



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2016 – 03:20 PM EDT

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

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

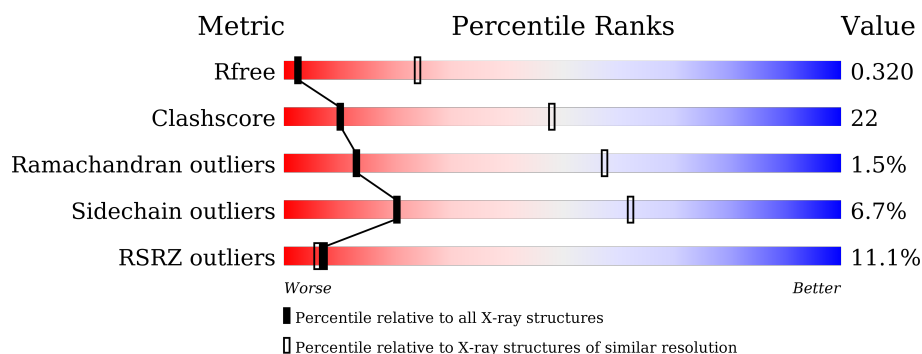
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1049	<div> <div>9%</div> <div>53%</div> <div>41%</div> <div>..</div> </div>
1	B	1049	<div> <div>7%</div> <div>56%</div> <div>39%</div> <div>..</div> </div>
1	C	1049	<div> <div>12%</div> <div>52%</div> <div>42%</div> <div>5% .</div> </div>
1	D	1049	<div> <div>11%</div> <div>55%</div> <div>39%</div> <div>5% .</div> </div>
1	E	1049	<div> <div>14%</div> <div>54%</div> <div>41%</div> <div>..</div> </div>
1	F	1049	<div> <div>14%</div> <div>54%</div> <div>41%</div> <div>.</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ERY	A	1101	-	-	-	X
2	ERY	D	1101	-	-	-	X
3	LMT	A	1102	-	-	-	X
3	LMT	A	1103	-	-	-	X
3	LMT	B	1101	X	-	-	X
3	LMT	C	1101	-	-	-	X
3	LMT	D	1103	-	-	-	X
3	LMT	E	1101	-	-	-	X
3	LMT	F	1101	-	-	-	X

2 Entry composition [i](#)

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

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

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

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

There are 18 discrepancies between the modelled and reference sequences:

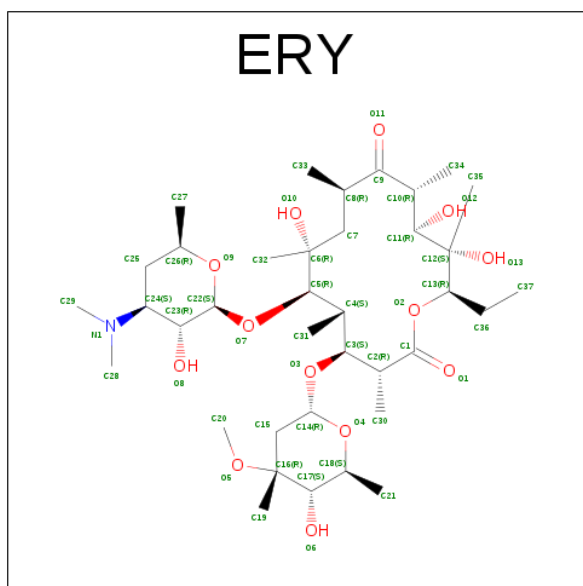
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	ALA	PHE	engineered mutation	UNP P31224
A	617	ALA	PHE	engineered mutation	UNP P31224
A	620	ALA	ARG	engineered mutation	UNP P31224
B	615	ALA	PHE	engineered mutation	UNP P31224
B	617	ALA	PHE	engineered mutation	UNP P31224
B	620	ALA	ARG	engineered mutation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

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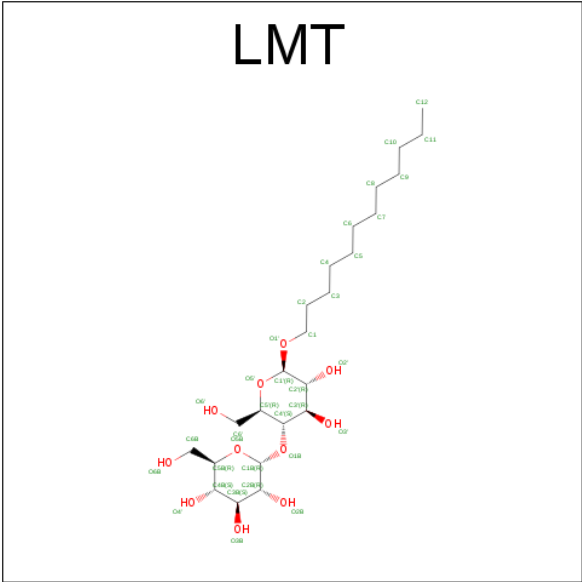
Chain	Residue	Modelled	Actual	Comment	Reference
F	620	ALA	ARG	engineered mutation	UNP P31224

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



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

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



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

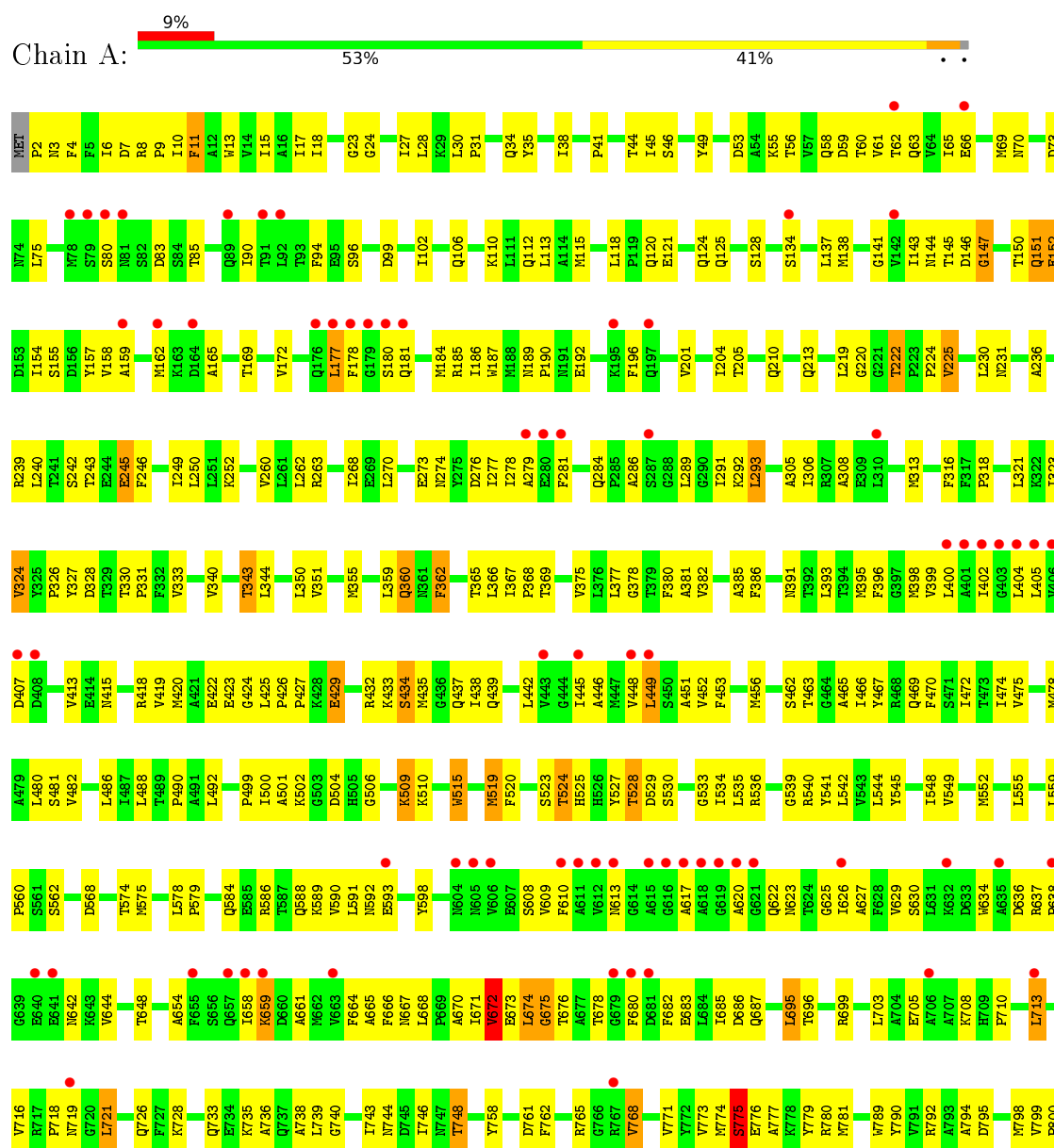
- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

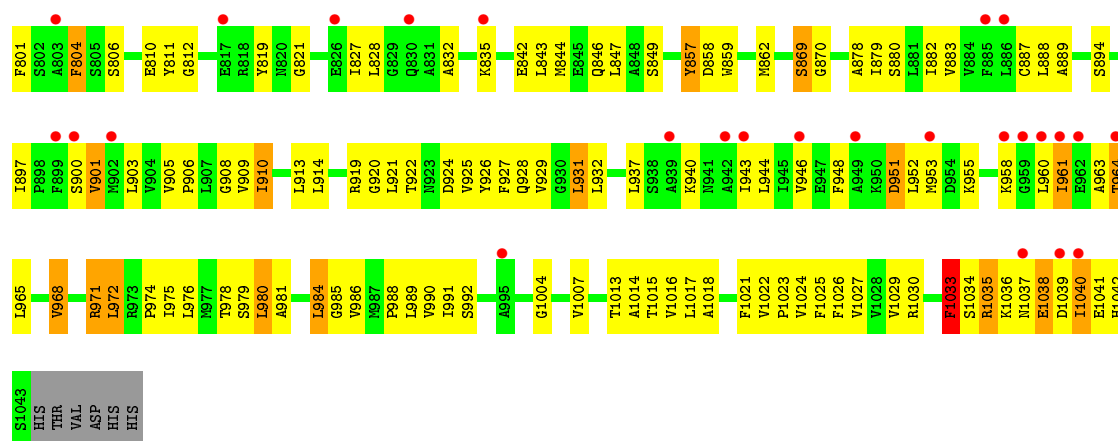
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	C	1	Total	Ni	0	0
			1	1		
4	E	1	Total	Ni	0	0
			1	1		

3 Residue-property plots

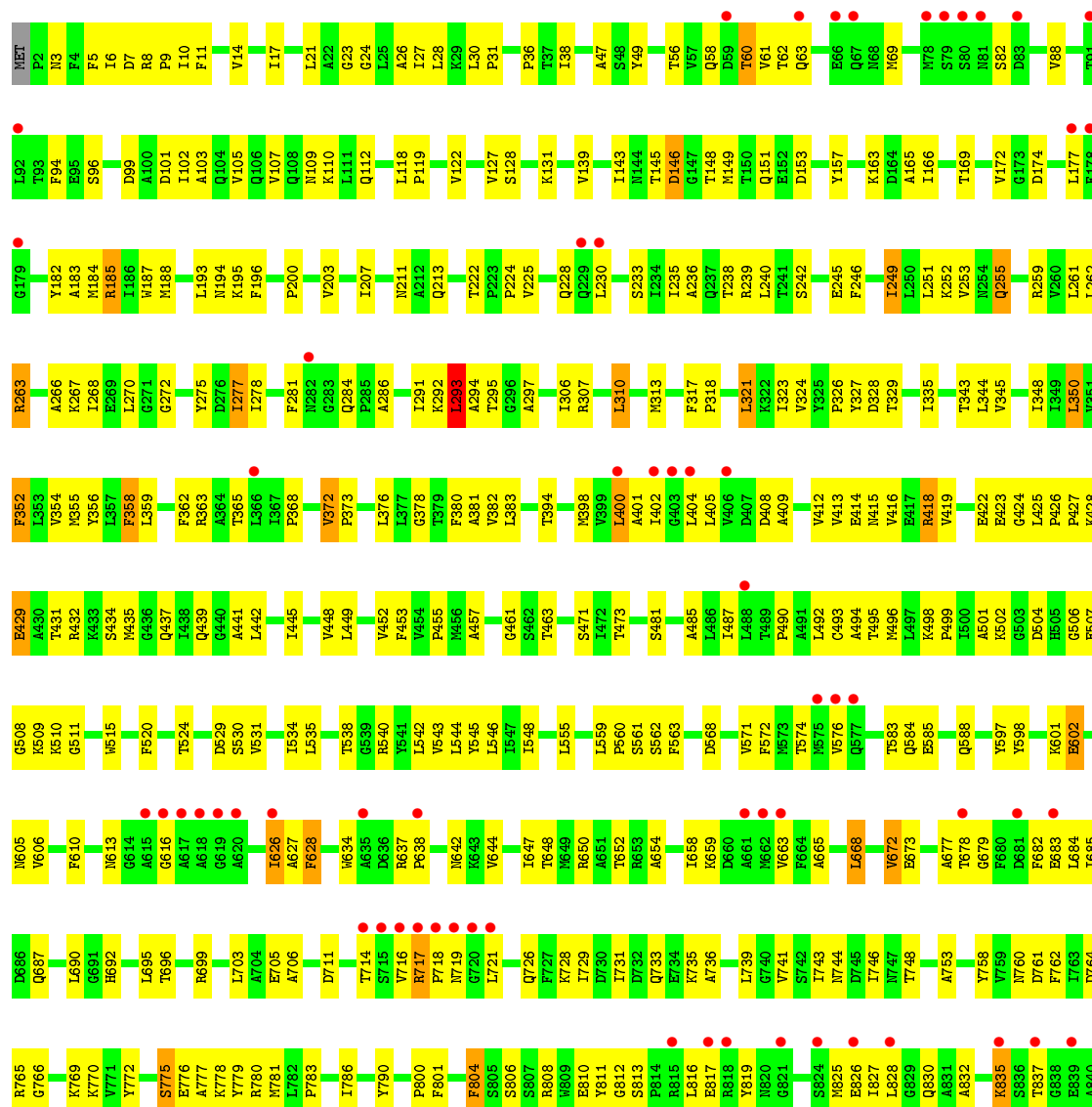
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

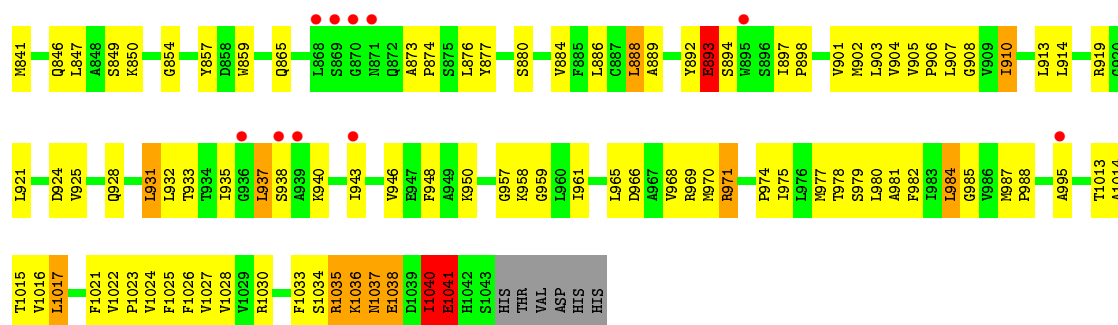
- Molecule 1: Multidrug efflux pump subunit AcrB



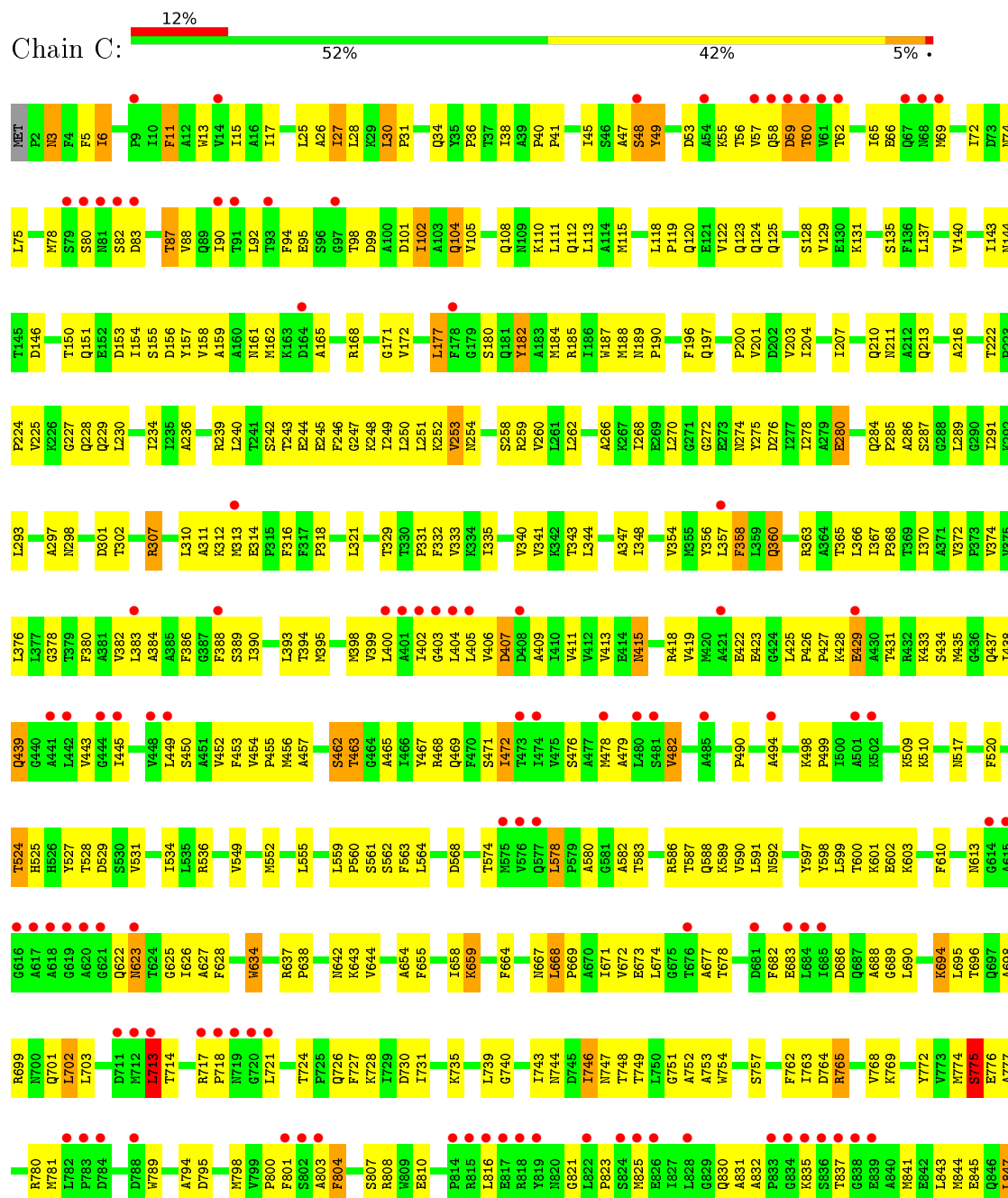


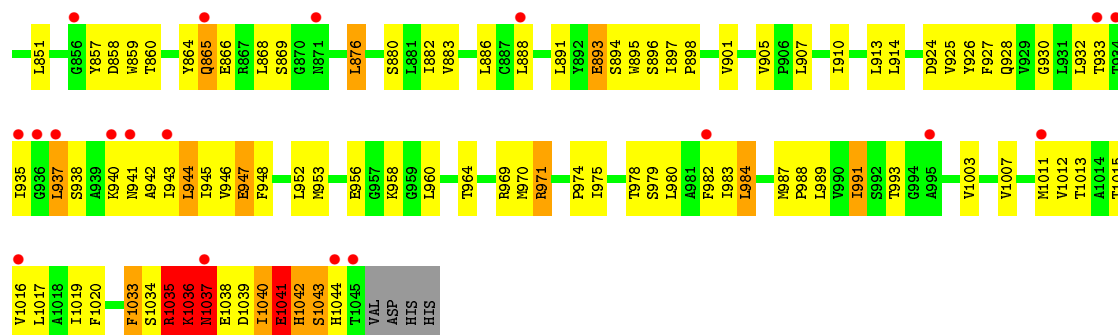
• Molecule 1: Multidrug efflux pump subunit AcrB



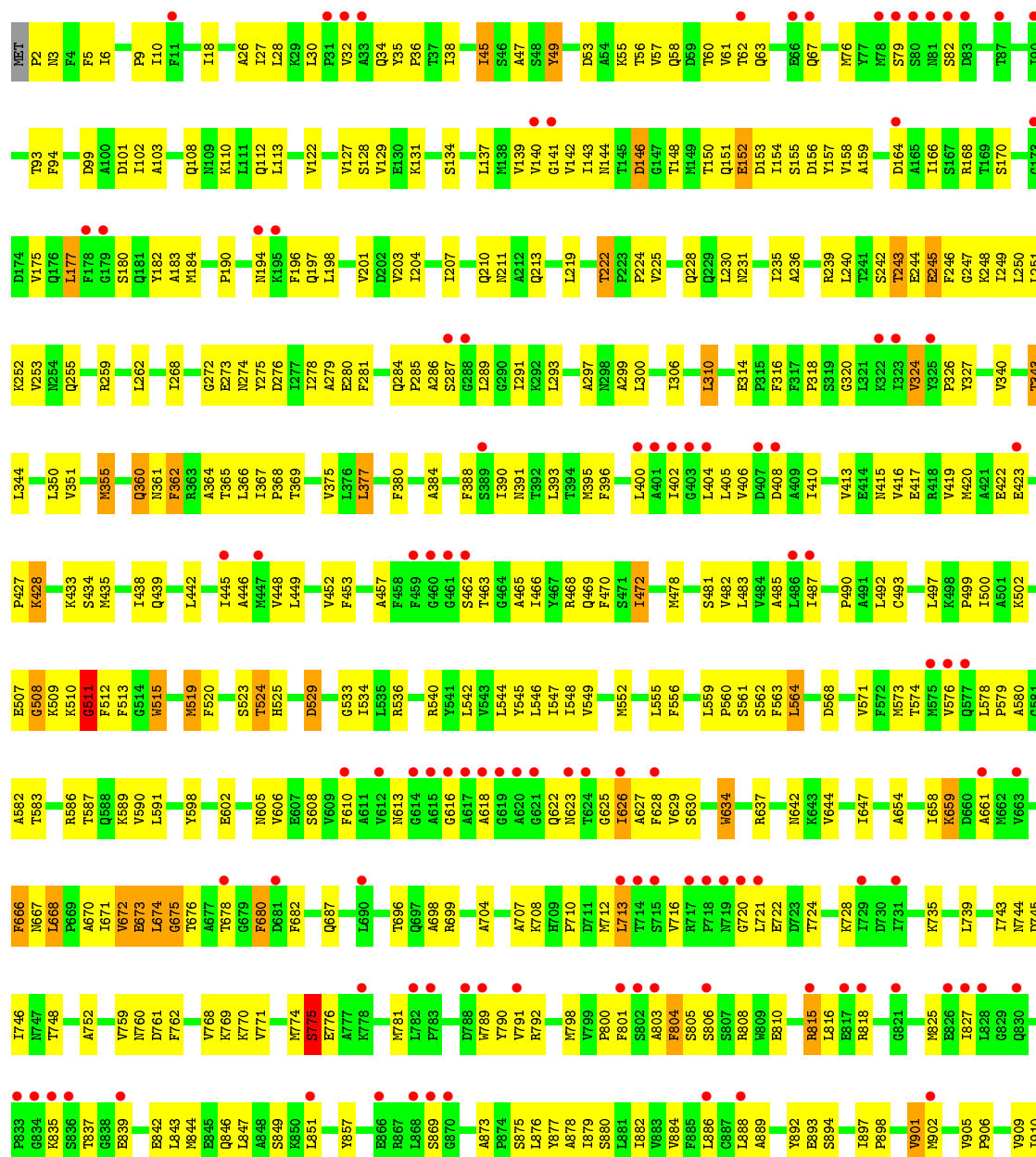


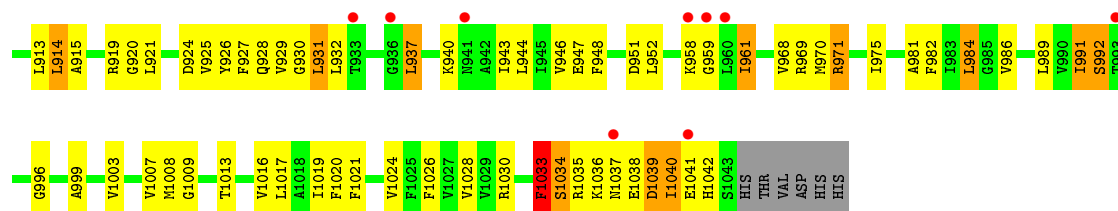
• Molecule 1: Multidrug efflux pump subunit AcrB



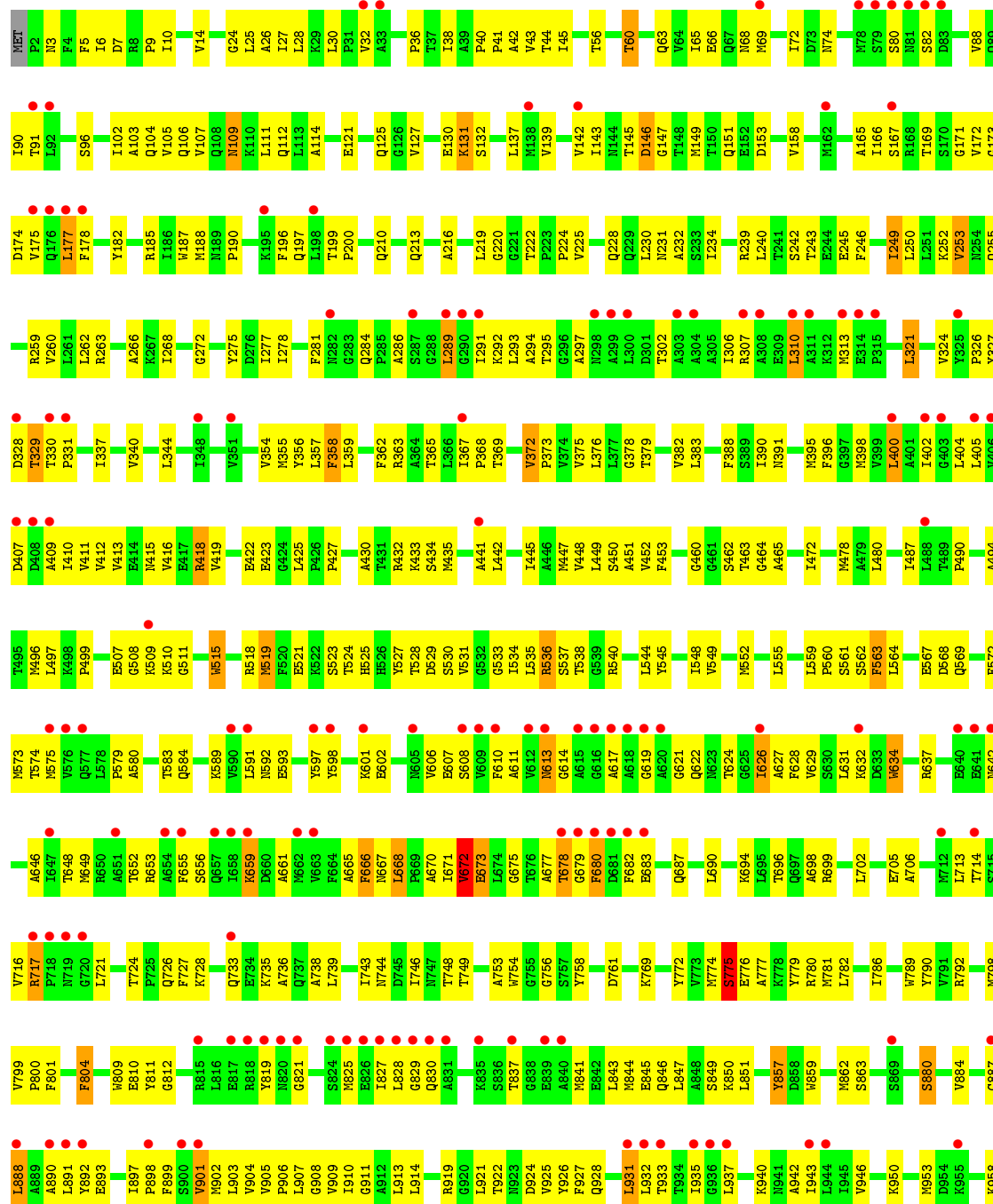


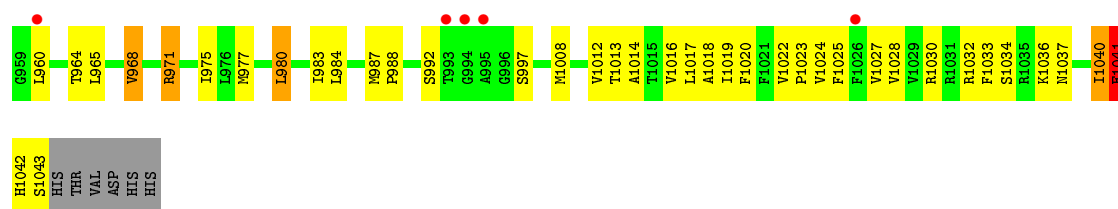
• Molecule 1: Multidrug efflux pump subunit AcrB



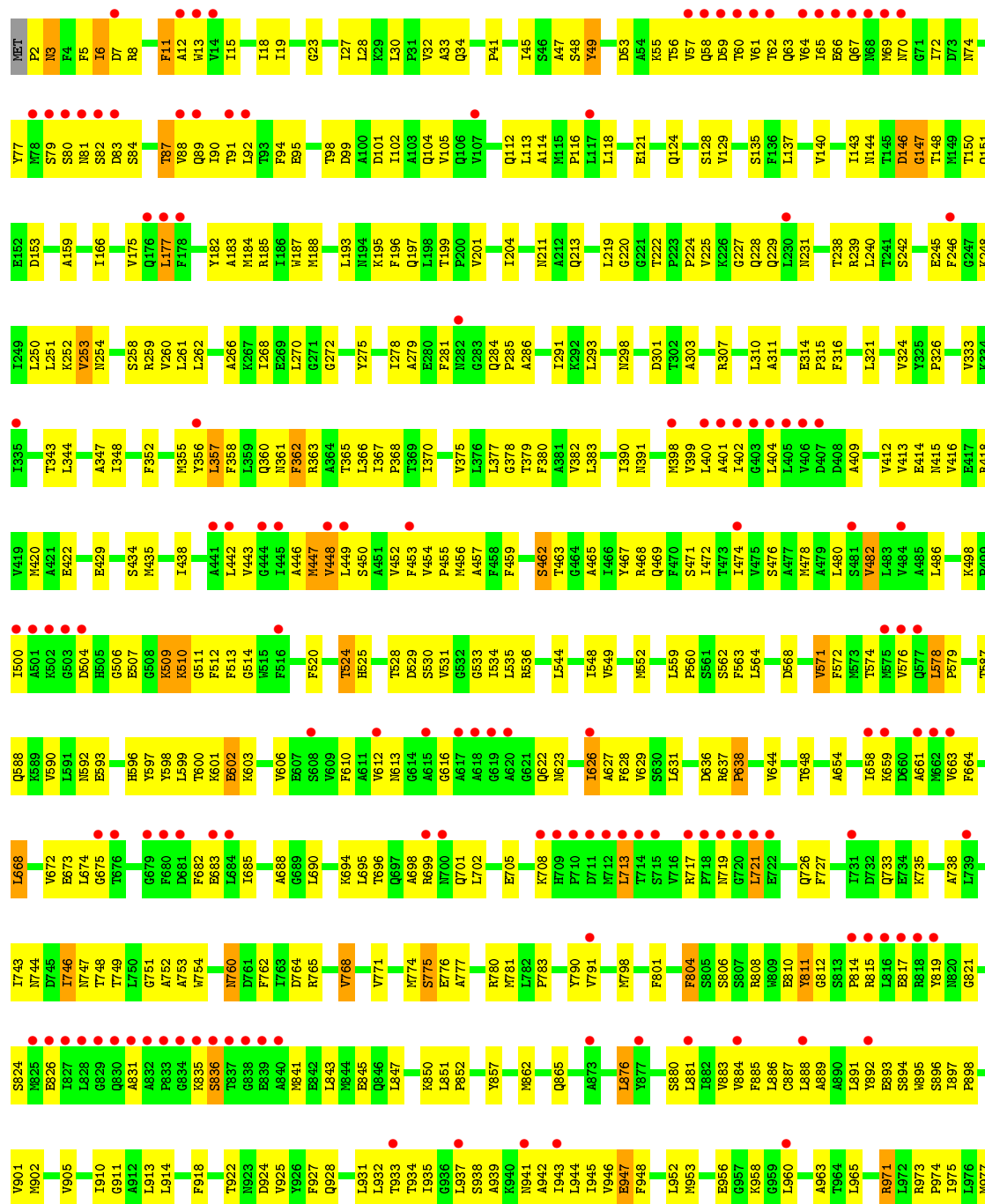


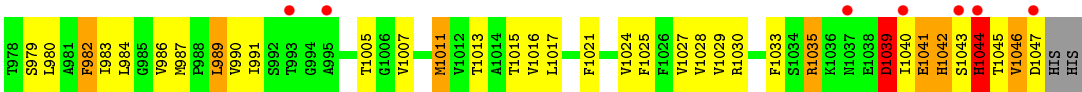
• Molecule 1: Multidrug efflux pump subunit AcrB





• Molecule 1: Multidrug efflux pump subunit AcrB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.18Å 156.77Å 218.17Å 90.00° 93.09° 90.00°	Depositor
Resolution (Å)	19.96 – 3.60 108.93 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.96-3.60) 97.1 (108.93-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.238 , 0.307 0.247 , 0.320	Depositor DCC
R_{free} test set	5666 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	101.2	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	47876	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.75 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2566e-04.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.59	1/8056 (0.0%)	0.81	5/10940 (0.0%)
1	B	0.59	0/8056	0.81	9/10940 (0.1%)
1	C	0.58	1/8074 (0.0%)	0.84	11/10965 (0.1%)
1	D	0.55	1/8056 (0.0%)	0.80	9/10940 (0.1%)
1	E	0.56	1/8056 (0.0%)	0.80	7/10940 (0.1%)
1	F	0.57	0/8089	0.83	6/10986 (0.1%)
All	All	0.57	4/48387 (0.0%)	0.82	47/65711 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
1	F	0	2
All	All	0	7

All (4) bond length outliers are listed below:

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

All (47) bond angle outliers are listed below:

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

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

There are no chirality outliers.

All (7) planarity outliers are listed below:

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

5.2 Too-close contacts

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:904:VAL:HG21	1:E:942:ALA:HB2	1.98	0.46
1:F:578:LEU:HB3	1:F:579:PRO:HD2	1.98	0.46
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.51	0.46
1:B:1026:PHE:O	1:B:1030:ARG:HB2	2.16	0.46
1:B:195:LYS:HB3	1:B:196:PHE:CD1	2.51	0.46
1:B:576:VAL:HG22	1:B:663:VAL:HG22	1.98	0.46
1:B:683:GLU:HG2	1:B:819:TYR:CG	2.51	0.46
1:C:187:TRP:HA	1:C:774:MET:O	2.16	0.46
1:D:897:ILE:HG12	1:D:1030:ARG:HD3	1.97	0.46
1:D:568:ASP:O	1:D:634:TRP:HZ3	1.98	0.46
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.98	0.46
1:D:919:ARG:HD3	1:D:921:LEU:HD23	1.98	0.46
1:F:572:PHE:CE1	1:F:648:THR:HG22	2.51	0.46
1:A:429:GLU:H	1:A:429:GLU:CD	2.18	0.45
1:B:405:LEU:HD22	1:B:481:SER:HB3	1.96	0.45
1:C:310:LEU:O	1:C:314:GLU:HG3	2.16	0.45
1:C:969:ARG:HH11	1:C:970:MET:HB3	1.81	0.45
1:D:610:PHE:O	1:D:627:ALA:HA	2.16	0.45
1:D:573:MET:HG2	1:D:628:PHE:CD1	2.51	0.45
1:E:356:TYR:C	1:E:358:PHE:H	2.19	0.45
1:E:418:ARG:O	1:E:422:GLU:HB2	2.15	0.45
1:E:425:LEU:HD12	1:E:430:ALA:HA	1.98	0.45
1:E:847:LEU:O	1:E:850:LYS:HB2	2.16	0.45
1:F:281:PHE:CE1	1:F:324:VAL:HG21	2.51	0.45
1:F:894:SER:HB3	1:F:897:ILE:HG12	1.98	0.45
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.97	0.45
1:F:953:MET:HE2	1:F:963:ALA:HB3	1.98	0.45
1:A:2:PRO:O	1:A:6:ILE:HG23	2.16	0.45
1:A:467:TYR:HE1	1:A:925:VAL:HG22	1.81	0.45
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.67	0.45
1:A:857:TYR:N	1:A:857:TYR:CD2	2.85	0.45
1:B:270:LEU:HA	1:B:270:LEU:HD12	1.78	0.45
1:B:520:PHE:O	1:B:524:THR:HG22	2.16	0.45
1:C:11:PHE:O	1:C:11:PHE:HD2	1.99	0.45
1:C:246:PHE:O	1:C:262:LEU:HD23	2.15	0.45
1:D:415:ASN:HB3	1:D:434:SER:HB2	1.98	0.45
1:D:442:LEU:HA	1:D:442:LEU:HD23	1.67	0.45
1:D:485:ALA:O	1:D:490:PRO:HD3	2.16	0.45
1:E:728:LYS:HB2	1:E:810:GLU:OE1	2.15	0.45
1:F:195:LYS:HB3	1:F:196:PHE:CD1	2.48	0.45
1:A:404:LEU:HD12	1:A:937:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:HA	1:A:880:SER:OG	2.15	0.45
1:A:926:TYR:H	1:A:926:TYR:HD1	1.64	0.45
1:A:985:GLY:O	1:A:988:PRO:HD2	2.17	0.45
1:C:165:ALA:HB3	1:C:313:MET:CE	2.46	0.45
1:C:382:VAL:O	1:C:386:PHE:HD2	1.99	0.45
1:C:658:ILE:O	1:C:658:ILE:HG13	2.17	0.45
1:C:563:PHE:HB2	1:C:866:GLU:HB2	1.97	0.45
1:D:225:VAL:HG22	1:E:781:MET:HE2	1.97	0.45
1:D:919:ARG:HG2	1:D:920:GLY:N	2.26	0.45
1:E:358:PHE:CD1	1:E:977:MET:HG2	2.51	0.45
1:F:504:ASP:C	1:F:506:GLY:N	2.70	0.45
1:A:172:VAL:CG2	1:A:306:ILE:HD11	2.46	0.45
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.51	0.45
1:B:294:ALA:HB3	1:B:297:ALA:HB2	1.97	0.45
1:B:957:GLY:O	1:B:1041:GLU:HA	2.16	0.45
1:D:310:LEU:O	1:D:314:GLU:HG3	2.17	0.45
1:E:398:MET:HB3	1:E:398:MET:HE3	1.87	0.45
1:E:515:TRP:O	1:E:519:MET:HG3	2.16	0.45
1:E:105:VAL:HB	1:F:105:VAL:HG13	1.99	0.45
1:F:3:ASN:N	1:F:3:ASN:OD1	2.49	0.45
1:F:459:PHE:CE1	1:F:876:LEU:HG	2.51	0.45
1:F:701:GLN:HE22	1:F:852:PRO:HD3	1.81	0.45
1:A:145:THR:C	1:A:147:GLY:H	2.20	0.45
1:A:574:THR:OG1	1:A:664:PHE:O	2.24	0.45
1:A:801:PHE:CD1	1:A:804:PHE:HE2	2.35	0.45
1:A:965:LEU:HD23	1:A:965:LEU:HA	1.64	0.45
1:C:280:GLU:HG3	1:C:285:PRO:HA	1.98	0.45
1:C:686:ASP:OD1	1:C:690:LEU:HB2	2.17	0.45
1:D:999:ALA:O	1:D:1003:VAL:HG23	2.16	0.45
1:D:542:LEU:O	1:D:546:LEU:HG	2.16	0.45
1:D:654:ALA:O	1:D:658:ILE:HG12	2.17	0.45
1:D:947:GLU:O	1:D:951:ASP:HB2	2.17	0.45
1:E:66:GLU:OE1	1:E:821:GLY:HA2	2.17	0.45
1:F:84:SER:HB3	1:F:814:PRO:HA	1.98	0.45
1:A:242:SER:OG	1:A:245:GLU:HG2	2.16	0.45
1:D:375:VAL:HG11	1:D:405:LEU:HD22	1.98	0.45
1:D:876:LEU:HD23	1:D:879:ILE:HD12	1.98	0.45
1:D:996:GLY:O	1:D:999:ALA:N	2.49	0.45
1:D:112:GLN:NE2	1:E:112:GLN:HB3	2.32	0.45
1:E:14:VAL:HG13	1:F:886:LEU:HD12	1.98	0.45
1:F:510:LYS:O	1:F:512:PHE:N	2.46	0.45

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1040/1049 (99%)	951 (91%)	75 (7%)	14 (1%)	15	60
1	B	1040/1049 (99%)	957 (92%)	70 (7%)	13 (1%)	15	60
1	C	1042/1049 (99%)	954 (92%)	72 (7%)	16 (2%)	13	57
1	D	1040/1049 (99%)	946 (91%)	79 (8%)	15 (1%)	14	59
1	E	1040/1049 (99%)	960 (92%)	63 (6%)	17 (2%)	12	56
1	F	1044/1049 (100%)	945 (90%)	83 (8%)	16 (2%)	13	57
All	All	6246/6294 (99%)	5713 (92%)	442 (7%)	91 (2%)	13	57

All (91) Ramachandran outliers are listed below:

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

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	845/852 (99%)	786 (93%)	59 (7%)	19	60
1	B	845/852 (99%)	788 (93%)	57 (7%)	20	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	847/852 (99%)	787 (93%)	60 (7%)	18	59
1	D	845/852 (99%)	795 (94%)	50 (6%)	24	66
1	E	845/852 (99%)	788 (93%)	57 (7%)	20	62
1	F	849/852 (100%)	791 (93%)	58 (7%)	20	61
All	All	5076/5112 (99%)	4735 (93%)	341 (7%)	20	62

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

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

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

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

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

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

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

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

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

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

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ERY	A	1101	-	53,53,53	1.26	4 (7%)	82,82,82	2.04	23 (28%)
3	LMT	A	1102	-	36,36,36	1.75	9 (25%)	47,47,47	1.18	5 (10%)
3	LMT	A	1103	-	36,36,36	1.88	8 (22%)	47,47,47	1.48	9 (19%)
3	LMT	B	1101	-	36,36,36	1.83	9 (25%)	47,47,47	1.95	11 (23%)
3	LMT	C	1101	-	36,36,36	1.72	9 (25%)	47,47,47	1.57	9 (19%)
2	ERY	D	1101	-	53,53,53	1.38	4 (7%)	82,82,82	2.02	22 (26%)
3	LMT	D	1102	-	36,36,36	1.81	10 (27%)	47,47,47	1.09	3 (6%)
3	LMT	D	1103	-	36,36,36	1.74	8 (22%)	47,47,47	1.60	10 (21%)
3	LMT	E	1101	-	36,36,36	1.81	10 (27%)	47,47,47	1.34	6 (12%)
3	LMT	F	1101	-	36,36,36	1.78	8 (22%)	47,47,47	1.38	8 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ERY	A	1101	-	-	0/72/107/107	0/3/3/3
3	LMT	A	1102	-	-	0/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	0/21/61/61	0/2/2/2

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

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1102	LMT	C6'-C5'	-3.24	1.40	1.51
3	F	1101	LMT	C6'-C5'	-3.11	1.40	1.51
3	E	1101	LMT	C3'-C2'	-3.10	1.44	1.52
3	D	1103	LMT	C6'-C5'	-3.04	1.41	1.51
3	A	1103	LMT	C6'-C5'	-2.96	1.41	1.51
3	C	1101	LMT	C6'-C5'	-2.90	1.41	1.51
3	A	1102	LMT	C6'-C5'	-2.85	1.41	1.51
3	E	1101	LMT	C6'-C5'	-2.73	1.42	1.51
3	B	1101	LMT	C6'-C5'	-2.72	1.42	1.51
3	C	1101	LMT	C3B-C2B	-2.42	1.46	1.52
3	F	1101	LMT	C3'-C2'	-2.38	1.46	1.52
3	E	1101	LMT	C3B-C2B	-2.33	1.46	1.52
3	D	1102	LMT	C3B-C2B	-2.27	1.46	1.52
3	C	1101	LMT	C3'-C2'	-2.15	1.46	1.52
3	A	1102	LMT	C3'-C2'	-2.12	1.46	1.52
3	D	1102	LMT	C3'-C2'	-2.11	1.46	1.52
3	E	1101	LMT	O2'-C2'	2.00	1.47	1.43
3	A	1102	LMT	C5-C4	2.04	1.63	1.51
2	A	1101	ERY	O11-C9	2.08	1.25	1.21
2	D	1101	ERY	O9-C22	2.11	1.47	1.41
2	A	1101	ERY	O6-C17	2.12	1.47	1.42
3	E	1101	LMT	C5-C4	2.19	1.64	1.51
3	B	1101	LMT	C5-C4	2.24	1.64	1.51
3	C	1101	LMT	O3'-C3'	2.28	1.48	1.43
3	F	1101	LMT	O2'-C2'	2.33	1.48	1.43
2	D	1101	ERY	O11-C9	2.33	1.25	1.21
3	D	1102	LMT	O3'-C3'	2.35	1.48	1.43
3	D	1103	LMT	O2'-C2'	2.38	1.48	1.43
3	D	1103	LMT	O3'-C3'	2.40	1.48	1.43
3	A	1102	LMT	O2'-C2'	2.40	1.48	1.43
3	A	1103	LMT	O2'-C2'	2.41	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1103	LMT	O3'-C3'	2.44	1.48	1.43
3	B	1101	LMT	O2'-C2'	2.47	1.48	1.43
2	A	1101	ERY	C25-C26	2.51	1.56	1.51
3	D	1102	LMT	O2'-C2'	2.52	1.48	1.43
3	C	1101	LMT	O2'-C2'	2.54	1.48	1.43
2	D	1101	ERY	C25-C26	2.63	1.56	1.51
3	B	1101	LMT	O3'-C3'	2.64	1.49	1.43
3	F	1101	LMT	O3B-C3B	2.78	1.49	1.43
3	A	1102	LMT	O5'-C1'	2.93	1.49	1.41
3	F	1101	LMT	O5B-C1B	2.96	1.49	1.41
3	D	1103	LMT	O3B-C3B	2.96	1.49	1.43
3	E	1101	LMT	O3B-C3B	2.98	1.50	1.43
3	A	1102	LMT	O3B-C3B	3.08	1.50	1.43
3	D	1103	LMT	O5'-C1'	3.17	1.49	1.41
3	A	1102	LMT	O1'-C1'	3.18	1.45	1.40
3	E	1101	LMT	O5B-C1B	3.22	1.50	1.41
3	D	1102	LMT	O5'-C5'	3.22	1.52	1.44
3	D	1102	LMT	O5'-C1'	3.24	1.50	1.41
3	A	1103	LMT	O1'-C1'	3.29	1.46	1.40
3	C	1101	LMT	O5B-C1B	3.34	1.50	1.41
3	D	1102	LMT	O3B-C3B	3.34	1.50	1.43
3	B	1101	LMT	O3B-C3B	3.35	1.50	1.43
3	C	1101	LMT	O5'-C1'	3.35	1.50	1.41
3	E	1101	LMT	O5'-C1'	3.38	1.50	1.41
3	D	1103	LMT	O1'-C1'	3.41	1.46	1.40
3	B	1101	LMT	O5'-C1'	3.48	1.50	1.41
3	A	1103	LMT	O3B-C3B	3.55	1.51	1.43
3	A	1102	LMT	O5B-C1B	3.56	1.51	1.41
3	C	1101	LMT	O1'-C1'	3.59	1.46	1.40
3	B	1101	LMT	O5'-C5'	3.62	1.53	1.44
3	F	1101	LMT	O5'-C1'	3.63	1.51	1.41
3	B	1101	LMT	O5B-C1B	3.63	1.51	1.41
3	A	1103	LMT	O5'-C1'	3.64	1.51	1.41
3	D	1102	LMT	O5B-C1B	3.65	1.51	1.41
3	F	1101	LMT	O1'-C1'	3.72	1.46	1.40
3	C	1101	LMT	O5'-C5'	3.73	1.53	1.44
3	D	1103	LMT	O5'-C5'	3.74	1.53	1.44
3	E	1101	LMT	O5'-C5'	3.74	1.53	1.44
3	A	1103	LMT	O5B-C1B	3.83	1.51	1.41
3	F	1101	LMT	O5'-C5'	3.88	1.54	1.44
3	D	1102	LMT	O1'-C1'	3.97	1.47	1.40
3	E	1101	LMT	O1'-C1'	4.00	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1101	LMT	O1'-C1'	4.01	1.47	1.40
3	A	1102	LMT	O5'-C5'	4.03	1.54	1.44
3	D	1103	LMT	O5B-C1B	4.23	1.52	1.41
3	A	1103	LMT	O5'-C5'	4.96	1.56	1.44
2	D	1101	ERY	O2-C1	5.23	1.46	1.34
2	A	1101	ERY	O2-C1	5.34	1.46	1.34

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	ERY	O2-C1-O1	-4.68	114.81	123.88
3	D	1103	LMT	C1'-O5'-C5'	-4.32	105.26	113.74
3	B	1101	LMT	O5'-C5'-C4'	-4.14	100.94	109.78
2	A	1101	ERY	C13-O2-C1	-4.10	111.23	118.10
2	D	1101	ERY	C25-C24-N1	-3.56	104.97	115.68
3	B	1101	LMT	C1'-O5'-C5'	-3.52	106.83	113.74
3	A	1103	LMT	C1B-O1B-C4'	-3.50	108.69	118.00
3	B	1101	LMT	C1B-O1B-C4'	-3.35	109.08	118.00
2	A	1101	ERY	C19-C16-C15	-3.25	104.57	110.21
3	C	1101	LMT	O2B-C2B-C1B	-3.22	102.88	110.01
3	D	1103	LMT	O5'-C5'-C4'	-3.14	103.07	109.78
3	D	1103	LMT	C3'-C4'-C5'	-2.88	104.27	110.85
2	A	1101	ERY	O7-C5-C4	-2.83	106.81	111.49
3	F	1101	LMT	O2B-C2B-C1B	-2.80	103.79	110.01
3	F	1101	LMT	O4'-C4B-C3B	-2.78	104.10	110.36
2	A	1101	ERY	O10-C6-C32	-2.75	102.30	108.58
2	D	1101	ERY	O10-C6-C5	-2.68	103.28	107.62
2	D	1101	ERY	C19-C16-C15	-2.63	105.64	110.21
2	A	1101	ERY	C33-C8-C7	-2.54	104.47	109.69
2	D	1101	ERY	C31-C4-C3	-2.52	106.76	111.45
3	E	1101	LMT	C1B-O1B-C4'	-2.45	111.48	118.00
2	D	1101	ERY	O3-C3-C4	-2.44	105.21	108.22
3	A	1102	LMT	C1B-O1B-C4'	-2.44	111.53	118.00
3	C	1101	LMT	C1B-O1B-C4'	-2.39	111.66	118.00
2	A	1101	ERY	O1-C1-C2	-2.36	118.45	124.27
2	D	1101	ERY	C3-C4-C5	-2.33	106.52	110.85
2	D	1101	ERY	O13-C12-C13	-2.22	103.61	107.10
3	A	1103	LMT	C2'-C3'-C4'	-2.21	104.75	109.63
2	A	1101	ERY	C35-C12-C11	-2.21	109.51	113.27
2	D	1101	ERY	C6-C5-C4	-2.18	111.03	114.12
2	D	1101	ERY	C33-C8-C7	-2.08	105.42	109.69
3	D	1102	LMT	O2B-C2B-C3B	-2.06	105.71	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1101	LMT	O3'-C3'-C4'	2.02	114.67	109.89
3	D	1103	LMT	O1B-C4'-C5'	2.02	114.70	109.33
2	A	1101	ERY	C35-C12-C13	2.02	114.32	111.23
2	A	1101	ERY	O2-C13-C12	2.03	110.66	107.17
2	A	1101	ERY	C22-O7-C5	2.08	120.13	116.36
3	F	1101	LMT	O5'-C5'-C6'	2.09	111.78	106.38
3	E	1101	LMT	C1-O1'-C1'	2.14	117.74	114.00
2	A	1101	ERY	C33-C8-C9	2.15	115.28	109.49
2	A	1101	ERY	C30-C2-C3	2.15	117.78	113.03
2	D	1101	ERY	O7-C22-C23	2.15	113.47	108.12
3	B	1101	LMT	C3B-C4B-C5B	2.17	114.10	110.23
3	D	1102	LMT	O5B-C1B-C2B	2.17	114.80	110.28
2	D	1101	ERY	O8-C23-C22	2.19	114.86	110.01
2	D	1101	ERY	C7-C6-C5	2.20	114.97	110.46
3	A	1103	LMT	O3'-C3'-C2'	2.20	115.33	110.36
3	D	1103	LMT	O1B-C4'-C3'	2.21	112.95	107.18
3	D	1103	LMT	O5'-C5'-C6'	2.28	112.30	106.38
3	F	1101	LMT	C1-O1'-C1'	2.30	118.03	114.00
3	A	1102	LMT	C1'-C2'-C3'	2.32	114.58	109.98
3	A	1103	LMT	C4B-C3B-C2B	2.35	115.11	110.79
2	D	1101	ERY	C26-C25-C24	2.35	114.83	110.44
3	D	1103	LMT	O5B-C5B-C6B	2.38	112.55	106.38
3	A	1103	LMT	O5'-C5'-C4'	2.40	114.90	109.78
3	B	1101	LMT	O2B-C2B-C3B	2.42	115.82	110.36
3	C	1101	LMT	O5'-C5'-C6'	2.44	112.70	106.38
2	A	1101	ERY	O4-C18-C21	2.46	111.80	106.57
3	A	1102	LMT	C2'-C3'-C4'	2.48	115.11	109.63
2	D	1101	ERY	C22-O9-C26	2.51	117.24	112.97
3	F	1101	LMT	O4'-C4B-C5B	2.51	115.84	109.23
3	A	1102	LMT	O1B-C1B-C2B	2.55	114.44	108.12
3	D	1103	LMT	O5B-C5B-C4B	2.57	114.57	109.67
3	B	1101	LMT	O1'-C1-C2	2.59	117.09	109.63
3	B	1101	LMT	O5B-C1B-C2B	2.64	115.76	110.28
3	C	1101	LMT	O1B-C4'-C3'	2.67	114.15	107.18
3	A	1103	LMT	C1'-O5'-C5'	2.69	119.02	113.74
3	B	1101	LMT	O5B-C5B-C4B	2.74	114.89	109.67
3	F	1101	LMT	O5B-C5B-C4B	2.74	114.89	109.67
3	A	1103	LMT	O1'-C1'-C2'	2.77	111.41	108.00
3	C	1101	LMT	C1B-O5B-C5B	2.85	119.33	113.74
2	D	1101	ERY	O13-C12-C11	2.85	114.58	109.21
3	F	1101	LMT	C4B-C3B-C2B	2.86	116.05	110.79
2	D	1101	ERY	O4-C18-C21	2.97	112.86	106.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1101	LMT	O5B-C5B-C4B	3.00	115.39	109.67
3	C	1101	LMT	O5B-C5B-C4B	3.02	115.43	109.67
3	E	1101	LMT	C3B-C4B-C5B	3.14	115.82	110.23
2	D	1101	ERY	O9-C26-C25	3.15	114.29	109.11
3	A	1103	LMT	O5B-C5B-C4B	3.16	115.70	109.67
2	A	1101	ERY	O7-C22-C23	3.18	116.02	108.12
3	A	1102	LMT	C1B-C2B-C3B	3.32	116.57	109.98
3	D	1103	LMT	C1'-C2'-C3'	3.40	116.72	109.98
3	E	1101	LMT	O5'-C5'-C6'	3.43	115.26	106.38
2	A	1101	ERY	O3-C3-C4	3.47	112.48	108.22
3	F	1101	LMT	C1B-C2B-C3B	3.57	117.06	109.98
2	A	1101	ERY	O2-C13-C36	3.57	113.95	107.37
3	E	1101	LMT	O1'-C1'-C2'	3.58	112.40	108.00
3	D	1103	LMT	O1'-C1'-C2'	3.64	112.47	108.00
3	B	1101	LMT	C4B-C3B-C2B	3.66	117.53	110.79
3	D	1102	LMT	O1'-C1'-C2'	3.77	112.64	108.00
3	A	1103	LMT	C3B-C4B-C5B	3.84	117.07	110.23
3	C	1101	LMT	C3B-C4B-C5B	3.91	117.20	110.23
2	A	1101	ERY	O2-C1-C2	3.97	119.63	111.44
2	A	1101	ERY	C29-N1-C24	4.11	125.18	113.14
2	D	1101	ERY	C29-N1-C24	4.18	125.41	113.14
3	C	1101	LMT	O1'-C1'-C2'	4.25	113.23	108.00
2	A	1101	ERY	O7-C5-C6	4.43	112.16	106.45
2	A	1101	ERY	C20-O5-C16	4.82	128.60	117.64
2	D	1101	ERY	C20-O5-C16	4.95	128.89	117.64
2	A	1101	ERY	O12-C11-C10	5.15	117.46	110.79
3	B	1101	LMT	O5'-C5'-C6'	5.22	119.89	106.38
2	A	1101	ERY	C15-C16-C17	5.48	114.81	107.82
2	D	1101	ERY	O7-C5-C6	5.63	113.71	106.45
3	B	1101	LMT	O1'-C1'-C2'	6.04	115.43	108.00
2	D	1101	ERY	O12-C11-C10	6.04	118.61	110.79
2	D	1101	ERY	C15-C16-C17	6.04	115.53	107.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1101	LMT	C3B

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 43 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1042/1049 (99%)	0.39	99 (9%) 10 8	49, 83, 120, 150	0
1	B	1042/1049 (99%)	0.28	70 (6%) 21 13	45, 81, 117, 154	0
1	C	1044/1049 (99%)	0.58	121 (11%) 6 5	40, 83, 120, 176	0
1	D	1042/1049 (99%)	0.53	117 (11%) 7 6	43, 94, 130, 161	0
1	E	1042/1049 (99%)	0.55	144 (13%) 4 4	57, 94, 125, 151	0
1	F	1046/1049 (99%)	0.66	144 (13%) 4 4	44, 89, 124, 158	0
All	All	6258/6294 (99%)	0.50	695 (11%) 7 6	40, 87, 124, 176	0

All (695) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	719	ASN	14.3
1	C	720	GLY	14.2
1	F	80	SER	11.4
1	F	720	GLY	10.9
1	C	618	ALA	9.8
1	B	869	SER	9.7
1	D	619	GLY	9.4
1	C	80	SER	9.3
1	F	835	LYS	9.1
1	C	83	ASP	8.9
1	C	619	GLY	8.9
1	C	719	ASN	8.8
1	D	720	GLY	8.6
1	F	82	SER	8.2
1	E	618	ALA	8.0
1	F	79	SER	8.0
1	F	618	ALA	8.0
1	F	826	GLU	7.9
1	F	83	ASP	7.7

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Mol	Chain	Res	Type	RSRZ
1	F	837	THR	7.7
1	D	719	ASN	7.6
1	E	681	ASP	7.3
1	D	869	SER	7.3
1	C	81	ASN	7.2
1	F	836	SER	7.0
1	C	79	SER	7.0
1	C	617	ALA	6.9
1	F	619	GLY	6.8
1	E	658	ILE	6.7
1	F	712	MET	6.7
1	C	836	SER	6.5
1	E	619	GLY	6.4
1	C	82	SER	6.4
1	B	618	ALA	6.4
1	D	618	ALA	6.3
1	E	80	SER	6.2
1	B	619	GLY	6.2
1	F	711	ASP	6.1
1	F	81	ASN	6.1
1	D	615	ALA	6.0
1	C	721	LEU	5.9
1	B	719	ASN	5.9
1	A	449	LEU	5.9
1	E	719	ASN	5.8
1	F	713	LEU	5.8
1	D	401	ALA	5.8
1	B	617	ALA	5.7
1	D	620	ALA	5.7
1	E	657	GLN	5.7
1	F	829	GLY	5.7
1	F	58	GLN	5.6
1	F	681	ASP	5.6
1	A	658	ILE	5.6
1	F	718	PRO	5.5
1	F	828	LEU	5.5
1	A	620	ALA	5.5
1	C	815	ARG	5.5
1	F	815	ARG	5.5
1	B	80	SER	5.5
1	D	178	PHE	5.5
1	E	655	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	619	GLY	5.5
1	B	817	GLU	5.4
1	E	291	ILE	5.4
1	F	817	GLU	5.4
1	D	616	GLY	5.4
1	E	615	ALA	5.4
1	E	617	ALA	5.4
1	D	460	GLY	5.3
1	F	60	THR	5.3
1	C	835	LYS	5.3
1	C	816	LEU	5.2
1	D	621	GLY	5.2
1	E	830	GLN	5.2
1	E	678	THR	5.2
1	E	290	GLY	5.2
1	F	617	ALA	5.2
1	C	712	MET	5.2
1	A	605	ASN	5.2
1	C	837	THR	5.1
1	D	826	GLU	5.1
1	F	676	THR	5.1
1	C	826	GLU	5.1
1	F	839	GLU	5.1
1	C	616	GLY	5.1
1	F	831	ALA	5.1
1	C	403	GLY	5.0
1	B	620	ALA	5.0
1	C	817	GLU	5.0
1	F	888	LEU	4.9
1	F	717	ARG	4.9
1	F	577	GLN	4.9
1	B	79	SER	4.9
1	F	402	ILE	4.8
1	E	78	MET	4.8
1	E	310	LEU	4.8
1	E	720	GLY	4.8
1	F	662	MET	4.8
1	C	449	LEU	4.7
1	E	659	LYS	4.7
1	A	617	ALA	4.7
1	E	307	ARG	4.7
1	F	834	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	943	ILE	4.7
1	F	840	ALA	4.7
1	D	617	ALA	4.6
1	F	620	ALA	4.6
1	F	69	MET	4.6
1	F	449	LEU	4.6
1	F	1037	ASN	4.6
1	E	826	GLU	4.6
1	A	1039	ASP	4.6
1	F	721	LEU	4.6
1	E	79	SER	4.5
1	D	681	ASP	4.5
1	C	494	ALA	4.5
1	F	832	ALA	4.5
1	E	81	ASN	4.4
1	F	500	ILE	4.4
1	A	615	ALA	4.4
1	D	461	GLY	4.3
1	F	59	ASP	4.3
1	C	445	ILE	4.3
1	D	81	ASN	4.3
1	F	62	THR	4.3
1	A	445	ILE	4.3
1	D	80	SER	4.3
1	B	577	GLN	4.3
1	A	179	GLY	4.3
1	E	616	GLY	4.3
1	C	818	ARG	4.2
1	A	618	ALA	4.2
1	D	83	ASP	4.2
1	B	818	ARG	4.2
1	C	615	ALA	4.2
1	F	481	SER	4.2
1	B	678	THR	4.2
1	C	681	ASP	4.2
1	A	92	LEU	4.2
1	B	616	GLY	4.2
1	D	721	LEU	4.1
1	E	620	ALA	4.1
1	F	501	ALA	4.1
1	B	720	GLY	4.1
1	B	662	MET	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	870	GLY	4.1
1	C	620	ALA	4.1
1	C	834	GLY	4.1
1	B	895	TRP	4.0
1	A	616	GLY	4.0
1	B	81	ASN	4.0
1	A	178	PHE	4.0
1	B	229	GLN	4.0
1	E	177	LEU	4.0
1	A	900	SER	4.0
1	E	900	SER	4.0
1	A	164	ASP	4.0
1	D	815	ARG	4.0
1	F	57	VAL	4.0
1	B	78	MET	4.0
1	C	1011	MET	3.9
1	D	79	SER	3.9
1	C	614	GLY	3.9
1	A	79	SER	3.9
1	E	888	LEU	3.9
1	E	818	ARG	3.9
1	C	62	THR	3.9
1	A	78	MET	3.9
1	D	78	MET	3.9
1	A	719	ASN	3.9
1	F	941	ASN	3.9
1	E	314	GLU	3.9
1	E	682	PHE	3.9
1	E	407	ASP	3.9
1	B	400	LEU	3.9
1	D	663	VAL	3.9
1	D	817	GLU	3.8
1	E	869	SER	3.8
1	E	933	THR	3.8
1	B	282	ASN	3.8
1	C	481	SER	3.8
1	C	833	PRO	3.8
1	F	68	ASN	3.8
1	E	993	THR	3.8
1	D	1041	GLU	3.8
1	F	400	LEU	3.8
1	A	1037	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	308	ALA	3.8
1	E	300	LEU	3.8
1	C	684	LEU	3.8
1	B	826	GLU	3.8
1	E	819	TYR	3.7
1	A	659	LYS	3.7
1	E	605	ASN	3.7
1	E	315	PRO	3.7
1	B	615	ALA	3.7
1	E	441	ALA	3.7
1	E	406	VAL	3.7
1	A	960	LEU	3.7
1	F	282	ASN	3.7
1	A	610	PHE	3.7
1	F	442	LEU	3.7
1	C	91	THR	3.7
1	C	442	LEU	3.7
1	C	404	LEU	3.6
1	B	718	PRO	3.6
1	F	680	PHE	3.6
1	F	830	GLN	3.6
1	D	389	SER	3.6
1	E	817	GLU	3.6
1	D	404	LEU	3.6
1	C	802	SER	3.6
1	A	663	VAL	3.6
1	B	715	SER	3.6
1	D	834	GLY	3.6
1	A	1040	ILE	3.6
1	A	959	GLY	3.6
1	A	681	ASP	3.6
1	F	404	LEU	3.6
1	A	611	ALA	3.5
1	C	444	GLY	3.5
1	A	400	LEU	3.5
1	D	462	SER	3.5
1	E	718	PRO	3.5
1	A	655	PHE	3.5
1	F	833	PRO	3.5
1	F	406	VAL	3.5
1	D	718	PRO	3.5
1	A	181	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	683	GLU	3.5
1	E	33	ALA	3.5
1	D	423	GLU	3.5
1	C	711	ASP	3.4
1	D	407	ASP	3.4
1	B	837	THR	3.4
1	A	402	ILE	3.4
1	D	400	LEU	3.4
1	F	576	VAL	3.4
1	B	681	ASP	3.4
1	E	712	MET	3.4
1	E	827	ILE	3.4
1	F	708	LYS	3.4
1	F	70	ASN	3.4
1	C	68	ASN	3.4
1	A	401	ALA	3.4
1	B	943	ILE	3.4
1	E	82	SER	3.4
1	A	641	GLU	3.4
1	F	65	ILE	3.4
1	F	66	GLU	3.3
1	F	504	ASP	3.3
1	E	663	VAL	3.3
1	B	67	GLN	3.3
1	F	827	ILE	3.3
1	C	838	GLY	3.3
1	D	886	LEU	3.3
1	E	328	ASP	3.3
1	E	839	GLU	3.3
1	F	699	ARG	3.3
1	E	299	ALA	3.3
1	F	818	ARG	3.3
1	A	612	VAL	3.3
1	C	441	ALA	3.3
1	D	828	LEU	3.3
1	E	944	LEU	3.3
1	C	825	MET	3.3
1	B	488	LEU	3.3
1	C	421	ALA	3.3
1	C	676	THR	3.3
1	F	659	LYS	3.3
1	E	831	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	835	LYS	3.3
1	E	287	SER	3.3
1	F	91	THR	3.3
1	C	888	LEU	3.2
1	D	614	GLY	3.2
1	D	866	GLU	3.2
1	C	402	ILE	3.2
1	E	576	VAL	3.2
1	F	502	LYS	3.2
1	F	1043	SER	3.2
1	D	678	THR	3.2
1	F	503	GLY	3.2
1	D	958	LYS	3.2
1	C	1044	HIS	3.2
1	E	403	GLY	3.2
1	F	13	TRP	3.2
1	C	400	LEU	3.2
1	F	825	MET	3.2
1	F	816	LEU	3.2
1	C	501	ALA	3.1
1	B	403	GLY	3.1
1	D	288	GLY	3.1
1	E	92	LEU	3.1
1	F	626	ILE	3.1
1	F	661	ALA	3.1
1	D	194	ASN	3.1
1	A	606	VAL	3.1
1	A	640	GLU	3.1
1	E	891	LEU	3.1
1	E	932	LEU	3.1
1	D	32	VAL	3.1
1	F	405	LEU	3.1
1	E	32	VAL	3.1
1	F	675	GLY	3.1
1	E	642	ASN	3.1
1	E	609	VAL	3.1
1	D	445	ILE	3.1
1	D	933	THR	3.1
1	A	80	SER	3.1
1	C	48	SER	3.1
1	C	936	GLY	3.1
1	E	679	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	404	LEU	3.1
1	E	640	GLU	3.1
1	E	612	VAL	3.1
1	E	488	LEU	3.0
1	F	933	THR	3.0
1	D	82	SER	3.0
1	A	403	GLY	3.0
1	D	839	GLU	3.0
1	B	63	GLN	3.0
1	E	683	GLU	3.0
1	D	322	LYS	3.0
1	A	964	THR	3.0
1	D	179	GLY	3.0
1	D	715	SER	3.0
1	C	575	MET	3.0
1	E	892	TYR	3.0
1	B	815	ARG	3.0
1	A	404	LEU	3.0
1	C	448	VAL	3.0
1	E	175	VAL	3.0
1	F	612	VAL	3.0
1	C	943	ILE	3.0
1	F	407	ASP	3.0
1	C	718	PRO	3.0
1	D	836	SER	2.9
1	E	936	GLY	2.9
1	F	78	MET	2.9
1	C	577	GLN	2.9
1	C	621	GLY	2.9
1	A	958	LYS	2.9
1	D	803	ALA	2.9
1	A	91	THR	2.9
1	C	937	LEU	2.9
1	A	657	GLN	2.9
1	F	474	ILE	2.9
1	C	713	LEU	2.9
1	C	935	ILE	2.9
1	E	303	ALA	2.9
1	C	388	PHE	2.9
1	D	870	GLY	2.9
1	B	91	THR	2.9
1	A	826	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	815	ARG	2.9
1	D	851	LEU	2.9
1	D	287	SER	2.9
1	F	877	TYR	2.9
1	E	994	GLY	2.9
1	D	11	PHE	2.9
1	C	783	PRO	2.9
1	D	713	LEU	2.9
1	A	632	LYS	2.8
1	C	822	LEU	2.8
1	A	134	SER	2.8
1	B	576	VAL	2.8
1	E	142	VAL	2.8
1	F	67	GLN	2.8
1	F	722	GLU	2.8
1	A	142	VAL	2.8
1	F	663	VAL	2.8
1	D	818	ARG	2.8
1	A	835	LYS	2.8
1	C	69	MET	2.8
1	C	856	GLY	2.8
1	E	820	ASN	2.8
1	E	601	LYS	2.8
1	D	402	ILE	2.8
1	D	1037	ASN	2.8
1	E	405	LEU	2.8
1	F	575	MET	2.8
1	B	871	ASN	2.8
1	D	960	LEU	2.8
1	D	888	LEU	2.8
1	A	961	ILE	2.7
1	C	401	ALA	2.7
1	C	57	VAL	2.7
1	D	830	GLN	2.7
1	D	788	ASP	2.7
1	C	405	LEU	2.7
1	A	830	GLN	2.7
1	D	323	ILE	2.7
1	A	767	ARG	2.7
1	A	949	ALA	2.7
1	F	615	ALA	2.7
1	F	658	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	840	ALA	2.7
1	A	817	GLU	2.7
1	B	683	GLU	2.7
1	B	868	LEU	2.7
1	F	731	ILE	2.7
1	E	613	ASN	2.7
1	F	246	PHE	2.7
1	A	613	ASN	2.7
1	E	91	THR	2.7
1	F	993	THR	2.7
1	E	509	LYS	2.7
1	C	784	ASP	2.7
1	E	821	GLY	2.7
1	A	195	LYS	2.6
1	B	661	ALA	2.6
1	B	828	LEU	2.6
1	C	60	THR	2.6
1	D	789	TRP	2.6
1	F	88	VAL	2.6
1	B	635	ALA	2.6
1	E	178	PHE	2.6
1	D	486	LEU	2.6
1	F	937	LEU	2.6
1	F	714	THR	2.6
1	C	717	ARG	2.6
1	D	801	PHE	2.6
1	B	939	ALA	2.6
1	C	14	VAL	2.6
1	D	173	GLY	2.6
1	E	83	ASP	2.6
1	F	683	GLU	2.6
1	F	398	MET	2.6
1	C	982	PHE	2.6
1	D	868	LEU	2.6
1	B	638	PRO	2.6
1	D	624	THR	2.6
1	D	487	ILE	2.6
1	C	828	LEU	2.6
1	E	680	PHE	2.6
1	A	942	ALA	2.6
1	B	663	VAL	2.6
1	F	92	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	474	ILE	2.6
1	A	162	MET	2.6
1	B	835	LYS	2.5
1	F	608	SER	2.5
1	E	662	MET	2.5
1	F	445	ILE	2.5
1	A	281	PHE	2.5
1	E	931	LEU	2.5
1	D	717	ARG	2.5
1	E	890	ALA	2.5
1	E	654	ALA	2.5
1	C	1037	ASN	2.5
1	B	714	THR	2.5
1	E	825	MET	2.5
1	A	406	VAL	2.5
1	C	58	GLN	2.5
1	A	902	MET	2.5
1	E	837	THR	2.5
1	F	995	ALA	2.5
1	A	176	GLN	2.5
1	C	54	ALA	2.5
1	C	97	GLY	2.5
1	C	178	PHE	2.5
1	F	178	PHE	2.5
1	B	821	GLY	2.5
1	E	162	MET	2.5
1	E	995	ALA	2.5
1	D	459	PHE	2.5
1	F	64	VAL	2.5
1	E	282	ASN	2.5
1	E	330	THR	2.5
1	E	717	ARG	2.5
1	A	408	ASP	2.4
1	A	621	GLY	2.4
1	E	400	LEU	2.4
1	C	788	ASP	2.4
1	D	140	VAL	2.4
1	C	941	ASN	2.4
1	D	628	PHE	2.4
1	C	473	THR	2.4
1	E	408	ASP	2.4
1	D	610	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	884	VAL	2.4
1	F	12	ALA	2.4
1	F	838	GLY	2.4
1	A	407	ASP	2.4
1	C	502	LYS	2.4
1	E	577	GLN	2.4
1	F	892	TYR	2.4
1	B	995	ALA	2.4
1	E	887	CYS	2.4
1	D	802	SER	2.4
1	E	641	GLU	2.4
1	A	81	ASN	2.4
1	C	478	MET	2.4
1	D	576	VAL	2.4
1	F	7	ASP	2.4
1	C	839	GLU	2.4
1	D	575	MET	2.4
1	D	325	TYR	2.4
1	B	178	PHE	2.4
1	A	177	LEU	2.4
1	F	401	ALA	2.4
1	C	814	PRO	2.4
1	B	230	LEU	2.4
1	C	803	ALA	2.4
1	E	367	ILE	2.4
1	A	962	GLU	2.4
1	B	66	GLU	2.4
1	C	685	ILE	2.4
1	A	679	GLY	2.4
1	B	575	MET	2.4
1	D	661	ALA	2.4
1	E	402	ILE	2.3
1	A	405	LEU	2.3
1	E	69	MET	2.3
1	F	403	GLY	2.3
1	A	443	VAL	2.3
1	A	803	ALA	2.3
1	B	406	VAL	2.3
1	E	598	TYR	2.3
1	E	733	GLN	2.3
1	F	441	ALA	2.3
1	C	576	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1045	THR	2.3
1	D	62	THR	2.3
1	F	61	VAL	2.3
1	A	180	SER	2.3
1	D	31	PRO	2.3
1	E	409	ALA	2.3
1	F	709	HIS	2.3
1	C	313	MET	2.3
1	C	59	ASP	2.3
1	D	806	SER	2.3
1	D	959	GLY	2.3
1	C	485	ALA	2.3
1	F	739	LEU	2.3
1	A	287	SER	2.3
1	D	791	VAL	2.3
1	B	717	ARG	2.3
1	D	33	ALA	2.3
1	F	873	ALA	2.3
1	F	117	LEU	2.3
1	F	89	GLN	2.3
1	C	933	THR	2.3
1	C	940	LYS	2.3
1	E	176	GLN	2.3
1	F	960	LEU	2.3
1	D	66	GLU	2.2
1	F	453	PHE	2.3
1	C	871	ASN	2.2
1	D	87	THR	2.2
1	E	348	ILE	2.2
1	F	448	VAL	2.2
1	E	714	THR	2.2
1	D	141	GLY	2.2
1	E	198	LEU	2.2
1	A	680	PHE	2.2
1	C	934	THR	2.2
1	D	993	THR	2.2
1	A	159	ALA	2.2
1	A	899	PHE	2.2
1	E	590	VAL	2.2
1	E	828	LEU	2.2
1	F	684	LEU	2.2
1	B	92	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	176	GLN	2.2
1	F	230	LEU	2.2
1	B	83	ASP	2.2
1	E	331	PRO	2.2
1	E	626	ILE	2.2
1	E	138	MET	2.2
1	A	197	GLN	2.2
1	D	714	THR	2.2
1	F	819	TYR	2.2
1	B	366	LEU	2.2
1	C	782	LEU	2.2
1	D	195	LYS	2.2
1	D	447	MET	2.2
1	D	835	LYS	2.2
1	E	313	MET	2.2
1	A	713	LEU	2.2
1	F	700	ASN	2.2
1	A	280	GLU	2.2
1	F	881	LEU	2.2
1	F	484	VAL	2.2
1	E	898	PRO	2.2
1	F	715	SER	2.2
1	D	731	ILE	2.2
1	E	829	GLY	2.2
1	E	304	ALA	2.2
1	E	651	ALA	2.2
1	D	164	ASP	2.2
1	F	1044	HIS	2.2
1	D	690	LEU	2.2
1	E	597	TYR	2.2
1	C	865	GLN	2.2
1	A	939	ALA	2.1
1	D	623	ASN	2.1
1	F	1047	ASP	2.1
1	A	66	GLU	2.1
1	C	90	ILE	2.1
1	D	90	ILE	2.1
1	B	721	LEU	2.1
1	D	403	GLY	2.1
1	F	679	GLY	2.1
1	A	953	MET	2.1
1	E	575	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	289	LEU	2.1
1	E	960	LEU	2.1
1	A	626	ILE	2.1
1	C	67	GLN	2.1
1	E	901	VAL	2.1
1	F	791	VAL	2.1
1	F	814	PRO	2.1
1	E	935	ILE	2.1
1	B	839	GLU	2.1
1	E	632	LYS	2.1
1	B	177	LEU	2.1
1	C	480	LEU	2.1
1	F	1040	ILE	2.1
1	F	444	GLY	2.1
1	A	448	VAL	2.1
1	E	351	VAL	2.1
1	F	516	PHE	2.1
1	C	357	LEU	2.1
1	C	623	ASN	2.1
1	D	941	ASN	2.1
1	B	626	ILE	2.1
1	B	936	GLY	2.1
1	E	937	LEU	2.1
1	E	325	TYR	2.1
1	D	778	LYS	2.1
1	E	298	ASN	2.1
1	C	824	SER	2.1
1	D	67	GLN	2.1
1	D	902	MET	2.1
1	E	610	PHE	2.1
1	D	729	ILE	2.1
1	B	179	GLY	2.1
1	C	429	GLU	2.1
1	D	782	LEU	2.1
1	A	885	PHE	2.1
1	A	638	PRO	2.1
1	C	164	ASP	2.1
1	D	408	ASP	2.1
1	F	710	PRO	2.1
1	C	383	LEU	2.1
1	D	626	ILE	2.1
1	B	824	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	593	GLU	2.1
1	B	59	ASP	2.1
1	D	783	PRO	2.1
1	A	706	ALA	2.1
1	E	955	LYS	2.1
1	A	62	THR	2.1
1	E	195	LYS	2.1
1	A	946	VAL	2.1
1	D	936	GLY	2.1
1	E	167	SER	2.1
1	F	14	VAL	2.1
1	E	311	ALA	2.1
1	D	827	ILE	2.1
1	B	716	VAL	2.1
1	D	821	GLY	2.1
1	A	604	ASN	2.0
1	A	886	LEU	2.0
1	F	177	LEU	2.0
1	E	608	SER	2.0
1	E	647	ILE	2.0
1	E	824	SER	2.0
1	F	943	ILE	2.0
1	B	402	ILE	2.0
1	C	61	VAL	2.0
1	C	1016	VAL	2.0
1	E	591	LEU	2.0
1	D	577	GLN	2.0
1	A	279	ALA	2.0
1	A	943	ILE	2.0
1	C	9	PRO	2.0
1	C	995	ALA	2.0
1	F	335	ILE	2.0
1	D	612	VAL	2.0
1	C	801	PHE	2.0
1	C	408	ASP	2.0
1	A	310	LEU	2.0
1	D	833	PRO	2.0
1	F	356	TYR	2.0
1	C	93	THR	2.0
1	F	107	VAL	2.0
1	E	1026	PHE	2.0
1	A	89	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	635	ALA	2.0
1	A	995	ALA	2.0
1	C	819	TYR	2.0
1	B	938	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	LMT	A	1103	35/35	0.84	1.05	6.48	58,93,104,107	0
2	ERY	A	1101	51/51	0.80	1.15	3.00	75,87,97,106	51
2	ERY	D	1101	51/51	0.67	1.13	2.62	73,92,103,104	51
3	LMT	F	1101	35/35	0.85	0.66	2.29	49,77,91,99	0
3	LMT	B	1101	35/35	0.84	0.57	1.87	49,76,101,110	0
3	LMT	A	1102	35/35	0.89	0.56	1.46	26,76,84,88	0
3	LMT	E	1101	35/35	0.83	0.54	1.05	57,76,88,116	0
3	LMT	D	1102	35/35	0.83	0.39	0.78	55,79,93,93	0
3	LMT	C	1101	35/35	0.81	0.46	0.73	55,72,93,98	0
3	LMT	D	1103	35/35	0.78	0.40	-0.17	79,94,108,110	0
4	NI	A	1104	1/1	0.99	0.15	-	54,54,54,54	0
4	NI	E	1102	1/1	0.98	0.13	-	94,94,94,94	0
4	NI	C	1102	1/1	0.99	0.12	-	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.