLN:NE2	1:B:109:ASN:O	2.34	0.60
1:A:134:SER:OG	2:A:1101:ERY:C32	2.48	0.60
1:B:225:VAL:HG12	1:C:777:ALA:HB1	1.84	0.60
1:B:744:ASN:O	1:B:748:THR:HG23	2.01	0.60
1:C:351:VAL:HG22	1:C:981:ALA:HB1	1.82	0.60
1:D:907:LEU:HD23	1:D:1017:LEU:HB3	1.83	0.60
1:F:185:ARG:HB3	1:F:187:TRP:NE1	2.16	0.60
1:F:672:VAL:O	1:F:674:LEU:N	2.32	0.60
1:F:961:ILE:HD12	1:F:961:ILE:H	1.65	0.60
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.82	0.60
1:B:452:VAL:HG23	1:B:453:PHE:HD2	1.65	0.60
1:C:222:THR:HA	1:C:224:PRO:HD3	1.83	0.60
1:F:291:ILE:HG21	1:F:306:ILE:HD11	1.81	0.60
1:F:576:VAL:HG22	1:F:663:VAL:HG13	1.82	0.60
1:F:744:ASN:O	1:F:748:THR:HG23	2.01	0.60
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.83	0.60
1:A:253:VAL:HG12	1:A:259:ARG:HG2	1.84	0.60
1:D:1013:THR:O	1:D:1017:LEU:HB2	2.00	0.60
1:A:112:GLN:HG3	1:B:112:GLN:OE1	2.01	0.60
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.84	0.60
1:B:979:SER:OG	1:B:1015:THR:HG21	2.02	0.60
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.65	0.60
1:A:1019:ILE:HG13	1:A:1020:PHE:CD1	2.37	0.60
1:B:1016:VAL:HG22	3:B:1101:LMT:H112	1.83	0.60
1:C:789:TRP:HB2	1:C:801:PHE:CD2	2.37	0.60
1:C:1038:GLU:HA	1:C:1039:ASP:CB	2.31	0.60
1:F:580:ALA:HB1	1:F:724:THR:HG22	1.83	0.60
1:D:61:VAL:HG22	1:D:118:LEU:HD22	1.82	0.60
1:E:531:VAL:O	1:E:534:ILE:HG13	2.02	0.60
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.83	0.60
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:HB2	1:B:246:PHE:CE1	2.37	0.60
1:D:58:GLN:HE21	1:D:63:GLN:HE21	1.48	0.60
1:E:281:PHE:CZ	1:E:324:VAL:HG21	2.36	0.60
1:A:211:ASN:O	1:A:760:ASN:ND2	2.35	0.60
1:D:272:GLY:N	1:D:275:TYR:OH	2.29	0.60
1:E:695:LEU:HD22	1:E:825:MET:SD	2.41	0.60
1:F:462:SER:HB3	1:F:865:GLN:HG2	1.84	0.60
1:B:405:LEU:HD22	1:B:481:SER:HB3	1.84	0.60
1:A:196:PHE:O	1:A:252:LYS:NZ	2.35	0.59
1:A:1030:ARG:HH12	1:A:1033:PHE:HB2	1.67	0.59
1:B:200:PRO:HB2	1:B:749:THR:HG22	1.82	0.59
1:B:277:ILE:HA	1:B:613:ASN:O	2.01	0.59
1:E:717:ARG:HD2	1:E:828:LEU:HB2	1.83	0.59
1:F:242:SER:HB2	1:F:245:GLU:HG3	1.84	0.59
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.84	0.59
1:C:465:ALA:HA	1:C:468:ARG:NH1	2.13	0.59
1:C:744:ASN:O	1:C:748:THR:HG23	2.02	0.59
1:D:699:ARG:NH2	1:D:722:GLU:OE1	2.35	0.59
1:E:26:ALA:O	1:E:30:LEU:HB2	2.02	0.59
1:A:360:GLN:HE22	1:A:513:PHE:HB3	1.67	0.59
1:E:971:ARG:HB3	1:E:971:ARG:CZ	2.32	0.59
1:F:104:GLN:NE2	1:F:108:GLN:OE1	2.35	0.59
1:A:388:PHE:CZ	1:A:472:ILE:HG12	2.37	0.59
1:B:1037:ASN:HB3	1:B:1040:ILE:HG12	1.84	0.59
1:D:239:ARG:NH1	1:D:761:ASP:O	2.36	0.59
1:E:399:VAL:O	1:E:402:ILE:HG12	2.01	0.59
1:E:1013:THR:O	1:E:1017:LEU:HB2	2.02	0.59
1:F:684:LEU:HD22	1:F:827:ILE:HD11	1.84	0.59
1:B:11:PHE:CE1	1:C:890:ALA:HB1	2.38	0.59
1:B:652:THR:HG23	1:B:665:ALA:H	1.68	0.59
1:C:623:ASN:N	1:C:623:ASN:OD1	2.27	0.59
1:C:948:PHE:HD2	1:C:970:MET:HE3	1.66	0.59
1:D:873:ALA:HB2	3:D:1103:LMT:H51	1.84	0.59
1:C:789:TRP:HB2	1:C:801:PHE:HD2	1.67	0.59
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.85	0.59
1:A:781:MET:CE	1:C:225:VAL:H	2.10	0.59
1:A:1037:ASN:CA	1:A:1038:GLU:HB2	2.30	0.59
1:C:156:ASP:OD1	1:C:765:ARG:NH2	2.35	0.59
1:D:897:ILE:HD13	1:D:950:LYS:HE3	1.85	0.59
1:E:9:PRO:HB3	1:E:495:THR:HG21	1.84	0.59
1:E:250:LEU:HD21	1:E:253:VAL:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:LEU:N	1:E:264:ASP:OD2	2.35	0.59
1:E:332:PHE:HD1	1:E:634:TRP:HH2	1.50	0.59
1:F:196:PHE:O	1:F:252:LYS:NZ	2.25	0.59
1:A:62:THR:HG21	1:A:818:ARG:HD3	1.83	0.59
1:D:309:GLU:O	1:D:312:LYS:HB2	2.02	0.59
1:D:457:ALA:O	1:D:468:ARG:NE	2.35	0.59
1:D:781:MET:HB3	1:F:228:GLN:HE22	1.68	0.59
1:F:888:LEU:HD21	1:F:943:ILE:HD11	1.85	0.59
1:D:344:LEU:HD21	1:D:399:VAL:HG22	1.83	0.59
1:C:200:PRO:HB2	1:C:749:THR:HG22	1.85	0.59
1:D:344:LEU:HD22	1:D:402:ILE:HD12	1.83	0.59
1:B:235:ILE:O	1:C:728:LYS:HD2	2.03	0.58
1:B:237:GLN:HG3	1:C:731:ILE:HD11	1.85	0.58
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.38	0.58
1:D:971:ARG:CZ	1:D:971:ARG:HB3	2.33	0.58
1:F:58:GLN:HA	1:F:62:THR:HB	1.85	0.58
1:F:698:ALA:O	1:F:701:GLN:HB3	2.03	0.58
1:F:1038:GLU:HB2	1:F:1039:ASP:CG	2.23	0.58
1:B:441:ALA:O	1:B:445:ILE:HG23	2.02	0.58
1:B:455:PRO:O	1:B:876:LEU:HD13	2.02	0.58
1:C:310:LEU:O	1:C:314:GLU:HG3	2.03	0.58
1:D:251:LEU:HD11	1:D:262:LEU:HA	1.84	0.58
1:A:928:GLN:OE1	3:A:1103:LMT:C6'	2.51	0.58
1:D:108:GLN:HE21	1:D:112:GLN:HE21	1.50	0.58
1:D:637:ARG:HD2	1:D:642:ASN:O	2.03	0.58
1:D:919:ARG:NH1	1:D:1005:THR:OG1	2.35	0.58
1:D:1031:ARG:HH12	1:D:1038:GLU:HG3	1.68	0.58
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.85	0.58
1:E:675:GLY:HA2	1:E:862:MET:HG3	1.84	0.58
1:A:456:MET:SD	1:A:932:LEU:HD11	2.44	0.58
1:A:1030:ARG:HH12	1:A:1033:PHE:CB	2.16	0.58
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.85	0.58
1:F:379:THR:HG23	1:F:476:SER:OG	2.03	0.58
1:C:945:ILE:HA	1:C:971:ARG:NH1	2.19	0.58
1:D:909:VAL:HG22	1:D:931:LEU:HD21	1.85	0.58
1:E:195:LYS:HZ1	1:E:196:PHE:HE1	1.52	0.58
1:E:240:LEU:HB2	1:E:246:PHE:CE1	2.38	0.58
1:E:703:LEU:HD21	1:E:718:PRO:HD3	1.86	0.58
1:F:538:THR:HG23	1:F:542:LEU:HD13	1.86	0.58
1:F:910:ILE:O	1:F:914:LEU:HB2	2.03	0.58
1:F:947:GLU:HG3	1:F:948:PHE:HD1	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:SER:HB3	1:B:90:ILE:HG12	1.85	0.58
1:C:83:ASP:HB2	1:C:87:THR:O	2.03	0.58
1:D:617:PHE:HA	2:D:1101:ERY:H351	1.85	0.58
1:F:343:THR:HG21	1:F:989:LEU:CD2	2.34	0.58
1:C:36:PRO:O	1:C:38:ILE:HG13	2.03	0.58
1:E:151:GLN:HE22	1:E:278:ILE:HA	1.68	0.58
1:A:584:GLN:HB2	1:A:622:GLN:HG2	1.84	0.58
1:C:81:ASN:OD1	1:C:815:ARG:NH1	2.37	0.58
1:E:165:ALA:HB3	1:E:313:MET:CE	2.33	0.58
1:E:671:ILE:HB	1:E:674:LEU:HG	1.86	0.58
1:F:578:LEU:HG	1:F:587:THR:HG22	1.86	0.58
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.39	0.58
1:B:99:ASP:HB3	1:B:102:ILE:HB	1.86	0.58
1:B:188:MET:HA	1:B:266:ALA:HB2	1.84	0.58
1:D:222:THR:HA	1:D:224:PRO:HD3	1.86	0.58
1:D:768:VAL:HG12	1:E:63:GLN:OE1	2.03	0.58
1:A:945:ILE:CG1	1:A:971:ARG:HH22	2.15	0.57
1:B:261:LEU:N	1:B:264:ASP:OD2	2.33	0.57
1:E:44:THR:HG1	1:E:91:THR:HG1	1.26	0.57
1:E:182:TYR:HB2	1:E:769:LYS:HZ2	1.69	0.57
1:C:58:GLN:O	1:C:62:THR:HB	2.03	0.57
1:C:190:PRO:HB3	1:C:789:TRP:CZ3	2.39	0.57
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.87	0.57
1:C:915:ALA:HB2	1:C:1009:GLY:HA3	1.86	0.57
1:D:344:LEU:HD21	1:D:399:VAL:HA	1.86	0.57
1:F:520:PHE:O	1:F:524:THR:HG22	2.02	0.57
1:F:1021:PHE:HB3	1:F:1025:PHE:CE1	2.39	0.57
1:F:1043:SER:OG	1:F:1044:HIS:N	2.37	0.57
1:C:463:THR:HG23	1:C:467:TYR:CE1	2.40	0.57
1:E:396:PHE:O	1:E:400:LEU:HB2	2.04	0.57
1:E:442:LEU:O	1:E:445:ILE:HG13	2.03	0.57
1:E:713:LEU:HD21	1:E:843:LEU:HD12	1.86	0.57
1:F:1034:SER:OG	1:F:1035:ARG:HA	2.04	0.57
1:A:544:LEU:O	1:A:548:ILE:HG13	2.04	0.57
1:B:559:LEU:HD23	1:B:560:PRO:CD	2.34	0.57
1:C:49:TYR:HD1	1:C:57:VAL:HG12	1.70	0.57
1:C:426:PRO:HD2	1:C:429:GLU:HB3	1.86	0.57
1:E:678:THR:HA	1:E:837:THR:OG1	2.03	0.57
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.86	0.57
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.85	0.57
1:A:242:SER:OG	1:A:245:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	1.87	0.57
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.39	0.57
1:C:201:VAL:HG22	1:C:748:THR:OG1	2.05	0.57
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.87	0.57
1:B:916:ALA:O	1:B:919:ARG:N	2.36	0.57
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.87	0.57
1:C:404:LEU:HB3	1:C:478:MET:SD	2.45	0.57
1:C:688:ALA:O	1:C:690:LEU:N	2.38	0.57
1:C:698:ALA:O	1:C:701:GLN:HB3	2.04	0.57
1:D:17:ILE:HG22	1:E:886:LEU:HD21	1.86	0.57
1:D:78:MET:O	1:D:820:ASN:N	2.26	0.57
1:F:358:PHE:CD2	1:F:977:MET:HG3	2.40	0.57
1:A:953:MET:HE2	1:A:963:ALA:HB3	1.85	0.57
1:B:985:GLY:O	1:B:988:PRO:HD2	2.04	0.57
1:D:919:ARG:HG2	1:D:920:GLY:H	1.69	0.57
1:E:441:ALA:HA	1:E:891:LEU:HD21	1.87	0.57
1:F:3:ASN:HD22	1:F:435:MET:CG	2.16	0.57
1:A:577:GLN:OE1	1:A:624:THR:HG22	2.05	0.57
1:B:28:LEU:HB3	1:B:29:LYS:HD2	1.87	0.57
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.40	0.57
1:B:668:LEU:H	1:B:668:LEU:CD2	2.14	0.57
1:D:415:ASN:HB3	1:D:434:SER:HB2	1.87	0.57
1:D:928:GLN:HG2	3:D:1103:LMT:H82	1.86	0.57
1:C:795:ASP:OD2	1:C:797:GLN:HG2	2.05	0.57
1:E:591:LEU:HD13	1:E:611:ALA:HB1	1.86	0.57
1:F:372:VAL:HG22	1:F:405:LEU:HD11	1.86	0.57
1:B:652:THR:CG2	1:B:665:ALA:H	2.18	0.57
1:C:57:VAL:HG23	1:C:82:SER:HB3	1.87	0.57
1:C:650:ARG:O	1:C:653:ARG:HB3	2.05	0.57
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.05	0.57
1:D:876:LEU:HD23	1:D:879:ILE:HD12	1.86	0.57
1:D:986:VAL:HG21	1:D:1007:VAL:HG11	1.86	0.57
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.87	0.57
1:A:801:PHE:HA	1:A:804:PHE:CE2	2.40	0.56
1:B:142:VAL:HG21	1:B:158:VAL:HG22	1.87	0.56
1:E:532:GLY:O	1:E:535:LEU:N	2.37	0.56
1:A:717:ARG:HE	1:A:828:LEU:HB2	1.69	0.56
1:A:777:ALA:HB1	1:C:225:VAL:HG12	1.86	0.56
1:B:695:LEU:HD22	1:B:825:MET:SD	2.45	0.56
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.86	0.56
1:C:228:GLN:NE2	1:C:230:LEU:H	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:815:ARG:HH21	2:D:1101:ERY:H291	1.70	0.56
1:F:113:LEU:O	1:F:116:PRO:HD2	2.05	0.56
1:A:154:ILE:O	1:A:157:TYR:N	2.38	0.56
1:A:644:VAL:CG1	1:A:667:ASN:HB2	2.32	0.56
1:A:728:LYS:HB2	1:A:810:GLU:OE1	2.05	0.56
1:C:990:VAL:HG13	1:C:1005:THR:OG1	2.05	0.56
1:D:59:ASP:HB3	1:F:763:ILE:HD11	1.87	0.56
1:E:733:GLN:HE22	1:E:743:ILE:HG21	1.69	0.56
1:F:64:VAL:HA	1:F:67:GLN:OE1	2.06	0.56
1:F:351:VAL:HG22	1:F:981:ALA:HB1	1.87	0.56
1:F:455:PRO:HG2	1:F:880:SER:HA	1.88	0.56
1:F:555:LEU:HB3	1:F:913:LEU:HB3	1.87	0.56
1:C:427:PRO:HD3	1:C:499:PRO:HB3	1.88	0.56
1:D:210:GLN:NE2	1:D:250:LEU:HB3	2.10	0.56
1:E:58:GLN:OE1	1:E:816:LEU:HD13	2.04	0.56
1:F:945:ILE:HA	1:F:971:ARG:NH1	2.20	0.56
1:A:49:TYR:HE1	1:A:60:THR:HG21	1.70	0.56
1:A:73:ASP:OD2	1:C:131:LYS:NZ	2.33	0.56
1:A:563:PHE:CE2	1:A:671:ILE:HD13	2.40	0.56
1:D:201:VAL:HA	1:D:204:ILE:HD12	1.86	0.56
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.88	0.56
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.86	0.56
1:B:545:TYR:HE2	1:B:907:LEU:HD11	1.70	0.56
1:C:47:ALA:HB3	1:C:88:VAL:HG13	1.88	0.56
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.71	0.56
1:C:959:GLY:HA2	1:C:1041:GLU:HA	1.87	0.56
1:D:317:PHE:HB3	1:D:321:LEU:HB3	1.87	0.56
1:E:901:VAL:HG23	1:E:942:ALA:HB3	1.87	0.56
1:F:587:THR:HG21	1:F:622:GLN:O	2.06	0.56
1:A:705:GLU:HB3	1:A:847:LEU:HD22	1.88	0.56
1:A:913:LEU:HD23	1:A:927:PHE:HZ	1.70	0.56
1:B:153:ASP:OD2	1:B:182:TYR:OH	2.23	0.56
1:C:380:PHE:CD2	1:C:383:LEU:HD12	2.40	0.56
1:D:3:ASN:HA	1:D:6:ILE:HG12	1.88	0.56
1:F:971:ARG:HB3	1:F:971:ARG:NH1	2.21	0.56
1:D:235:ILE:O	1:E:728:LYS:HD2	2.06	0.56
1:E:575:MET:HA	1:E:626:ILE:HG13	1.87	0.56
1:D:276:ASP:OD1	1:F:222:THR:HG21	2.05	0.56
1:E:758:TYR:HE1	1:E:770:LYS:HG2	1.71	0.56
1:F:53:ASP:OD1	1:F:56:THR:OG1	2.17	0.56
1:A:530:SER:CB	3:A:1102:LMT:H2O2	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.31	0.56
1:D:644:VAL:HG11	1:D:667:ASN:HB2	1.87	0.56
1:D:682:PHE:HD2	1:D:683:GLU:N	2.04	0.56
1:E:380:PHE:HA	1:E:383:LEU:HD12	1.88	0.56
1:F:1035:ARG:NH1	1:F:1038:GLU:OE1	2.39	0.56
1:A:186:ILE:HB	1:A:773:VAL:HG22	1.88	0.55
1:C:746:ILE:HG13	1:C:747:ASN:N	2.21	0.55
1:C:966:ASP:OD1	1:C:969:ARG:NH2	2.39	0.55
1:F:187:TRP:HA	1:F:774:MET:O	2.06	0.55
1:F:579:PRO:HD3	1:F:661:ALA:HB2	1.87	0.55
1:C:898:PRO:HA	1:C:901:VAL:HG12	1.89	0.55
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.89	0.55
1:E:582:ALA:HA	1:E:586:ARG:HH21	1.71	0.55
1:E:710:PRO:HA	1:E:713:LEU:O	2.06	0.55
1:F:101:ASP:OD1	1:F:131:LYS:NZ	2.27	0.55
1:F:343:THR:HG21	1:F:989:LEU:HD21	1.87	0.55
1:C:585:GLU:O	1:C:589:LYS:HG3	2.07	0.55
1:C:762:PHE:CE1	1:C:764:ASP:HB2	2.41	0.55
1:C:945:ILE:HG12	1:C:971:ARG:HH22	1.70	0.55
1:E:156:ASP:OD1	1:E:765:ARG:NH2	2.39	0.55
1:E:216:ALA:HB1	1:E:234:ILE:HG22	1.87	0.55
1:E:516:PHE:CA	1:E:519:MET:HG3	2.34	0.55
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.88	0.55
1:A:159:ALA:HB2	1:A:177:LEU:HD11	1.88	0.55
1:A:459:PHE:CZ	1:A:873:ALA:HA	2.40	0.55
1:B:400:LEU:HD12	1:B:933:THR:HG21	1.89	0.55
1:C:187:TRP:HA	1:C:774:MET:O	2.05	0.55
1:C:752:ALA:O	1:C:774:MET:HA	2.07	0.55
1:D:683:GLU:HG2	1:D:819:TYR:CG	2.41	0.55
1:F:382:VAL:HG21	1:F:476:SER:HB2	1.89	0.55
1:A:935:ILE:HG21	3:A:1103:LMT:H112	1.88	0.55
1:B:616:GLY:HA2	1:B:626:ILE:HB	1.87	0.55
1:C:764:ASP:OD1	1:C:765:ARG:HG3	2.07	0.55
1:E:632:LYS:O	1:E:637:ARG:NE	2.36	0.55
1:E:987:MET:HA	1:E:1008:MET:HE3	1.89	0.55
1:A:535:LEU:HD21	1:A:1027:VAL:HG21	1.89	0.55
1:A:781:MET:HE1	1:C:225:VAL:HG13	1.88	0.55
1:A:790:TYR:HB3	1:A:798:MET:HB3	1.88	0.55
1:D:637:ARG:HB3	1:D:642:ASN:HB3	1.87	0.55
1:E:80:SER:CB	1:E:90:ILE:HG12	2.36	0.55
1:E:415:ASN:HD22	1:E:434:SER:CB	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:613:ASN:HD22	1:E:614:GLY:N	2.05	0.55
1:F:144:ASN:OD1	1:F:148:THR:HA	2.07	0.55
1:F:944:LEU:HB3	1:F:971:ARG:NE	2.22	0.55
1:F:1042:HIS:CG	1:F:1043:SER:N	2.75	0.55
1:A:897:ILE:HA	1:A:1029:VAL:CG1	2.37	0.55
1:B:344:LEU:HD23	1:B:402:ILE:HD11	1.88	0.55
1:B:733:GLN:HE22	1:B:743:ILE:HG21	1.71	0.55
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.88	0.55
1:D:359:LEU:O	1:D:361:ASN:N	2.40	0.55
1:E:545:TYR:OH	1:E:903:LEU:O	2.18	0.55
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.88	0.55
1:F:947:GLU:HG3	1:F:948:PHE:N	2.21	0.55
1:A:420:MET:HB3	1:A:500:ILE:HB	1.88	0.55
1:F:877:TYR:O	1:F:881:LEU:HG	2.07	0.55
1:A:229:GLN:HE21	1:B:586:ARG:HD3	1.71	0.55
1:B:238:THR:OG1	1:C:728:LYS:NZ	2.39	0.55
1:B:415:ASN:OD1	1:B:418:ARG:NH1	2.36	0.55
1:C:187:TRP:HE3	1:C:775:SER:O	1.90	0.55
1:C:393:LEU:HD13	1:C:466:ILE:HG23	1.89	0.55
1:C:801:PHE:HA	1:C:804:PHE:CE2	2.42	0.55
1:C:961:ILE:HD12	1:C:961:ILE:H	1.72	0.55
1:D:109:ASN:ND2	1:F:129:VAL:HG23	2.22	0.55
1:D:112:GLN:HG3	1:E:112:GLN:OE1	2.07	0.55
1:D:568:ASP:OD1	1:D:637:ARG:NH1	2.26	0.55
1:F:447:MET:HG2	1:F:891:LEU:HD22	1.89	0.55
1:D:944:LEU:HB3	1:D:971:ARG:CZ	2.37	0.54
1:E:143:ILE:HG22	1:E:286:ALA:HB2	1.90	0.54
1:F:568:ASP:OD1	1:F:637:ARG:NH1	2.39	0.54
1:A:459:PHE:HZ	1:A:873:ALA:HA	1.72	0.54
1:A:535:LEU:CD2	1:A:1027:VAL:HG21	2.37	0.54
1:B:119:PRO:HG2	1:B:122:VAL:HB	1.87	0.54
1:D:658:ILE:HG13	1:D:659:LYS:NZ	2.23	0.54
1:E:343:THR:HG22	1:E:344:LEU:HD23	1.88	0.54
1:F:45:ILE:HB	1:F:90:ILE:HG12	1.89	0.54
1:F:99:ASP:HB3	1:F:102:ILE:HB	1.89	0.54
1:F:253:VAL:HG22	1:F:259:ARG:HG2	1.90	0.54
1:F:404:LEU:HB3	1:F:478:MET:SD	2.47	0.54
1:A:169:THR:HG21	1:A:306:ILE:HG13	1.89	0.54
1:A:453:PHE:CE2	1:A:932:LEU:HB3	2.42	0.54
1:A:622:GLN:HE21	1:C:222:THR:HG22	1.72	0.54
1:A:976:LEU:O	1:A:980:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:GLN:NE2	1:B:812:GLY:HA3	2.23	0.54
1:B:1042:HIS:CG	1:B:1043:SER:H	2.25	0.54
1:C:144:ASN:O	1:C:284:GLN:NE2	2.40	0.54
1:C:943:ILE:O	1:C:947:GLU:HB3	2.07	0.54
1:E:344:LEU:HD22	1:E:402:ILE:HG21	1.89	0.54
1:F:184:MET:HB2	1:F:762:PHE:CE2	2.42	0.54
1:F:751:GLY:O	1:F:753:ALA:N	2.41	0.54
1:C:418:ARG:O	1:C:422:GLU:HB2	2.07	0.54
1:C:586:ARG:O	1:C:589:LYS:HB2	2.08	0.54
1:D:441:ALA:O	1:D:445:ILE:HG23	2.07	0.54
1:F:277:ILE:HA	1:F:613:ASN:O	2.07	0.54
1:F:617:PHE:CE1	1:F:626:ILE:HD11	2.42	0.54
1:A:726:GLN:OE1	1:A:812:GLY:HA3	2.07	0.54
1:B:415:ASN:CG	1:B:418:ARG:HH12	2.10	0.54
1:D:744:ASN:O	1:D:748:THR:HG23	2.07	0.54
1:D:834:GLY:O	1:D:835:LYS:HD2	2.07	0.54
1:F:699:ARG:HD3	1:F:825:MET:SD	2.48	0.54
1:A:42:ALA:HB2	1:A:93:THR:HG23	1.89	0.54
1:C:674:LEU:HD22	1:C:861:GLY:HA2	1.90	0.54
1:C:703:LEU:HD11	1:C:718:PRO:HD3	1.88	0.54
1:C:941:ASN:HD21	1:C:1015:THR:HG22	1.72	0.54
1:F:519:MET:O	1:F:523:SER:OG	2.18	0.54
1:F:563:PHE:CE2	1:F:564:LEU:HD22	2.43	0.54
1:B:671:ILE:HB	1:B:674:LEU:HD12	1.89	0.54
1:C:360:GLN:OE1	1:C:517:ASN:ND2	2.33	0.54
1:D:946:VAL:HG13	1:D:1026:PHE:CE1	2.43	0.54
1:E:911:GLY:HA2	1:E:1013:THR:HG21	1.89	0.54
1:B:706:ALA:CB	1:B:716:VAL:HG11	2.38	0.54
1:D:352:PHE:HD2	1:D:353:LEU:HD23	1.72	0.54
1:F:20:MET:HG2	1:F:374:VAL:HA	1.90	0.54
1:F:945:ILE:HA	1:F:971:ARG:HH12	1.72	0.54
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.88	0.54
1:B:575:MET:HA	1:B:626:ILE:HG13	1.89	0.54
1:B:919:ARG:HB3	1:B:921:LEU:HD23	1.89	0.54
1:C:571:VAL:N	1:C:631:LEU:HD12	2.22	0.54
1:C:579:PRO:HD3	1:C:661:ALA:CB	2.36	0.54
1:D:70:ASN:HB2	1:F:167:SER:HB2	1.90	0.54
1:E:32:VAL:HG21	1:E:300:LEU:HD13	1.89	0.54
1:E:54:ALA:HB2	1:E:84:SER:HB3	1.89	0.54
1:F:563:PHE:HB2	1:F:866:GLU:HG3	1.89	0.54
1:F:1043:SER:HB2	1:F:1044:HIS:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:SER:HB3	1:A:814:PRO:HA	1.89	0.54
1:A:419:VAL:HG11	1:A:433:LYS:HG2	1.90	0.54
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.89	0.54
1:C:559:LEU:HD23	1:C:560:PRO:HD2	1.90	0.54
1:D:10:ILE:HG13	1:E:895:TRP:CE2	2.42	0.54
1:E:519:MET:O	1:E:523:SER:OG	2.23	0.54
1:F:599:LEU:O	1:F:603:LYS:HG2	2.08	0.54
1:A:330:THR:HB	1:A:331:PRO:HD3	1.90	0.53
1:A:1040:ILE:HG13	1:A:1041:GLU:N	2.22	0.53
1:C:801:PHE:HD1	1:C:804:PHE:HE2	1.55	0.53
1:D:274:ASN:ND2	1:D:276:ASP:OD2	2.30	0.53
1:D:391:ASN:O	1:D:395:MET:HG2	2.07	0.53
1:E:790:TYR:CE1	1:E:800:PRO:HB3	2.43	0.53
1:F:376:LEU:O	1:F:379:THR:N	2.41	0.53
1:F:549:VAL:O	1:F:552:MET:HB3	2.08	0.53
1:A:591:LEU:HD11	1:A:625:GLY:HA3	1.90	0.53
1:A:960:LEU:O	1:A:964:THR:HG23	2.09	0.53
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.90	0.53
1:B:910:ILE:O	1:B:914:LEU:HB2	2.08	0.53
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.43	0.53
1:F:616:GLY:HA2	1:F:626:ILE:HD12	1.89	0.53
1:F:800:PRO:HG2	1:F:803:ALA:HB2	1.90	0.53
1:F:817:GLU:HB2	1:F:824:SER:O	2.08	0.53
1:F:915:ALA:HB2	1:F:1009:GLY:HA3	1.89	0.53
1:F:952:LEU:O	1:F:956:GLU:HB2	2.08	0.53
1:A:932:LEU:HD23	3:A:1103:LMT:H71	1.89	0.53
1:B:44:THR:OG1	1:B:91:THR:OG1	2.24	0.53
1:B:775:SER:OG	1:B:780:ARG:HG2	2.07	0.53
1:E:453:PHE:O	1:E:471:SER:OG	2.14	0.53
1:F:507:GLU:HG2	1:F:518:ARG:HG3	1.90	0.53
1:A:836:SER:HB3	1:A:839:GLU:CD	2.28	0.53
1:C:244:GLU:HG2	1:C:248:LYS:HE3	1.89	0.53
1:E:196:PHE:N	1:E:196:PHE:HD1	2.06	0.53
1:C:178:PHE:HE2	1:C:615:PHE:CD1	2.25	0.53
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.89	0.53
1:C:531:VAL:HG21	1:C:968:VAL:HG11	1.90	0.53
1:E:160:ALA:HA	1:E:767:ARG:NH2	2.23	0.53
1:F:80:SER:HB3	1:F:90:ILE:HG22	1.91	0.53
1:A:146:ASP:OD2	1:A:146:ASP:N	2.39	0.53
1:B:272:GLY:N	1:B:275:TYR:OH	2.34	0.53
1:B:362:PHE:O	1:B:365:THR:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:PHE:HE1	1:C:857:TYR:HB2	1.70	0.53
1:D:355:MET:HA	1:D:355:MET:HE2	1.91	0.53
3:E:1101:LMT:H5B	3:E:1101:LMT:H6D	1.89	0.53
1:F:686:ASP:OD2	1:F:823:PRO:HD2	2.09	0.53
1:A:352:PHE:HD2	1:A:353:LEU:HD23	1.74	0.53
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.08	0.53
1:E:104:GLN:HE21	1:F:109:ASN:HD22	1.55	0.53
1:E:196:PHE:N	1:E:196:PHE:CD1	2.77	0.53
1:A:453:PHE:CD2	1:A:932:LEU:HD13	2.44	0.53
1:A:781:MET:HE1	1:C:225:VAL:N	2.11	0.53
1:B:52:ALA:HB1	1:B:56:THR:HB	1.91	0.53
1:B:415:ASN:HD22	1:B:434:SER:CB	2.19	0.53
1:B:644:VAL:O	1:B:648:THR:HG23	2.08	0.53
1:E:511:GLY:HA2	1:E:515:TRP:HD1	1.73	0.53
1:E:1037:ASN:H	1:E:1038:GLU:HA	1.74	0.53
1:F:548:ILE:HD13	1:F:1017:LEU:HD21	1.91	0.53
1:F:555:LEU:HD11	1:F:914:LEU:HD12	1.90	0.53
1:A:533:GLY:HA2	1:A:536:ARG:HH11	1.73	0.53
1:B:11:PHE:HE1	1:C:890:ALA:HB1	1.74	0.53
1:C:5:PHE:HD2	1:C:6:ILE:HG12	1.74	0.53
1:C:253:VAL:HG22	1:C:259:ARG:HG2	1.90	0.53
1:D:316:PHE:CD1	1:E:687:GLN:HG2	2.43	0.53
1:B:363:ARG:HD3	1:B:496:MET:O	2.09	0.53
1:B:614:GLY:HA2	1:B:621:GLY:O	2.09	0.53
1:D:14:VAL:HG11	1:E:890:ALA:HB2	1.91	0.53
1:F:897:ILE:HG23	1:F:946:VAL:CG1	2.39	0.53
1:A:520:PHE:O	1:A:524:THR:HG22	2.09	0.52
1:B:508:GLY:CA	1:B:518:ARG:HH21	2.22	0.52
1:C:178:PHE:HE2	1:C:615:PHE:HD1	1.57	0.52
1:C:356:TYR:O	1:C:358:PHE:N	2.41	0.52
1:D:727:PHE:HD1	1:D:809:TRP:CE2	2.27	0.52
1:E:42:ALA:HB3	1:E:132:SER:HB3	1.91	0.52
1:E:415:ASN:OD1	1:E:418:ARG:NH1	2.40	0.52
1:E:888:LEU:HD21	1:E:943:ILE:HD11	1.92	0.52
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.44	0.52
1:A:34:GLN:HB2	1:A:333:VAL:HG22	1.90	0.52
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.27	0.52
1:A:448:VAL:O	1:A:451:ALA:HB3	2.09	0.52
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.90	0.52
1:F:568:ASP:CG	1:F:637:ARG:HH12	2.12	0.52
1:F:720:GLY:HA2	1:F:815:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:801:PHE:HA	1:F:804:PHE:CE2	2.45	0.52
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.44	0.52
1:B:378:GLY:O	1:B:382:VAL:HG23	2.09	0.52
1:B:894:SER:HB2	1:B:897:ILE:HD12	1.91	0.52
1:C:945:ILE:HA	1:C:971:ARG:HH12	1.75	0.52
1:D:72:ILE:HD13	1:D:107:VAL:HA	1.90	0.52
1:D:159:ALA:HB2	1:D:177:LEU:HD11	1.89	0.52
1:D:957:GLY:O	1:D:1040:ILE:HB	2.09	0.52
1:C:250:LEU:HD21	1:C:253:VAL:HG23	1.91	0.52
1:C:352:PHE:CD2	1:C:353:LEU:HD23	2.44	0.52
1:C:414:GLU:OE1	1:C:973:ARG:HD3	2.09	0.52
1:C:971:ARG:HB3	1:C:971:ARG:NH1	2.24	0.52
1:D:17:ILE:CG2	1:E:886:LEU:HD21	2.40	0.52
1:E:228:GLN:NE2	1:E:230:LEU:O	2.39	0.52
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.39	0.52
1:A:715:SER:O	1:A:717:ARG:HD3	2.10	0.52
1:D:563:PHE:CD1	3:D:1103:LMT:H5B	2.45	0.52
1:E:344:LEU:HD21	1:E:399:VAL:HA	1.91	0.52
1:E:484:VAL:HG13	1:E:488:LEU:HB3	1.91	0.52
1:E:682:PHE:CZ	1:E:857:TYR:HB2	2.45	0.52
1:F:876:LEU:O	1:F:880:SER:HB2	2.08	0.52
1:A:595:THR:O	1:A:599:LEU:HG	2.10	0.52
1:A:958:LYS:C	1:A:1040:ILE:HG12	2.30	0.52
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.90	0.52
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.92	0.52
1:C:30:LEU:HD23	1:C:390:ILE:HD11	1.91	0.52
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.40	0.52
1:C:587:THR:HG21	1:C:622:GLN:O	2.09	0.52
1:D:400:LEU:HD23	1:D:929:VAL:HG12	1.91	0.52
1:D:418:ARG:HD3	1:D:422:GLU:OE1	2.10	0.52
1:D:945:ILE:HG13	1:D:971:ARG:NH2	2.24	0.52
1:E:42:ALA:O	1:E:132:SER:N	2.39	0.52
1:E:49:TYR:CE1	1:E:60:THR:HG21	2.43	0.52
1:F:352:PHE:CD2	1:F:353:LEU:HD23	2.45	0.52
1:A:361:ASN:HD21	1:A:498:LYS:HB2	1.74	0.52
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.90	0.52
1:C:455:PRO:HG2	1:C:880:SER:HA	1.92	0.52
1:C:885:PHE:HD2	1:C:886:LEU:HD22	1.75	0.52
1:F:244:GLU:HG2	1:F:248:LYS:HE3	1.92	0.52
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.38	0.52
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.92	0.52
1:D:362:PHE:O	1:D:366:LEU:HG	2.09	0.52
1:F:45:ILE:HD12	1:F:90:ILE:HG13	1.92	0.52
1:A:195:LYS:HG2	1:A:196:PHE:CE2	2.45	0.52
1:A:404:LEU:HD12	1:A:937:LEU:CD2	2.40	0.52
1:A:897:ILE:HD13	1:A:950:LYS:HE3	1.91	0.52
1:A:919:ARG:HG2	1:A:920:GLY:H	1.74	0.52
1:B:327:TYR:HD1	1:B:628:PHE:CZ	2.27	0.52
1:C:356:TYR:C	1:C:358:PHE:N	2.63	0.52
1:F:34:GLN:CB	1:F:333:VAL:HG22	2.36	0.52
1:F:82:SER:HB2	1:F:816:LEU:HB2	1.92	0.52
1:F:380:PHE:HD2	1:F:383:LEU:HD12	1.74	0.52
1:F:574:THR:HG23	1:F:627:ALA:HB3	1.92	0.52
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.92	0.52
1:C:443:VAL:O	1:C:447:MET:HB3	2.10	0.52
1:C:664:PHE:CD2	1:C:717:ARG:HD2	2.38	0.52
1:D:449:LEU:HB3	1:D:478:MET:SD	2.50	0.52
1:F:469:GLN:O	1:F:472:ILE:HG22	2.10	0.52
1:F:945:ILE:CG1	1:F:971:ARG:HH22	2.23	0.52
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.43	0.51
1:B:501:ALA:O	1:B:504:ASP:HB2	2.10	0.51
1:C:78:MET:HG3	1:C:92:LEU:HD13	1.92	0.51
1:C:587:THR:HG21	1:C:623:ASN:HA	1.93	0.51
1:C:982:PHE:HD2	1:C:1011:MET:HG2	1.74	0.51
1:F:66:GLU:OE1	1:F:821:GLY:HA2	2.09	0.51
1:F:911:GLY:HA3	1:F:1010:GLY:HA2	1.92	0.51
1:A:775:SER:OG	1:A:780:ARG:HG2	2.10	0.51
1:B:139:VAL:O	1:B:326:PRO:HD2	2.09	0.51
1:C:23:GLY:HA3	1:C:377:LEU:O	2.10	0.51
1:C:987:MET:HG3	1:C:1008:MET:HE1	1.92	0.51
1:D:58:GLN:HE21	1:D:63:GLN:NE2	2.07	0.51
1:D:712:MET:O	1:D:832:ALA:N	2.37	0.51
1:D:728:LYS:HB2	1:D:810:GLU:OE1	2.09	0.51
1:D:817:GLU:OE1	2:D:1101:ERY:H282	2.10	0.51
1:A:30:LEU:HD11	1:A:384:ALA:HA	1.91	0.51
1:C:727:PHE:HD1	1:C:809:TRP:CE2	2.28	0.51
1:D:31:PRO:O	1:D:389:SER:HB2	2.10	0.51
1:D:559:LEU:HD23	1:D:560:PRO:HD2	1.92	0.51
1:E:932:LEU:HD23	1:E:935:ILE:HD12	1.92	0.51
1:F:104:GLN:HG3	1:F:105:VAL:N	2.24	0.51
1:A:725:PRO:HA	1:A:810:GLU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.46	0.51
1:B:1026:PHE:O	1:B:1030:ARG:HB2	2.09	0.51
1:C:940:LYS:HZ1	1:C:978:THR:HG21	1.74	0.51
1:D:573:MET:HB3	1:D:666:PHE:CE1	2.44	0.51
1:D:815:ARG:NH2	2:D:1101:ERY:H291	2.25	0.51
1:E:740:GLY:O	1:E:794:ALA:N	2.43	0.51
1:F:898:PRO:HA	1:F:901:VAL:HG12	1.93	0.51
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.91	0.51
1:C:2:PRO:O	1:C:5:PHE:HB3	2.09	0.51
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.92	0.51
1:C:188:MET:HA	1:C:266:ALA:HB2	1.93	0.51
1:C:694:LYS:HD3	1:C:694:LYS:N	2.23	0.51
1:C:897:ILE:HG23	1:C:946:VAL:CG1	2.41	0.51
1:D:728:LYS:HB2	1:D:810:GLU:CD	2.31	0.51
1:D:246:PHE:HA	1:D:249:ILE:HG13	1.93	0.51
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.46	0.51
1:A:960:LEU:HD21	1:A:1027:VAL:HG13	1.92	0.51
1:B:54:ALA:HB2	1:B:84:SER:HB3	1.93	0.51
1:C:1034:SER:OG	1:C:1037:ASN:HB3	2.11	0.51
1:E:715:SER:O	1:E:717:ARG:HG3	2.11	0.51
1:F:801:PHE:CD1	1:F:804:PHE:HE2	2.29	0.51
1:F:960:LEU:HD23	1:F:1031:ARG:HH21	1.76	0.51
1:A:190:PRO:HG3	1:A:779:TYR:HB3	1.92	0.51
1:B:418:ARG:O	1:B:422:GLU:HB2	2.10	0.51
1:B:534:ILE:CD1	1:B:1024:VAL:HG22	2.41	0.51
1:C:743:ILE:H	1:C:743:ILE:HD12	1.76	0.51
1:D:246:PHE:O	1:D:262:LEU:HD23	2.11	0.51
1:D:415:ASN:ND2	1:D:434:SER:HB2	2.15	0.51
1:D:617:PHE:CD2	2:D:1101:ERY:H361	2.43	0.51
1:E:584:GLN:HB2	1:E:622:GLN:HG2	1.91	0.51
1:A:935:ILE:CG2	3:A:1103:LMT:H112	2.41	0.51
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.92	0.51
1:C:841:MET:SD	1:C:863:SER:HB3	2.51	0.51
1:D:358:PHE:O	1:D:359:LEU:HD23	2.11	0.51
1:D:910:ILE:O	1:D:914:LEU:HB2	2.11	0.51
1:F:455:PRO:HB3	1:F:879:ILE:HG22	1.93	0.51
1:F:525:HIS:O	1:F:528:THR:HG22	2.11	0.51
1:C:66:GLU:OE1	1:C:821:GLY:HA2	2.11	0.51
1:C:196:PHE:HD1	1:C:260:VAL:CG1	2.24	0.51
1:C:702:LEU:HD12	1:C:851:LEU:HD11	1.92	0.51
1:C:945:ILE:CG1	1:C:971:ARG:HH22	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:VAL:HG21	1:E:406:VAL:HG11	1.94	0.51
1:E:448:VAL:HG21	1:E:888:LEU:HD21	1.93	0.51
1:E:658:ILE:HG13	1:E:659:LYS:HD2	1.93	0.51
1:E:658:ILE:O	1:E:659:LYS:HD2	2.11	0.51
1:E:858:ASP:OD1	1:E:859:TRP:N	2.39	0.51
1:F:11:PHE:CE2	1:F:15:ILE:HD11	2.46	0.51
1:F:188:MET:HA	1:F:266:ALA:HB2	1.93	0.51
1:A:61:VAL:HG21	1:A:122:VAL:HG21	1.92	0.50
1:A:225:VAL:HG12	1:B:777:ALA:CB	2.40	0.50
1:A:897:ILE:HA	1:A:1029:VAL:HG11	1.93	0.50
1:A:937:LEU:O	1:A:940:LYS:HB3	2.12	0.50
1:A:959:GLY:HA2	1:A:1040:ILE:HB	1.91	0.50
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.46	0.50
1:C:372:VAL:HG22	1:C:405:LEU:HD11	1.93	0.50
1:F:509:LYS:HE2	1:F:513:PHE:HD1	1.75	0.50
1:F:947:GLU:HG3	1:F:948:PHE:CD1	2.45	0.50
1:B:129:VAL:O	1:C:113:LEU:HD21	2.10	0.50
1:B:636:ASP:O	1:B:638:PRO:HD3	2.10	0.50
1:C:239:ARG:NH1	1:C:761:ASP:HB2	2.27	0.50
1:C:509:LYS:HE2	1:C:513:PHE:CD1	2.46	0.50
1:D:425:LEU:HD12	1:D:425:LEU:H	1.76	0.50
1:E:84:SER:HB3	1:E:814:PRO:HA	1.93	0.50
1:E:1019:ILE:HG13	1:E:1020:PHE:HD1	1.76	0.50
1:A:17:ILE:HG22	1:B:886:LEU:HD21	1.94	0.50
1:A:545:TYR:HB2	1:A:1021:PHE:CE2	2.47	0.50
1:A:865:GLN:O	1:A:868:LEU:HB2	2.11	0.50
1:A:944:LEU:O	1:A:947:GLU:HB3	2.11	0.50
1:C:186:ILE:HG22	1:C:773:VAL:HG23	1.93	0.50
1:C:944:LEU:HD22	1:C:971:ARG:HD2	1.93	0.50
1:C:979:SER:HA	1:C:1011:MET:HE3	1.93	0.50
1:D:62:THR:OG1	1:D:88:VAL:HG21	2.11	0.50
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.47	0.50
1:F:572:PHE:HD1	1:F:666:PHE:O	1.95	0.50
1:F:686:ASP:HB3	1:F:823:PRO:O	2.11	0.50
1:F:841:MET:HG2	1:F:859:TRP:CH2	2.47	0.50
1:A:1031:ARG:O	1:A:1032:ARG:HG3	2.11	0.50
1:B:583:THR:HG22	1:B:585:GLU:H	1.76	0.50
1:C:61:VAL:HA	1:C:118:LEU:CD2	2.42	0.50
1:C:990:VAL:HG21	1:C:1008:MET:SD	2.51	0.50
1:D:623:ASN:OD1	1:D:623:ASN:N	2.27	0.50
1:E:104:GLN:OE1	1:E:131:LYS:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:PHE:CE2	1:E:323:ILE:HD13	2.46	0.50
1:F:13:TRP:CH2	1:F:370:ILE:HD13	2.46	0.50
1:F:418:ARG:HD3	1:F:422:GLU:OE2	2.10	0.50
1:F:545:TYR:OH	1:F:903:LEU:O	2.22	0.50
1:F:584:GLN:HB2	1:F:622:GLN:HG2	1.92	0.50
1:A:4:PHE:HB3	1:A:8:ARG:NH1	2.27	0.50
1:B:154:ILE:HG22	1:B:287:SER:HB3	1.92	0.50
1:D:281:PHE:CE1	1:D:608:SER:HB2	2.47	0.50
1:D:900:SER:HB3	1:D:1029:VAL:HG21	1.94	0.50
1:E:144:ASN:HA	1:E:320:GLY:O	2.11	0.50
1:E:156:ASP:OD2	1:E:769:LYS:NZ	2.42	0.50
1:E:175:VAL:HG23	1:F:70:ASN:HD22	1.77	0.50
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.42	0.50
1:E:901:VAL:HG23	1:E:942:ALA:CB	2.41	0.50
1:A:401:ALA:O	1:A:405:LEU:HG	2.12	0.50
1:A:530:SER:OG	3:A:1102:LMT:O2'	1.93	0.50
1:A:582:ALA:HA	1:A:586:ARG:HH21	1.77	0.50
1:B:61:VAL:HG21	1:B:122:VAL:HG21	1.94	0.50
1:C:195:LYS:HG2	1:C:196:PHE:CE2	2.47	0.50
1:D:282:ASN:HD21	1:D:608:SER:HA	1.75	0.50
1:D:351:VAL:HG22	1:D:981:ALA:HB1	1.94	0.50
1:F:210:GLN:HE22	1:F:250:LEU:H	1.59	0.50
1:B:848:ALA:HA	1:B:851:LEU:HG	1.93	0.50
1:D:10:ILE:HG13	1:E:895:TRP:CZ2	2.47	0.50
1:D:31:PRO:HB2	1:D:389:SER:CB	2.40	0.50
1:D:393:LEU:HD22	1:D:470:PHE:HE1	1.76	0.50
1:D:690:LEU:O	1:D:694:LYS:HB2	2.11	0.50
1:E:537:SER:OG	1:E:540:ARG:NH2	2.43	0.50
1:E:762:PHE:CE1	1:E:764:ASP:HB2	2.46	0.50
1:E:897:ILE:N	1:E:898:PRO:HD2	2.27	0.50
1:F:362:PHE:O	1:F:366:LEU:HG	2.11	0.50
1:F:435:MET:O	1:F:439:GLN:HG2	2.11	0.50
1:A:533:GLY:HA2	1:A:536:ARG:NH1	2.27	0.50
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.77	0.50
1:A:1016:VAL:O	1:A:1016:VAL:HG12	2.12	0.50
1:B:220:GLY:HA3	1:B:230:LEU:O	2.12	0.50
1:C:58:GLN:HA	1:C:62:THR:HB	1.93	0.50
1:C:376:LEU:O	1:C:379:THR:N	2.45	0.50
1:D:170:SER:OG	1:E:74:ASN:N	2.39	0.50
1:E:795:ASP:OD2	1:E:796:GLY:N	2.45	0.50
1:F:13:TRP:HH2	1:F:370:ILE:HD13	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.27	0.50
1:B:165:ALA:HB3	1:B:313:MET:CE	2.42	0.50
1:C:520:PHE:CZ	1:C:973:ARG:HG3	2.47	0.50
1:C:983:ILE:HG13	1:C:1011:MET:HG3	1.94	0.50
1:D:16:ALA:HB2	1:D:488:LEU:HD13	1.93	0.50
1:D:591:LEU:HD13	1:D:611:ALA:HB1	1.92	0.50
1:E:451:ALA:O	1:E:880:SER:OG	2.26	0.50
1:E:888:LEU:HD13	1:E:901:VAL:HG13	1.93	0.50
1:A:801:PHE:CD1	1:A:804:PHE:HE2	2.30	0.49
1:B:108:GLN:OE1	1:C:112:GLN:HB3	2.12	0.49
1:B:801:PHE:CD1	1:B:804:PHE:HE2	2.30	0.49
1:C:34:GLN:HG3	1:C:333:VAL:HA	1.93	0.49
1:C:138:MET:HE1	1:C:325:TYR:HD2	1.77	0.49
1:C:343:THR:HG21	1:C:989:LEU:HD23	1.94	0.49
1:C:678:THR:O	1:C:830:GLN:HG2	2.12	0.49
1:C:897:ILE:O	1:C:901:VAL:HG12	2.13	0.49
1:E:211:ASN:OD1	1:E:240:LEU:N	2.41	0.49
1:E:837:THR:HG22	1:E:841:MET:SD	2.52	0.49
1:A:53:ASP:OD1	1:A:56:THR:OG1	2.16	0.49
1:A:415:ASN:HD22	1:A:434:SER:HB2	1.77	0.49
1:A:650:ARG:O	1:A:653:ARG:HB3	2.12	0.49
1:C:386:PHE:CD1	1:C:472:ILE:HD11	2.47	0.49
1:E:575:MET:HG3	1:E:664:PHE:HB2	1.93	0.49
1:F:23:GLY:HA3	1:F:377:LEU:HB3	1.95	0.49
1:A:220:GLY:HA3	1:A:230:LEU:O	2.13	0.49
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.47	0.49
1:B:244:GLU:HG2	1:B:248:LYS:HE3	1.94	0.49
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.94	0.49
1:B:520:PHE:O	1:B:524:THR:HG22	2.11	0.49
1:C:139:VAL:HB	1:C:327:TYR:HB3	1.93	0.49
1:C:668:LEU:H	1:C:668:LEU:CD2	2.23	0.49
1:C:940:LYS:HZ2	1:C:978:THR:HG21	1.77	0.49
1:D:31:PRO:HB2	1:D:389:SER:HB3	1.94	0.49
1:D:322:LYS:HG2	1:D:323:ILE:O	2.13	0.49
1:D:634:TRP:CD1	1:D:634:TRP:N	2.81	0.49
1:D:832:ALA:HB3	1:D:835:LYS:HD3	1.92	0.49
1:F:527:TYR:OH	1:F:968:VAL:HG13	2.13	0.49
1:A:568:ASP:O	1:A:634:TRP:HZ3	1.96	0.49
1:C:20:MET:HG2	1:C:374:VAL:HA	1.94	0.49
1:C:228:GLN:HE21	1:C:230:LEU:H	1.59	0.49
1:E:636:ASP:O	1:E:638:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:GLN:OE1	1:F:620:ARG:NH2	2.26	0.49
1:F:623:ASN:N	1:F:623:ASN:OD1	2.40	0.49
1:A:685:ILE:HD11	1:A:819:TYR:CD2	2.48	0.49
1:A:893:GLU:OE2	1:C:8:ARG:HB3	2.11	0.49
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.78	0.49
1:C:352:PHE:HZ	1:C:362:PHE:CE1	2.30	0.49
1:E:530:SER:O	1:E:534:ILE:HG23	2.12	0.49
1:E:790:TYR:HE1	1:E:800:PRO:HB3	1.77	0.49
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.94	0.49
1:A:190:PRO:HB2	1:A:788:ASP:O	2.13	0.49
1:A:605:ASN:ND2	1:A:647:ILE:HD11	2.25	0.49
1:A:795:ASP:OD2	1:A:796:GLY:N	2.44	0.49
1:B:327:TYR:HB2	1:B:628:PHE:CE2	2.48	0.49
1:C:584:GLN:N	1:C:622:GLN:HB3	2.28	0.49
1:C:800:PRO:HG2	1:C:803:ALA:HB2	1.93	0.49
1:C:904:VAL:HG21	1:C:942:ALA:HB2	1.95	0.49
1:C:1038:GLU:CA	1:C:1039:ASP:HB2	2.43	0.49
1:D:344:LEU:HD22	1:D:402:ILE:CD1	2.41	0.49
1:D:699:ARG:O	1:D:703:LEU:HG	2.13	0.49
1:D:713:LEU:HD21	1:D:843:LEU:CD1	2.40	0.49
1:E:190:PRO:HG3	1:E:779:TYR:HB3	1.94	0.49
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.94	0.49
1:A:668:LEU:HD23	1:A:668:LEU:H	1.76	0.49
1:B:946:VAL:HG13	1:B:1026:PHE:CE1	2.47	0.49
1:D:1030:ARG:HA	1:D:1030:ARG:NH1	2.27	0.49
1:F:3:ASN:ND2	1:F:435:MET:HG3	2.18	0.49
1:A:860:THR:HG21	2:A:1101:ERY:H281	1.95	0.49
1:D:678:THR:HA	1:D:837:THR:OG1	2.12	0.49
1:D:982:PHE:HD2	1:D:1011:MET:HG3	1.78	0.49
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.94	0.49
1:A:1038:GLU:HB3	1:A:1039:ASP:C	2.33	0.49
3:B:1101:LMT:H6E	3:B:1101:LMT:O5B	2.13	0.49
1:C:230:LEU:HG	1:C:231:ASN:N	2.28	0.49
1:C:860:THR:HA	1:C:864:TYR:HB2	1.95	0.49
1:D:309:GLU:HA	1:D:312:LYS:HD2	1.95	0.49
1:E:102:ILE:O	1:E:106:GLN:HG3	2.11	0.49
1:E:182:TYR:HB2	1:E:769:LYS:NZ	2.27	0.49
1:A:182:TYR:HB2	1:A:769:LYS:NZ	2.27	0.49
1:D:132:SER:OG	1:D:133:SER:N	2.46	0.49
1:D:141:GLY:HA3	1:D:324:VAL:HG12	1.95	0.49
1:E:327:TYR:HB2	1:E:628:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:375:VAL:HB	1:E:405:LEU:HD13	1.95	0.49
1:E:973:ARG:O	1:E:977:MET:HG3	2.13	0.49
1:A:424:GLY:CA	1:A:502:LYS:HB3	2.37	0.48
1:A:444:GLY:O	1:A:448:VAL:HG23	2.13	0.48
1:A:914:LEU:O	1:A:918:PHE:HB2	2.13	0.48
1:A:945:ILE:HG13	1:A:971:ARG:NH2	2.24	0.48
1:B:485:ALA:HA	1:B:489:THR:HG23	1.95	0.48
1:B:485:ALA:O	1:B:490:PRO:HD3	2.13	0.48
1:D:216:ALA:HB1	1:D:234:ILE:HG22	1.95	0.48
1:D:279:ALA:HB3	1:D:286:ALA:O	2.13	0.48
1:D:568:ASP:O	1:D:634:TRP:HZ3	1.96	0.48
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.95	0.48
1:E:142:VAL:HG13	1:E:323:ILE:HD12	1.95	0.48
1:E:584:GLN:N	1:E:622:GLN:HB3	2.28	0.48
1:F:510:LYS:HG2	1:F:511:GLY:N	2.28	0.48
1:F:563:PHE:HE2	1:F:564:LEU:HD22	1.78	0.48
1:A:261:LEU:N	1:A:264:ASP:OD2	2.44	0.48
1:A:426:PRO:O	1:A:429:GLU:HG2	2.13	0.48
1:B:573:MET:HE3	1:B:628:PHE:HB2	1.95	0.48
1:C:55:LYS:HD2	1:C:55:LYS:O	2.13	0.48
1:C:545:TYR:OH	1:C:903:LEU:O	2.19	0.48
1:C:841:MET:HG2	1:C:859:TRP:CH2	2.48	0.48
1:C:940:LYS:HE2	1:C:941:ASN:OD1	2.13	0.48
1:E:132:SER:O	1:E:132:SER:OG	2.24	0.48
1:E:175:VAL:HG23	1:F:70:ASN:ND2	2.28	0.48
1:E:218:GLN:HG3	1:E:221:GLY:HA2	1.95	0.48
1:A:56:THR:O	1:A:60:THR:HG22	2.13	0.48
1:A:534:ILE:HG23	3:A:1102:LMT:H1'	1.95	0.48
1:A:905:VAL:HG13	1:A:935:ILE:HD13	1.95	0.48
1:C:382:VAL:HG11	1:C:476:SER:HB3	1.95	0.48
1:E:587:THR:OG1	1:E:622:GLN:O	2.26	0.48
1:F:944:LEU:HD12	1:F:975:ILE:HG12	1.96	0.48
1:B:80:SER:CB	1:B:90:ILE:HG12	2.44	0.48
1:B:538:THR:O	1:B:541:TYR:HB2	2.13	0.48
1:B:774:MET:HG2	1:B:775:SER:N	2.27	0.48
1:B:897:ILE:N	1:B:898:PRO:HD2	2.29	0.48
1:C:34:GLN:HE21	1:C:333:VAL:CG2	2.21	0.48
1:C:414:GLU:HG2	1:C:973:ARG:NH1	2.28	0.48
1:C:636:ASP:O	1:C:638:PRO:HD3	2.12	0.48
1:C:947:GLU:HG3	1:C:948:PHE:N	2.27	0.48
1:D:146:ASP:HB2	1:D:148:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:ASN:N	1:D:605:ASN:OD1	2.46	0.48
1:E:30:LEU:HD12	1:E:31:PRO:HD2	1.95	0.48
1:F:246:PHE:O	1:F:262:LEU:HD23	2.14	0.48
1:F:669:PRO:HB2	1:F:862:MET:SD	2.54	0.48
1:F:979:SER:CB	1:F:1015:THR:HG21	2.43	0.48
1:A:576:VAL:HG21	1:A:591:LEU:CD2	2.44	0.48
1:A:712:MET:O	1:A:832:ALA:N	2.45	0.48
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.47	0.48
1:A:982:PHE:O	1:A:985:GLY:N	2.46	0.48
1:B:404:LEU:HD21	1:B:449:LEU:HD22	1.96	0.48
1:C:694:LYS:HA	1:C:697:GLN:OE1	2.13	0.48
1:D:351:VAL:O	1:D:355:MET:HB2	2.13	0.48
1:D:602:GLU:HG3	1:D:605:ASN:ND2	2.28	0.48
1:E:24:GLY:O	1:E:28:LEU:HB2	2.13	0.48
1:E:744:ASN:O	1:E:748:THR:HG23	2.13	0.48
1:E:846:GLN:O	1:E:849:SER:OG	2.22	0.48
1:F:835:LYS:HG2	1:F:836:SER:N	2.28	0.48
1:A:5:PHE:HE2	1:A:11:PHE:CD1	2.31	0.48
1:B:562:SER:HB3	1:B:924:ASP:HB3	1.96	0.48
1:C:201:VAL:HG23	1:C:749:THR:CG2	2.44	0.48
1:C:940:LYS:O	1:C:943:ILE:HB	2.14	0.48
1:D:750:LEU:HD12	1:D:754:TRP:CD1	2.48	0.48
1:D:913:LEU:HD23	1:D:927:PHE:HZ	1.78	0.48
3:D:1102:LMT:H5B	3:D:1102:LMT:H6E	1.94	0.48
1:E:732:ASP:OD1	1:E:735:LYS:HG3	2.13	0.48
1:E:909:VAL:HG12	1:E:913:LEU:HG	1.95	0.48
1:E:1037:ASN:HB2	1:E:1038:GLU:O	2.14	0.48
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.94	0.48
1:A:80:SER:CB	1:A:90:ILE:HG12	2.42	0.48
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.95	0.48
1:A:172:VAL:CG2	1:A:306:ILE:HD11	2.43	0.48
1:B:1020:PHE:O	1:B:1023:PRO:HG2	2.13	0.48
1:C:398:MET:HG2	1:C:473:THR:HG21	1.96	0.48
1:D:762:PHE:CE1	1:D:764:ASP:HB2	2.49	0.48
1:D:894:SER:HB2	1:D:897:ILE:HD12	1.94	0.48
1:A:891:LEU:HD23	1:A:892:TYR:CE1	2.48	0.48
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.95	0.48
1:A:1040:ILE:HG13	1:A:1041:GLU:H	1.79	0.48
1:C:214:VAL:HB	1:C:236:ALA:HB3	1.95	0.48
1:E:186:ILE:HB	1:E:773:VAL:HG23	1.96	0.48
1:A:382:VAL:HG11	1:A:476:SER:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1101:ERY:H71	2:A:1101:ERY:H10	1.62	0.48
1:B:459:PHE:O	1:B:464:GLY:HA3	2.14	0.48
1:C:525:HIS:HA	1:C:528:THR:HG22	1.96	0.48
1:C:531:VAL:O	1:C:534:ILE:HG13	2.13	0.48
1:C:817:GLU:OE2	1:C:825:MET:HA	2.14	0.48
1:D:726:GLN:O	1:D:810:GLU:HG2	2.14	0.48
1:D:781:MET:CE	1:F:225:VAL:H	2.26	0.48
1:D:953:MET:HE1	1:D:960:LEU:HD12	1.95	0.48
1:E:39:ALA:HA	1:E:462:SER:OG	2.14	0.48
1:F:761:ASP:OD1	1:F:770:LYS:HA	2.14	0.48
1:A:683:GLU:HG2	1:A:819:TYR:CG	2.49	0.48
1:C:44:THR:OG1	1:C:91:THR:OG1	2.24	0.48
1:C:156:ASP:OD2	1:C:182:TYR:HB2	2.14	0.48
1:C:358:PHE:O	1:C:359:LEU:HD23	2.14	0.48
1:C:391:ASN:OD1	1:C:393:LEU:HB2	2.14	0.48
1:D:352:PHE:CD2	1:D:353:LEU:HD23	2.49	0.48
1:D:571:VAL:N	1:D:631:LEU:HD12	2.29	0.48
1:D:680:PHE:HD1	1:D:859:TRP:HZ3	1.61	0.48
1:D:801:PHE:HA	1:D:804:PHE:CE2	2.49	0.48
1:E:525:HIS:HA	1:E:528:THR:HG22	1.96	0.48
1:E:1016:VAL:O	1:E:1016:VAL:HG12	2.14	0.48
1:A:7:ASP:O	1:A:8:ARG:HG3	2.13	0.47
1:A:376:LEU:O	1:A:379:THR:N	2.47	0.47
1:A:559:LEU:HD22	1:A:923:ASN:H	1.79	0.47
1:A:702:LEU:HD22	1:A:827:ILE:HD13	1.96	0.47
1:A:832:ALA:CB	1:A:835:LYS:HD3	2.38	0.47
1:C:682:PHE:CZ	1:C:857:TYR:HB2	2.49	0.47
1:D:277:ILE:HA	1:D:613:ASN:O	2.13	0.47
1:E:169:THR:HG21	1:E:306:ILE:HG13	1.95	0.47
1:E:289:LEU:HA	1:E:289:LEU:HD23	1.66	0.47
1:E:507:GLU:HG2	1:E:518:ARG:HA	1.96	0.47
1:F:492:LEU:O	1:F:496:MET:HG2	2.14	0.47
1:F:911:GLY:HA2	1:F:1013:THR:HG21	1.96	0.47
1:A:902:MET:O	1:A:905:VAL:HG23	2.14	0.47
1:B:188:MET:HA	1:B:266:ALA:CB	2.44	0.47
1:C:527:TYR:OH	1:C:968:VAL:HG13	2.14	0.47
1:D:26:ALA:O	1:D:30:LEU:HB2	2.14	0.47
1:D:58:GLN:NE2	1:D:818:ARG:NH1	2.61	0.47
1:D:423:GLU:O	1:D:502:LYS:HB3	2.14	0.47
1:D:1030:ARG:HA	1:D:1030:ARG:HH11	1.79	0.47
1:E:196:PHE:HD2	1:E:260:VAL:HG22	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:462:SER:H	1:E:865:GLN:HE21	1.62	0.47
1:E:534:ILE:HD11	1:E:1024:VAL:HG22	1.95	0.47
1:F:42:ALA:HB2	1:F:93:THR:HG23	1.95	0.47
1:F:74:ASN:HB2	1:F:98:THR:HG21	1.96	0.47
1:F:146:ASP:O	1:F:148:THR:N	2.47	0.47
1:F:158:VAL:HG22	1:F:162:MET:HE3	1.96	0.47
1:F:614:GLY:O	1:F:620:ARG:HA	2.14	0.47
1:F:775:SER:OG	1:F:780:ARG:HG2	2.14	0.47
1:A:63:GLN:OE1	1:C:768:VAL:HG12	2.14	0.47
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.95	0.47
1:C:75:LEU:HD11	1:C:92:LEU:HB3	1.96	0.47
1:C:348:ILE:HG13	1:C:402:ILE:CD1	2.42	0.47
1:C:586:ARG:HA	1:C:589:LYS:HD2	1.96	0.47
1:D:508:GLY:H	1:D:518:ARG:HG3	1.78	0.47
1:A:648:THR:HB	1:A:665:ALA:O	2.13	0.47
1:A:909:VAL:HA	1:A:931:LEU:HD21	1.96	0.47
1:A:1007:VAL:HG12	1:A:1008:MET:N	2.28	0.47
1:B:904:VAL:HG13	1:B:907:LEU:HD22	1.96	0.47
1:C:382:VAL:HG11	1:C:476:SER:CB	2.44	0.47
1:C:449:LEU:HD21	1:C:937:LEU:HD23	1.96	0.47
1:C:877:TYR:O	1:C:881:LEU:HG	2.14	0.47
1:D:198:LEU:HD11	1:D:252:LYS:HB2	1.97	0.47
1:E:255:GLN:OE1	1:E:256:ASP:N	2.47	0.47
1:E:659:LYS:HE3	1:E:659:LYS:HA	1.97	0.47
1:A:172:VAL:HG22	1:A:306:ILE:HD11	1.94	0.47
1:A:210:GLN:HE22	1:A:250:LEU:N	2.13	0.47
1:B:32:VAL:HG12	1:B:390:ILE:HD12	1.96	0.47
1:B:270:LEU:HA	1:B:270:LEU:HD12	1.63	0.47
1:B:317:PHE:CE2	1:B:323:ILE:HD13	2.50	0.47
1:B:344:LEU:HD13	1:B:376:LEU:HD13	1.96	0.47
1:B:583:THR:HB	1:B:586:ARG:H	1.79	0.47
1:C:244:GLU:CG	1:C:248:LYS:HE3	2.45	0.47
1:C:637:ARG:HD2	1:C:642:ASN:O	2.13	0.47
1:C:682:PHE:HE2	1:C:702:LEU:HD11	1.80	0.47
1:D:203:VAL:O	1:D:206:ALA:HB3	2.15	0.47
1:D:890:ALA:HB1	1:F:11:PHE:CD1	2.50	0.47
1:E:2:PRO:O	1:E:6:ILE:HD12	2.14	0.47
1:F:73:ASP:OD2	1:F:106:GLN:NE2	2.33	0.47
1:A:379:THR:HA	1:A:382:VAL:HG23	1.96	0.47
1:B:9:PRO:HB3	1:B:495:THR:HG21	1.96	0.47
1:B:442:LEU:O	1:B:445:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ALA:HA	1:B:468:ARG:NH1	2.30	0.47
1:D:535:LEU:CD2	1:D:1027:VAL:HG21	2.45	0.47
1:D:559:LEU:HD23	1:D:560:PRO:CD	2.45	0.47
1:D:1040:ILE:HG22	1:D:1041:GLU:N	2.29	0.47
1:F:227:GLY:O	1:F:229:GLN:HG3	2.14	0.47
1:F:996:GLY:O	1:F:999:ALA:N	2.48	0.47
1:B:534:ILE:HG22	3:B:1101:LMT:H5'	1.97	0.47
1:B:836:SER:OG	1:B:839:GLU:HG3	2.14	0.47
1:B:907:LEU:HG	1:B:1017:LEU:HD23	1.96	0.47
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.97	0.47
1:D:58:GLN:HA	1:D:62:THR:HB	1.97	0.47
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.49	0.47
1:D:417:GLU:OE1	1:D:497:LEU:HD21	2.14	0.47
1:D:562:SER:HB2	1:D:924:ASP:HB3	1.97	0.47
1:D:708:LYS:C	1:D:710:PRO:HD3	2.35	0.47
1:D:754:TRP:CZ3	1:F:219:LEU:HD23	2.49	0.47
1:D:888:LEU:HB2	1:D:898:PRO:HB3	1.97	0.47
1:D:1031:ARG:O	1:D:1032:ARG:HG3	2.14	0.47
1:D:1035:ARG:NH2	1:D:1036:LYS:HG3	2.30	0.47
1:E:652:THR:HG23	1:E:665:ALA:CB	2.42	0.47
1:E:904:VAL:HG21	1:E:942:ALA:CB	2.45	0.47
1:F:900:SER:HB3	1:F:1029:VAL:HG21	1.96	0.47
1:A:367:ILE:HG12	1:A:492:LEU:HB3	1.96	0.47
1:A:690:LEU:HD11	1:A:853:THR:O	2.15	0.47
1:A:751:GLY:O	1:A:753:ALA:N	2.48	0.47
1:B:222:THR:HA	1:B:224:PRO:HD3	1.96	0.47
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.96	0.47
1:D:30:LEU:HD12	1:D:31:PRO:HD2	1.96	0.47
1:D:944:LEU:O	1:D:947:GLU:HB3	2.14	0.47
1:E:187:TRP:NE1	1:E:269:GLU:OE2	2.48	0.47
1:F:220:GLY:HA3	1:F:230:LEU:O	2.15	0.47
1:F:672:VAL:C	1:F:674:LEU:H	2.18	0.47
1:A:375:VAL:HB	1:A:405:LEU:HD13	1.96	0.47
1:A:420:MET:HB2	1:A:500:ILE:HD12	1.96	0.47
1:A:971:ARG:C	1:A:974:PRO:HD2	2.35	0.47
1:C:63:GLN:O	1:C:67:GLN:HG3	2.15	0.47
1:C:801:PHE:CD1	1:C:804:PHE:HE2	2.31	0.47
1:C:1016:VAL:HG13	3:C:1101:LMT:H112	1.96	0.47
1:D:125:GLN:OE1	1:D:770:LYS:HE3	2.15	0.47
1:E:213:GLN:HE21	1:E:239:ARG:HG3	1.80	0.47
1:E:764:ASP:OD1	1:E:765:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:ARG:HB3	1:F:187:TRP:HE1	1.79	0.47
1:F:311:ALA:O	1:F:314:GLU:HB2	2.14	0.47
1:F:514:GLY:HA2	1:F:517:ASN:OD1	2.14	0.47
1:F:696:THR:HG23	1:F:699:ARG:HH12	1.80	0.47
1:A:127:VAL:HB	1:B:113:LEU:HD22	1.96	0.47
1:A:602:GLU:OE2	1:A:650:ARG:NH1	2.48	0.47
1:A:937:LEU:HD23	1:A:937:LEU:HA	1.74	0.47
1:A:1039:ASP:H	1:A:1040:ILE:HD13	1.80	0.47
1:B:189:ASN:OD1	1:B:190:PRO:HD2	2.14	0.47
1:B:783:PRO:O	1:B:786:ILE:HG12	2.15	0.47
1:B:961:ILE:H	1:B:961:ILE:HG13	1.52	0.47
1:C:214:VAL:CG2	1:C:237:GLN:HB2	2.45	0.47
1:C:371:ALA:O	1:C:375:VAL:HG23	2.14	0.47
1:C:600:THR:O	1:C:603:LYS:HG3	2.15	0.47
1:C:922:THR:O	1:C:924:ASP:N	2.48	0.47
1:C:953:MET:HE1	1:C:960:LEU:HD12	1.97	0.47
1:D:388:PHE:CE2	1:D:472:ILE:HD12	2.50	0.47
1:D:549:VAL:HG22	1:D:906:PRO:HG2	1.97	0.47
1:E:416:VAL:HG21	1:E:493:CYS:SG	2.55	0.47
1:E:508:GLY:H	1:E:518:ARG:HE	1.63	0.47
1:E:736:ALA:HB1	1:E:741:VAL:HG23	1.96	0.47
1:A:525:HIS:HA	1:A:528:THR:HG22	1.96	0.46
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.51	0.46
1:B:244:GLU:O	1:B:247:GLY:N	2.48	0.46
1:C:196:PHE:N	1:C:196:PHE:CD2	2.83	0.46
1:C:455:PRO:HG3	1:C:883:VAL:HG21	1.97	0.46
1:C:559:LEU:HD23	1:C:560:PRO:CD	2.46	0.46
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.79	0.46
1:E:32:VAL:HA	1:E:390:ILE:O	2.15	0.46
1:E:615:PHE:HD2	1:E:620:ARG:HG2	1.81	0.46
1:E:775:SER:HB3	1:E:780:ARG:HD3	1.98	0.46
1:E:960:LEU:O	1:E:964:THR:HG23	2.15	0.46
1:F:356:TYR:CA	1:F:365:THR:HG21	2.39	0.46
1:A:574:THR:CG2	1:A:627:ALA:HB3	2.46	0.46
1:B:259:ARG:O	1:B:259:ARG:HG2	2.13	0.46
1:B:554:TYR:CZ	1:B:558:ARG:HG3	2.50	0.46
1:C:124:GLN:HG3	1:C:125:GLN:N	2.27	0.46
1:D:83:ASP:HB2	1:D:87:THR:O	2.15	0.46
1:D:165:ALA:HB3	1:D:313:MET:HE1	1.96	0.46
1:D:189:ASN:HB3	1:D:192:GLU:HB2	1.96	0.46
1:D:350:LEU:HD23	1:D:350:LEU:HA	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:676:THR:OG1	1:D:679:GLY:HA3	2.15	0.46
1:D:682:PHE:CD2	1:D:683:GLU:N	2.83	0.46
1:E:795:ASP:OD2	1:E:797:GLN:N	2.47	0.46
1:E:818:ARG:HH12	1:E:823:PRO:HG3	1.80	0.46
1:F:391:ASN:OD1	1:F:393:LEU:HB2	2.15	0.46
1:F:671:ILE:CG2	1:F:674:LEU:HB2	2.45	0.46
1:F:743:ILE:H	1:F:743:ILE:HD12	1.81	0.46
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.60	0.46
1:A:34:GLN:HB2	1:A:333:VAL:CG2	2.45	0.46
1:A:244:GLU:O	1:A:247:GLY:N	2.48	0.46
1:A:531:VAL:HG12	1:A:535:LEU:HD12	1.96	0.46
1:A:929:VAL:O	1:A:932:LEU:HB2	2.15	0.46
1:B:184:MET:HB3	1:B:771:VAL:HG13	1.97	0.46
1:B:242:SER:HB2	1:B:245:GLU:HG3	1.98	0.46
1:B:525:HIS:HA	1:B:528:THR:HG22	1.96	0.46
1:B:801:PHE:HA	1:B:804:PHE:CE2	2.51	0.46
1:C:971:ARG:C	1:C:974:PRO:HD2	2.36	0.46
1:D:198:LEU:HD23	1:D:792:ARG:HH21	1.81	0.46
1:E:623:ASN:O	1:E:623:ASN:ND2	2.48	0.46
1:E:726:GLN:NE2	1:E:812:GLY:HA3	2.30	0.46
1:F:945:ILE:HG13	1:F:971:ARG:HH22	1.80	0.46
1:B:61:VAL:HG22	1:B:118:LEU:HD22	1.96	0.46
1:C:39:ALA:CB	1:C:673:GLU:HG2	2.46	0.46
1:C:216:ALA:HB1	1:C:234:ILE:HG22	1.97	0.46
1:C:568:ASP:O	1:C:634:TRP:HZ3	1.99	0.46
1:D:520:PHE:O	1:D:524:THR:HG22	2.16	0.46
1:E:177:LEU:HG	1:E:289:LEU:HD21	1.97	0.46
1:E:195:LYS:NZ	1:E:196:PHE:HE1	2.13	0.46
1:E:367:ILE:HB	1:E:368:PRO:HD3	1.98	0.46
1:E:892:TYR:O	1:E:893:GLU:HB2	2.15	0.46
1:F:449:LEU:HD23	1:F:449:LEU:HA	1.73	0.46
1:F:946:VAL:HG13	1:F:1026:PHE:CE1	2.51	0.46
1:A:222:THR:HG23	1:B:275:TYR:HB2	1.97	0.46
1:A:382:VAL:O	1:A:385:ALA:HB3	2.15	0.46
1:A:583:THR:HG21	1:C:228:GLN:HG3	1.97	0.46
1:B:185:ARG:HB3	1:B:187:TRP:NE1	2.31	0.46
1:B:715:SER:O	1:B:717:ARG:HG3	2.15	0.46
1:C:45:ILE:HD12	1:C:90:ILE:HB	1.96	0.46
1:C:101:ASP:O	1:C:105:VAL:HG23	2.15	0.46
1:C:332:PHE:CD1	1:C:634:TRP:CH2	3.04	0.46
1:C:966:ASP:O	1:C:970:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:781:MET:HB3	1:F:228:GLN:NE2	2.30	0.46
1:E:559:LEU:HD12	1:E:923:ASN:HB2	1.98	0.46
1:E:904:VAL:HG21	1:E:942:ALA:HB2	1.97	0.46
1:F:752:ALA:O	1:F:774:MET:HA	2.16	0.46
1:F:1038:GLU:HB2	1:F:1039:ASP:OD1	2.14	0.46
1:A:586:ARG:O	1:A:590:VAL:HG23	2.16	0.46
1:A:641:GLU:HB2	1:A:650:ARG:NH2	2.31	0.46
1:B:535:LEU:HD22	1:B:1027:VAL:HG11	1.98	0.46
1:C:425:LEU:HD13	1:C:429:GLU:HG3	1.97	0.46
1:C:577:GLN:HG3	1:C:624:THR:HG22	1.98	0.46
1:C:671:ILE:HB	1:C:862:MET:SD	2.55	0.46
1:D:457:ALA:HB1	1:D:468:ARG:HG3	1.97	0.46
1:D:538:THR:HG21	1:D:1028:VAL:HG21	1.97	0.46
1:E:104:GLN:NE2	1:F:109:ASN:HD22	2.14	0.46
1:E:149:MET:HB2	1:E:153:ASP:CB	2.45	0.46
1:E:203:VAL:O	1:E:207:ILE:HG13	2.16	0.46
1:E:242:SER:OG	1:E:245:GLU:HG3	2.16	0.46
1:E:415:ASN:HB3	1:E:434:SER:HB2	1.97	0.46
1:F:351:VAL:HG11	1:F:406:VAL:HG11	1.96	0.46
1:F:1025:PHE:O	1:F:1029:VAL:HG23	2.15	0.46
1:A:16:ALA:HB2	1:A:488:LEU:HD13	1.98	0.46
1:A:187:TRP:HE3	1:A:775:SER:O	1.97	0.46
1:A:768:VAL:HG12	1:B:63:GLN:OE1	2.15	0.46
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.96	0.46
1:C:354:VAL:HG23	1:C:984:LEU:HD12	1.98	0.46
1:C:456:MET:HA	1:C:459:PHE:CD1	2.51	0.46
1:C:743:ILE:HA	1:C:746:ILE:HG23	1.97	0.46
1:F:352:PHE:HA	1:F:355:MET:CE	2.41	0.46
1:F:673:GLU:H	1:F:673:GLU:CD	2.19	0.46
1:C:898:PRO:O	1:C:901:VAL:N	2.49	0.46
1:E:57:VAL:HB	1:E:88:VAL:CG2	2.46	0.46
1:E:196:PHE:CD2	1:E:260:VAL:HG22	2.51	0.46
1:F:344:LEU:O	1:F:348:ILE:HG13	2.15	0.46
1:A:228:GLN:NE2	1:A:230:LEU:O	2.47	0.46
1:A:623:ASN:OD1	1:A:623:ASN:N	2.42	0.46
1:A:669:PRO:HG2	1:A:676:THR:HG22	1.97	0.46
1:B:61:VAL:CG2	1:B:122:VAL:HG21	2.45	0.46
1:B:888:LEU:HA	1:B:888:LEU:HD23	1.53	0.46
1:C:340:VAL:HG11	1:C:395:MET:CB	2.33	0.46
1:D:76:MET:HB2	1:D:93:THR:O	2.16	0.46
1:D:723:ASP:HA	1:D:812:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.98	0.46
1:F:183:ALA:O	1:F:270:LEU:HD12	2.16	0.46
1:F:418:ARG:O	1:F:422:GLU:HB2	2.16	0.46
1:F:483:LEU:HA	1:F:483:LEU:HD23	1.77	0.46
1:F:774:MET:HG2	1:F:775:SER:N	2.31	0.46
1:A:427:PRO:CD	1:A:499:PRO:HB3	2.39	0.46
1:B:578:LEU:HD22	1:B:661:ALA:CB	2.45	0.46
1:B:774:MET:HG2	1:B:775:SER:H	1.81	0.46
1:C:555:LEU:HD11	1:C:914:LEU:HD12	1.98	0.46
1:C:973:ARG:HG2	1:C:977:MET:CE	2.46	0.46
1:E:142:VAL:HG12	1:E:321:LEU:HD11	1.98	0.46
1:E:447:MET:HB3	1:E:887:CYS:SG	2.56	0.46
1:E:1042:HIS:HB3	1:E:1043:SER:HB3	1.96	0.46
1:F:74:ASN:O	1:F:94:PHE:HD2	1.98	0.46
1:F:186:ILE:HG12	1:F:268:ILE:HG12	1.97	0.46
1:F:506:GLY:C	1:F:508:GLY:H	2.19	0.46
1:F:953:MET:HE2	1:F:963:ALA:HB3	1.97	0.46
1:A:513:PHE:O	1:A:516:PHE:HB3	2.16	0.45
1:A:987:MET:HA	1:A:1008:MET:HE3	1.98	0.45
1:B:355:MET:HG2	1:B:365:THR:HA	1.97	0.45
1:B:398:MET:HE3	1:B:398:MET:HB3	1.82	0.45
1:C:188:MET:HA	1:C:266:ALA:CB	2.47	0.45
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.46	0.45
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.51	0.45
1:D:605:ASN:HD22	1:D:647:ILE:HD11	1.81	0.45
1:D:754:TRP:CH2	1:D:780:ARG:HA	2.51	0.45
1:E:712:MET:SD	1:E:835:LYS:HG2	2.56	0.45
1:F:75:LEU:HD11	1:F:92:LEU:HD12	1.97	0.45
1:F:420:MET:HB3	1:F:500:ILE:HB	1.98	0.45
1:A:1039:ASP:N	1:A:1040:ILE:HD13	2.32	0.45
1:B:897:ILE:HD13	1:B:950:LYS:HE3	1.98	0.45
1:D:865:GLN:HE21	1:D:865:GLN:HA	1.82	0.45
1:E:65:ILE:O	1:E:69:MET:HG2	2.17	0.45
1:E:455:PRO:O	1:E:876:LEU:HD13	2.15	0.45
1:E:713:LEU:HD11	1:E:843:LEU:HD12	1.98	0.45
1:E:888:LEU:HD13	1:E:901:VAL:CG1	2.45	0.45
1:F:668:LEU:H	1:F:668:LEU:HG	1.22	0.45
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.16	0.45
1:A:577:GLN:O	1:A:661:ALA:HB1	2.16	0.45
1:A:800:PRO:O	1:A:803:ALA:HB3	2.15	0.45
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:ASP:OD1	1:B:859:TRP:N	2.48	0.45
1:D:576:VAL:HG21	1:D:591:LEU:HD23	1.98	0.45
1:D:674:LEU:HD22	1:D:675:GLY:H	1.80	0.45
1:D:953:MET:HE1	1:D:960:LEU:HA	1.98	0.45
1:E:637:ARG:HB3	1:E:642:ASN:HB3	1.99	0.45
1:E:987:MET:CA	1:E:1008:MET:HE3	2.46	0.45
1:F:24:GLY:O	1:F:27:ILE:HG13	2.16	0.45
1:F:58:GLN:HG2	1:F:63:GLN:NE2	2.30	0.45
1:F:164:ASP:HB3	1:F:168:ARG:HH22	1.81	0.45
1:F:858:ASP:OD2	1:F:859:TRP:N	2.40	0.45
1:A:446:ALA:CB	1:A:482:VAL:HG21	2.45	0.45
1:B:453:PHE:O	1:B:471:SER:OG	2.27	0.45
1:C:429:GLU:O	1:C:433:LYS:HB2	2.16	0.45
1:D:678:THR:HG21	1:D:835:LYS:O	2.17	0.45
1:E:844:MET:HE2	1:E:847:LEU:HB2	1.99	0.45
1:F:680:PHE:CD2	1:F:859:TRP:HZ3	2.34	0.45
1:F:776:GLU:HB2	1:F:779:TYR:CE1	2.52	0.45
1:F:898:PRO:O	1:F:901:VAL:N	2.48	0.45
1:A:74:ASN:O	1:A:94:PHE:HD2	2.00	0.45
1:A:636:ASP:O	1:A:638:PRO:HD3	2.17	0.45
1:A:1039:ASP:CA	1:A:1040:ILE:HB	2.43	0.45
1:B:541:TYR:CD1	1:B:541:TYR:N	2.85	0.45
1:B:564:LEU:HD13	1:B:671:ILE:HD12	1.99	0.45
1:C:354:VAL:HG22	1:C:980:LEU:HD23	1.98	0.45
1:C:379:THR:HG23	1:C:476:SER:OG	2.16	0.45
1:D:159:ALA:HB2	1:D:177:LEU:CD1	2.47	0.45
1:D:522:LYS:O	1:D:525:HIS:HB3	2.17	0.45
1:D:876:LEU:HD23	1:D:876:LEU:HA	1.82	0.45
1:F:644:VAL:O	1:F:648:THR:HG23	2.16	0.45
1:A:80:SER:O	1:A:817:GLU:HA	2.17	0.45
1:A:418:ARG:NH2	1:A:948:PHE:HE2	2.15	0.45
1:A:511:GLY:HA2	1:A:515:TRP:CD1	2.51	0.45
1:B:946:VAL:HG13	1:B:1026:PHE:CD1	2.52	0.45
1:C:53:ASP:O	1:C:56:THR:HB	2.17	0.45
1:C:567:GLU:OE1	1:C:996:GLY:HA2	2.17	0.45
1:D:112:GLN:OE1	1:D:112:GLN:HA	2.16	0.45
1:D:400:LEU:CD2	1:D:929:VAL:HG12	2.47	0.45
1:E:166:ILE:HD11	1:E:310:LEU:CD1	2.46	0.45
1:F:948:PHE:HD2	1:F:970:MET:HE2	1.81	0.45
1:A:705:GLU:HA	1:A:708:LYS:HD3	1.99	0.45
1:A:876:LEU:HD23	1:A:876:LEU:HA	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:LEU:HD23	1:C:555:LEU:HA	1.62	0.45
1:C:730:ASP:OD1	1:C:808:ARG:NE	2.34	0.45
1:D:20:MET:HG2	1:D:374:VAL:HA	1.98	0.45
1:D:658:ILE:HG13	1:D:659:LYS:HZ1	1.80	0.45
1:D:888:LEU:HD22	1:D:901:VAL:HG11	1.99	0.45
1:D:907:LEU:O	1:D:1013:THR:OG1	2.30	0.45
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.42	0.45
1:E:775:SER:OG	1:E:776:GLU:N	2.49	0.45
1:F:165:ALA:HB3	1:F:313:MET:HE1	1.98	0.45
1:F:293:LEU:HD11	1:F:299:ALA:HA	1.97	0.45
1:F:578:LEU:HD22	1:F:661:ALA:CB	2.47	0.45
1:F:638:PRO:HB2	1:F:639:GLY:H	1.64	0.45
1:F:684:LEU:HD23	1:F:825:MET:HB2	1.98	0.45
1:F:841:MET:O	1:F:845:GLU:HG2	2.17	0.45
1:F:971:ARG:HH21	1:F:975:ILE:HD11	1.82	0.45
1:A:541:TYR:N	1:A:541:TYR:CD1	2.82	0.45
1:A:617:PHE:CZ	2:A:1101:ERY:H312	2.52	0.45
1:A:750:LEU:HD12	1:A:754:TRP:CD1	2.52	0.45
1:A:1030:ARG:HA	1:A:1030:ARG:NH1	2.30	0.45
1:B:149:MET:HG3	1:B:154:ILE:HG13	1.98	0.45
1:B:259:ARG:HG3	1:B:261:LEU:HG	1.97	0.45
1:B:407:ASP:OD2	1:B:940:LYS:NZ	2.46	0.45
1:B:584:GLN:HB2	1:B:622:GLN:HG2	1.99	0.45
1:B:634:TRP:CD1	1:B:634:TRP:N	2.72	0.45
1:D:240:LEU:HD12	1:D:246:PHE:CZ	2.52	0.45
1:D:598:TYR:CE2	1:D:629:VAL:HG21	2.52	0.45
1:D:674:LEU:HD22	1:D:862:MET:HB3	1.99	0.45
1:D:695:LEU:HD22	1:D:825:MET:SD	2.57	0.45
2:D:1101:ERY:H5	2:D:1101:ERY:C18	2.44	0.45
1:E:578:LEU:HB2	1:E:623:ASN:O	2.16	0.45
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.99	0.45
1:F:94:PHE:CE1	1:F:103:ALA:HB1	2.51	0.45
1:F:249:ILE:O	1:F:262:LEU:N	2.48	0.45
1:A:344:LEU:HD11	1:A:398:MET:CB	2.47	0.45
1:D:162:MET:O	1:D:164:ASP:N	2.50	0.45
1:D:878:ALA:O	1:D:882:ILE:HG12	2.16	0.45
1:D:925:VAL:O	1:D:928:GLN:N	2.50	0.45
1:D:987:MET:HA	1:D:1008:MET:HE3	1.99	0.45
1:E:189:ASN:OD1	1:E:190:PRO:HD2	2.16	0.45
1:E:1041:GLU:OE1	1:E:1041:GLU:N	2.50	0.45
1:F:32:VAL:HG22	1:F:390:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:MET:HG3	1:F:95:GLU:CD	2.38	0.45
1:F:318:PRO:HG2	1:F:321:LEU:HG	1.98	0.45
1:F:463:THR:HG22	1:F:467:TYR:CZ	2.52	0.45
1:F:561:SER:O	1:F:838:GLY:HA3	2.17	0.45
1:F:937:LEU:HD11	1:F:982:PHE:HE2	1.80	0.45
1:A:354:VAL:HG21	1:A:981:ALA:HA	1.99	0.45
1:A:584:GLN:N	1:A:622:GLN:HB3	2.32	0.45
1:B:58:GLN:HA	1:B:62:THR:HB	1.98	0.45
1:B:310:LEU:HD23	1:B:325:TYR:OH	2.17	0.45
1:C:196:PHE:HD1	1:C:260:VAL:HG13	1.82	0.45
1:C:399:VAL:HG11	1:C:989:LEU:HD21	1.98	0.45
1:C:960:LEU:HB3	1:C:1040:ILE:HG23	1.99	0.45
1:D:470:PHE:HD2	1:D:929:VAL:HG11	1.80	0.45
1:D:1019:ILE:HG13	1:D:1020:PHE:CD1	2.51	0.45
1:D:1040:ILE:HG22	1:D:1041:GLU:H	1.81	0.45
1:E:187:TRP:HE3	1:E:775:SER:O	2.00	0.45
1:E:291:ILE:HG21	1:E:306:ILE:HD11	1.99	0.45
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.99	0.45
1:E:463:THR:OG1	1:E:464:GLY:N	2.50	0.45
1:E:563:PHE:HE1	1:E:866:GLU:OE2	2.00	0.45
1:A:4:PHE:O	1:A:8:ARG:HD2	2.17	0.44
1:A:680:PHE:CE2	1:A:829:GLY:HA3	2.53	0.44
1:B:154:ILE:O	1:B:157:TYR:N	2.49	0.44
1:D:23:GLY:HA3	1:D:377:LEU:O	2.17	0.44
1:D:456:MET:SD	1:D:932:LEU:HD11	2.56	0.44
1:D:886:LEU:HD13	1:F:18:ILE:HG13	1.99	0.44
1:D:948:PHE:O	1:D:952:LEU:HG	2.17	0.44
1:E:1038:GLU:C	1:E:1040:ILE:N	2.71	0.44
1:F:219:LEU:HD13	1:F:230:LEU:HD21	1.98	0.44
1:F:888:LEU:HD13	1:F:901:VAL:HG11	1.98	0.44
1:A:158:VAL:HA	1:A:162:MET:HE3	1.99	0.44
1:A:909:VAL:HG22	1:A:935:ILE:HD11	1.98	0.44
1:B:758:TYR:HE1	1:B:770:LYS:CG	2.30	0.44
1:C:167:SER:HB3	1:C:175:VAL:HG21	1.98	0.44
1:C:240:LEU:HD12	1:C:246:PHE:CD1	2.52	0.44
1:D:270:LEU:HD12	1:D:270:LEU:HA	1.57	0.44
1:D:658:ILE:O	1:D:659:LYS:HD3	2.17	0.44
1:D:922:THR:O	1:D:924:ASP:N	2.50	0.44
1:E:30:LEU:HG	1:E:31:PRO:HD2	1.99	0.44
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.98	0.44
1:E:438:ILE:HG22	1:E:948:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:619:GLY:HA2	1:E:815:ARG:NH1	2.31	0.44
1:E:937:LEU:HD23	1:E:937:LEU:HA	1.69	0.44
1:F:69:MET:SD	1:F:72:ILE:HD11	2.57	0.44
1:F:177:LEU:HD23	1:F:289:LEU:HD23	1.99	0.44
1:F:272:GLY:N	1:F:275:TYR:OH	2.35	0.44
1:F:508:GLY:O	1:F:509:LYS:HB2	2.16	0.44
1:F:683:GLU:HG2	1:F:819:TYR:CG	2.53	0.44
1:A:58:GLN:OE1	1:A:816:LEU:HD13	2.16	0.44
1:A:377:LEU:HA	1:A:377:LEU:HD23	1.77	0.44
1:A:671:ILE:HD12	1:A:674:LEU:O	2.18	0.44
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.32	0.44
1:D:335:ILE:O	1:D:339:GLU:HG2	2.18	0.44
1:E:40:PRO:HD3	1:E:462:SER:OG	2.16	0.44
1:E:412:VAL:HG22	1:E:438:ILE:HD11	1.99	0.44
1:E:1040:ILE:O	1:E:1041:GLU:HB3	2.17	0.44
1:F:81:ASN:HD21	1:F:815:ARG:NH1	2.15	0.44
1:F:302:THR:O	1:F:305:ALA:HB3	2.17	0.44
1:F:1034:SER:HB3	1:F:1035:ARG:HB3	1.99	0.44
1:A:775:SER:HG	1:A:780:ARG:HG2	1.81	0.44
1:B:699:ARG:NH2	1:B:722:GLU:OE1	2.50	0.44
1:B:808:ARG:NH1	1:B:810:GLU:OE2	2.51	0.44
1:C:24:GLY:O	1:C:27:ILE:HG13	2.17	0.44
1:C:546:LEU:HD23	1:C:546:LEU:HA	1.83	0.44
1:D:572:PHE:CE1	1:D:648:THR:HG22	2.52	0.44
1:D:885:PHE:CE1	1:D:898:PRO:HB2	2.53	0.44
1:D:900:SER:HA	1:D:1025:PHE:HB3	2.00	0.44
1:D:904:VAL:CG1	1:D:938:SER:HB3	2.48	0.44
1:E:146:ASP:OD1	1:E:148:THR:OG1	2.35	0.44
1:E:525:HIS:O	1:E:526:HIS:C	2.55	0.44
1:E:950:LYS:HZ1	1:E:1030:ARG:NE	2.15	0.44
1:F:378:GLY:O	1:F:382:VAL:HG23	2.17	0.44
1:F:514:GLY:C	1:F:516:PHE:H	2.21	0.44
1:A:185:ARG:HB3	1:A:187:TRP:NE1	2.32	0.44
1:A:391:ASN:O	1:A:395:MET:HG2	2.18	0.44
1:B:758:TYR:HE1	1:B:770:LYS:HG2	1.82	0.44
1:B:800:PRO:HG2	1:B:803:ALA:HB2	2.00	0.44
1:C:182:TYR:O	1:C:769:LYS:HD3	2.18	0.44
1:C:380:PHE:HA	1:C:383:LEU:HD12	1.99	0.44
1:C:1016:VAL:HG12	1:C:1016:VAL:O	2.18	0.44
1:D:154:ILE:CG2	1:D:287:SER:HB3	2.45	0.44
1:D:866:GLU:HB2	3:D:1103:LMT:O2B	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:SER:O	1:E:133:SER:OG	2.36	0.44
1:E:375:VAL:HG13	1:E:480:LEU:HB3	1.99	0.44
1:A:158:VAL:HA	1:A:162:MET:CE	2.47	0.44
1:A:239:ARG:HB2	1:A:763:ILE:HD12	1.99	0.44
1:A:559:LEU:HD23	1:A:560:PRO:CD	2.45	0.44
1:B:190:PRO:HG3	1:B:779:TYR:HB3	1.99	0.44
1:C:293:LEU:HD11	1:C:297:ALA:O	2.17	0.44
1:C:363:ARG:H	1:C:363:ARG:HG2	1.66	0.44
1:C:636:ASP:C	1:C:638:PRO:HD3	2.38	0.44
1:C:888:LEU:HD23	1:C:888:LEU:HA	1.78	0.44
1:D:893:GLU:OE2	1:F:8:ARG:HB3	2.16	0.44
1:E:743:ILE:H	1:E:743:ILE:HD12	1.82	0.44
1:E:910:ILE:O	1:E:914:LEU:HB2	2.16	0.44
1:F:100:ALA:O	1:F:103:ALA:HB3	2.17	0.44
1:F:340:VAL:CG1	1:F:395:MET:HB3	2.47	0.44
1:A:187:TRP:HA	1:A:774:MET:O	2.17	0.44
1:A:360:GLN:HE21	1:A:360:GLN:HB3	1.58	0.44
1:A:549:VAL:O	1:A:552:MET:HB3	2.18	0.44
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.99	0.44
1:C:568:ASP:OD1	1:C:644:VAL:HG23	2.18	0.44
1:C:597:TYR:HD2	1:C:598:TYR:CD1	2.35	0.44
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.99	0.44
1:D:357:LEU:HD23	1:D:357:LEU:O	2.16	0.44
1:D:795:ASP:OD2	1:D:796:GLY:N	2.50	0.44
1:D:938:SER:OG	1:D:1014:ALA:HB1	2.17	0.44
1:E:894:SER:HB3	1:E:897:ILE:HB	1.99	0.44
1:A:404:LEU:HD12	1:A:937:LEU:HD21	2.00	0.44
1:A:729:ILE:HG22	1:A:731:ILE:HD11	2.00	0.44
1:A:752:ALA:O	1:A:774:MET:HA	2.17	0.44
1:B:383:LEU:O	1:B:386:PHE:N	2.51	0.44
1:B:602:GLU:HB3	1:B:606:VAL:HG23	1.99	0.44
1:C:185:ARG:HD3	1:C:185:ARG:HA	1.71	0.44
1:C:680:PHE:CD2	1:C:859:TRP:HZ3	2.35	0.44
1:C:785:ASP:HA	1:C:788:ASP:OD2	2.18	0.44
1:C:905:VAL:HB	1:C:906:PRO:HD3	2.00	0.44
1:D:54:ALA:HB2	1:D:84:SER:HB3	1.99	0.44
1:D:102:ILE:HD12	1:F:101:ASP:HB3	2.00	0.44
1:D:218:GLN:HG2	1:D:233:SER:HA	1.98	0.44
1:D:893:GLU:OE2	1:F:11:PHE:HB2	2.18	0.44
1:D:984:LEU:HD23	1:D:984:LEU:HA	1.77	0.44
1:D:1016:VAL:O	1:D:1016:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:459:PHE:O	1:E:464:GLY:HA3	2.18	0.44
1:E:520:PHE:O	1:E:524:THR:HG22	2.17	0.44
1:E:739:LEU:HD13	1:E:799:VAL:HG11	1.99	0.44
1:F:669:PRO:HG2	1:F:675:GLY:HA3	2.00	0.44
1:F:898:PRO:O	1:F:901:VAL:HG12	2.18	0.44
1:A:30:LEU:HD12	1:A:31:PRO:HD2	2.00	0.44
1:A:80:SER:HA	1:A:89:GLN:O	2.18	0.44
1:A:672:VAL:HB	1:A:673:GLU:OE2	2.18	0.44
1:A:986:VAL:HG21	1:A:1007:VAL:CG1	2.45	0.44
1:B:249:ILE:HG12	1:B:262:LEU:HB2	1.99	0.44
1:B:484:VAL:O	1:B:489:THR:HG23	2.18	0.44
1:B:555:LEU:HA	1:B:555:LEU:HD23	1.75	0.44
1:C:542:LEU:HA	1:C:542:LEU:HD12	1.69	0.44
1:C:652:THR:OG1	1:C:665:ALA:N	2.46	0.44
1:D:915:ALA:HB2	1:D:1009:GLY:HA3	1.99	0.44
1:E:314:GLU:N	1:E:315:PRO:HD2	2.32	0.44
1:E:568:ASP:O	1:E:634:TRP:CZ3	2.69	0.44
1:E:588:GLN:HE21	1:E:592:ASN:ND2	2.14	0.44
1:E:775:SER:OG	1:E:780:ARG:HG2	2.17	0.44
1:E:1019:ILE:HG13	1:E:1020:PHE:CD1	2.53	0.44
1:F:33:ALA:O	1:F:391:ASN:HA	2.17	0.44
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.74	0.43
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.52	0.43
1:B:376:LEU:HA	1:B:376:LEU:HD23	1.52	0.43
1:B:894:SER:HB3	1:B:897:ILE:H	1.83	0.43
1:C:159:ALA:HB2	1:C:177:LEU:HD11	1.99	0.43
1:C:706:ALA:HB1	1:C:713:LEU:HD22	1.99	0.43
1:C:723:ASP:OD1	1:C:813:SER:HB3	2.18	0.43
1:D:393:LEU:HD12	1:D:469:GLN:HG3	2.00	0.43
1:D:644:VAL:CG1	1:D:667:ASN:HB2	2.48	0.43
1:E:35:TYR:HE2	1:E:393:LEU:HD21	1.82	0.43
1:E:789:TRP:HB2	1:E:801:PHE:CE2	2.53	0.43
1:E:1032:ARG:HA	1:E:1033:PHE:HB3	2.00	0.43
1:F:110:LYS:O	1:F:113:LEU:HB2	2.18	0.43
1:F:645:GLU:O	1:F:649:MET:HB2	2.17	0.43
1:A:225:VAL:HG13	1:B:781:MET:HE1	2.01	0.43
1:A:781:MET:CE	1:C:228:GLN:HB2	2.47	0.43
1:C:396:PHE:CD1	1:C:1003:VAL:HG21	2.53	0.43
1:C:483:LEU:HA	1:C:483:LEU:HD23	1.71	0.43
1:C:535:LEU:HD21	1:C:1027:VAL:HG21	2.00	0.43
1:D:182:TYR:HD1	1:D:182:TYR:HA	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LEU:HD13	1:D:200:PRO:HD3	2.01	0.43
1:D:462:SER:O	1:D:466:ILE:HG12	2.18	0.43
1:D:514:GLY:HA2	1:D:517:ASN:ND2	2.33	0.43
1:D:563:PHE:O	1:D:564:LEU:HD12	2.18	0.43
1:E:55:LYS:HG2	1:E:59:ASP:OD2	2.18	0.43
1:E:588:GLN:HG3	1:E:592:ASN:HD21	1.82	0.43
1:E:644:VAL:HG11	1:E:667:ASN:ND2	2.33	0.43
1:E:717:ARG:HD2	1:E:717:ARG:O	2.18	0.43
1:E:877:TYR:HD2	1:E:877:TYR:HA	1.60	0.43
1:F:359:LEU:O	1:F:361:ASN:N	2.51	0.43
1:F:578:LEU:CG	1:F:587:THR:HG22	2.46	0.43
1:F:905:VAL:HB	1:F:906:PRO:HD3	1.99	0.43
1:F:1021:PHE:HB3	1:F:1025:PHE:CZ	2.53	0.43
1:A:27:ILE:HG12	1:A:380:PHE:CD2	2.53	0.43
1:A:216:ALA:HB1	1:A:234:ILE:HG22	1.98	0.43
1:A:699:ARG:HD2	1:A:718:PRO:HB3	2.00	0.43
1:A:857:TYR:HE2	1:C:312:LYS:NZ	2.17	0.43
1:B:174:ASP:HB3	1:B:292:LYS:HB2	1.99	0.43
1:B:520:PHE:O	1:B:523:SER:OG	2.28	0.43
1:B:682:PHE:CE2	1:B:857:TYR:HB2	2.53	0.43
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.99	0.43
1:C:201:VAL:O	1:C:204:ILE:HB	2.18	0.43
1:C:510:LYS:HG2	1:C:511:GLY:N	2.33	0.43
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.53	0.43
1:D:555:LEU:HD11	1:D:914:LEU:HD12	2.00	0.43
1:D:752:ALA:O	1:D:774:MET:HA	2.19	0.43
1:D:937:LEU:HD12	1:D:1011:MET:SD	2.58	0.43
1:E:184:MET:HB2	1:E:762:PHE:CE2	2.53	0.43
1:E:545:TYR:CE2	1:E:1025:PHE:HZ	2.36	0.43
1:E:574:THR:CG2	1:E:627:ALA:HB3	2.47	0.43
1:F:445:ILE:HG12	1:F:940:LYS:HG3	2.00	0.43
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.52	0.43
1:A:344:LEU:HD11	1:A:398:MET:HB2	2.00	0.43
1:B:203:VAL:O	1:B:207:ILE:HG13	2.19	0.43
1:B:1042:HIS:CG	1:B:1043:SER:N	2.86	0.43
1:C:3:ASN:C	1:C:5:PHE:N	2.71	0.43
1:C:159:ALA:HB2	1:C:177:LEU:CD1	2.49	0.43
1:C:359:LEU:HB2	1:C:365:THR:HG23	2.00	0.43
1:C:602:GLU:OE2	1:C:650:ARG:NH1	2.51	0.43
1:C:931:LEU:O	1:C:934:THR:HB	2.18	0.43
1:D:332:PHE:HB2	1:D:634:TRP:HH2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:MET:HB3	1:D:713:LEU:HD22	2.00	0.43
1:D:945:ILE:CG1	1:D:971:ARG:HH22	2.31	0.43
1:E:355:MET:CE	1:E:410:ILE:HG12	2.49	0.43
1:E:572:PHE:CE1	1:E:648:THR:HG22	2.53	0.43
1:F:200:PRO:HB2	1:F:749:THR:HG22	1.99	0.43
1:F:277:ILE:CD1	1:F:620:ARG:HH11	2.32	0.43
1:F:702:LEU:HB2	1:F:851:LEU:HD11	2.00	0.43
1:F:760:ASN:O	1:F:771:VAL:HB	2.19	0.43
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.99	0.43
1:A:767:ARG:HH12	1:B:67:GLN:CD	2.22	0.43
1:B:83:ASP:HB2	1:B:87:THR:O	2.17	0.43
1:B:717:ARG:CD	1:B:828:LEU:HB2	2.46	0.43
1:B:721:LEU:HB3	1:B:814:PRO:HG2	1.99	0.43
1:C:227:GLY:O	1:C:229:GLN:HG3	2.19	0.43
1:D:182:TYR:O	1:D:769:LYS:HB3	2.17	0.43
1:D:422:GLU:HB3	1:D:423:GLU:HG3	2.00	0.43
1:D:768:VAL:HG13	1:E:67:GLN:HE22	1.84	0.43
1:D:912:ALA:O	1:D:915:ALA:N	2.51	0.43
1:E:104:GLN:HE21	1:F:109:ASN:ND2	2.15	0.43
1:F:447:MET:HE3	1:F:887:CYS:HB3	2.00	0.43
1:F:602:GLU:HB3	1:F:606:VAL:HG23	2.00	0.43
1:F:669:PRO:CG	1:F:675:GLY:HA3	2.49	0.43
1:A:376:LEU:O	1:A:377:LEU:C	2.56	0.43
1:A:429:GLU:CD	1:A:429:GLU:H	2.21	0.43
1:A:483:LEU:HD13	1:A:487:ILE:HD12	2.01	0.43
1:A:946:VAL:HG13	1:A:1026:PHE:CD1	2.53	0.43
1:B:545:TYR:HE2	1:B:907:LEU:CD1	2.30	0.43
1:B:953:MET:HE2	1:B:963:ALA:HB3	1.99	0.43
1:D:240:LEU:HD12	1:D:246:PHE:CE1	2.54	0.43
1:D:615:PHE:CZ	2:D:1101:ERY:H343	2.53	0.43
1:D:908:GLY:HA2	1:D:1014:ALA:HB2	1.98	0.43
1:E:512:PHE:HB3	1:E:513:PHE:CD1	2.54	0.43
1:E:1038:GLU:C	1:E:1040:ILE:H	2.21	0.43
1:F:49:TYR:HD1	1:F:57:VAL:HG12	1.81	0.43
1:F:782:LEU:O	1:F:785:ASP:HB2	2.18	0.43
1:F:960:LEU:O	1:F:964:THR:HG23	2.19	0.43
1:A:445:ILE:HD12	1:A:446:ALA:N	2.33	0.43
1:B:23:GLY:HA3	1:B:377:LEU:O	2.19	0.43
1:B:187:TRP:HE3	1:B:775:SER:O	2.02	0.43
1:B:470:PHE:HZ	1:B:926:TYR:HE2	1.67	0.43
1:B:675:GLY:C	1:B:677:ALA:H	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1037:ASN:HA	1:B:1038:GLU:CG	2.48	0.43
1:C:181:GLN:OE1	1:C:767:ARG:NH2	2.49	0.43
1:D:800:PRO:O	1:D:803:ALA:HB3	2.19	0.43
1:E:178:PHE:O	1:E:287:SER:OG	2.26	0.43
1:E:959:GLY:O	1:E:963:ALA:N	2.41	0.43
1:F:284:GLN:CG	1:F:285:PRO:HD2	2.49	0.43
1:A:133:SER:OG	1:A:135:SER:O	2.36	0.43
1:A:712:MET:HG2	1:A:843:LEU:HG	2.01	0.43
1:A:961:ILE:H	1:A:961:ILE:HG13	1.38	0.43
1:B:5:PHE:CE1	1:B:487:ILE:HG12	2.54	0.43
1:B:175:VAL:HG23	1:C:70:ASN:HD22	1.83	0.43
1:B:196:PHE:N	1:B:196:PHE:CD1	2.87	0.43
1:B:356:TYR:HE1	1:B:362:PHE:HA	1.83	0.43
1:B:511:GLY:HA2	1:B:515:TRP:HE1	1.84	0.43
1:B:721:LEU:HD12	1:B:721:LEU:HA	1.91	0.43
1:B:1019:ILE:HG13	1:B:1020:PHE:CD1	2.53	0.43
1:C:146:ASP:O	1:C:148:THR:N	2.51	0.43
1:C:412:VAL:CG2	1:C:442:LEU:HD11	2.49	0.43
1:C:520:PHE:CE2	1:C:973:ARG:HG3	2.53	0.43
1:C:787:GLY:O	1:C:789:TRP:N	2.52	0.43
1:C:938:SER:HB3	1:C:1014:ALA:HB1	2.01	0.43
1:C:960:LEU:O	1:C:964:THR:HG23	2.19	0.43
1:D:63:GLN:O	1:D:67:GLN:HG3	2.17	0.43
1:E:213:GLN:HG2	1:E:239:ARG:HG3	2.00	0.43
1:E:508:GLY:HA2	1:E:518:ARG:NE	2.34	0.43
1:E:1042:HIS:HB3	1:E:1043:SER:CB	2.49	0.43
1:F:608:SER:OG	1:F:630:SER:HB3	2.18	0.43
1:A:66:GLU:OE1	1:A:821:GLY:HA2	2.18	0.43
1:A:132:SER:OG	1:A:133:SER:N	2.51	0.43
1:A:189:ASN:OD1	1:A:190:PRO:HD2	2.19	0.43
1:A:428:LYS:HG3	1:A:429:GLU:OE2	2.19	0.43
1:B:332:PHE:C	1:B:332:PHE:CD2	2.93	0.43
1:B:898:PRO:O	1:B:901:VAL:HG12	2.19	0.43
1:C:332:PHE:HD1	1:C:634:TRP:CH2	2.37	0.43
1:D:101:ASP:OD1	1:D:101:ASP:N	2.48	0.43
1:D:137:LEU:HD23	1:D:291:ILE:HG22	2.01	0.43
1:D:897:ILE:HA	1:D:1029:VAL:HG11	2.01	0.43
1:E:244:GLU:O	1:E:247:GLY:N	2.51	0.43
1:E:658:ILE:C	1:E:659:LYS:HD2	2.39	0.43
1:E:894:SER:HB2	1:E:897:ILE:HD12	2.00	0.43
1:E:905:VAL:HB	1:E:906:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:GLN:HB2	1:F:333:VAL:HG13	1.99	0.43
1:F:355:MET:HG2	1:F:410:ILE:HD11	1.99	0.43
1:F:578:LEU:HB3	1:F:579:PRO:HD2	2.01	0.43
1:F:889:ALA:HB2	1:F:898:PRO:HG2	2.00	0.43
1:A:81:ASN:OD1	2:A:1101:ERY:H272	2.19	0.43
1:A:177:LEU:HA	1:A:177:LEU:HD23	1.69	0.43
1:A:196:PHE:CD1	1:A:260:VAL:HG13	2.53	0.43
1:A:890:ALA:HB2	1:C:14:VAL:HG11	2.01	0.43
1:A:910:ILE:O	1:A:910:ILE:HG13	2.19	0.43
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.84	0.43
1:B:356:TYR:HD1	1:B:365:THR:HG21	1.84	0.43
1:B:393:LEU:HD22	1:B:470:PHE:HE1	1.84	0.43
1:C:166:ILE:O	1:C:169:THR:HB	2.19	0.43
1:C:445:ILE:HG12	1:C:940:LYS:CG	2.49	0.43
1:D:30:LEU:HD12	1:D:30:LEU:HA	1.80	0.43
1:D:38:ILE:CG2	1:D:462:SER:HB2	2.38	0.43
1:D:428:LYS:H	1:D:428:LYS:HG2	1.21	0.43
1:D:531:VAL:HG21	1:D:968:VAL:HG11	2.00	0.43
1:D:572:PHE:CD1	1:D:648:THR:HG22	2.53	0.43
1:D:897:ILE:HG12	1:D:1030:ARG:HD2	2.00	0.43
1:E:40:PRO:HA	1:E:41:PRO:HD3	1.75	0.43
1:E:459:PHE:CD2	1:E:876:LEU:HD12	2.53	0.43
1:E:539:GLY:O	1:E:542:LEU:HB2	2.19	0.43
1:F:187:TRP:NE1	1:F:269:GLU:OE1	2.52	0.43
1:F:382:VAL:HG11	1:F:476:SER:HB2	2.00	0.43
1:F:571:VAL:HG12	1:F:668:LEU:HD11	2.01	0.43
1:A:11:PHE:HE1	1:A:15:ILE:HD11	1.84	0.42
1:A:352:PHE:CD2	1:A:353:LEU:HD23	2.53	0.42
1:A:726:GLN:O	1:A:810:GLU:HG2	2.19	0.42
1:A:1018:ALA:O	1:A:1022:VAL:HG23	2.19	0.42
1:B:211:ASN:O	1:B:760:ASN:ND2	2.52	0.42
1:B:352:PHE:CD2	1:B:353:LEU:HD23	2.49	0.42
1:C:42:ALA:HB2	1:C:93:THR:HG23	2.01	0.42
1:C:516:PHE:HA	1:C:519:MET:HE3	2.01	0.42
1:C:686:ASP:HB3	1:C:823:PRO:HB2	2.01	0.42
1:D:484:VAL:HG13	1:D:488:LEU:HB3	2.01	0.42
1:D:702:LEU:HD22	1:D:827:ILE:HD13	2.01	0.42
1:E:239:ARG:NH1	1:E:761:ASP:HB2	2.34	0.42
1:E:675:GLY:C	1:E:677:ALA:H	2.22	0.42
1:F:382:VAL:HG11	1:F:476:SER:CB	2.48	0.42
1:F:984:LEU:HA	1:F:984:LEU:HD23	1.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:SER:HB3	1:A:180:SER:N	2.28	0.42
1:A:362:PHE:CD2	1:A:362:PHE:N	2.85	0.42
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.57	0.42
1:A:893:GLU:CD	1:C:8:ARG:HB3	2.39	0.42
1:B:401:ALA:O	1:B:405:LEU:HG	2.19	0.42
1:B:690:LEU:HD11	1:B:854:GLY:HA3	2.00	0.42
1:B:813:SER:HA	1:B:814:PRO:HD3	1.93	0.42
1:B:817:GLU:OE1	1:B:826:GLU:N	2.52	0.42
1:C:311:ALA:O	1:C:315:PRO:HD3	2.19	0.42
1:C:913:LEU:HD23	1:C:927:PHE:HZ	1.84	0.42
1:D:156:ASP:OD1	1:D:765:ARG:NH2	2.52	0.42
1:E:174:ASP:CB	1:E:292:LYS:HB2	2.46	0.42
1:F:144:ASN:HA	1:F:320:GLY:O	2.19	0.42
1:F:659:LYS:HD3	1:F:659:LYS:HA	1.82	0.42
1:F:776:GLU:HB2	1:F:779:TYR:CD1	2.54	0.42
1:A:210:GLN:HE22	1:A:250:LEU:H	1.66	0.42
1:B:144:ASN:HA	1:B:320:GLY:O	2.20	0.42
1:C:425:LEU:HD22	1:C:429:GLU:HG2	2.00	0.42
1:C:536:ARG:HD2	3:C:1101:LMT:O4'	2.19	0.42
1:D:441:ALA:HB2	1:D:947:GLU:OE2	2.19	0.42
1:D:467:TYR:CE2	1:D:925:VAL:HG22	2.54	0.42
1:E:766:GLY:O	1:F:59:ASP:HB2	2.20	0.42
1:E:801:PHE:CD1	1:E:804:PHE:HE2	2.38	0.42
1:E:1007:VAL:HG12	1:E:1008:MET:N	2.35	0.42
1:E:1037:ASN:HB2	1:E:1038:GLU:CA	2.50	0.42
1:F:181:GLN:HG2	1:F:182:TYR:N	2.34	0.42
1:F:546:LEU:HD23	1:F:546:LEU:HA	1.69	0.42
1:F:971:ARG:C	1:F:974:PRO:HD2	2.40	0.42
1:A:1026:PHE:CE2	1:A:1030:ARG:HG3	2.55	0.42
1:B:984:LEU:HD23	1:B:984:LEU:HA	1.63	0.42
1:C:453:PHE:HZ	1:C:933:THR:OG1	2.02	0.42
1:C:680:PHE:HA	1:C:863:SER:OG	2.20	0.42
1:C:787:GLY:C	1:C:789:TRP:H	2.23	0.42
1:D:997:SER:HA	1:D:1000:GLN:HB2	2.01	0.42
1:F:73:ASP:HB2	1:F:106:GLN:OE1	2.19	0.42
1:F:356:TYR:C	1:F:358:PHE:H	2.23	0.42
1:F:455:PRO:HG3	1:F:883:VAL:HG21	2.00	0.42
1:F:913:LEU:HD23	1:F:927:PHE:HZ	1.85	0.42
1:F:985:GLY:O	1:F:988:PRO:HD2	2.19	0.42
1:B:888:LEU:HD11	1:B:943:ILE:HD11	2.02	0.42
1:C:64:VAL:CG1	1:C:117:LEU:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:GLY:HA3	1:C:302:THR:OG1	2.19	0.42
1:C:246:PHE:O	1:C:262:LEU:HD23	2.19	0.42
1:D:108:GLN:NE2	1:E:109:ASN:O	2.53	0.42
1:D:190:PRO:HB3	1:D:789:TRP:CZ3	2.54	0.42
1:D:239:ARG:HH12	1:D:761:ASP:HB2	1.85	0.42
1:D:292:LYS:NZ	2:D:1101:ERY:O11	2.52	0.42
1:D:361:ASN:HB3	1:D:364:ALA:HB3	2.02	0.42
1:D:851:LEU:HB3	1:D:852:PRO:HD2	2.00	0.42
1:E:230:LEU:HG	1:E:231:ASN:N	2.33	0.42
1:E:355:MET:SD	1:E:365:THR:HA	2.60	0.42
1:E:519:MET:H	1:E:519:MET:HG2	1.59	0.42
1:E:549:VAL:O	1:E:552:MET:HB3	2.19	0.42
1:E:582:ALA:HA	1:E:586:ARG:NH2	2.33	0.42
1:E:971:ARG:C	1:E:974:PRO:HD2	2.40	0.42
1:F:277:ILE:HD11	1:F:620:ARG:HH11	1.84	0.42
1:F:340:VAL:HG11	1:F:395:MET:HB3	2.00	0.42
1:F:680:PHE:HB2	1:F:859:TRP:CZ3	2.54	0.42
1:A:375:VAL:HG22	1:A:484:VAL:HG21	2.02	0.42
1:A:604:ASN:O	1:A:632:LYS:HD2	2.20	0.42
1:B:47:ALA:HB2	1:B:127:VAL:HG13	2.01	0.42
1:C:647:ILE:O	1:C:650:ARG:N	2.53	0.42
1:D:577:GLN:OE1	1:D:624:THR:HG22	2.18	0.42
1:D:636:ASP:N	1:D:636:ASP:OD1	2.51	0.42
1:F:185:ARG:HH12	1:F:774:MET:HE2	1.85	0.42
1:F:509:LYS:O	1:F:518:ARG:NH1	2.52	0.42
1:F:617:PHE:CD1	1:F:626:ILE:HD11	2.55	0.42
1:F:1019:ILE:HG13	1:F:1020:PHE:CD1	2.54	0.42
1:A:30:LEU:HD23	1:A:390:ILE:HG13	2.01	0.42
1:A:578:LEU:HB2	1:A:623:ASN:O	2.19	0.42
1:A:787:GLY:O	1:A:789:TRP:N	2.52	0.42
1:A:857:TYR:N	1:A:857:TYR:CD2	2.88	0.42
1:B:201:VAL:HG23	1:B:749:THR:HG23	2.02	0.42
1:C:411:VAL:O	1:C:415:ASN:HB2	2.19	0.42
1:C:445:ILE:HG12	1:C:940:LYS:HG3	2.02	0.42
1:D:418:ARG:HH22	1:D:948:PHE:HE2	1.65	0.42
1:E:318:PRO:HG2	1:E:321:LEU:HB2	2.00	0.42
1:E:572:PHE:HA	1:E:668:LEU:CD2	2.47	0.42
1:E:678:THR:O	1:E:678:THR:OG1	2.27	0.42
1:E:925:VAL:O	1:E:928:GLN:N	2.53	0.42
1:F:15:ILE:O	1:F:19:ILE:HG13	2.20	0.42
1:F:443:VAL:HG12	1:F:891:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:540:ARG:O	1:F:543:VAL:HB	2.20	0.42
1:F:575:MET:HG2	1:F:666:PHE:HE1	1.85	0.42
1:A:102:ILE:HD13	1:A:102:ILE:HA	1.91	0.42
1:C:75:LEU:CD1	1:C:92:LEU:HB3	2.49	0.42
1:C:706:ALA:HB2	1:C:847:LEU:HD23	2.00	0.42
1:C:800:PRO:HB2	1:C:802:SER:OG	2.19	0.42
1:C:835:LYS:HG2	1:C:836:SER:N	2.35	0.42
1:D:546:LEU:HD23	1:D:546:LEU:HA	1.82	0.42
1:E:154:ILE:HG22	1:E:287:SER:HB3	2.02	0.42
1:E:789:TRP:HB2	1:E:801:PHE:HE2	1.83	0.42
1:E:818:ARG:NH1	1:E:823:PRO:HG3	2.34	0.42
1:E:1026:PHE:O	1:E:1030:ARG:HB2	2.20	0.42
1:F:584:GLN:N	1:F:622:GLN:HB3	2.35	0.42
1:F:742:SER:O	1:F:745:ASP:HB2	2.20	0.42
1:A:3:ASN:O	1:A:4:PHE:C	2.58	0.42
1:A:94:PHE:CE1	1:A:103:ALA:HB1	2.55	0.42
1:A:618:ALA:C	1:A:815:ARG:HH22	2.22	0.42
1:A:634:TRP:CD1	1:A:634:TRP:N	2.85	0.42
1:B:57:VAL:HB	1:B:88:VAL:HG23	2.02	0.42
1:B:143:ILE:HG22	1:B:286:ALA:HB2	2.01	0.42
1:B:572:PHE:HD1	1:B:666:PHE:O	2.02	0.42
1:B:712:MET:CE	1:B:839:GLU:HB3	2.50	0.42
1:B:841:MET:HG2	1:B:859:TRP:CH2	2.55	0.42
1:B:913:LEU:HD23	1:B:927:PHE:HZ	1.85	0.42
1:C:270:LEU:HA	1:C:270:LEU:HD12	1.56	0.42
1:C:337:ILE:HG13	1:C:392:THR:HG23	2.02	0.42
1:C:456:MET:HB3	1:C:876:LEU:HD21	2.02	0.42
1:C:886:LEU:HD13	1:C:886:LEU:HA	1.71	0.42
1:D:343:THR:O	1:D:346:GLU:HB2	2.20	0.42
1:D:544:LEU:O	1:D:548:ILE:HG13	2.19	0.42
1:E:589:LYS:O	1:E:592:ASN:HB2	2.20	0.42
1:F:892:TYR:C	1:F:894:SER:H	2.22	0.42
1:F:973:ARG:HG2	1:F:977:MET:HE2	2.01	0.42
1:C:692:HIS:CD2	1:C:692:HIS:C	2.93	0.42
1:E:185:ARG:HD3	1:E:185:ARG:HA	1.90	0.42
1:E:310:LEU:HA	1:E:310:LEU:HD12	1.84	0.42
1:E:685:ILE:HG22	1:E:687:GLN:OE1	2.20	0.42
1:F:931:LEU:O	1:F:935:ILE:HG13	2.19	0.42
1:A:472:ILE:HG22	1:A:473:THR:N	2.34	0.41
1:A:545:TYR:HB2	1:A:1021:PHE:HE2	1.85	0.41
1:A:644:VAL:O	1:A:648:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ILE:HG12	1:A:1030:ARG:HD2	2.01	0.41
1:B:514:GLY:C	1:B:516:PHE:H	2.23	0.41
1:B:990:VAL:HG22	1:B:1004:GLY:C	2.40	0.41
1:C:580:ALA:HB1	1:C:724:THR:CG2	2.48	0.41
1:C:587:THR:OG1	1:C:613:ASN:ND2	2.51	0.41
1:C:671:ILE:CG2	1:C:674:LEU:HB2	2.49	0.41
1:D:542:LEU:HD12	1:D:542:LEU:HA	1.82	0.41
1:D:583:THR:CG2	1:F:229:GLN:HA	2.45	0.41
1:D:675:GLY:H	1:D:862:MET:HB3	1.84	0.41
1:D:961:ILE:H	1:D:961:ILE:HD12	1.85	0.41
1:E:249:ILE:HD11	1:E:262:LEU:HD22	2.02	0.41
1:E:520:PHE:O	1:E:523:SER:OG	2.38	0.41
1:E:752:ALA:O	1:E:774:MET:HA	2.19	0.41
1:E:776:GLU:CG	1:E:777:ALA:H	2.32	0.41
1:A:58:GLN:HG3	1:A:818:ARG:HD2	2.03	0.41
1:A:900:SER:HB3	1:A:1029:VAL:HG21	2.01	0.41
1:A:985:GLY:O	1:A:988:PRO:HD2	2.20	0.41
1:B:969:ARG:NH1	1:B:970:MET:HB3	2.34	0.41
1:B:1015:THR:C	1:B:1017:LEU:H	2.24	0.41
1:C:39:ALA:HB3	1:C:673:GLU:HG2	2.01	0.41
1:C:356:TYR:CA	1:C:365:THR:HG21	2.41	0.41
1:C:564:LEU:HD23	1:C:670:ALA:HB3	2.01	0.41
1:D:190:PRO:HB3	1:D:789:TRP:CE3	2.54	0.41
1:D:262:LEU:HD12	1:D:265:VAL:CG2	2.50	0.41
1:D:699:ARG:HD2	1:D:718:PRO:HB3	2.02	0.41
1:D:708:LYS:HE3	1:D:708:LYS:HB3	1.84	0.41
1:D:946:VAL:HG13	1:D:1026:PHE:CD1	2.55	0.41
1:E:754:TRP:CH2	1:E:780:ARG:HA	2.56	0.41
1:F:894:SER:CB	1:F:897:ILE:HG12	2.48	0.41
1:F:944:LEU:HB3	1:F:971:ARG:HE	1.83	0.41
1:A:228:GLN:NE2	1:A:230:LEU:H	2.17	0.41
1:B:5:PHE:HE2	1:B:11:PHE:HD2	1.68	0.41
1:B:425:LEU:HB2	1:B:430:ALA:HB2	2.02	0.41
1:B:459:PHE:CB	1:B:464:GLY:HA2	2.51	0.41
1:C:564:LEU:HG	1:C:565:PRO:HD2	2.01	0.41
1:D:6:ILE:HG13	1:D:7:ASP:N	2.34	0.41
1:D:375:VAL:HG21	1:D:481:SER:HA	2.02	0.41
1:D:401:ALA:O	1:D:405:LEU:HG	2.20	0.41
1:D:448:VAL:HG22	1:D:887:CYS:CB	2.44	0.41
1:D:764:ASP:OD1	1:D:765:ARG:HG3	2.20	0.41
1:D:961:ILE:H	1:D:961:ILE:CD1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:PHE:CZ	1:E:103:ALA:HB1	2.55	0.41
1:E:119:PRO:HG2	1:E:122:VAL:HB	2.02	0.41
1:E:445:ILE:HG12	1:E:940:LYS:HE3	2.01	0.41
1:E:459:PHE:CE2	1:E:876:LEU:HD12	2.55	0.41
1:E:536:ARG:NE	3:E:1101:LMT:O3B	2.53	0.41
1:F:187:TRP:HE3	1:F:775:SER:O	2.03	0.41
1:F:352:PHE:HD1	1:F:369:THR:OG1	2.04	0.41
1:F:369:THR:O	1:F:373:PRO:HD2	2.20	0.41
1:A:78:MET:HG3	1:A:92:LEU:HG	2.01	0.41
1:A:183:ALA:HB2	1:A:273:GLU:HG3	2.01	0.41
1:A:832:ALA:HB3	1:A:835:LYS:CD	2.41	0.41
1:A:1040:ILE:HD11	1:A:1042:HIS:HB2	2.01	0.41
1:B:255:GLN:H	1:B:255:GLN:HG3	1.59	0.41
1:C:591:LEU:HD11	1:C:625:GLY:HA3	2.01	0.41
1:D:160:ALA:HA	1:D:767:ARG:NE	2.35	0.41
1:D:452:VAL:HG12	1:D:880:SER:OG	2.20	0.41
1:D:841:MET:O	1:D:845:GLU:HG3	2.20	0.41
1:D:1018:ALA:O	1:D:1022:VAL:HG23	2.20	0.41
1:E:273:GLU:OE1	1:E:770:LYS:HD2	2.21	0.41
1:E:534:ILE:HG22	3:E:1101:LMT:C5'	2.49	0.41
1:E:891:LEU:HA	1:E:891:LEU:HD12	1.68	0.41
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.76	0.41
1:B:14:VAL:HG22	1:C:886:LEU:CD1	2.42	0.41
1:B:185:ARG:HD3	1:B:185:ARG:HA	1.84	0.41
1:B:237:GLN:CG	1:C:731:ILE:HD11	2.50	0.41
1:B:359:LEU:HD13	1:B:417:GLU:HG3	2.01	0.41
1:B:684:LEU:HD12	1:B:684:LEU:HA	1.64	0.41
1:C:443:VAL:HG12	1:C:891:LEU:CD2	2.50	0.41
1:C:525:HIS:CD2	1:C:525:HIS:C	2.92	0.41
1:C:674:LEU:HD23	1:C:674:LEU:HA	1.91	0.41
1:C:713:LEU:HD21	1:C:844:MET:SD	2.60	0.41
1:D:57:VAL:HG21	1:D:86:GLY:HA2	2.02	0.41
1:E:362:PHE:O	1:E:366:LEU:HG	2.21	0.41
1:E:588:GLN:NE2	1:E:592:ASN:HD21	2.14	0.41
1:E:617:PHE:HD1	1:E:617:PHE:HA	1.75	0.41
1:F:34:GLN:HB2	1:F:333:VAL:CG2	2.35	0.41
1:F:149:MET:HG3	1:F:154:ILE:HG13	2.03	0.41
1:F:795:ASP:OD2	1:F:797:GLN:HG2	2.21	0.41
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.84	0.41
1:A:847:LEU:HD23	1:A:847:LEU:HA	1.86	0.41
1:B:5:PHE:CE2	1:B:11:PHE:HD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:TYR:C	1:B:358:PHE:H	2.24	0.41
1:B:937:LEU:HD23	1:B:937:LEU:HA	1.73	0.41
1:B:987:MET:HA	1:B:1008:MET:HE3	2.03	0.41
1:C:61:VAL:HG21	1:C:122:VAL:HG21	2.03	0.41
1:C:574:THR:HG23	1:C:627:ALA:HB3	2.03	0.41
1:C:644:VAL:CG1	1:C:667:ASN:HB2	2.50	0.41
1:C:858:ASP:OD2	1:C:859:TRP:N	2.50	0.41
1:D:136:PHE:CD2	1:D:292:LYS:HG3	2.56	0.41
1:D:356:TYR:C	1:D:358:PHE:H	2.23	0.41
1:D:420:MET:HB2	1:D:420:MET:HE3	1.93	0.41
1:D:527:TYR:CE2	1:D:968:VAL:HG13	2.56	0.41
1:D:682:PHE:CE2	1:D:857:TYR:HB2	2.56	0.41
1:D:801:PHE:CD1	1:D:804:PHE:HE2	2.39	0.41
1:E:32:VAL:HG12	1:E:390:ILE:HB	2.01	0.41
1:E:189:ASN:HB3	1:E:192:GLU:HB2	2.02	0.41
1:E:537:SER:OG	1:E:540:ARG:NE	2.50	0.41
1:E:597:TYR:CD1	1:E:601:LYS:HD2	2.56	0.41
1:E:997:SER:HA	1:E:1000:GLN:HB2	2.03	0.41
1:F:897:ILE:HD11	1:F:950:LYS:HE2	2.02	0.41
1:F:1043:SER:HB2	1:F:1044:HIS:ND1	2.36	0.41
1:A:127:VAL:O	1:B:113:LEU:HD13	2.21	0.41
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.89	0.41
1:A:735:LYS:O	1:A:738:ALA:HB3	2.20	0.41
1:B:352:PHE:CZ	1:B:362:PHE:HE1	2.39	0.41
1:B:459:PHE:HB3	1:B:464:GLY:HA2	2.02	0.41
1:B:594:VAL:HG22	1:B:655:PHE:CZ	2.56	0.41
1:B:950:LYS:HE2	1:B:950:LYS:HB2	1.73	0.41
1:D:314:GLU:OE1	1:D:323:ILE:HD12	2.20	0.41
1:D:605:ASN:O	1:D:632:LYS:N	2.45	0.41
1:D:684:LEU:HD12	1:D:684:LEU:HA	1.93	0.41
1:A:10:ILE:HG13	1:B:895:TRP:CE2	2.56	0.41
1:A:211:ASN:CG	1:A:240:LEU:HG	2.40	0.41
1:A:706:ALA:HB1	1:A:713:LEU:HD23	2.03	0.41
1:A:944:LEU:HD23	1:A:944:LEU:HA	1.89	0.41
1:B:77:TYR:OH	1:B:861:GLY:HA2	2.20	0.41
1:B:847:LEU:HD23	1:B:847:LEU:HA	1.88	0.41
1:C:594:VAL:HG22	1:C:655:PHE:CE2	2.56	0.41
1:C:751:GLY:O	1:C:753:ALA:N	2.54	0.41
1:D:108:GLN:NE2	1:E:109:ASN:HB2	2.35	0.41
1:D:360:GLN:H	1:D:360:GLN:HG2	1.69	0.41
1:D:388:PHE:CZ	1:D:472:ILE:HD12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:727:PHE:CD1	1:D:809:TRP:CE2	3.07	0.41
1:E:544:LEU:O	1:E:547:ILE:HB	2.21	0.41
1:F:578:LEU:HA	1:F:661:ALA:HB1	2.03	0.41
1:A:163:LYS:HD2	1:A:177:LEU:HG	2.03	0.41
1:A:245:GLU:O	1:A:249:ILE:HG13	2.20	0.41
1:A:310:LEU:O	1:A:314:GLU:HG3	2.21	0.41
1:A:530:SER:CB	3:A:1102:LMT:O2'	2.66	0.41
1:A:648:THR:HB	1:A:665:ALA:C	2.41	0.41
1:A:1041:GLU:H	1:A:1042:HIS:HA	1.86	0.41
1:B:164:ASP:OD2	1:C:67:GLN:HG2	2.21	0.41
1:B:291:ILE:HG21	1:B:306:ILE:HD11	2.02	0.41
1:B:574:THR:HG21	1:B:598:TYR:HE2	1.85	0.41
1:B:876:LEU:HD23	1:B:879:ILE:HD12	2.03	0.41
1:C:937:LEU:HD13	1:C:1011:MET:HE2	2.01	0.41
1:C:952:LEU:HD11	1:C:970:MET:HE2	2.03	0.41
1:C:971:ARG:HH21	1:C:975:ILE:HD11	1.86	0.41
1:D:424:GLY:HA3	1:D:502:LYS:HB3	2.03	0.41
1:D:451:ALA:HB1	1:D:883:VAL:HG12	2.03	0.41
1:D:545:TYR:HB2	1:D:1021:PHE:CE2	2.56	0.41
1:D:584:GLN:HB2	1:D:622:GLN:HG2	2.03	0.41
1:D:597:TYR:CD2	1:D:598:TYR:CD1	3.09	0.41
1:D:641:GLU:HG2	1:D:642:ASN:N	2.36	0.41
1:D:682:PHE:O	1:D:826:GLU:HA	2.21	0.41
1:E:354:VAL:O	1:E:358:PHE:HB2	2.20	0.41
1:E:514:GLY:C	1:E:516:PHE:H	2.22	0.41
1:E:675:GLY:HA2	1:E:862:MET:SD	2.61	0.41
1:E:699:ARG:HE	1:E:718:PRO:HG3	1.85	0.41
1:E:750:LEU:HD12	1:E:754:TRP:CD1	2.56	0.41
1:E:839:GLU:O	1:E:842:GLU:HB3	2.21	0.41
1:E:841:MET:O	1:E:845:GLU:HG3	2.21	0.41
1:E:887:CYS:O	1:E:890:ALA:HB3	2.21	0.41
1:E:922:THR:O	1:E:924:ASP:N	2.53	0.41
1:F:36:PRO:HD3	1:F:391:ASN:CG	2.42	0.41
1:F:72:ILE:HD13	1:F:72:ILE:HG21	1.87	0.41
1:F:172:VAL:HG13	1:F:291:ILE:HG23	2.02	0.41
1:F:888:LEU:CD1	1:F:901:VAL:HG11	2.50	0.41
1:A:246:PHE:HA	1:A:249:ILE:HG13	2.02	0.41
1:A:682:PHE:CE2	1:A:857:TYR:HB2	2.56	0.41
1:A:902:MET:C	1:A:904:VAL:H	2.25	0.41
1:B:993:THR:O	1:B:997:SER:HB3	2.21	0.41
1:C:671:ILE:HG21	1:C:674:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:VAL:HG23	1:D:749:THR:HG23	2.02	0.41
1:D:375:VAL:HG11	1:D:405:LEU:HD22	2.03	0.41
1:D:538:THR:HG21	1:D:1028:VAL:CG2	2.51	0.41
1:D:636:ASP:O	1:D:638:PRO:HD3	2.21	0.41
1:D:1007:VAL:HG12	1:D:1008:MET:N	2.36	0.41
1:E:166:ILE:O	1:E:169:THR:HB	2.20	0.41
1:E:200:PRO:HA	1:E:203:VAL:HG23	2.03	0.41
1:E:680:PHE:CE1	1:E:682:PHE:HB2	2.56	0.41
1:F:49:TYR:HB3	1:F:57:VAL:HG12	2.02	0.41
1:F:151:GLN:NE2	1:F:279:ALA:O	2.54	0.41
1:F:382:VAL:O	1:F:386:PHE:HD2	2.04	0.41
1:A:67:GLN:HG2	1:C:767:ARG:HH12	1.85	0.40
1:A:525:HIS:O	1:A:528:THR:HG22	2.21	0.40
1:A:1030:ARG:HA	1:A:1030:ARG:HH11	1.86	0.40
1:B:242:SER:HB2	1:B:245:GLU:H	1.87	0.40
1:B:448:VAL:HG13	1:B:884:VAL:CG2	2.49	0.40
1:B:459:PHE:HD1	1:B:467:TYR:CD1	2.39	0.40
1:B:535:LEU:HA	1:B:535:LEU:HD23	1.78	0.40
1:B:982:PHE:CD2	1:B:1011:MET:HG3	2.56	0.40
1:C:13:TRP:HH2	1:C:370:ILE:HD13	1.86	0.40
1:C:307:ARG:NE	1:C:325:TYR:OH	2.54	0.40
1:C:365:THR:O	1:C:368:PRO:HD2	2.21	0.40
1:C:396:PHE:O	1:C:400:LEU:HB2	2.21	0.40
1:C:687:GLN:HG3	1:C:688:ALA:N	2.36	0.40
1:D:467:TYR:HE2	1:D:925:VAL:HG22	1.85	0.40
1:D:485:ALA:O	1:D:490:PRO:HD3	2.21	0.40
1:D:671:ILE:H	1:D:671:ILE:HG13	1.59	0.40
1:D:678:THR:HG22	1:D:837:THR:N	2.36	0.40
1:D:890:ALA:HB1	1:F:11:PHE:CE1	2.56	0.40
1:D:894:SER:HB3	1:D:897:ILE:HB	2.03	0.40
1:D:1034:SER:HG	1:D:1035:ARG:H	1.60	0.40
1:F:459:PHE:CE2	1:F:872:GLN:HB3	2.56	0.40
1:F:560:PRO:HB2	1:F:836:SER:OG	2.21	0.40
1:F:979:SER:OG	1:F:1015:THR:HG21	2.20	0.40
1:A:680:PHE:CZ	1:A:829:GLY:HA3	2.57	0.40
1:A:801:PHE:HA	1:A:804:PHE:HE2	1.84	0.40
1:C:950:LYS:HG3	1:C:951:ASP:N	2.36	0.40
1:D:144:ASN:HA	1:D:320:GLY:O	2.21	0.40
1:D:332:PHE:O	1:D:336:SER:HB2	2.21	0.40
1:D:574:THR:HG23	1:D:627:ALA:HB3	2.03	0.40
1:D:602:GLU:OE1	1:D:650:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:LYS:HG2	1:E:196:PHE:CE1	2.56	0.40
1:E:555:LEU:HD23	1:E:555:LEU:HA	1.82	0.40
1:F:329:THR:O	1:F:333:VAL:HG23	2.21	0.40
1:F:414:GLU:HG2	1:F:973:ARG:NH1	2.36	0.40
1:F:931:LEU:HD23	1:F:931:LEU:HA	1.72	0.40
1:F:1032:ARG:O	1:F:1033:PHE:HB2	2.21	0.40
1:A:144:ASN:HA	1:A:320:GLY:O	2.21	0.40
1:A:344:LEU:HD22	1:A:402:ILE:CD1	2.52	0.40
1:B:172:VAL:HG13	1:B:291:ILE:HG23	2.02	0.40
1:B:729:ILE:HG22	1:B:731:ILE:HD13	2.03	0.40
1:B:915:ALA:CB	1:B:1009:GLY:HA3	2.41	0.40
1:C:263:ARG:O	1:C:263:ARG:HG2	2.22	0.40
1:C:445:ILE:HG23	1:C:940:LYS:HG3	2.03	0.40
1:C:594:VAL:O	1:C:597:TYR:N	2.55	0.40
1:D:377:LEU:O	1:D:380:PHE:HB2	2.21	0.40
1:D:710:PRO:HA	1:D:713:LEU:O	2.21	0.40
1:D:948:PHE:N	1:D:948:PHE:CD1	2.89	0.40
1:E:6:ILE:HD11	1:E:435:MET:HG3	2.02	0.40
1:E:30:LEU:CD1	1:E:31:PRO:HD2	2.50	0.40
1:E:267:LYS:HD3	1:E:776:GLU:OE2	2.21	0.40
1:E:294:ALA:HB3	1:E:297:ALA:HB2	2.02	0.40
1:E:416:VAL:HG11	1:E:497:LEU:HD23	2.04	0.40
1:E:639:GLY:O	1:E:643:LYS:HG3	2.21	0.40
1:F:102:ILE:HD13	1:F:102:ILE:HA	1.84	0.40
1:F:321:LEU:HD23	1:F:321:LEU:HA	1.75	0.40
1:F:510:LYS:H	1:F:510:LYS:HD3	1.85	0.40
1:F:701:GLN:HE22	1:F:852:PRO:HD3	1.86	0.40
1:F:703:LEU:HD21	1:F:716:VAL:HG12	2.04	0.40
1:A:400:LEU:CD2	1:A:929:VAL:HG12	2.50	0.40
1:A:505:HIS:O	1:A:507:GLU:N	2.55	0.40
1:A:682:PHE:HD2	1:A:683:GLU:N	2.19	0.40
1:A:686:ASP:O	1:A:822:LEU:HD13	2.22	0.40
1:B:137:LEU:HD12	1:B:329:THR:HG22	2.03	0.40
1:B:195:LYS:HB3	1:B:196:PHE:HD1	1.86	0.40
1:B:655:PHE:HB3	1:B:663:VAL:HB	2.03	0.40
1:B:871:ASN:N	1:B:871:ASN:OD1	2.54	0.40
1:B:904:VAL:HG21	1:B:942:ALA:HB2	2.03	0.40
1:B:944:LEU:HD23	1:B:944:LEU:HA	1.78	0.40
1:C:459:PHE:CZ	1:C:876:LEU:HA	2.56	0.40
1:C:591:LEU:HD23	1:C:591:LEU:HA	1.92	0.40
1:C:735:LYS:O	1:C:738:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ASN:OD1	1:D:70:ASN:N	2.54	0.40
1:D:414:GLU:CG	1:D:974:PRO:HG3	2.52	0.40
1:D:666:PHE:N	1:D:666:PHE:CD1	2.89	0.40
2:D:1101:ERY:H313	2:D:1101:ERY:C20	2.52	0.40
1:E:641:GLU:HB2	1:E:650:ARG:NH2	2.37	0.40
1:E:950:LYS:NZ	1:E:953:MET:SD	2.94	0.40
1:F:118:LEU:HA	1:F:119:PRO:HD3	1.94	0.40
1:F:783:PRO:O	1:F:786:ILE:HG12	2.21	0.40
1:A:453:PHE:HE2	1:A:932:LEU:HB3	1.83	0.40
1:A:895:TRP:CE2	1:C:10:ILE:HG12	2.56	0.40
1:A:926:TYR:HE1	1:A:999:ALA:HB1	1.86	0.40
1:A:953:MET:HG3	1:A:958:LYS:O	2.22	0.40
1:B:143:ILE:O	1:B:321:LEU:HA	2.21	0.40
1:B:591:LEU:HD11	1:B:625:GLY:HA3	2.04	0.40
1:B:1016:VAL:HG12	1:B:1016:VAL:O	2.21	0.40
1:C:15:ILE:O	1:C:19:ILE:HG13	2.22	0.40
1:C:65:ILE:HG23	1:C:111:LEU:HD23	2.03	0.40
1:D:201:VAL:O	1:D:204:ILE:HB	2.22	0.40
1:D:666:PHE:N	1:D:666:PHE:HD1	2.20	0.40
3:D:1103:LMT:H21	3:D:1103:LMT:H1'	1.78	0.40
1:E:31:PRO:HB2	1:E:389:SER:HB2	2.02	0.40
1:F:588:GLN:NE2	1:F:592:ASN:OD1	2.52	0.40
1:F:986:VAL:CG1	1:F:1008:MET:HB2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1042/1049 (99%)	943 (90%)	86 (8%)	13 (1%)	<b>13</b> 47
1	B	1040/1049 (99%)	955 (92%)	68 (6%)	17 (2%)	<b>9</b> 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1040/1049 (99%)	934 (90%)	88 (8%)	18 (2%)	9	40
1	D	1040/1049 (99%)	943 (91%)	83 (8%)	14 (1%)	12	45
1	E	1040/1049 (99%)	947 (91%)	72 (7%)	21 (2%)	7	37
1	F	1041/1049 (99%)	932 (90%)	81 (8%)	28 (3%)	5	31
All	All	6243/6294 (99%)	5654 (91%)	478 (8%)	111 (2%)	8	38

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	508	GLY
1	B	360	GLN
1	B	509	LYS
1	B	673	GLU
1	B	677	ALA
1	B	1038	GLU
1	C	360	GLN
1	C	893	GLU
1	C	1037	ASN
1	C	1041	GLU
1	D	360	GLN
1	D	508	GLY
1	D	675	GLY
1	D	677	ALA
1	E	358	PHE
1	E	360	GLN
1	E	509	LYS
1	E	673	GLU
1	E	893	GLU
1	E	1039	ASP
1	E	1041	GLU
1	F	134	SER
1	F	360	GLN
1	F	509	LYS
1	F	673	GLU
1	F	691	GLY
1	F	836	SER
1	F	893	GLU
1	F	1033	PHE
1	F	1036	LYS
1	F	1038	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	1043	SER
1	A	991	ILE
1	A	1037	ASN
1	B	638	PRO
1	B	672	VAL
1	B	689	GLY
1	B	893	GLU
1	B	1040	ILE
1	C	146	ASP
1	C	147	GLY
1	C	509	LYS
1	C	689	GLY
1	C	836	SER
1	C	871	ASN
1	D	1036	LYS
1	D	1042	HIS
1	E	638	PRO
1	E	672	VAL
1	E	677	ALA
1	E	1040	ILE
1	F	133	SER
1	F	147	GLY
1	F	511	GLY
1	F	638	PRO
1	F	639	GLY
1	F	689	GLY
1	F	1040	ILE
1	A	133	SER
1	A	263	ARG
1	A	923	ASN
1	A	992	SER
1	A	1043	SER
1	B	263	ARG
1	B	833	PRO
1	C	775	SER
1	C	870	GLY
1	C	1035	ARG
1	D	163	LYS
1	D	775	SER
1	E	511	GLY
1	E	775	SER
1	F	146	ASP

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Mol	Chain	Res	Type
1	F	862	MET
1	B	775	SER
1	C	62	THR
1	D	1034	SER
1	E	134	SER
1	E	263	ARG
1	E	1036	LYS
1	F	263	ARG
1	F	775	SER
1	B	892	TYR
1	B	923	ASN
1	C	6	ILE
1	C	357	LEU
1	D	62	THR
1	D	960	LEU
1	D	1033	PHE
1	E	903	LEU
1	F	507	GLU
1	F	536	ARG
1	F	752	ALA
1	B	676	THR
1	D	133	SER
1	E	62	THR
1	A	1040	ILE
1	C	658	ILE
1	D	751	GLY
1	E	508	GLY
1	F	751	GLY
1	E	639	GLY
1	A	1016	VAL
1	B	639	GLY
1	C	751	GLY
1	E	1016	VAL
1	F	658	ILE
1	A	427	PRO
1	A	910	ILE
1	F	6	ILE

### 5.3.2 Protein sidechains [i](#)

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	850/855 (99%)	788 (93%)	62 (7%)	14	44
1	B	848/855 (99%)	781 (92%)	67 (8%)	12	40
1	C	848/855 (99%)	780 (92%)	68 (8%)	12	40
1	D	848/855 (99%)	775 (91%)	73 (9%)	10	37
1	E	848/855 (99%)	771 (91%)	77 (9%)	9	34
1	F	849/855 (99%)	761 (90%)	88 (10%)	7	29
All	All	5091/5130 (99%)	4656 (92%)	435 (8%)	10	37

All (435) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	21	LEU
1	A	45	ILE
1	A	48	SER
1	A	49	TYR
1	A	93	THR
1	A	151	GLN
1	A	205	THR
1	A	222	THR
1	A	225	VAL
1	A	243	THR
1	A	293	LEU
1	A	310	LEU
1	A	321	LEU
1	A	324	VAL
1	A	336	SER
1	A	343	THR
1	A	360	GLN
1	A	362	PHE
1	A	400	LEU
1	A	428	LYS
1	A	462	SER
1	A	463	THR
1	A	483	LEU
1	A	489	THR
1	A	519	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	523	SER
1	A	524	THR
1	A	538	THR
1	A	559	LEU
1	A	561	SER
1	A	575	MET
1	A	634	TRP
1	A	662	MET
1	A	664	PHE
1	A	666	PHE
1	A	671	ILE
1	A	674	LEU
1	A	682	PHE
1	A	687	GLN
1	A	697	GLN
1	A	713	LEU
1	A	716	VAL
1	A	717	ARG
1	A	721	LEU
1	A	748	THR
1	A	760	ASN
1	A	768	VAL
1	A	797	GLN
1	A	804	PHE
1	A	815	ARG
1	A	817	GLU
1	A	843	LEU
1	A	857	TYR
1	A	961	ILE
1	A	964	THR
1	A	968	VAL
1	A	980	LEU
1	A	984	LEU
1	A	986	VAL
1	A	1007	VAL
1	A	1041	GLU
1	B	25	LEU
1	B	28	LEU
1	B	29	LYS
1	B	105	VAL
1	B	128	SER
1	B	131	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	145	THR
1	B	146	ASP
1	B	151	GLN
1	B	196	PHE
1	B	225	VAL
1	B	243	THR
1	B	255	GLN
1	B	259	ARG
1	B	277	ILE
1	B	295	THR
1	B	310	LEU
1	B	321	LEU
1	B	324	VAL
1	B	332	PHE
1	B	336	SER
1	B	353	LEU
1	B	355	MET
1	B	360	GLN
1	B	372	VAL
1	B	400	LEU
1	B	459	PHE
1	B	472	ILE
1	B	489	THR
1	B	519	MET
1	B	524	THR
1	B	561	SER
1	B	571	VAL
1	B	578	LEU
1	B	592	ASN
1	B	602	GLU
1	B	617	PHE
1	B	626	ILE
1	B	634	TRP
1	B	652	THR
1	B	653	ARG
1	B	659	LYS
1	B	672	VAL
1	B	673	GLU
1	B	682	PHE
1	B	687	GLN
1	B	694	LYS
1	B	695	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	708	LYS
1	B	717	ARG
1	B	721	LEU
1	B	748	THR
1	B	768	VAL
1	B	775	SER
1	B	804	PHE
1	B	806	SER
1	B	811	TYR
1	B	835	LYS
1	B	914	LEU
1	B	958	LYS
1	B	961	ILE
1	B	968	VAL
1	B	971	ARG
1	B	980	LEU
1	B	1007	VAL
1	B	1041	GLU
1	B	1043	SER
1	C	3	ASN
1	C	6	ILE
1	C	34	GLN
1	C	44	THR
1	C	48	SER
1	C	49	TYR
1	C	59	ASP
1	C	87	THR
1	C	93	THR
1	C	102	ILE
1	C	104	GLN
1	C	112	GLN
1	C	115	MET
1	C	151	GLN
1	C	174	ASP
1	C	177	LEU
1	C	222	THR
1	C	243	THR
1	C	274	ASN
1	C	300	LEU
1	C	336	SER
1	C	358	PHE
1	C	415	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	432	ARG
1	C	447	MET
1	C	462	SER
1	C	463	THR
1	C	472	ILE
1	C	482	VAL
1	C	489	THR
1	C	510	LYS
1	C	519	MET
1	C	524	THR
1	C	538	THR
1	C	540	ARG
1	C	542	LEU
1	C	561	SER
1	C	571	VAL
1	C	578	LEU
1	C	596	HIS
1	C	602	GLU
1	C	626	ILE
1	C	634	TRP
1	C	657	GLN
1	C	659	LYS
1	C	668	LEU
1	C	672	VAL
1	C	674	LEU
1	C	681	ASP
1	C	694	LYS
1	C	714	THR
1	C	716	VAL
1	C	721	LEU
1	C	724	THR
1	C	746	ILE
1	C	775	SER
1	C	804	PHE
1	C	807	SER
1	C	847	LEU
1	C	860	THR
1	C	876	LEU
1	C	895	TRP
1	C	947	GLU
1	C	950	LYS
1	C	958	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	980	LEU
1	C	991	ILE
1	C	1032	ARG
1	D	3	ASN
1	D	21	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	182	TYR
1	D	205	THR
1	D	243	THR
1	D	255	GLN
1	D	293	LEU
1	D	324	VAL
1	D	336	SER
1	D	355	MET
1	D	360	GLN
1	D	362	PHE
1	D	439	GLN
1	D	463	THR
1	D	472	ILE
1	D	483	LEU
1	D	519	MET
1	D	523	SER
1	D	524	THR
1	D	538	THR
1	D	564	LEU
1	D	566	ASP
1	D	571	VAL
1	D	575	MET
1	D	602	GLU
1	D	605	ASN
1	D	626	ILE
1	D	634	TRP
1	D	659	LYS
1	D	662	MET
1	D	666	PHE
1	D	668	LEU
1	D	671	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	674	LEU
1	D	682	PHE
1	D	687	GLN
1	D	697	GLN
1	D	713	LEU
1	D	714	THR
1	D	717	ARG
1	D	721	LEU
1	D	726	GLN
1	D	743	ILE
1	D	748	THR
1	D	757	SER
1	D	768	VAL
1	D	775	SER
1	D	797	GLN
1	D	804	PHE
1	D	806	SER
1	D	815	ARG
1	D	857	TYR
1	D	862	MET
1	D	865	GLN
1	D	901	VAL
1	D	918	PHE
1	D	922	THR
1	D	931	LEU
1	D	958	LYS
1	D	961	ILE
1	D	968	VAL
1	D	980	LEU
1	D	986	VAL
1	D	1007	VAL
1	D	1033	PHE
1	D	1041	GLU
1	D	1042	HIS
1	E	3	ASN
1	E	6	ILE
1	E	25	LEU
1	E	28	LEU
1	E	48	SER
1	E	49	TYR
1	E	60	THR
1	E	93	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	105	VAL
1	E	109	ASN
1	E	128	SER
1	E	145	THR
1	E	151	GLN
1	E	174	ASP
1	E	175	VAL
1	E	177	LEU
1	E	196	PHE
1	E	225	VAL
1	E	230	LEU
1	E	255	GLN
1	E	259	ARG
1	E	277	ILE
1	E	293	LEU
1	E	295	THR
1	E	324	VAL
1	E	329	THR
1	E	343	THR
1	E	355	MET
1	E	358	PHE
1	E	372	VAL
1	E	439	GLN
1	E	513	PHE
1	E	519	MET
1	E	523	SER
1	E	524	THR
1	E	526	HIS
1	E	540	ARG
1	E	559	LEU
1	E	561	SER
1	E	563	PHE
1	E	569	GLN
1	E	613	ASN
1	E	626	ILE
1	E	630	SER
1	E	634	TRP
1	E	659	LYS
1	E	662	MET
1	E	668	LEU
1	E	672	VAL
1	E	673	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	678	THR
1	E	687	GLN
1	E	694	LYS
1	E	695	LEU
1	E	697	GLN
1	E	699	ARG
1	E	708	LYS
1	E	713	LEU
1	E	714	THR
1	E	717	ARG
1	E	760	ASN
1	E	775	SER
1	E	804	PHE
1	E	806	SER
1	E	843	LEU
1	E	880	SER
1	E	958	LYS
1	E	961	ILE
1	E	968	VAL
1	E	971	ARG
1	E	980	LEU
1	E	986	VAL
1	E	1007	VAL
1	E	1032	ARG
1	E	1033	PHE
1	E	1041	GLU
1	E	1043	SER
1	F	3	ASN
1	F	6	ILE
1	F	28	LEU
1	F	34	GLN
1	F	45	ILE
1	F	48	SER
1	F	49	TYR
1	F	76	MET
1	F	81	ASN
1	F	87	THR
1	F	88	VAL
1	F	90	ILE
1	F	93	THR
1	F	96	SER
1	F	104	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	112	GLN
1	F	129	VAL
1	F	151	GLN
1	F	174	ASP
1	F	177	LEU
1	F	182	TYR
1	F	189	ASN
1	F	222	THR
1	F	243	THR
1	F	274	ASN
1	F	293	LEU
1	F	300	LEU
1	F	307	ARG
1	F	321	LEU
1	F	336	SER
1	F	362	PHE
1	F	418	ARG
1	F	432	ARG
1	F	447	MET
1	F	448	VAL
1	F	462	SER
1	F	472	ILE
1	F	482	VAL
1	F	489	THR
1	F	493	CYS
1	F	510	LYS
1	F	515	TRP
1	F	519	MET
1	F	524	THR
1	F	538	THR
1	F	540	ARG
1	F	559	LEU
1	F	564	LEU
1	F	571	VAL
1	F	578	LEU
1	F	596	HIS
1	F	602	GLU
1	F	615	PHE
1	F	626	ILE
1	F	630	SER
1	F	634	TRP
1	F	649	MET

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Mol	Chain	Res	Type
1	F	659	LYS
1	F	668	LEU
1	F	672	VAL
1	F	674	LEU
1	F	683	GLU
1	F	695	LEU
1	F	697	GLN
1	F	703	LEU
1	F	721	LEU
1	F	730	ASP
1	F	743	ILE
1	F	775	SER
1	F	804	PHE
1	F	806	SER
1	F	811	TYR
1	F	843	LEU
1	F	853	THR
1	F	862	MET
1	F	865	GLN
1	F	895	TRP
1	F	947	GLU
1	F	958	LYS
1	F	971	ARG
1	F	980	LEU
1	F	986	VAL
1	F	991	ILE
1	F	993	THR
1	F	1033	PHE
1	F	1035	ARG
1	F	1038	GLU
1	F	1044	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	229	GLN
1	A	231	ASN
1	A	361	ASN
1	A	605	ASN
1	B	34	GLN
1	B	228	GLN

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Mol	Chain	Res	Type
1	B	744	ASN
1	C	34	GLN
1	C	622	GLN
1	D	58	GLN
1	D	108	GLN
1	D	109	ASN
1	D	210	GLN
1	D	415	ASN
1	D	517	ASN
1	D	865	GLN
1	D	1037	ASN
1	E	67	GLN
1	E	104	GLN
1	E	231	ASN
1	E	588	GLN
1	E	592	ASN
1	E	667	ASN
1	F	81	ASN
1	F	104	GLN
1	F	108	GLN
1	F	210	GLN
1	F	228	GLN
1	F	231	ASN
1	F	439	GLN
1	F	692	HIS
1	F	726	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	LMT	E	1101	-	36,36,36	1.81	10 (27%)	47,47,47	1.69	11 (23%)
2	ERY	D	1101	-	53,53,53	1.27	2 (3%)	82,82,82	1.95	20 (24%)
3	LMT	A	1102	-	36,36,36	1.76	8 (22%)	47,47,47	1.43	7 (14%)
3	LMT	D	1102	-	36,36,36	1.78	9 (25%)	47,47,47	1.06	2 (4%)
3	LMT	D	1103	-	36,36,36	1.87	10 (27%)	47,47,47	1.45	5 (10%)
3	LMT	C	1101	-	36,36,36	1.76	9 (25%)	47,47,47	1.11	4 (8%)
2	ERY	A	1101	-	53,53,53	1.22	3 (5%)	82,82,82	2.05	23 (28%)
3	LMT	B	1101	-	36,36,36	1.85	11 (30%)	47,47,47	1.58	10 (21%)
3	LMT	A	1103	-	36,36,36	1.79	8 (22%)	47,47,47	1.60	10 (21%)
3	LMT	F	1101	-	36,36,36	1.84	9 (25%)	47,47,47	1.16	4 (8%)

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	E	1101	-	-	14/21/61/61	0/2/2/2
2	ERY	D	1101	-	-	24/72/107/107	1/3/3/3
3	LMT	A	1102	-	-	8/21/61/61	0/2/2/2
3	LMT	D	1102	-	-	11/21/61/61	0/2/2/2
3	LMT	D	1103	-	-	10/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	9/21/61/61	0/2/2/2
2	ERY	A	1101	-	-	35/72/107/107	0/3/3/3
3	LMT	B	1101	-	-	12/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	13/21/61/61	0/2/2/2
3	LMT	F	1101	-	-	8/21/61/61	0/2/2/2

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	ERY	O2-C1	5.97	1.48	1.34
2	A	1101	ERY	O2-C1	5.12	1.46	1.34
3	E	1101	LMT	O1 <sup>2</sup> -C1'	4.71	1.48	1.40
3	B	1101	LMT	O1 <sup>2</sup> -C1'	4.53	1.47	1.40
3	F	1101	LMT	O1 <sup>2</sup> -C1'	4.30	1.47	1.40
3	D	1103	LMT	O1 <sup>2</sup> -C1'	4.28	1.47	1.40
3	A	1103	LMT	O5B-C1B	4.26	1.52	1.41
3	D	1103	LMT	O5 <sup>2</sup> -C5'	4.23	1.54	1.44
3	D	1102	LMT	O1 <sup>2</sup> -C1'	4.12	1.47	1.40
3	D	1103	LMT	O5B-C1B	4.12	1.52	1.41
3	C	1101	LMT	O5 <sup>2</sup> -C5'	4.02	1.54	1.44
3	A	1102	LMT	O5 <sup>2</sup> -C5'	3.92	1.53	1.44
3	B	1101	LMT	O5B-C1B	3.88	1.51	1.41
3	D	1102	LMT	O5 <sup>2</sup> -C5'	3.88	1.53	1.44
3	F	1101	LMT	O5 <sup>2</sup> -C5'	3.81	1.53	1.44
3	A	1103	LMT	O1 <sup>2</sup> -C1'	3.73	1.46	1.40
3	A	1102	LMT	O5B-C1B	3.71	1.51	1.41
3	F	1101	LMT	O5B-C1B	3.70	1.51	1.41
3	A	1102	LMT	O1 <sup>2</sup> -C1'	3.58	1.46	1.40
3	B	1101	LMT	O5 <sup>2</sup> -C5'	3.53	1.52	1.44
3	D	1103	LMT	O5 <sup>2</sup> -C1'	3.52	1.50	1.41
3	C	1101	LMT	O1 <sup>2</sup> -C1'	3.52	1.46	1.40
3	D	1103	LMT	O3B-C3B	3.48	1.51	1.43
3	D	1102	LMT	O5B-C1B	3.43	1.50	1.41
3	E	1101	LMT	O5 <sup>2</sup> -C5'	3.41	1.52	1.44
3	A	1103	LMT	O3B-C3B	3.40	1.51	1.43
3	D	1102	LMT	C6 <sup>2</sup> -C5'	-3.36	1.40	1.51
3	A	1103	LMT	O5 <sup>2</sup> -C5'	3.35	1.52	1.44
3	A	1103	LMT	C6 <sup>2</sup> -C5'	-3.35	1.40	1.51
3	C	1101	LMT	O5 <sup>2</sup> -C1'	3.33	1.50	1.41
3	E	1101	LMT	C6 <sup>2</sup> -C5'	-3.24	1.41	1.51
3	C	1101	LMT	O5B-C1B	3.21	1.50	1.41
3	D	1102	LMT	O5 <sup>2</sup> -C1'	3.14	1.49	1.41
3	E	1101	LMT	O5 <sup>2</sup> -C1'	3.13	1.49	1.41
3	B	1101	LMT	O5 <sup>2</sup> -C1'	3.12	1.49	1.41
3	E	1101	LMT	O5B-C1B	3.09	1.49	1.41
3	B	1101	LMT	C6 <sup>2</sup> -C5'	-3.08	1.41	1.51
3	F	1101	LMT	O5 <sup>2</sup> -C1'	3.08	1.49	1.41
3	C	1101	LMT	C6 <sup>2</sup> -C5'	-3.05	1.41	1.51
3	A	1102	LMT	C6 <sup>2</sup> -C5'	-3.02	1.41	1.51
3	F	1101	LMT	C6 <sup>2</sup> -C5'	-3.01	1.41	1.51
3	E	1101	LMT	O3B-C3B	2.94	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	LMT	O5'-C1'	2.90	1.49	1.41
3	D	1102	LMT	O3B-C3B	2.89	1.49	1.43
3	A	1102	LMT	O3B-C3B	2.84	1.49	1.43
3	D	1103	LMT	O2'-C2'	2.84	1.49	1.43
3	D	1103	LMT	C6'-C5'	-2.67	1.42	1.51
3	B	1101	LMT	O2'-C2'	2.66	1.49	1.43
3	F	1101	LMT	O3B-C3B	2.65	1.49	1.43
3	A	1103	LMT	O2'-C2'	2.64	1.49	1.43
3	A	1103	LMT	O5'-C1'	2.63	1.48	1.41
3	C	1101	LMT	O2'-C2'	2.61	1.49	1.43
2	D	1101	ERY	O9-C22	2.48	1.48	1.41
3	B	1101	LMT	O3B-C3B	2.43	1.48	1.43
3	B	1101	LMT	O3'-C3'	2.43	1.48	1.43
3	C	1101	LMT	O3B-C3B	2.41	1.48	1.43
3	D	1102	LMT	O2'-C2'	2.39	1.48	1.43
3	A	1102	LMT	O2'-C2'	2.37	1.48	1.43
3	E	1101	LMT	O2'-C2'	2.32	1.48	1.43
3	C	1101	LMT	C3B-C2B	-2.29	1.46	1.52
3	D	1102	LMT	O3'-C3'	2.25	1.48	1.43
3	E	1101	LMT	C3B-C2B	-2.22	1.46	1.52
3	A	1103	LMT	O3'-C3'	2.22	1.48	1.43
3	B	1101	LMT	C3'-C2'	-2.21	1.46	1.52
3	C	1101	LMT	C3'-C2'	-2.21	1.46	1.52
3	F	1101	LMT	C3'-C2'	-2.20	1.46	1.52
3	E	1101	LMT	O3'-C3'	2.17	1.48	1.43
2	A	1101	ERY	C23-C24	2.15	1.58	1.53
3	D	1103	LMT	O3'-C3'	2.15	1.48	1.43
3	B	1101	LMT	C5-C4	2.09	1.63	1.51
3	F	1101	LMT	O3'-C3'	2.08	1.47	1.43
3	E	1101	LMT	C3'-C2'	-2.06	1.47	1.52
3	F	1101	LMT	C5-C4	2.06	1.63	1.51
3	D	1103	LMT	C4'-C5'	2.05	1.58	1.52
2	A	1101	ERY	O6-C17	2.04	1.46	1.42
3	D	1102	LMT	C5-C4	2.03	1.63	1.51
3	D	1103	LMT	C5-C4	2.03	1.63	1.51
3	A	1102	LMT	C5-C4	2.02	1.62	1.51
3	B	1101	LMT	C3B-C2B	-2.01	1.47	1.52

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	ERY	C20-O5-C16	6.02	130.12	117.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	ERY	O7-C5-C4	-5.93	102.66	111.54
2	D	1101	ERY	O12-C11-C10	5.44	118.84	110.71
2	D	1101	ERY	C22-O7-C5	5.29	125.44	116.25
2	D	1101	ERY	C29-N1-C24	4.95	128.00	113.11
2	A	1101	ERY	O2-C1-O1	-4.87	114.85	123.94
3	E	1101	LMT	C1'-C2'-C3'	4.82	120.04	110.00
2	D	1101	ERY	C33-C8-C7	-4.74	101.10	109.81
3	A	1102	LMT	C1'-C2'-C3'	4.57	119.52	110.00
3	A	1103	LMT	C1'-O5'-C5'	-4.55	104.76	113.69
2	A	1101	ERY	C22-O7-C5	4.51	124.09	116.25
2	A	1101	ERY	C13-O2-C1	-4.40	110.35	118.18
3	A	1102	LMT	C2'-C3'-C4'	4.40	119.73	109.68
3	B	1101	LMT	O1'-C1'-C2'	4.26	114.95	108.30
2	A	1101	ERY	C19-C16-C15	-4.22	102.96	110.49
3	F	1101	LMT	O5B-C5B-C4B	4.10	117.15	109.69
2	D	1101	ERY	O2-C13-C36	4.08	115.17	107.40
3	E	1101	LMT	O5B-C5B-C4B	3.97	116.89	109.69
3	E	1101	LMT	O1'-C1'-C2'	3.94	114.45	108.30
2	D	1101	ERY	C20-O5-C16	3.90	125.70	117.55
3	A	1103	LMT	C2'-C3'-C4'	3.90	118.59	109.68
2	D	1101	ERY	C25-C24-N1	-3.74	105.11	115.67
3	B	1101	LMT	C1B-O1B-C4'	-3.69	108.83	117.96
3	A	1103	LMT	C1'-C2'-C3'	3.66	117.61	110.00
3	A	1103	LMT	C3B-C4B-C5B	3.61	116.68	110.24
3	E	1101	LMT	O2'-C2'-C3'	-3.56	102.12	110.35
3	D	1103	LMT	C1'-C2'-C3'	3.51	117.30	110.00
3	B	1101	LMT	C3B-C4B-C5B	3.41	116.32	110.24
3	D	1103	LMT	C3B-C4B-C5B	3.37	116.25	110.24
3	F	1101	LMT	C1-O1'-C1'	3.35	119.40	113.84
2	A	1101	ERY	O2-C13-C12	3.32	112.70	107.29
3	C	1101	LMT	C6B-C5B-C4B	-3.20	105.51	113.00
2	A	1101	ERY	C29-N1-C24	3.20	122.73	113.11
3	E	1101	LMT	C1B-C2B-C3B	-3.20	103.33	110.00
3	D	1103	LMT	C1B-O1B-C4'	-3.19	110.06	117.96
2	D	1101	ERY	C3-C4-C5	3.15	117.96	111.19
2	A	1101	ERY	C3-C4-C5	3.10	117.86	111.19
3	D	1102	LMT	C1'-C2'-C3'	3.09	116.44	110.00
3	C	1101	LMT	C1B-O1B-C4'	-3.05	110.42	117.96
3	E	1101	LMT	C2'-C3'-C4'	3.04	116.63	109.68
2	A	1101	ERY	O7-C22-C23	3.04	115.98	108.10
2	A	1101	ERY	O7-C5-C6	3.01	110.11	106.39
2	D	1101	ERY	C22-O9-C26	2.99	117.65	112.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1103	LMT	C2'-C3'-C4'	2.99	116.50	109.68
3	B	1101	LMT	O5B-C5B-C4B	2.94	115.04	109.69
3	B	1101	LMT	C6B-C5B-C4B	-2.91	106.19	113.00
3	C	1101	LMT	O5B-C5B-C4B	2.88	114.92	109.69
3	B	1101	LMT	O3B-C3B-C2B	-2.87	103.71	110.35
2	D	1101	ERY	O7-C5-C4	-2.85	107.27	111.54
2	D	1101	ERY	O9-C26-C27	2.84	112.91	106.88
3	B	1101	LMT	C4B-C3B-C2B	2.83	115.76	110.82
2	D	1101	ERY	O4-C18-C21	2.79	112.73	106.70
3	A	1102	LMT	C1B-O1B-C4'	-2.77	111.10	117.96
2	D	1101	ERY	C33-C8-C9	2.77	116.08	109.44
2	D	1101	ERY	C36-C13-C12	-2.75	109.99	115.20
2	D	1101	ERY	C31-C4-C3	-2.69	106.57	111.40
2	A	1101	ERY	O2-C1-C2	2.66	117.40	111.56
2	A	1101	ERY	C31-C4-C3	-2.65	106.66	111.40
3	A	1103	LMT	O5B-C5B-C6B	2.62	112.95	106.44
2	D	1101	ERY	O5-C16-C17	2.55	107.58	103.81
2	D	1101	ERY	C30-C2-C3	2.53	118.65	112.92
3	A	1103	LMT	O1'-C1'-C2'	2.53	112.25	108.30
3	E	1101	LMT	C1B-O1B-C4'	-2.52	111.73	117.96
3	A	1103	LMT	O5B-C5B-C4B	2.50	114.24	109.69
3	F	1101	LMT	C1'-C2'-C3'	2.48	115.16	110.00
3	C	1101	LMT	O3B-C3B-C2B	-2.47	104.64	110.35
2	A	1101	ERY	O12-C11-C10	2.45	114.38	110.71
2	A	1101	ERY	O4-C18-C21	2.45	111.99	106.70
3	D	1102	LMT	O2B-C2B-C1B	-2.44	104.12	110.05
2	A	1101	ERY	O9-C26-C27	2.43	112.04	106.88
2	A	1101	ERY	O10-C6-C32	-2.42	102.89	108.47
2	A	1101	ERY	C15-C16-C17	2.39	111.95	107.67
3	D	1103	LMT	O1B-C1B-C2B	2.38	114.27	108.10
3	E	1101	LMT	O5'-C5'-C6'	2.37	112.34	106.44
3	E	1101	LMT	O5B-C1B-C2B	-2.37	105.34	110.35
3	B	1101	LMT	C1B-O5B-C5B	2.35	118.31	113.69
3	A	1102	LMT	O5B-C5B-C4B	2.31	113.88	109.69
3	E	1101	LMT	O5'-C5'-C4'	-2.30	104.91	109.75
3	A	1102	LMT	O1'-C1'-C2'	2.27	111.85	108.30
2	A	1101	ERY	C7-C8-C9	-2.24	109.47	113.32
2	A	1101	ERY	C35-C12-C13	2.21	114.42	111.31
3	F	1101	LMT	C6B-C5B-C4B	-2.21	107.83	113.00
3	B	1101	LMT	O3B-C3B-C4B	-2.20	105.26	110.35
3	A	1102	LMT	O2'-C2'-C3'	-2.20	105.26	110.35
3	A	1103	LMT	C4B-C3B-C2B	2.19	114.64	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	LMT	O5'-C5'-C6'	2.18	111.86	106.44
3	A	1103	LMT	O5'-C5'-C4'	-2.15	105.23	109.75
2	A	1101	ERY	C30-C2-C3	2.13	117.75	112.92
3	A	1103	LMT	C1B-O5B-C5B	2.12	117.85	113.69
2	A	1101	ERY	C25-C24-N1	-2.12	109.69	115.67
2	A	1101	ERY	O6-C17-C16	2.12	115.08	111.12
2	D	1101	ERY	O13-C12-C13	-2.09	103.92	107.28
2	D	1101	ERY	C16-C17-C18	-2.07	107.96	111.14
3	E	1101	LMT	O5'-C1'-C2'	2.04	114.67	110.35
3	B	1101	LMT	C3'-C4'-C5'	2.02	115.55	110.93
2	D	1101	ERY	O11-C9-C10	-2.00	117.76	120.60

There are no chirality outliers.

All (144) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	ERY	C9-C10-C11-C12
2	A	1101	ERY	C34-C10-C11-C12
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	C11-C12-C13-C36
2	A	1101	ERY	O13-C12-C13-O2
2	A	1101	ERY	C2-C1-O2-C13
2	A	1101	ERY	O1-C1-C2-C3
2	A	1101	ERY	C6-C5-O7-C22
2	A	1101	ERY	C32-C6-C7-C8
2	A	1101	ERY	O10-C6-C7-C8
2	A	1101	ERY	C23-C24-N1-C29
2	A	1101	ERY	C25-C24-N1-C29
2	D	1101	ERY	C9-C10-C11-C12
2	D	1101	ERY	C34-C10-C11-C12
2	D	1101	ERY	C10-C11-C12-C13
2	D	1101	ERY	C10-C11-C12-C35
2	D	1101	ERY	C10-C11-C12-O13
2	D	1101	ERY	O12-C11-C12-C35
2	D	1101	ERY	O12-C11-C12-O13
2	D	1101	ERY	O1-C1-O2-C13

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Mol	Chain	Res	Type	Atoms
2	D	1101	ERY	C33-C8-C9-C10
2	D	1101	ERY	C33-C8-C9-O11
2	D	1101	ERY	C23-C24-N1-C29
2	D	1101	ERY	C25-C24-N1-C29
3	A	1103	LMT	C2'-C1'-O1'-C1
3	A	1103	LMT	O5'-C1'-O1'-C1
3	C	1101	LMT	C2'-C1'-O1'-C1
3	C	1101	LMT	O5'-C1'-O1'-C1
3	D	1102	LMT	C2'-C1'-O1'-C1
3	E	1101	LMT	C2'-C1'-O1'-C1
3	E	1101	LMT	O5'-C1'-O1'-C1
3	E	1101	LMT	O5'-C5'-C6'-O6'
3	D	1103	LMT	O5B-C1B-O1B-C4'
2	D	1101	ERY	C2-C1-O2-C13
3	D	1103	LMT	C2-C3-C4-C5
3	D	1102	LMT	C3-C4-C5-C6
3	E	1101	LMT	C3-C4-C5-C6
3	A	1103	LMT	O5B-C1B-O1B-C4'
3	E	1101	LMT	C4'-C5'-C6'-O6'
3	F	1101	LMT	C4B-C5B-C6B-O6B
3	D	1102	LMT	C4B-C5B-C6B-O6B
2	A	1101	ERY	C25-C24-N1-C28
3	C	1101	LMT	O5'-C5'-C6'-O6'
3	E	1101	LMT	C4B-C5B-C6B-O6B
3	A	1103	LMT	C4B-C5B-C6B-O6B
3	B	1101	LMT	C4B-C5B-C6B-O6B
3	C	1101	LMT	C4'-C5'-C6'-O6'
3	D	1103	LMT	C4-C5-C6-C7
3	F	1101	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	C5-C6-C7-C8
3	C	1101	LMT	C6-C7-C8-C9
3	D	1102	LMT	O5B-C5B-C6B-O6B
3	D	1102	LMT	O5'-C1'-O1'-C1
3	A	1102	LMT	O1'-C1-C2-C3
2	A	1101	ERY	O1-C1-O2-C13
3	E	1101	LMT	O1'-C1-C2-C3
3	A	1103	LMT	O5'-C5'-C6'-O6'
3	B	1101	LMT	C4'-C5'-C6'-O6'
3	C	1101	LMT	O1'-C1-C2-C3
3	B	1101	LMT	O5'-C5'-C6'-O6'
2	A	1101	ERY	O2-C13-C36-C37
3	B	1101	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	1101	LMT	C3-C4-C5-C6
3	A	1102	LMT	C2'-C1'-O1'-C1
3	D	1102	LMT	C11-C10-C9-C8
3	C	1101	LMT	C2-C1-O1'-C1'
3	E	1101	LMT	C2-C1-O1'-C1'
3	E	1101	LMT	C5-C6-C7-C8
2	A	1101	ERY	C4-C5-O7-C22
3	A	1103	LMT	C2-C3-C4-C5
3	B	1101	LMT	O5B-C5B-C6B-O6B
2	A	1101	ERY	C2-C3-C4-C31
3	F	1101	LMT	O1'-C1-C2-C3
2	A	1101	ERY	O3-C3-C4-C5
3	A	1102	LMT	O5'-C1'-O1'-C1
3	E	1101	LMT	C6-C7-C8-C9
2	A	1101	ERY	C35-C12-C13-C36
2	D	1101	ERY	C35-C12-C13-O2
3	D	1103	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	C1-C2-C3-C4
3	B	1101	LMT	C11-C10-C9-C8
3	D	1102	LMT	O1'-C1-C2-C3
3	E	1101	LMT	C9-C10-C11-C12
3	A	1103	LMT	C4'-C5'-C6'-O6'
3	F	1101	LMT	C7-C8-C9-C10
2	D	1101	ERY	O12-C11-C12-C13
3	B	1101	LMT	C4-C5-C6-C7
3	B	1101	LMT	C9-C10-C11-C12
2	A	1101	ERY	O4-C14-O3-C3
3	F	1101	LMT	C4-C5-C6-C7
3	D	1102	LMT	C1-C2-C3-C4
2	A	1101	ERY	C7-C8-C9-C10
3	F	1101	LMT	C3-C4-C5-C6
3	D	1103	LMT	C2-C1-O1'-C1'
2	A	1101	ERY	O3-C3-C4-C31
3	D	1103	LMT	C6-C7-C8-C9
3	F	1101	LMT	C1-C2-C3-C4
3	D	1102	LMT	C6-C7-C8-C9
2	A	1101	ERY	C34-C10-C11-O12
3	B	1101	LMT	C5-C6-C7-C8
3	A	1103	LMT	C4-C5-C6-C7
3	D	1103	LMT	C7-C8-C9-C10
3	A	1103	LMT	O5B-C5B-C6B-O6B
3	A	1103	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	D	1102	LMT	C5-C6-C7-C8
3	E	1101	LMT	O5B-C5B-C6B-O6B
3	A	1103	LMT	C5-C6-C7-C8
2	D	1101	ERY	C11-C12-C13-O2
2	A	1101	ERY	C2-C3-C4-C5
3	B	1101	LMT	C6-C7-C8-C9
2	A	1101	ERY	C7-C8-C9-O11
2	D	1101	ERY	C4-C5-O7-C22
2	D	1101	ERY	C6-C5-O7-C22
2	D	1101	ERY	O4-C14-O3-C3
3	A	1103	LMT	C6-C7-C8-C9
3	D	1103	LMT	C3-C4-C5-C6
2	A	1101	ERY	C6-C7-C8-C33
2	D	1101	ERY	C7-C8-C9-C10
3	D	1103	LMT	C1-C2-C3-C4
3	D	1102	LMT	C9-C10-C11-C12
2	A	1101	ERY	C12-C13-C36-C37
2	D	1101	ERY	C32-C6-C7-C8
3	E	1101	LMT	C11-C10-C9-C8
3	A	1102	LMT	C11-C10-C9-C8
3	A	1102	LMT	C2-C3-C4-C5
3	E	1101	LMT	C4-C5-C6-C7
2	D	1101	ERY	C34-C10-C11-O12
2	A	1101	ERY	C9-C10-C11-O12
2	D	1101	ERY	C9-C10-C11-O12
3	C	1101	LMT	C4-C5-C6-C7
2	A	1101	ERY	C6-C7-C8-C9
3	C	1101	LMT	C7-C8-C9-C10
3	D	1103	LMT	C9-C10-C11-C12
3	F	1101	LMT	C4'-C5'-C6'-O6'
3	A	1103	LMT	C1-C2-C3-C4
2	D	1101	ERY	C7-C8-C9-O11
3	A	1102	LMT	C2-C1-O1'-C1'
3	A	1102	LMT	C3-C4-C5-C6

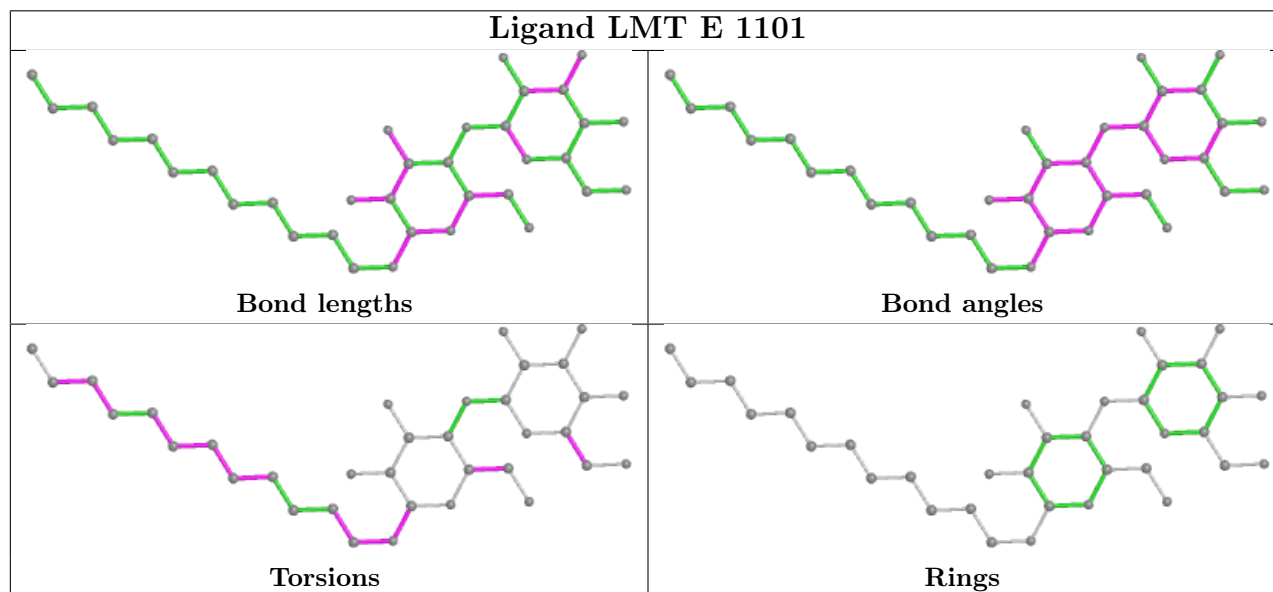
All (1) ring outliers are listed below:

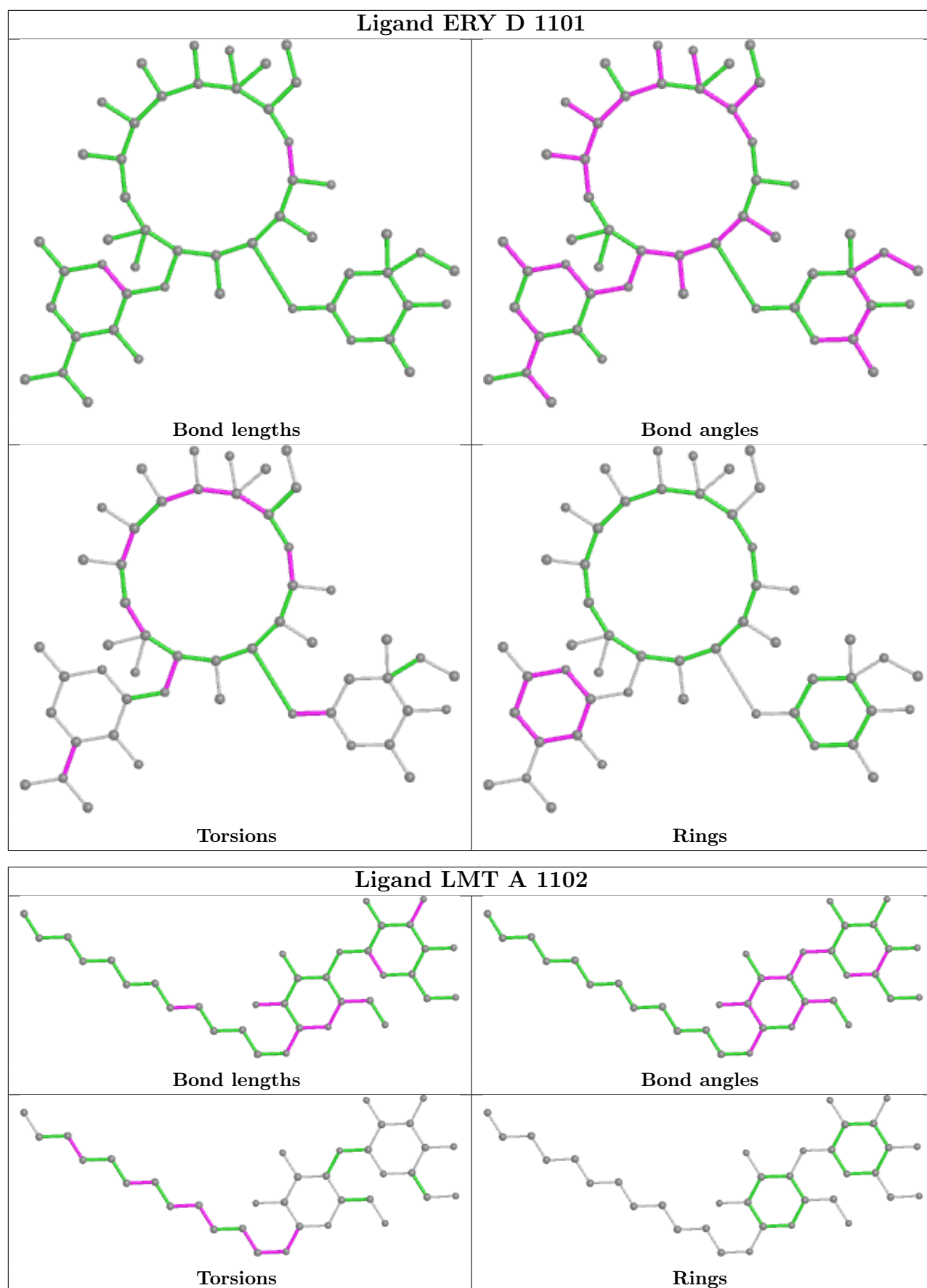
Mol	Chain	Res	Type	Atoms
2	D	1101	ERY	C22-C23-C24-C25-C26-O9

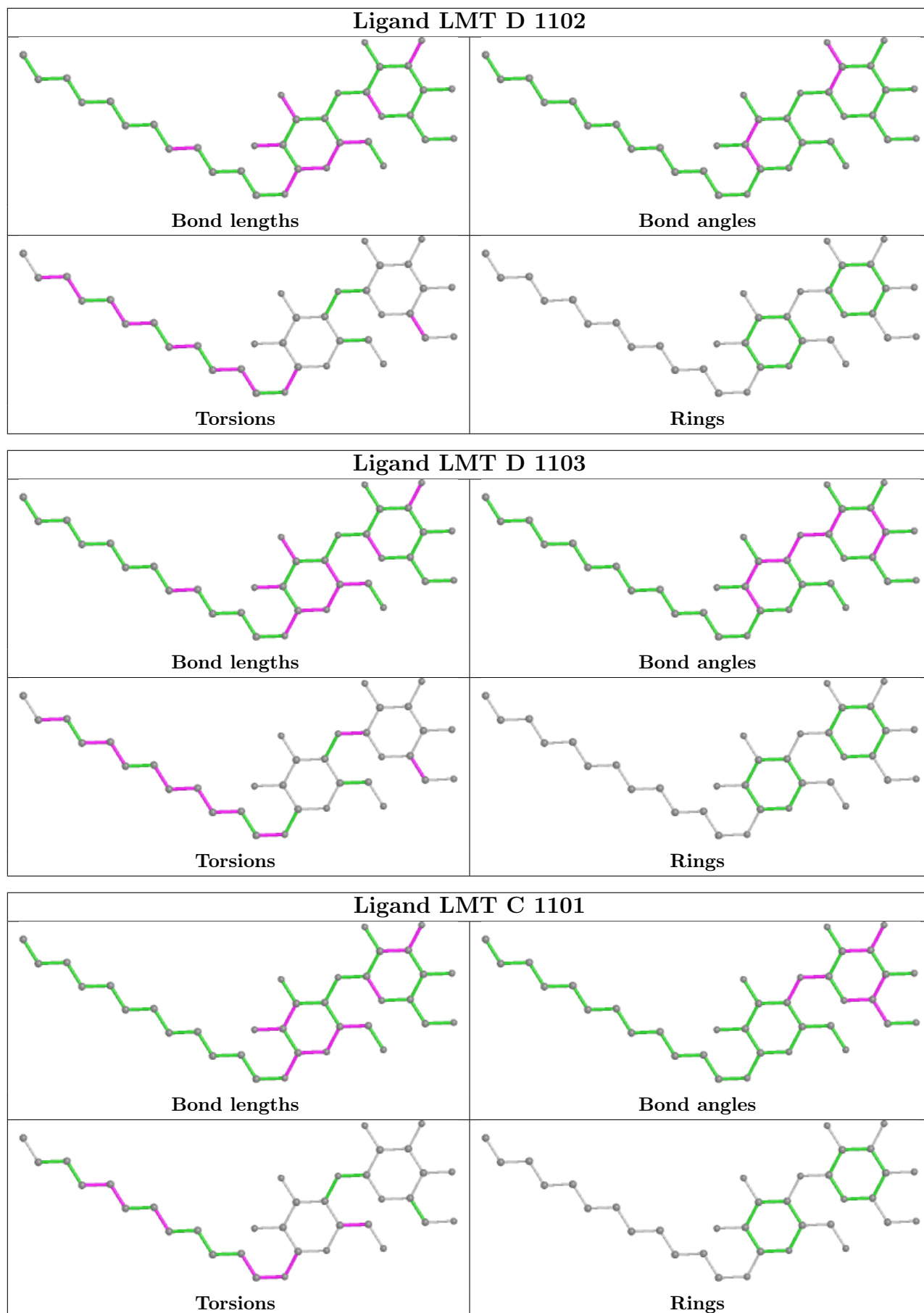
9 monomers are involved in 50 short contacts:

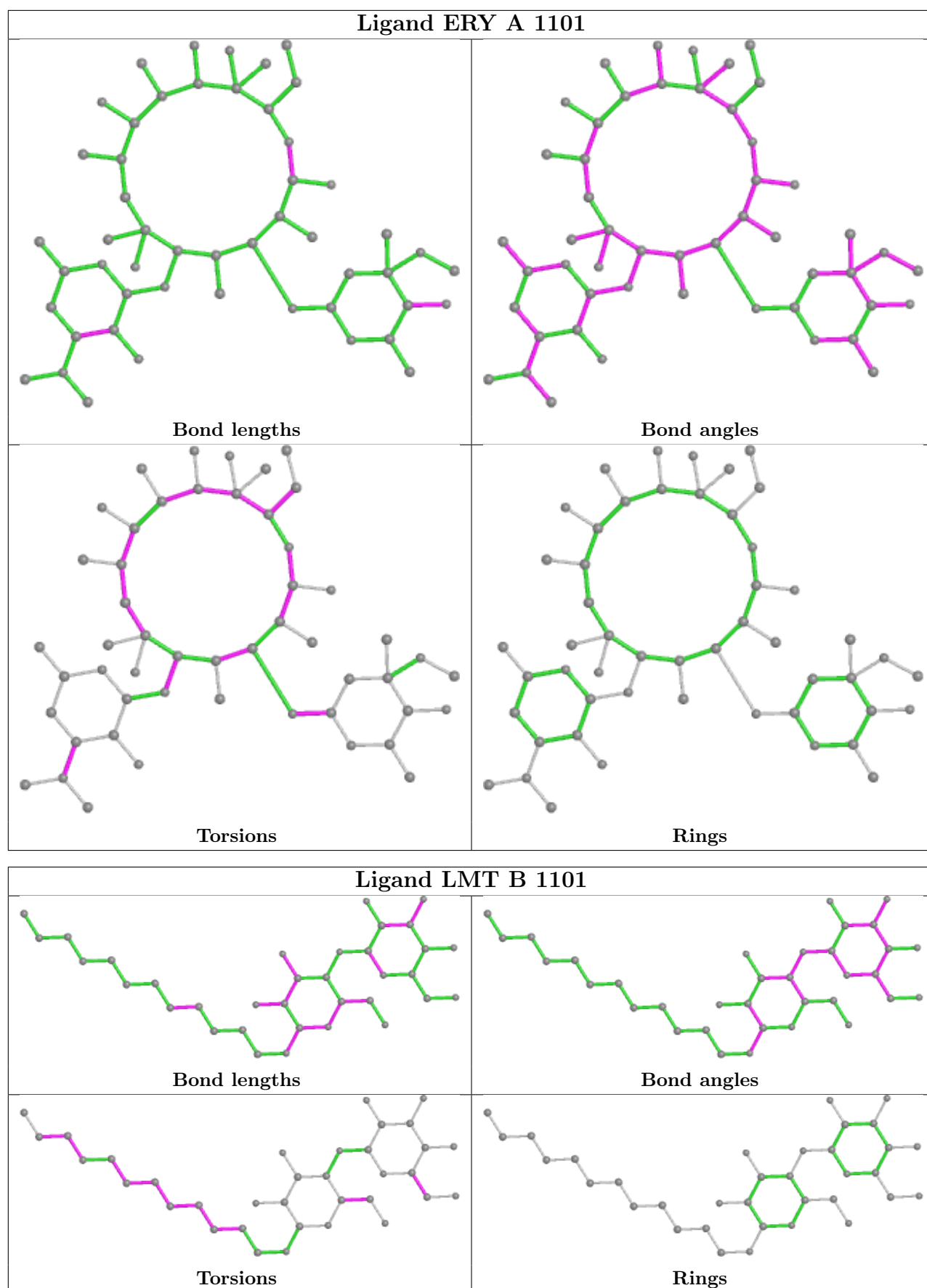
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1101	LMT	5	0
2	D	1101	ERY	12	0
3	A	1102	LMT	5	0
3	D	1102	LMT	1	0
3	D	1103	LMT	5	0
3	C	1101	LMT	2	0
2	A	1101	ERY	6	0
3	B	1101	LMT	5	0
3	A	1103	LMT	9	0

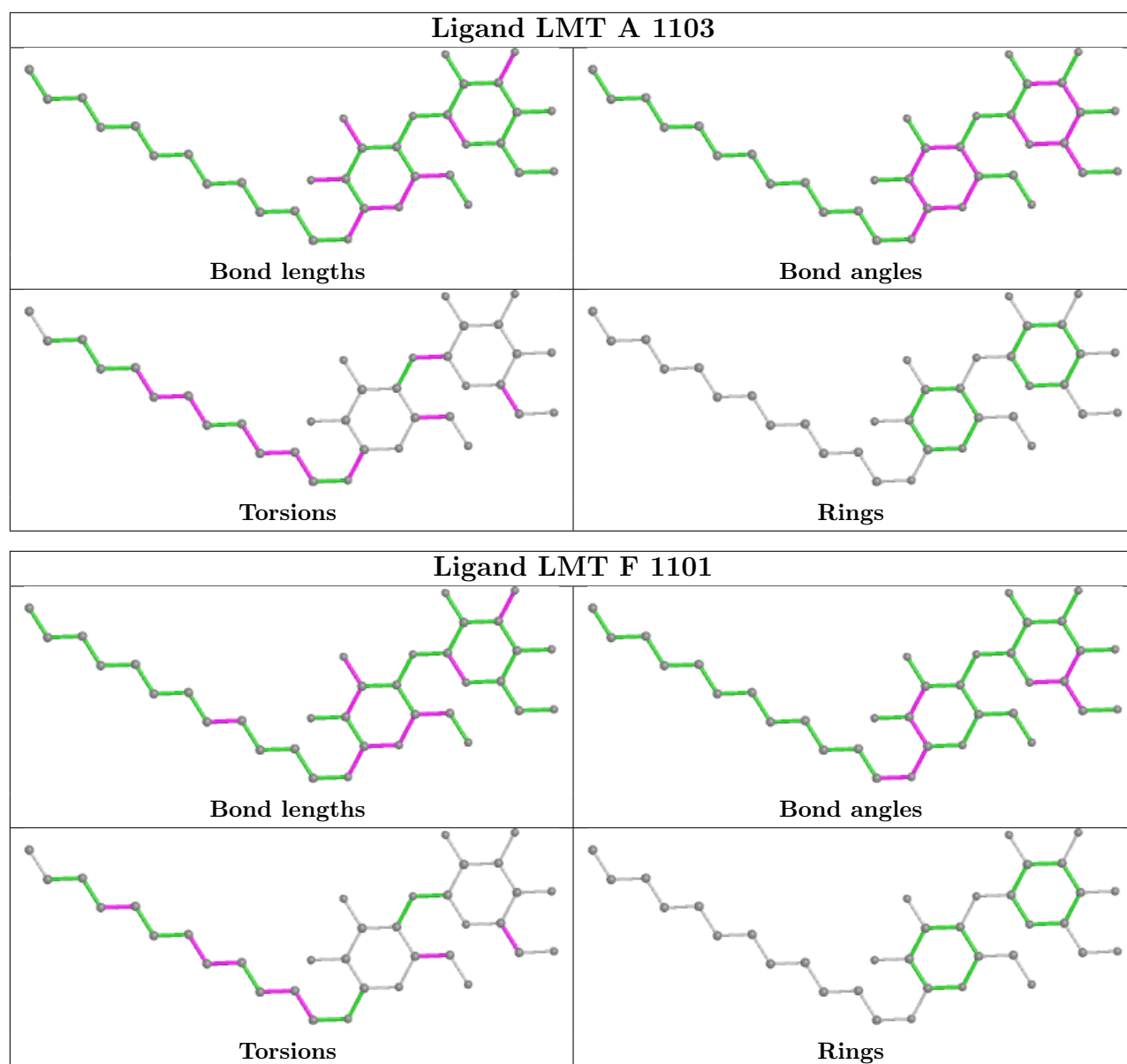
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1044/1049 (99%)	0.65	141 (13%) 3 4	46, 78, 106, 147	0
1	B	1042/1049 (99%)	0.65	140 (13%) 3 4	50, 76, 102, 148	0
1	C	1042/1049 (99%)	0.89	169 (16%) 1 2	43, 77, 103, 155	0
1	D	1042/1049 (99%)	0.83	162 (15%) 2 3	45, 86, 112, 147	0
1	E	1042/1049 (99%)	0.82	180 (17%) 1 2	55, 86, 108, 147	0
1	F	1043/1049 (99%)	0.96	212 (20%) 1 1	52, 82, 106, 158	0
All	All	6255/6294 (99%)	0.80	1004 (16%) 1 2	43, 81, 107, 158	0

All (1004) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	720	GLY	16.8
1	F	48	SER	14.6
1	C	719	ASN	14.1
1	F	719	ASN	13.5
1	F	720	GLY	12.3
1	D	619	GLY	11.9
1	C	80	SER	11.2
1	F	79	SER	10.6
1	D	621	GLY	9.5
1	E	291	ILE	9.5
1	E	719	ASN	9.3
1	D	463	THR	9.2
1	E	81	ASN	9.2
1	E	720	GLY	8.9
1	E	618	ALA	8.9
1	E	617	PHE	8.9
1	B	620	ARG	8.7
1	A	619	GLY	8.6
1	B	869	SER	8.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	617	PHE	8.5
1	F	80	SER	8.2
1	F	442	LEU	8.2
1	F	676	THR	8.1
1	F	9	PRO	8.0
1	D	620	ARG	8.0
1	C	815	ARG	7.8
1	E	681	ASP	7.8
1	F	91	THR	7.6
1	C	836	SER	7.6
1	B	895	TRP	7.5
1	D	462	SER	7.5
1	F	712	MET	7.4
1	F	618	ALA	7.3
1	E	619	GLY	7.3
1	A	618	ALA	7.3
1	C	83	ASP	7.2
1	B	615	PHE	7.1
1	C	79	SER	7.1
1	A	615	PHE	7.1
1	D	615	PHE	7.1
1	E	290	GLY	7.1
1	D	866	GLU	7.1
1	D	459	PHE	7.0
1	F	503	GLY	7.0
1	D	719	ASN	7.0
1	B	870	GLY	7.0
1	A	400	LEU	7.0
1	D	460	GLY	6.9
1	D	720	GLY	6.9
1	C	619	GLY	6.9
1	F	675	GLY	6.9
1	A	13	TRP	6.8
1	C	618	ALA	6.8
1	D	1038	GLU	6.8
1	C	501	ALA	6.8
1	E	943	ILE	6.7
1	C	9	PRO	6.7
1	D	869	SER	6.6
1	F	836	SER	6.6
1	E	615	PHE	6.6
1	C	721	LEU	6.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	47	ALA	6.6
1	E	488	LEU	6.5
1	C	872	GLN	6.5
1	C	835	LYS	6.5
1	B	617	PHE	6.5
1	F	406	VAL	6.4
1	C	617	PHE	6.4
1	B	488	LEU	6.3
1	F	405	LEU	6.3
1	B	229	GLN	6.3
1	F	865	GLN	6.3
1	F	46	SER	6.2
1	C	826	GLU	6.2
1	D	618	ALA	6.2
1	F	619	GLY	6.2
1	F	81	ASN	6.2
1	F	711	ASP	6.2
1	F	721	LEU	6.1
1	F	826	GLU	6.0
1	F	617	PHE	6.0
1	D	323	ILE	6.0
1	A	620	ARG	6.0
1	C	871	ASN	6.0
1	A	403	GLY	5.9
1	A	719	ASN	5.9
1	B	79	SER	5.9
1	F	10	ILE	5.9
1	B	403	GLY	5.9
1	C	81	ASN	5.9
1	D	663	VAL	5.9
1	F	69	MET	5.8
1	C	1038	GLU	5.8
1	F	835	LYS	5.8
1	B	943	ILE	5.8
1	F	713	LEU	5.7
1	D	1037	ASN	5.7
1	E	91	THR	5.7
1	C	1039	ASP	5.7
1	D	870	GLY	5.7
1	E	620	ARG	5.7
1	F	815	ARG	5.6
1	C	888	LEU	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	486	LEU	5.6
1	E	79	SER	5.6
1	B	618	ALA	5.6
1	F	230	LEU	5.5
1	A	621	GLY	5.5
1	E	80	SER	5.5
1	F	481	SER	5.5
1	F	13	TRP	5.5
1	F	837	THR	5.5
1	E	680	PHE	5.5
1	D	895	TRP	5.5
1	D	960	LEU	5.5
1	F	407	ASP	5.5
1	C	837	THR	5.5
1	C	445	ILE	5.4
1	E	314	GLU	5.4
1	F	869	SER	5.4
1	B	619	GLY	5.4
1	F	410	ILE	5.4
1	A	404	LEU	5.4
1	F	107	VAL	5.4
1	C	712	MET	5.4
1	A	445	ILE	5.4
1	E	901	VAL	5.3
1	F	620	ARG	5.3
1	E	495	THR	5.3
1	F	473	THR	5.3
1	F	445	ILE	5.3
1	E	308	ALA	5.3
1	F	403	GLY	5.2
1	C	782	LEU	5.2
1	E	315	PRO	5.2
1	B	621	GLY	5.2
1	D	617	PHE	5.2
1	D	681	ASP	5.1
1	B	714	THR	5.1
1	F	888	LEU	5.1
1	F	449	LEU	5.1
1	B	716	VAL	5.1
1	C	494	ALA	5.1
1	F	398	MET	5.1
1	B	715	SER	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	82	SER	5.1
1	F	501	ALA	5.1
1	E	87	THR	5.0
1	C	620	ARG	5.0
1	A	89	GLN	5.0
1	E	944	LEU	5.0
1	B	230	LEU	5.0
1	E	826	GLU	5.0
1	A	449	LEU	5.0
1	F	516	PHE	5.0
1	B	624	THR	4.9
1	D	614	GLY	4.9
1	F	89	GLN	4.9
1	D	11	PHE	4.9
1	A	1040	ILE	4.9
1	C	405	LEU	4.9
1	F	448	VAL	4.9
1	F	840	ALA	4.9
1	C	57	VAL	4.8
1	B	719	ASN	4.8
1	E	92	LEU	4.8
1	A	92	LEU	4.8
1	A	486	LEU	4.8
1	E	496	MET	4.8
1	E	406	VAL	4.8
1	A	938	SER	4.8
1	F	541	TYR	4.8
1	C	681	ASP	4.8
1	A	605	ASN	4.8
1	B	613	ASN	4.8
1	A	946	VAL	4.8
1	E	366	LEU	4.8
1	B	91	THR	4.7
1	B	315	PRO	4.7
1	D	9	PRO	4.7
1	E	489	THR	4.7
1	C	783	PRO	4.7
1	C	834	GLY	4.7
1	F	615	PHE	4.7
1	D	461	GLY	4.7
1	A	410	ILE	4.7
1	E	616	GLY	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	441	ALA	4.7
1	A	494	ALA	4.7
1	B	678	THR	4.6
1	C	739	LEU	4.6
1	D	81	ASN	4.6
1	E	487	ILE	4.6
1	E	888	LEU	4.6
1	B	80	SER	4.6
1	D	508	GLY	4.6
1	E	83	ASP	4.6
1	A	942	ALA	4.6
1	E	89	GLN	4.6
1	F	488	LEU	4.5
1	C	48	SER	4.5
1	D	577	GLN	4.5
1	C	448	VAL	4.5
1	C	868	LEU	4.5
1	A	408	ASP	4.5
1	C	711	ASP	4.5
1	A	368	PRO	4.5
1	B	404	LEU	4.5
1	D	782	LEU	4.5
1	F	839	GLU	4.5
1	F	60	THR	4.5
1	F	937	LEU	4.4
1	A	401	ALA	4.4
1	D	815	ARG	4.4
1	B	487	ILE	4.4
1	A	939	ALA	4.4
1	B	894	SER	4.4
1	A	616	GLY	4.4
1	A	943	ILE	4.4
1	F	231	ASN	4.4
1	C	804	PHE	4.4
1	A	407	ASP	4.4
1	D	400	LEU	4.3
1	A	402	ILE	4.3
1	F	938	SER	4.3
1	E	408	ASP	4.3
1	E	678	THR	4.3
1	F	901	VAL	4.3
1	C	684	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	937	LEU	4.3
1	B	225	VAL	4.3
1	E	682	PHE	4.3
1	E	892	TYR	4.3
1	C	70	ASN	4.3
1	C	310	LEU	4.2
1	F	941	ASN	4.2
1	D	834	GLY	4.2
1	C	10	ILE	4.2
1	E	815	ARG	4.2
1	D	576	VAL	4.2
1	F	897	ILE	4.2
1	F	892	TYR	4.2
1	A	714	THR	4.2
1	E	138	MET	4.1
1	B	400	LEU	4.1
1	F	895	TRP	4.1
1	F	402	ILE	4.1
1	F	3	ASN	4.1
1	C	504	ASP	4.1
1	F	474	ILE	4.1
1	F	502	LYS	4.1
1	F	868	LEU	4.1
1	C	615	PHE	4.1
1	F	679	GLY	4.1
1	E	405	LEU	4.1
1	D	493	CYS	4.1
1	E	741	VAL	4.1
1	F	708	LYS	4.1
1	D	626	ILE	4.1
1	A	397	GLY	4.0
1	F	57	VAL	4.0
1	F	889	ALA	4.0
1	C	403	GLY	4.0
1	C	402	ILE	4.0
1	E	310	LEU	4.0
1	C	362	PHE	4.0
1	C	449	LEU	4.0
1	B	486	LEU	4.0
1	C	833	PRO	4.0
1	D	504	ASP	4.0
1	C	511	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	370	ILE	4.0
1	E	679	GLY	4.0
1	B	439	GLN	3.9
1	C	839	GLU	3.9
1	E	632	LYS	3.9
1	D	894	SER	3.9
1	C	13	TRP	3.9
1	C	510	LYS	3.9
1	D	401	ALA	3.9
1	A	87	THR	3.9
1	C	503	GLY	3.9
1	D	837	THR	3.9
1	B	616	GLY	3.9
1	F	681	ASP	3.9
1	E	933	THR	3.8
1	F	404	LEU	3.8
1	E	834	GLY	3.8
1	A	640	GLU	3.8
1	A	43	VAL	3.8
1	E	677	ALA	3.8
1	E	78	MET	3.8
1	E	362	PHE	3.8
1	E	939	ALA	3.8
1	E	307	ARG	3.8
1	F	709	HIS	3.8
1	F	902	MET	3.8
1	E	367	ILE	3.8
1	A	1039	ASP	3.8
1	C	54	ALA	3.8
1	F	484	VAL	3.8
1	F	825	MET	3.8
1	D	656	SER	3.7
1	B	407	ASP	3.7
1	B	720	GLY	3.7
1	F	7	ASP	3.7
1	C	683	GLU	3.7
1	E	400	LEU	3.7
1	F	817	GLU	3.7
1	F	306	ILE	3.7
1	E	492	LEU	3.7
1	F	943	ILE	3.7
1	E	900	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	435	MET	3.7
1	B	623	ASN	3.7
1	D	322	LYS	3.7
1	D	79	SER	3.7
1	B	78	MET	3.7
1	D	12	ALA	3.7
1	B	89	GLN	3.7
1	A	91	THR	3.7
1	C	621	GLY	3.6
1	D	92	LEU	3.6
1	C	935	ILE	3.6
1	C	937	LEU	3.6
1	C	500	ILE	3.6
1	D	662	MET	3.6
1	A	656	SER	3.6
1	A	10	ILE	3.6
1	F	577	GLN	3.6
1	D	661	ALA	3.6
1	E	175	VAL	3.6
1	C	314	GLU	3.6
1	E	432	ARG	3.6
1	A	496	MET	3.6
1	E	657	GLN	3.6
1	A	369	THR	3.6
1	A	9	PRO	3.6
1	E	613	ASN	3.6
1	C	663	VAL	3.5
1	C	869	SER	3.5
1	F	540	ARG	3.5
1	E	817	GLU	3.5
1	F	83	ASP	3.5
1	B	534	ILE	3.5
1	B	408	ASP	3.5
1	D	83	ASP	3.5
1	D	897	ILE	3.5
1	F	512	PHE	3.5
1	D	613	ASN	3.5
1	C	444	GLY	3.5
1	D	893	GLU	3.5
1	C	68	ASN	3.5
1	C	791	VAL	3.5
1	D	993	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	713	LEU	3.5
1	D	90	ILE	3.5
1	D	791	VAL	3.5
1	C	722	GLU	3.4
1	B	291	ILE	3.4
1	D	10	ILE	3.4
1	B	830	GLN	3.4
1	B	492	LEU	3.4
1	B	889	ALA	3.4
1	B	866	GLU	3.4
1	B	412	VAL	3.4
1	C	401	ALA	3.4
1	E	32	VAL	3.4
1	B	90	ILE	3.4
1	D	833	PRO	3.4
1	C	889	ALA	3.4
1	D	624	THR	3.4
1	E	88	VAL	3.4
1	B	5	PHE	3.4
1	F	718	PRO	3.4
1	F	624	THR	3.4
1	F	848	ALA	3.4
1	B	577	GLN	3.4
1	C	865	GLN	3.4
1	D	731	ILE	3.4
1	E	683	GLU	3.4
1	A	81	ASN	3.4
1	E	576	VAL	3.4
1	E	904	VAL	3.4
1	F	485	ALA	3.4
1	E	934	THR	3.4
1	D	622	GLN	3.4
1	B	177	LEU	3.4
1	A	680	PHE	3.4
1	F	896	SER	3.4
1	A	443	VAL	3.4
1	B	92	LEU	3.4
1	D	678	THR	3.4
1	F	504	ASP	3.4
1	F	706	ALA	3.4
1	C	463	THR	3.4
1	F	942	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	400	LEU	3.3
1	B	401	ALA	3.3
1	D	627	ALA	3.3
1	E	441	ALA	3.3
1	B	837	THR	3.3
1	D	804	PHE	3.3
1	D	729	ILE	3.3
1	F	832	ALA	3.3
1	C	838	GLY	3.3
1	A	489	THR	3.3
1	D	809	TRP	3.3
1	A	398	MET	3.3
1	A	90	ILE	3.3
1	A	613	ASN	3.3
1	F	408	ASP	3.3
1	E	605	ASN	3.3
1	E	513	PHE	3.3
1	E	866	GLU	3.3
1	A	894	SER	3.3
1	A	634	TRP	3.3
1	F	463	THR	3.3
1	A	892	TYR	3.3
1	F	828	LEU	3.3
1	B	81	ASN	3.2
1	F	44	THR	3.2
1	E	633	ASP	3.2
1	D	5	PHE	3.2
1	C	69	MET	3.2
1	F	444	GLY	3.2
1	A	88	VAL	3.2
1	E	869	SER	3.2
1	D	80	SER	3.2
1	F	462	SER	3.2
1	A	935	ILE	3.2
1	D	487	ILE	3.2
1	F	443	VAL	3.2
1	A	396	PHE	3.2
1	D	727	PHE	3.2
1	C	817	GLU	3.2
1	D	835	LYS	3.2
1	F	849	SER	3.2
1	E	357	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	827	ILE	3.2
1	E	292	LYS	3.2
1	A	961	ILE	3.2
1	E	721	LEU	3.2
1	F	626	ILE	3.2
1	A	866	GLU	3.2
1	F	390	ILE	3.2
1	D	89	GLN	3.2
1	F	401	ALA	3.2
1	C	892	TYR	3.2
1	B	901	VAL	3.2
1	E	439	GLN	3.2
1	C	577	GLN	3.2
1	A	681	ASP	3.2
1	A	575	MET	3.1
1	C	390	ILE	3.1
1	A	873	ALA	3.1
1	C	488	LEU	3.1
1	A	635	ALA	3.1
1	F	576	VAL	3.1
1	C	624	THR	3.1
1	A	399	VAL	3.1
1	E	929	VAL	3.1
1	F	831	ALA	3.1
1	A	246	PHE	3.1
1	B	11	PHE	3.1
1	C	941	ASN	3.1
1	F	834	GLY	3.1
1	D	888	LEU	3.1
1	F	310	LEU	3.1
1	C	388	PHE	3.1
1	F	621	GLY	3.1
1	C	576	VAL	3.1
1	B	495	THR	3.1
1	A	655	PHE	3.1
1	A	134	SER	3.1
1	E	938	SER	3.1
1	E	409	ALA	3.1
1	A	164	ASP	3.0
1	D	616	GLY	3.0
1	C	91	THR	3.0
1	D	606	VAL	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	839	GLU	3.0
1	E	993	THR	3.0
1	D	575	MET	3.0
1	A	874	PRO	3.0
1	E	902	MET	3.0
1	D	178	PHE	3.0
1	D	889	ALA	3.0
1	C	718	PRO	3.0
1	E	331	PRO	3.0
1	E	62	THR	3.0
1	D	385	ALA	3.0
1	E	891	LEU	3.0
1	B	494	ALA	3.0
1	E	71	GLY	3.0
1	D	167	SER	3.0
1	C	421	ALA	3.0
1	D	961	ILE	3.0
1	E	837	THR	3.0
1	A	657	GLN	3.0
1	C	713	LEU	3.0
1	F	409	ALA	3.0
1	C	778	LYS	3.0
1	A	83	ASP	3.0
1	B	897	ILE	3.0
1	F	482	VAL	3.0
1	F	872	GLN	3.0
1	C	938	SER	3.0
1	A	899	PHE	3.0
1	E	396	PHE	3.0
1	A	355	MET	3.0
1	F	496	MET	3.0
1	D	403	GLY	3.0
1	D	623	ASN	3.0
1	E	897	ILE	2.9
1	F	739	LEU	2.9
1	C	801	PHE	2.9
1	F	62	THR	2.9
1	A	945	ILE	2.9
1	C	867	ARG	2.9
1	A	900	SER	2.9
1	C	742	SER	2.9
1	A	44	THR	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	405	LEU	2.9
1	C	563	PHE	2.9
1	D	892	TYR	2.9
1	A	178	PHE	2.9
1	F	110	LYS	2.9
1	B	231	ASN	2.9
1	E	311	ALA	2.9
1	E	624	THR	2.9
1	E	835	LYS	2.9
1	A	376	LEU	2.9
1	D	404	LEU	2.9
1	E	828	LEU	2.9
1	C	676	THR	2.9
1	E	936	GLY	2.9
1	B	88	VAL	2.9
1	E	626	ILE	2.9
1	C	498	LYS	2.9
1	D	959	GLY	2.9
1	E	289	LEU	2.9
1	A	762	PHE	2.9
1	D	982	PHE	2.9
1	B	836	SER	2.9
1	E	940	LYS	2.9
1	E	438	ILE	2.9
1	F	175	VAL	2.9
1	D	610	PHE	2.9
1	E	942	ALA	2.9
1	F	838	GLY	2.9
1	E	1007	VAL	2.9
1	F	809	TRP	2.9
1	D	665	ALA	2.9
1	E	746	ILE	2.8
1	B	933	THR	2.8
1	E	369	THR	2.8
1	F	940	LYS	2.8
1	F	90	ILE	2.8
1	A	12	ALA	2.8
1	D	733	GLN	2.8
1	F	936	GLY	2.8
1	C	945	ILE	2.8
1	D	306	ILE	2.8
1	F	127	VAL	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	895	TRP	2.8
1	C	166	ILE	2.8
1	D	467	TYR	2.8
1	B	211	ASN	2.8
1	B	829	GLY	2.8
1	E	404	LEU	2.8
1	C	410	ILE	2.8
1	F	855	VAL	2.8
1	C	496	MET	2.8
1	D	449	LEU	2.8
1	A	167	SER	2.8
1	C	674	LEU	2.8
1	D	91	THR	2.8
1	B	711	ASP	2.8
1	D	141	GLY	2.8
1	F	65	ILE	2.8
1	E	33	ALA	2.8
1	E	890	ALA	2.8
1	A	976	LEU	2.8
1	D	87	THR	2.8
1	D	510	LYS	2.8
1	D	664	PHE	2.8
1	C	502	LYS	2.8
1	A	607	GLU	2.7
1	F	746	ILE	2.7
1	C	516	PHE	2.7
1	E	831	ALA	2.7
1	C	207	ILE	2.7
1	E	229	GLN	2.7
1	F	846	GLN	2.7
1	B	83	ASP	2.7
1	E	13	TRP	2.7
1	D	402	ILE	2.7
1	A	442	LEU	2.7
1	B	591	LEU	2.7
1	C	816	LEU	2.7
1	F	59	ASP	2.7
1	F	841	MET	2.7
1	D	49	TYR	2.7
1	D	578	LEU	2.7
1	A	444	GLY	2.7
1	B	815	ARG	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	558	ARG	2.7
1	F	8	ARG	2.7
1	C	67	GLN	2.7
1	F	515	TRP	2.7
1	B	175	VAL	2.7
1	A	82	SER	2.7
1	E	296	GLY	2.7
1	B	663	VAL	2.7
1	E	819	TYR	2.7
1	F	495	THR	2.7
1	F	843	LEU	2.7
1	B	938	SER	2.7
1	E	246	PHE	2.7
1	B	942	ALA	2.7
1	F	159	ALA	2.7
1	F	845	GLU	2.7
1	F	782	LEU	2.7
1	A	508	GLY	2.7
1	C	398	MET	2.7
1	F	246	PHE	2.7
1	B	576	VAL	2.7
1	B	246	PHE	2.7
1	C	741	VAL	2.7
1	F	704	ALA	2.7
1	E	714	THR	2.7
1	B	841	MET	2.7
1	C	814	PRO	2.7
1	A	79	SER	2.6
1	A	371	ALA	2.7
1	E	824	SER	2.6
1	F	613	ASN	2.6
1	A	516	PHE	2.6
1	E	830	GLN	2.6
1	A	453	PHE	2.6
1	B	298	ASN	2.6
1	E	73	ASP	2.6
1	E	407	ASP	2.6
1	B	891	LEU	2.6
1	E	402	ILE	2.6
1	B	428	LYS	2.6
1	C	708	LYS	2.6
1	D	1039	ASP	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	641	GLU	2.6
1	C	622	GLN	2.6
1	F	707	ALA	2.6
1	C	982	PHE	2.6
1	C	127	VAL	2.6
1	D	59	ASP	2.6
1	B	491	ALA	2.6
1	E	86	GLY	2.6
1	E	712	MET	2.6
1	E	636	ASP	2.6
1	F	477	ALA	2.6
1	C	406	VAL	2.6
1	A	492	LEU	2.6
1	E	782	LEU	2.6
1	A	815	ARG	2.6
1	C	446	ALA	2.6
1	F	877	TYR	2.6
1	F	45	ILE	2.6
1	F	851	LEU	2.6
1	C	932	LEU	2.6
1	A	467	TYR	2.6
1	B	758	TYR	2.6
1	C	12	ALA	2.6
1	E	889	ALA	2.6
1	D	164	ASP	2.6
1	F	715	SER	2.6
1	D	590	VAL	2.6
1	F	88	VAL	2.6
1	E	860	THR	2.6
1	B	835	LYS	2.6
1	D	142	VAL	2.6
1	F	82	SER	2.6
1	F	856	GLY	2.6
1	A	591	LEU	2.6
1	D	246	PHE	2.5
1	D	386	PHE	2.5
1	A	632	LYS	2.5
1	C	507	GLU	2.5
1	A	80	SER	2.5
1	E	769	LYS	2.5
1	B	406	VAL	2.5
1	B	937	LEU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	891	LEU	2.5
1	C	389	SER	2.5
1	E	727	PHE	2.5
1	A	406	VAL	2.5
1	F	106	GLN	2.5
1	C	404	LEU	2.5
1	E	75	LEU	2.5
1	C	575	MET	2.5
1	F	867	ARG	2.5
1	E	778	LYS	2.5
1	F	70	ASN	2.5
1	F	680	PHE	2.5
1	F	612	VAL	2.5
1	A	871	ASN	2.5
1	F	446	ALA	2.5
1	F	489	THR	2.5
1	B	48	SER	2.5
1	E	833	PRO	2.5
1	D	828	LEU	2.5
1	E	541	TYR	2.5
1	E	328	ASP	2.5
1	B	844	MET	2.5
1	E	642	ASN	2.5
1	A	801	PHE	2.5
1	B	899	PHE	2.5
1	D	943	ILE	2.5
1	F	487	ILE	2.5
1	C	578	LEU	2.5
1	C	497	LEU	2.4
1	D	886	LEU	2.4
1	C	993	THR	2.4
1	F	294	ALA	2.4
1	E	762	PHE	2.4
1	F	164	ASP	2.4
1	A	895	TRP	2.4
1	B	888	LEU	2.4
1	B	431	THR	2.4
1	A	835	LYS	2.4
1	F	111	LEU	2.4
1	A	885	PHE	2.4
1	F	884	VAL	2.4
1	B	409	ALA	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	939	ALA	2.4
1	F	682	PHE	2.4
1	C	90	ILE	2.4
1	C	746	ILE	2.4
1	B	240	LEU	2.4
1	A	367	ILE	2.4
1	D	935	ILE	2.4
1	A	357	LEU	2.4
1	D	591	LEU	2.4
1	B	762	PHE	2.4
1	D	640	GLU	2.4
1	E	46	SER	2.4
1	C	587	THR	2.4
1	D	431	THR	2.4
1	F	357	LEU	2.4
1	E	47	ALA	2.4
1	B	900	SER	2.4
1	E	486	LEU	2.4
1	C	655	PHE	2.4
1	E	655	PHE	2.4
1	D	713	LEU	2.4
1	B	32	VAL	2.4
1	B	176	GLN	2.4
1	C	616	GLY	2.4
1	D	573	MET	2.4
1	D	801	PHE	2.4
1	C	518	ARG	2.4
1	D	494	ALA	2.4
1	F	12	ALA	2.4
1	D	507	GLU	2.4
1	F	211	ASN	2.4
1	B	461	GLY	2.3
1	C	745	ASP	2.3
1	A	893	GLU	2.3
1	B	292	LYS	2.3
1	E	177	LEU	2.3
1	F	400	LEU	2.3
1	A	411	VAL	2.3
1	C	62	THR	2.3
1	B	59	ASP	2.3
1	F	1021	PHE	2.3
1	E	398	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	462	SER	2.3
1	B	741	VAL	2.3
1	C	809	TRP	2.3
1	C	870	GLY	2.3
1	E	5	PHE	2.3
1	B	828	LEU	2.3
1	B	531	VAL	2.3
1	D	933	THR	2.3
1	C	848	ALA	2.3
1	E	10	ILE	2.3
1	F	500	ILE	2.3
1	C	512	PHE	2.3
1	D	355	MET	2.3
1	F	121	GLU	2.3
1	A	47	ALA	2.3
1	A	488	LEU	2.3
1	C	897	ILE	2.3
1	F	92	LEU	2.3
1	F	578	LEU	2.3
1	F	710	PRO	2.3
1	B	44	THR	2.3
1	E	658	ILE	2.3
1	F	14	VAL	2.3
1	F	399	VAL	2.3
1	E	607	GLU	2.3
1	A	310	LEU	2.3
1	B	310	LEU	2.3
1	A	568	ASP	2.3
1	A	661	ALA	2.3
1	D	407	ASP	2.3
1	E	706	ALA	2.3
1	F	1026	PHE	2.3
1	D	900	SER	2.3
1	D	743	ILE	2.3
1	F	1037	ASN	2.3
1	D	814	PRO	2.3
1	A	606	VAL	2.3
1	C	33	ALA	2.3
1	D	926	TYR	2.3
1	F	372	VAL	2.3
1	E	614	GLY	2.3
1	A	519	MET	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	828	LEU	2.3
1	D	946	VAL	2.3
1	F	494	ALA	2.3
1	A	463	THR	2.3
1	F	1023	PRO	2.3
1	F	163	LYS	2.3
1	C	942	ALA	2.3
1	F	240	LEU	2.2
1	D	778	LYS	2.2
1	B	680	PHE	2.2
1	D	389	SER	2.2
1	A	405	LEU	2.2
1	B	442	LEU	2.2
1	B	944	LEU	2.2
1	C	230	LEU	2.2
1	D	310	LEU	2.2
1	A	624	THR	2.2
1	C	623	ASN	2.2
1	D	324	VAL	2.2
1	E	925	VAL	2.2
1	E	429	GLU	2.2
1	A	1037	ASN	2.2
1	C	278	ILE	2.2
1	E	90	ILE	2.2
1	B	484	VAL	2.2
1	B	1022	VAL	2.2
1	A	614	GLY	2.2
1	B	290	GLY	2.2
1	B	536	ARG	2.2
1	B	995	ALA	2.2
1	C	846	GLN	2.2
1	C	198	LEU	2.2
1	D	977	MET	2.2
1	C	1019	ILE	2.2
1	F	396	PHE	2.2
1	F	762	PHE	2.2
1	B	174	ASP	2.2
1	A	330	THR	2.2
1	D	307	ARG	2.2
1	C	989	LEU	2.2
1	E	198	LEU	2.2
1	F	1020	PHE	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	612	VAL	2.2
1	B	892	TYR	2.2
1	B	947	GLU	2.2
1	D	854	GLY	2.2
1	E	440	GLY	2.2
1	D	140	VAL	2.2
1	D	464	GLY	2.2
1	E	325	TYR	2.2
1	F	939	ALA	2.2
1	A	587	THR	2.2
1	E	442	LEU	2.2
1	F	169	THR	2.2
1	F	684	LEU	2.2
1	F	808	ARG	2.2
1	A	626	ILE	2.2
1	B	411	VAL	2.2
1	B	443	VAL	2.2
1	D	836	SER	2.2
1	F	699	ARG	2.2
1	A	470	PHE	2.2
1	D	563	PHE	2.2
1	C	32	VAL	2.2
1	F	827	ILE	2.2
1	F	683	GLU	2.2
1	E	930	GLY	2.2
1	C	657	GLN	2.2
1	C	976	LEU	2.2
1	C	980	LEU	2.2
1	E	12	ALA	2.2
1	F	483	LEU	2.2
1	F	558	ARG	2.2
1	B	3	ASN	2.2
1	F	68	ASN	2.2
1	E	994	GLY	2.2
1	A	441	ALA	2.2
1	D	690	LEU	2.2
1	D	868	LEU	2.2
1	A	830	GLN	2.2
1	B	237	GLN	2.2
1	C	1023	PRO	2.2
1	D	746	ILE	2.2
1	B	982	PHE	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	718	PRO	2.2
1	C	1037	ASN	2.2
1	E	330	THR	2.2
1	C	356	TYR	2.1
1	A	490	PRO	2.1
1	B	402	ILE	2.1
1	D	367	ILE	2.1
1	D	612	VAL	2.1
1	D	497	LEU	2.1
1	E	211	ASN	2.1
1	A	727	PHE	2.1
1	D	628	PHE	2.1
1	B	896	SER	2.1
1	C	291	ILE	2.1
1	F	731	ILE	2.1
1	F	86	GLY	2.1
1	F	662	MET	2.1
1	D	230	LEU	2.1
1	A	982	PHE	2.1
1	C	1026	PHE	2.1
1	E	634	TRP	2.1
1	C	940	LYS	2.1
1	D	940	LYS	2.1
1	C	626	ILE	2.1
1	E	577	GLN	2.1
1	B	718	PRO	2.1
1	B	289	LEU	2.1
1	E	711	ASP	2.1
1	D	853	THR	2.1
1	E	760	ASN	2.1
1	F	933	THR	2.1
1	B	626	ILE	2.1
1	F	278	ILE	2.1
1	A	48	SER	2.1
1	B	219	LEU	2.1
1	D	976	LEU	2.1
1	A	958	LYS	2.1
1	D	789	TRP	2.1
1	C	426	PRO	2.1
1	F	128	SER	2.1
1	B	926	TYR	2.1
1	A	372	VAL	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	741	VAL	2.1
1	D	585	GLU	2.1
1	D	278	ILE	2.1
1	D	929	VAL	2.1
1	F	929	VAL	2.1
1	C	936	GLY	2.1
1	B	73	ASP	2.1
1	B	43	VAL	2.1
1	F	225	VAL	2.1
1	B	112	GLN	2.1
1	B	440	GLY	2.1
1	F	816	LEU	2.1
1	B	178	PHE	2.1
1	A	962	GLU	2.1
1	D	433	LYS	2.1
1	E	210	GLN	2.1
1	F	162	MET	2.1
1	B	964	THR	2.1
1	A	817	GLU	2.1
1	B	839	GLU	2.1
1	E	661	ALA	2.1
1	A	493	CYS	2.1
1	A	181	GLN	2.1
1	A	136	PHE	2.1
1	E	1026	PHE	2.1
1	D	509	LYS	2.1
1	F	43	VAL	2.1
1	C	306	ILE	2.1
1	C	323	ILE	2.1
1	D	390	ILE	2.1
1	A	193	LEU	2.1
1	B	278	ILE	2.1
1	B	886	LEU	2.1
1	C	112	GLN	2.0
1	D	784	ASP	2.1
1	E	174	ASP	2.1
1	F	890	ALA	2.0
1	B	935	ILE	2.0
1	E	625	GLY	2.0
1	D	518	ARG	2.0
1	E	1011	MET	2.0
1	F	453	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	612	VAL	2.0
1	D	736	ALA	2.0
1	E	85	THR	2.0
1	F	945	ILE	2.0
1	C	818	ARG	2.0
1	D	396	PHE	2.0
1	C	14	VAL	2.0
1	A	323	ILE	2.0
1	E	494	ALA	2.0
1	C	736	ALA	2.0
1	F	932	LEU	2.0
1	D	725	PRO	2.0
1	B	859	TRP	2.0
1	C	522	LYS	2.0
1	E	297	ALA	2.0
1	A	953	MET	2.0
1	E	312	LYS	2.0
1	C	960	LEU	2.0
1	E	905	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

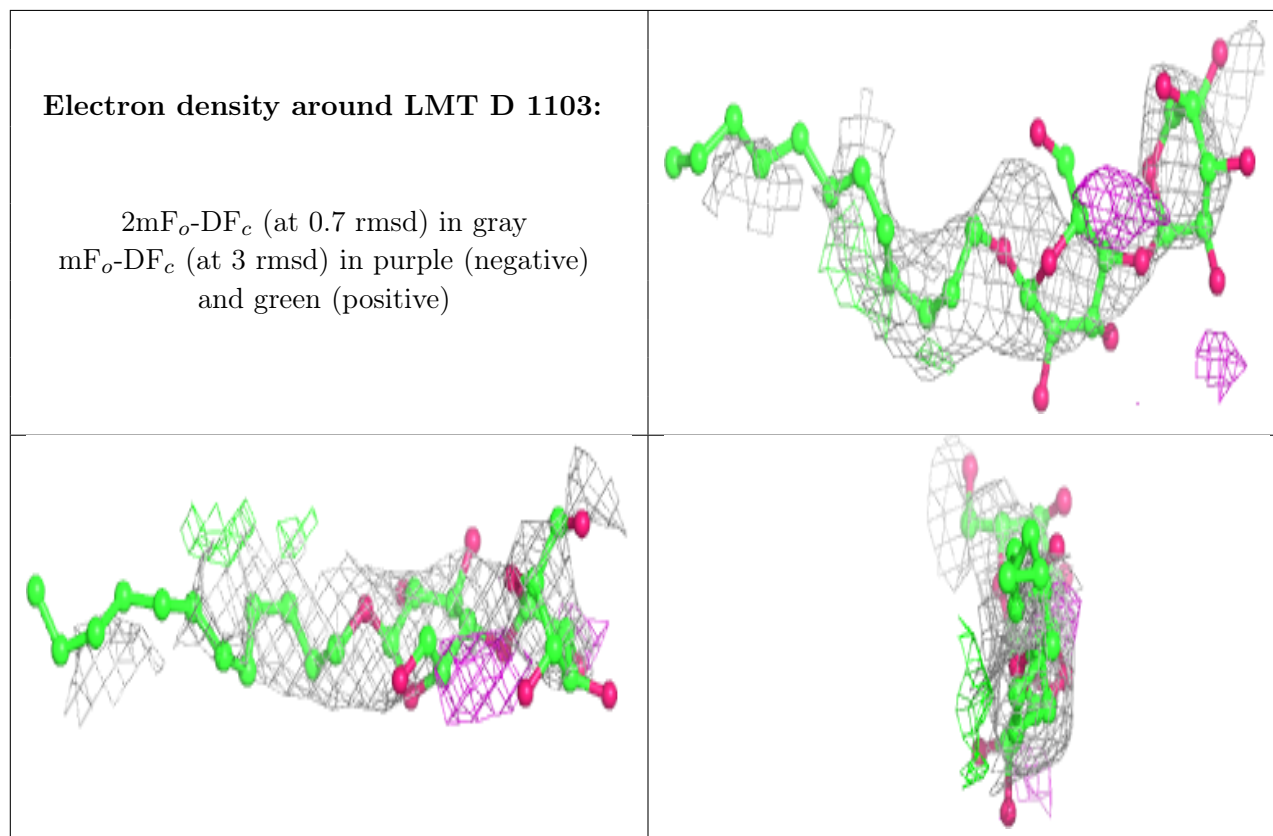
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LMT	D	1103	35/35	0.66	0.79	79,95,103,110	0
3	LMT	A	1103	35/35	0.68	1.09	82,95,107,111	0
2	ERY	D	1101	51/51	0.75	1.07	71,84,96,107	51
3	LMT	B	1101	35/35	0.82	0.78	53,82,105,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ERY	A	1101	51/51	0.84	1.20	70,79,90,95	51
3	LMT	E	1101	35/35	0.85	0.47	45,79,97,125	0
3	LMT	F	1101	35/35	0.85	0.98	48,88,105,110	0
3	LMT	D	1102	35/35	0.86	0.56	64,82,96,102	0
3	LMT	C	1101	35/35	0.86	0.52	64,84,95,96	0
3	LMT	A	1102	35/35	0.89	0.54	28,83,89,94	0
4	NI	A	1104	1/1	0.98	0.09	61,61,61,61	0
4	NI	C	1102	1/1	0.99	0.12	72,72,72,72	0
4	NI	E	1102	1/1	0.99	0.13	79,79,79,79	0

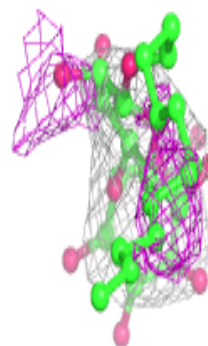
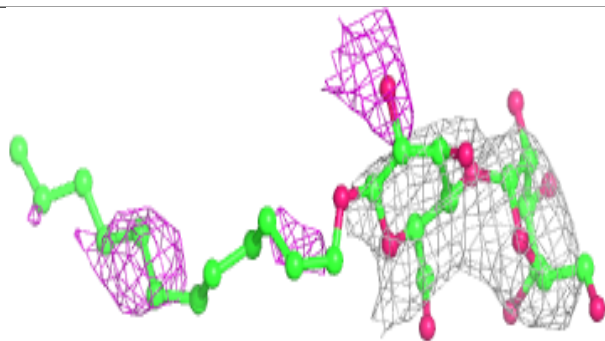
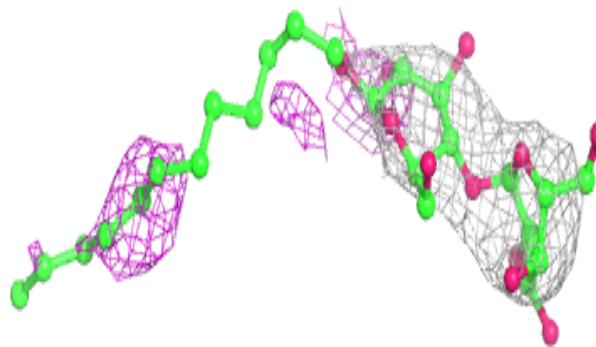
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





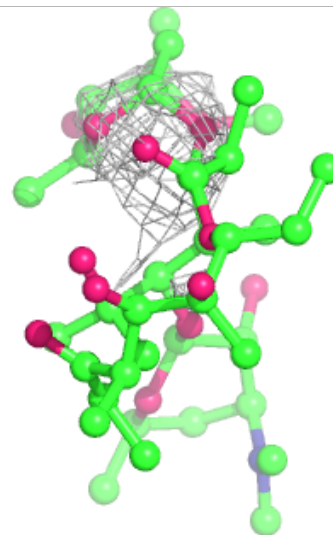
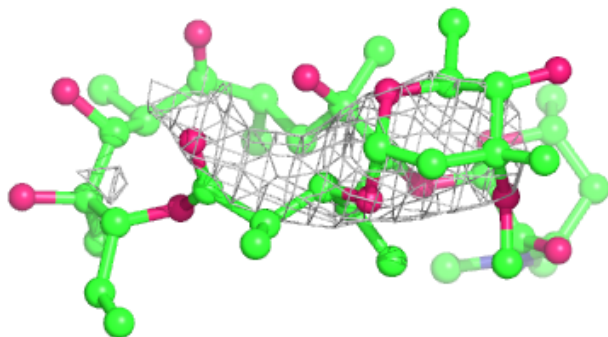
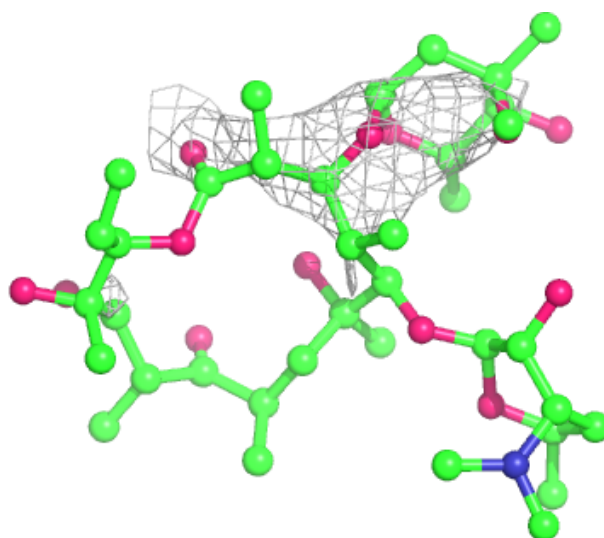
**Electron density around LMT A 1103:**

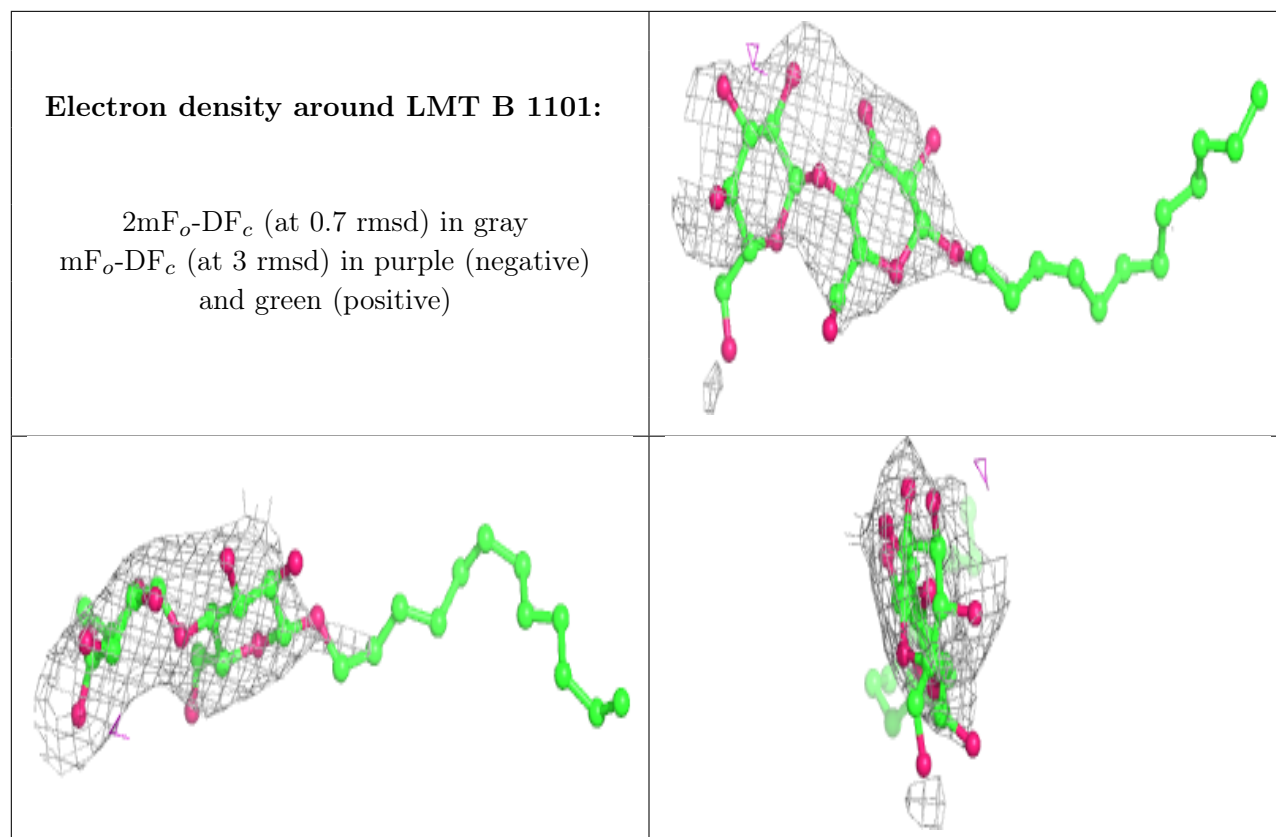
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ERY D 1101:**

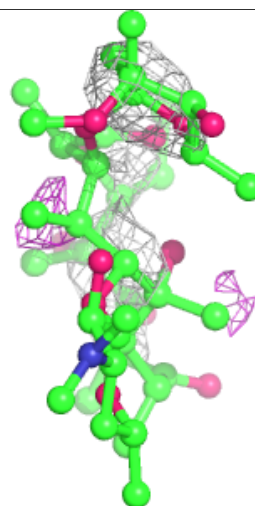
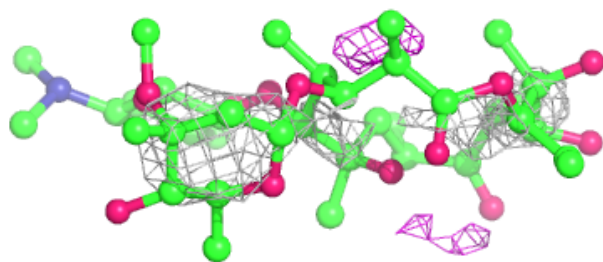
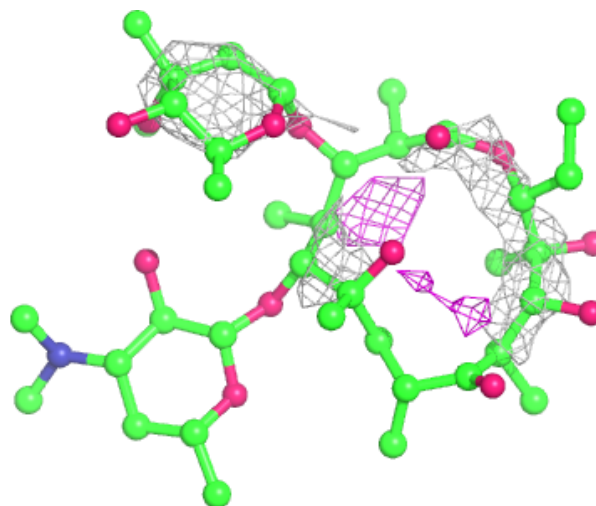
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

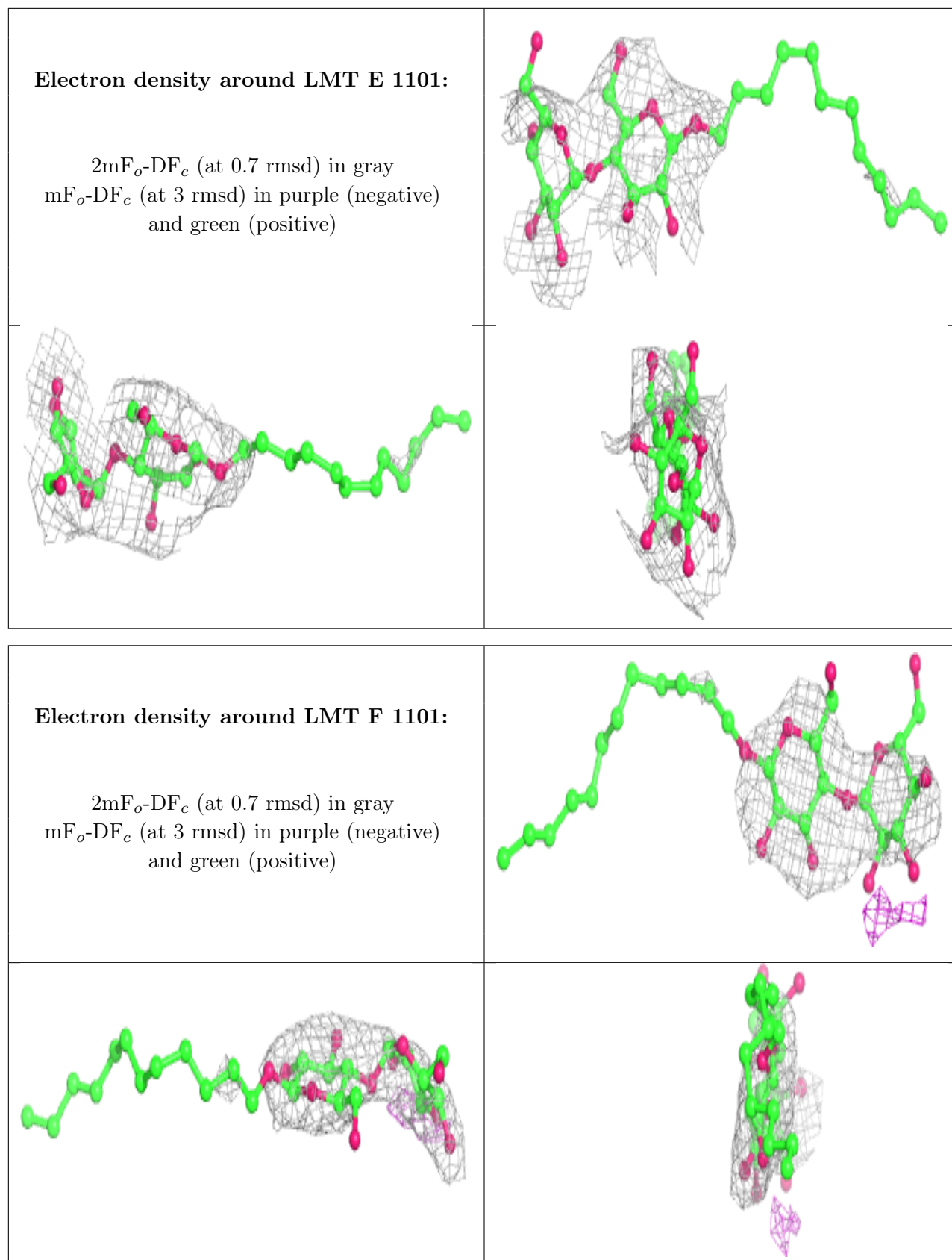




**Electron density around ERY A 1101:**

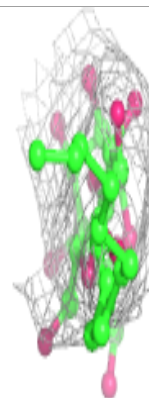
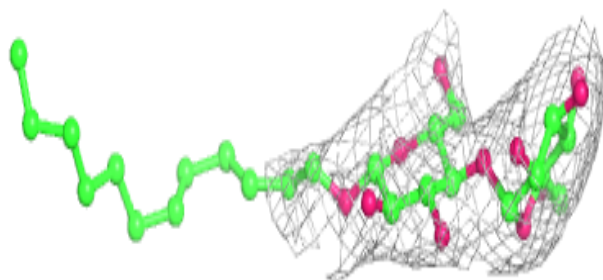
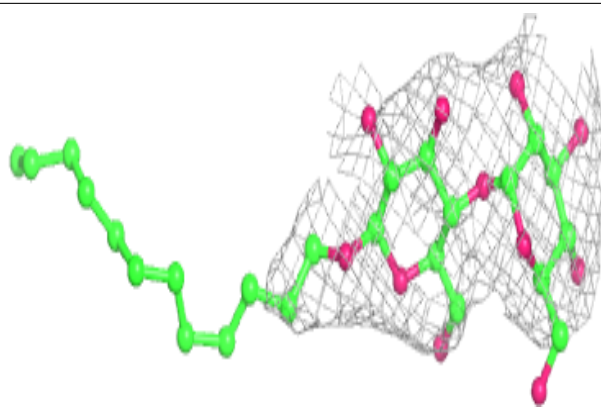
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



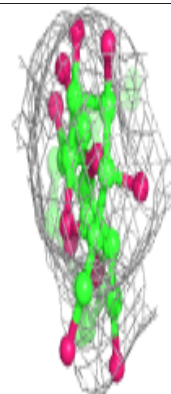
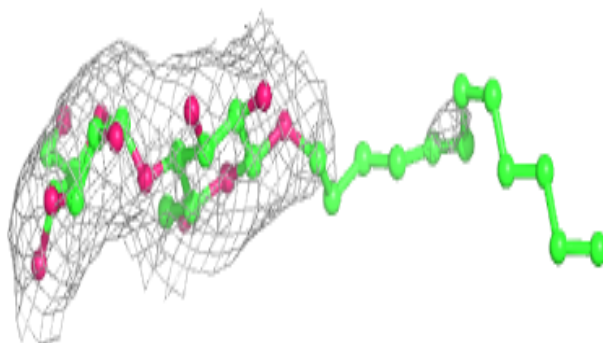
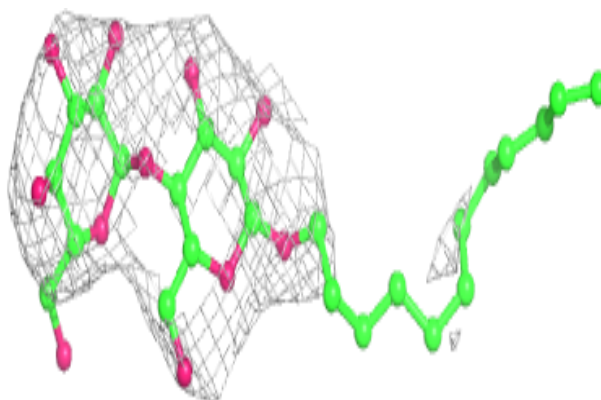


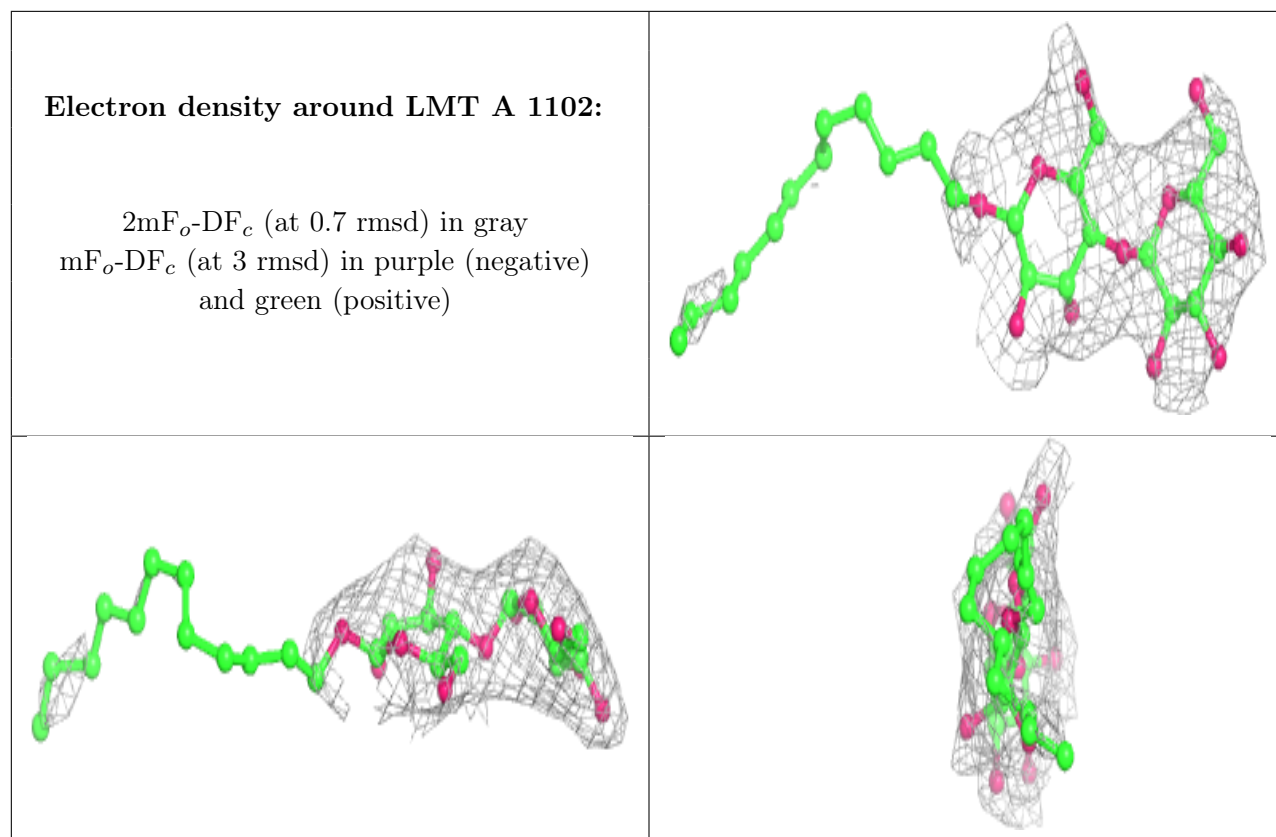
**Electron density around LMT D 1102:**

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

**Electron density around LMT 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.