



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:00 AM UTC

PDB ID : 4ZJQ / pdb_00004zjq
Title : Crystal structure of AcrB deletion mutant in complex with antibiotic in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-29
Resolution : 3.59 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

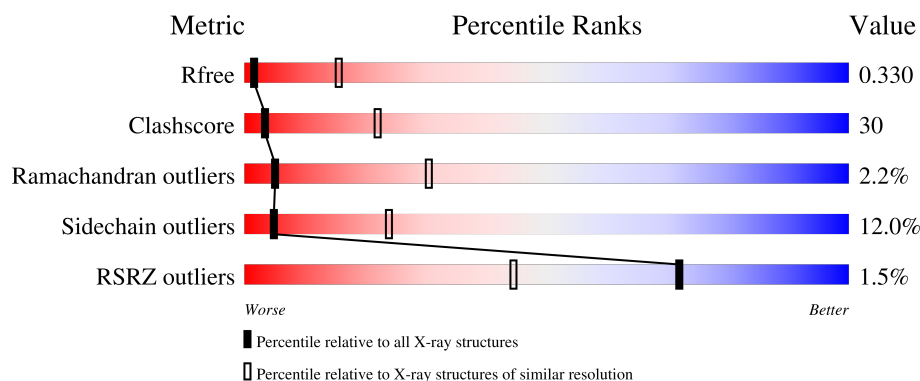
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	1044	% 46% 45% 8% .
1	B	1044	44% 47% 8% .
1	C	1044	2% 40% 49% 9% ..
1	D	1044	% 43% 47% 8% ..
1	E	1044	% 45% 46% 8% .

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Mol	Chain	Length	Quality of chain
1	F	1044	3% 39% 50% 9% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 47697 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	B	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			
1	C	1036	Total	C	N	O	S	0	0	0
			7877	5063	1302	1469	43			
1	D	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	E	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			
1	F	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			

There are 36 discrepancies between the modelled and reference sequences:

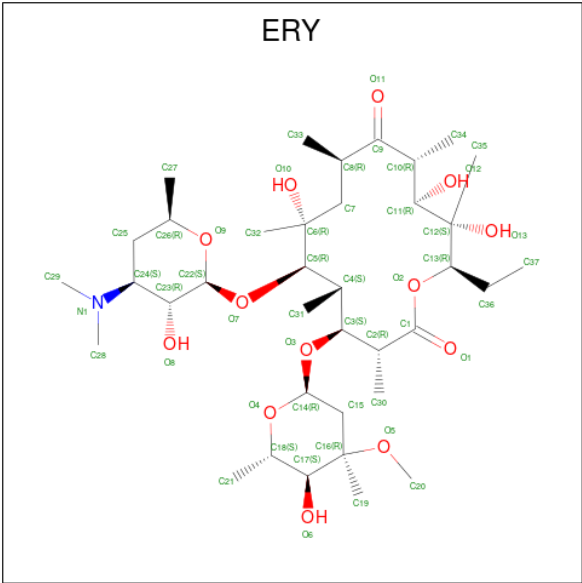
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	GLY	PHE	engineered mutation	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	PHE	deletion	UNP P31224
A	?	-	ALA	deletion	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	ARG	deletion	UNP P31224
B	?	GLY	PHE	engineered mutation	UNP P31224
B	?	-	GLY	deletion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

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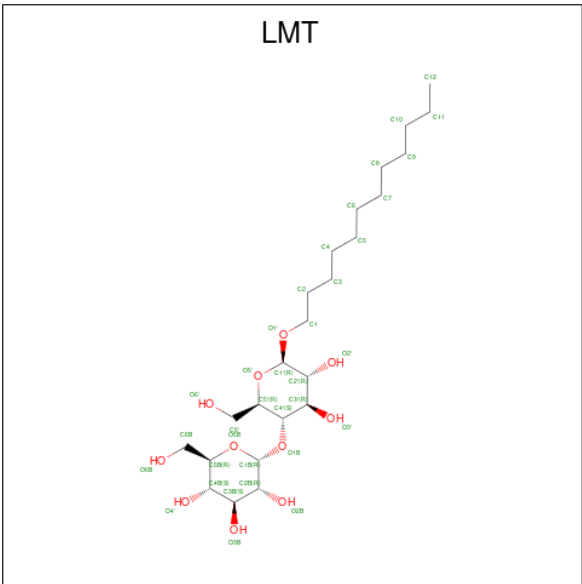
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P31224
D	?	GLY	PHE	engineered mutation	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	PHE	deletion	UNP P31224
D	?	-	ALA	deletion	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	ARG	deletion	UNP P31224
E	?	GLY	PHE	engineered mutation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

- Molecule 2 is ERYTHROMYCIN A (CCD ID: ERY) (formula: C₃₇H₆₇NO₁₃).



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

- Molecule 3 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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		

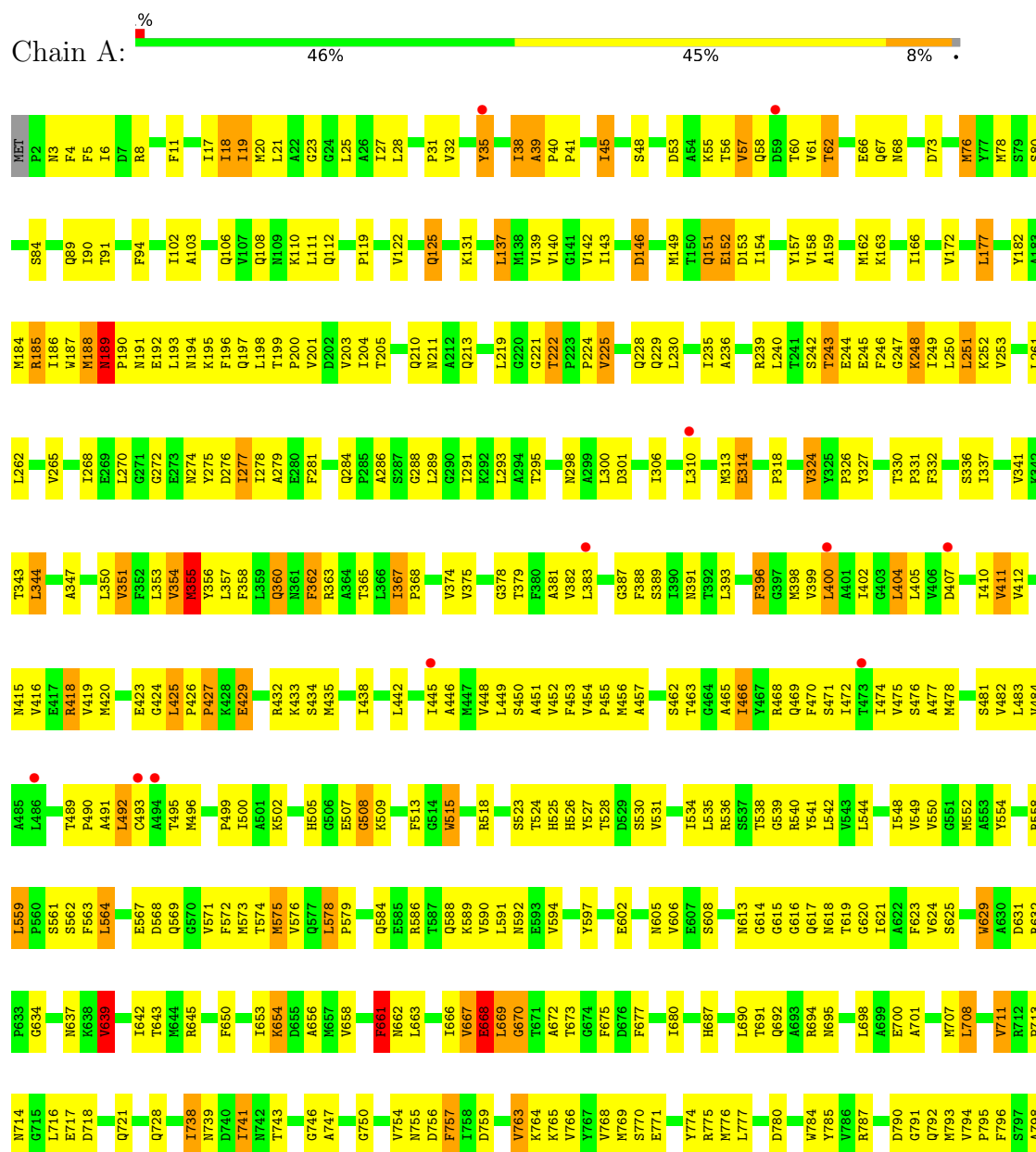
- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

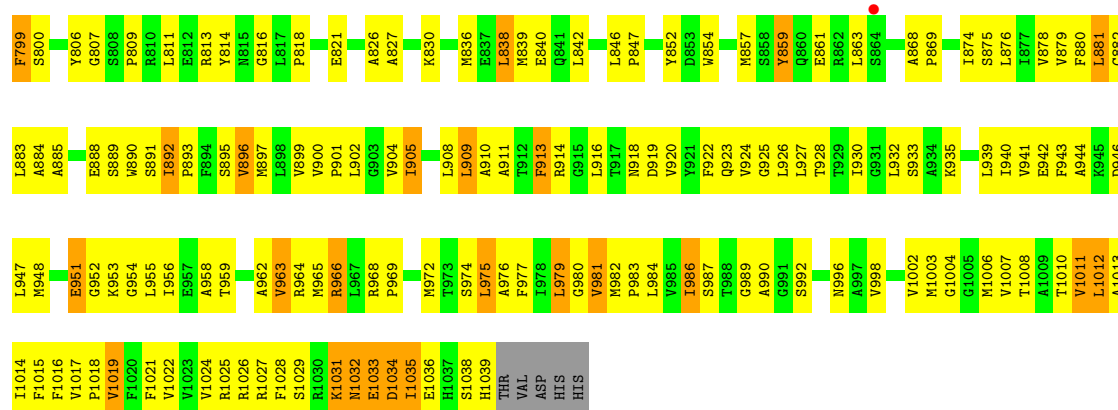
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ni	0	0
			1	1		
4	C	1	Total	Ni	0	0
			1	1		
4	E	1	Total	Ni	0	0
			1	1		

3 Residue-property plots

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

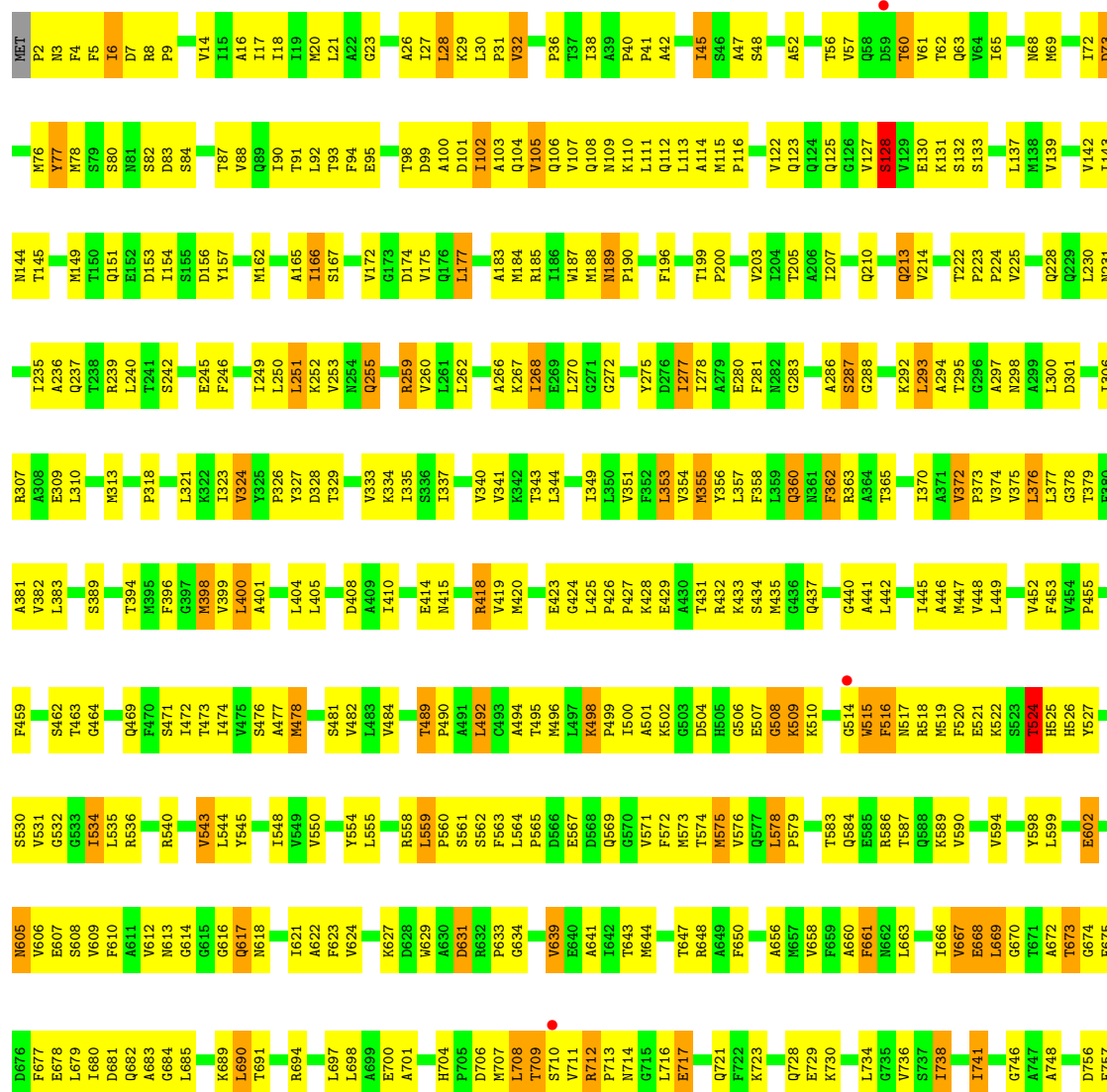
• Molecule 1: Multidrug efflux pump subunit AcrB

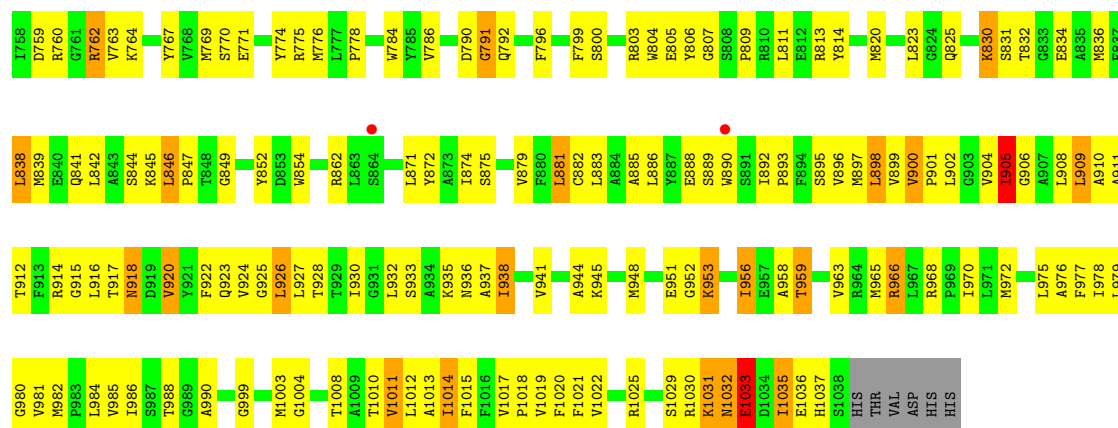




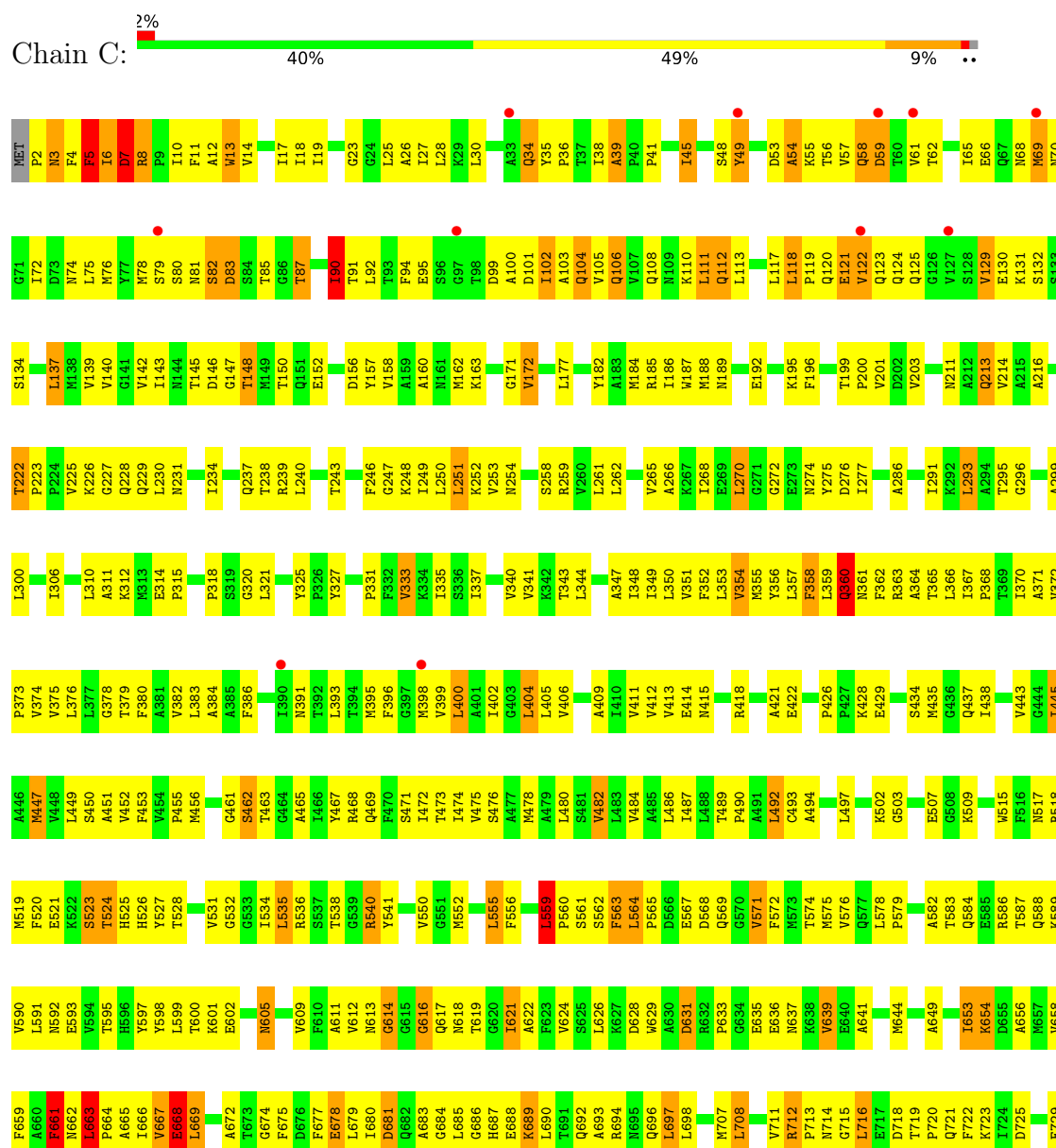
Molecule 1: Multidrug efflux pump subunit AcrB

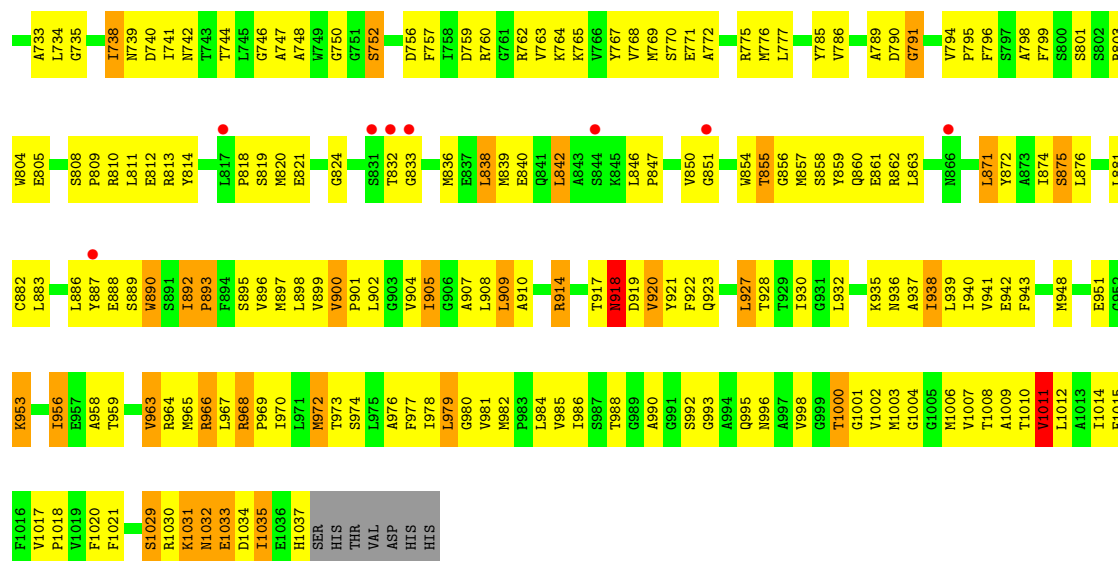
Chain B: 44% 47% 8%



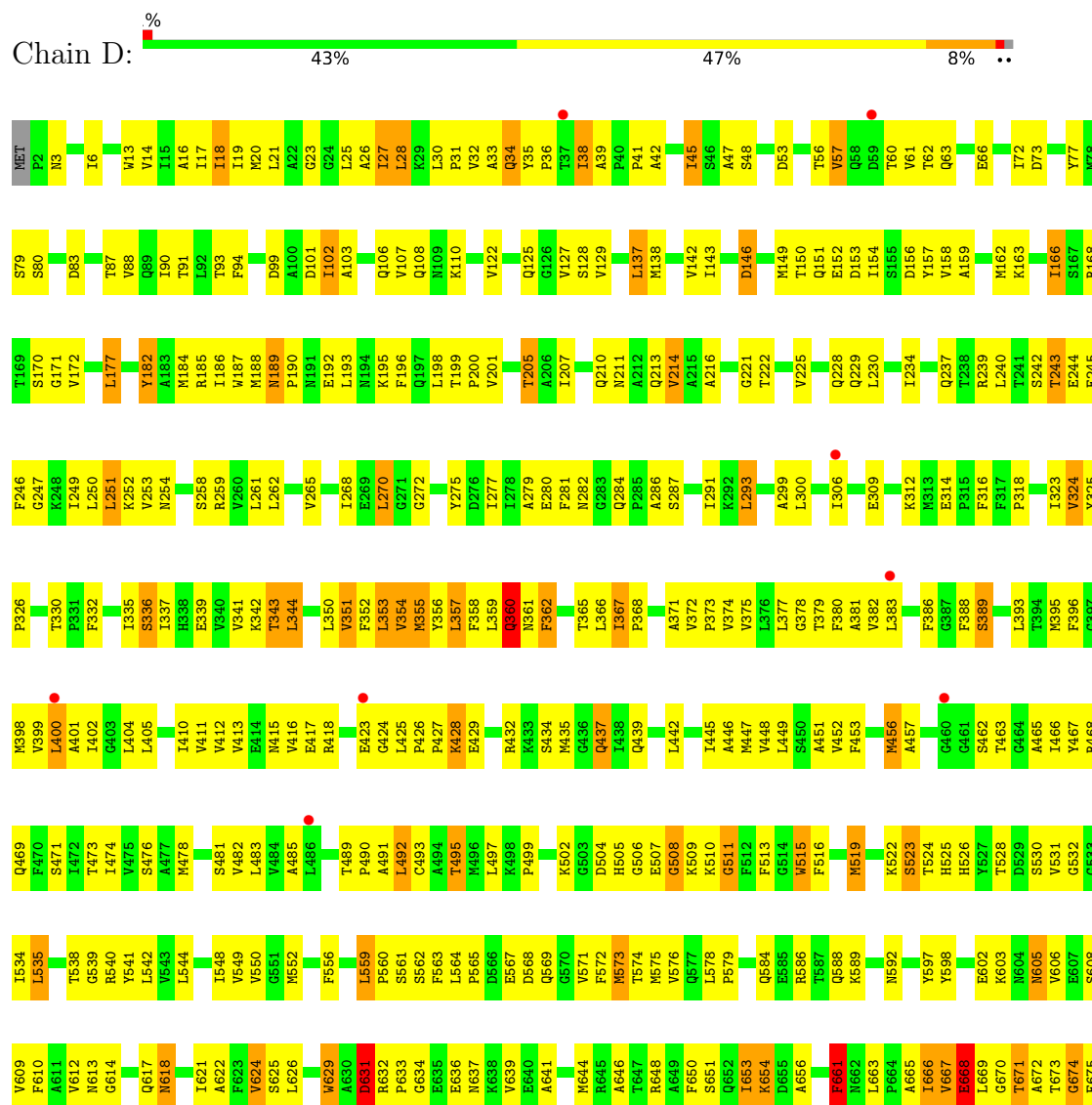


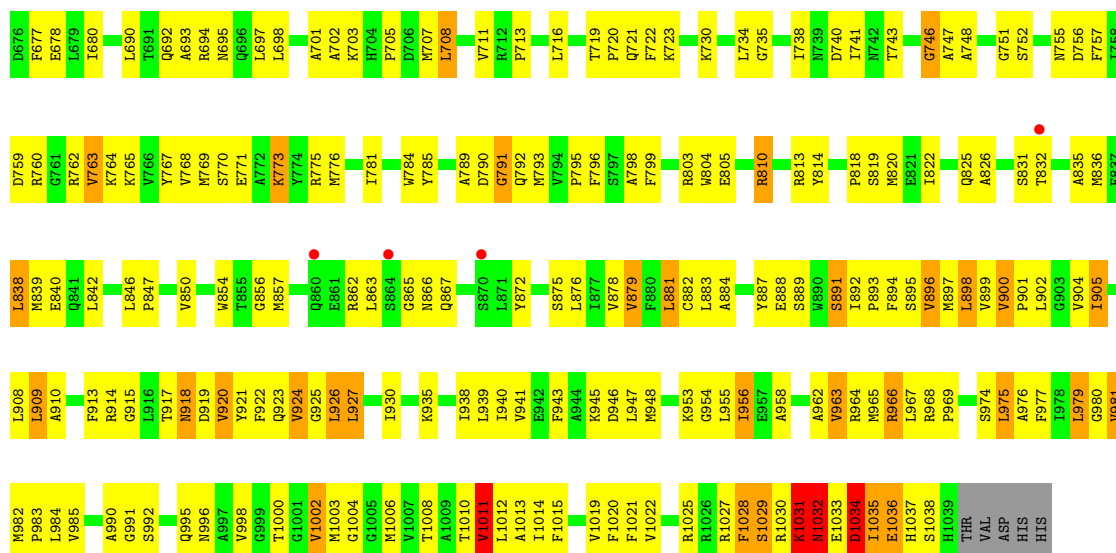
• Molecule 1: Multidrug efflux pump subunit AcrB



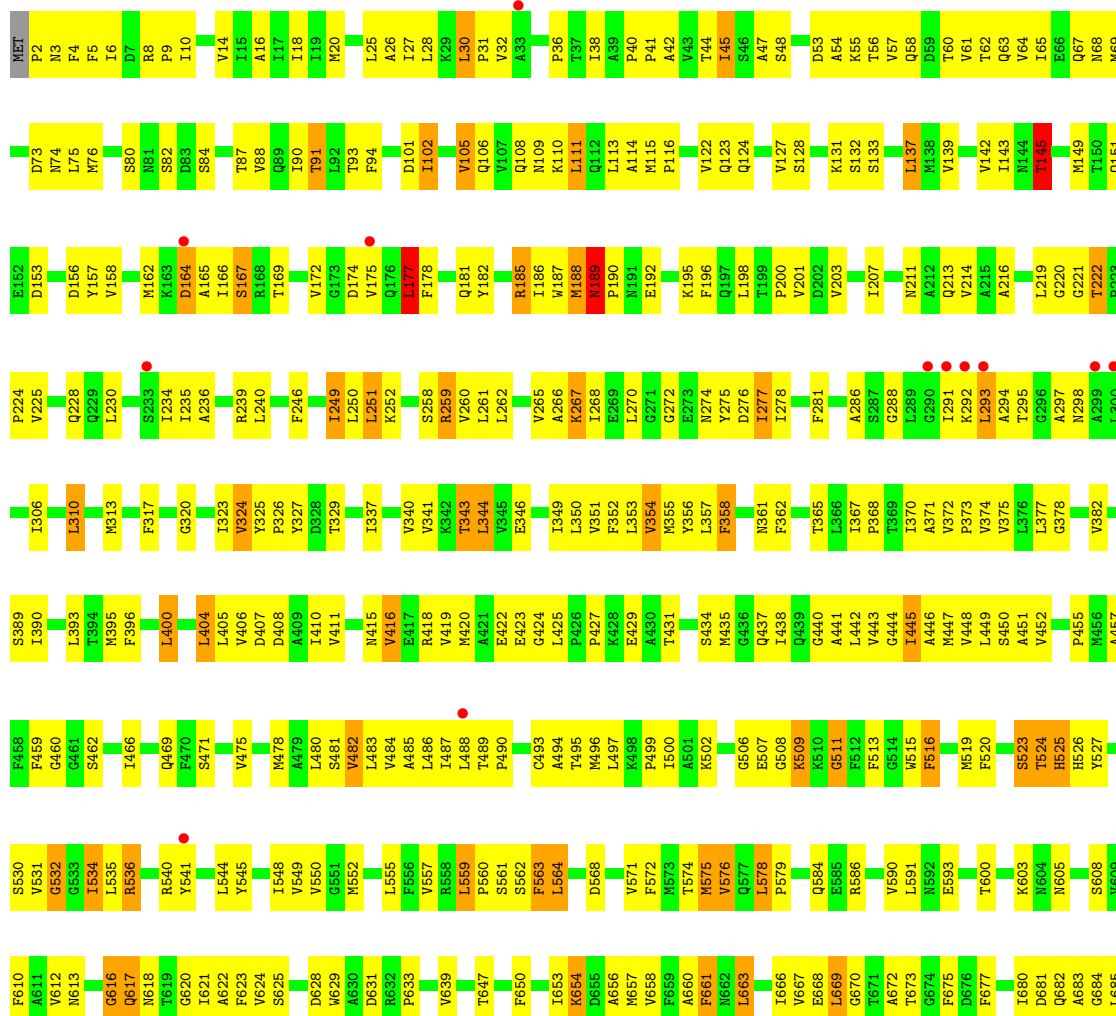
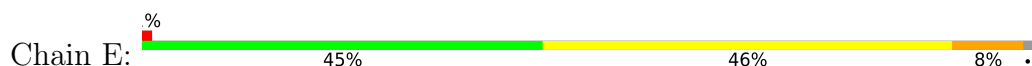


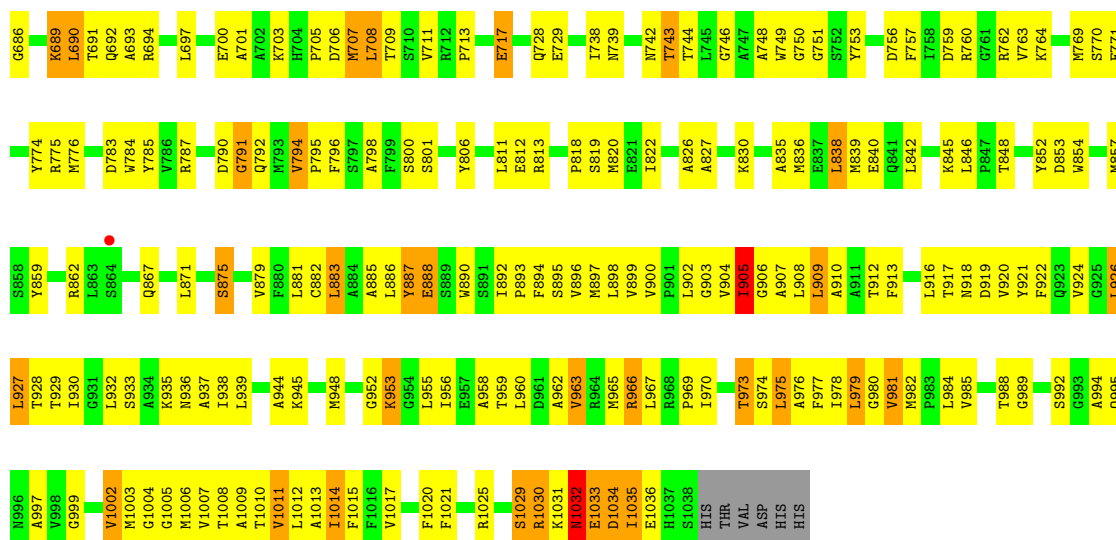
● Molecule 1: Multidrug efflux pump subunit AcrB



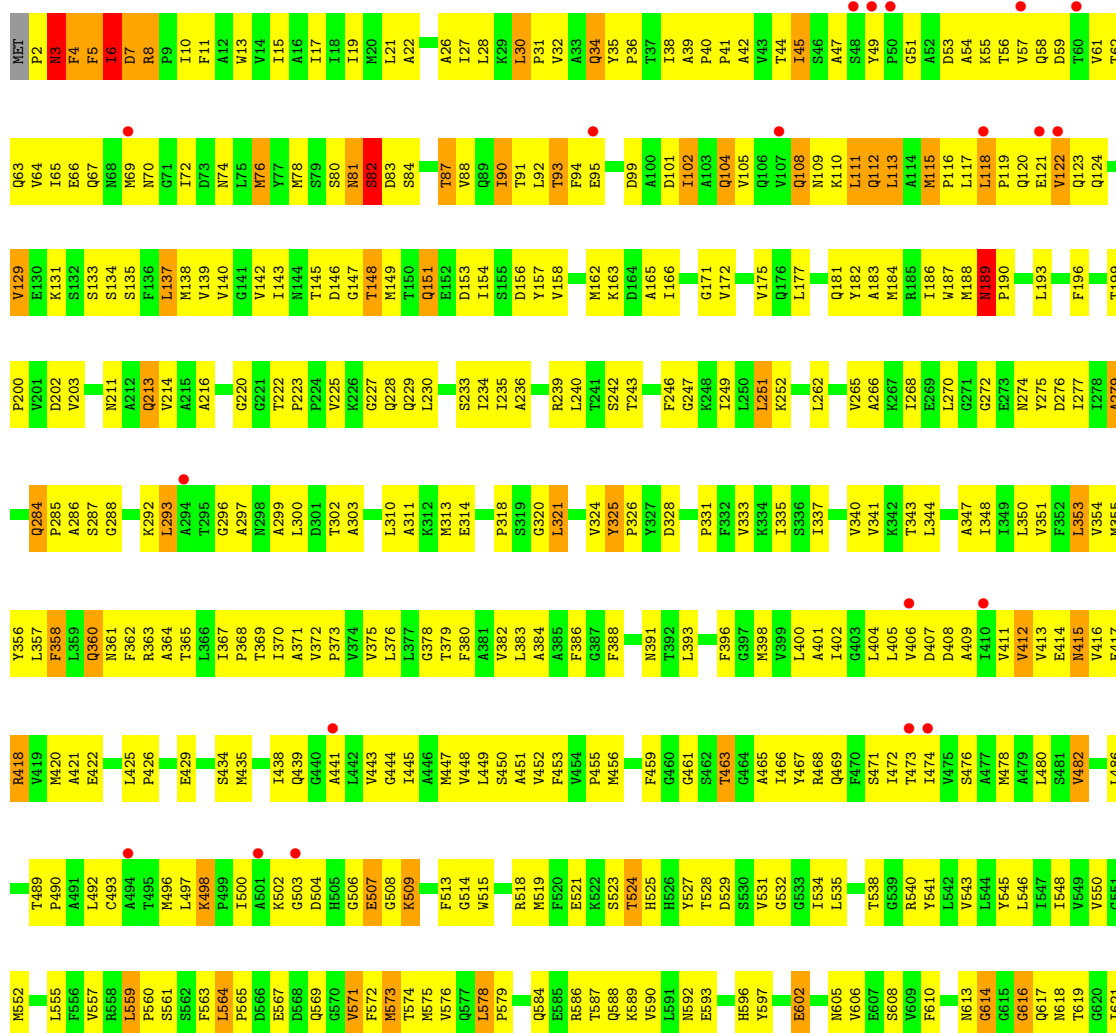


• Molecule 1: Multidrug efflux pump subunit AcrB





• 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	150.06Å 154.57Å 215.74Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	19.96 – 3.59 19.96 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.96-3.59) 95.8 (19.96-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.246 , 0.319 0.264 , 0.330	Depositor DCC
R_{free} test set	5715 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	110.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.055 for -k,-h,-l 0.070 for k,h,-l 0.068 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	47697	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9200e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	2/8043 (0.0%)	1.22	39/10922 (0.4%)
1	B	0.80	5/8032 (0.1%)	1.18	32/10907 (0.3%)
1	C	0.82	3/8026 (0.0%)	1.29	78/10899 (0.7%)
1	D	0.75	1/8043 (0.0%)	1.18	39/10922 (0.4%)
1	E	0.76	1/8032 (0.0%)	1.18	36/10907 (0.3%)
1	F	0.77	1/8032 (0.0%)	1.23	57/10907 (0.5%)
All	All	0.78	13/48208 (0.0%)	1.22	281/65464 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
1	F	0	2
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	900	VAL	CA-CB	10.18	1.59	1.54
1	B	372	VAL	CA-CB	9.89	1.59	1.54
1	A	1017	VAL	CA-CB	-9.55	1.49	1.54
1	B	900	VAL	CA-CB	6.75	1.57	1.54
1	C	122	VAL	CA-CB	5.84	1.61	1.54
1	C	563	PHE	CA-C	-5.84	1.45	1.52
1	B	673	THR	CA-CB	5.64	1.60	1.52
1	B	418	ARG	CA-C	-5.57	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1035	ILE	CA-CB	5.51	1.60	1.54
1	F	426	PRO	CA-C	5.35	1.57	1.52
1	E	673	THR	CA-CB	5.26	1.59	1.52
1	A	892	ILE	CA-C	5.24	1.57	1.52
1	D	900	VAL	CA-CB	5.00	1.56	1.54

All (281) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	559	LEU	CA-C-N	13.01	133.16	119.76
1	E	559	LEU	C-N-CA	13.01	133.16	119.76
1	F	118	LEU	CA-C-N	11.24	133.89	119.84
1	F	118	LEU	C-N-CA	11.24	133.89	119.84
1	C	118	LEU	CA-C-N	10.89	133.45	119.84
1	C	118	LEU	C-N-CA	10.89	133.45	119.84
1	C	892	ILE	CA-C-N	-10.52	108.03	118.97
1	C	892	ILE	C-N-CA	-10.52	108.03	118.97
1	F	8	ARG	CA-C-N	10.28	130.46	119.05
1	F	8	ARG	C-N-CA	10.28	130.46	119.05
1	E	532	GLY	N-CA-C	-9.52	101.46	112.50
1	A	35	TYR	CA-C-N	-9.47	108.00	119.84
1	A	35	TYR	C-N-CA	-9.47	108.00	119.84
1	A	39	ALA	CA-C-N	9.38	130.04	120.38
1	A	39	ALA	C-N-CA	9.38	130.04	120.38
1	C	8	ARG	CA-C-N	9.33	129.54	119.28
1	C	8	ARG	C-N-CA	9.33	129.54	119.28
1	E	288	GLY	N-CA-C	9.08	124.35	111.10
1	B	559	LEU	CA-C-N	8.82	129.35	119.83
1	B	559	LEU	C-N-CA	8.82	129.35	119.83
1	A	989	GLY	N-CA-C	-8.77	99.16	110.38
1	D	189	ASN	CA-C-N	8.71	128.34	118.85
1	D	189	ASN	C-N-CA	8.71	128.34	118.85
1	C	296	GLY	N-CA-C	8.60	124.92	114.69
1	C	515	TRP	N-CA-C	-8.52	101.69	110.97
1	B	1035	ILE	N-CA-C	8.45	119.01	110.23
1	F	172	VAL	N-CA-C	8.16	119.91	107.99
1	C	663	LEU	CA-C-N	7.98	127.93	120.03
1	C	663	LEU	C-N-CA	7.98	127.93	120.03
1	E	30	LEU	CA-C-N	7.78	127.77	119.76
1	E	30	LEU	C-N-CA	7.78	127.77	119.76
1	A	668	GLU	N-CA-C	7.77	122.10	112.47
1	F	189	ASN	CA-C-N	7.75	127.41	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	189	ASN	C-N-CA	7.75	127.41	119.19
1	F	7	ASP	N-CA-C	-7.62	104.40	112.93
1	D	668	GLU	N-CA-C	7.56	121.84	112.47
1	B	288	GLY	N-CA-C	7.51	122.11	111.14
1	D	325	TYR	CA-C-N	7.48	127.01	118.85
1	D	325	TYR	C-N-CA	7.48	127.01	118.85
1	C	39	ALA	CA-C-N	7.44	125.02	119.66
1	C	39	ALA	C-N-CA	7.44	125.02	119.66
1	C	559	LEU	CA-C-N	7.40	127.82	119.83
1	C	559	LEU	C-N-CA	7.40	127.82	119.83
1	C	846	LEU	CA-C-N	7.38	129.06	119.84
1	C	846	LEU	C-N-CA	7.38	129.06	119.84
1	F	1033	GLU	N-CA-C	7.35	121.19	108.76
1	D	38	ILE	N-CA-C	-7.28	105.68	112.96
1	F	3	ASN	N-CA-C	-7.23	103.40	111.28
1	E	177	LEU	N-CA-C	7.15	120.17	108.52
1	B	890	TRP	N-CA-C	-7.12	102.94	111.69
1	C	564	LEU	CA-C-N	-7.11	110.95	119.84
1	C	564	LEU	C-N-CA	-7.11	110.95	119.84
1	C	83	ASP	N-CA-C	7.10	121.02	109.59
1	E	1032	ASN	CA-C-N	7.07	134.43	121.70
1	E	1032	ASN	C-N-CA	7.07	134.43	121.70
1	A	515	TRP	N-CA-C	-7.07	103.58	111.71
1	F	30	LEU	CA-C-N	7.00	126.97	119.76
1	F	30	LEU	C-N-CA	7.00	126.97	119.76
1	F	892	ILE	CA-C-N	-6.99	111.10	119.84
1	F	892	ILE	C-N-CA	-6.99	111.10	119.84
1	B	846	LEU	CA-C-N	6.94	128.52	119.84
1	B	846	LEU	C-N-CA	6.94	128.52	119.84
1	C	1000	THR	N-CA-C	6.81	119.33	111.02
1	A	754	VAL	CB-CA-C	-6.78	105.94	111.71
1	C	4	PHE	N-CA-C	-6.69	103.23	111.33
1	F	719	THR	CA-C-N	6.67	126.90	119.90
1	F	719	THR	C-N-CA	6.67	126.90	119.90
1	C	172	VAL	N-CA-C	6.66	117.71	107.99
1	E	189	ASN	CA-C-N	6.63	126.08	118.85
1	E	189	ASN	C-N-CA	6.63	126.08	118.85
1	F	559	LEU	CA-C-N	6.62	126.98	119.83
1	F	559	LEU	C-N-CA	6.62	126.98	119.83
1	E	959	THR	N-CA-C	-6.59	104.02	111.07
1	F	213	GLN	N-CA-C	-6.59	99.56	110.17
1	B	287	SER	CA-C-N	-6.57	116.30	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	SER	C-N-CA	-6.57	116.30	121.82
1	E	669	LEU	N-CA-C	6.57	124.79	110.80
1	D	819	SER	N-CA-C	6.56	118.73	108.96
1	D	867	GLN	N-CA-C	6.56	121.32	113.12
1	C	58	GLN	N-CA-C	6.55	119.25	111.71
1	C	213	GLN	N-CA-C	-6.54	99.64	110.17
1	D	293	LEU	N-CA-C	6.53	119.75	109.96
1	B	177	LEU	N-CA-C	6.51	119.13	108.52
1	C	968	ARG	CA-C-N	-6.48	111.86	119.05
1	C	968	ARG	C-N-CA	-6.48	111.86	119.05
1	A	892	ILE	CB-CA-C	-6.45	107.52	114.35
1	C	661	PHE	N-CA-C	6.42	118.53	108.96
1	B	532	GLY	N-CA-C	-6.42	105.05	112.50
1	F	820	MET	N-CA-C	6.42	120.05	108.69
1	F	498	LYS	CA-C-N	-6.42	113.34	119.76
1	F	498	LYS	C-N-CA	-6.42	113.34	119.76
1	C	680	ILE	N-CA-C	6.41	117.15	108.17
1	B	132	SER	N-CA-C	6.41	119.71	108.56
1	B	959	THR	N-CA-C	-6.39	104.23	111.07
1	C	325	TYR	CA-C-N	6.39	125.96	119.19
1	C	325	TYR	C-N-CA	6.39	125.96	119.19
1	E	361	ASN	N-CA-C	6.38	117.88	107.23
1	D	576	VAL	N-CA-C	6.34	117.16	107.77
1	D	515	TRP	N-CA-C	-6.31	104.45	111.71
1	E	482	VAL	N-CA-C	6.31	116.46	110.53
1	A	576	VAL	N-CA-C	6.22	117.08	108.12
1	A	754	VAL	N-CA-C	6.21	117.32	111.48
1	E	101	ASP	N-CA-C	6.20	118.04	111.28
1	F	325	TYR	CA-C-N	6.18	125.74	119.19
1	F	325	TYR	C-N-CA	6.18	125.74	119.19
1	F	81	ASN	N-CA-C	6.17	119.01	109.07
1	F	777	LEU	CA-C-N	6.15	127.52	119.84
1	F	777	LEU	C-N-CA	6.15	127.52	119.84
1	B	607	GLU	N-CA-C	-6.14	105.44	113.12
1	F	416	VAL	N-CA-C	6.14	116.26	110.30
1	C	150	THR	N-CA-C	6.13	119.86	110.36
1	C	484	VAL	N-CA-C	6.12	116.28	110.53
1	D	661	PHE	N-CA-C	6.10	118.04	108.96
1	A	38	ILE	N-CA-C	-6.09	106.87	112.96
1	F	652	GLN	N-CA-C	-6.08	103.98	111.40
1	B	189	ASN	CA-C-N	6.08	125.47	118.85
1	B	189	ASN	C-N-CA	6.08	125.47	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	635	GLU	N-CA-C	-6.08	105.36	112.89
1	F	529	ASP	N-CA-C	-6.06	103.83	111.11
1	C	243	THR	N-CA-C	-6.06	104.79	111.82
1	A	466	ILE	N-CA-C	6.05	116.72	110.36
1	C	445	ILE	CB-CA-C	-6.05	104.09	112.02
1	F	808	SER	N-CA-C	-6.05	101.96	110.31
1	C	893	PRO	CA-C-O	-6.02	111.30	120.03
1	C	7	ASP	CA-C-N	6.00	131.20	122.98
1	C	7	ASP	C-N-CA	6.00	131.20	122.98
1	B	624	VAL	N-CA-C	6.00	117.08	107.73
1	B	213	GLN	N-CA-C	-5.97	100.56	110.17
1	A	892	ILE	N-CA-C	5.96	121.25	112.61
1	E	661	PHE	N-CA-C	5.94	117.81	108.96
1	A	277	ILE	N-CA-C	5.93	116.41	107.80
1	E	445	ILE	N-CA-C	-5.93	104.57	110.62
1	D	447	MET	N-CA-C	5.91	119.68	112.23
1	D	336	SER	N-CA-C	5.90	117.40	110.97
1	C	5	PHE	N-CA-C	-5.89	104.77	111.14
1	F	792	GLN	N-CA-C	5.89	119.08	109.59
1	F	697	LEU	N-CA-C	5.88	117.49	111.14
1	E	794	VAL	CA-C-N	5.87	125.84	120.03
1	E	794	VAL	C-N-CA	5.87	125.84	120.03
1	C	482	VAL	CB-CA-C	-5.87	104.46	111.97
1	E	576	VAL	N-CA-C	5.86	116.44	107.77
1	C	54	ALA	N-CA-C	5.85	117.33	111.07
1	B	498	LYS	CA-C-N	5.83	125.59	119.76
1	B	498	LYS	C-N-CA	5.83	125.59	119.76
1	E	525	HIS	N-CA-C	-5.79	104.65	110.97
1	A	559	LEU	CA-C-N	5.79	126.08	119.83
1	A	559	LEU	C-N-CA	5.79	126.08	119.83
1	F	90	ILE	N-CA-C	5.79	115.08	106.85
1	C	333	VAL	CB-CA-C	-5.78	104.58	111.97
1	C	752	SER	N-CA-C	5.76	118.05	108.13
1	A	425	LEU	CA-C-N	5.76	126.31	120.38
1	A	425	LEU	C-N-CA	5.76	126.31	120.38
1	D	163	LYS	N-CA-C	5.75	118.29	111.33
1	F	113	LEU	CA-CB-CG	5.74	136.39	116.30
1	C	668	GLU	N-CA-C	5.74	119.59	112.59
1	A	367	ILE	CA-C-N	-5.73	113.86	119.64
1	A	367	ILE	C-N-CA	-5.73	113.86	119.64
1	C	993	GLY	N-CA-C	-5.72	105.57	112.49
1	F	493	CYS	N-CA-C	-5.72	104.74	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	THR	N-CA-C	-5.71	106.36	113.15
1	B	1032	ASN	CA-C-N	5.70	131.96	121.70
1	B	1032	ASN	C-N-CA	5.70	131.96	121.70
1	F	649	ALA	N-CA-C	5.70	117.35	111.03
1	D	367	ILE	CA-C-N	-5.68	113.90	119.64
1	D	367	ILE	C-N-CA	-5.68	113.90	119.64
1	F	1027	ARG	N-CA-C	-5.67	103.97	112.54
1	B	128	SER	N-CA-C	5.67	118.78	109.72
1	C	777	LEU	CA-C-N	5.65	126.91	119.84
1	C	777	LEU	C-N-CA	5.65	126.91	119.84
1	E	416	VAL	N-CA-C	5.62	115.75	110.30
1	D	330	THR	N-CA-C	5.62	119.81	112.17
1	A	951	GLU	N-CA-C	-5.59	104.10	112.54
1	F	296	GLY	N-CA-C	5.55	121.29	114.69
1	B	514	GLY	N-CA-C	5.55	126.33	113.18
1	A	1017	VAL	CB-CA-C	-5.53	108.44	113.70
1	C	719	THR	CA-C-N	5.53	125.71	119.90
1	C	719	THR	C-N-CA	5.53	125.71	119.90
1	F	32	VAL	N-CA-C	5.52	116.69	108.46
1	A	288	GLY	N-CA-C	5.52	119.16	111.10
1	C	23	GLY	N-CA-C	5.51	119.82	112.77
1	C	90	ILE	N-CA-C	5.49	115.45	106.72
1	B	516	PHE	N-CA-C	5.48	117.97	111.33
1	E	133	SER	N-CA-C	-5.48	100.86	109.25
1	D	1034	ASP	CA-C-N	5.46	131.53	121.70
1	D	1034	ASP	C-N-CA	5.46	131.53	121.70
1	C	662	ASN	N-CA-C	5.46	118.38	109.59
1	F	444	GLY	N-CA-C	5.46	119.49	112.83
1	A	355	MET	CB-CG-SD	5.45	129.06	112.70
1	D	773	LYS	N-CA-C	5.45	117.98	111.71
1	C	163	LYS	N-CA-C	5.45	117.65	111.11
1	F	288	GLY	N-CA-C	5.44	119.05	111.10
1	F	852	TYR	N-CA-C	5.44	117.45	109.24
1	C	134	SER	N-CA-C	-5.43	104.06	111.56
1	C	833	GLY	N-CA-C	5.42	119.70	112.77
1	D	34	GLN	N-CA-C	-5.40	105.47	111.36
1	D	389	SER	N-CA-C	5.40	117.39	109.24
1	A	188	MET	N-CA-C	5.38	118.24	110.28
1	B	268	ILE	N-CA-C	5.38	115.64	108.11
1	D	361	ASN	N-CA-C	5.37	116.20	107.23
1	E	1029	SER	N-CA-C	5.36	122.22	110.80
1	F	965	MET	N-CA-C	-5.36	105.48	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	ASP	N-CA-C	5.34	117.98	109.96
1	D	73	ASP	N-CA-C	5.33	118.24	109.76
1	F	122	VAL	N-CA-C	-5.33	105.31	110.42
1	B	125	GLN	N-CA-C	-5.31	106.30	112.89
1	C	132	SER	N-CA-C	5.31	117.56	108.90
1	E	516	PHE	N-CA-C	5.31	117.75	111.33
1	B	524	THR	N-CA-C	-5.30	105.67	111.82
1	D	846	LEU	CA-C-N	5.30	126.46	119.84
1	D	846	LEU	C-N-CA	5.30	126.46	119.84
1	C	106	GLN	N-CA-C	5.28	117.12	111.36
1	E	513	PHE	N-CA-C	-5.28	106.89	113.38
1	A	125	GLN	N-CA-C	-5.27	106.35	112.89
1	C	708	LEU	N-CA-C	5.25	118.15	109.85
1	D	359	LEU	N-CA-C	-5.24	105.61	113.89
1	D	618	ASN	N-CA-C	5.23	118.92	112.54
1	F	21	LEU	N-CA-C	-5.23	105.66	111.36
1	A	515	TRP	CA-CB-CG	5.23	123.53	113.60
1	B	478	MET	N-CA-C	5.23	116.83	111.03
1	C	733	ALA	N-CA-C	5.22	116.83	111.03
1	B	133	SER	N-CA-C	-5.22	103.02	110.59
1	A	396	PHE	N-CA-C	-5.22	106.42	112.89
1	C	824	GLY	N-CA-C	5.22	118.10	110.38
1	A	859	TYR	N-CA-C	-5.22	105.03	111.40
1	E	145	THR	N-CA-C	5.21	117.04	111.36
1	A	314	GLU	N-CA-C	5.20	121.30	109.81
1	F	4	PHE	N-CA-C	-5.20	105.04	111.33
1	C	122	VAL	N-CA-C	-5.17	105.46	110.42
1	A	661	PHE	N-CA-C	5.17	116.66	108.96
1	F	279	ALA	N-CA-C	5.17	117.32	108.90
1	E	258	SER	N-CA-C	-5.17	102.64	110.28
1	C	482	VAL	N-CA-CB	5.16	116.59	110.55
1	C	697	LEU	N-CA-C	5.16	116.72	111.14
1	D	924	VAL	N-CA-C	-5.16	105.36	110.62
1	A	564	LEU	CA-C-N	-5.15	113.40	119.84
1	A	564	LEU	C-N-CA	-5.15	113.40	119.84
1	C	489	THR	CA-C-N	-5.15	113.33	119.05
1	C	489	THR	C-N-CA	-5.15	113.33	119.05
1	E	848	THR	N-CA-C	5.15	117.63	109.96
1	F	993	GLY	N-CA-C	-5.15	106.26	112.49
1	A	163	LYS	N-CA-C	5.15	117.56	111.33
1	B	260	VAL	N-CA-C	5.14	115.17	107.51
1	F	284	GLN	CA-C-N	-5.14	114.44	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	284	GLN	C-N-CA	-5.14	114.44	119.99
1	D	631	ASP	N-CA-C	-5.13	106.79	113.16
1	F	51	GLY	N-CA-C	5.13	121.94	115.42
1	A	1035	ILE	N-CA-C	5.12	120.00	109.34
1	C	914	ARG	N-CA-C	-5.12	102.00	109.63
1	E	883	LEU	CA-CB-CG	-5.12	98.39	116.30
1	C	19	ILE	N-CA-C	5.11	115.73	110.36
1	A	189	ASN	CA-C-N	5.11	124.61	119.19
1	A	189	ASN	C-N-CA	5.11	124.61	119.19
1	C	223	PRO	CA-C-N	-5.11	115.47	120.52
1	C	223	PRO	C-N-CA	-5.11	115.47	120.52
1	C	1032	ASN	N-CA-C	5.11	117.83	111.24
1	F	824	GLY	N-CA-C	5.11	117.94	110.38
1	F	968	ARG	CA-C-N	-5.10	113.29	118.85
1	F	968	ARG	C-N-CA	-5.10	113.29	118.85
1	A	757	PHE	N-CA-C	5.10	117.61	109.81
1	C	49	TYR	CA-C-N	5.09	126.21	119.84
1	C	49	TYR	C-N-CA	5.09	126.21	119.84
1	D	674	GLY	N-CA-C	5.09	121.23	111.31
1	E	167	SER	N-CA-C	-5.08	107.05	113.20
1	C	130	GLU	N-CA-C	5.08	116.79	109.07
1	D	371	ALA	CA-C-N	5.07	124.39	120.33
1	D	371	ALA	C-N-CA	5.07	124.39	120.33
1	D	519	MET	CB-CG-SD	5.07	127.92	112.70
1	D	386	PHE	N-CA-C	-5.07	106.78	113.17
1	E	680	ILE	N-CA-C	5.07	115.27	108.17
1	F	82	SER	N-CA-C	5.07	116.96	107.99
1	D	891	SER	CA-C-N	5.07	123.43	120.24
1	D	891	SER	C-N-CA	5.07	123.43	120.24
1	C	34	GLN	N-CA-C	-5.06	105.84	111.36
1	C	1001	GLY	N-CA-C	-5.05	106.64	112.50
1	E	371	ALA	N-CA-C	5.05	116.63	111.03
1	F	54	ALA	N-CA-C	5.04	117.15	111.11
1	C	959	THR	N-CA-C	-5.03	105.69	111.07
1	C	786	VAL	N-CA-C	5.03	115.15	108.11
1	D	125	GLN	N-CA-C	-5.03	106.66	112.89
1	E	534	ILE	N-CA-C	-5.02	104.71	111.44
1	E	188	MET	N-CA-C	5.02	117.71	110.28

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1034	ASP	Peptide
1	B	1033	GLU	Peptide
1	D	1032	ASN	Peptide
1	F	1033	GLU	Peptide
1	F	1034	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7893	0	8034	472	0
1	B	7883	0	8027	470	0
1	C	7877	0	8022	521	0
1	D	7893	0	8034	500	0
1	E	7883	0	8027	497	0
1	F	7883	0	8027	535	0
2	A	51	0	67	5	0
2	D	51	0	67	4	0
3	A	70	0	92	7	0
3	B	35	0	46	7	0
3	C	35	0	46	1	0
3	D	70	0	92	13	0
3	E	35	0	46	11	0
3	F	35	0	46	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	47697	0	48673	2908	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (2908) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.45	0.98
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.44	0.96
1:C:893:PRO:HA	1:C:896:VAL:HG12	1.43	0.96
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.47	0.93
1:C:887:TYR:O	1:C:889:SER:N	2.01	0.93
1:A:427:PRO:HD3	1:A:499:PRO:HB3	1.51	0.92
1:A:351:VAL:HG22	1:A:976:ALA:HB1	1.51	0.92
1:F:741:ILE:HG22	1:F:786:VAL:HG21	1.52	0.92
1:A:708:LEU:HD21	1:A:838:LEU:HD12	1.52	0.90
1:F:404:LEU:HG	1:F:449:LEU:HD13	1.52	0.90
1:B:356:TYR:O	1:B:358:PHE:N	2.05	0.90
1:C:196:PHE:O	1:C:252:LYS:NZ	2.06	0.89
1:A:874:ILE:HD13	1:C:25:LEU:HD21	1.54	0.89
1:A:445:ILE:HD13	1:A:935:LYS:HE3	1.54	0.89
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.55	0.88
1:C:343:THR:HG21	1:C:984:LEU:HD21	1.55	0.88
1:C:932:LEU:HD13	1:C:1006:MET:HE2	1.53	0.88
1:E:1032:ASN:N	1:E:1033:GLU:HB2	1.88	0.88
1:A:562:SER:HB2	1:A:919:ASP:HB3	1.54	0.87
1:C:356:TYR:HA	1:C:365:THR:HG21	1.55	0.87
1:B:896:VAL:HG21	1:B:938:ILE:HG13	1.55	0.87
1:C:914:ARG:NH2	1:C:985:VAL:O	2.08	0.87
1:F:262:LEU:HG	1:F:268:ILE:HD11	1.54	0.87
1:F:186:ILE:HG12	1:F:268:ILE:HG12	1.57	0.86
1:D:196:PHE:O	1:D:252:LYS:NZ	2.07	0.86
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.56	0.86
1:C:360:GLN:OE1	1:C:517:ASN:ND2	2.09	0.86
1:E:530:SER:OG	3:E:1101:LMT:H1'	1.76	0.85
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.54	0.85
1:F:932:LEU:HD13	1:F:1006:MET:HE2	1.58	0.85
1:A:948:MET:HE2	1:A:958:ALA:HB3	1.59	0.85
1:E:707:MET:HG2	1:E:838:LEU:HG	1.59	0.84
1:A:579:PRO:HD3	1:A:656:ALA:HB2	1.57	0.84
1:F:1034:ASP:HA	1:F:1035:ILE:HG12	1.59	0.83
1:D:158:VAL:HA	1:D:162:MET:HE3	1.60	0.83
1:A:108:GLN:NE2	1:B:109:ASN:O	2.12	0.83
1:A:350:LEU:HD22	1:A:979:LEU:HB3	1.58	0.83
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.58	0.82
1:D:1015:PHE:HE2	3:D:1102:LMT:H32	1.43	0.82
1:A:272:GLY:N	1:A:275:TYR:OH	2.12	0.82
1:B:189:ASN:HD22	1:B:267:LYS:HE2	1.44	0.82
1:B:196:PHE:O	1:B:252:LYS:NZ	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:VAL:HG22	1:E:976:ALA:HB1	1.60	0.82
1:C:59:ASP:OD2	1:C:59:ASP:N	2.09	0.82
1:C:156:ASP:OD1	1:C:760:ARG:NH2	2.13	0.82
1:C:351:VAL:HG22	1:C:976:ALA:HB1	1.60	0.81
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.60	0.81
1:A:632:ARG:NH1	1:A:637:ASN:O	2.14	0.81
1:C:939:LEU:HB3	1:C:966:ARG:HD2	1.62	0.80
1:D:669:LEU:HD12	1:D:670:GLY:H	1.43	0.80
1:C:918:ASN:HD21	1:C:923:GLN:HE21	1.27	0.80
1:C:380:PHE:HD2	1:C:383:LEU:HD12	1.43	0.80
1:C:428:LYS:HG2	1:C:494:ALA:HB1	1.63	0.80
1:D:23:GLY:HA2	1:D:381:ALA:HB2	1.62	0.80
1:D:6:ILE:HD12	1:D:432:ARG:HG2	1.63	0.80
1:C:356:TYR:C	1:C:358:PHE:H	1.90	0.80
1:A:584:GLN:HB2	1:A:617:GLN:HG2	1.64	0.79
1:E:404:LEU:HD21	1:E:449:LEU:HD22	1.63	0.79
1:F:83:ASP:HB2	1:F:87:THR:O	1.82	0.79
1:A:908:LEU:HD23	1:A:922:PHE:HZ	1.46	0.79
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.63	0.79
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.65	0.79
1:C:893:PRO:O	1:C:896:VAL:N	2.15	0.79
1:B:56:THR:O	1:B:60:THR:OG1	1.99	0.79
1:E:446:ALA:HB2	1:E:482:VAL:HG21	1.65	0.79
1:A:53:ASP:OD1	1:A:56:THR:OG1	2.00	0.79
1:B:415:ASN:OD1	1:B:418:ARG:NH1	2.14	0.78
1:E:272:GLY:N	1:E:275:TYR:OH	2.15	0.78
1:B:102:ILE:O	1:B:106:GLN:HG3	1.83	0.78
1:D:516:PHE:HA	1:D:519:MET:HE2	1.64	0.78
1:F:398:MET:HG2	1:F:473:THR:HG21	1.65	0.78
1:F:698:LEU:HD11	1:F:713:PRO:HD3	1.64	0.78
1:E:356:TYR:C	1:E:358:PHE:H	1.92	0.78
1:A:941:VAL:HG13	1:A:1021:PHE:CD1	2.19	0.78
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.64	0.78
1:B:310:LEU:HD23	1:B:323:ILE:HG21	1.65	0.77
1:E:262:LEU:HG	1:E:268:ILE:HD11	1.64	0.77
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.66	0.77
1:E:896:VAL:HG21	1:E:938:ILE:HG13	1.66	0.77
1:B:156:ASP:OD1	1:B:760:ARG:NH2	2.18	0.77
1:B:966:ARG:O	1:B:970:ILE:HG12	1.85	0.77
1:C:659:PHE:CD2	1:C:712:ARG:HD2	2.20	0.77
1:D:108:GLN:NE2	1:E:109:ASN:O	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:893:PRO:O	1:F:896:VAL:N	2.18	0.77
1:F:896:VAL:HG23	1:F:937:ALA:HB3	1.67	0.77
1:D:519:MET:O	1:D:523:SER:OG	2.02	0.77
1:F:966:ARG:HB3	1:F:966:ARG:CZ	2.14	0.77
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.67	0.77
1:A:73:ASP:OD2	1:C:131:LYS:NZ	2.16	0.77
1:D:963:VAL:HA	1:D:966:ARG:HH22	1.50	0.76
1:E:73:ASP:H	1:E:106:GLN:HE22	1.32	0.76
1:E:974:SER:OG	1:E:1010:THR:HG21	1.84	0.76
1:C:984:LEU:O	1:C:996:ASN:ND2	2.18	0.76
1:A:400:LEU:HD21	1:A:925:GLY:HA2	1.66	0.76
1:C:396:PHE:CD1	1:C:998:VAL:HG21	2.20	0.76
1:C:892:ILE:HG23	1:C:941:VAL:HG11	1.68	0.76
1:D:253:VAL:HG12	1:D:259:ARG:HG2	1.66	0.76
1:D:1014:ILE:HG13	1:D:1015:PHE:HD1	1.51	0.76
1:E:102:ILE:O	1:E:106:GLN:HG3	1.85	0.76
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.66	0.76
1:E:448:VAL:HG13	1:E:879:VAL:HG22	1.67	0.76
1:E:356:TYR:O	1:E:358:PHE:N	2.17	0.76
1:C:356:TYR:O	1:C:358:PHE:N	2.19	0.76
1:F:5:PHE:O	1:F:7:ASP:N	2.19	0.76
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.67	0.75
1:C:3:ASN:N	1:C:3:ASN:OD1	2.17	0.75
1:C:414:GLU:HG2	1:C:968:ARG:HH11	1.51	0.75
1:E:1032:ASN:H	1:E:1033:GLU:HB2	1.49	0.75
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.68	0.75
1:D:424:GLY:HA3	1:D:502:LYS:HB3	1.67	0.75
1:D:908:LEU:HD23	1:D:922:PHE:HZ	1.52	0.75
1:E:156:ASP:OD1	1:E:760:ARG:NH2	2.19	0.75
1:E:827:ALA:HB3	1:E:830:LYS:HD3	1.67	0.75
1:A:225:VAL:HG22	1:B:776:MET:HE2	1.67	0.75
1:A:977:PHE:O	1:A:980:GLY:N	2.19	0.75
1:D:677:PHE:HB3	1:D:822:ILE:HB	1.68	0.75
1:F:400:LEU:HB3	1:F:474:ILE:HD11	1.69	0.75
1:A:1032:ASN:HA	1:A:1035:ILE:HD11	1.69	0.75
1:D:60:THR:HG23	1:D:61:VAL:HG23	1.67	0.75
1:E:530:SER:OG	3:E:1101:LMT:O2'	2.04	0.75
1:A:453:PHE:O	1:A:471:SER:OG	2.04	0.74
1:F:228:GLN:NE2	1:F:230:LEU:O	2.19	0.74
1:C:714:ASN:HB3	1:C:821:GLU:HB3	1.69	0.74
1:B:762:ARG:HG2	1:B:762:ARG:HH11	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:VAL:HG12	1:E:390:ILE:HB	1.67	0.74
1:E:62:THR:HG21	1:E:813:ARG:HD3	1.67	0.74
1:E:694:ARG:HH11	1:E:820:MET:HE1	1.52	0.74
1:A:400:LEU:HD23	1:A:924:VAL:HG12	1.69	0.74
1:A:827:ALA:HB3	1:A:830:LYS:HD3	1.69	0.74
1:C:120:GLN:HA	1:C:123:GLN:HB2	1.68	0.74
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.69	0.74
1:A:382:VAL:HG11	1:A:476:SER:HB2	1.69	0.74
1:A:974:SER:OG	1:A:1010:THR:HG21	1.86	0.74
1:B:356:TYR:C	1:B:358:PHE:H	1.96	0.74
1:D:883:LEU:HD13	1:D:896:VAL:HG13	1.70	0.74
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.69	0.74
1:D:400:LEU:HD23	1:D:924:VAL:HG12	1.70	0.73
1:E:228:GLN:NE2	1:E:230:LEU:O	2.21	0.73
1:D:977:PHE:O	1:D:980:GLY:N	2.22	0.73
1:E:185:ARG:HH12	1:E:769:MET:HE3	1.53	0.73
1:E:396:PHE:O	1:E:400:LEU:HB2	1.88	0.73
1:E:1034:ASP:O	1:E:1036:GLU:N	2.20	0.73
1:A:694:ARG:NH2	1:A:717:GLU:OE1	2.21	0.73
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.69	0.73
1:D:225:VAL:HG22	1:E:776:MET:HE2	1.70	0.73
1:A:984:LEU:O	1:A:996:ASN:ND2	2.22	0.73
1:F:356:TYR:O	1:F:358:PHE:N	2.22	0.73
1:B:762:ARG:HH12	1:C:117:LEU:HD13	1.53	0.73
1:D:770:SER:OG	1:D:771:GLU:O	2.06	0.73
1:C:507:GLU:HG2	1:C:518:ARG:HG3	1.71	0.72
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.71	0.72
1:C:449:LEU:HD21	1:C:932:LEU:HD23	1.71	0.72
1:D:456:MET:HG3	1:D:927:LEU:HD11	1.71	0.72
1:D:735:GLY:O	1:D:789:ALA:N	2.23	0.72
1:B:142:VAL:HG11	1:B:162:MET:HE1	1.72	0.72
1:E:60:THR:HG23	1:E:61:VAL:HG23	1.69	0.72
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.71	0.72
1:E:694:ARG:HD2	1:E:713:PRO:HB3	1.69	0.72
1:C:239:ARG:HH12	1:C:756:ASP:H	1.37	0.72
1:D:355:MET:HB3	1:D:365:THR:OG1	1.90	0.72
1:F:99:ASP:HB3	1:F:102:ILE:HB	1.72	0.72
1:B:362:PHE:O	1:B:365:THR:HG22	1.90	0.72
1:C:79:SER:HB3	1:C:814:TYR:HD1	1.54	0.72
1:A:728:GLN:HE22	1:A:738:ILE:HG21	1.54	0.72
1:C:426:PRO:HD2	1:C:429:GLU:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:PHE:O	1:D:471:SER:OG	2.07	0.71
1:A:491:ALA:O	1:A:495:THR:OG1	2.08	0.71
1:B:73:ASP:H	1:B:106:GLN:HE22	1.38	0.71
1:B:663:LEU:HD23	1:B:663:LEU:H	1.56	0.71
1:C:66:GLU:OE2	1:C:80:SER:OG	2.08	0.71
1:F:563:PHE:HB2	1:F:861:GLU:HG3	1.71	0.71
1:B:166:ILE:HD11	1:B:310:LEU:HD11	1.71	0.71
1:B:236:ALA:O	1:C:723:LYS:NZ	2.24	0.71
1:C:13:TRP:HH2	1:C:370:ILE:HD13	1.54	0.71
1:C:663:LEU:H	1:C:663:LEU:HD23	1.55	0.71
1:C:977:PHE:O	1:C:980:GLY:N	2.23	0.71
1:D:170:SER:HB2	1:E:75:LEU:H	1.55	0.71
1:B:165:ALA:HB3	1:B:313:MET:HE2	1.73	0.71
1:B:680:ILE:HD11	1:B:814:TYR:HD2	1.54	0.71
1:B:404:LEU:HD23	1:B:478:MET:HG3	1.73	0.71
1:C:683:ALA:O	1:C:685:LEU:N	2.24	0.71
1:C:943:PHE:HD2	1:C:965:MET:HE3	1.56	0.71
1:A:923:GLN:HG2	3:A:1103:LMT:H12	1.71	0.71
1:A:186:ILE:HB	1:A:768:VAL:HG22	1.70	0.71
1:B:26:ALA:O	1:B:30:LEU:HB2	1.91	0.71
1:B:700:GLU:HB3	1:B:842:LEU:HD22	1.72	0.71
1:E:44:THR:HG1	1:E:91:THR:HG1	1.35	0.71
1:C:889:SER:HB3	1:C:892:ILE:HG12	1.71	0.70
1:E:142:VAL:HG11	1:E:162:MET:HE1	1.74	0.70
1:E:362:PHE:O	1:E:365:THR:HG22	1.91	0.70
1:E:593:GLU:OE1	1:E:654:LYS:NZ	2.23	0.70
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.73	0.70
1:B:555:LEU:HD11	1:B:909:LEU:HD12	1.72	0.70
1:D:272:GLY:N	1:D:275:TYR:OH	2.23	0.70
1:C:803:ARG:NH1	1:C:805:GLU:OE2	2.25	0.70
1:D:708:LEU:HD21	1:D:838:LEU:HD12	1.73	0.70
1:F:770:SER:OG	1:F:771:GLU:O	2.10	0.70
1:F:887:TYR:O	1:F:889:SER:N	2.24	0.70
1:C:669:LEU:HD13	1:C:856:GLY:HA2	1.74	0.70
1:D:157:TYR:CZ	1:D:318:PRO:HD3	2.26	0.70
1:F:659:PHE:CD2	1:F:712:ARG:HD2	2.27	0.70
1:D:382:VAL:HG11	1:D:476:SER:HB2	1.74	0.70
1:E:706:ASP:O	1:E:830:LYS:NZ	2.24	0.70
1:B:448:VAL:HG13	1:B:879:VAL:HG22	1.74	0.70
1:B:452:VAL:HG23	1:B:453:PHE:CD2	2.27	0.70
1:D:80:SER:HB3	1:D:90:ILE:HG23	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:422:GLU:O	1:F:502:LYS:HG3	1.92	0.70
1:D:1014:ILE:HG13	1:D:1015:PHE:CD1	2.25	0.70
1:E:530:SER:HG	3:E:1101:LMT:C2'	2.05	0.70
1:A:1014:ILE:HG13	1:A:1015:PHE:HD1	1.55	0.70
1:D:967:LEU:HD11	3:D:1102:LMT:H123	1.72	0.70
1:A:883:LEU:HD13	1:A:896:VAL:HG13	1.74	0.69
1:D:904:VAL:HG13	1:D:926:LEU:HD11	1.74	0.69
1:E:378:GLY:O	1:E:382:VAL:HG23	1.92	0.69
1:A:530:SER:CB	3:A:1102:LMT:H2O2	2.03	0.69
1:D:910:ALA:HB2	1:D:1004:GLY:HA3	1.74	0.69
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.75	0.69
1:F:348:ILE:HG13	1:F:402:ILE:HD13	1.74	0.69
1:D:562:SER:HB2	1:D:919:ASP:HB3	1.74	0.69
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.27	0.69
1:A:230:LEU:HD21	1:B:804:TRP:HH2	1.57	0.69
1:C:380:PHE:CD2	1:C:383:LEU:HD12	2.27	0.69
1:E:691:THR:HG23	1:E:694:ARG:HH12	1.57	0.69
1:A:274:ASN:ND2	1:A:276:ASP:OD2	2.20	0.69
1:A:451:ALA:HB1	1:A:878:VAL:HG12	1.73	0.69
1:C:902:LEU:HD23	1:C:1012:LEU:HB3	1.73	0.69
1:A:355:MET:HB3	1:A:365:THR:OG1	1.90	0.69
1:A:1008:THR:O	1:A:1012:LEU:HB2	1.93	0.69
1:B:445:ILE:HG21	1:B:935:LYS:HD2	1.74	0.69
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.27	0.69
1:C:519:MET:O	1:C:523:SER:OG	2.08	0.69
1:D:39:ALA:HB2	1:D:668:GLU:HG3	1.73	0.69
1:E:562:SER:OG	1:E:563:PHE:N	2.24	0.69
1:A:158:VAL:HA	1:A:162:MET:HE3	1.75	0.69
1:A:277:ILE:HG12	1:A:614:GLY:HA3	1.75	0.69
1:C:902:LEU:HG	1:C:1012:LEU:HD23	1.74	0.69
1:E:442:LEU:O	1:E:445:ILE:HG13	1.93	0.69
1:F:196:PHE:O	1:F:252:LYS:NZ	2.24	0.69
1:F:382:VAL:HG11	1:F:476:SER:HB2	1.75	0.69
1:A:424:GLY:HA3	1:A:502:LYS:HB3	1.75	0.68
1:C:855:THR:HA	1:C:859:TYR:HB2	1.75	0.68
1:B:6:ILE:O	1:B:428:LYS:NZ	2.26	0.68
1:B:101:ASP:OD1	1:B:131:LYS:NZ	2.24	0.68
1:E:663:LEU:HD23	1:E:663:LEU:H	1.59	0.68
1:E:683:ALA:O	1:E:685:LEU:N	2.26	0.68
1:F:461:GLY:HA3	1:F:863:LEU:HD21	1.74	0.68
1:F:908:LEU:HD23	1:F:922:PHE:HZ	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ARG:HD3	1:B:496:MET:O	1.92	0.68
1:C:104:GLN:OE1	1:C:108:GLN:NE2	2.27	0.68
1:B:188:MET:HE1	1:B:200:PRO:HG3	1.75	0.68
1:F:108:GLN:HB2	1:F:129:VAL:HG21	1.75	0.68
1:F:452:VAL:O	1:F:455:PRO:HD2	1.93	0.68
1:D:776:MET:HE3	1:F:228:GLN:OE1	1.94	0.68
1:E:41:PRO:HG2	1:E:94:PHE:HB2	1.76	0.68
1:E:770:SER:OG	1:E:771:GLU:O	2.11	0.68
1:C:158:VAL:HA	1:C:162:MET:HE3	1.74	0.68
1:C:918:ASN:ND2	1:C:923:GLN:HE21	1.90	0.68
1:D:609:VAL:HG22	1:D:624:VAL:HG13	1.75	0.68
1:D:617:GLN:NE2	1:F:220:GLY:O	2.25	0.68
1:A:969:PRO:HA	1:A:972:MET:HE3	1.76	0.68
1:A:770:SER:OG	1:A:771:GLU:O	2.10	0.68
1:B:41:PRO:HG2	1:B:94:PHE:HB2	1.76	0.68
1:C:982:MET:HG3	1:C:1003:MET:HE1	1.76	0.68
1:A:25:LEU:HD21	1:B:874:ILE:HD11	1.76	0.68
1:F:42:ALA:HB2	1:F:93:THR:HG23	1.74	0.68
1:A:435:MET:HG3	1:A:490:PRO:HB3	1.75	0.67
1:A:1014:ILE:HG13	1:A:1015:PHE:CD1	2.29	0.67
1:D:568:ASP:OD1	1:D:632:ARG:NH1	2.17	0.67
1:D:914:ARG:NH1	1:D:1000:THR:OG1	2.26	0.67
2:D:1101:ERY:H302	2:D:1101:ERY:H151	1.75	0.67
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.76	0.67
1:D:1015:PHE:CE2	3:D:1102:LMT:H32	2.28	0.67
1:F:936:ASN:HD21	1:F:1010:THR:HG22	1.59	0.67
1:B:335:ILE:HG21	1:B:990:ALA:HB3	1.77	0.67
1:A:210:GLN:HE22	1:A:250:LEU:H	1.42	0.67
1:C:452:VAL:HG23	1:C:453:PHE:HD1	1.60	0.67
1:D:316:PHE:CD1	1:E:682:GLN:HG2	2.29	0.67
1:E:404:LEU:HD23	1:E:478:MET:HG3	1.76	0.67
1:B:272:GLY:N	1:B:275:TYR:OH	2.21	0.67
1:D:1030:ARG:O	1:D:1031:LYS:HE2	1.94	0.67
1:E:165:ALA:HB3	1:E:313:MET:CE	2.24	0.67
1:A:663:LEU:HD23	1:A:663:LEU:H	1.60	0.67
1:C:6:ILE:HG21	1:C:487:ILE:HG23	1.76	0.67
1:E:853:ASP:OD1	1:E:854:TRP:N	2.27	0.67
1:B:1014:ILE:HG13	1:B:1015:PHE:CD1	2.29	0.67
1:E:174:ASP:HB3	1:E:292:LYS:HB2	1.77	0.67
1:A:3:ASN:O	1:A:6:ILE:HG12	1.94	0.67
1:C:738:ILE:O	1:C:741:ILE:HG13	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:535:LEU:HD21	1:D:1022:VAL:HG21	1.76	0.67
1:E:324:VAL:HG13	1:E:326:PRO:HD3	1.76	0.67
1:B:536:ARG:NH2	3:B:2100:LMT:O3B	2.28	0.67
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.77	0.67
1:E:375:VAL:HG11	1:E:405:LEU:HD22	1.75	0.67
1:F:700:GLU:HA	1:F:703:LYS:HE3	1.77	0.67
3:B:2100:LMT:H6E	3:B:2100:LMT:H5B	1.77	0.66
1:D:400:LEU:HD11	1:D:1002:VAL:HG21	1.77	0.66
1:D:771:GLU:HG2	1:D:773:LYS:HG2	1.77	0.66
1:E:143:ILE:HG22	1:E:286:ALA:HB2	1.77	0.66
1:E:435:MET:SD	1:E:490:PRO:HB3	2.34	0.66
1:E:441:ALA:HA	1:E:886:LEU:HD21	1.76	0.66
1:A:31:PRO:HB2	1:A:389:SER:HB2	1.78	0.66
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.77	0.66
1:B:69:MET:HE1	1:B:107:VAL:HG13	1.77	0.66
1:C:723:LYS:HG2	1:C:803:ARG:CZ	2.25	0.66
1:E:26:ALA:O	1:E:30:LEU:HB2	1.95	0.66
1:F:586:ARG:HA	1:F:589:LYS:HD2	1.77	0.66
1:F:629:TRP:H	1:F:629:TRP:CD1	2.11	0.66
1:B:770:SER:OG	1:B:771:GLU:O	2.13	0.66
1:C:614:GLY:HA2	1:C:616:GLY:N	2.10	0.66
1:C:940:ILE:HD13	1:C:963:VAL:HG22	1.76	0.66
1:E:977:PHE:O	1:E:980:GLY:N	2.28	0.66
1:A:17:ILE:HG22	1:B:881:LEU:HD21	1.77	0.66
1:A:977:PHE:HD2	1:A:1006:MET:HE2	1.60	0.66
1:B:378:GLY:O	1:B:382:VAL:HG23	1.95	0.66
1:C:735:GLY:O	1:C:789:ALA:N	2.28	0.66
1:D:897:MET:O	1:D:900:VAL:HG23	1.96	0.66
1:F:356:TYR:C	1:F:358:PHE:H	2.04	0.66
1:C:1014:ILE:HG13	1:C:1015:PHE:CD1	2.31	0.66
1:D:586:ARG:O	1:D:589:LYS:HB3	1.96	0.66
1:B:455:PRO:O	1:B:871:LEU:HD13	1.95	0.66
1:C:101:ASP:OD1	1:C:131:LYS:NZ	2.24	0.66
1:C:228:GLN:NE2	1:C:230:LEU:O	2.28	0.66
1:C:404:LEU:HB3	1:C:478:MET:SD	2.36	0.66
1:F:954:GLY:HA2	1:F:1035:ILE:HG13	1.78	0.66
1:A:281:PHE:HE1	1:A:608:SER:HB2	1.61	0.66
1:C:53:ASP:O	1:C:56:THR:HB	1.96	0.66
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.78	0.66
1:F:616:GLY:HA3	1:F:617:GLN:C	2.20	0.66
1:A:140:VAL:HB	1:A:289:LEU:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:THR:HB	1:A:826:ALA:HB3	1.77	0.66
1:D:293:LEU:HD11	1:D:299:ALA:HA	1.78	0.66
1:D:663:LEU:HD23	1:D:663:LEU:H	1.61	0.66
1:E:981:VAL:HG21	1:E:1002:VAL:HG11	1.76	0.66
1:C:414:GLU:HG2	1:C:968:ARG:NH1	2.10	0.65
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.78	0.65
1:D:730:LYS:O	1:D:734:LEU:HG	1.97	0.65
1:E:578:LEU:HD21	1:E:590:VAL:HG21	1.79	0.65
1:B:143:ILE:HG22	1:B:286:ALA:HB2	1.78	0.65
1:B:225:VAL:HG12	1:C:772:ALA:HB1	1.77	0.65
1:C:300:LEU:HD11	1:C:333:VAL:HG11	1.77	0.65
1:E:53:ASP:OD1	1:E:56:THR:OG1	2.11	0.65
1:E:629:TRP:CD1	1:E:629:TRP:H	2.15	0.65
1:B:14:VAL:HG22	1:C:881:LEU:HD13	1.79	0.65
1:B:100:ALA:HB1	1:B:131:LYS:HE3	1.79	0.65
1:B:166:ILE:HD11	1:B:310:LEU:CD1	2.26	0.65
1:B:562:SER:OG	1:B:563:PHE:N	2.26	0.65
1:C:836:MET:O	1:C:840:GLU:HG2	1.96	0.65
1:A:897:MET:O	1:A:900:VAL:HG23	1.97	0.65
1:B:883:LEU:HD13	1:B:896:VAL:HG11	1.76	0.65
1:C:372:VAL:HA	1:C:405:LEU:HD11	1.76	0.65
1:F:356:TYR:HA	1:F:365:THR:HG21	1.78	0.65
1:F:685:LEU:O	1:F:689:LYS:HB2	1.96	0.65
1:A:790:ASP:OD2	1:A:791:GLY:N	2.28	0.65
1:B:554:TYR:CZ	1:B:558:ARG:HG3	2.31	0.65
1:C:182:TYR:HB2	1:C:764:LYS:HZ3	1.61	0.65
1:D:695:ASN:HA	1:D:698:LEU:HD12	1.78	0.65
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.79	0.65
1:F:398:MET:HG2	1:F:473:THR:CG2	2.27	0.65
1:D:309:GLU:HA	1:D:312:LYS:HD2	1.79	0.65
1:E:691:THR:HG23	1:E:694:ARG:NH1	2.12	0.65
1:F:66:GLU:OE1	1:F:816:GLY:HA2	1.97	0.65
1:F:443:VAL:HG12	1:F:886:LEU:HD21	1.79	0.65
1:F:940:ILE:HA	1:F:966:ARG:NH1	2.12	0.65
1:A:18:ILE:HG13	1:B:881:LEU:HD23	1.79	0.65
1:F:940:ILE:HG12	1:F:966:ARG:HH22	1.62	0.65
1:A:112:GLN:HG3	1:B:112:GLN:OE1	1.96	0.64
1:D:992:SER:HA	1:D:995:GLN:HB2	1.79	0.64
1:E:14:VAL:HG22	1:F:881:LEU:HD13	1.80	0.64
1:E:219:LEU:HD13	1:F:778:PRO:HG3	1.77	0.64
1:A:1032:ASN:O	1:A:1033:GLU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:GLY:HA2	1:B:518:ARG:HE	1.61	0.64
1:F:614:GLY:HA2	1:F:616:GLY:N	2.11	0.64
1:A:4:PHE:HB3	1:A:8:ARG:NH1	2.13	0.64
1:A:531:VAL:HG11	1:A:963:VAL:HG11	1.79	0.64
1:C:274:ASN:ND2	1:C:276:ASP:OD2	2.30	0.64
1:C:351:VAL:HG11	1:C:406:VAL:HG21	1.79	0.64
1:C:452:VAL:HG23	1:C:453:PHE:CD1	2.31	0.64
1:D:795:PRO:HG2	1:D:798:ALA:HB2	1.80	0.64
1:D:974:SER:OG	1:D:1010:THR:HG21	1.97	0.64
1:F:187:TRP:HB3	1:F:771:GLU:HA	1.80	0.64
1:C:1029:SER:OG	1:C:1030:ARG:N	2.30	0.64
1:F:578:LEU:HB2	1:F:618:ASN:O	1.98	0.64
1:C:616:GLY:HA3	1:C:617:GLN:C	2.23	0.64
1:F:455:PRO:HB3	1:F:874:ILE:HG22	1.80	0.64
1:F:593:GLU:OE1	1:F:654:LYS:NZ	2.23	0.64
1:D:914:ARG:NH2	1:D:985:VAL:O	2.24	0.64
1:A:465:ALA:O	1:A:469:GLN:HG2	1.98	0.64
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.77	0.64
1:C:78:MET:HG3	1:C:92:LEU:HD13	1.80	0.64
1:C:586:ARG:HA	1:C:589:LYS:HD2	1.80	0.64
1:E:367:ILE:HB	1:E:368:PRO:HD3	1.80	0.64
1:F:587:THR:OG1	1:F:613:ASN:ND2	2.31	0.64
1:A:157:TYR:CZ	1:A:318:PRO:HD3	2.33	0.64
1:B:408:ASP:OD1	1:B:935:LYS:NZ	2.25	0.64
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.80	0.64
1:E:196:PHE:O	1:E:252:LYS:NZ	2.20	0.64
1:E:536:ARG:HG3	3:E:1101:LMT:O3B	1.96	0.64
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.78	0.63
1:B:709:THR:HG22	1:B:825:GLN:HG3	1.80	0.63
1:D:442:LEU:O	1:D:445:ILE:HG13	1.98	0.63
1:F:379:THR:HG23	1:F:476:SER:OG	1.98	0.63
1:D:18:ILE:HG13	1:E:881:LEU:HD23	1.78	0.63
1:F:343:THR:HG21	1:F:984:LEU:HD21	1.79	0.63
1:F:380:PHE:HD2	1:F:383:LEU:HD12	1.63	0.63
1:D:146:ASP:OD2	1:D:146:ASP:N	2.31	0.63
1:D:187:TRP:HH2	1:F:223:PRO:HD2	1.63	0.63
1:E:441:ALA:O	1:E:445:ILE:HG23	1.99	0.63
1:E:544:LEU:O	1:E:548:ILE:HG13	1.98	0.63
1:A:883:LEU:HB2	1:A:893:PRO:HB3	1.80	0.63
1:D:221:GLY:H	1:E:775:ARG:HH12	1.45	0.63
1:E:1030:ARG:HH11	1:E:1030:ARG:H	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:HG23	1:A:462:SER:HB2	1.81	0.63
1:B:57:VAL:HG23	1:B:82:SER:HB3	1.81	0.63
1:B:340:VAL:HG22	1:B:396:PHE:HE1	1.63	0.63
1:C:396:PHE:O	1:C:400:LEU:HB2	1.97	0.63
1:A:796:PHE:HD1	1:A:799:PHE:HE2	1.46	0.63
1:C:521:GLU:O	1:C:524:THR:HG23	1.99	0.63
1:C:890:TRP:CE3	1:C:890:TRP:HA	2.33	0.63
1:D:170:SER:OG	1:E:74:ASN:N	2.28	0.63
1:D:210:GLN:HE22	1:D:250:LEU:HB3	1.63	0.63
1:D:584:GLN:HB2	1:D:617:GLN:HG2	1.81	0.63
1:D:982:MET:HA	1:D:1003:MET:HE1	1.80	0.63
1:E:1008:THR:O	1:E:1012:LEU:HB2	1.99	0.63
1:D:31:PRO:O	1:D:389:SER:HB2	1.99	0.63
1:E:327:TYR:HB2	1:E:623:PHE:CZ	2.33	0.63
1:F:82:SER:HB2	1:F:811:LEU:HB2	1.80	0.63
1:A:66:GLU:OE1	1:A:816:GLY:HA2	1.99	0.63
1:A:669:LEU:HD22	1:A:670:GLY:H	1.63	0.63
1:D:981:VAL:HG12	1:D:1003:MET:HE3	1.81	0.63
1:B:644:MET:HE2	1:B:648:ARG:HE	1.64	0.63
1:D:678:GLU:HG2	1:D:814:TYR:CG	2.33	0.63
1:F:588:GLN:O	1:F:592:ASN:ND2	2.32	0.63
1:A:575:MET:HA	1:A:621:ILE:HG13	1.81	0.62
1:B:584:GLN:HB2	1:B:617:GLN:HG2	1.79	0.62
1:C:272:GLY:N	1:C:275:TYR:OH	2.26	0.62
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.80	0.62
1:F:348:ILE:HG12	1:F:372:VAL:HG11	1.80	0.62
1:A:228:GLN:NE2	1:A:230:LEU:O	2.32	0.62
1:A:400:LEU:HD11	1:A:1002:VAL:HG21	1.81	0.62
1:D:790:ASP:OD2	1:D:791:GLY:N	2.31	0.62
1:D:1029:SER:OG	1:D:1030:ARG:N	2.30	0.62
1:F:893:PRO:HA	1:F:896:VAL:HG12	1.79	0.62
1:B:1008:THR:O	1:B:1012:LEU:HB2	2.00	0.62
1:C:896:VAL:HG23	1:C:937:ALA:HB3	1.79	0.62
1:D:103:ALA:HA	1:D:106:GLN:HE21	1.64	0.62
1:D:966:ARG:C	1:D:969:PRO:HD2	2.24	0.62
1:A:67:GLN:OE1	1:C:762:ARG:NH1	2.32	0.62
1:A:243:THR:HG23	1:A:268:ILE:HG22	1.82	0.62
1:A:573:MET:HE3	1:A:623:PHE:HE1	1.63	0.62
1:B:900:VAL:HG13	1:B:930:ILE:HG23	1.80	0.62
1:C:674:GLY:HA2	1:C:832:THR:HG23	1.80	0.62
1:E:351:VAL:HG21	1:E:406:VAL:HG11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.80	0.62
1:A:244:GLU:HG2	1:A:248:LYS:HE2	1.81	0.62
1:B:945:LYS:HZ2	1:B:1025:ARG:NH2	1.98	0.62
1:C:386:PHE:CD2	1:C:472:ILE:HD11	2.34	0.62
1:F:404:LEU:HB3	1:F:478:MET:SD	2.39	0.62
1:F:939:LEU:HB3	1:F:966:ARG:NE	2.14	0.62
1:A:795:PRO:HG2	1:A:798:ALA:HB2	1.80	0.62
1:A:941:VAL:HG13	1:A:1021:PHE:HD1	1.65	0.62
1:F:380:PHE:CD2	1:F:383:LEU:HD12	2.35	0.62
1:F:952:GLY:O	1:F:1036:GLU:HA	2.00	0.62
1:F:1014:ILE:HG13	1:F:1015:PHE:CD1	2.34	0.62
1:D:344:LEU:HD21	1:D:399:VAL:HA	1.80	0.62
1:D:457:ALA:O	1:D:468:ARG:NE	2.33	0.62
1:F:251:LEU:HD11	1:F:262:LEU:HA	1.81	0.62
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.80	0.62
1:C:629:TRP:CD1	1:C:629:TRP:H	2.16	0.62
1:E:188:MET:HE1	1:E:200:PRO:HG3	1.81	0.62
1:B:507:GLU:O	1:B:509:LYS:N	2.33	0.62
1:C:616:GLY:HA3	1:C:618:ASN:N	2.15	0.62
1:C:939:LEU:HB3	1:C:966:ARG:CD	2.29	0.62
1:D:182:TYR:HB2	1:D:764:LYS:HZ3	1.62	0.62
1:F:506:GLY:O	1:F:508:GLY:N	2.29	0.62
1:A:770:SER:HB3	1:A:775:ARG:HD3	1.81	0.62
1:A:785:TYR:HB3	1:A:793:MET:HB3	1.82	0.62
1:B:770:SER:HB3	1:B:775:ARG:HD3	1.81	0.61
1:B:1014:ILE:HG13	1:B:1015:PHE:HD1	1.63	0.61
1:C:693:ALA:O	1:C:696:GLN:HB3	2.00	0.61
1:F:36:PRO:HD3	1:F:391:ASN:CG	2.25	0.61
1:A:84:SER:HB3	1:A:809:PRO:HA	1.82	0.61
1:A:948:MET:HE1	1:A:955:LEU:HD12	1.82	0.61
1:B:36:PRO:HD2	1:B:38:ILE:HD11	1.81	0.61
1:B:691:THR:HG23	1:B:694:ARG:NH1	2.15	0.61
1:B:977:PHE:O	1:B:980:GLY:N	2.32	0.61
1:D:556:PHE:HD1	1:D:908:LEU:HD21	1.64	0.61
1:E:115:MET:O	1:E:123:GLN:NE2	2.33	0.61
1:F:120:GLN:HA	1:F:123:GLN:HB2	1.82	0.61
1:F:324:VAL:HG23	1:F:326:PRO:HD3	1.82	0.61
1:F:455:PRO:HG3	1:F:878:VAL:HG21	1.82	0.61
1:C:443:VAL:HG12	1:C:886:LEU:HD21	1.82	0.61
1:C:614:GLY:HA2	1:C:616:GLY:H	1.66	0.61
1:C:897:MET:O	1:C:900:VAL:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:892:ILE:HG23	1:F:941:VAL:HG11	1.81	0.61
1:A:80:SER:HB3	1:A:90:ILE:HG23	1.82	0.61
1:B:707:MET:HE3	1:B:834:GLU:HB3	1.82	0.61
1:B:803:ARG:NH1	1:B:805:GLU:OE2	2.33	0.61
1:C:918:ASN:HD22	1:C:918:ASN:C	2.08	0.61
1:E:187:TRP:HB3	1:E:771:GLU:HA	1.82	0.61
1:E:1015:PHE:HE2	3:E:1101:LMT:H11	1.65	0.61
1:B:647:THR:CG2	1:B:660:ALA:H	2.14	0.61
1:D:776:MET:HE1	1:F:225:VAL:H	1.64	0.61
1:E:892:ILE:O	1:E:895:SER:OG	2.16	0.61
1:F:545:TYR:OH	1:F:898:LEU:O	2.06	0.61
1:C:649:ALA:O	1:C:653:ILE:HG12	1.99	0.61
1:C:985:VAL:HG13	1:C:1000:THR:OG1	1.99	0.61
1:F:425:LEU:HD22	1:F:429:GLU:HG2	1.82	0.61
1:A:228:GLN:OE1	1:B:776:MET:HE3	2.01	0.61
1:A:966:ARG:C	1:A:969:PRO:HD2	2.26	0.61
1:D:56:THR:O	1:D:60:THR:HG22	2.01	0.61
1:E:58:GLN:HG3	1:E:813:ARG:HD2	1.83	0.61
1:E:690:LEU:HD22	1:E:820:MET:SD	2.41	0.61
1:A:881:LEU:HD11	1:C:17:ILE:CG2	2.31	0.61
1:B:108:GLN:OE1	1:C:112:GLN:HB3	2.01	0.61
1:B:420:MET:HB3	1:B:500:ILE:HB	1.82	0.61
1:B:683:ALA:O	1:B:685:LEU:N	2.32	0.61
1:B:762:ARG:HG2	1:B:762:ARG:NH1	2.15	0.61
1:C:184:MET:HA	1:C:184:MET:HE3	1.83	0.61
1:C:398:MET:HG2	1:C:473:THR:HG21	1.83	0.61
1:C:447:MET:HE1	1:C:882:CYS:HB3	1.82	0.61
1:D:351:VAL:HG22	1:D:976:ALA:HB1	1.83	0.61
1:F:576:VAL:HG22	1:F:658:VAL:HG13	1.82	0.61
1:F:746:GLY:O	1:F:750:GLY:N	2.29	0.61
1:A:588:GLN:HE21	1:A:592:ASN:HD21	1.49	0.61
1:A:885:ALA:HB2	1:C:14:VAL:HG11	1.83	0.61
1:B:61:VAL:CG2	1:B:122:VAL:HG21	2.31	0.61
1:C:80:SER:HB3	1:C:90:ILE:HG23	1.81	0.61
1:C:404:LEU:HD11	1:C:932:LEU:HD21	1.82	0.61
1:D:182:TYR:HB2	1:D:764:LYS:NZ	2.16	0.61
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.82	0.61
1:F:163:LYS:HD2	1:F:177:LEU:HD23	1.81	0.61
1:A:776:MET:HE2	1:C:225:VAL:HG22	1.81	0.60
1:B:262:LEU:HG	1:B:268:ILE:HD11	1.82	0.60
1:B:900:VAL:HB	1:B:901:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ILE:HD12	1:C:75:LEU:HD22	1.83	0.60
1:C:871:LEU:HD22	1:C:927:LEU:HD11	1.83	0.60
1:C:935:LYS:HZ1	1:C:973:THR:HG21	1.65	0.60
1:D:186:ILE:HB	1:D:768:VAL:HG22	1.81	0.60
1:D:448:VAL:HG22	1:D:882:CYS:HB3	1.83	0.60
1:E:355:MET:SD	1:E:365:THR:HA	2.40	0.60
1:F:69:MET:HB3	1:F:72:ILE:HD11	1.81	0.60
1:F:563:PHE:HD2	1:F:564:LEU:HB2	1.66	0.60
1:F:614:GLY:HA2	1:F:616:GLY:H	1.66	0.60
1:B:545:TYR:OH	1:B:898:LEU:O	2.16	0.60
1:B:1010:THR:O	1:B:1012:LEU:N	2.35	0.60
1:C:465:ALA:HA	1:C:468:ARG:HH11	1.66	0.60
1:E:574:THR:HG23	1:E:622:ALA:HB3	1.82	0.60
1:F:184:MET:HA	1:F:184:MET:HE3	1.83	0.60
1:B:73:ASP:H	1:B:106:GLN:NE2	1.98	0.60
1:B:404:LEU:HD21	1:B:449:LEU:HD22	1.82	0.60
1:B:574:THR:HG23	1:B:622:ALA:HB3	1.82	0.60
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.37	0.60
1:E:677:PHE:CZ	1:E:852:TYR:HB2	2.37	0.60
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.83	0.60
1:C:61:VAL:HA	1:C:118:LEU:CD2	2.31	0.60
1:D:770:SER:HB3	1:D:775:ARG:HD3	1.84	0.60
1:A:567:GLU:O	1:A:569:GLN:HG3	2.01	0.60
1:A:739:ASN:O	1:A:743:THR:HG23	2.00	0.60
1:A:939:LEU:HB3	1:A:966:ARG:HD2	1.82	0.60
1:B:414:GLU:OE1	1:B:968:ARG:NH1	2.35	0.60
1:B:674:GLY:HA2	1:B:825:GLN:HA	1.82	0.60
1:C:890:TRP:HA	1:C:890:TRP:HE3	1.66	0.60
1:E:73:ASP:H	1:E:106:GLN:NE2	1.98	0.60
1:F:902:LEU:HD23	1:F:1012:LEU:HB3	1.82	0.60
1:B:629:TRP:CD1	1:B:629:TRP:H	2.18	0.60
1:D:184:MET:HB2	1:D:757:PHE:CE2	2.37	0.60
1:E:56:THR:O	1:E:60:THR:HG22	2.00	0.60
1:F:683:ALA:O	1:F:685:LEU:N	2.35	0.60
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.83	0.60
1:C:137:LEU:HD22	1:C:293:LEU:HG	1.82	0.60
1:F:902:LEU:HG	1:F:1012:LEU:HD23	1.83	0.60
1:B:355:MET:HE1	1:B:410:ILE:HG12	1.82	0.60
1:D:790:ASP:OD2	1:D:792:GLN:HG3	2.01	0.60
1:D:962:ALA:C	1:D:966:ARG:HH12	2.10	0.60
1:E:813:ARG:HH12	1:E:818:PRO:HG3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:904:VAL:O	1:E:907:ALA:N	2.35	0.60
1:F:507:GLU:HG2	1:F:518:ARG:HG3	1.83	0.60
1:A:694:ARG:HD2	1:A:713:PRO:HB3	1.84	0.59
1:A:790:ASP:OD2	1:A:792:GLN:N	2.31	0.59
1:B:281:PHE:CE2	1:B:324:VAL:HG21	2.36	0.59
1:C:714:ASN:O	1:C:810:ARG:NH2	2.33	0.59
1:E:181:GLN:OE1	1:E:762:ARG:NH2	2.35	0.59
1:F:883:LEU:HD21	1:F:938:ILE:HD11	1.84	0.59
1:B:559:LEU:HG	1:B:560:PRO:HD2	1.83	0.59
1:B:694:ARG:HD3	1:B:820:MET:HE2	1.84	0.59
1:B:1032:ASN:HB3	1:B:1035:ILE:HG22	1.82	0.59
1:C:69:MET:HG2	1:C:92:LEU:HD11	1.82	0.59
1:C:239:ARG:NH1	1:C:756:ASP:H	1.99	0.59
1:C:586:ARG:O	1:C:589:LYS:HB2	2.02	0.59
1:E:355:MET:HE1	1:E:368:PRO:HG2	1.84	0.59
1:E:650:PHE:HA	1:E:654:LYS:HD3	1.83	0.59
1:F:277:ILE:HG12	1:F:614:GLY:O	2.02	0.59
1:F:563:PHE:CD2	1:F:564:LEU:HB2	2.37	0.59
1:A:941:VAL:HG22	1:A:1021:PHE:HB2	1.84	0.59
1:C:455:PRO:HG2	1:C:875:SER:HA	1.84	0.59
1:D:723:LYS:NZ	1:F:236:ALA:O	2.34	0.59
1:A:119:PRO:HB2	1:A:122:VAL:HB	1.83	0.59
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.85	0.59
1:F:445:ILE:HG23	1:F:935:LYS:HG3	1.83	0.59
1:F:693:ALA:O	1:F:696:GLN:HB3	2.02	0.59
1:B:899:VAL:HG13	1:B:902:LEU:HD22	1.84	0.59
1:E:251:LEU:HD11	1:E:265:VAL:HG21	1.84	0.59
1:E:982:MET:HG3	1:E:1003:MET:HE1	1.84	0.59
1:F:421:ALA:O	1:F:503:GLY:N	2.32	0.59
1:F:1033:GLU:HG3	1:F:1034:ASP:HB2	1.83	0.59
1:D:343:THR:HG21	1:D:984:LEU:HD21	1.85	0.59
1:E:893:PRO:O	1:E:896:VAL:N	2.35	0.59
1:F:563:PHE:HE2	1:F:564:LEU:HD22	1.67	0.59
1:A:412:VAL:HG11	1:A:489:THR:HG22	1.84	0.59
1:A:839:MET:HE2	1:A:839:MET:HA	1.83	0.59
1:A:908:LEU:HD23	1:A:922:PHE:CZ	2.33	0.59
1:B:327:TYR:HB2	1:B:623:PHE:CZ	2.38	0.59
1:B:610:PHE:HB3	1:B:623:PHE:HB3	1.85	0.59
1:C:404:LEU:HG	1:C:449:LEU:HD13	1.84	0.59
1:C:1034:ASP:O	1:C:1035:ILE:HG12	2.02	0.59
1:D:707:MET:HG2	1:D:838:LEU:HG	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:872:TYR:CE1	3:D:1103:LMT:H92	2.37	0.59
1:D:914:ARG:HG2	1:D:915:GLY:H	1.67	0.59
1:E:686:GLY:H	1:E:689:LYS:HE3	1.67	0.59
1:E:936:ASN:ND2	1:E:970:ILE:HG23	2.18	0.59
1:F:3:ASN:OD1	1:F:3:ASN:N	2.22	0.59
1:E:236:ALA:O	1:F:723:LYS:NZ	2.29	0.59
1:E:444:GLY:HA3	1:E:886:LEU:HD22	1.84	0.59
1:B:139:VAL:O	1:B:326:PRO:HD2	2.02	0.59
1:C:528:THR:HG21	1:C:964:ARG:HG3	1.85	0.59
1:A:426:PRO:HB2	1:A:429:GLU:OE2	2.03	0.59
1:B:62:THR:HG21	1:B:813:ARG:HD3	1.84	0.59
1:C:689:LYS:HE3	1:C:689:LYS:H	1.68	0.59
1:C:734:LEU:HD12	1:C:794:VAL:HG11	1.85	0.59
1:D:137:LEU:HD22	1:D:293:LEU:HG	1.84	0.59
1:D:400:LEU:HD21	1:D:925:GLY:HA2	1.83	0.59
1:D:426:PRO:HB3	1:D:428:LYS:NZ	2.18	0.59
1:E:899:VAL:HG21	1:E:937:ALA:HB2	1.85	0.59
1:F:563:PHE:HB2	1:F:861:GLU:CG	2.33	0.59
1:B:48:SER:HB3	1:B:87:THR:HG22	1.85	0.58
1:D:813:ARG:HH12	1:D:818:PRO:HG3	1.68	0.58
1:F:158:VAL:HA	1:F:162:MET:HE3	1.85	0.58
1:F:723:LYS:HG2	1:F:803:ARG:CZ	2.33	0.58
1:A:448:VAL:HG22	1:A:882:CYS:HB3	1.85	0.58
1:B:578:LEU:HB2	1:B:618:ASN:O	2.03	0.58
1:C:34:GLN:HG2	1:C:333:VAL:HA	1.85	0.58
1:C:251:LEU:HD12	1:C:265:VAL:HG11	1.84	0.58
1:D:198:LEU:HD11	1:D:252:LYS:HB2	1.85	0.58
2:D:1101:ERY:H352	2:D:1101:ERY:H2	1.85	0.58
1:E:164:ASP:OD1	1:E:164:ASP:N	2.36	0.58
1:E:1014:ILE:HG13	1:E:1015:PHE:HD1	1.68	0.58
1:A:1032:ASN:O	1:A:1032:ASN:ND2	2.33	0.58
1:B:383:LEU:HD21	1:B:473:THR:HA	1.84	0.58
1:B:442:LEU:O	1:B:445:ILE:HG13	2.03	0.58
1:B:647:THR:HG22	1:B:660:ALA:H	1.67	0.58
1:B:896:VAL:HG23	1:B:937:ALA:HB3	1.85	0.58
1:C:376:LEU:O	1:C:379:THR:N	2.36	0.58
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.85	0.58
1:A:757:PHE:CE1	1:A:759:ASP:HB2	2.38	0.58
1:B:905:ILE:O	1:B:909:LEU:HB2	2.03	0.58
1:F:574:THR:HG23	1:F:622:ALA:HB3	1.85	0.58
1:A:918:ASN:OD1	1:A:923:GLN:NE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:738:ILE:HD12	1:C:738:ILE:H	1.68	0.58
1:D:356:TYR:O	1:D:358:PHE:N	2.36	0.58
1:F:940:ILE:HD12	1:F:1017:VAL:HB	1.86	0.58
1:F:977:PHE:O	1:F:980:GLY:N	2.37	0.58
1:A:423:GLU:HB2	1:A:425:LEU:HD13	1.86	0.58
1:A:573:MET:HE3	1:A:623:PHE:CE1	2.37	0.58
1:B:185:ARG:HH11	1:B:767:TYR:HB3	1.68	0.58
1:C:910:ALA:HB2	1:C:1004:GLY:HA3	1.85	0.58
1:E:900:VAL:O	1:E:904:VAL:HG23	2.03	0.58
1:A:396:PHE:CD2	1:A:998:VAL:HG21	2.38	0.58
1:B:362:PHE:HA	1:B:365:THR:HG22	1.85	0.58
1:B:535:LEU:HD22	1:B:1022:VAL:HG11	1.84	0.58
1:D:883:LEU:HB2	1:D:893:PRO:HB3	1.86	0.58
1:E:169:THR:HG21	1:E:306:ILE:HG13	1.85	0.58
1:E:213:GLN:HG2	1:E:239:ARG:HG3	1.85	0.58
1:E:214:VAL:HG11	1:F:742:ASN:HB3	1.85	0.58
1:F:6:ILE:C	1:F:8:ARG:H	2.12	0.58
1:A:151:GLN:HE21	1:A:152:GLU:HA	1.69	0.58
1:A:159:ALA:HB2	1:A:177:LEU:HD11	1.85	0.58
1:B:189:ASN:ND2	1:B:267:LYS:HE2	2.14	0.58
1:C:796:PHE:HA	1:C:799:PHE:CE2	2.38	0.58
1:C:1014:ILE:HG13	1:C:1015:PHE:HD1	1.68	0.58
1:D:210:GLN:HE22	1:D:250:LEU:H	1.50	0.58
1:D:568:ASP:O	1:D:629:TRP:HZ3	1.87	0.58
1:E:576:VAL:HG22	1:E:658:VAL:HG13	1.86	0.58
1:F:396:PHE:O	1:F:400:LEU:HB2	2.04	0.58
1:F:909:LEU:O	1:F:913:PHE:HB2	2.03	0.58
1:A:35:TYR:CZ	1:A:564:LEU:HD23	2.38	0.58
1:A:578:LEU:HB2	1:A:618:ASN:O	2.04	0.58
1:B:62:THR:OG1	1:B:88:VAL:HG21	2.04	0.58
1:B:363:ARG:HD2	1:B:498:LYS:HB2	1.86	0.58
1:B:240:LEU:HB2	1:B:246:PHE:CE1	2.39	0.57
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.28	0.57
1:D:1031:LYS:HG3	1:D:1033:GLU:CD	2.29	0.57
1:E:32:VAL:HG22	1:E:298:ASN:ND2	2.19	0.57
1:E:693:ALA:HB1	1:E:846:LEU:HD13	1.86	0.57
1:F:2:PRO:HD2	1:F:4:PHE:HD1	1.69	0.57
1:A:6:ILE:HD11	1:A:432:ARG:HE	1.68	0.57
1:A:198:LEU:HD23	1:A:787:ARG:HH21	1.68	0.57
1:C:415:ASN:ND2	1:C:438:ILE:HG21	2.19	0.57
1:D:262:LEU:HG	1:D:268:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447:MET:HB3	1:E:882:CYS:SG	2.43	0.57
1:A:6:ILE:CD1	1:A:432:ARG:HE	2.16	0.57
1:B:14:VAL:HG13	1:C:881:LEU:HD12	1.86	0.57
1:B:573:MET:HB2	1:B:661:PHE:HE2	1.68	0.57
1:C:452:VAL:O	1:C:455:PRO:HD2	2.04	0.57
1:C:675:PHE:HE2	1:C:839:MET:HE2	1.67	0.57
1:F:65:ILE:HG21	1:F:90:ILE:HG13	1.86	0.57
1:F:274:ASN:OD1	1:F:275:TYR:N	2.37	0.57
1:F:447:MET:HG2	1:F:886:LEU:HD22	1.84	0.57
1:A:62:THR:HG21	1:A:813:ARG:HD3	1.85	0.57
1:B:1010:THR:C	1:B:1012:LEU:H	2.13	0.57
1:C:182:TYR:HB2	1:C:764:LYS:NZ	2.18	0.57
1:E:31:PRO:HB2	1:E:389:SER:HB2	1.85	0.57
1:A:457:ALA:O	1:A:468:ARG:NE	2.38	0.57
1:D:357:LEU:HD23	1:D:358:PHE:CD1	2.40	0.57
1:D:887:TYR:CD2	1:D:892:ILE:HG22	2.39	0.57
1:E:416:VAL:HG21	1:E:493:CYS:SG	2.44	0.57
1:F:880:PHE:C	1:F:880:PHE:CD2	2.83	0.57
1:B:376:LEU:O	1:B:379:THR:N	2.38	0.57
1:B:560:PRO:HG2	1:B:917:THR:HA	1.85	0.57
1:C:659:PHE:CE2	1:C:712:ARG:HB3	2.39	0.57
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.87	0.57
1:E:757:PHE:CE1	1:E:759:ASP:HB2	2.39	0.57
1:F:414:GLU:HG2	1:F:968:ARG:NH1	2.20	0.57
1:A:210:GLN:HE22	1:A:250:LEU:N	2.03	0.57
1:A:225:VAL:H	1:B:776:MET:HE1	1.69	0.57
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.87	0.57
1:C:752:SER:O	1:C:767:TYR:HA	2.05	0.57
1:D:72:ILE:HG21	1:D:107:VAL:HG23	1.86	0.57
1:D:72:ILE:HD13	1:D:107:VAL:HG22	1.86	0.57
1:D:99:ASP:HB3	1:D:102:ILE:HB	1.85	0.57
1:E:728:GLN:HE22	1:E:738:ILE:HG21	1.69	0.57
1:F:5:PHE:C	1:F:7:ASP:H	2.09	0.57
1:F:193:LEU:HD23	1:F:265:VAL:HB	1.86	0.57
1:A:56:THR:O	1:A:60:THR:HG22	2.03	0.57
1:A:146:ASP:OD2	1:A:146:ASP:N	2.29	0.57
1:B:41:PRO:HD2	1:B:94:PHE:O	2.04	0.57
1:B:83:ASP:HB2	1:B:87:THR:O	2.04	0.57
1:A:196:PHE:O	1:A:252:LYS:NZ	2.25	0.57
1:C:583:THR:HA	1:C:617:GLN:OE1	2.04	0.57
1:C:681:ASP:HB3	1:C:818:PRO:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:SD	1:A:410:ILE:HG12	2.45	0.57
1:A:470:PHE:CG	1:A:924:VAL:HG21	2.39	0.57
1:A:568:ASP:CG	1:A:632:ARG:HH22	2.12	0.57
1:C:576:VAL:HG22	1:C:658:VAL:HG13	1.86	0.57
1:E:415:ASN:ND2	1:E:437:GLN:OE1	2.38	0.57
1:E:1014:ILE:HG13	1:E:1015:PHE:CD1	2.40	0.57
1:F:796:PHE:HA	1:F:799:PHE:CE2	2.39	0.57
1:A:895:SER:HB3	1:A:1024:VAL:HG21	1.87	0.56
1:B:741:ILE:HG22	1:B:796:PHE:HE1	1.70	0.56
1:C:677:PHE:HD2	1:C:678:GLU:N	2.03	0.56
1:D:416:VAL:HG21	1:D:493:CYS:SG	2.45	0.56
1:D:1008:THR:O	1:D:1012:LEU:HB2	2.05	0.56
1:E:137:LEU:HD12	1:E:329:THR:HG22	1.87	0.56
1:E:670:GLY:HA2	1:E:857:MET:SD	2.44	0.56
1:F:670:GLY:HA3	1:F:857:MET:HG2	1.87	0.56
1:D:943:PHE:O	1:D:947:LEU:HG	2.05	0.56
1:E:1015:PHE:CE2	3:E:1101:LMT:H32	2.40	0.56
1:F:757:PHE:CE1	1:F:759:ASP:HB2	2.39	0.56
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.32	0.56
1:A:981:VAL:HG12	1:A:1003:MET:HE3	1.87	0.56
1:B:190:PRO:HB3	1:B:784:TRP:CH2	2.41	0.56
1:C:65:ILE:HG23	1:C:111:LEU:HD23	1.88	0.56
1:C:277:ILE:HG12	1:C:614:GLY:O	2.06	0.56
1:C:447:MET:O	1:C:451:ALA:HB2	2.04	0.56
1:D:465:ALA:O	1:D:469:GLN:HG2	2.05	0.56
1:D:540:ARG:HG3	1:D:541:TYR:CD1	2.40	0.56
1:D:629:TRP:CD1	1:D:629:TRP:H	2.22	0.56
1:E:48:SER:HB3	1:E:87:THR:HG22	1.86	0.56
1:E:108:GLN:HE22	1:F:112:GLN:HB3	1.70	0.56
1:E:408:ASP:OD1	1:E:935:LYS:NZ	2.37	0.56
1:F:356:TYR:C	1:F:358:PHE:N	2.63	0.56
1:F:482:VAL:O	1:F:486:LEU:HG	2.06	0.56
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.39	0.56
1:B:650:PHE:HB3	1:B:658:VAL:HB	1.87	0.56
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.87	0.56
1:C:935:LYS:NZ	1:C:973:THR:HG21	2.20	0.56
1:D:368:PRO:HG3	1:D:413:VAL:HG21	1.87	0.56
1:D:926:LEU:O	1:D:930:ILE:HG13	2.06	0.56
1:E:650:PHE:HB3	1:E:658:VAL:HB	1.87	0.56
1:F:119:PRO:HB2	1:F:122:VAL:HB	1.88	0.56
1:B:23:GLY:HA2	1:B:381:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:VAL:HG21	1:B:122:VAL:HG21	1.87	0.56
1:B:156:ASP:OD2	1:B:764:LYS:NZ	2.39	0.56
1:C:39:ALA:HB2	1:C:668:GLU:HG2	1.87	0.56
1:C:770:SER:OG	1:C:775:ARG:HG2	2.04	0.56
1:E:575:MET:HA	1:E:621:ILE:HG13	1.87	0.56
1:E:906:GLY:HA3	1:E:1008:THR:OG1	2.05	0.56
1:F:101:ASP:OD1	1:F:131:LYS:NZ	2.39	0.56
1:F:202:ASP:OD2	1:F:787:ARG:NH2	2.39	0.56
1:F:351:VAL:HG11	1:F:406:VAL:HG21	1.88	0.56
1:F:453:PHE:HZ	1:F:928:THR:HG1	1.53	0.56
1:F:956:ILE:H	1:F:956:ILE:HD12	1.71	0.56
1:D:23:GLY:HA3	1:D:377:LEU:O	2.06	0.56
1:A:362:PHE:O	1:A:365:THR:HG22	2.06	0.56
1:A:632:ARG:HB3	1:A:637:ASN:HB3	1.87	0.56
1:A:880:PHE:CE1	1:A:893:PRO:HB2	2.41	0.56
1:A:881:LEU:HD11	1:C:17:ILE:HG22	1.88	0.56
1:A:1013:ALA:C	1:A:1015:PHE:H	2.12	0.56
1:C:1032:ASN:N	1:C:1033:GLU:HB2	2.20	0.56
1:D:427:PRO:HD2	1:D:428:LYS:HZ3	1.71	0.56
1:F:13:TRP:HH2	1:F:370:ILE:HD13	1.70	0.56
1:B:898:LEU:HB3	1:B:1020:PHE:CZ	2.40	0.56
1:D:277:ILE:HA	1:D:613:ASN:O	2.05	0.56
1:E:156:ASP:OD2	1:E:764:LYS:NZ	2.38	0.56
1:E:225:VAL:HG12	1:F:772:ALA:HB1	1.87	0.56
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.88	0.56
1:E:751:GLY:HA2	1:E:769:MET:HG3	1.88	0.56
1:E:790:ASP:OD2	1:E:792:GLN:N	2.39	0.56
1:F:227:GLY:O	1:F:229:GLN:HG3	2.06	0.56
1:F:883:LEU:HD12	1:F:896:VAL:HG11	1.88	0.56
1:A:225:VAL:H	1:B:776:MET:CE	2.19	0.56
1:B:453:PHE:O	1:B:471:SER:OG	2.16	0.56
1:C:6:ILE:CG2	1:C:12:ALA:HB2	2.36	0.56
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.88	0.56
1:C:892:ILE:HG23	1:C:941:VAL:CG1	2.35	0.56
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.88	0.56
1:D:920:VAL:O	1:D:923:GLN:N	2.38	0.56
1:E:424:GLY:HA3	1:E:502:LYS:HB2	1.88	0.56
1:E:902:LEU:HG	1:E:1012:LEU:HD23	1.88	0.56
1:E:905:ILE:O	1:E:909:LEU:HB2	2.06	0.56
1:F:675:PHE:CD2	1:F:854:TRP:HZ3	2.23	0.56
1:A:400:LEU:HD21	1:A:925:GLY:CA	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ARG:O	1:A:589:LYS:HB3	2.06	0.56
1:B:796:PHE:HA	1:B:799:PHE:CE2	2.41	0.56
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.41	0.56
1:C:531:VAL:HG21	1:C:963:VAL:HG11	1.87	0.56
1:D:17:ILE:HG22	1:E:881:LEU:HD21	1.88	0.56
1:E:111:LEU:HD11	1:E:127:VAL:HB	1.88	0.56
1:A:211:ASN:CG	1:A:240:LEU:HG	2.31	0.55
1:A:591:LEU:HD11	1:A:620:GLY:HA3	1.86	0.55
1:B:1015:PHE:CE2	3:B:2100:LMT:H21	2.41	0.55
1:D:35:TYR:HB3	1:D:38:ILE:HD11	1.88	0.55
1:D:426:PRO:HD2	1:D:429:GLU:CG	2.37	0.55
1:A:32:VAL:HB	1:A:300:LEU:HD22	1.87	0.55
1:A:187:TRP:HB3	1:A:771:GLU:HA	1.88	0.55
1:A:776:MET:HE1	1:C:225:VAL:H	1.71	0.55
1:B:3:ASN:O	1:B:6:ILE:HB	2.06	0.55
1:B:400:LEU:HG	1:B:924:VAL:HG12	1.88	0.55
1:B:400:LEU:HD11	1:B:925:GLY:HA2	1.87	0.55
1:D:27:ILE:HD11	1:D:380:PHE:CE1	2.40	0.55
1:E:555:LEU:HD11	1:E:909:LEU:HD12	1.88	0.55
1:F:540:ARG:HG3	1:F:541:TYR:CD1	2.41	0.55
1:F:662:ASN:O	1:F:673:THR:OG1	2.21	0.55
1:F:855:THR:HA	1:F:859:TYR:HB2	1.88	0.55
1:A:249:ILE:HD12	1:A:262:LEU:HD23	1.87	0.55
1:C:318:PRO:HG2	1:C:321:LEU:CB	2.37	0.55
1:E:45:ILE:HD11	1:E:69:MET:HE2	1.88	0.55
1:E:985:VAL:HG22	1:E:999:GLY:HA3	1.88	0.55
1:F:371:ALA:O	1:F:375:VAL:HG23	2.06	0.55
1:A:982:MET:O	1:A:986:ILE:HG12	2.05	0.55
1:B:836:MET:HE1	1:B:862:ARG:HG3	1.89	0.55
1:C:340:VAL:HG22	1:C:995:GLN:HE21	1.71	0.55
1:C:966:ARG:HB3	1:C:966:ARG:CZ	2.36	0.55
1:D:388:PHE:HE1	1:D:469:GLN:HE22	1.53	0.55
1:D:966:ARG:HB3	1:D:966:ARG:NH1	2.21	0.55
1:A:420:MET:HB3	1:A:500:ILE:HB	1.88	0.55
1:A:470:PHE:CD2	1:A:924:VAL:HG11	2.41	0.55
1:B:106:GLN:HA	1:B:109:ASN:ND2	2.22	0.55
1:B:899:VAL:HG21	1:B:937:ALA:CB	2.37	0.55
1:C:616:GLY:HA3	1:C:619:THR:H	1.71	0.55
1:D:34:GLN:NE2	1:D:332:PHE:HE2	2.04	0.55
1:E:239:ARG:HD3	1:E:756:ASP:O	2.07	0.55
1:E:559:LEU:HD21	1:E:917:THR:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:701:ALA:HB3	1:E:711:VAL:HG11	1.88	0.55
1:F:616:GLY:HA3	1:F:618:ASN:N	2.21	0.55
1:A:172:VAL:HG22	1:A:306:ILE:HD11	1.88	0.55
1:A:425:LEU:HD23	1:A:429:GLU:HB2	1.88	0.55
1:A:427:PRO:CD	1:A:499:PRO:HB3	2.33	0.55
1:C:139:VAL:HB	1:C:327:TYR:HB3	1.87	0.55
1:C:240:LEU:HD11	1:C:249:ILE:HD11	1.88	0.55
1:C:785:TYR:CE2	1:C:795:PRO:HB3	2.41	0.55
1:C:1031:LYS:HE3	1:C:1035:ILE:HD13	1.89	0.55
1:D:31:PRO:HB2	1:D:389:SER:HB3	1.89	0.55
1:E:40:PRO:HD3	1:E:462:SER:OG	2.06	0.55
1:E:790:ASP:OD2	1:E:791:GLY:N	2.40	0.55
1:C:53:ASP:OD1	1:C:56:THR:OG1	2.21	0.55
1:C:456:MET:HB3	1:C:871:LEU:HD21	1.89	0.55
1:C:540:ARG:HG3	1:C:541:TYR:HD1	1.72	0.55
1:D:187:TRP:HB3	1:D:771:GLU:HA	1.89	0.55
1:D:908:LEU:HD23	1:D:922:PHE:CZ	2.37	0.55
1:F:187:TRP:HA	1:F:769:MET:O	2.06	0.55
1:F:836:MET:O	1:F:840:GLU:HG2	2.07	0.55
1:A:963:VAL:HG21	1:A:1018:PRO:HG3	1.89	0.55
1:D:396:PHE:CD1	1:D:998:VAL:HG21	2.42	0.55
1:E:425:LEU:HD22	1:E:429:GLU:HG2	1.89	0.55
1:E:700:GLU:HB3	1:E:842:LEU:HD22	1.88	0.55
1:E:900:VAL:HG13	1:E:930:ILE:HG23	1.88	0.55
1:F:463:THR:HG23	1:F:920:VAL:HG22	1.88	0.55
1:A:914:ARG:HH12	1:A:996:ASN:HB3	1.71	0.55
1:C:75:LEU:HD21	1:C:78:MET:HB2	1.89	0.55
1:D:355:MET:HB3	1:D:365:THR:HG1	1.72	0.55
1:E:116:PRO:HA	1:E:123:GLN:HE22	1.71	0.55
1:E:250:LEU:HD11	1:E:259:ARG:HB2	1.89	0.55
1:E:530:SER:OG	3:E:1101:LMT:C1'	2.54	0.55
1:F:753:TYR:OH	1:F:756:ASP:OD2	2.25	0.55
1:F:1014:ILE:HG13	1:F:1015:PHE:HD1	1.71	0.55
1:A:653:ILE:HG13	1:A:654:LYS:HE2	1.88	0.54
1:A:892:ILE:HA	1:A:1024:VAL:CG1	2.37	0.54
1:B:394:THR:O	1:B:473:THR:HG21	2.07	0.54
1:B:697:LEU:HB2	1:B:846:LEU:HD11	1.89	0.54
1:D:962:ALA:O	1:D:965:MET:HG2	2.07	0.54
1:E:3:ASN:HA	1:E:6:ILE:HD12	1.89	0.54
1:E:795:PRO:HG2	1:E:798:ALA:HB2	1.88	0.54
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:PRO:HD3	1:B:656:ALA:HB2	1.88	0.54
1:C:119:PRO:O	1:C:123:GLN:HG3	2.06	0.54
1:C:678:GLU:HG2	1:C:814:TYR:CD2	2.42	0.54
1:D:172:VAL:HG13	1:D:291:ILE:HG23	1.89	0.54
1:D:379:THR:HG23	1:D:476:SER:OG	2.08	0.54
1:D:762:ARG:NH1	1:E:67:GLN:HE21	2.05	0.54
1:E:291:ILE:HG21	1:E:306:ILE:HD11	1.88	0.54
1:E:748:ALA:O	1:E:770:SER:HB3	2.07	0.54
1:A:562:SER:HB2	1:A:919:ASP:CB	2.31	0.54
1:A:701:ALA:HB3	1:A:711:VAL:HG11	1.89	0.54
1:A:857:MET:HG2	2:A:1101:ERY:H202	1.88	0.54
1:A:1031:LYS:HE2	1:A:1035:ILE:HG23	1.90	0.54
1:B:80:SER:HB3	1:B:90:ILE:HG23	1.88	0.54
1:B:354:VAL:O	1:B:358:PHE:HB2	2.07	0.54
1:B:545:TYR:HE2	1:B:902:LEU:HD11	1.72	0.54
1:B:910:ALA:HB2	1:B:1004:GLY:HA3	1.87	0.54
1:C:34:GLN:CB	1:C:333:VAL:HG22	2.34	0.54
1:C:270:LEU:HD21	1:C:759:ASP:OD2	2.07	0.54
1:D:839:MET:HE2	1:D:839:MET:HA	1.90	0.54
1:E:530:SER:HG	3:E:1101:LMT:C1'	2.20	0.54
1:E:893:PRO:O	1:E:896:VAL:HG12	2.08	0.54
1:E:955:LEU:HD13	1:E:1025:ARG:HG2	1.89	0.54
1:E:966:ARG:O	1:E:970:ILE:HG12	2.07	0.54
1:F:171:GLY:O	1:F:293:LEU:HD23	2.08	0.54
1:F:914:ARG:NH2	1:F:985:VAL:O	2.40	0.54
1:A:187:TRP:HA	1:A:769:MET:O	2.06	0.54
1:C:103:ALA:O	1:C:106:GLN:N	2.39	0.54
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.89	0.54
1:C:1008:THR:O	1:C:1012:LEU:HB2	2.08	0.54
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.90	0.54
1:E:281:PHE:CZ	1:E:324:VAL:HG21	2.42	0.54
1:A:38:ILE:HG12	1:A:466:ILE:HD11	1.90	0.54
1:A:796:PHE:HD1	1:A:799:PHE:CE2	2.26	0.54
1:A:902:LEU:HG	1:A:1012:LEU:HD23	1.89	0.54
1:B:250:LEU:HD11	1:B:259:ARG:HB2	1.89	0.54
1:C:409:ALA:O	1:C:413:VAL:HG23	2.07	0.54
1:C:757:PHE:CE1	1:C:759:ASP:HB2	2.43	0.54
1:C:889:SER:CB	1:C:892:ILE:HG12	2.38	0.54
1:D:189:ASN:HB3	1:D:192:GLU:HB2	1.88	0.54
1:D:427:PRO:HD2	1:D:428:LYS:NZ	2.22	0.54
1:D:748:ALA:O	1:D:770:SER:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:891:SER:OG	1:D:1028:PHE:HB3	2.07	0.54
1:D:941:VAL:HG13	1:D:1021:PHE:CD1	2.42	0.54
1:E:42:ALA:HB2	1:E:93:THR:HG23	1.90	0.54
1:E:530:SER:HG	3:E:1101:LMT:H1'	1.70	0.54
1:F:78:MET:HG3	1:F:92:LEU:HD13	1.89	0.54
1:F:941:VAL:HG13	1:F:1021:PHE:CD1	2.43	0.54
1:B:327:TYR:HD1	1:B:623:PHE:CZ	2.25	0.54
3:B:2100:LMT:H6E	3:B:2100:LMT:C5B	2.38	0.54
1:C:520:PHE:O	1:C:524:THR:HG22	2.08	0.54
1:C:770:SER:HB3	1:C:775:ARG:HD3	1.89	0.54
1:D:221:GLY:N	1:E:775:ARG:HH12	2.06	0.54
1:F:584:GLN:HB2	1:F:617:GLN:HG2	1.89	0.54
1:F:938:ILE:O	1:F:942:GLU:HB3	2.08	0.54
1:B:548:ILE:HG23	1:B:905:ILE:HD13	1.89	0.54
1:C:156:ASP:OD2	1:C:764:LYS:NZ	2.38	0.54
1:C:453:PHE:HB3	1:C:471:SER:HA	1.90	0.54
1:E:211:ASN:CG	1:E:240:LEU:HG	2.33	0.54
1:E:317:PHE:HE2	1:E:323:ILE:HG12	1.73	0.54
1:C:723:LYS:HG2	1:C:803:ARG:NH2	2.22	0.54
1:E:572:PHE:HA	1:E:663:LEU:CD2	2.37	0.54
1:F:49:TYR:HD1	1:F:57:VAL:HG12	1.71	0.54
1:F:770:SER:OG	1:F:775:ARG:HG2	2.08	0.54
1:F:941:VAL:HG13	1:F:1021:PHE:CE1	2.42	0.54
1:A:251:LEU:HD12	1:A:265:VAL:HG11	1.88	0.54
1:A:629:TRP:H	1:A:629:TRP:CD1	2.26	0.54
1:C:382:VAL:HG11	1:C:476:SER:HB2	1.88	0.54
1:C:716:LEU:CD2	1:C:810:ARG:HE	2.20	0.54
1:D:142:VAL:HG11	1:D:162:MET:HE1	1.89	0.54
1:D:1033:GLU:HB3	1:D:1035:ILE:HG12	1.90	0.54
1:E:108:GLN:NE2	1:F:112:GLN:HB3	2.23	0.54
1:E:139:VAL:O	1:E:326:PRO:HD2	2.08	0.54
1:E:584:GLN:HB2	1:E:617:GLN:HG2	1.88	0.54
1:E:686:GLY:O	1:E:689:LYS:N	2.40	0.54
1:F:528:THR:HG21	1:F:964:ARG:HG3	1.88	0.54
1:F:871:LEU:HD22	1:F:927:LEU:HD11	1.89	0.54
1:A:108:GLN:NE2	1:B:109:ASN:HB2	2.23	0.54
1:A:388:PHE:CE1	1:A:472:ILE:HG21	2.43	0.54
1:A:941:VAL:HG13	1:A:1021:PHE:CE1	2.43	0.54
1:E:175:VAL:HG23	1:F:70:ASN:ND2	2.23	0.54
1:F:892:ILE:HG23	1:F:941:VAL:CG1	2.38	0.54
1:C:770:SER:HG	1:C:775:ARG:HG2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:677:PHE:HD2	1:D:678:GLU:N	2.06	0.53
1:E:836:MET:O	1:E:840:GLU:HG3	2.08	0.53
1:E:929:THR:O	1:E:933:SER:OG	2.23	0.53
1:F:527:TYR:HB2	3:F:2100:LMT:H82	1.90	0.53
1:A:707:MET:HB3	1:A:708:LEU:HD22	1.88	0.53
1:C:62:THR:HG21	1:C:813:ARG:HD3	1.90	0.53
1:D:905:ILE:O	1:D:909:LEU:HB2	2.08	0.53
1:E:166:ILE:O	1:E:169:THR:HB	2.07	0.53
1:F:908:LEU:HD23	1:F:922:PHE:CZ	2.41	0.53
1:C:677:PHE:CD1	1:C:839:MET:HE3	2.44	0.53
1:C:747:ALA:O	1:C:769:MET:HA	2.08	0.53
1:D:3:ASN:HA	1:D:6:ILE:HD11	1.89	0.53
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.90	0.53
1:F:65:ILE:HG23	1:F:111:LEU:HD23	1.90	0.53
1:F:189:ASN:CG	1:F:774:TYR:HH	2.10	0.53
1:F:748:ALA:O	1:F:770:SER:HB3	2.07	0.53
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.43	0.53
1:B:521:GLU:O	1:B:524:THR:HG23	2.08	0.53
1:C:892:ILE:O	1:C:895:SER:OG	2.27	0.53
1:E:166:ILE:HD11	1:E:310:LEU:CD1	2.38	0.53
1:E:186:ILE:HD13	1:E:262:LEU:HD21	1.89	0.53
1:E:356:TYR:C	1:E:358:PHE:N	2.60	0.53
1:E:407:ASP:OD1	1:E:973:THR:OG1	2.20	0.53
1:E:559:LEU:HD12	1:E:912:THR:OG1	2.09	0.53
1:F:587:THR:HG21	1:F:617:GLN:O	2.09	0.53
1:F:639:VAL:O	1:F:643:THR:HG23	2.07	0.53
1:A:796:PHE:HA	1:A:799:PHE:CE2	2.43	0.53
1:B:183:ALA:O	1:B:270:LEU:HD12	2.09	0.53
1:C:540:ARG:HG3	1:C:541:TYR:CD1	2.44	0.53
1:C:661:PHE:N	1:C:661:PHE:CD1	2.76	0.53
1:D:528:THR:HG21	1:D:964:ARG:HG3	1.89	0.53
1:D:757:PHE:CE1	1:D:759:ASP:HB2	2.42	0.53
1:E:978:ILE:O	1:E:982:MET:HB2	2.09	0.53
1:F:563:PHE:CE2	1:F:564:LEU:HD22	2.43	0.53
1:F:588:GLN:OE1	1:F:592:ASN:ND2	2.41	0.53
1:A:201:VAL:HA	1:A:204:ILE:HD12	1.90	0.53
1:A:650:PHE:HB3	1:A:658:VAL:HB	1.91	0.53
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.91	0.53
1:C:411:VAL:O	1:C:415:ASN:ND2	2.41	0.53
1:D:151:GLN:H	1:D:151:GLN:CD	2.16	0.53
1:B:28:LEU:HD12	1:B:29:LYS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:GLY:C	1:D:249:ILE:H	2.16	0.53
1:E:393:LEU:HD12	1:E:469:GLN:HG3	1.90	0.53
1:F:331:PRO:O	1:F:335:ILE:HG22	2.08	0.53
1:F:919:ASP:OD1	1:F:921:TYR:N	2.41	0.53
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.90	0.53
1:A:452:VAL:HA	1:A:875:SER:OG	2.09	0.53
1:B:415:ASN:ND2	1:B:434:SER:HB2	2.24	0.53
1:C:688:GLU:HB3	1:C:689:LYS:HE2	1.89	0.53
1:C:707:MET:SD	1:C:838:LEU:HB2	2.49	0.53
1:E:105:VAL:HG23	1:F:109:ASN:HD21	1.73	0.53
1:A:45:ILE:HD12	1:A:90:ILE:HB	1.91	0.53
1:A:222:THR:HG23	1:B:275:TYR:HB2	1.91	0.53
1:A:982:MET:HB3	1:A:983:PRO:HD3	1.91	0.53
1:B:908:LEU:HD23	1:B:922:PHE:HZ	1.73	0.53
1:C:350:LEU:HD23	1:C:979:LEU:HB3	1.90	0.53
1:C:661:PHE:N	1:C:661:PHE:HD1	2.06	0.53
1:D:150:THR:N	1:D:153:ASP:OD1	2.27	0.53
1:E:415:ASN:O	1:E:419:VAL:HG23	2.09	0.53
1:E:694:ARG:NH2	1:E:717:GLU:OE1	2.42	0.53
1:E:909:LEU:O	1:E:913:PHE:HB2	2.07	0.53
1:F:239:ARG:HD3	1:F:756:ASP:O	2.08	0.53
1:A:418:ARG:NH2	1:A:943:PHE:HE2	2.07	0.53
1:A:528:THR:HG21	1:A:964:ARG:HG3	1.90	0.53
1:B:210:GLN:NE2	1:B:250:LEU:O	2.42	0.53
1:B:694:ARG:HD2	1:B:713:PRO:HB3	1.91	0.53
1:D:32:VAL:HB	1:D:300:LEU:HD22	1.91	0.53
1:D:240:LEU:HD12	1:D:246:PHE:CD2	2.44	0.53
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.89	0.53
1:D:675:PHE:CD1	1:D:854:TRP:HZ3	2.27	0.53
1:E:16:ALA:HB2	1:E:488:LEU:HD13	1.91	0.53
1:E:246:PHE:O	1:E:249:ILE:HG23	2.08	0.53
1:F:567:GLU:O	1:F:569:GLN:HG3	2.09	0.53
1:F:610:PHE:HB3	1:F:623:PHE:HB2	1.90	0.53
1:F:668:GLU:CD	1:F:668:GLU:H	2.15	0.53
1:F:955:LEU:HD21	1:F:1022:VAL:HA	1.91	0.53
1:A:721:GLN:OE1	1:A:807:GLY:HA3	2.09	0.52
1:B:893:PRO:O	1:B:896:VAL:HG12	2.08	0.52
1:C:450:SER:HB2	1:C:475:VAL:HA	1.90	0.52
1:C:720:PRO:HA	1:C:805:GLU:O	2.09	0.52
1:D:362:PHE:O	1:D:365:THR:HG22	2.08	0.52
1:E:612:VAL:N	1:E:621:ILE:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:401:ALA:O	1:F:404:LEU:N	2.42	0.52
1:F:905:ILE:O	1:F:909:LEU:HB2	2.09	0.52
1:F:939:LEU:HD12	1:F:970:ILE:HG12	1.91	0.52
1:A:53:ASP:O	1:A:56:THR:HB	2.09	0.52
1:A:242:SER:OG	1:A:245:GLU:HG3	2.08	0.52
1:A:563:PHE:C	1:A:564:LEU:HD12	2.34	0.52
1:B:678:GLU:HG2	1:B:814:TYR:CG	2.43	0.52
1:B:904:VAL:HG22	1:B:926:LEU:HD21	1.91	0.52
1:A:453:PHE:CE2	1:A:474:ILE:HD13	2.44	0.52
1:B:115:MET:O	1:B:123:GLN:NE2	2.42	0.52
1:E:563:PHE:O	1:E:564:LEU:HD12	2.09	0.52
1:F:146:ASP:OD2	1:F:320:GLY:HA3	2.10	0.52
1:F:492:LEU:HD13	1:F:496:MET:SD	2.49	0.52
1:F:670:GLY:CA	1:F:857:MET:HG2	2.39	0.52
1:F:721:GLN:OE1	1:F:807:GLY:HA3	2.08	0.52
1:F:932:LEU:HD11	1:F:977:PHE:CE2	2.45	0.52
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.92	0.52
1:A:701:ALA:HB2	1:A:839:MET:HE1	1.90	0.52
1:A:882:CYS:O	1:A:885:ALA:HB3	2.09	0.52
1:B:343:THR:OG1	1:B:984:LEU:HD21	2.10	0.52
1:B:704:HIS:HB2	1:B:708:LEU:HD12	1.91	0.52
1:D:207:ILE:O	1:D:211:ASN:HB3	2.09	0.52
1:D:228:GLN:NE2	1:D:230:LEU:O	2.38	0.52
1:D:723:LYS:HD2	1:F:235:ILE:O	2.09	0.52
1:E:36:PRO:HD2	1:E:38:ILE:HD11	1.92	0.52
1:E:927:LEU:HA	1:E:930:ILE:HD12	1.91	0.52
1:F:61:VAL:HA	1:F:118:LEU:CD2	2.39	0.52
1:F:565:PRO:HG2	1:F:567:GLU:OE2	2.09	0.52
1:B:680:ILE:HD11	1:B:814:TYR:CD2	2.40	0.52
1:C:605:ASN:OD1	1:C:637:ASN:ND2	2.42	0.52
1:C:855:THR:CA	1:C:859:TYR:HB2	2.38	0.52
1:D:963:VAL:HA	1:D:966:ARG:NH2	2.23	0.52
1:F:509:LYS:HG2	1:F:513:PHE:HB2	1.92	0.52
1:A:310:LEU:O	1:A:314:GLU:HG3	2.09	0.52
1:A:948:MET:SD	1:A:955:LEU:HA	2.50	0.52
1:C:465:ALA:HA	1:C:468:ARG:NH1	2.24	0.52
1:C:908:LEU:HD23	1:C:922:PHE:HZ	1.74	0.52
1:D:351:VAL:O	1:D:355:MET:HB2	2.10	0.52
1:E:355:MET:HG2	1:E:365:THR:OG1	2.10	0.52
1:F:597:TYR:CD2	1:F:650:PHE:HZ	2.28	0.52
1:B:578:LEU:HG	1:B:587:THR:OG1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:ILE:HG22	1:B:796:PHE:CE1	2.44	0.52
1:C:966:ARG:NE	1:C:966:ARG:O	2.43	0.52
1:D:426:PRO:HB3	1:D:428:LYS:HZ3	1.74	0.52
1:D:584:GLN:N	1:D:617:GLN:HB3	2.24	0.52
1:E:54:ALA:HB2	1:E:84:SER:HB3	1.90	0.52
1:E:106:GLN:HA	1:E:109:ASN:ND2	2.24	0.52
1:F:939:LEU:HD22	1:F:966:ARG:HD2	1.92	0.52
1:A:453:PHE:CD2	1:A:474:ILE:HG21	2.45	0.52
1:B:327:TYR:HD1	1:B:623:PHE:CE1	2.27	0.52
1:B:690:LEU:HD22	1:B:820:MET:SD	2.50	0.52
1:C:524:THR:O	1:C:527:TYR:HB3	2.09	0.52
1:C:746:GLY:O	1:C:750:GLY:N	2.36	0.52
1:D:184:MET:HA	1:D:184:MET:HE3	1.91	0.52
1:D:360:GLN:NE2	1:D:513:PHE:O	2.43	0.52
1:D:1031:LYS:HG3	1:D:1033:GLU:OE1	2.09	0.52
1:E:343:THR:OG1	1:E:984:LEU:HD21	2.10	0.52
1:E:813:ARG:NH1	1:E:818:PRO:HG3	2.25	0.52
1:F:893:PRO:O	1:F:896:VAL:HG12	2.09	0.52
1:A:184:MET:HE1	1:A:243:THR:OG1	2.10	0.52
1:A:261:LEU:O	1:A:265:VAL:HG13	2.10	0.52
1:A:400:LEU:CD2	1:A:924:VAL:HG12	2.40	0.52
1:C:555:LEU:HD11	1:C:909:LEU:HD12	1.92	0.52
1:D:776:MET:CE	1:F:225:VAL:H	2.23	0.52
1:E:490:PRO:O	1:E:493:CYS:HB2	2.10	0.52
1:F:113:LEU:O	1:F:116:PRO:HD2	2.10	0.52
1:F:571:VAL:HG12	1:F:663:LEU:HD11	1.91	0.52
1:B:578:LEU:HD21	1:B:590:VAL:HG21	1.92	0.52
1:B:631:ASP:C	1:B:633:PRO:HD3	2.34	0.52
1:C:563:PHE:HB2	1:C:861:GLU:HB2	1.90	0.52
1:D:396:PHE:HD1	1:D:921:TYR:CE2	2.28	0.52
1:D:756:ASP:HB3	1:D:763:VAL:HG23	1.91	0.52
1:E:9:PRO:HG2	1:E:10:ILE:HD13	1.92	0.52
1:E:372:VAL:HG23	1:E:373:PRO:CD	2.38	0.52
1:E:457:ALA:HB2	1:E:471:SER:OG	2.10	0.52
1:E:507:GLU:O	1:E:509:LYS:N	2.43	0.52
1:F:944:ALA:O	1:F:948:MET:HE3	2.10	0.52
1:A:836:MET:O	1:A:840:GLU:HG3	2.09	0.51
1:B:68:ASN:CB	1:B:114:ALA:HB2	2.41	0.51
1:C:563:PHE:CE2	1:C:666:ILE:HD11	2.45	0.51
1:D:149:MET:HB2	1:D:153:ASP:HB2	1.90	0.51
1:E:404:LEU:HD12	1:E:932:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:826:ALA:HB2	1:E:835:ALA:HB2	1.91	0.51
1:E:883:LEU:HD13	1:E:896:VAL:HG11	1.91	0.51
1:F:11:PHE:O	1:F:15:ILE:HG13	2.10	0.51
1:A:680:ILE:HD11	1:A:814:TYR:HD2	1.74	0.51
1:A:1013:ALA:C	1:A:1015:PHE:N	2.68	0.51
1:C:146:ASP:O	1:C:148:THR:N	2.43	0.51
1:C:211:ASN:OD1	1:C:240:LEU:N	2.38	0.51
1:C:348:ILE:HG12	1:C:372:VAL:HG11	1.91	0.51
1:C:917:THR:O	1:C:919:ASP:N	2.43	0.51
1:F:182:TYR:HD2	1:F:760:ARG:HH22	1.58	0.51
1:F:616:GLY:HA3	1:F:619:THR:H	1.74	0.51
1:A:184:MET:HB3	1:A:766:VAL:HG13	1.92	0.51
1:A:539:GLY:O	1:A:542:LEU:HB2	2.10	0.51
1:B:575:MET:HE3	1:B:621:ILE:HD12	1.92	0.51
1:B:639:VAL:O	1:B:643:THR:HG23	2.10	0.51
1:C:184:MET:HB2	1:C:757:PHE:CE2	2.45	0.51
1:C:992:SER:HA	1:C:995:GLN:HB2	1.91	0.51
1:E:1030:ARG:HD3	1:E:1030:ARG:N	2.26	0.51
1:F:451:ALA:O	1:F:878:VAL:HG11	2.11	0.51
1:F:555:LEU:HD11	1:F:909:LEU:HD12	1.92	0.51
1:F:561:SER:O	1:F:833:GLY:HA3	2.10	0.51
1:F:1030:ARG:C	1:F:1032:ASN:H	2.18	0.51
1:A:184:MET:HB2	1:A:757:PHE:CE2	2.45	0.51
1:A:236:ALA:O	1:B:723:LYS:NZ	2.43	0.51
1:A:888:GLU:CD	1:C:8:ARG:HB3	2.36	0.51
1:B:605:ASN:O	1:B:627:LYS:N	2.40	0.51
1:B:1032:ASN:CB	1:B:1033:GLU:HB2	2.40	0.51
1:C:839:MET:HA	1:C:842:LEU:HD22	1.91	0.51
1:D:213:GLN:HG2	1:D:239:ARG:HG2	1.92	0.51
1:D:425:LEU:HD23	1:D:429:GLU:HB2	1.92	0.51
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.91	0.51
1:A:677:PHE:CZ	1:A:852:TYR:HB2	2.45	0.51
1:A:892:ILE:HG12	1:A:1025:ARG:HD3	1.93	0.51
1:B:872:TYR:HA	1:B:875:SER:HB3	1.93	0.51
1:D:900:VAL:HB	1:D:901:PRO:HD3	1.92	0.51
1:D:918:ASN:OD1	1:D:923:GLN:NE2	2.38	0.51
1:E:281:PHE:HB2	1:E:610:PHE:CD1	2.46	0.51
1:E:974:SER:HG	1:E:1010:THR:HG21	1.76	0.51
1:E:1031:LYS:HD3	1:E:1035:ILE:HG13	1.93	0.51
1:A:796:PHE:O	1:A:800:SER:OG	2.13	0.51
1:C:251:LEU:HD21	1:C:262:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:919:ASP:OD1	1:C:921:TYR:N	2.43	0.51
1:D:393:LEU:HD13	1:D:466:ILE:HA	1.92	0.51
1:E:647:THR:HG22	1:E:660:ALA:H	1.75	0.51
1:F:188:MET:HE1	1:F:200:PRO:HG3	1.91	0.51
1:F:638:LYS:HG2	1:F:640:GLU:H	1.76	0.51
1:F:694:ARG:HD3	1:F:820:MET:SD	2.50	0.51
1:B:698:LEU:HD21	1:B:713:PRO:HD3	1.92	0.51
1:C:461:GLY:HA3	1:C:863:LEU:HD21	1.92	0.51
1:C:584:GLN:HB2	1:C:617:GLN:HG2	1.92	0.51
1:C:613:ASN:HD22	1:C:614:GLY:N	2.08	0.51
1:C:756:ASP:OD1	1:C:765:LYS:HA	2.11	0.51
1:D:243:THR:HG23	1:D:268:ILE:HG22	1.92	0.51
1:D:435:MET:SD	1:D:490:PRO:HB3	2.50	0.51
1:D:883:LEU:HD22	1:D:896:VAL:HG11	1.92	0.51
1:F:64:VAL:HG13	1:F:117:LEU:HB2	1.93	0.51
1:B:190:PRO:HG3	1:B:774:TYR:HB3	1.92	0.51
1:B:441:ALA:O	1:B:445:ILE:HG23	2.11	0.51
1:C:13:TRP:CZ2	1:C:492:LEU:HD21	2.45	0.51
1:C:588:GLN:O	1:C:592:ASN:ND2	2.43	0.51
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.46	0.51
1:D:41:PRO:HG2	1:D:94:PHE:HB2	1.92	0.51
1:D:94:PHE:CE2	1:D:103:ALA:HB1	2.46	0.51
1:D:251:LEU:HD11	1:D:262:LEU:HA	1.93	0.51
1:D:747:ALA:O	1:D:769:MET:HA	2.11	0.51
1:E:32:VAL:HG22	1:E:298:ASN:HD21	1.75	0.51
1:E:80:SER:HB3	1:E:90:ILE:HG23	1.93	0.51
1:F:211:ASN:CG	1:F:240:LEU:HG	2.36	0.51
1:A:691:THR:HG23	1:A:694:ARG:HH12	1.75	0.51
1:B:7:ASP:CG	1:B:432:ARG:HH21	2.16	0.51
1:C:379:THR:HG23	1:C:476:SER:OG	2.10	0.51
1:C:872:TYR:OH	1:C:923:GLN:HG2	2.10	0.51
1:E:375:VAL:HG13	1:E:480:LEU:HB3	1.92	0.51
1:E:897:MET:O	1:E:900:VAL:HG23	2.11	0.51
1:E:1010:THR:OG1	1:E:1011:VAL:N	2.44	0.51
1:B:372:VAL:O	1:B:375:VAL:N	2.44	0.51
1:B:1015:PHE:HE2	3:B:2100:LMT:H21	1.75	0.51
1:C:663:LEU:H	1:C:663:LEU:CD2	2.24	0.51
1:C:939:LEU:HD12	1:C:970:ILE:HG12	1.91	0.51
1:D:33:ALA:HA	1:D:300:LEU:HD13	1.92	0.51
1:D:418:ARG:CZ	1:D:965:MET:HE2	2.41	0.51
1:D:578:LEU:HB2	1:D:618:ASN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:796:PHE:HA	1:D:799:PHE:CE2	2.46	0.51
1:F:112:GLN:OE1	1:F:115:MET:HE2	2.11	0.51
1:A:35:TYR:OH	1:A:564:LEU:HD23	2.11	0.50
1:A:388:PHE:CE2	1:A:472:ILE:HD13	2.46	0.50
1:B:459:PHE:HB3	1:B:464:GLY:HA2	1.93	0.50
1:C:110:LYS:O	1:C:113:LEU:HB2	2.11	0.50
1:C:977:PHE:HD2	1:C:1006:MET:HG2	1.75	0.50
1:D:485:ALA:HA	1:D:489:THR:HB	1.92	0.50
1:D:977:PHE:HD2	1:D:1006:MET:HG3	1.76	0.50
1:E:310:LEU:HD23	1:E:323:ILE:HG21	1.92	0.50
1:E:459:PHE:CD2	1:E:871:LEU:HD12	2.46	0.50
1:E:610:PHE:HB3	1:E:623:PHE:HB3	1.92	0.50
1:A:982:MET:SD	1:A:1003:MET:HE1	2.51	0.50
1:B:31:PRO:HB2	1:B:389:SER:HB2	1.93	0.50
1:B:351:VAL:HG22	1:B:976:ALA:HB1	1.94	0.50
1:C:35:TYR:HE1	1:C:665:ALA:HB1	1.76	0.50
1:C:100:ALA:HB2	1:C:295:THR:HG21	1.93	0.50
1:C:631:ASP:C	1:C:633:PRO:HD3	2.36	0.50
1:D:210:GLN:NE2	1:D:250:LEU:HB3	2.27	0.50
1:D:540:ARG:HG3	1:D:541:TYR:HD1	1.75	0.50
1:D:894:PHE:HA	1:D:897:MET:HE2	1.93	0.50
1:E:200:PRO:HD2	1:E:744:THR:HG22	1.92	0.50
1:F:675:PHE:HB2	1:F:854:TRP:CZ3	2.46	0.50
1:A:31:PRO:HB2	1:A:389:SER:CB	2.40	0.50
1:B:1032:ASN:CA	1:B:1033:GLU:HB2	2.41	0.50
1:C:83:ASP:HB2	1:C:87:THR:O	2.11	0.50
1:C:465:ALA:O	1:C:468:ARG:HB3	2.11	0.50
1:C:1032:ASN:HB3	1:C:1033:GLU:HA	1.94	0.50
1:D:462:SER:O	1:D:466:ILE:HG12	2.11	0.50
1:D:982:MET:HB3	1:D:983:PRO:HD3	1.94	0.50
1:E:532:GLY:O	1:E:535:LEU:N	2.45	0.50
1:F:608:SER:OG	1:F:625:SER:HB3	2.11	0.50
1:F:770:SER:HB3	1:F:775:ARG:HD3	1.94	0.50
1:A:354:VAL:HG21	1:A:975:LEU:HB3	1.92	0.50
1:B:3:ASN:HA	1:B:6:ILE:HD13	1.94	0.50
1:B:300:LEU:HD11	1:B:333:VAL:HG12	1.93	0.50
1:B:534:ILE:HG13	1:B:535:LEU:N	2.27	0.50
1:B:576:VAL:HG22	1:B:658:VAL:HG22	1.93	0.50
1:B:952:GLY:O	1:B:1035:ILE:HG13	2.12	0.50
1:C:948:MET:HE2	1:C:958:ALA:HB3	1.92	0.50
1:E:149:MET:HB2	1:E:153:ASP:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ILE:HG12	1:E:268:ILE:HG12	1.93	0.50
1:E:1021:PHE:HD2	1:E:1021:PHE:O	1.95	0.50
1:F:184:MET:HB2	1:F:757:PHE:CE2	2.47	0.50
1:F:409:ALA:O	1:F:413:VAL:HG23	2.12	0.50
1:F:900:VAL:HB	1:F:901:PRO:HD3	1.92	0.50
1:A:579:PRO:HD3	1:A:656:ALA:CB	2.34	0.50
1:A:884:ALA:N	1:A:893:PRO:HG3	2.26	0.50
1:C:905:ILE:O	1:C:909:LEU:HB2	2.12	0.50
1:E:415:ASN:HB3	1:E:434:SER:HB2	1.92	0.50
1:F:156:ASP:OD1	1:F:760:ARG:NH2	2.45	0.50
1:F:187:TRP:HE3	1:F:770:SER:O	1.94	0.50
1:F:344:LEU:HD22	1:F:402:ILE:HD11	1.93	0.50
1:F:388:PHE:HD1	1:F:469:GLN:HE22	1.58	0.50
1:F:415:ASN:HB3	1:F:434:SER:HB2	1.92	0.50
1:F:772:ALA:O	1:F:776:MET:HE3	2.11	0.50
1:F:936:ASN:ND2	1:F:1010:THR:HG22	2.26	0.50
1:A:790:ASP:OD2	1:A:792:GLN:HG3	2.11	0.50
1:B:105:VAL:HG21	1:C:105:VAL:HG13	1.94	0.50
1:B:106:GLN:HA	1:B:109:ASN:HD21	1.77	0.50
1:B:294:ALA:HB3	1:B:297:ALA:HB2	1.94	0.50
1:B:796:PHE:CD1	1:B:799:PHE:HE2	2.30	0.50
1:C:942:GLU:HG3	1:C:943:PHE:N	2.26	0.50
1:D:509:LYS:HG2	1:D:510:LYS:HG3	1.93	0.50
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.46	0.50
1:D:836:MET:O	1:D:840:GLU:HG3	2.12	0.50
1:F:363:ARG:HE	1:F:498:LYS:HD2	1.76	0.50
1:F:453:PHE:O	1:F:471:SER:OG	2.30	0.50
1:A:602:GLU:OE2	1:A:645:ARG:NH1	2.45	0.50
1:A:776:MET:HE3	1:C:228:GLN:OE1	2.11	0.50
1:B:525:HIS:O	1:B:526:HIS:C	2.53	0.50
1:B:759:ASP:OD1	1:B:760:ARG:HG3	2.11	0.50
1:C:358:PHE:O	1:C:359:LEU:HD23	2.12	0.50
1:D:485:ALA:O	1:D:490:PRO:HD3	2.10	0.50
1:F:572:PHE:HD1	1:F:661:PHE:O	1.94	0.50
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.19	0.50
1:A:324:VAL:HG12	1:A:326:PRO:HD3	1.94	0.50
1:A:350:LEU:HD13	1:A:980:GLY:HA2	1.93	0.50
1:A:891:SER:OG	1:A:1028:PHE:HB2	2.12	0.50
1:B:424:GLY:HA3	1:B:502:LYS:HB2	1.93	0.50
1:B:897:MET:O	1:B:900:VAL:HG23	2.12	0.50
1:B:1010:THR:OG1	1:B:1011:VAL:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:CYS:HA	1:C:497:LEU:HB2	1.93	0.50
1:D:940:ILE:HD13	1:D:963:VAL:HG23	1.93	0.50
1:E:520:PHE:O	1:E:524:THR:HG22	2.12	0.50
1:E:578:LEU:HB2	1:E:618:ASN:O	2.11	0.50
1:A:190:PRO:HG3	1:A:784:TRP:CH2	2.46	0.50
1:A:404:LEU:HD21	1:A:449:LEU:HD22	1.94	0.50
1:A:893:PRO:O	1:A:896:VAL:HG13	2.12	0.50
1:A:1033:GLU:H	1:A:1035:ILE:HG13	1.77	0.50
1:B:469:GLN:O	1:B:473:THR:OG1	2.29	0.50
1:B:644:MET:HE3	1:B:644:MET:O	2.11	0.50
1:B:667:VAL:HB	1:B:668:GLU:OE2	2.12	0.50
1:C:34:GLN:CG	1:C:333:VAL:HG22	2.42	0.50
1:C:525:HIS:O	1:C:526:HIS:C	2.53	0.50
1:D:281:PHE:CE1	1:D:608:SER:HB2	2.46	0.50
1:D:400:LEU:CD2	1:D:924:VAL:HG12	2.41	0.50
1:D:448:VAL:HG13	1:D:879:VAL:HG22	1.94	0.50
1:D:785:TYR:HB3	1:D:793:MET:HB3	1.93	0.50
1:E:647:THR:HG23	1:E:660:ALA:HB3	1.93	0.50
1:E:966:ARG:C	1:E:969:PRO:HD2	2.37	0.50
1:F:2:PRO:O	1:F:5:PHE:HB3	2.12	0.50
1:F:139:VAL:O	1:F:326:PRO:HD2	2.12	0.50
1:A:445:ILE:CD1	1:A:935:LYS:HE3	2.36	0.49
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.94	0.49
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.93	0.49
1:D:225:VAL:H	1:E:776:MET:CE	2.25	0.49
1:E:440:GLY:O	1:E:886:LEU:HD11	2.12	0.49
1:F:121:GLU:O	1:F:124:GLN:HG2	2.12	0.49
1:F:239:ARG:NH1	1:F:756:ASP:H	2.10	0.49
1:F:573:MET:SD	1:F:623:PHE:HD1	2.34	0.49
1:F:896:VAL:HG23	1:F:937:ALA:CB	2.40	0.49
1:F:963:VAL:O	1:F:967:LEU:HB2	2.11	0.49
1:A:535:LEU:CD2	1:A:1022:VAL:HG21	2.41	0.49
1:A:776:MET:CE	1:C:225:VAL:H	2.26	0.49
1:B:340:VAL:HG22	1:B:396:PHE:CE1	2.45	0.49
1:B:899:VAL:HG21	1:B:937:ALA:HB2	1.93	0.49
1:B:1013:ALA:C	1:B:1015:PHE:H	2.19	0.49
1:C:1010:THR:C	1:C:1012:LEU:H	2.20	0.49
1:D:210:GLN:NE2	1:D:250:LEU:H	2.08	0.49
1:D:277:ILE:HG12	1:D:614:GLY:HA3	1.92	0.49
1:D:672:ALA:O	1:D:832:THR:OG1	2.26	0.49
1:D:990:ALA:O	1:D:992:SER:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1006:MET:O	1:D:1010:THR:HG23	2.12	0.49
1:E:190:PRO:HG3	1:E:774:TYR:HB3	1.93	0.49
1:E:485:ALA:HA	1:E:489:THR:OG1	2.11	0.49
1:E:657:MET:HA	1:E:657:MET:HE3	1.93	0.49
1:A:959:THR:HG21	1:A:1022:VAL:HG22	1.93	0.49
1:B:564:LEU:CD1	1:B:666:ILE:HD12	2.42	0.49
1:B:573:MET:HB2	1:B:661:PHE:CE2	2.47	0.49
1:B:746:GLY:O	1:B:748:ALA:N	2.46	0.49
1:C:588:GLN:HG3	1:C:592:ASN:HD21	1.77	0.49
1:D:210:GLN:HE22	1:D:250:LEU:N	2.10	0.49
1:D:356:TYR:C	1:D:358:PHE:H	2.20	0.49
1:D:632:ARG:HD2	1:D:637:ASN:O	2.12	0.49
1:E:1013:ALA:C	1:E:1015:PHE:H	2.20	0.49
1:F:602:GLU:HB3	1:F:606:VAL:HG23	1.94	0.49
1:A:687:HIS:HE2	1:A:718:ASP:CG	2.20	0.49
1:A:900:VAL:O	1:A:904:VAL:HG23	2.12	0.49
1:B:447:MET:HB3	1:B:882:CYS:SG	2.52	0.49
1:B:922:PHE:O	1:B:926:LEU:HB2	2.12	0.49
1:D:72:ILE:HG23	1:D:106:GLN:CB	2.41	0.49
1:D:452:VAL:HG12	1:D:875:SER:OG	2.12	0.49
1:D:945:LYS:NZ	1:D:1025:ARG:HH21	2.10	0.49
1:E:4:PHE:CE1	1:E:8:ARG:NE	2.80	0.49
1:E:189:ASN:HB3	1:E:192:GLU:HB2	1.95	0.49
1:E:445:ILE:HG21	1:E:935:LYS:HD2	1.92	0.49
1:E:653:ILE:HG13	1:E:654:LYS:HD2	1.94	0.49
1:E:675:PHE:C	1:E:675:PHE:CD1	2.90	0.49
1:E:927:LEU:HD23	1:E:930:ILE:HD12	1.94	0.49
1:A:475:VAL:O	1:A:478:MET:HB3	2.12	0.49
1:B:16:ALA:O	1:B:20:MET:HG3	2.12	0.49
1:C:13:TRP:CE3	1:C:13:TRP:HA	2.46	0.49
1:D:770:SER:OG	1:D:775:ARG:HG2	2.12	0.49
1:E:145:THR:OG1	1:E:320:GLY:O	2.30	0.49
1:E:953:LYS:O	1:E:1035:ILE:HD13	2.13	0.49
1:E:1032:ASN:H	1:E:1032:ASN:ND2	2.10	0.49
1:F:679:LEU:HD22	1:F:822:ILE:HD11	1.92	0.49
1:F:855:THR:CA	1:F:859:TYR:HB2	2.42	0.49
1:F:880:PHE:HB2	1:F:897:MET:SD	2.53	0.49
1:A:347:ALA:HA	1:A:350:LEU:HD12	1.94	0.49
1:A:954:GLY:HA2	1:A:1033:GLU:HA	1.93	0.49
1:A:955:LEU:HD23	1:A:1026:ARG:CZ	2.42	0.49
1:A:1025:ARG:NH1	1:A:1028:PHE:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:MET:HE3	1:B:95:GLU:HA	1.94	0.49
1:B:673:THR:HA	1:B:832:THR:OG1	2.12	0.49
1:B:706:ASP:O	1:B:830:LYS:HD3	2.12	0.49
1:B:790:ASP:OD2	1:B:791:GLY:N	2.45	0.49
1:C:250:LEU:HD13	1:C:259:ARG:HD2	1.92	0.49
3:D:1102:LMT:H31	3:D:1102:LMT:O2'	2.13	0.49
1:E:259:ARG:H	1:E:259:ARG:HD3	1.77	0.49
1:E:527:TYR:CZ	1:E:967:LEU:HD23	2.47	0.49
1:E:568:ASP:O	1:E:629:TRP:HZ3	1.95	0.49
1:F:3:ASN:HD22	1:F:435:MET:HG3	1.77	0.49
1:F:165:ALA:HB3	1:F:313:MET:HE1	1.93	0.49
1:F:363:ARG:HH21	1:F:498:LYS:HD2	1.77	0.49
1:F:509:LYS:HE2	1:F:513:PHE:CD1	2.48	0.49
1:F:1031:LYS:O	1:F:1031:LYS:HD3	2.12	0.49
1:A:584:GLN:N	1:A:617:GLN:HB3	2.27	0.49
1:B:280:GLU:HG2	1:B:283:GLY:O	2.12	0.49
1:B:355:MET:HE2	1:B:972:MET:SD	2.52	0.49
1:B:728:GLN:HE22	1:B:738:ILE:HG21	1.78	0.49
1:C:687:HIS:NE2	1:C:718:ASP:OD1	2.32	0.49
1:D:190:PRO:HG3	1:D:784:TRP:CZ2	2.48	0.49
1:D:872:TYR:CD1	3:D:1103:LMT:H92	2.48	0.49
1:E:354:VAL:O	1:E:358:PHE:HB2	2.12	0.49
1:E:1010:THR:C	1:E:1012:LEU:H	2.21	0.49
1:A:151:GLN:OE1	1:A:278:ILE:HG22	2.13	0.49
1:A:356:TYR:O	1:A:360:GLN:N	2.41	0.49
1:A:455:PRO:HG2	1:A:875:SER:HB2	1.94	0.49
1:A:910:ALA:HB2	1:A:1004:GLY:HA3	1.94	0.49
3:A:1102:LMT:H52	3:A:1102:LMT:H82	1.56	0.49
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.48	0.49
1:C:453:PHE:HZ	1:C:928:THR:OG1	1.96	0.49
1:C:556:PHE:HD1	1:C:908:LEU:HD21	1.77	0.49
1:C:579:PRO:HD3	1:C:656:ALA:HB2	1.93	0.49
1:D:275:TYR:CD1	1:F:223:PRO:HD3	2.47	0.49
1:D:670:GLY:HA2	1:D:857:MET:HE3	1.94	0.49
1:E:169:THR:HG21	1:E:306:ILE:CG1	2.41	0.49
1:E:903:GLY:O	1:E:1005:GLY:HA2	2.12	0.49
1:E:1006:MET:O	1:E:1010:THR:HG23	2.13	0.49
1:F:368:PRO:O	1:F:371:ALA:HB3	2.13	0.49
1:F:504:ASP:C	1:F:506:GLY:H	2.18	0.49
1:A:131:LYS:HB2	1:A:295:THR:HB	1.95	0.49
1:A:251:LEU:HD21	1:A:262:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:GLY:O	1:A:1036:GLU:N	2.44	0.49
1:C:27:ILE:HA	1:C:30:LEU:HD22	1.94	0.49
1:C:532:GLY:O	1:C:535:LEU:N	2.46	0.49
1:C:653:ILE:HG13	1:C:654:LYS:HE2	1.95	0.49
1:C:940:ILE:HA	1:C:966:ARG:NH1	2.27	0.49
1:D:187:TRP:HH2	1:F:223:PRO:CD	2.26	0.49
1:D:362:PHE:CD1	1:D:362:PHE:N	2.80	0.49
1:D:567:GLU:O	1:D:569:GLN:HG3	2.13	0.49
1:D:1034:ASP:HA	1:D:1035:ILE:C	2.37	0.49
1:E:246:PHE:O	1:E:262:LEU:HD23	2.12	0.49
1:F:747:ALA:O	1:F:769:MET:HA	2.13	0.49
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.48	0.49
1:A:404:LEU:HD12	1:A:932:LEU:CD2	2.43	0.49
1:B:748:ALA:O	1:B:770:SER:HB3	2.13	0.49
1:B:1032:ASN:OD1	1:B:1033:GLU:HB2	2.12	0.49
1:B:1035:ILE:HG13	1:B:1036:GLU:N	2.28	0.49
1:C:230:LEU:HG	1:C:231:ASN:N	2.28	0.49
1:C:935:LYS:NZ	1:C:936:ASN:OD1	2.38	0.49
1:D:452:VAL:HG23	1:D:453:PHE:CD1	2.47	0.49
1:D:667:VAL:HB	1:D:668:GLU:CD	2.38	0.49
1:D:720:PRO:HA	1:D:805:GLU:O	2.13	0.49
1:D:872:TYR:CD2	3:D:1103:LMT:H111	2.48	0.49
1:E:187:TRP:HA	1:E:769:MET:O	2.13	0.49
1:E:446:ALA:CB	1:E:482:VAL:HG21	2.38	0.49
1:E:978:ILE:HD13	1:E:1007:VAL:HG22	1.95	0.49
1:F:943:PHE:HD2	1:F:965:MET:HE3	1.77	0.49
1:A:357:LEU:HD23	1:A:358:PHE:CD1	2.47	0.48
1:C:160:ALA:HB1	1:C:762:ARG:HD3	1.95	0.48
1:C:368:PRO:O	1:C:371:ALA:HB3	2.13	0.48
1:D:1033:GLU:OE1	1:D:1035:ILE:HG23	2.12	0.48
1:E:988:THR:HG22	1:E:989:GLY:H	1.78	0.48
1:A:573:MET:HG3	1:A:661:PHE:CE1	2.49	0.48
1:B:902:LEU:HG	1:B:1012:LEU:HD23	1.94	0.48
1:C:58:GLN:OE1	1:C:811:LEU:HB3	2.13	0.48
1:C:598:TYR:CE2	1:C:624:VAL:HG21	2.48	0.48
1:D:101:ASP:OD1	1:D:101:ASP:N	2.46	0.48
1:D:279:ALA:HB3	1:D:286:ALA:O	2.13	0.48
1:D:401:ALA:O	1:D:405:LEU:HG	2.13	0.48
1:D:437:GLN:O	1:D:437:GLN:NE2	2.46	0.48
1:D:574:THR:HG23	1:D:622:ALA:HB3	1.95	0.48
1:D:776:MET:HB3	1:F:228:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:438:ILE:O	1:E:441:ALA:HB3	2.13	0.48
1:E:631:ASP:OD1	1:E:631:ASP:N	2.45	0.48
1:F:540:ARG:HG3	1:F:541:TYR:HD1	1.78	0.48
1:F:883:LEU:CD2	1:F:938:ILE:HD11	2.43	0.48
1:F:900:VAL:HG13	1:F:930:ILE:HG23	1.96	0.48
1:F:985:VAL:HG13	1:F:1000:THR:OG1	2.13	0.48
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.48	0.48
1:A:535:LEU:HD21	1:A:1022:VAL:HG21	1.96	0.48
1:A:784:TRP:HB2	1:A:796:PHE:CD2	2.48	0.48
1:A:794:VAL:HG12	1:A:798:ALA:HB3	1.95	0.48
1:A:926:LEU:O	1:A:930:ILE:HG13	2.13	0.48
1:C:227:GLY:O	1:C:229:GLN:HG3	2.12	0.48
1:C:876:LEU:HD21	1:C:930:ILE:HD13	1.95	0.48
1:D:211:ASN:O	1:D:755:ASN:ND2	2.44	0.48
1:D:350:LEU:HD13	1:D:979:LEU:C	2.39	0.48
1:D:984:LEU:O	1:D:996:ASN:ND2	2.40	0.48
1:E:977:PHE:CD2	1:E:1006:MET:HG3	2.49	0.48
1:F:63:GLN:HG2	1:F:67:GLN:OE1	2.13	0.48
1:F:455:PRO:HB3	1:F:874:ILE:CG2	2.42	0.48
1:C:185:ARG:HB3	1:C:187:TRP:NE1	2.27	0.48
1:C:900:VAL:O	1:C:904:VAL:HG23	2.14	0.48
1:D:380:PHE:CE2	1:D:398:MET:HE3	2.48	0.48
1:D:549:VAL:O	1:D:552:MET:HB3	2.14	0.48
1:D:1011:VAL:O	1:D:1012:LEU:HD12	2.14	0.48
1:E:201:VAL:HG22	1:E:743:THR:OG1	2.13	0.48
1:F:506:GLY:C	1:F:508:GLY:H	2.18	0.48
1:F:509:LYS:HE2	1:F:513:PHE:HB2	1.94	0.48
1:F:714:ASN:HB3	1:F:821:GLU:HB3	1.95	0.48
1:A:508:GLY:H	1:A:518:ARG:HG3	1.77	0.48
1:B:239:ARG:HD3	1:B:756:ASP:O	2.13	0.48
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.48	0.48
1:C:247:GLY:C	1:C:249:ILE:H	2.21	0.48
1:C:697:LEU:HD21	1:C:839:MET:HE1	1.93	0.48
1:D:270:LEU:HD21	1:D:759:ASP:OD1	2.14	0.48
1:D:631:ASP:C	1:D:633:PRO:HD3	2.38	0.48
1:D:673:THR:HB	1:D:826:ALA:H	1.78	0.48
1:D:674:GLY:HA2	1:D:825:GLN:HG2	1.96	0.48
1:D:981:VAL:HG21	1:D:1002:VAL:HG11	1.95	0.48
1:E:839:MET:HA	1:E:839:MET:HE2	1.95	0.48
1:E:883:LEU:HD13	1:E:896:VAL:CG1	2.43	0.48
1:E:910:ALA:HB2	1:E:1004:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:560:PRO:O	1:F:917:THR:OG1	2.20	0.48
1:A:360:GLN:OE1	1:A:513:PHE:HB3	2.14	0.48
1:A:530:SER:CB	3:A:1102:LMT:O2'	2.56	0.48
1:A:738:ILE:HA	1:A:741:ILE:HG13	1.95	0.48
1:B:188:MET:HA	1:B:266:ALA:CB	2.43	0.48
1:B:231:ASN:OD1	1:C:617:GLN:NE2	2.47	0.48
1:B:573:MET:SD	1:B:623:PHE:HD1	2.36	0.48
1:B:1017:VAL:N	1:B:1018:PRO:HD2	2.28	0.48
1:D:343:THR:HG22	1:D:344:LEU:HD23	1.95	0.48
1:D:400:LEU:HA	1:D:400:LEU:HD12	1.46	0.48
1:E:102:ILE:O	1:E:105:VAL:HG12	2.13	0.48
1:E:992:SER:HA	1:E:995:GLN:HB2	1.95	0.48
1:F:251:LEU:HD21	1:F:262:LEU:HB2	1.95	0.48
1:F:318:PRO:HG2	1:F:321:LEU:HG	1.95	0.48
1:F:579:PRO:HD3	1:F:656:ALA:HB2	1.95	0.48
1:F:939:LEU:HB3	1:F:966:ARG:CD	2.44	0.48
1:F:974:SER:OG	1:F:1010:THR:HG21	2.13	0.48
1:B:936:ASN:ND2	1:B:970:ILE:HG23	2.29	0.48
1:D:884:ALA:HA	1:D:889:SER:O	2.14	0.48
1:E:225:VAL:HG13	1:F:776:MET:SD	2.54	0.48
1:E:281:PHE:CE1	1:E:608:SER:HB2	2.49	0.48
1:F:80:SER:OG	1:F:90:ILE:HG23	2.13	0.48
1:F:183:ALA:O	1:F:270:LEU:HD12	2.13	0.48
1:F:521:GLU:O	1:F:524:THR:HG23	2.13	0.48
1:A:187:TRP:HE3	1:A:770:SER:O	1.97	0.48
1:A:393:LEU:HD22	1:A:470:PHE:CE1	2.49	0.48
1:A:575:MET:HE2	1:A:575:MET:HB2	1.77	0.48
1:B:154:ILE:HG22	1:B:287:SER:HB3	1.96	0.48
1:B:281:PHE:HE1	1:B:608:SER:HB2	1.79	0.48
1:B:770:SER:HG	1:B:775:ARG:HG2	1.78	0.48
1:C:200:PRO:HB2	1:C:744:THR:HG22	1.96	0.48
1:C:422:GLU:O	1:C:502:LYS:HG3	2.14	0.48
1:C:559:LEU:HG	1:C:560:PRO:HD2	1.96	0.48
1:D:251:LEU:HD21	1:D:262:LEU:HB2	1.96	0.48
1:D:344:LEU:HD21	1:D:399:VAL:HG22	1.96	0.48
1:F:351:VAL:HG12	1:F:355:MET:HE2	1.95	0.48
1:F:459:PHE:CE1	1:F:871:LEU:HG	2.49	0.48
1:F:463:THR:HG22	1:F:467:TYR:CZ	2.48	0.48
1:F:939:LEU:O	1:F:966:ARG:NH1	2.47	0.48
1:A:184:MET:HG2	1:A:246:PHE:CE2	2.49	0.48
1:A:549:VAL:O	1:A:552:MET:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:THR:HG21	1:A:830:LYS:O	2.14	0.48
1:B:36:PRO:O	1:B:38:ILE:HG13	2.14	0.48
1:B:948:MET:HE3	1:B:948:MET:HB2	1.65	0.48
1:D:25:LEU:HA	1:D:28:LEU:HD12	1.95	0.48
1:D:110:LYS:HD3	1:D:110:LYS:HA	1.58	0.48
1:D:356:TYR:C	1:D:358:PHE:N	2.72	0.48
1:E:564:LEU:CD1	1:E:666:ILE:HD12	2.43	0.48
1:F:138:MET:HE1	1:F:325:TYR:HD2	1.79	0.48
1:F:149:MET:HG3	1:F:154:ILE:HG13	1.96	0.48
1:F:631:ASP:C	1:F:633:PRO:HD3	2.38	0.48
1:F:642:ILE:HA	1:F:645:ARG:NH1	2.29	0.48
1:F:1006:MET:O	1:F:1009:ALA:HB3	2.14	0.48
1:A:125:GLN:OE1	1:A:765:LYS:HE3	2.13	0.48
1:A:186:ILE:HG12	1:A:268:ILE:HG12	1.96	0.48
1:A:757:PHE:HE1	1:A:759:ASP:HB2	1.78	0.48
1:B:144:ASN:ND2	1:B:149:MET:HE3	2.29	0.48
1:B:708:LEU:HD22	1:B:839:MET:HE3	1.95	0.48
1:C:966:ARG:HB3	1:C:966:ARG:NH1	2.28	0.48
1:D:17:ILE:CG2	1:E:881:LEU:HD21	2.44	0.48
1:D:228:GLN:OE1	1:E:776:MET:HE3	2.14	0.48
1:E:796:PHE:O	1:E:800:SER:OG	2.19	0.48
1:F:455:PRO:HG2	1:F:875:SER:HA	1.96	0.48
1:F:951:GLU:O	1:F:953:LYS:N	2.47	0.48
1:A:687:HIS:O	1:A:691:THR:OG1	2.20	0.47
1:A:859:TYR:O	1:A:863:LEU:HG	2.14	0.47
1:B:116:PRO:HA	1:B:123:GLN:HE22	1.78	0.47
1:B:423:GLU:OE1	1:B:433:LYS:HE3	2.14	0.47
1:B:534:ILE:HD11	1:B:1019:VAL:HG21	1.96	0.47
1:B:1021:PHE:O	1:B:1025:ARG:HB2	2.13	0.47
1:C:356:TYR:C	1:C:358:PHE:N	2.59	0.47
1:C:372:VAL:HB	1:C:373:PRO:CD	2.44	0.47
1:C:575:MET:HA	1:C:621:ILE:HG13	1.96	0.47
1:C:795:PRO:HG2	1:C:798:ALA:HB2	1.96	0.47
1:D:213:GLN:HA	1:D:237:GLN:O	2.14	0.47
1:D:532:GLY:HA2	1:D:535:LEU:HB2	1.96	0.47
1:D:895:SER:HA	1:D:1020:PHE:HB3	1.96	0.47
1:E:367:ILE:HD11	1:E:497:LEU:HD13	1.96	0.47
1:F:274:ASN:OD1	1:F:276:ASP:N	2.42	0.47
1:F:725:ASP:OD1	1:F:803:ARG:NH2	2.43	0.47
1:F:1020:PHE:O	1:F:1024:VAL:HG23	2.14	0.47
1:A:140:VAL:N	1:A:289:LEU:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:MET:HE1	1:A:200:PRO:HG3	1.96	0.47
1:A:330:THR:HB	1:A:331:PRO:HD3	1.95	0.47
1:A:344:LEU:HD11	1:A:398:MET:CB	2.44	0.47
1:A:429:GLU:H	1:A:429:GLU:CD	2.22	0.47
1:A:527:TYR:O	1:A:531:VAL:HG23	2.13	0.47
1:B:796:PHE:O	1:B:800:SER:OG	2.31	0.47
1:C:343:THR:HG21	1:C:984:LEU:CD2	2.34	0.47
1:C:715:GLY:HA2	1:C:810:ARG:NH2	2.29	0.47
1:D:826:ALA:HB2	1:D:835:ALA:HB2	1.95	0.47
1:D:927:LEU:HA	1:D:930:ILE:HD12	1.95	0.47
1:E:515:TRP:O	1:E:519:MET:HG3	2.13	0.47
1:E:677:PHE:CE1	1:E:852:TYR:HB2	2.49	0.47
1:E:746:GLY:O	1:E:750:GLY:N	2.43	0.47
1:F:45:ILE:HD12	1:F:90:ILE:HB	1.96	0.47
1:F:402:ILE:O	1:F:406:VAL:HG22	2.14	0.47
1:F:472:ILE:HG23	1:F:473:THR:N	2.29	0.47
1:F:555:LEU:HB3	1:F:908:LEU:HB3	1.95	0.47
1:F:737:SER:O	1:F:740:ASP:HB2	2.14	0.47
1:F:775:ARG:O	1:F:776:MET:HE2	2.14	0.47
1:A:17:ILE:CG2	1:B:881:LEU:HD21	2.43	0.47
1:B:1010:THR:C	1:B:1012:LEU:N	2.72	0.47
1:C:565:PRO:HG2	1:C:567:GLU:OE2	2.14	0.47
1:D:41:PRO:HD2	1:D:94:PHE:O	2.14	0.47
1:D:522:LYS:O	1:D:525:HIS:HB3	2.15	0.47
1:D:530:SER:OG	3:D:1102:LMT:H1'	2.14	0.47
1:E:310:LEU:HG	1:E:323:ILE:HG13	1.96	0.47
1:F:3:ASN:HD21	1:F:439:GLN:HG3	1.80	0.47
1:F:137:LEU:HD11	1:F:303:ALA:HB2	1.96	0.47
1:F:242:SER:O	1:F:246:PHE:HD1	1.96	0.47
1:F:369:THR:O	1:F:373:PRO:HD2	2.14	0.47
1:A:902:LEU:HD21	1:A:1016:PHE:HB2	1.96	0.47
1:B:165:ALA:HB3	1:B:313:MET:CE	2.41	0.47
1:B:515:TRP:O	1:B:519:MET:HG3	2.14	0.47
1:C:146:ASP:OD2	1:C:320:GLY:HA3	2.15	0.47
1:C:171:GLY:O	1:C:293:LEU:HD23	2.14	0.47
1:D:216:ALA:HB1	1:D:234:ILE:HG22	1.96	0.47
1:D:504:ASP:C	1:D:506:GLY:H	2.22	0.47
1:D:1028:PHE:O	1:D:1029:SER:HB2	2.15	0.47
1:E:675:PHE:CE2	1:E:839:MET:HG3	2.48	0.47
1:E:932:LEU:HA	1:E:932:LEU:HD23	1.51	0.47
1:F:376:LEU:HD22	1:F:398:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASP:OD2	1:A:182:TYR:OH	2.32	0.47
1:A:210:GLN:NE2	1:A:250:LEU:H	2.09	0.47
1:A:379:THR:OG1	1:A:477:ALA:HA	2.14	0.47
1:B:5:PHE:C	1:B:8:ARG:H	2.22	0.47
1:B:32:VAL:HG22	1:B:298:ASN:ND2	2.30	0.47
1:B:555:LEU:HB3	1:B:908:LEU:HB3	1.95	0.47
1:D:941:VAL:HG13	1:D:1021:PHE:CE1	2.49	0.47
1:E:5:PHE:CE1	1:E:487:ILE:HG12	2.50	0.47
1:E:948:MET:HE2	1:E:958:ALA:HB3	1.97	0.47
1:F:311:ALA:O	1:F:314:GLU:HB2	2.14	0.47
1:F:564:LEU:HD23	1:F:665:ALA:HB3	1.95	0.47
1:F:685:LEU:HD22	1:F:689:LYS:NZ	2.30	0.47
1:A:76:MET:HE2	1:A:859:TYR:HE2	1.79	0.47
1:A:900:VAL:HB	1:A:901:PRO:HD3	1.97	0.47
1:A:1015:PHE:HE2	3:A:1102:LMT:H21	1.79	0.47
1:B:956:ILE:H	1:B:956:ILE:HG13	1.49	0.47
1:C:211:ASN:CG	1:C:240:LEU:HG	2.39	0.47
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.50	0.47
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.96	0.47
1:D:188:MET:HE1	1:D:200:PRO:HG3	1.96	0.47
1:D:353:LEU:HD22	1:D:353:LEU:HA	1.70	0.47
1:D:948:MET:HE2	1:D:958:ALA:HB3	1.96	0.47
1:D:1027:ARG:O	1:D:1028:PHE:HB2	2.15	0.47
1:E:250:LEU:HD13	1:E:261:LEU:HD23	1.96	0.47
1:E:352:PHE:CE1	1:E:365:THR:HG23	2.50	0.47
1:F:382:VAL:HG11	1:F:476:SER:CB	2.44	0.47
1:F:935:LYS:NZ	1:F:973:THR:HG21	2.30	0.47
1:A:221:GLY:HA3	1:B:775:ARG:HH12	1.79	0.47
1:A:449:LEU:O	1:A:453:PHE:HD1	1.97	0.47
1:A:763:VAL:HG12	1:B:63:GLN:OE1	2.15	0.47
1:A:962:ALA:O	1:A:965:MET:HG2	2.15	0.47
1:B:137:LEU:HD12	1:B:329:THR:HG22	1.96	0.47
1:B:520:PHE:O	1:B:524:THR:HG22	2.14	0.47
1:B:932:LEU:O	1:B:933:SER:C	2.58	0.47
1:B:944:ALA:O	1:B:948:MET:HE3	2.14	0.47
1:C:587:THR:HG21	1:C:618:ASN:HA	1.96	0.47
1:C:722:PHE:HD1	1:C:804:TRP:CD2	2.33	0.47
1:C:739:ASN:O	1:C:742:ASN:HB2	2.14	0.47
1:C:918:ASN:ND2	1:C:918:ASN:O	2.41	0.47
1:D:21:LEU:HD13	1:D:21:LEU:HA	1.74	0.47
1:D:166:ILE:HD13	1:D:309:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:PHE:HD2	1:D:353:LEU:HD23	1.80	0.47
1:D:356:TYR:O	1:D:360:GLN:N	2.42	0.47
1:D:673:THR:HA	1:D:832:THR:OG1	2.14	0.47
1:D:697:LEU:HD23	1:D:822:ILE:HD13	1.97	0.47
1:D:884:ALA:N	1:D:893:PRO:HG3	2.30	0.47
1:E:44:THR:OG1	1:E:91:THR:OG1	2.13	0.47
1:E:343:THR:HG22	1:E:344:LEU:HD23	1.97	0.47
1:E:346:GLU:O	1:E:349:ILE:N	2.48	0.47
1:F:110:LYS:O	1:F:113:LEU:HB2	2.15	0.47
1:F:151:GLN:NE2	1:F:279:ALA:O	2.47	0.47
1:F:190:PRO:HB3	1:F:784:TRP:CH2	2.50	0.47
1:F:696:GLN:HG2	1:F:846:LEU:HD22	1.96	0.47
1:F:704:HIS:CE1	1:F:842:LEU:HD11	2.50	0.47
1:F:876:LEU:HD21	1:F:930:ILE:HD13	1.96	0.47
1:F:910:ALA:HB2	1:F:1004:GLY:HA3	1.96	0.47
1:A:966:ARG:HB3	1:A:966:ARG:HH11	1.80	0.47
1:B:701:ALA:HB3	1:B:711:VAL:HG11	1.96	0.47
1:B:897:MET:O	1:B:899:VAL:N	2.47	0.47
1:B:904:VAL:O	1:B:906:GLY:N	2.48	0.47
1:C:54:ALA:HB3	1:C:808:SER:O	2.15	0.47
1:C:293:LEU:HD11	1:C:299:ALA:HA	1.96	0.47
1:C:527:TYR:O	1:C:531:VAL:HG23	2.15	0.47
1:D:445:ILE:HD13	1:D:935:LYS:HE3	1.96	0.47
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.80	0.47
1:E:355:MET:CE	1:E:368:PRO:HG2	2.44	0.47
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.96	0.47
1:F:355:MET:SD	1:F:368:PRO:HB2	2.55	0.47
1:F:756:ASP:OD1	1:F:765:LYS:HA	2.15	0.47
1:F:759:ASP:OD1	1:F:760:ARG:HG3	2.14	0.47
1:F:899:VAL:HA	1:F:902:LEU:HD13	1.97	0.47
1:A:211:ASN:O	1:A:755:ASN:ND2	2.45	0.47
1:A:544:LEU:O	1:A:548:ILE:HG13	2.14	0.47
1:C:121:GLU:O	1:C:124:GLN:HG2	2.15	0.47
1:C:261:LEU:O	1:C:265:VAL:HG13	2.15	0.47
1:C:1010:THR:OG1	1:C:1011:VAL:N	2.46	0.47
1:C:1010:THR:O	1:C:1012:LEU:N	2.48	0.47
1:D:579:PRO:HD3	1:D:656:ALA:HB2	1.96	0.47
1:D:785:TYR:CB	1:D:793:MET:HB3	2.45	0.47
1:D:893:PRO:O	1:D:896:VAL:HG13	2.15	0.47
1:E:47:ALA:HB2	1:E:127:VAL:HG13	1.97	0.47
1:E:220:GLY:HA3	1:E:230:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:ILE:HG21	1:F:111:LEU:HG	1.96	0.47
1:F:146:ASP:OD2	1:F:146:ASP:N	2.40	0.47
1:F:876:LEU:CD2	1:F:930:ILE:HG21	2.45	0.47
1:A:438:ILE:O	1:A:442:LEU:HG	2.15	0.47
1:A:695:ASN:HA	1:A:698:LEU:HD12	1.97	0.47
1:A:977:PHE:CD2	1:A:1006:MET:HE2	2.45	0.47
1:B:151:GLN:OE1	1:B:278:ILE:HA	2.16	0.47
1:B:396:PHE:O	1:B:400:LEU:HB2	2.14	0.47
1:B:408:ASP:OD2	1:B:481:SER:OG	2.22	0.47
1:B:594:VAL:HG22	1:B:650:PHE:CZ	2.50	0.47
1:B:663:LEU:H	1:B:663:LEU:CD2	2.25	0.47
1:C:254:ASN:HB2	1:C:258:SER:OG	2.15	0.47
1:D:72:ILE:HG23	1:D:106:GLN:HB2	1.97	0.47
1:E:697:LEU:HD23	1:E:822:ILE:HD13	1.97	0.47
1:F:669:LEU:HA	1:F:669:LEU:HD23	1.72	0.47
1:F:746:GLY:O	1:F:748:ALA:N	2.48	0.47
1:B:36:PRO:HG3	1:B:469:GLN:HG3	1.98	0.46
1:B:401:ALA:O	1:B:405:LEU:HG	2.15	0.46
1:B:545:TYR:CE2	1:B:1020:PHE:HZ	2.32	0.46
1:B:986:ILE:O	1:B:986:ILE:HG22	2.15	0.46
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.97	0.46
1:C:239:ARG:HD3	1:C:756:ASP:O	2.15	0.46
1:C:318:PRO:HG2	1:C:321:LEU:HG	1.97	0.46
1:D:45:ILE:HD12	1:D:90:ILE:HB	1.96	0.46
1:D:199:THR:HG23	1:D:793:MET:HE1	1.97	0.46
1:D:544:LEU:O	1:D:548:ILE:HG13	2.15	0.46
1:D:694:ARG:HD2	1:D:713:PRO:HB3	1.97	0.46
1:D:701:ALA:HB3	1:D:711:VAL:HG11	1.97	0.46
1:D:881:LEU:HD11	1:F:17:ILE:CG2	2.45	0.46
1:E:326:PRO:O	1:E:623:PHE:HE2	1.98	0.46
1:E:350:LEU:HD13	1:E:980:GLY:HA2	1.97	0.46
1:E:908:LEU:HD23	1:E:922:PHE:HZ	1.81	0.46
1:F:58:GLN:HA	1:F:62:THR:HB	1.96	0.46
1:F:723:LYS:HB3	1:F:803:ARG:HG3	1.98	0.46
1:F:955:LEU:O	1:F:958:ALA:N	2.48	0.46
1:A:222:THR:HA	1:A:224:PRO:HD3	1.97	0.46
1:A:525:HIS:O	1:A:526:HIS:C	2.58	0.46
1:A:541:TYR:N	1:A:541:TYR:CD1	2.80	0.46
1:B:157:TYR:CZ	1:B:318:PRO:HD3	2.51	0.46
1:B:356:TYR:C	1:B:358:PHE:N	2.63	0.46
1:C:378:GLY:O	1:C:382:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:LEU:O	1:C:490:PRO:HG2	2.15	0.46
1:D:383:LEU:HB3	1:D:388:PHE:HB2	1.98	0.46
1:D:451:ALA:HB1	1:D:878:VAL:HG12	1.98	0.46
1:D:892:ILE:HG12	1:D:1025:ARG:CD	2.46	0.46
1:E:151:GLN:NE2	1:E:277:ILE:O	2.48	0.46
1:E:200:PRO:O	1:E:203:VAL:N	2.48	0.46
1:E:899:VAL:HG21	1:E:937:ALA:CB	2.45	0.46
1:F:15:ILE:O	1:F:19:ILE:HG13	2.15	0.46
1:F:240:LEU:HD12	1:F:246:PHE:CD2	2.50	0.46
1:A:239:ARG:NH1	1:A:756:ASP:HB2	2.30	0.46
1:A:813:ARG:HH12	1:A:818:PRO:HG3	1.79	0.46
1:B:326:PRO:O	1:B:623:PHE:HE2	1.98	0.46
1:B:435:MET:HG3	1:B:490:PRO:HB3	1.97	0.46
1:C:246:PHE:HA	1:C:249:ILE:HG12	1.97	0.46
1:D:588:GLN:HB2	1:D:613:ASN:HD22	1.80	0.46
1:E:143:ILE:HG22	1:E:286:ALA:CB	2.45	0.46
1:E:251:LEU:HD12	1:E:265:VAL:HG11	1.98	0.46
1:F:135:SER:HB3	1:F:668:GLU:HB3	1.97	0.46
1:F:284:GLN:HG3	1:F:285:PRO:HD2	1.98	0.46
1:F:375:VAL:HB	1:F:405:LEU:HD22	1.97	0.46
1:A:470:PHE:CD1	1:A:924:VAL:HG21	2.49	0.46
1:B:418:ARG:CZ	1:B:965:MET:HE2	2.46	0.46
1:B:712:ARG:CD	1:B:823:LEU:HB2	2.46	0.46
1:B:889:SER:HB3	1:B:892:ILE:HB	1.96	0.46
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.96	0.46
1:D:412:VAL:HG11	1:D:489:THR:HG22	1.97	0.46
1:D:415:ASN:OD1	1:D:434:SER:HB2	2.15	0.46
1:D:423:GLU:HB2	1:D:425:LEU:HD13	1.97	0.46
1:D:955:LEU:HD21	1:D:1022:VAL:HG13	1.98	0.46
1:E:76:MET:HG2	1:E:859:TYR:OH	2.14	0.46
1:E:355:MET:CE	1:E:410:ILE:HG12	2.45	0.46
1:F:104:GLN:HG3	1:F:105:VAL:N	2.24	0.46
1:F:367:ILE:HG21	1:F:489:THR:HG23	1.97	0.46
1:F:940:ILE:HA	1:F:966:ARG:HH12	1.79	0.46
1:A:419:VAL:HG13	1:A:423:GLU:CD	2.40	0.46
1:A:423:GLU:OE2	1:A:433:LYS:HE2	2.16	0.46
1:A:770:SER:OG	1:A:775:ARG:HG2	2.15	0.46
1:A:770:SER:HG	1:A:775:ARG:HG2	1.79	0.46
2:A:1101:ERY:H321	2:A:1101:ERY:H8	1.74	0.46
1:B:685:LEU:HD11	1:B:849:GLY:HA3	1.98	0.46
1:C:142:VAL:HG21	1:C:162:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:LEU:HD12	1:D:246:PHE:CE2	2.50	0.46
1:D:457:ALA:HA	1:D:468:ARG:HA	1.97	0.46
1:D:836:MET:HE1	1:D:862:ARG:HB2	1.97	0.46
1:E:416:VAL:HG11	1:E:497:LEU:HD23	1.97	0.46
1:E:434:SER:O	1:E:437:GLN:HB2	2.15	0.46
1:F:358:PHE:CD1	1:F:972:MET:HG2	2.51	0.46
1:F:375:VAL:HG21	1:F:405:LEU:HD13	1.97	0.46
1:F:450:SER:HB3	1:F:478:MET:HB2	1.98	0.46
1:A:142:VAL:HG21	1:A:158:VAL:HG22	1.98	0.46
1:A:190:PRO:HD3	1:A:774:TYR:CD1	2.51	0.46
1:A:449:LEU:HB3	1:A:478:MET:SD	2.56	0.46
1:B:631:ASP:OD1	1:B:631:ASP:N	2.48	0.46
1:B:911:ALA:O	1:B:915:GLY:N	2.48	0.46
1:C:5:PHE:C	1:C:5:PHE:CD2	2.93	0.46
1:C:5:PHE:C	1:C:7:ASP:H	2.22	0.46
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.97	0.46
1:C:562:SER:HB2	1:C:919:ASP:HB3	1.97	0.46
1:C:948:MET:HE3	1:C:948:MET:HB2	1.61	0.46
1:D:149:MET:HG3	1:D:154:ILE:HG13	1.97	0.46
1:D:563:PHE:CE1	3:D:1103:LMT:H5B	2.50	0.46
1:D:810:ARG:O	1:D:810:ARG:HG3	2.14	0.46
1:E:187:TRP:HE3	1:E:770:SER:O	1.97	0.46
1:E:274:ASN:ND2	1:E:276:ASP:OD2	2.30	0.46
1:F:300:LEU:HD11	1:F:333:VAL:HG11	1.98	0.46
1:F:504:ASP:C	1:F:506:GLY:N	2.67	0.46
1:F:531:VAL:HG21	1:F:963:VAL:HG11	1.98	0.46
1:F:891:SER:HB3	1:F:1028:PHE:CD2	2.50	0.46
1:A:407:ASP:OD2	1:A:935:LYS:HG2	2.15	0.46
1:B:382:VAL:HG11	1:B:476:SER:OG	2.16	0.46
1:B:440:GLY:O	1:B:886:LEU:HD11	2.16	0.46
1:B:679:LEU:HD12	1:B:679:LEU:HA	1.80	0.46
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.46	0.46
1:C:748:ALA:O	1:C:770:SER:HB3	2.15	0.46
1:D:187:TRP:CH2	1:F:223:PRO:HD2	2.48	0.46
1:E:926:LEU:O	1:E:930:ILE:HG13	2.15	0.46
1:F:364:ALA:HA	1:F:367:ILE:HD12	1.98	0.46
1:F:465:ALA:HA	1:F:468:ARG:NH1	2.31	0.46
1:F:940:ILE:HG12	1:F:966:ARG:NH2	2.29	0.46
1:A:20:MET:SD	1:A:374:VAL:HG22	2.55	0.46
1:A:110:LYS:HD3	1:A:110:LYS:HA	1.58	0.46
1:A:462:SER:O	1:A:466:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:GLY:N	1:A:616:GLY:HA2	2.31	0.46
1:A:667:VAL:HG12	1:A:668:GLU:OE1	2.16	0.46
1:B:149:MET:HB2	1:B:153:ASP:HB2	1.97	0.46
1:B:277:ILE:HA	1:B:613:ASN:O	2.16	0.46
1:B:530:SER:O	1:B:534:ILE:HG23	2.16	0.46
1:B:563:PHE:O	1:B:564:LEU:HD12	2.15	0.46
1:C:344:LEU:HA	1:C:399:VAL:HG22	1.97	0.46
1:C:790:ASP:OD2	1:C:791:GLY:N	2.49	0.46
1:D:149:MET:HB2	1:D:153:ASP:CB	2.45	0.46
1:D:365:THR:O	1:D:368:PRO:HD2	2.16	0.46
1:D:597:TYR:CD2	1:D:650:PHE:CZ	3.04	0.46
1:D:1032:ASN:HB3	1:D:1033:GLU:H	1.44	0.46
1:E:57:VAL:HG23	1:E:82:SER:HB3	1.98	0.46
1:F:635:GLU:O	1:F:638:LYS:HB3	2.16	0.46
1:A:450:SER:HB3	1:A:478:MET:HE1	1.98	0.46
1:B:293:LEU:HD13	1:B:294:ALA:O	2.15	0.46
1:B:906:GLY:O	1:B:910:ALA:N	2.49	0.46
1:B:941:VAL:HG13	1:B:1021:PHE:CE1	2.51	0.46
1:B:948:MET:HE2	1:B:958:ALA:HB3	1.98	0.46
1:C:142:VAL:HG21	1:C:158:VAL:HG22	1.98	0.46
1:C:182:TYR:HD2	1:C:760:ARG:HH22	1.64	0.46
1:C:449:LEU:HD12	1:C:478:MET:HE2	1.98	0.46
1:C:571:VAL:N	1:C:626:LEU:HD12	2.30	0.46
1:C:899:VAL:HG21	1:C:937:ALA:HB2	1.98	0.46
1:F:211:ASN:OD1	1:F:240:LEU:N	2.45	0.46
1:F:659:PHE:HE2	1:F:712:ARG:HB3	1.80	0.46
1:F:669:LEU:HD13	1:F:856:GLY:C	2.40	0.46
1:A:102:ILE:HG21	1:C:101:ASP:HB3	1.98	0.46
1:A:391:ASN:OD1	1:A:393:LEU:N	2.48	0.46
1:A:505:HIS:O	1:A:507:GLU:N	2.49	0.46
1:A:554:TYR:CZ	1:A:558:ARG:HG3	2.51	0.46
1:B:242:SER:HB2	1:B:245:GLU:HG3	1.98	0.46
1:B:404:LEU:HD12	1:B:932:LEU:HD21	1.97	0.46
1:B:509:LYS:HD3	1:B:510:LYS:HE2	1.97	0.46
1:B:522:LYS:O	1:B:525:HIS:HB3	2.16	0.46
1:B:941:VAL:HG13	1:B:1021:PHE:CD1	2.51	0.46
1:C:685:LEU:O	1:C:689:LYS:NZ	2.38	0.46
1:D:449:LEU:HB3	1:D:478:MET:SD	2.56	0.46
1:D:636:GLU:OE1	1:D:636:GLU:N	2.42	0.46
1:E:350:LEU:CD1	1:E:980:GLY:HA2	2.46	0.46
1:E:545:TYR:HE2	1:E:902:LEU:HD11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:906:GLY:HA2	1:E:1008:THR:HG21	1.97	0.46
1:F:272:GLY:N	1:F:275:TYR:OH	2.28	0.46
1:F:378:GLY:O	1:F:382:VAL:HG23	2.16	0.46
1:B:4:PHE:CE1	1:B:8:ARG:NE	2.84	0.45
1:B:594:VAL:HG22	1:B:650:PHE:CE2	2.52	0.45
1:C:908:LEU:HD23	1:C:922:PHE:CZ	2.50	0.45
1:C:956:ILE:H	1:C:956:ILE:HD12	1.81	0.45
1:D:16:ALA:O	1:D:20:MET:HG3	2.17	0.45
1:D:275:TYR:HB2	1:F:222:THR:HB	1.99	0.45
1:D:667:VAL:O	1:D:668:GLU:HG2	2.16	0.45
1:D:763:VAL:HG12	1:E:63:GLN:OE1	2.15	0.45
1:D:963:VAL:CA	1:D:966:ARG:HH22	2.25	0.45
1:D:982:MET:CA	1:D:1003:MET:HE1	2.47	0.45
1:E:525:HIS:O	1:E:526:HIS:C	2.57	0.45
1:E:531:VAL:HG11	1:E:963:VAL:HG11	1.98	0.45
1:E:631:ASP:C	1:E:633:PRO:HD3	2.41	0.45
1:E:1010:THR:O	1:E:1012:LEU:N	2.50	0.45
1:F:677:PHE:O	1:F:821:GLU:HA	2.15	0.45
1:A:247:GLY:C	1:A:249:ILE:H	2.24	0.45
1:A:405:LEU:CD2	1:A:481:SER:HB3	2.37	0.45
1:A:759:ASP:HB3	1:A:764:LYS:HE3	1.99	0.45
1:B:78:MET:HG3	1:B:92:LEU:HG	1.97	0.45
1:B:111:LEU:HD11	1:B:127:VAL:HB	1.98	0.45
1:B:527:TYR:O	1:B:531:VAL:HG23	2.16	0.45
1:C:351:VAL:HG12	1:C:355:MET:HE2	1.98	0.45
1:C:519:MET:HE3	1:C:519:MET:HB3	1.90	0.45
1:C:552:MET:HE2	1:C:552:MET:HB3	1.87	0.45
1:C:871:LEU:O	1:C:875:SER:HB2	2.17	0.45
1:C:900:VAL:HB	1:C:901:PRO:HD3	1.98	0.45
1:C:920:VAL:HG12	1:C:921:TYR:N	2.31	0.45
1:C:920:VAL:O	1:C:923:GLN:HB2	2.16	0.45
1:D:309:GLU:O	1:D:312:LYS:HB2	2.17	0.45
1:D:881:LEU:HD11	1:F:17:ILE:HG22	1.97	0.45
1:E:58:GLN:OE1	1:E:811:LEU:HD13	2.16	0.45
1:E:557:VAL:C	1:E:559:LEU:H	2.24	0.45
1:E:935:LYS:O	1:E:936:ASN:C	2.59	0.45
1:F:216:ALA:HB1	1:F:234:ILE:HG22	1.97	0.45
1:F:531:VAL:O	1:F:534:ILE:HG13	2.16	0.45
1:A:200:PRO:O	1:A:203:VAL:N	2.48	0.45
1:A:707:MET:O	1:A:827:ALA:N	2.49	0.45
1:A:981:VAL:HG11	1:A:1003:MET:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:932:LEU:HD23	1:B:932:LEU:HA	1.76	0.45
1:C:667:VAL:HB	1:C:668:GLU:OE2	2.16	0.45
1:D:30:LEU:HD12	1:D:30:LEU:HA	1.83	0.45
1:D:79:SER:HA	1:D:813:ARG:O	2.15	0.45
1:D:1010:THR:OG1	1:D:1011:VAL:N	2.49	0.45
1:E:2:PRO:O	1:E:6:ILE:HG13	2.16	0.45
1:E:327:TYR:HD1	1:E:623:PHE:CE1	2.33	0.45
1:F:575:MET:HE3	1:F:575:MET:HB3	1.78	0.45
1:F:653:ILE:O	1:F:654:LYS:HE2	2.16	0.45
1:A:53:ASP:O	1:A:57:VAL:HG23	2.16	0.45
1:A:448:VAL:O	1:A:451:ALA:HB3	2.17	0.45
1:A:457:ALA:HB1	1:A:468:ARG:HG3	1.97	0.45
1:B:69:MET:CE	1:B:107:VAL:HG13	2.43	0.45
1:B:104:GLN:HG3	1:B:131:LYS:HG3	1.98	0.45
1:B:187:TRP:HA	1:B:769:MET:O	2.16	0.45
1:C:45:ILE:HD12	1:C:90:ILE:HB	1.98	0.45
1:D:261:LEU:O	1:D:265:VAL:HG13	2.16	0.45
1:D:491:ALA:O	1:D:495:THR:OG1	2.26	0.45
1:E:235:ILE:N	1:F:722:PHE:O	2.45	0.45
1:E:291:ILE:HD13	1:E:306:ILE:HD13	1.96	0.45
1:E:370:ILE:O	1:E:374:VAL:HG23	2.16	0.45
1:F:3:ASN:ND2	1:F:435:MET:HG3	2.31	0.45
1:F:400:LEU:HD12	1:F:400:LEU:HA	1.69	0.45
1:F:527:TYR:CD1	3:F:2100:LMT:H71	2.51	0.45
1:F:977:PHE:O	1:F:978:ILE:C	2.60	0.45
1:A:184:MET:HE3	1:A:184:MET:HA	1.98	0.45
1:A:889:SER:HB3	1:A:892:ILE:HB	1.97	0.45
1:B:157:TYR:CD2	1:B:162:MET:HE2	2.51	0.45
1:B:300:LEU:HD11	1:B:333:VAL:CG1	2.46	0.45
1:B:372:VAL:HG12	1:B:405:LEU:HB3	1.99	0.45
1:B:501:ALA:O	1:B:504:ASP:HB2	2.17	0.45
1:B:675:PHE:CD1	1:B:854:TRP:HZ3	2.34	0.45
1:C:310:LEU:O	1:C:314:GLU:HG3	2.17	0.45
1:E:524:THR:O	1:E:527:TYR:HB3	2.17	0.45
1:E:896:VAL:HG21	1:E:938:ILE:CG1	2.42	0.45
1:F:142:VAL:HG12	1:F:321:LEU:HD22	1.99	0.45
1:F:216:ALA:HB1	1:F:234:ILE:CG2	2.46	0.45
1:F:826:ALA:HB3	1:F:830:LYS:HG3	1.97	0.45
1:F:1010:THR:C	1:F:1012:LEU:H	2.25	0.45
1:A:795:PRO:O	1:A:798:ALA:HB3	2.16	0.45
1:A:944:ALA:HB2	1:A:959:THR:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LEU:HD23	1:B:113:LEU:HA	1.80	0.45
1:B:572:PHE:CE1	1:B:643:THR:HG22	2.51	0.45
1:D:383:LEU:HD11	1:D:473:THR:HG23	1.97	0.45
1:D:573:MET:HG3	1:D:661:PHE:CE1	2.52	0.45
1:E:9:PRO:HB3	1:E:495:THR:HG21	1.99	0.45
1:E:449:LEU:HD23	1:E:449:LEU:HA	1.86	0.45
1:E:527:TYR:CE2	1:E:967:LEU:HD23	2.52	0.45
1:E:1030:ARG:O	1:E:1030:ARG:HG2	2.17	0.45
1:F:53:ASP:O	1:F:56:THR:OG1	2.25	0.45
1:F:154:ILE:HG22	1:F:287:SER:HB3	1.99	0.45
1:F:247:GLY:C	1:F:249:ILE:H	2.24	0.45
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.98	0.45
1:F:978:ILE:HG23	1:F:1003:MET:HE3	1.99	0.45
1:F:1013:ALA:C	1:F:1015:PHE:H	2.24	0.45
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.74	0.45
1:A:639:VAL:HG11	1:A:662:ASN:HB2	1.99	0.45
1:A:675:PHE:CD1	1:A:854:TRP:HZ3	2.35	0.45
1:A:1033:GLU:O	1:A:1034:ASP:HB2	2.15	0.45
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.98	0.45
1:B:738:ILE:HA	1:B:741:ILE:HG13	1.99	0.45
1:C:187:TRP:HA	1:C:769:MET:O	2.17	0.45
1:C:463:THR:HG23	1:C:920:VAL:HG22	1.98	0.45
1:C:595:THR:HG23	1:C:609:VAL:HB	1.99	0.45
1:C:675:PHE:CE2	1:C:839:MET:HE2	2.50	0.45
1:C:677:PHE:CD2	1:C:678:GLU:N	2.85	0.45
1:D:190:PRO:HG3	1:D:784:TRP:CH2	2.52	0.45
1:D:693:ALA:HB1	1:D:850:VAL:HG11	1.97	0.45
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.46	0.45
1:B:47:ALA:HB2	1:B:127:VAL:HA	1.98	0.45
1:C:714:ASN:N	1:C:821:GLU:O	2.50	0.45
1:C:847:PRO:HG2	1:C:850:VAL:HG21	1.97	0.45
1:D:214:VAL:HG23	1:D:237:GLN:HB3	1.99	0.45
1:D:350:LEU:HD22	1:D:979:LEU:HB3	1.99	0.45
1:D:375:VAL:HG21	1:D:481:SER:HA	1.99	0.45
1:E:198:LEU:HD23	1:E:787:ARG:HH21	1.82	0.45
1:E:562:SER:HB3	1:E:919:ASP:HB3	1.97	0.45
1:F:69:MET:CB	1:F:72:ILE:HD11	2.46	0.45
1:F:293:LEU:HD22	1:F:297:ALA:HB3	1.99	0.45
1:F:769:MET:HG2	1:F:770:SER:N	2.31	0.45
1:F:982:MET:HE2	1:F:982:MET:HB3	1.57	0.45
1:A:796:PHE:HA	1:A:799:PHE:HE2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1035:ILE:HG13	1:B:1036:GLU:H	1.81	0.45
1:C:694:ARG:HD3	1:C:820:MET:SD	2.57	0.45
1:D:254:ASN:ND2	1:D:258:SER:OG	2.44	0.45
1:D:339:GLU:OE1	1:D:342:LYS:HD3	2.17	0.45
1:D:424:GLY:CA	1:D:502:LYS:HB3	2.43	0.45
1:D:584:GLN:H	1:D:617:GLN:HB3	1.82	0.45
1:D:680:ILE:HD11	1:D:814:TYR:HD2	1.82	0.45
1:D:1010:THR:C	1:D:1012:LEU:H	2.24	0.45
1:E:770:SER:HB3	1:E:775:ARG:HD3	1.98	0.45
1:E:883:LEU:HD23	1:E:883:LEU:HA	1.64	0.45
1:E:905:ILE:O	1:E:905:ILE:HG13	2.16	0.45
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.99	0.45
1:F:166:ILE:HG22	1:F:175:VAL:HG21	1.99	0.45
1:F:368:PRO:O	1:F:406:VAL:HG12	2.16	0.45
1:F:368:PRO:HB3	1:F:409:ALA:HB3	1.99	0.45
1:F:725:ASP:CG	1:F:803:ARG:HH21	2.24	0.45
1:A:383:LEU:O	1:A:387:GLY:N	2.51	0.45
1:A:525:HIS:O	1:A:528:THR:N	2.49	0.45
1:B:139:VAL:HB	1:B:327:TYR:HB3	1.97	0.45
1:B:516:PHE:HA	1:B:519:MET:HE2	1.99	0.45
1:B:669:LEU:CD2	1:B:670:GLY:H	2.30	0.45
1:B:920:VAL:O	1:B:923:GLN:N	2.48	0.45
1:C:531:VAL:O	1:C:534:ILE:HG13	2.17	0.45
1:D:378:GLY:O	1:D:382:VAL:HG23	2.16	0.45
1:D:923:GLN:CD	3:D:1103:LMT:H32	2.42	0.45
1:F:39:ALA:HB2	1:F:668:GLU:HG2	1.98	0.45
1:F:200:PRO:HB2	1:F:744:THR:HG22	1.98	0.45
1:A:239:ARG:HH12	1:A:756:ASP:HB2	1.82	0.44
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.98	0.44
1:A:939:LEU:O	1:A:942:GLU:HB3	2.17	0.44
1:A:943:PHE:O	1:A:947:LEU:HG	2.17	0.44
1:A:966:ARG:HB3	1:A:966:ARG:NH1	2.32	0.44
1:B:184:MET:HA	1:B:184:MET:HE3	1.99	0.44
1:B:841:GLN:O	1:B:844:SER:OG	2.33	0.44
1:B:883:LEU:HD21	1:B:938:ILE:HD11	1.99	0.44
1:C:185:ARG:HB3	1:C:187:TRP:HE1	1.82	0.44
1:C:584:GLN:HB2	1:C:584:GLN:HE21	1.56	0.44
1:C:677:PHE:O	1:C:821:GLU:HA	2.17	0.44
1:D:26:ALA:O	1:D:30:LEU:HB2	2.17	0.44
1:E:281:PHE:HB2	1:E:610:PHE:CE1	2.52	0.44
1:E:739:ASN:O	1:E:742:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:MET:HA	1:F:266:ALA:CB	2.47	0.44
1:F:412:VAL:HG13	1:F:435:MET:HE1	1.99	0.44
1:F:519:MET:HE3	1:F:519:MET:HB3	1.65	0.44
1:A:367:ILE:HG12	1:A:492:LEU:HB3	1.99	0.44
1:A:559:LEU:HD11	1:A:911:ALA:HB3	1.98	0.44
1:B:52:ALA:HB1	1:B:56:THR:HB	2.00	0.44
1:B:185:ARG:NH1	1:B:767:TYR:HB3	2.31	0.44
1:B:559:LEU:CG	1:B:560:PRO:HD2	2.46	0.44
1:B:770:SER:OG	1:B:775:ARG:HG2	2.17	0.44
1:C:574:THR:HG23	1:C:622:ALA:HB3	1.99	0.44
1:D:14:VAL:HG11	1:E:885:ALA:HB2	1.99	0.44
1:D:83:ASP:HB2	1:D:87:THR:O	2.17	0.44
1:D:435:MET:HE3	1:D:435:MET:HB3	1.84	0.44
1:D:539:GLY:O	1:D:542:LEU:HB2	2.17	0.44
1:D:588:GLN:NE2	1:D:592:ASN:OD1	2.50	0.44
1:D:677:PHE:CD2	1:D:678:GLU:N	2.85	0.44
1:D:781:ILE:HA	1:D:781:ILE:HD13	1.81	0.44
1:D:897:MET:C	1:D:899:VAL:H	2.26	0.44
1:D:923:GLN:NE2	3:D:1103:LMT:H32	2.32	0.44
1:E:6:ILE:HD13	1:E:431:THR:HG22	1.99	0.44
1:E:64:VAL:O	1:E:68:ASN:ND2	2.50	0.44
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.97	0.44
1:E:466:ILE:HD13	1:E:564:LEU:HD11	1.98	0.44
1:F:200:PRO:O	1:F:203:VAL:N	2.50	0.44
1:F:239:ARG:HH12	1:F:756:ASP:H	1.65	0.44
1:F:350:LEU:O	1:F:353:LEU:N	2.49	0.44
1:F:412:VAL:CG1	1:F:435:MET:HE1	2.47	0.44
1:F:456:MET:HE3	1:F:467:TYR:O	2.16	0.44
1:F:555:LEU:HD23	1:F:555:LEU:HA	1.67	0.44
1:F:948:MET:HE3	1:F:948:MET:HB2	1.66	0.44
1:A:78:MET:HE2	1:A:78:MET:HB3	1.74	0.44
1:A:457:ALA:HB2	1:A:471:SER:OG	2.16	0.44
1:A:746:GLY:O	1:A:750:GLY:N	2.43	0.44
1:A:771:GLU:HB3	1:A:774:TYR:CE1	2.53	0.44
1:B:530:SER:OG	3:B:2100:LMT:H1'	2.17	0.44
1:B:710:SER:O	1:B:712:ARG:HG3	2.17	0.44
1:C:186:ILE:O	1:C:768:VAL:HG23	2.17	0.44
1:C:450:SER:CB	1:C:475:VAL:HA	2.47	0.44
1:C:631:ASP:N	1:C:631:ASP:OD1	2.49	0.44
1:C:636:GLU:OE2	1:C:636:GLU:N	2.47	0.44
1:C:974:SER:OG	1:C:1010:THR:HG21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:GLN:HE22	1:D:250:LEU:CB	2.28	0.44
1:D:945:LYS:NZ	1:D:1025:ARG:NH2	2.65	0.44
1:E:771:GLU:HB3	1:E:774:TYR:CD1	2.52	0.44
1:E:944:ALA:O	1:E:948:MET:HE3	2.17	0.44
1:F:199:THR:HG22	1:F:785:TYR:O	2.18	0.44
1:F:393:LEU:HD22	1:F:466:ILE:HG23	1.98	0.44
1:F:926:LEU:O	1:F:929:THR:HB	2.18	0.44
1:F:1034:ASP:H	1:F:1035:ILE:HG23	1.83	0.44
1:A:955:LEU:HD21	1:A:1022:VAL:HG13	1.98	0.44
1:A:1025:ARG:HA	1:A:1025:ARG:HD2	1.78	0.44
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.39	0.44
1:B:441:ALA:HA	1:B:886:LEU:HD21	1.99	0.44
1:B:559:LEU:HD22	1:B:918:ASN:HB2	1.99	0.44
1:B:1030:ARG:NH1	1:B:1031:LYS:HB2	2.32	0.44
1:C:253:VAL:HG22	1:C:259:ARG:HG2	1.98	0.44
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.99	0.44
1:C:415:ASN:CG	1:C:438:ILE:HG21	2.42	0.44
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.99	0.44
1:D:532:GLY:O	1:D:535:LEU:N	2.51	0.44
1:D:831:SER:OG	1:D:832:THR:N	2.47	0.44
1:E:6:ILE:HG23	1:E:494:ALA:HB2	2.00	0.44
1:E:68:ASN:CB	1:E:114:ALA:HB2	2.46	0.44
1:E:190:PRO:HB3	1:E:784:TRP:CE3	2.52	0.44
1:F:353:LEU:HD22	1:F:353:LEU:HA	1.71	0.44
1:F:889:SER:CB	1:F:892:ILE:HG12	2.46	0.44
1:B:102:ILE:O	1:B:105:VAL:HG12	2.18	0.44
1:B:842:LEU:O	1:B:845:LYS:HB2	2.18	0.44
1:C:2:PRO:O	1:C:5:PHE:HB3	2.18	0.44
1:C:65:ILE:HG21	1:C:90:ILE:HD12	1.98	0.44
1:C:102:ILE:HA	1:C:102:ILE:HD13	1.76	0.44
1:C:456:MET:CB	1:C:871:LEU:HD21	2.46	0.44
1:C:687:HIS:HE2	1:C:718:ASP:CG	2.20	0.44
1:C:967:LEU:O	1:C:970:ILE:HB	2.17	0.44
1:D:332:PHE:O	1:D:336:SER:HB3	2.18	0.44
1:E:182:TYR:HB2	1:E:764:LYS:NZ	2.32	0.44
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.47	0.44
1:E:451:ALA:O	1:E:875:SER:OG	2.25	0.44
1:F:361:ASN:O	1:F:362:PHE:C	2.61	0.44
1:F:418:ARG:HB3	1:F:418:ARG:NH1	2.32	0.44
1:F:860:GLN:O	1:F:863:LEU:HB3	2.17	0.44
1:B:895:SER:HA	1:B:1020:PHE:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ASP:O	1:C:157:TYR:C	2.60	0.44
1:C:421:ALA:O	1:C:503:GLY:N	2.35	0.44
1:D:156:ASP:OD1	1:D:760:ARG:NH2	2.50	0.44
1:D:189:ASN:HA	1:D:190:PRO:HD3	1.72	0.44
1:D:756:ASP:OD1	1:D:765:LYS:HA	2.18	0.44
1:D:1015:PHE:HZ	3:D:1102:LMT:H52	1.82	0.44
1:E:20:MET:HA	1:E:377:LEU:HD13	1.99	0.44
1:E:549:VAL:O	1:E:552:MET:HB3	2.18	0.44
1:F:78:MET:HG3	1:F:92:LEU:CD1	2.46	0.44
1:F:438:ILE:HG22	1:F:943:PHE:CZ	2.53	0.44
1:A:344:LEU:HD11	1:A:398:MET:HB2	2.00	0.44
1:A:363:ARG:O	1:A:496:MET:HE2	2.17	0.44
1:A:888:GLU:OE2	1:C:11:PHE:HB2	2.18	0.44
1:B:40:PRO:HD3	1:B:462:SER:OG	2.17	0.44
1:B:167:SER:HB2	1:C:70:ASN:CG	2.43	0.44
1:B:199:THR:O	1:B:203:VAL:HG23	2.18	0.44
1:B:573:MET:CB	1:B:661:PHE:HE2	2.31	0.44
1:C:331:PRO:O	1:C:335:ILE:HG22	2.17	0.44
1:D:424:GLY:HA3	1:D:502:LYS:CB	2.42	0.44
1:D:435:MET:O	1:D:439:GLN:HB2	2.18	0.44
1:D:605:ASN:O	1:D:626:LEU:HD23	2.18	0.44
1:D:702:ALA:HB2	1:D:711:VAL:HG21	1.98	0.44
1:D:721:GLN:HG2	1:F:233:SER:HB2	2.00	0.44
1:D:902:LEU:HD23	1:D:1012:LEU:HB3	2.00	0.44
1:D:966:ARG:HB3	1:D:966:ARG:HH11	1.83	0.44
1:E:579:PRO:HD3	1:E:656:ALA:HB2	2.00	0.44
1:F:11:PHE:CE2	1:F:15:ILE:HD11	2.53	0.44
1:F:246:PHE:O	1:F:262:LEU:HD23	2.17	0.44
1:F:434:SER:O	1:F:438:ILE:HG12	2.17	0.44
1:F:572:PHE:HA	1:F:663:LEU:HD21	2.00	0.44
1:F:666:ILE:HB	1:F:857:MET:SD	2.58	0.44
1:A:211:ASN:OD1	1:A:240:LEU:HG	2.18	0.44
1:A:277:ILE:HA	1:A:613:ASN:O	2.17	0.44
1:A:701:ALA:CB	1:A:711:VAL:HG11	2.48	0.44
1:A:785:TYR:CE1	1:A:795:PRO:HB3	2.53	0.44
1:B:398:MET:HE3	1:B:398:MET:HB3	1.55	0.44
1:B:544:LEU:O	1:B:548:ILE:HG13	2.18	0.44
1:B:599:LEU:HA	1:B:599:LEU:HD23	1.73	0.44
1:C:590:VAL:O	1:C:593:GLU:HB2	2.18	0.44
1:D:1013:ALA:C	1:D:1015:PHE:H	2.26	0.44
1:E:216:ALA:HB1	1:E:234:ILE:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:978:ILE:HG23	1:E:1003:MET:HE2	1.98	0.44
1:F:889:SER:HB3	1:F:892:ILE:HG12	2.00	0.44
1:B:116:PRO:HA	1:B:123:GLN:NE2	2.33	0.44
1:B:143:ILE:O	1:B:321:LEU:HA	2.18	0.44
1:B:811:LEU:HD23	1:B:811:LEU:HA	1.85	0.44
1:B:930:ILE:H	1:B:930:ILE:HG13	1.69	0.44
1:C:81:ASN:CG	1:C:810:ARG:HH11	2.25	0.44
1:C:455:PRO:HB3	1:C:874:ILE:HG22	2.00	0.44
1:C:883:LEU:CD2	1:C:938:ILE:HD11	2.48	0.44
1:D:270:LEU:HD12	1:D:270:LEU:HA	1.77	0.44
1:D:525:HIS:O	1:D:526:HIS:C	2.61	0.44
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.82	0.44
1:E:842:LEU:O	1:E:845:LYS:HB2	2.18	0.44
1:E:887:TYR:O	1:E:888:GLU:HB2	2.17	0.44
1:F:420:MET:HB3	1:F:500:ILE:HB	2.00	0.44
1:F:773:LYS:HE2	1:F:774:TYR:CE2	2.52	0.44
1:F:825:GLN:HB3	1:F:830:LYS:NZ	2.32	0.44
1:A:191:ASN:O	1:A:194:ASN:N	2.51	0.43
1:B:379:THR:OG1	1:B:477:ALA:HA	2.18	0.43
1:B:978:ILE:HG23	1:B:1003:MET:HE2	2.00	0.43
1:B:985:VAL:HG22	1:B:999:GLY:HA3	2.00	0.43
1:C:664:PRO:HD3	1:C:672:ALA:C	2.43	0.43
1:D:201:VAL:HG21	1:D:740:ASP:OD2	2.18	0.43
1:D:242:SER:OG	1:D:245:GLU:HG3	2.18	0.43
1:D:770:SER:HG	1:D:775:ARG:HG2	1.83	0.43
1:E:203:VAL:O	1:E:207:ILE:HG13	2.18	0.43
1:E:443:VAL:O	1:E:446:ALA:HB3	2.18	0.43
1:E:584:GLN:N	1:E:617:GLN:HB3	2.33	0.43
1:E:600:THR:O	1:E:603:LYS:HB2	2.18	0.43
1:E:1013:ALA:O	1:E:1015:PHE:N	2.51	0.43
1:F:35:TYR:CG	1:F:38:ILE:HD12	2.52	0.43
1:F:532:GLY:O	1:F:535:LEU:N	2.51	0.43
1:F:812:GLU:O	1:F:818:PRO:HA	2.18	0.43
1:A:219:LEU:HD13	1:B:778:PRO:HG3	1.99	0.43
1:A:327:TYR:OH	1:A:663:LEU:HD13	2.18	0.43
1:B:255:GLN:H	1:B:255:GLN:HG3	1.43	0.43
1:B:400:LEU:HD13	1:B:400:LEU:HA	1.86	0.43
1:B:425:LEU:HD11	1:B:433:LYS:HE2	1.99	0.43
1:B:641:ALA:O	1:B:644:MET:HB3	2.18	0.43
1:C:39:ALA:HB2	1:C:668:GLU:CG	2.48	0.43
1:C:412:VAL:CG1	1:C:435:MET:HE1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ILE:O	1:D:106:GLN:HG3	2.18	0.43
1:D:372:VAL:O	1:D:373:PRO:C	2.61	0.43
1:D:690:LEU:HD22	1:D:820:MET:SD	2.58	0.43
1:D:968:ARG:HB3	1:D:969:PRO:HD3	2.00	0.43
1:E:531:VAL:O	1:E:534:ILE:HG13	2.18	0.43
1:F:1013:ALA:C	1:F:1015:PHE:N	2.76	0.43
1:A:355:MET:HB3	1:A:365:THR:HG1	1.80	0.43
1:B:235:ILE:HD11	1:C:721:GLN:CD	2.43	0.43
1:B:414:GLU:OE1	1:B:968:ARG:HD3	2.17	0.43
1:B:691:THR:HG23	1:B:694:ARG:HH12	1.84	0.43
1:B:721:GLN:CD	1:B:807:GLY:HA3	2.42	0.43
1:C:579:PRO:HD3	1:C:656:ALA:CB	2.49	0.43
1:C:725:ASP:HB3	1:C:801:SER:HB3	2.00	0.43
1:C:893:PRO:HA	1:C:896:VAL:CG1	2.31	0.43
1:C:972:MET:HE2	1:C:972:MET:HB2	1.73	0.43
1:E:372:VAL:O	1:E:373:PRO:C	2.62	0.43
1:E:584:GLN:N	1:E:617:GLN:OE1	2.33	0.43
1:E:1013:ALA:C	1:E:1015:PHE:N	2.76	0.43
1:F:143:ILE:HG22	1:F:286:ALA:HB2	2.00	0.43
1:F:367:ILE:CG2	1:F:489:THR:HG23	2.49	0.43
1:F:597:TYR:CD2	1:F:650:PHE:CZ	3.06	0.43
1:A:58:GLN:HG3	1:A:813:ARG:HD2	1.99	0.43
1:A:137:LEU:HD22	1:A:293:LEU:HG	1.99	0.43
1:A:235:ILE:HD11	1:B:721:GLN:HB2	2.00	0.43
1:A:654:LYS:HD3	1:A:654:LYS:HA	1.80	0.43
1:A:897:MET:O	1:A:899:VAL:N	2.51	0.43
1:B:172:VAL:HG22	1:B:306:ILE:HD11	1.99	0.43
1:B:418:ARG:NE	1:B:965:MET:HE2	2.33	0.43
1:C:351:VAL:O	1:C:355:MET:HE2	2.19	0.43
1:C:974:SER:O	1:C:978:ILE:HG13	2.18	0.43
1:D:159:ALA:HB2	1:D:177:LEU:HD11	2.01	0.43
1:E:422:GLU:HB3	1:E:423:GLU:HG3	2.00	0.43
1:E:883:LEU:HD21	1:E:938:ILE:HD11	1.99	0.43
1:E:922:PHE:O	1:E:926:LEU:HB2	2.18	0.43
1:E:952:GLY:O	1:E:1035:ILE:HB	2.18	0.43
1:F:34:GLN:HB2	1:F:333:VAL:CG2	2.33	0.43
1:F:456:MET:HB3	1:F:871:LEU:HD21	1.99	0.43
1:F:535:LEU:HD21	1:F:1022:VAL:HG21	2.01	0.43
1:F:572:PHE:C	1:F:573:MET:HG2	2.43	0.43
1:F:1008:THR:O	1:F:1012:LEU:HB2	2.18	0.43
1:A:190:PRO:HG3	1:A:784:TRP:CZ2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASP:OD1	1:C:222:THR:HG21	2.18	0.43
1:A:416:VAL:HG21	1:A:493:CYS:SG	2.58	0.43
1:B:65:ILE:O	1:B:69:MET:HG2	2.17	0.43
1:B:573:MET:O	1:B:661:PHE:HD2	2.01	0.43
1:C:493:CYS:SG	1:C:497:LEU:HD22	2.58	0.43
1:C:564:LEU:HD12	1:C:564:LEU:HA	1.83	0.43
1:C:602:GLU:HG3	1:C:605:ASN:HD22	1.84	0.43
1:C:641:ALA:O	1:C:644:MET:HB3	2.18	0.43
1:C:772:ALA:O	1:C:776:MET:HE3	2.18	0.43
1:C:901:PRO:O	1:C:905:ILE:HG22	2.19	0.43
1:C:936:ASN:ND2	1:C:1010:THR:HG22	2.33	0.43
1:D:45:ILE:HD12	1:D:90:ILE:HD12	2.00	0.43
1:D:62:THR:OG1	1:D:88:VAL:HG21	2.18	0.43
1:E:415:ASN:OD1	1:E:418:ARG:NH1	2.52	0.43
1:E:757:PHE:HE1	1:E:759:ASP:HB2	1.79	0.43
1:F:11:PHE:C	1:F:11:PHE:CD2	2.97	0.43
1:F:328:ASP:O	1:F:331:PRO:HD2	2.19	0.43
1:F:525:HIS:O	1:F:528:THR:N	2.51	0.43
1:A:700:GLU:HB3	1:A:842:LEU:HD22	1.99	0.43
1:A:926:LEU:HD22	3:A:1103:LMT:C4	2.48	0.43
1:B:602:GLU:HB3	1:B:606:VAL:HG23	1.99	0.43
1:C:38:ILE:HG23	1:C:462:SER:HB2	2.00	0.43
1:C:83:ASP:HA	1:C:809:PRO:O	2.19	0.43
1:C:659:PHE:HE2	1:C:712:ARG:HB3	1.83	0.43
1:D:229:GLN:HG2	1:E:586:ARG:HE	1.84	0.43
1:D:559:LEU:HG	1:D:560:PRO:HD2	1.99	0.43
1:D:572:PHE:CE2	1:D:624:VAL:HB	2.54	0.43
1:D:898:LEU:HB3	1:D:1020:PHE:CE2	2.54	0.43
1:D:939:LEU:HD23	1:D:939:LEU:HA	1.67	0.43
1:E:106:GLN:HA	1:E:109:ASN:HD21	1.83	0.43
1:E:483:LEU:O	1:E:487:ILE:N	2.49	0.43
1:F:30:LEU:HA	1:F:31:PRO:HD3	1.92	0.43
1:F:171:GLY:HA3	1:F:302:THR:HG23	2.01	0.43
1:F:666:ILE:CG2	1:F:669:LEU:HB2	2.49	0.43
1:F:898:LEU:HD13	1:F:1020:PHE:CD2	2.54	0.43
1:F:935:LYS:HZ2	1:F:973:THR:HG21	1.82	0.43
1:F:1017:VAL:O	1:F:1020:PHE:HB2	2.18	0.43
1:A:152:GLU:H	1:A:152:GLU:HG2	1.29	0.43
1:A:631:ASP:OD1	1:A:631:ASP:N	2.51	0.43
1:A:881:LEU:HD12	1:C:18:ILE:HG13	2.00	0.43
1:A:939:LEU:HD23	1:A:939:LEU:HA	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:ARG:HG2	1:A:972:MET:HE2	2.01	0.43
1:B:203:VAL:O	1:B:207:ILE:HG13	2.19	0.43
1:C:370:ILE:O	1:C:374:VAL:HG23	2.18	0.43
1:C:398:MET:HE3	1:C:398:MET:HB3	1.75	0.43
1:C:990:ALA:O	1:C:992:SER:N	2.51	0.43
1:D:490:PRO:O	1:D:493:CYS:HB2	2.19	0.43
1:D:509:LYS:O	1:D:511:GLY:N	2.50	0.43
1:F:240:LEU:HD12	1:F:246:PHE:CG	2.54	0.43
1:F:649:ALA:O	1:F:653:ILE:HG12	2.19	0.43
1:F:948:MET:HE2	1:F:958:ALA:HB3	2.01	0.43
1:A:534:ILE:CD1	1:A:1019:VAL:HG22	2.49	0.43
1:B:200:PRO:O	1:B:203:VAL:N	2.52	0.43
1:B:418:ARG:HD2	1:B:965:MET:HB2	1.99	0.43
1:B:419:VAL:HG21	1:B:434:SER:HB3	2.00	0.43
1:B:576:VAL:HG22	1:B:658:VAL:HG13	2.00	0.43
1:C:355:MET:HE3	1:C:355:MET:HB2	1.72	0.43
1:D:20:MET:HG2	1:D:374:VAL:HA	2.00	0.43
1:D:45:ILE:HA	1:D:128:SER:O	2.19	0.43
1:D:314:GLU:OE1	1:D:323:ILE:HD12	2.19	0.43
1:D:362:PHE:O	1:D:366:LEU:HG	2.18	0.43
1:D:568:ASP:O	1:D:629:TRP:CZ3	2.70	0.43
1:D:641:ALA:HA	1:D:644:MET:HE3	2.01	0.43
1:D:648:ARG:O	1:D:651:SER:OG	2.32	0.43
1:D:1025:ARG:HA	1:D:1025:ARG:HD2	1.86	0.43
1:E:647:THR:CG2	1:E:660:ALA:H	2.32	0.43
1:E:701:ALA:CB	1:E:711:VAL:HG11	2.47	0.43
1:F:393:LEU:HD13	1:F:466:ILE:HA	2.00	0.43
1:F:408:ASP:OD2	1:F:445:ILE:HD12	2.19	0.43
1:F:602:GLU:HB3	1:F:606:VAL:CG2	2.48	0.43
1:F:704:HIS:HE1	1:F:842:LEU:HD11	1.83	0.43
1:A:375:VAL:HG22	1:A:484:VAL:HG21	2.01	0.43
1:A:399:VAL:HG11	1:A:984:LEU:HD11	2.00	0.43
1:A:527:TYR:OH	1:A:963:VAL:HG22	2.19	0.43
1:A:531:VAL:HG12	1:A:535:LEU:HD12	1.99	0.43
1:A:1007:VAL:HG12	1:A:1008:THR:N	2.33	0.43
1:B:300:LEU:HD23	1:B:334:LYS:HG2	2.00	0.43
1:B:492:LEU:O	1:B:496:MET:HG2	2.18	0.43
1:B:598:TYR:HB2	1:B:609:VAL:HG21	2.01	0.43
1:B:694:ARG:NH2	1:B:717:GLU:OE1	2.52	0.43
1:C:188:MET:HE3	1:C:188:MET:HB2	1.79	0.43
1:C:213:GLN:HE22	1:C:238:THR:HG23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:PHE:HD2	1:C:972:MET:SD	2.41	0.43
1:C:371:ALA:O	1:C:375:VAL:HG23	2.18	0.43
1:C:759:ASP:OD1	1:C:760:ARG:HG3	2.19	0.43
1:C:812:GLU:HB2	1:C:819:SER:O	2.18	0.43
1:D:207:ILE:CD1	1:D:768:VAL:HG21	2.49	0.43
1:D:507:GLU:O	1:D:508:GLY:C	2.61	0.43
1:D:836:MET:HE1	1:D:862:ARG:HG3	2.01	0.43
2:D:1101:ERY:H312	2:D:1101:ERY:H303	2.00	0.43
1:E:157:TYR:CD2	1:E:162:MET:HE2	2.54	0.43
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.56	0.43
1:F:76:MET:HG3	1:F:95:GLU:CD	2.44	0.43
1:F:146:ASP:O	1:F:148:THR:N	2.51	0.43
1:F:435:MET:SD	1:F:490:PRO:HG3	2.59	0.43
1:F:438:ILE:HG22	1:F:943:PHE:HZ	1.83	0.43
1:F:897:MET:O	1:F:900:VAL:HG23	2.18	0.43
1:A:251:LEU:HD11	1:A:265:VAL:HG21	2.00	0.43
1:A:897:MET:C	1:A:899:VAL:H	2.26	0.43
1:B:540:ARG:O	1:B:543:VAL:HB	2.19	0.43
1:B:701:ALA:CB	1:B:711:VAL:HG11	2.49	0.43
1:B:1013:ALA:C	1:B:1015:PHE:N	2.76	0.43
1:C:200:PRO:O	1:C:203:VAL:N	2.52	0.43
1:C:393:LEU:O	1:C:396:PHE:HB2	2.19	0.43
1:D:53:ASP:OD1	1:D:56:THR:OG1	2.26	0.43
1:D:63:GLN:HE21	1:F:763:VAL:HG12	1.84	0.43
1:D:66:GLU:OE2	1:D:80:SER:OG	2.24	0.43
1:D:350:LEU:HD13	1:D:979:LEU:HB3	1.99	0.43
1:D:597:TYR:OH	1:D:646:ALA:HA	2.19	0.43
1:E:400:LEU:HG	1:E:924:VAL:HG12	2.01	0.43
1:E:591:LEU:HD11	1:E:620:GLY:HA3	2.00	0.43
1:E:738:ILE:H	1:E:738:ILE:HD12	1.83	0.43
1:E:936:ASN:CG	1:E:970:ILE:HD12	2.44	0.43
1:E:945:LYS:HZ2	1:E:1025:ARG:NH2	2.16	0.43
1:E:982:MET:CB	1:E:1003:MET:HE1	2.49	0.43
1:F:153:ASP:O	1:F:156:ASP:HB3	2.18	0.43
1:A:21:LEU:HA	1:A:21:LEU:HD13	1.70	0.42
1:A:162:MET:HG2	1:A:313:MET:SD	2.59	0.42
1:A:210:GLN:NE2	1:A:250:LEU:O	2.52	0.42
1:B:730:LYS:O	1:B:734:LEU:HG	2.19	0.42
1:C:362:PHE:CE2	1:C:366:LEU:HD21	2.53	0.42
1:C:898:LEU:HB3	1:C:1020:PHE:CE2	2.54	0.42
1:D:72:ILE:HD13	1:D:107:VAL:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:GLY:O	1:D:293:LEU:HD23	2.19	0.42
1:D:531:VAL:HG21	1:D:963:VAL:HG11	2.00	0.42
1:D:694:ARG:NH1	1:D:820:MET:SD	2.91	0.42
1:D:703:LYS:C	1:D:705:PRO:HD3	2.43	0.42
1:E:221:GLY:HA3	1:F:775:ARG:HH12	1.83	0.42
1:E:973:THR:HG22	1:E:974:SER:N	2.34	0.42
1:E:994:ALA:O	1:E:997:ALA:N	2.52	0.42
1:E:1021:PHE:C	1:E:1021:PHE:CD2	2.97	0.42
1:F:274:ASN:ND2	1:F:276:ASP:OD2	2.52	0.42
1:F:361:ASN:O	1:F:364:ALA:N	2.52	0.42
1:F:639:VAL:HG11	1:F:662:ASN:OD1	2.19	0.42
1:A:955:LEU:O	1:A:959:THR:HG23	2.19	0.42
1:B:72:ILE:HG23	1:B:106:GLN:HB3	2.00	0.42
1:B:251:LEU:HD21	1:B:262:LEU:HB2	2.00	0.42
1:B:517:ASN:O	1:B:521:GLU:HB2	2.19	0.42
1:C:5:PHE:C	1:C:5:PHE:HD2	2.27	0.42
1:E:139:VAL:HG13	1:E:178:PHE:CE1	2.54	0.42
1:F:452:VAL:HG13	1:F:879:VAL:HG23	2.02	0.42
1:A:279:ALA:HB3	1:A:286:ALA:O	2.19	0.42
1:B:45:ILE:HA	1:B:128:SER:O	2.19	0.42
1:B:62:THR:O	1:B:65:ILE:N	2.52	0.42
1:B:210:GLN:HE22	1:B:250:LEU:N	2.18	0.42
1:B:228:GLN:O	1:C:583:THR:HG21	2.19	0.42
1:B:353:LEU:HD22	1:B:353:LEU:HA	1.78	0.42
1:B:714:ASN:HB2	1:B:823:LEU:HG	2.01	0.42
1:B:738:ILE:HA	1:B:741:ILE:CD1	2.49	0.42
1:C:6:ILE:O	1:C:6:ILE:HG22	2.19	0.42
1:C:27:ILE:HD13	1:C:27:ILE:HG21	1.85	0.42
1:C:104:GLN:HG3	1:C:105:VAL:N	2.33	0.42
1:C:354:VAL:O	1:C:358:PHE:HB2	2.20	0.42
1:C:1006:MET:O	1:C:1009:ALA:HB3	2.19	0.42
1:D:669:LEU:CD1	1:D:670:GLY:H	2.24	0.42
1:D:752:SER:O	1:D:767:TYR:HA	2.20	0.42
1:E:222:THR:HA	1:E:224:PRO:HD3	2.00	0.42
1:E:975:LEU:O	1:E:979:LEU:HG	2.19	0.42
1:F:398:MET:HE3	1:F:398:MET:HB3	1.58	0.42
1:F:880:PHE:C	1:F:880:PHE:HD2	2.27	0.42
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.76	0.42
1:A:569:GLN:NE2	1:A:663:LEU:HG	2.34	0.42
1:A:777:LEU:O	1:A:780:ASP:N	2.44	0.42
1:B:21:LEU:HD23	1:B:21:LEU:HA	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:ARG:HH11	1:B:820:MET:CE	2.33	0.42
1:B:708:LEU:HD11	1:B:838:LEU:HD12	2.00	0.42
1:C:36:PRO:O	1:C:38:ILE:HG13	2.20	0.42
1:C:124:GLN:HG3	1:C:125:GLN:N	2.30	0.42
1:C:172:VAL:HG13	1:C:291:ILE:HG23	2.01	0.42
1:C:226:LYS:NZ	1:C:226:LYS:HB3	2.34	0.42
1:C:572:PHE:CE2	1:C:624:VAL:HB	2.53	0.42
1:C:675:PHE:HB2	1:C:854:TRP:CZ3	2.55	0.42
1:C:708:LEU:HD13	1:C:838:LEU:HD12	2.01	0.42
1:D:53:ASP:O	1:D:56:THR:HB	2.19	0.42
1:D:605:ASN:OD1	1:D:637:ASN:ND2	2.52	0.42
1:D:671:THR:OG1	1:D:674:GLY:HA3	2.20	0.42
1:D:1035:ILE:HB	1:D:1036:GLU:H	1.43	0.42
1:E:293:LEU:HD11	1:E:297:ALA:O	2.19	0.42
1:E:408:ASP:OD2	1:E:481:SER:OG	2.19	0.42
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.84	0.42
1:E:482:VAL:O	1:E:486:LEU:HG	2.19	0.42
1:E:516:PHE:HA	1:E:519:MET:HE2	2.00	0.42
1:E:540:ARG:HB2	1:E:541:TYR:HD1	1.84	0.42
1:E:1003:MET:HB2	1:E:1003:MET:HE3	1.83	0.42
1:F:19:ILE:O	1:F:22:ALA:HB3	2.19	0.42
1:F:631:ASP:OD1	1:F:631:ASP:N	2.51	0.42
1:F:636:GLU:N	1:F:636:GLU:OE2	2.52	0.42
1:F:638:LYS:HE2	1:F:640:GLU:HG3	2.00	0.42
1:F:796:PHE:CD1	1:F:799:PHE:HE2	2.36	0.42
1:F:939:LEU:HB3	1:F:966:ARG:HD2	2.01	0.42
1:A:139:VAL:HB	1:A:327:TYR:HB3	2.00	0.42
1:A:963:VAL:CG2	1:A:1018:PRO:HG3	2.49	0.42
1:B:228:GLN:NE2	1:B:230:LEU:O	2.49	0.42
1:B:251:LEU:HD11	1:B:262:LEU:HA	2.02	0.42
1:C:187:TRP:HE3	1:C:770:SER:O	2.03	0.42
1:C:893:PRO:O	1:C:895:SER:N	2.52	0.42
1:D:143:ILE:HG22	1:D:286:ALA:CB	2.49	0.42
1:D:168:ARG:HB3	1:E:75:LEU:HD22	2.02	0.42
1:D:182:TYR:HD1	1:D:182:TYR:HA	1.69	0.42
1:D:889:SER:HB2	1:D:892:ILE:HD12	2.00	0.42
1:D:990:ALA:C	1:D:992:SER:H	2.27	0.42
1:E:53:ASP:OD2	1:E:55:LYS:N	2.50	0.42
1:E:196:PHE:HB3	1:E:252:LYS:HE2	2.01	0.42
1:E:527:TYR:OH	1:E:1014:ILE:HB	2.20	0.42
1:E:576:VAL:HB	1:E:620:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:977:PHE:HD2	1:E:1006:MET:HG3	1.85	0.42
1:F:140:VAL:HG11	1:F:310:LEU:HD21	2.01	0.42
1:F:376:LEU:O	1:F:379:THR:N	2.51	0.42
1:A:61:VAL:HG21	1:A:122:VAL:HG21	2.01	0.42
1:A:151:GLN:HE21	1:A:152:GLU:CA	2.30	0.42
1:A:244:GLU:CG	1:A:248:LYS:HE2	2.47	0.42
1:B:214:VAL:HG11	1:C:742:ASN:HB3	2.02	0.42
1:C:188:MET:HA	1:C:266:ALA:HB2	2.00	0.42
1:C:352:PHE:CD2	1:C:352:PHE:C	2.97	0.42
1:C:613:ASN:HD22	1:C:613:ASN:C	2.28	0.42
1:C:693:ALA:HB1	1:C:850:VAL:HG11	2.00	0.42
1:C:1010:THR:C	1:C:1012:LEU:N	2.76	0.42
1:D:13:TRP:CE2	1:D:492:LEU:HD21	2.55	0.42
1:D:923:GLN:HG2	3:D:1103:LMT:H52	2.01	0.42
1:E:435:MET:HE1	1:E:485:ALA:O	2.19	0.42
1:E:681:ASP:HB3	1:E:818:PRO:O	2.20	0.42
1:E:748:ALA:HB3	1:E:749:TRP:HD1	1.84	0.42
1:E:836:MET:HG2	1:E:854:TRP:CH2	2.55	0.42
1:E:982:MET:HB3	1:E:982:MET:HE2	1.69	0.42
1:F:27:ILE:HG23	1:F:380:PHE:HB3	2.02	0.42
1:F:552:MET:HE2	1:F:552:MET:HB3	1.89	0.42
1:F:610:PHE:O	1:F:623:PHE:N	2.43	0.42
1:A:39:ALA:HA	1:A:40:PRO:HD2	1.68	0.42
1:A:94:PHE:CZ	1:A:103:ALA:HB1	2.55	0.42
1:A:229:GLN:HE21	1:B:586:ARG:HD3	1.83	0.42
1:A:505:HIS:C	1:A:507:GLU:N	2.78	0.42
1:A:770:SER:HB2	1:A:784:TRP:CH2	2.55	0.42
1:B:370:ILE:O	1:B:374:VAL:HG23	2.20	0.42
1:B:559:LEU:HD12	1:B:912:THR:OG1	2.19	0.42
1:C:108:GLN:HB3	1:C:129:VAL:HG11	2.01	0.42
1:C:201:VAL:HG21	1:C:740:ASP:OD1	2.19	0.42
1:C:698:LEU:CD1	1:C:713:PRO:HD3	2.49	0.42
1:D:417:GLU:OE1	1:D:497:LEU:HD11	2.20	0.42
2:D:1101:ERY:H4	2:D:1101:ERY:H71	1.41	0.42
1:E:267:LYS:HD3	1:E:771:GLU:OE2	2.20	0.42
1:E:293:LEU:HD13	1:E:294:ALA:O	2.20	0.42
1:E:654:LYS:HE3	1:E:654:LYS:HB3	1.78	0.42
1:E:812:GLU:HB2	1:E:819:SER:O	2.19	0.42
1:F:509:LYS:HB3	1:F:514:GLY:HA3	2.02	0.42
1:F:736:VAL:HG11	1:F:786:VAL:HB	2.02	0.42
1:A:57:VAL:HA	1:A:60:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASN:O	1:A:110:LYS:HB3	2.19	0.42
1:A:298:ASN:HB3	1:A:301:ASP:HB2	2.02	0.42
1:A:905:ILE:O	1:A:905:ILE:HG13	2.19	0.42
1:B:185:ARG:NH1	1:B:767:TYR:HD1	2.18	0.42
1:B:564:LEU:HD11	1:B:666:ILE:HD12	2.00	0.42
1:B:674:GLY:H	1:B:832:THR:HG23	1.85	0.42
1:C:311:ALA:O	1:C:315:PRO:HD3	2.19	0.42
1:C:707:MET:HG3	1:C:838:LEU:HG	2.02	0.42
1:C:836:MET:HG2	1:C:854:TRP:CH2	2.55	0.42
1:C:887:TYR:C	1:C:889:SER:H	2.19	0.42
1:D:354:VAL:HG21	1:D:975:LEU:HB3	2.00	0.42
1:D:813:ARG:NH2	1:D:818:PRO:HD3	2.34	0.42
1:E:249:ILE:O	1:E:262:LEU:N	2.48	0.42
1:E:390:ILE:HG23	1:E:395:MET:SD	2.59	0.42
1:E:520:PHE:O	1:E:523:SER:OG	2.38	0.42
1:F:11:PHE:O	1:F:11:PHE:HD2	2.01	0.42
1:F:13:TRP:NE1	1:F:492:LEU:HD21	2.34	0.42
1:F:543:VAL:O	1:F:546:LEU:HB2	2.20	0.42
1:F:669:LEU:HD22	1:F:856:GLY:HA2	2.02	0.42
1:A:351:VAL:O	1:A:355:MET:HB2	2.20	0.42
1:A:738:ILE:H	1:A:738:ILE:HD12	1.84	0.42
1:A:1035:ILE:HG22	1:A:1036:GLU:O	2.19	0.42
1:B:294:ALA:HB3	1:B:297:ALA:CB	2.49	0.42
1:B:453:PHE:CD1	1:B:474:ILE:HG22	2.55	0.42
1:C:152:GLU:HG2	1:C:275:TYR:HE2	1.84	0.42
1:C:654:LYS:HD3	1:C:654:LYS:HA	1.60	0.42
1:C:876:LEU:HD23	1:C:876:LEU:HA	1.70	0.42
1:C:941:VAL:HG13	1:C:1021:PHE:CD1	2.54	0.42
1:C:966:ARG:C	1:C:969:PRO:HD2	2.45	0.42
1:D:251:LEU:CD1	1:D:265:VAL:HG21	2.50	0.42
1:D:448:VAL:O	1:D:451:ALA:HB3	2.20	0.42
1:D:574:THR:CG2	1:D:622:ALA:HB3	2.49	0.42
1:D:610:PHE:O	1:D:622:ALA:HA	2.19	0.42
1:D:654:LYS:HA	1:D:654:LYS:HD3	1.70	0.42
1:D:795:PRO:O	1:D:798:ALA:HB3	2.20	0.42
1:E:3:ASN:HA	1:E:6:ILE:CD1	2.50	0.42
1:E:455:PRO:O	1:E:871:LEU:HD13	2.20	0.42
1:E:694:ARG:HD3	1:E:820:MET:HE2	2.01	0.42
1:E:917:THR:O	1:E:919:ASP:N	2.52	0.42
1:F:5:PHE:C	1:F:5:PHE:CD2	2.98	0.42
1:F:486:LEU:O	1:F:490:PRO:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:769:MET:HG2	1:F:770:SER:H	1.85	0.42
1:A:821:GLU:OE1	2:A:1101:ERY:H24	2.20	0.42
1:A:1021:PHE:CZ	1:A:1025:ARG:HG3	2.55	0.42
1:B:98:THR:HG22	1:B:99:ASP:N	2.35	0.42
1:B:130:GLU:HG2	1:C:113:LEU:HD21	2.02	0.42
1:B:281:PHE:HB2	1:B:610:PHE:CD1	2.55	0.42
1:B:484:VAL:O	1:B:489:THR:HG23	2.19	0.42
1:B:675:PHE:CE1	1:B:677:PHE:HB2	2.54	0.42
1:B:831:SER:OG	1:B:834:GLU:HG3	2.20	0.42
1:B:982:MET:HB3	1:B:982:MET:HE2	1.46	0.42
1:C:887:TYR:C	1:C:889:SER:N	2.75	0.42
1:C:935:LYS:O	1:C:938:ILE:HB	2.19	0.42
1:D:1002:VAL:HG12	1:D:1003:MET:N	2.35	0.42
1:E:30:LEU:HD12	1:E:30:LEU:HA	1.93	0.42
1:E:310:LEU:HD23	1:E:325:TYR:OH	2.20	0.42
1:E:559:LEU:HG	1:E:560:PRO:HD2	2.02	0.42
1:F:447:MET:O	1:F:451:ALA:HB2	2.20	0.42
1:F:452:VAL:HG23	1:F:453:PHE:CD1	2.55	0.42
1:F:590:VAL:O	1:F:593:GLU:HB2	2.19	0.42
1:F:708:LEU:HD13	1:F:838:LEU:HD12	2.02	0.42
1:F:757:PHE:HE1	1:F:759:ASP:HB2	1.85	0.42
1:F:1010:THR:O	1:F:1012:LEU:N	2.53	0.42
1:A:80:SER:HA	1:A:89:GLN:O	2.20	0.41
1:A:378:GLY:O	1:A:381:ALA:HB3	2.19	0.41
1:A:420:MET:HE3	1:A:500:ILE:HD12	2.02	0.41
1:A:454:VAL:O	1:A:457:ALA:HB3	2.20	0.41
1:A:456:MET:HE1	1:A:924:VAL:HG22	2.02	0.41
1:A:642:ILE:HA	1:A:645:ARG:NH1	2.35	0.41
1:B:277:ILE:HG22	1:B:614:GLY:HA3	2.00	0.41
1:B:373:PRO:O	1:B:376:LEU:HB2	2.19	0.41
1:C:55:LYS:HE2	1:C:55:LYS:HB3	1.91	0.41
1:C:143:ILE:O	1:C:321:LEU:HD22	2.20	0.41
1:C:156:ASP:OD2	1:C:182:TYR:HB2	2.19	0.41
1:D:723:LYS:HG2	1:D:803:ARG:CZ	2.50	0.41
1:D:746:GLY:O	1:D:748:ALA:N	2.53	0.41
1:D:776:MET:HE2	1:F:225:VAL:HG22	2.01	0.41
1:E:110:LYS:HD3	1:E:110:LYS:HA	1.53	0.41
1:E:124:GLN:NE2	1:E:753:TYR:HD2	2.18	0.41
1:E:250:LEU:HD12	1:E:260:VAL:O	2.19	0.41
1:F:344:LEU:HD11	1:F:376:LEU:HD13	2.01	0.41
1:F:453:PHE:CE2	1:F:474:ILE:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:509:LYS:CG	1:F:513:PHE:HB2	2.50	0.41
1:A:185:ARG:HB3	1:A:187:TRP:NE1	2.35	0.41
1:A:425:LEU:HB3	1:A:429:GLU:HG3	2.01	0.41
1:A:574:THR:HG21	1:A:594:VAL:HG11	2.01	0.41
1:A:940:ILE:HG12	1:A:966:ARG:NH2	2.35	0.41
1:B:524:THR:O	1:B:527:TYR:HB3	2.19	0.41
1:B:1031:LYS:HA	1:B:1032:ASN:HA	1.76	0.41
1:C:415:ASN:OD1	1:C:418:ARG:NH2	2.51	0.41
1:C:536:ARG:NH1	3:C:1101:LMT:O4'	2.53	0.41
1:D:31:PRO:HB2	1:D:389:SER:CB	2.50	0.41
1:D:324:VAL:HG12	1:D:326:PRO:HD3	2.01	0.41
1:D:434:SER:O	1:D:437:GLN:N	2.53	0.41
1:D:977:PHE:CD2	1:D:1006:MET:HG3	2.54	0.41
1:E:36:PRO:O	1:E:38:ILE:HG13	2.19	0.41
1:E:65:ILE:O	1:E:69:MET:HG2	2.19	0.41
1:E:75:LEU:HG	1:E:76:MET:N	2.35	0.41
1:F:812:GLU:HB2	1:F:819:SER:O	2.19	0.41
1:B:9:PRO:HB3	1:B:495:THR:OG1	2.21	0.41
1:B:76:MET:HB3	1:B:77:TYR:HD2	1.85	0.41
1:B:115:MET:HB2	1:B:116:PRO:HD3	2.02	0.41
1:B:298:ASN:HB3	1:B:301:ASP:HB2	2.02	0.41
1:B:736:VAL:HG11	1:B:786:VAL:HB	2.01	0.41
1:B:910:ALA:O	1:B:914:ARG:HB2	2.20	0.41
1:C:69:MET:O	1:C:72:ILE:HD11	2.19	0.41
1:C:360:GLN:HE21	1:C:360:GLN:HB3	1.66	0.41
1:C:567:GLU:O	1:C:569:GLN:HG3	2.20	0.41
1:C:966:ARG:O	1:C:969:PRO:HG2	2.21	0.41
1:C:1017:VAL:N	1:C:1018:PRO:HD2	2.36	0.41
1:E:68:ASN:HB3	1:E:114:ALA:HB2	2.01	0.41
1:E:340:VAL:HG11	1:E:395:MET:HE3	2.02	0.41
1:E:784:TRP:C	1:E:785:TYR:HD2	2.29	0.41
1:F:966:ARG:O	1:F:970:ILE:HG13	2.21	0.41
1:A:61:VAL:CG2	1:A:122:VAL:HG21	2.51	0.41
1:A:149:MET:HG3	1:A:154:ILE:HG13	2.01	0.41
1:A:914:ARG:HD3	1:A:916:LEU:HD23	2.01	0.41
1:B:42:ALA:HB2	1:B:93:THR:HG23	2.01	0.41
1:B:157:TYR:HD2	1:B:162:MET:HE2	1.85	0.41
1:B:190:PRO:HB3	1:B:784:TRP:CZ3	2.55	0.41
1:B:431:THR:O	1:B:432:ARG:C	2.63	0.41
1:C:3:ASN:ND2	1:C:435:MET:HG3	2.34	0.41
1:C:36:PRO:HD3	1:C:391:ASN:CG	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ASN:HD22	1:C:276:ASP:CG	2.28	0.41
1:C:716:LEU:HD23	1:C:810:ARG:HE	1.84	0.41
1:D:888:GLU:OE1	1:F:8:ARG:HB3	2.20	0.41
1:D:1034:ASP:HA	1:D:1035:ILE:O	2.19	0.41
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.50	0.41
1:E:939:LEU:HD23	1:E:939:LEU:HA	1.76	0.41
1:F:40:PRO:HA	1:F:41:PRO:HD3	1.94	0.41
1:F:133:SER:HB2	1:F:292:LYS:HD3	2.02	0.41
1:F:143:ILE:HG22	1:F:286:ALA:CB	2.50	0.41
1:F:417:GLU:OE2	1:F:497:LEU:HD11	2.21	0.41
1:F:959:THR:O	1:F:960:LEU:C	2.62	0.41
1:A:5:PHE:HE2	1:A:11:PHE:CD1	2.39	0.41
1:A:536:ARG:NH1	3:A:1102:LMT:O4'	2.53	0.41
1:A:955:LEU:HD23	1:A:1026:ARG:NH2	2.35	0.41
1:A:990:ALA:O	1:A:992:SER:N	2.54	0.41
1:B:707:MET:CE	1:B:834:GLU:HB3	2.49	0.41
1:B:882:CYS:O	1:B:885:ALA:HB3	2.21	0.41
1:C:110:LYS:HA	1:C:110:LYS:HD3	1.61	0.41
1:C:398:MET:HG2	1:C:473:THR:CG2	2.49	0.41
1:C:978:ILE:O	1:C:982:MET:HB2	2.20	0.41
1:D:35:TYR:HE1	1:D:665:ALA:HB1	1.84	0.41
1:D:36:PRO:O	1:D:38:ILE:HG13	2.20	0.41
1:D:405:LEU:HD23	1:D:481:SER:HB3	2.02	0.41
1:D:631:ASP:N	1:D:631:ASP:OD1	2.53	0.41
1:D:653:ILE:HG13	1:D:654:LYS:HE2	2.02	0.41
1:D:784:TRP:HB2	1:D:796:PHE:CD2	2.56	0.41
1:D:948:MET:CE	1:D:955:LEU:HA	2.50	0.41
1:E:158:VAL:CG1	1:E:177:LEU:HD21	2.51	0.41
1:E:165:ALA:HB3	1:E:313:MET:HE3	1.97	0.41
1:E:564:LEU:HD13	1:E:666:ILE:HD12	2.01	0.41
1:E:677:PHE:HB3	1:E:822:ILE:HB	2.03	0.41
1:E:751:GLY:CA	1:E:769:MET:HG3	2.50	0.41
1:E:794:VAL:HG12	1:E:798:ALA:HB3	2.02	0.41
1:E:890:TRP:O	1:E:893:PRO:HD2	2.20	0.41
1:E:904:VAL:O	1:E:906:GLY:N	2.53	0.41
1:E:919:ASP:OD1	1:E:921:TYR:N	2.53	0.41
1:F:157:TYR:CD2	1:F:162:MET:HE2	2.55	0.41
1:F:438:ILE:O	1:F:441:ALA:HB3	2.21	0.41
1:F:569:GLN:HA	1:F:629:TRP:HH2	1.86	0.41
1:F:632:ARG:HA	1:F:637:ASN:HD22	1.84	0.41
1:A:58:GLN:OE1	1:A:811:LEU:HD13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ASN:OD1	1:A:619:THR:HG23	2.21	0.41
1:B:586:ARG:O	1:B:589:LYS:HB3	2.21	0.41
1:B:757:PHE:CE1	1:B:759:ASP:HB2	2.56	0.41
1:D:72:ILE:HG23	1:D:106:GLN:HB3	2.02	0.41
1:D:210:GLN:HE22	1:D:250:LEU:CA	2.34	0.41
1:D:467:TYR:CE2	1:D:920:VAL:HG22	2.56	0.41
1:D:534:ILE:HD11	1:D:1019:VAL:HG22	2.03	0.41
1:E:32:VAL:H	1:E:298:ASN:ND2	2.18	0.41
1:E:188:MET:HE3	1:E:784:TRP:HZ3	1.85	0.41
1:E:956:ILE:O	1:E:960:LEU:HB2	2.20	0.41
1:F:84:SER:HB3	1:F:809:PRO:HA	2.02	0.41
1:F:948:MET:HE1	1:F:1021:PHE:HE2	1.86	0.41
1:A:139:VAL:O	1:A:139:VAL:HG12	2.20	0.41
1:A:426:PRO:HB2	1:A:429:GLU:CD	2.45	0.41
1:B:99:ASP:HB3	1:B:102:ILE:HB	2.02	0.41
1:B:213:GLN:HA	1:B:237:GLN:O	2.21	0.41
1:B:222:THR:HA	1:B:224:PRO:HD3	2.02	0.41
1:B:647:THR:HG23	1:B:660:ALA:HB3	2.02	0.41
1:B:712:ARG:HD2	1:B:823:LEU:HB2	2.03	0.41
1:B:985:VAL:HG22	1:B:999:GLY:CA	2.51	0.41
1:C:27:ILE:HA	1:C:30:LEU:HB2	2.02	0.41
1:C:375:VAL:HA	1:C:480:LEU:HD13	2.03	0.41
1:C:456:MET:HE3	1:C:467:TYR:O	2.20	0.41
1:C:914:ARG:HD2	1:C:1000:THR:HG21	2.01	0.41
1:C:940:ILE:HG12	1:C:966:ARG:NH2	2.35	0.41
1:C:982:MET:HB3	1:C:982:MET:HE2	1.64	0.41
1:D:47:ALA:HB2	1:D:127:VAL:HG13	2.03	0.41
1:D:137:LEU:HG	1:D:138:MET:HG2	2.02	0.41
1:D:156:ASP:O	1:D:157:TYR:C	2.61	0.41
1:D:201:VAL:O	1:D:205:THR:OG1	2.34	0.41
1:D:563:PHE:CD2	1:D:666:ILE:HD13	2.56	0.41
1:E:113:LEU:HD23	1:E:113:LEU:HA	1.92	0.41
1:E:143:ILE:HG21	1:E:281:PHE:CD2	2.56	0.41
1:E:452:VAL:HA	1:E:875:SER:OG	2.21	0.41
1:E:530:SER:CB	3:E:1101:LMT:O2'	2.69	0.41
1:E:1015:PHE:HE2	3:E:1101:LMT:C1	2.33	0.41
1:F:181:GLN:HG2	1:F:182:TYR:N	2.35	0.41
1:F:738:ILE:H	1:F:738:ILE:HD12	1.85	0.41
1:A:154:ILE:O	1:A:157:TYR:N	2.54	0.41
1:A:410:ILE:O	1:A:411:VAL:C	2.64	0.41
1:A:602:GLU:HB3	1:A:606:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:ALA:N	1:A:869:PRO:HD2	2.36	0.41
1:A:955:LEU:HB2	1:A:1032:ASN:O	2.20	0.41
1:B:916:LEU:HD13	1:B:916:LEU:HA	1.83	0.41
3:B:2100:LMT:H6E	3:B:2100:LMT:O5B	2.21	0.41
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.86	0.41
1:D:335:ILE:O	1:D:339:GLU:HG2	2.20	0.41
1:D:559:LEU:HD22	1:D:918:ASN:HB2	2.03	0.41
1:D:722:PHE:HD1	1:D:804:TRP:CE2	2.39	0.41
1:D:865:GLY:O	1:D:866:ASN:HB2	2.21	0.41
1:D:941:VAL:HG22	1:D:1021:PHE:HB2	2.02	0.41
1:D:954:GLY:HA2	1:D:1033:GLU:O	2.21	0.41
1:E:211:ASN:OD1	1:E:239:ARG:HA	2.20	0.41
1:E:240:LEU:HB2	1:E:246:PHE:CZ	2.56	0.41
1:E:496:MET:HE3	1:E:496:MET:HB2	1.83	0.41
1:F:382:VAL:O	1:F:386:PHE:HD2	2.03	0.41
1:F:548:ILE:O	1:F:905:ILE:HD13	2.21	0.41
1:F:811:LEU:HA	1:F:811:LEU:HD23	1.83	0.41
1:F:914:ARG:HD2	1:F:1000:THR:HG21	2.03	0.41
1:A:191:ASN:O	1:A:193:LEU:N	2.54	0.41
1:A:332:PHE:O	1:A:336:SER:HB3	2.21	0.41
1:A:355:MET:HE3	1:A:355:MET:HA	2.02	0.41
1:A:398:MET:O	1:A:402:ILE:HG13	2.21	0.41
1:A:714:ASN:N	1:A:821:GLU:O	2.51	0.41
1:A:846:LEU:HB3	1:A:847:PRO:HD2	2.02	0.41
1:A:932:LEU:O	1:A:933:SER:C	2.64	0.41
1:A:980:GLY:O	1:A:983:PRO:HD2	2.20	0.41
1:B:426:PRO:HD2	1:B:429:GLU:HB3	2.02	0.41
1:B:534:ILE:HD11	1:B:1019:VAL:CG2	2.50	0.41
1:B:616:GLY:O	1:B:618:ASN:N	2.54	0.41
1:B:771:GLU:O	1:B:775:ARG:HG2	2.21	0.41
1:B:790:ASP:OD2	1:B:792:GLN:N	2.53	0.41
1:B:883:LEU:HD23	1:B:883:LEU:HA	1.60	0.41
1:B:945:LYS:NZ	1:B:1025:ARG:NH2	2.68	0.41
1:C:6:ILE:C	1:C:8:ARG:H	2.28	0.41
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.99	0.41
1:C:358:PHE:CD2	1:C:972:MET:SD	3.14	0.41
1:C:474:ILE:O	1:C:475:VAL:C	2.62	0.41
1:C:599:LEU:HD23	1:C:599:LEU:HA	1.90	0.41
1:C:602:GLU:HG3	1:C:605:ASN:ND2	2.36	0.41
1:C:977:PHE:O	1:C:978:ILE:C	2.63	0.41
1:D:17:ILE:HG23	1:D:21:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:THR:OG1	1:E:275:TYR:O	2.39	0.41
1:D:360:GLN:HE21	1:D:360:GLN:HB3	1.68	0.41
1:D:395:MET:HE3	1:D:395:MET:HB3	1.85	0.41
1:D:410:ILE:O	1:D:411:VAL:C	2.63	0.41
1:D:602:GLU:HB3	1:D:606:VAL:HG23	2.03	0.41
1:D:722:PHE:CD1	1:D:804:TRP:CE2	3.09	0.41
1:D:956:ILE:H	1:D:956:ILE:HG13	1.47	0.41
1:E:460:GLY:N	1:E:867:GLN:OE1	2.44	0.41
1:E:886:LEU:HA	1:E:886:LEU:HD12	1.80	0.41
1:E:893:PRO:O	1:E:894:PHE:C	2.64	0.41
1:E:1010:THR:C	1:E:1012:LEU:N	2.76	0.41
1:E:1032:ASN:OD1	1:E:1033:GLU:HA	2.21	0.41
1:F:13:TRP:HE1	1:F:492:LEU:HD21	1.86	0.41
1:F:408:ASP:O	1:F:412:VAL:HG23	2.20	0.41
1:F:548:ILE:HD13	1:F:1012:LEU:HD21	2.03	0.41
1:F:557:VAL:C	1:F:559:LEU:H	2.29	0.41
1:F:572:PHE:CE1	1:F:643:THR:HG22	2.56	0.41
1:F:716:LEU:HD13	1:F:716:LEU:HA	1.93	0.41
1:F:770:SER:HG	1:F:775:ARG:HG2	1.85	0.41
1:F:897:MET:HE3	1:F:897:MET:HB3	1.86	0.41
1:F:967:LEU:O	1:F:970:ILE:HB	2.21	0.41
1:F:974:SER:CB	1:F:1010:THR:HG21	2.50	0.41
1:F:1017:VAL:N	1:F:1018:PRO:HD2	2.35	0.41
1:A:668:GLU:HA	2:A:1101:ERY:H213	2.02	0.41
1:A:909:LEU:O	1:A:913:PHE:HB2	2.21	0.41
1:B:2:PRO:O	1:B:6:ILE:HD12	2.21	0.41
1:B:376:LEU:O	1:B:377:LEU:C	2.63	0.41
1:B:572:PHE:HD1	1:B:661:PHE:O	2.03	0.41
1:B:842:LEU:HD23	1:B:842:LEU:HA	1.85	0.41
1:B:1019:VAL:H	1:B:1019:VAL:HG23	1.56	0.41
1:C:26:ALA:HB1	1:C:384:ALA:CB	2.51	0.41
1:C:79:SER:HB3	1:C:814:TYR:CD1	2.44	0.41
1:C:216:ALA:HB1	1:C:234:ILE:HG22	2.03	0.41
1:C:361:ASN:O	1:C:364:ALA:N	2.51	0.41
1:C:872:TYR:O	1:C:876:LEU:HG	2.20	0.41
1:C:968:ARG:HG2	1:C:972:MET:HE2	2.01	0.41
1:C:1007:VAL:HG12	1:C:1008:THR:N	2.34	0.41
1:D:189:ASN:O	1:D:193:LEU:HG	2.21	0.41
1:E:188:MET:HA	1:E:266:ALA:CB	2.51	0.41
1:E:190:PRO:HB2	1:E:783:ASP:O	2.20	0.41
1:E:616:GLY:O	1:E:618:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:ALA:HB2	1:F:668:GLU:CG	2.51	0.41
1:F:407:ASP:HB2	1:F:973:THR:OG1	2.21	0.41
1:F:414:GLU:HG2	1:F:968:ARG:HH11	1.85	0.41
1:F:697:LEU:HD21	1:F:839:MET:HE1	2.03	0.41
1:F:723:LYS:HG2	1:F:803:ARG:NH1	2.36	0.41
1:F:927:LEU:HD22	1:F:930:ILE:HD12	2.04	0.41
1:A:575:MET:HE2	1:A:621:ILE:HD12	2.03	0.40
1:B:567:GLU:O	1:B:569:GLN:HG3	2.21	0.40
1:C:434:SER:O	1:C:437:GLN:N	2.51	0.40
1:C:587:THR:HG21	1:C:617:GLN:O	2.22	0.40
1:C:951:GLU:O	1:C:953:LYS:N	2.54	0.40
1:D:182:TYR:O	1:D:764:LYS:HB3	2.21	0.40
1:D:446:ALA:HB2	1:D:482:VAL:HG21	2.03	0.40
1:D:511:GLY:HA2	1:D:515:TRP:NE1	2.36	0.40
1:D:917:THR:O	1:D:919:ASP:N	2.54	0.40
1:D:920:VAL:HG12	1:D:921:TYR:N	2.36	0.40
1:E:240:LEU:HD12	1:E:246:PHE:CD2	2.56	0.40
1:E:405:LEU:HD23	1:E:481:SER:HB3	2.03	0.40
1:E:694:ARG:NH1	1:E:820:MET:HE1	2.28	0.40
1:F:5:PHE:C	1:F:7:ASP:N	2.73	0.40
1:F:402:ILE:HD13	1:F:402:ILE:HG21	1.88	0.40
1:A:396:PHE:O	1:A:400:LEU:HB2	2.22	0.40
1:A:939:LEU:CB	1:A:966:ARG:HD2	2.50	0.40
1:A:1025:ARG:C	1:A:1027:ARG:H	2.28	0.40
1:B:174:ASP:HB3	1:B:292:LYS:HB2	2.04	0.40
1:B:555:LEU:HA	1:B:555:LEU:HD23	1.73	0.40
1:B:951:GLU:O	1:B:953:LYS:N	2.54	0.40
1:C:152:GLU:HG2	1:C:275:TYR:CE2	2.56	0.40
1:C:188:MET:HE1	1:C:200:PRO:HG3	2.02	0.40
1:C:591:LEU:HB3	1:C:611:ALA:HB1	2.03	0.40
1:C:600:THR:C	1:C:602:GLU:H	2.29	0.40
1:D:42:ALA:HB2	1:D:93:THR:HG22	2.03	0.40
1:D:225:VAL:H	1:E:776:MET:HE1	1.85	0.40
1:D:393:LEU:HD11	1:D:466:ILE:HD12	2.03	0.40
1:E:445:ILE:HG22	1:E:938:ILE:HG21	2.02	0.40
1:E:574:THR:CG2	1:E:622:ALA:HB3	2.50	0.40
1:E:705:PRO:HA	1:E:708:LEU:O	2.21	0.40
1:E:770:SER:OG	1:E:775:ARG:HG2	2.22	0.40
1:E:1021:PHE:HD2	1:E:1021:PHE:C	2.29	0.40
1:F:162:MET:HG2	1:F:313:MET:SD	2.62	0.40
1:F:738:ILE:O	1:F:741:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:902:LEU:HD21	1:F:1016:PHE:HB2	2.03	0.40
1:F:969:PRO:O	1:F:970:ILE:C	2.65	0.40
1:A:184:MET:HG2	1:A:246:PHE:CD2	2.56	0.40
1:A:572:PHE:CE1	1:A:643:THR:HG22	2.56	0.40
1:A:776:MET:HE3	1:A:776:MET:HB3	1.97	0.40
1:B:84:SER:HB3	1:B:809:PRO:HA	2.03	0.40
1:C:568:ASP:OD1	1:C:639:VAL:HG23	2.21	0.40
1:C:666:ILE:HB	1:C:857:MET:SD	2.61	0.40
1:C:675:PHE:CD2	1:C:854:TRP:HZ3	2.40	0.40
1:C:907:ALA:O	1:C:910:ALA:HB3	2.20	0.40
1:C:974:SER:CB	1:C:1010:THR:HG21	2.51	0.40
1:D:504:ASP:C	1:D:506:GLY:N	2.77	0.40
1:D:751:GLY:HA2	1:D:769:MET:HG3	2.04	0.40
1:D:842:LEU:HD23	1:D:842:LEU:HA	1.99	0.40
1:D:1010:THR:O	1:D:1012:LEU:N	2.55	0.40
1:E:251:LEU:CD1	1:E:265:VAL:HG21	2.50	0.40
1:E:420:MET:HB3	1:E:500:ILE:HB	2.03	0.40
1:E:557:VAL:O	1:E:559:LEU:N	2.54	0.40
1:E:887:TYR:CD2	1:E:892:ILE:HG22	2.57	0.40
1:E:903:GLY:HA2	1:E:1009:ALA:HB2	2.04	0.40
1:E:962:ALA:O	1:E:965:MET:N	2.54	0.40
1:E:994:ALA:O	1:E:995:GLN:C	2.63	0.40
1:E:1017:VAL:O	1:E:1020:PHE:HB2	2.21	0.40
1:A:19:ILE:HD13	1:A:19:ILE:HG21	1.80	0.40
1:A:455:PRO:HG2	1:A:875:SER:CB	2.51	0.40
1:A:597:TYR:CD2	1:A:650:PHE:CZ	3.10	0.40
1:A:955:LEU:H	1:A:1033:GLU:HA	1.85	0.40
2:A:1101:ERY:H26	2:A:1101:ERY:O6	2.20	0.40
1:B:309:GLU:O	1:B:313:MET:HG3	2.22	0.40
1:B:434:SER:O	1:B:437:GLN:HB2	2.21	0.40
1:B:677:PHE:CZ	1:B:852:TYR:HB2	2.57	0.40
1:B:746:GLY:C	1:B:748:ALA:N	2.76	0.40
1:C:368:PRO:O	1:C:406:VAL:HG12	2.21	0.40
1:C:445:ILE:HG23	1:C:935:LYS:HG3	2.03	0.40
1:C:1034:ASP:CG	1:C:1035:ILE:H	2.30	0.40
1:D:53:ASP:O	1:D:57:VAL:HG23	2.21	0.40
1:D:77:TYR:OH	1:D:856:GLY:HA2	2.21	0.40
1:D:249:ILE:HD12	1:D:262:LEU:HD23	2.02	0.40
1:D:282:ASN:C	1:D:284:GLN:H	2.29	0.40
1:D:412:VAL:O	1:D:416:VAL:HG23	2.22	0.40
1:E:407:ASP:O	1:E:411:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:450:SER:HB3	1:E:478:MET:HE1	2.03	0.40
1:E:527:TYR:O	1:E:531:VAL:HG23	2.22	0.40
1:E:882:CYS:O	1:E:885:ALA:HB3	2.21	0.40
1:E:982:MET:CG	1:E:1003:MET:HE1	2.50	0.40
1:F:35:TYR:CD1	1:F:38:ILE:HD12	2.56	0.40
1:F:188:MET:HA	1:F:266:ALA:HB2	2.02	0.40
1:F:340:VAL:HG22	1:F:396:PHE:HE2	1.86	0.40
1:F:790:ASP:OD2	1:F:791:GLY:N	2.53	0.40
1:A:435:MET:HE3	1:A:435:MET:HB3	1.72	0.40
1:A:747:ALA:O	1:A:769:MET:HA	2.21	0.40
1:A:890:TRP:CZ2	1:C:10:ILE:HG23	2.56	0.40
1:A:948:MET:HG2	1:A:1035:ILE:HD12	2.02	0.40
1:B:478:MET:HE3	1:B:478:MET:HB3	1.87	0.40
1:B:681:ASP:HB2	1:B:690:LEU:HG	2.04	0.40
1:B:899:VAL:HA	1:B:902:LEU:HD13	2.04	0.40
1:B:1036:GLU:O	1:B:1037:HIS:ND1	2.54	0.40
1:C:3:ASN:HB3	1:C:490:PRO:HG2	2.03	0.40
1:C:57:VAL:HG23	1:C:82:SER:HB3	2.03	0.40
1:C:434:SER:O	1:C:438:ILE:HG12	2.22	0.40
1:C:679:LEU:HD12	1:C:851:GLY:O	2.21	0.40
1:C:686:GLY:HA3	1:C:689:LYS:NZ	2.36	0.40
1:C:883:LEU:HD23	1:C:883:LEU:HA	1.76	0.40
1:C:883:LEU:CD1	1:C:938:ILE:HD11	2.52	0.40
1:C:939:LEU:CD1	1:C:970:ILE:HG12	2.51	0.40
1:C:1017:VAL:O	1:C:1020:PHE:HB2	2.21	0.40
1:D:19:ILE:HD13	1:D:19:ILE:HG21	1.89	0.40
1:D:20:MET:HB3	1:D:377:LEU:HD13	2.03	0.40
1:D:108:GLN:OE1	1:D:129:VAL:HB	2.21	0.40
1:D:193:LEU:HD13	1:D:200:PRO:HD3	2.03	0.40
1:E:9:PRO:HB3	1:E:495:THR:CG2	2.51	0.40
1:E:419:VAL:HG21	1:E:434:SER:HB3	2.04	0.40
1:E:471:SER:O	1:E:475:VAL:HG23	2.20	0.40
1:E:478:MET:HE3	1:E:478:MET:HB3	1.83	0.40
1:F:11:PHE:C	1:F:11:PHE:HD2	2.30	0.40
1:F:26:ALA:HB1	1:F:384:ALA:CB	2.52	0.40
1:F:375:VAL:HA	1:F:480:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1036/1044 (99%)	902 (87%)	117 (11%)	17 (2%)	7	36
1	B	1035/1044 (99%)	896 (87%)	117 (11%)	22 (2%)	5	31
1	C	1034/1044 (99%)	896 (87%)	119 (12%)	19 (2%)	6	34
1	D	1036/1044 (99%)	894 (86%)	116 (11%)	26 (2%)	4	28
1	E	1035/1044 (99%)	894 (86%)	116 (11%)	25 (2%)	4	29
1	F	1035/1044 (99%)	891 (86%)	118 (11%)	26 (2%)	4	28
All	All	6211/6264 (99%)	5373 (86%)	703 (11%)	135 (2%)	5	30

All (135) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	E	888	GLU
1	E	1029	SER
1	E	1033	GLU
1	E	1035	ILE
1	F	6	ILE
1	F	134	SER
1	F	357	LEU
1	F	509	LYS
1	F	684	GLY
1	F	888	GLU
1	F	1034	ASP
1	F	1036	GLU
1	A	360	GLN
1	A	508	GLY
1	A	509	LYS
1	A	670	GLY
1	A	1038	SER
1	B	509	LYS
1	C	147	GLY
1	C	684	GLY
1	C	1031	LYS
1	C	1033	GLU
1	D	511	GLY
1	D	1031	LYS
1	E	508	GLY
1	E	509	LYS
1	E	669	LEU
1	E	672	ALA
1	E	684	GLY
1	F	147	GLY
1	F	675	PHE
1	F	918	ASN
1	A	986	ILE
1	A	1029	SER
1	B	360	GLN
1	B	684	GLY
1	B	905	ILE
1	B	918	ASN
1	C	360	GLN
1	C	614	GLY
1	C	1029	SER
1	D	918	ASN

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Mol	Chain	Res	Type
1	D	1034	ASP
1	D	1038	SER
1	E	358	PHE
1	E	616	GLY
1	F	299	ALA
1	F	507	GLU
1	F	1035	ILE
1	A	62	THR
1	A	248	LYS
1	B	617	GLN
1	B	898	LEU
1	B	1031	LYS
1	C	6	ILE
1	C	918	ASN
1	D	360	GLN
1	D	671	THR
1	D	898	LEU
1	E	506	GLY
1	E	617	GLN
1	E	918	ASN
1	E	1034	ASP
1	F	148	THR
1	F	616	GLY
1	F	1031	LYS
1	A	672	ALA
1	A	1011	VAL
1	B	376	LEU
1	B	1011	VAL
1	C	148	THR
1	C	248	LYS
1	D	505	HIS
1	D	634	GLY
1	D	1036	GLU
1	E	132	SER
1	E	511	GLY
1	E	887	TYR
1	E	898	LEU
1	F	360	GLN
1	F	633	PRO
1	F	1037	HIS
1	C	616	GLY
1	D	847	PRO

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Mol	Chain	Res	Type
1	D	863	LEU
1	F	5	PHE
1	A	634	GLY
1	C	1011	VAL
1	D	1011	VAL
1	F	1011	VAL
1	C	653	ILE
1	D	791	GLY
1	A	427	PRO
1	B	1014	ILE
1	C	791	GLY
1	D	991	GLY
1	E	639	VAL
1	E	905	ILE
1	E	1011	VAL
1	E	1014	ILE
1	A	639	VAL
1	B	506	GLY
1	B	565	PRO
1	D	565	PRO
1	D	653	ILE
1	D	746	GLY
1	E	791	GLY
1	F	412	VAL
1	F	614	GLY
1	F	905	ILE
1	A	666	ILE
1	B	634	GLY
1	B	791	GLY
1	B	847	PRO
1	F	791	GLY

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	846/852 (99%)	742 (88%)	104 (12%)	4 23
1	B	845/852 (99%)	751 (89%)	94 (11%)	6 27
1	C	844/852 (99%)	736 (87%)	108 (13%)	4 22
1	D	846/852 (99%)	743 (88%)	103 (12%)	5 23
1	E	845/852 (99%)	754 (89%)	91 (11%)	6 28
1	F	845/852 (99%)	735 (87%)	110 (13%)	4 21
All	All	5071/5112 (99%)	4461 (88%)	610 (12%)	5 24

All (610) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	19	ILE
1	A	27	ILE
1	A	28	LEU
1	A	45	ILE
1	A	48	SER
1	A	57	VAL
1	A	76	MET
1	A	91	THR
1	A	111	LEU
1	A	137	LEU
1	A	146	ASP
1	A	151	GLN
1	A	152	GLU
1	A	166	ILE
1	A	177	LEU
1	A	185	ARG
1	A	189	ASN
1	A	195	LYS
1	A	197	GLN
1	A	199	THR
1	A	205	THR
1	A	222	THR
1	A	225	VAL
1	A	243	THR
1	A	251	LEU
1	A	253	VAL

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Mol	Chain	Res	Type
1	A	270	LEU
1	A	284	GLN
1	A	324	VAL
1	A	337	ILE
1	A	341	VAL
1	A	343	THR
1	A	344	LEU
1	A	351	VAL
1	A	353	LEU
1	A	354	VAL
1	A	355	MET
1	A	362	PHE
1	A	400	LEU
1	A	404	LEU
1	A	411	VAL
1	A	418	ARG
1	A	429	GLU
1	A	463	THR
1	A	483	LEU
1	A	492	LEU
1	A	515	TRP
1	A	523	SER
1	A	524	THR
1	A	538	THR
1	A	540	ARG
1	A	550	VAL
1	A	561	SER
1	A	571	VAL
1	A	575	MET
1	A	578	LEU
1	A	605	ASN
1	A	624	VAL
1	A	625	SER
1	A	629	TRP
1	A	639	VAL
1	A	654	LYS
1	A	661	PHE
1	A	667	VAL
1	A	668	GLU
1	A	669	LEU
1	A	690	LEU
1	A	692	GLN

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Mol	Chain	Res	Type
1	A	708	LEU
1	A	711	VAL
1	A	716	LEU
1	A	738	ILE
1	A	741	ILE
1	A	763	VAL
1	A	799	PHE
1	A	806	TYR
1	A	838	LEU
1	A	861	GLU
1	A	876	LEU
1	A	879	VAL
1	A	881	LEU
1	A	896	VAL
1	A	905	ILE
1	A	909	LEU
1	A	913	PHE
1	A	920	VAL
1	A	927	LEU
1	A	928	THR
1	A	946	ASP
1	A	951	GLU
1	A	953	LYS
1	A	956	ILE
1	A	963	VAL
1	A	966	ARG
1	A	975	LEU
1	A	979	LEU
1	A	981	VAL
1	A	1011	VAL
1	A	1012	LEU
1	A	1019	VAL
1	A	1031	LYS
1	A	1032	ASN
1	A	1039	HIS
1	B	6	ILE
1	B	17	ILE
1	B	18	ILE
1	B	27	ILE
1	B	28	LEU
1	B	32	VAL
1	B	45	ILE

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Mol	Chain	Res	Type
1	B	60	THR
1	B	77	TYR
1	B	91	THR
1	B	102	ILE
1	B	105	VAL
1	B	128	SER
1	B	145	THR
1	B	166	ILE
1	B	175	VAL
1	B	177	LEU
1	B	205	THR
1	B	249	ILE
1	B	251	LEU
1	B	253	VAL
1	B	255	GLN
1	B	259	ARG
1	B	277	ILE
1	B	293	LEU
1	B	295	THR
1	B	324	VAL
1	B	337	ILE
1	B	341	VAL
1	B	344	LEU
1	B	349	ILE
1	B	353	LEU
1	B	355	MET
1	B	360	GLN
1	B	362	PHE
1	B	398	MET
1	B	399	VAL
1	B	400	LEU
1	B	463	THR
1	B	472	ILE
1	B	489	THR
1	B	492	LEU
1	B	515	TRP
1	B	524	THR
1	B	534	ILE
1	B	543	VAL
1	B	550	VAL
1	B	561	SER
1	B	571	VAL

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Mol	Chain	Res	Type
1	B	575	MET
1	B	578	LEU
1	B	583	THR
1	B	602	GLU
1	B	605	ASN
1	B	612	VAL
1	B	631	ASP
1	B	639	VAL
1	B	661	PHE
1	B	667	VAL
1	B	668	GLU
1	B	669	LEU
1	B	682	GLN
1	B	689	LYS
1	B	690	LEU
1	B	708	LEU
1	B	709	THR
1	B	712	ARG
1	B	716	LEU
1	B	717	GLU
1	B	729	GLU
1	B	738	ILE
1	B	741	ILE
1	B	762	ARG
1	B	763	VAL
1	B	806	TYR
1	B	830	LYS
1	B	838	LEU
1	B	881	LEU
1	B	905	ILE
1	B	909	LEU
1	B	920	VAL
1	B	926	LEU
1	B	927	LEU
1	B	928	THR
1	B	938	ILE
1	B	953	LYS
1	B	956	ILE
1	B	959	THR
1	B	963	VAL
1	B	966	ARG
1	B	975	LEU

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Mol	Chain	Res	Type
1	B	979	LEU
1	B	981	VAL
1	B	988	THR
1	C	3	ASN
1	C	5	PHE
1	C	7	ASP
1	C	13	TRP
1	C	28	LEU
1	C	45	ILE
1	C	48	SER
1	C	59	ASP
1	C	68	ASN
1	C	69	MET
1	C	76	MET
1	C	82	SER
1	C	87	THR
1	C	90	ILE
1	C	91	THR
1	C	102	ILE
1	C	104	GLN
1	C	111	LEU
1	C	112	GLN
1	C	121	GLU
1	C	122	VAL
1	C	129	VAL
1	C	137	LEU
1	C	145	THR
1	C	177	LEU
1	C	195	LYS
1	C	199	THR
1	C	222	THR
1	C	251	LEU
1	C	270	LEU
1	C	293	LEU
1	C	312	LYS
1	C	337	ILE
1	C	341	VAL
1	C	349	ILE
1	C	353	LEU
1	C	354	VAL
1	C	358	PHE
1	C	360	GLN

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Mol	Chain	Res	Type
1	C	363	ARG
1	C	400	LEU
1	C	404	LEU
1	C	447	MET
1	C	462	SER
1	C	482	VAL
1	C	492	LEU
1	C	523	SER
1	C	524	THR
1	C	535	LEU
1	C	538	THR
1	C	540	ARG
1	C	550	VAL
1	C	555	LEU
1	C	559	LEU
1	C	561	SER
1	C	571	VAL
1	C	578	LEU
1	C	605	ASN
1	C	612	VAL
1	C	621	ILE
1	C	628	ASP
1	C	631	ASP
1	C	639	VAL
1	C	654	LYS
1	C	661	PHE
1	C	663	LEU
1	C	667	VAL
1	C	668	GLU
1	C	669	LEU
1	C	678	GLU
1	C	681	ASP
1	C	689	LYS
1	C	690	LEU
1	C	692	GLN
1	C	711	VAL
1	C	712	ARG
1	C	716	LEU
1	C	729	GLU
1	C	738	ILE
1	C	763	VAL
1	C	771	GLU

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Mol	Chain	Res	Type
1	C	838	LEU
1	C	842	LEU
1	C	855	THR
1	C	858	SER
1	C	860	GLN
1	C	862	ARG
1	C	871	LEU
1	C	875	SER
1	C	890	TRP
1	C	905	ILE
1	C	909	LEU
1	C	918	ASN
1	C	920	VAL
1	C	927	LEU
1	C	938	ILE
1	C	953	LYS
1	C	956	ILE
1	C	963	VAL
1	C	966	ARG
1	C	972	MET
1	C	979	LEU
1	C	981	VAL
1	C	986	ILE
1	C	988	THR
1	C	1002	VAL
1	C	1011	VAL
1	C	1037	HIS
1	D	18	ILE
1	D	27	ILE
1	D	28	LEU
1	D	45	ILE
1	D	48	SER
1	D	57	VAL
1	D	91	THR
1	D	102	ILE
1	D	122	VAL
1	D	137	LEU
1	D	146	ASP
1	D	152	GLU
1	D	166	ILE
1	D	177	LEU
1	D	182	TYR

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Mol	Chain	Res	Type
1	D	185	ARG
1	D	195	LYS
1	D	205	THR
1	D	214	VAL
1	D	243	THR
1	D	244	GLU
1	D	251	LEU
1	D	270	LEU
1	D	280	GLU
1	D	324	VAL
1	D	337	ILE
1	D	341	VAL
1	D	343	THR
1	D	344	LEU
1	D	351	VAL
1	D	353	LEU
1	D	354	VAL
1	D	355	MET
1	D	360	GLN
1	D	362	PHE
1	D	400	LEU
1	D	404	LEU
1	D	428	LYS
1	D	437	GLN
1	D	456	MET
1	D	463	THR
1	D	474	ILE
1	D	483	LEU
1	D	492	LEU
1	D	495	THR
1	D	523	SER
1	D	524	THR
1	D	535	LEU
1	D	538	THR
1	D	550	VAL
1	D	559	LEU
1	D	561	SER
1	D	564	LEU
1	D	571	VAL
1	D	573	MET
1	D	575	MET
1	D	603	LYS

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Mol	Chain	Res	Type
1	D	605	ASN
1	D	612	VAL
1	D	621	ILE
1	D	624	VAL
1	D	625	SER
1	D	629	TRP
1	D	631	ASP
1	D	639	VAL
1	D	654	LYS
1	D	661	PHE
1	D	666	ILE
1	D	667	VAL
1	D	668	GLU
1	D	692	GLN
1	D	708	LEU
1	D	716	LEU
1	D	719	THR
1	D	738	ILE
1	D	741	ILE
1	D	743	THR
1	D	763	VAL
1	D	810	ARG
1	D	838	LEU
1	D	876	LEU
1	D	879	VAL
1	D	881	LEU
1	D	896	VAL
1	D	905	ILE
1	D	909	LEU
1	D	913	PHE
1	D	920	VAL
1	D	926	LEU
1	D	927	LEU
1	D	938	ILE
1	D	946	ASP
1	D	953	LYS
1	D	956	ILE
1	D	963	VAL
1	D	966	ARG
1	D	975	LEU
1	D	979	LEU
1	D	981	VAL

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Mol	Chain	Res	Type
1	D	1002	VAL
1	D	1011	VAL
1	D	1031	LYS
1	D	1032	ASN
1	E	18	ILE
1	E	25	LEU
1	E	27	ILE
1	E	28	LEU
1	E	45	ILE
1	E	88	VAL
1	E	91	THR
1	E	102	ILE
1	E	105	VAL
1	E	111	LEU
1	E	122	VAL
1	E	128	SER
1	E	131	LYS
1	E	137	LEU
1	E	145	THR
1	E	164	ASP
1	E	177	LEU
1	E	185	ARG
1	E	189	ASN
1	E	195	LYS
1	E	222	THR
1	E	249	ILE
1	E	251	LEU
1	E	259	ARG
1	E	267	LYS
1	E	270	LEU
1	E	277	ILE
1	E	293	LEU
1	E	295	THR
1	E	310	LEU
1	E	324	VAL
1	E	337	ILE
1	E	341	VAL
1	E	343	THR
1	E	344	LEU
1	E	353	LEU
1	E	354	VAL
1	E	400	LEU

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Mol	Chain	Res	Type
1	E	404	LEU
1	E	523	SER
1	E	524	THR
1	E	536	ARG
1	E	550	VAL
1	E	561	SER
1	E	563	PHE
1	E	564	LEU
1	E	571	VAL
1	E	575	MET
1	E	578	LEU
1	E	605	ASN
1	E	624	VAL
1	E	625	SER
1	E	628	ASP
1	E	654	LYS
1	E	661	PHE
1	E	663	LEU
1	E	667	VAL
1	E	668	GLU
1	E	689	LYS
1	E	690	LEU
1	E	692	GLN
1	E	703	LYS
1	E	707	MET
1	E	708	LEU
1	E	709	THR
1	E	717	GLU
1	E	729	GLU
1	E	743	THR
1	E	763	VAL
1	E	801	SER
1	E	806	TYR
1	E	838	LEU
1	E	862	ARG
1	E	875	SER
1	E	905	ILE
1	E	909	LEU
1	E	916	LEU
1	E	920	VAL
1	E	926	LEU
1	E	927	LEU

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Mol	Chain	Res	Type
1	E	928	THR
1	E	953	LYS
1	E	963	VAL
1	E	966	ARG
1	E	973	THR
1	E	975	LEU
1	E	979	LEU
1	E	981	VAL
1	E	1002	VAL
1	E	1030	ARG
1	E	1032	ASN
1	F	3	ASN
1	F	6	ILE
1	F	10	ILE
1	F	28	LEU
1	F	34	GLN
1	F	44	THR
1	F	45	ILE
1	F	55	LYS
1	F	59	ASP
1	F	76	MET
1	F	81	ASN
1	F	82	SER
1	F	87	THR
1	F	91	THR
1	F	93	THR
1	F	102	ILE
1	F	104	GLN
1	F	108	GLN
1	F	111	LEU
1	F	112	GLN
1	F	115	MET
1	F	129	VAL
1	F	137	LEU
1	F	145	THR
1	F	151	GLN
1	F	189	ASN
1	F	214	VAL
1	F	243	THR
1	F	251	LEU
1	F	293	LEU
1	F	321	LEU

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Mol	Chain	Res	Type
1	F	337	ILE
1	F	341	VAL
1	F	353	LEU
1	F	354	VAL
1	F	358	PHE
1	F	360	GLN
1	F	411	VAL
1	F	415	ASN
1	F	418	ARG
1	F	448	VAL
1	F	463	THR
1	F	482	VAL
1	F	515	TRP
1	F	523	SER
1	F	524	THR
1	F	538	THR
1	F	550	VAL
1	F	564	LEU
1	F	571	VAL
1	F	573	MET
1	F	578	LEU
1	F	596	HIS
1	F	602	GLU
1	F	605	ASN
1	F	621	ILE
1	F	628	ASP
1	F	631	ASP
1	F	639	VAL
1	F	644	MET
1	F	652	GLN
1	F	661	PHE
1	F	663	LEU
1	F	667	VAL
1	F	668	GLU
1	F	669	LEU
1	F	681	ASP
1	F	690	LEU
1	F	692	GLN
1	F	698	LEU
1	F	716	LEU
1	F	717	GLU
1	F	738	ILE

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Mol	Chain	Res	Type
1	F	763	VAL
1	F	771	GLU
1	F	783	ASP
1	F	785	TYR
1	F	801	SER
1	F	806	TYR
1	F	838	LEU
1	F	842	LEU
1	F	860	GLN
1	F	862	ARG
1	F	871	LEU
1	F	875	SER
1	F	879	VAL
1	F	880	PHE
1	F	881	LEU
1	F	890	TRP
1	F	905	ILE
1	F	909	LEU
1	F	913	PHE
1	F	916	LEU
1	F	920	VAL
1	F	927	LEU
1	F	938	ILE
1	F	953	LYS
1	F	963	VAL
1	F	966	ARG
1	F	975	LEU
1	F	979	LEU
1	F	981	VAL
1	F	986	ILE
1	F	988	THR
1	F	1002	VAL
1	F	1011	VAL
1	F	1028	PHE
1	F	1031	LYS
1	F	1035	ILE
1	F	1037	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN

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Mol	Chain	Res	Type
1	A	197	GLN
1	A	210	GLN
1	A	229	GLN
1	A	588	GLN
1	A	592	ASN
1	A	613	ASN
1	A	704	HIS
1	A	728	GLN
1	A	739	ASN
1	B	106	GLN
1	B	123	GLN
1	B	189	ASN
1	B	194	ASN
1	B	213	GLN
1	C	58	GLN
1	C	63	GLN
1	C	81	ASN
1	C	104	GLN
1	C	108	GLN
1	C	181	GLN
1	C	274	ASN
1	C	588	GLN
1	C	592	ASN
1	C	613	ASN
1	C	704	HIS
1	C	728	GLN
1	C	742	ASN
1	C	815	ASN
1	C	860	GLN
1	C	918	ASN
1	C	923	GLN
1	D	58	GLN
1	D	63	GLN
1	D	68	ASN
1	D	89	GLN
1	D	112	GLN
1	D	120	GLN
1	D	210	GLN
1	D	211	ASN
1	D	218	GLN
1	D	229	GLN
1	D	237	GLN

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Mol	Chain	Res	Type
1	D	298	ASN
1	D	437	GLN
1	D	439	GLN
1	D	469	GLN
1	D	588	GLN
1	D	592	ASN
1	D	613	ASN
1	D	704	HIS
1	E	34	GLN
1	E	67	GLN
1	E	123	GLN
1	E	218	GLN
1	E	298	ASN
1	E	577	GLN
1	E	996	ASN
1	E	1032	ASN
1	F	34	GLN
1	F	70	ASN
1	F	109	ASN
1	F	181	GLN
1	F	191	ASN
1	F	569	GLN
1	F	577	GLN
1	F	652	GLN
1	F	728	GLN

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 oligosaccharides 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	1.16	3 (5%)	82,82,82	1.91	18 (21%)
3	LMT	D	1102	-	36,36,36	1.80	9 (25%)	47,47,47	1.42	7 (14%)
3	LMT	E	1101	-	36,36,36	1.89	10 (27%)	47,47,47	1.63	8 (17%)
2	ERY	D	1101	-	53,53,53	1.29	3 (5%)	82,82,82	2.08	31 (37%)
3	LMT	C	1101	-	36,36,36	1.78	9 (25%)	47,47,47	1.43	6 (12%)
3	LMT	B	2100	-	36,36,36	1.72	10 (27%)	47,47,47	1.94	14 (29%)
3	LMT	F	2100	-	36,36,36	1.73	9 (25%)	47,47,47	1.12	2 (4%)
3	LMT	A	1102	-	36,36,36	1.76	10 (27%)	47,47,47	1.15	4 (8%)
3	LMT	D	1103	-	36,36,36	1.91	9 (25%)	47,47,47	1.32	8 (17%)
3	LMT	A	1103	-	36,36,36	1.87	9 (25%)	47,47,47	1.60	9 (19%)

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	-	-	33/72/107/107	0/3/3/3
3	LMT	D	1102	-	-	11/21/61/61	0/2/2/2
3	LMT	E	1101	-	-	10/21/61/61	0/2/2/2
2	ERY	D	1101	-	-	47/72/107/107	0/3/3/3
3	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
3	LMT	B	2100	-	-	11/21/61/61	0/2/2/2
3	LMT	F	2100	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	12/21/61/61	0/2/2/2
3	LMT	D	1103	-	-	15/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	14/21/61/61	0/2/2/2

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	ERY	O2-C1	5.54	1.47	1.34
2	A	1101	ERY	O2-C1	5.27	1.46	1.34
3	A	1103	LMT	O5'-C5'	4.54	1.55	1.44
3	D	1103	LMT	O5'-C5'	4.47	1.55	1.44
3	E	1101	LMT	O1'-C1'	4.32	1.47	1.40
3	E	1101	LMT	O5B-C1B	4.26	1.52	1.41
3	D	1102	LMT	O3B-C3B	4.15	1.53	1.43
3	D	1103	LMT	O5B-C1B	4.13	1.52	1.41
3	D	1103	LMT	O1'-C1'	4.07	1.47	1.40
3	B	2100	LMT	O5B-C1B	3.88	1.51	1.41
3	F	2100	LMT	O5'-C5'	3.87	1.53	1.44
3	A	1103	LMT	O1'-C1'	3.82	1.46	1.40
3	D	1103	LMT	O3B-C3B	3.76	1.52	1.43
3	A	1102	LMT	O5B-C1B	3.75	1.51	1.41
3	E	1101	LMT	O5'-C5'	3.70	1.53	1.44
3	C	1101	LMT	O5'-C5'	3.66	1.53	1.44
3	D	1102	LMT	O1'-C1'	3.65	1.46	1.40
3	A	1102	LMT	O5'-C5'	3.59	1.53	1.44
3	A	1102	LMT	O1'-C1'	3.54	1.46	1.40
3	D	1103	LMT	O5'-C1'	3.50	1.50	1.41
3	B	2100	LMT	C6'-C5'	-3.49	1.40	1.51
3	D	1102	LMT	C6'-C5'	-3.48	1.40	1.51
3	C	1101	LMT	O1'-C1'	3.45	1.46	1.40
3	A	1103	LMT	O3B-C3B	3.44	1.51	1.43
3	C	1101	LMT	O3B-C3B	3.43	1.51	1.43
3	F	2100	LMT	O5'-C1'	3.38	1.50	1.41
3	C	1101	LMT	C6'-C5'	-3.37	1.40	1.51
3	A	1102	LMT	C6'-C5'	-3.29	1.40	1.51
3	A	1103	LMT	O5B-C1B	3.28	1.50	1.41
3	A	1103	LMT	O5'-C1'	3.27	1.50	1.41
3	F	2100	LMT	C6'-C5'	-3.26	1.40	1.51
3	B	2100	LMT	O1'-C1'	3.26	1.45	1.40
3	D	1102	LMT	O5'-C5'	3.24	1.52	1.44
3	A	1103	LMT	C6'-C5'	-3.23	1.41	1.51
3	F	2100	LMT	O1'-C1'	3.23	1.45	1.40
3	F	2100	LMT	O5B-C1B	3.19	1.50	1.41
3	E	1101	LMT	C6'-C5'	-3.17	1.41	1.51
3	C	1101	LMT	O5'-C1'	3.11	1.49	1.41
3	D	1103	LMT	C6'-C5'	-3.05	1.41	1.51
3	F	2100	LMT	O3B-C3B	3.04	1.50	1.43
3	B	2100	LMT	O5'-C5'	2.96	1.51	1.44
3	D	1103	LMT	O2'-C2'	2.90	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1101	LMT	O5'-C1'	2.89	1.49	1.41
3	D	1102	LMT	C3'-C2'	-2.87	1.44	1.52
3	D	1102	LMT	O5'-C1'	2.86	1.49	1.41
3	B	2100	LMT	O2'-C2'	2.80	1.49	1.43
3	A	1102	LMT	O5'-C1'	2.70	1.48	1.41
3	C	1101	LMT	O5B-C1B	2.65	1.48	1.41
3	E	1101	LMT	C3B-C2B	-2.64	1.45	1.52
3	A	1102	LMT	C3'-C2'	-2.62	1.45	1.52
2	D	1101	ERY	O11-C9	2.55	1.25	1.21
3	A	1102	LMT	O3B-C3B	2.54	1.49	1.43
3	E	1101	LMT	O2'-C2'	2.51	1.49	1.43
3	F	2100	LMT	O2'-C2'	2.51	1.49	1.43
3	A	1102	LMT	C3B-C2B	-2.47	1.45	1.52
3	C	1101	LMT	O2'-C2'	2.46	1.49	1.43
3	B	2100	LMT	O3B-C3B	2.46	1.49	1.43
3	A	1102	LMT	O2'-C2'	2.44	1.49	1.43
3	D	1102	LMT	O5B-C1B	2.39	1.48	1.41
3	D	1103	LMT	O3'-C3'	2.36	1.48	1.43
3	F	2100	LMT	C3'-C2'	-2.35	1.46	1.52
3	D	1102	LMT	O2'-C2'	2.34	1.48	1.43
3	B	2100	LMT	O3'-C3'	2.33	1.48	1.43
3	B	2100	LMT	O5'-C1'	2.28	1.47	1.41
3	C	1101	LMT	C3'-C2'	-2.24	1.46	1.52
3	E	1101	LMT	C5-C4	2.23	1.62	1.51
3	D	1103	LMT	C5-C4	2.22	1.62	1.51
3	A	1103	LMT	O2'-C2'	2.21	1.48	1.43
3	E	1101	LMT	O5B-C5B	2.20	1.49	1.44
3	F	2100	LMT	C5-C4	2.20	1.62	1.51
2	A	1101	ERY	C25-C26	2.20	1.55	1.52
3	D	1102	LMT	O1B-C1B	-2.15	1.35	1.41
3	A	1103	LMT	C3'-C2'	-2.15	1.46	1.52
3	C	1101	LMT	C5-C4	2.14	1.62	1.51
3	A	1102	LMT	C5-C4	2.08	1.62	1.51
3	B	2100	LMT	C3'-C2'	-2.07	1.47	1.52
3	E	1101	LMT	C3'-C2'	-2.05	1.47	1.52
3	A	1103	LMT	O2B-C2B	2.05	1.48	1.43
2	D	1101	ERY	C25-C26	2.02	1.55	1.52
2	A	1101	ERY	O11-C9	2.01	1.24	1.21
3	B	2100	LMT	C5-C4	2.01	1.61	1.51

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	LMT	O5B-C5B-C4B	5.57	119.73	109.70
3	E	1101	LMT	C1B-C2B-C3B	-5.46	98.53	110.01
2	D	1101	ERY	C20-O5-C16	5.39	128.48	117.51
3	C	1101	LMT	C4B-C3B-C2B	5.04	119.67	110.83
2	D	1101	ERY	C12-C11-C10	5.00	122.25	116.40
2	A	1101	ERY	C20-O5-C16	4.86	127.40	117.51
3	B	2100	LMT	O5B-C5B-C4B	4.62	118.03	109.70
2	A	1101	ERY	O2-C13-C12	4.61	114.55	107.28
2	D	1101	ERY	O2-C13-C36	4.59	115.88	107.36
3	B	2100	LMT	C4B-C3B-C2B	4.54	118.81	110.83
2	D	1101	ERY	O2-C1-C2	4.52	121.19	111.53
3	C	1101	LMT	C1B-C2B-C3B	4.48	119.44	110.01
3	D	1102	LMT	C4B-C3B-C2B	4.47	118.68	110.83
2	D	1101	ERY	O2-C1-O1	-4.25	116.27	123.95
2	A	1101	ERY	O12-C11-C10	4.22	116.75	110.77
3	B	2100	LMT	C1B-C2B-C3B	4.07	118.57	110.01
2	A	1101	ERY	C29-N1-C24	4.03	124.77	113.15
3	B	2100	LMT	O3B-C3B-C4B	-3.99	100.98	110.38
2	A	1101	ERY	O7-C5-C6	3.99	111.15	106.40
2	A	1101	ERY	C26-C25-C24	3.95	117.20	110.46
3	E	1101	LMT	C1B-O5B-C5B	3.95	121.43	113.72
2	A	1101	ERY	C22-C23-C24	3.86	115.34	109.15
2	D	1101	ERY	O4-C18-C21	3.76	115.09	106.74
2	A	1101	ERY	C15-C16-C17	3.65	113.88	107.64
3	A	1103	LMT	C3B-C4B-C5B	3.60	116.76	110.23
3	E	1101	LMT	O1'-C1'-C2'	3.56	113.68	108.27
3	F	2100	LMT	O5B-C5B-C4B	3.52	116.04	109.70
3	B	2100	LMT	C3B-C4B-C5B	3.49	116.55	110.23
3	A	1103	LMT	O1B-C1B-C2B	3.47	116.63	108.09
2	D	1101	ERY	O12-C11-C10	3.43	115.63	110.77
2	A	1101	ERY	C35-C12-C13	3.40	115.86	111.26
2	A	1101	ERY	C25-C24-C23	3.39	114.89	110.02
3	E	1101	LMT	O5B-C5B-C4B	3.35	115.73	109.70
2	D	1101	ERY	C29-N1-C24	3.33	122.74	113.15
3	D	1102	LMT	C3B-C4B-C5B	3.25	116.12	110.23
2	D	1101	ERY	O7-C22-C23	3.23	116.03	108.09
3	D	1103	LMT	C1B-C2B-C3B	3.23	116.80	110.01
2	D	1101	ERY	C22-O7-C5	3.22	121.74	116.26
3	D	1102	LMT	C1B-C2B-C3B	3.14	116.62	110.01
2	A	1101	ERY	O9-C26-C25	3.14	113.83	109.34
2	D	1101	ERY	O11-C9-C8	-3.13	115.65	121.30
3	E	1101	LMT	O1B-C1B-C2B	-3.06	100.55	108.09
2	A	1101	ERY	O12-C11-C12	-3.06	100.95	106.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1103	LMT	O1B-C4'-C3'	3.05	115.00	107.23
3	F	2100	LMT	C1B-O1B-C4'	-3.04	110.78	117.98
3	B	2100	LMT	O5B-C1B-C2B	3.03	116.59	110.37
2	D	1101	ERY	O8-C23-C22	2.98	117.17	110.08
2	A	1101	ERY	C19-C16-C15	-2.96	105.47	110.64
2	A	1101	ERY	O4-C18-C21	2.94	113.26	106.74
2	D	1101	ERY	O12-C11-C12	-2.94	101.18	106.57
3	B	2100	LMT	C1B-O5B-C5B	2.93	119.44	113.72
2	D	1101	ERY	C25-C24-N1	-2.86	107.54	115.59
2	D	1101	ERY	C35-C12-C13	2.85	115.11	111.26
3	B	2100	LMT	O5'-C1'-O1'	-2.85	103.32	110.04
2	A	1101	ERY	O10-C6-C5	-2.83	102.38	107.60
3	C	1101	LMT	O1'-C1'-C2'	-2.82	103.99	108.27
3	B	2100	LMT	C6B-C5B-C4B	-2.80	106.15	113.02
3	A	1103	LMT	C1'-O5'-C5'	2.78	119.15	113.72
2	A	1101	ERY	O6-C17-C18	-2.68	104.84	109.46
2	D	1101	ERY	C34-C10-C11	-2.65	110.94	114.30
3	D	1103	LMT	O5B-C5B-C6B	2.65	113.00	106.44
2	D	1101	ERY	C3-C2-C1	2.62	115.23	109.93
3	C	1101	LMT	C1B-O1B-C4'	-2.62	111.76	117.98
3	E	1101	LMT	C1'-C2'-C3'	2.61	115.50	110.01
3	D	1102	LMT	C1'-O5'-C5'	2.55	118.71	113.72
3	A	1103	LMT	O1'-C1'-C2'	2.51	112.09	108.27
3	A	1103	LMT	O2B-C2B-C1B	2.49	116.02	110.08
2	D	1101	ERY	O3-C3-C4	2.48	111.16	108.23
2	A	1101	ERY	C33-C8-C7	-2.47	105.29	109.88
3	B	2100	LMT	O2B-C2B-C1B	-2.46	104.22	110.08
3	D	1102	LMT	C1B-O5B-C5B	-2.45	108.94	113.72
2	D	1101	ERY	C30-C2-C3	2.45	118.47	113.00
3	A	1103	LMT	O5B-C1B-C2B	-2.44	105.35	110.37
3	A	1103	LMT	O5'-C5'-C4'	2.44	114.76	109.72
2	D	1101	ERY	C11-C10-C9	2.41	113.35	109.48
2	D	1101	ERY	C19-C16-C15	-2.41	106.44	110.64
2	D	1101	ERY	C29-N1-C28	2.40	117.55	110.49
3	A	1102	LMT	O3'-C3'-C2'	-2.38	104.77	110.38
3	B	2100	LMT	O1B-C1B-C2B	-2.36	102.29	108.09
3	A	1103	LMT	C1B-O1B-C4'	-2.35	112.40	117.98
3	A	1102	LMT	O5B-C5B-C4B	2.32	113.88	109.70
3	A	1102	LMT	C1'-O5'-C5'	2.32	118.25	113.72
2	D	1101	ERY	C3-C4-C5	2.29	115.94	111.17
3	C	1101	LMT	O3B-C3B-C4B	-2.27	105.02	110.38
3	D	1103	LMT	O5B-C5B-C4B	2.26	113.77	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2100	LMT	C3'-C4'-C5'	2.25	115.92	110.93
3	E	1101	LMT	C2'-C3'-C4'	2.25	114.78	109.68
3	D	1102	LMT	O5B-C1B-C2B	2.19	114.86	110.37
3	D	1102	LMT	O4'-C4B-C3B	-2.19	105.22	110.38
3	D	1103	LMT	C4B-C3B-C2B	2.19	114.67	110.83
2	D	1101	ERY	O6-C17-C18	-2.16	105.75	109.46
3	D	1103	LMT	C1'-C2'-C3'	2.14	114.51	110.01
3	E	1101	LMT	O5'-C5'-C6'	2.13	111.71	106.44
3	B	2100	LMT	O3B-C3B-C2B	-2.12	105.38	110.38
3	A	1102	LMT	C2'-C3'-C4'	2.11	114.46	109.68
2	D	1101	ERY	C15-C16-C17	2.10	111.24	107.64
3	B	2100	LMT	C1-O1'-C1'	2.10	117.26	113.68
2	D	1101	ERY	C34-C10-C9	2.08	111.72	108.09
2	D	1101	ERY	C16-C15-C14	-2.06	111.52	114.99
2	D	1101	ERY	O10-C6-C5	-2.05	103.82	107.60
2	D	1101	ERY	O11-C9-C10	2.04	123.47	120.64
3	D	1103	LMT	C1'-O5'-C5'	2.03	117.69	113.72
3	D	1103	LMT	O1B-C1B-O5B	2.03	116.03	110.69
3	C	1101	LMT	O3B-C3B-C2B	-2.02	105.61	110.38
2	A	1101	ERY	C30-C2-C3	2.02	117.51	113.00
2	D	1101	ERY	C13-C12-C11	-2.02	104.35	108.21
2	D	1101	ERY	O9-C26-C27	2.01	110.65	106.88

There are no chirality outliers.

All (176) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	ERY	C11-C12-C13-O2
2	A	1101	ERY	C11-C12-C13-C36
2	A	1101	ERY	C35-C12-C13-O2
2	A	1101	ERY	C35-C12-C13-C36
2	A	1101	ERY	O13-C12-C13-O2
2	A	1101	ERY	O13-C12-C13-C36
2	A	1101	ERY	C12-C13-O2-C1
2	A	1101	ERY	O2-C13-C36-C37
2	A	1101	ERY	C2-C1-O2-C13
2	A	1101	ERY	O2-C1-C2-C3
2	A	1101	ERY	C4-C5-C6-C7
2	A	1101	ERY	C4-C5-C6-O10
2	A	1101	ERY	O7-C5-C6-C7
2	A	1101	ERY	O7-C5-C6-C32
2	A	1101	ERY	O7-C5-C6-O10

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Mol	Chain	Res	Type	Atoms
2	A	1101	ERY	C15-C14-O3-C3
2	A	1101	ERY	O4-C14-O3-C3
2	A	1101	ERY	C17-C16-O5-C20
2	D	1101	ERY	C9-C10-C11-C12
2	D	1101	ERY	C10-C11-C12-C13
2	D	1101	ERY	C10-C11-C12-C35
2	D	1101	ERY	C10-C11-C12-O13
2	D	1101	ERY	O12-C11-C12-C13
2	D	1101	ERY	O12-C11-C12-C35
2	D	1101	ERY	O12-C11-C12-O13
2	D	1101	ERY	C2-C1-O2-C13
2	D	1101	ERY	O1-C1-O2-C13
2	D	1101	ERY	C4-C5-C6-C7
2	D	1101	ERY	C4-C5-C6-C32
2	D	1101	ERY	C4-C5-C6-O10
2	D	1101	ERY	O7-C5-C6-C7
2	D	1101	ERY	O7-C5-C6-C32
2	D	1101	ERY	O7-C5-C6-O10
2	D	1101	ERY	C5-C6-C7-C8
2	D	1101	ERY	C32-C6-C7-C8
2	D	1101	ERY	C7-C8-C9-C10
2	D	1101	ERY	C7-C8-C9-O11
2	D	1101	ERY	O4-C14-O3-C3
2	D	1101	ERY	C15-C16-O5-C20
2	D	1101	ERY	C19-C16-O5-C20
3	A	1102	LMT	C2'-C1'-O1'-C1
3	A	1103	LMT	O5'-C1'-O1'-C1
3	B	2100	LMT	C2-C1-O1'-C1'
3	D	1103	LMT	C2'-C1'-O1'-C1
2	D	1101	ERY	O9-C22-O7-C5
3	D	1103	LMT	O5B-C5B-C6B-O6B
3	C	1101	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	C4B-C5B-C6B-O6B
3	F	2100	LMT	C3-C4-C5-C6
3	A	1102	LMT	O5B-C5B-C6B-O6B
3	E	1101	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	O5'-C1'-O1'-C1
3	D	1103	LMT	O5'-C1'-O1'-C1
3	D	1102	LMT	O5B-C5B-C6B-O6B
2	A	1101	ERY	O3-C3-C4-C31
3	C	1101	LMT	C1-C2-C3-C4
2	A	1101	ERY	C2-C3-C4-C31

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Mol	Chain	Res	Type	Atoms
2	A	1101	ERY	O3-C3-C4-C5
2	A	1101	ERY	C2-C3-C4-C5
3	B	2100	LMT	C4B-C5B-C6B-O6B
3	A	1103	LMT	C5-C6-C7-C8
2	D	1101	ERY	C15-C14-O3-C3
2	A	1101	ERY	O1-C1-O2-C13
3	E	1101	LMT	O5'-C5'-C6'-O6'
3	F	2100	LMT	C4'-C5'-C6'-O6'
3	D	1102	LMT	C4B-C5B-C6B-O6B
3	A	1103	LMT	C4B-C5B-C6B-O6B
3	C	1101	LMT	C4B-C5B-C6B-O6B
3	A	1103	LMT	O5'-C5'-C6'-O6'
2	D	1101	ERY	C36-C13-O2-C1
3	E	1101	LMT	C4B-C5B-C6B-O6B
3	B	2100	LMT	C4-C5-C6-C7
3	B	2100	LMT	O5B-C1B-O1B-C4'
3	F	2100	LMT	O5'-C5'-C6'-O6'
2	A	1101	ERY	O1-C1-C2-C3
3	A	1102	LMT	C5-C6-C7-C8
3	C	1101	LMT	C4'-C5'-C6'-O6'
3	E	1101	LMT	O1'-C1-C2-C3
3	D	1103	LMT	C4B-C5B-C6B-O6B
3	B	2100	LMT	O5B-C5B-C6B-O6B
2	D	1101	ERY	C25-C24-N1-C29
3	A	1102	LMT	C4'-C5'-C6'-O6'
3	C	1101	LMT	C2'-C1'-O1'-C1
3	C	1101	LMT	O5'-C5'-C6'-O6'
3	E	1101	LMT	C4'-C5'-C6'-O6'
3	C	1101	LMT	O5'-C1'-O1'-C1
3	C	1101	LMT	O1'-C1-C2-C3
2	D	1101	ERY	C23-C24-N1-C28
2	D	1101	ERY	C23-C24-N1-C29
3	D	1102	LMT	C11-C10-C9-C8
3	F	2100	LMT	O1'-C1-C2-C3
3	D	1103	LMT	C3-C4-C5-C6
3	F	2100	LMT	C6-C7-C8-C9
3	A	1103	LMT	C1-C2-C3-C4
3	D	1103	LMT	C1-C2-C3-C4
3	E	1101	LMT	C11-C10-C9-C8
2	D	1101	ERY	C25-C24-N1-C28
3	A	1103	LMT	C3-C4-C5-C6
3	C	1101	LMT	C6-C7-C8-C9

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

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Mol	Chain	Res	Type	Atoms
2	D	1101	ERY	C34-C10-C11-C12
3	D	1103	LMT	C4-C5-C6-C7
3	A	1103	LMT	C6-C7-C8-C9
3	E	1101	LMT	C2B-C1B-O1B-C4'
2	A	1101	ERY	C15-C16-O5-C20
3	D	1103	LMT	O5'-C5'-C6'-O6'
3	A	1102	LMT	C3-C4-C5-C6
2	A	1101	ERY	C6-C7-C8-C33
2	D	1101	ERY	C6-C7-C8-C33
3	A	1103	LMT	O5B-C5B-C6B-O6B
2	D	1101	ERY	C1-C2-C3-O3
3	A	1102	LMT	C2-C3-C4-C5
3	D	1103	LMT	C3'-C4'-O1B-C1B
3	C	1101	LMT	C2-C1-O1'-C1'
3	D	1103	LMT	C5'-C4'-O1B-C1B
2	D	1101	ERY	C30-C2-C3-C4
2	D	1101	ERY	C9-C10-C11-O12
3	E	1101	LMT	O5B-C1B-O1B-C4'
3	E	1101	LMT	C9-C10-C11-C12
3	D	1102	LMT	C9-C10-C11-C12
2	A	1101	ERY	O1-C1-C2-C30
3	F	2100	LMT	O5B-C5B-C6B-O6B
2	D	1101	ERY	C2-C3-O3-C14
2	A	1101	ERY	C6-C7-C8-C9
2	D	1101	ERY	C6-C7-C8-C9
2	D	1101	ERY	C34-C10-C9-O11
2	D	1101	ERY	O13-C12-C13-C36
3	D	1102	LMT	C2'-C1'-O1'-C1
3	F	2100	LMT	C2'-C1'-O1'-C1
3	B	2100	LMT	C2B-C1B-O1B-C4'
2	D	1101	ERY	C1-C2-C3-C4
2	D	1101	ERY	C33-C8-C9-C10
3	D	1102	LMT	O5'-C1'-O1'-C1
2	A	1101	ERY	O2-C1-C2-C30
3	D	1103	LMT	O5B-C1B-O1B-C4'

There are no ring outliers.

10 monomers are involved in 50 short contacts:

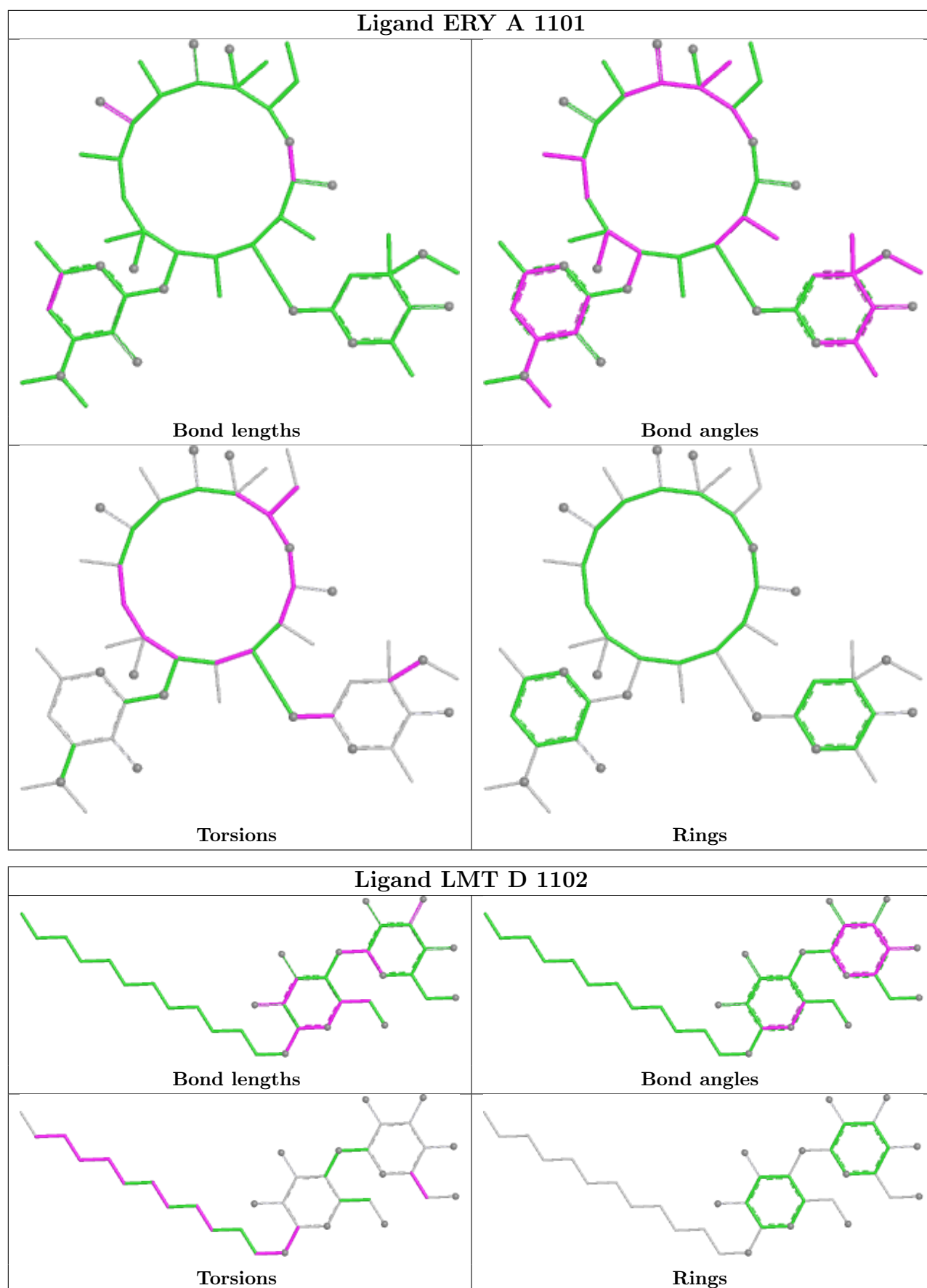
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ERY	5	0
3	D	1102	LMT	6	0

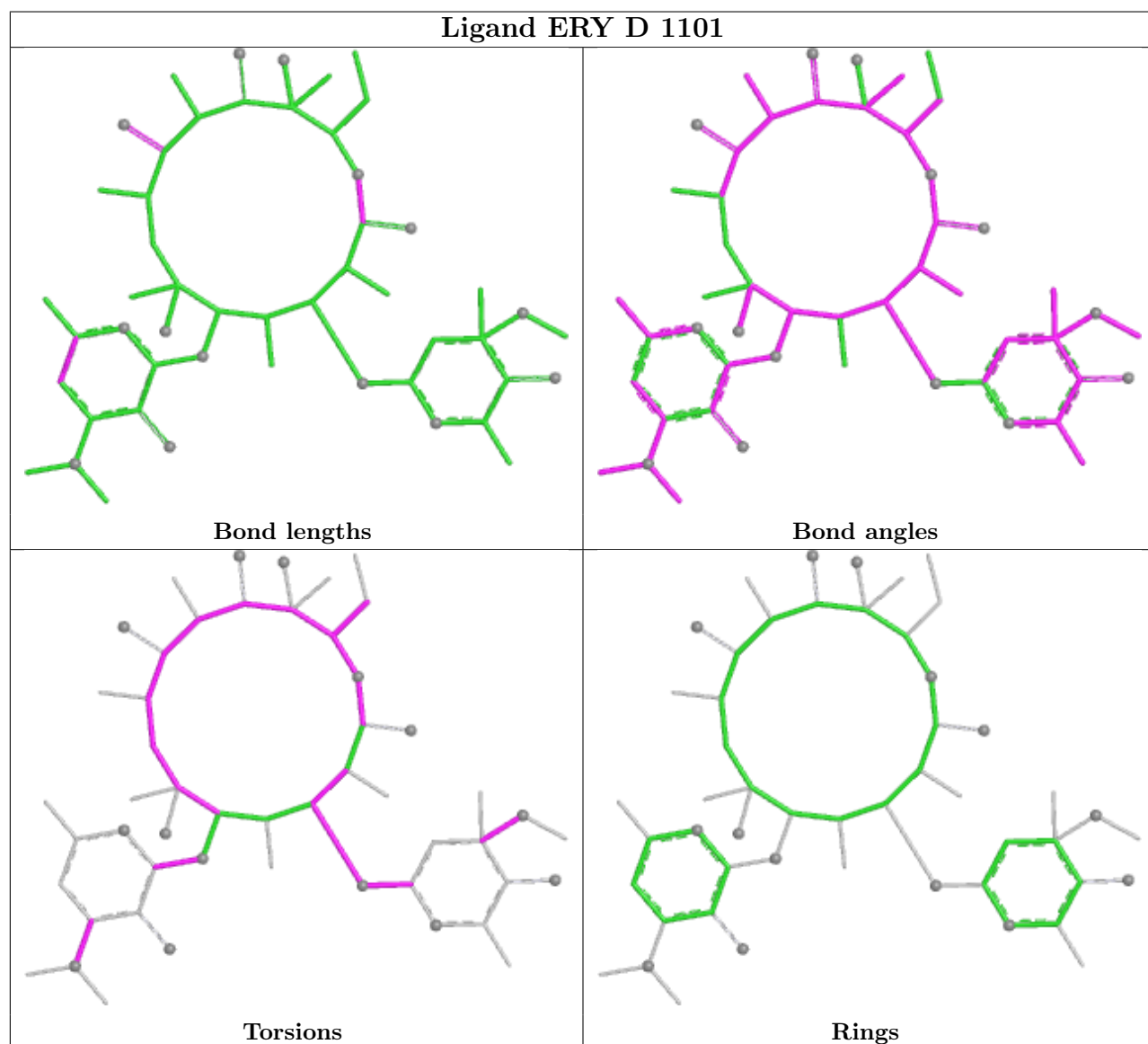
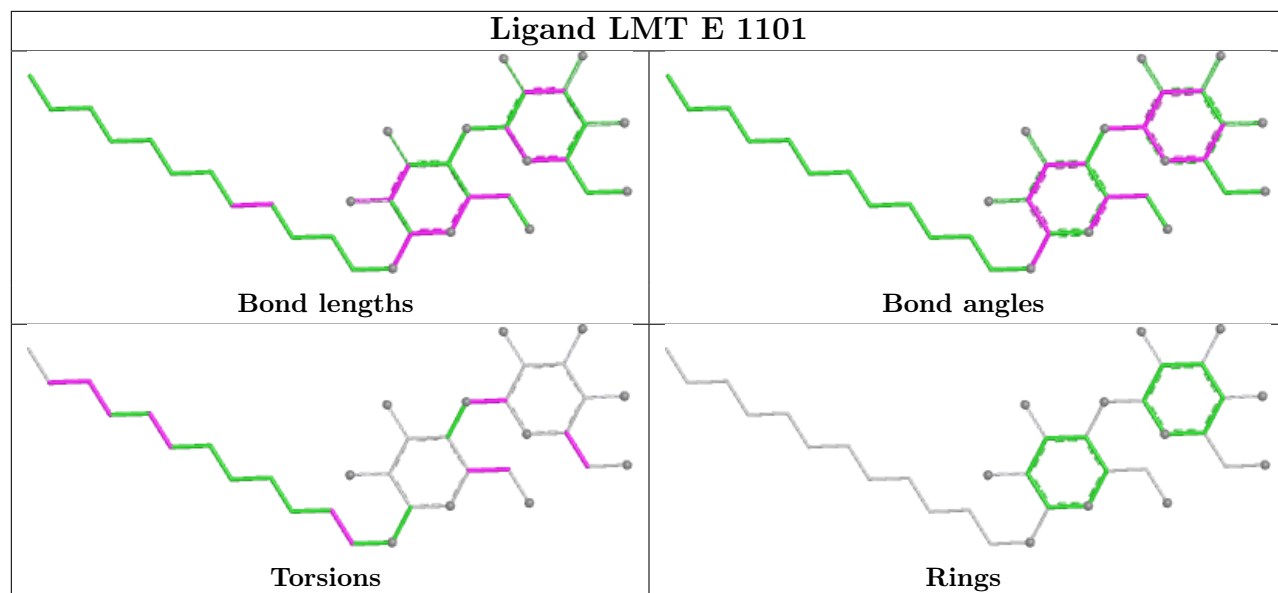
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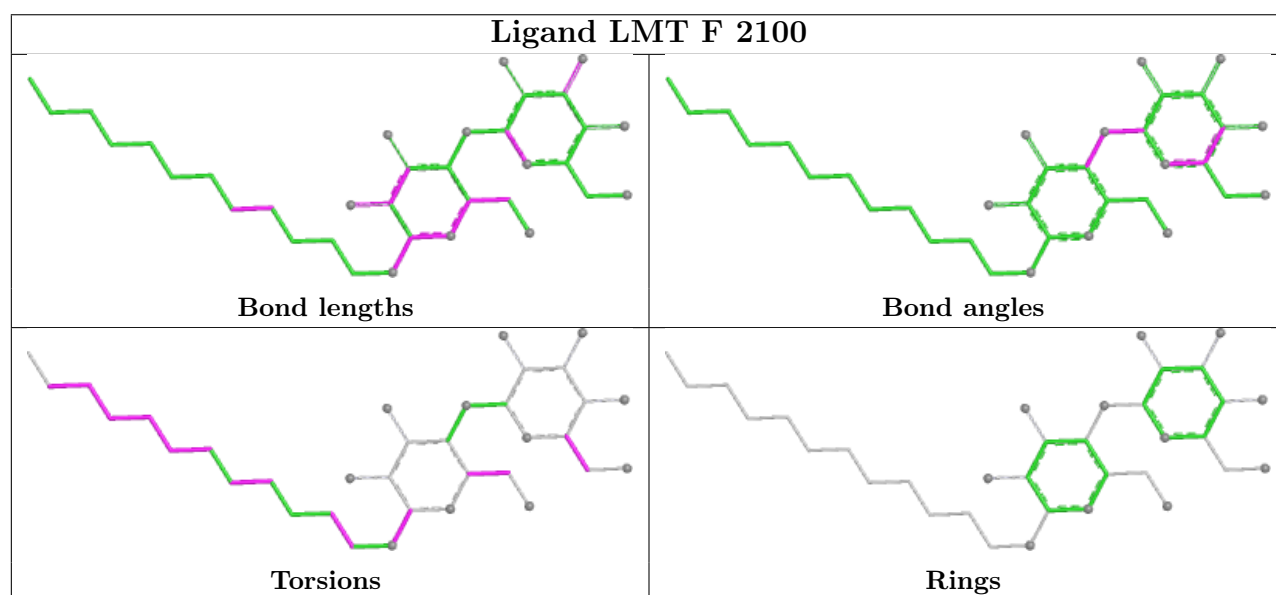
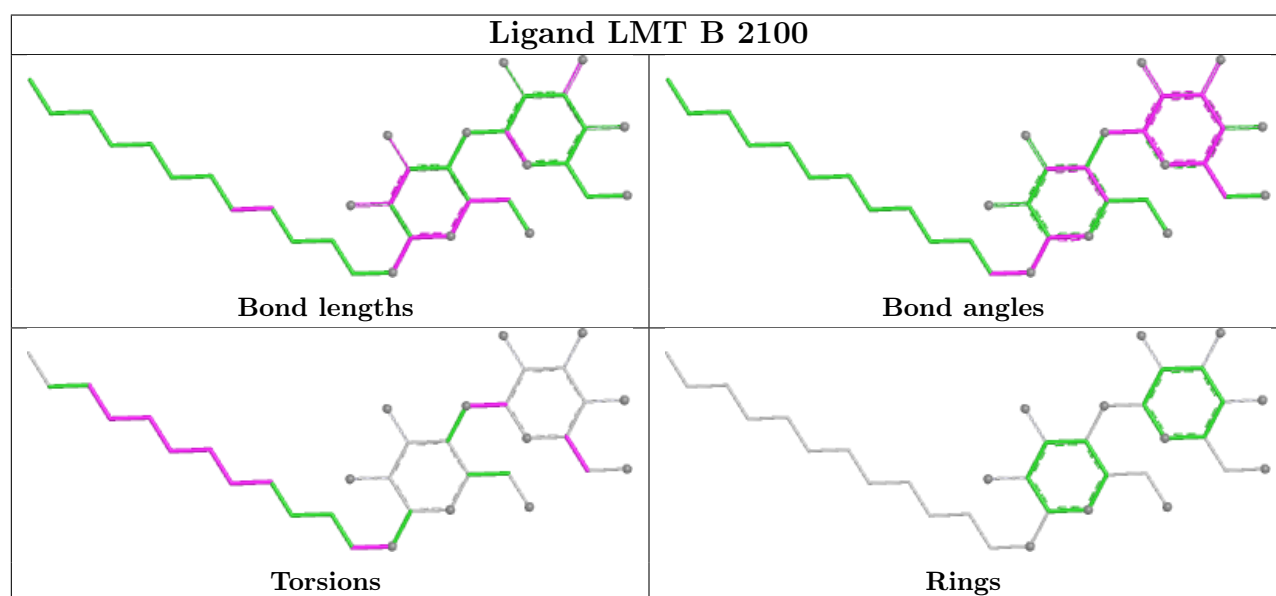
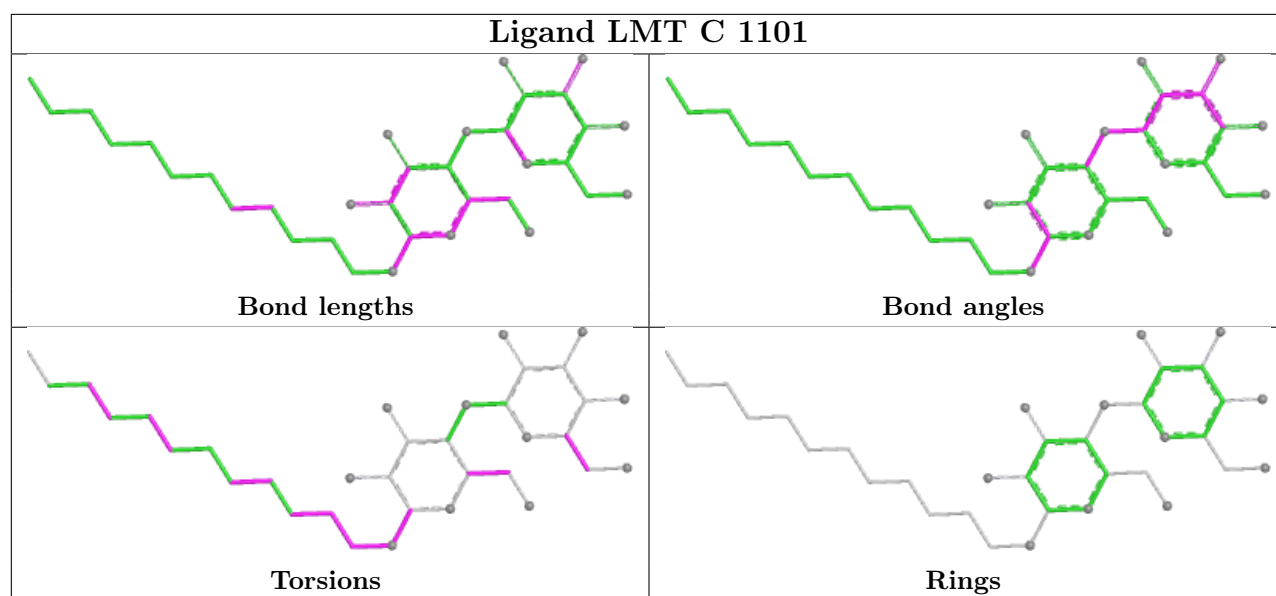
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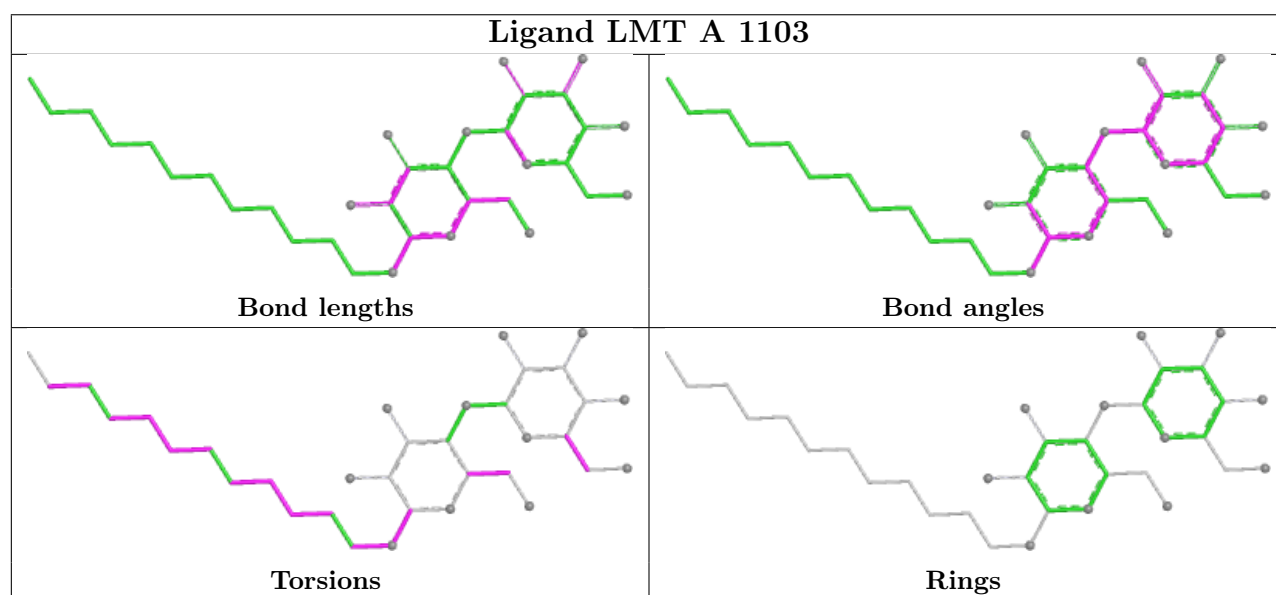
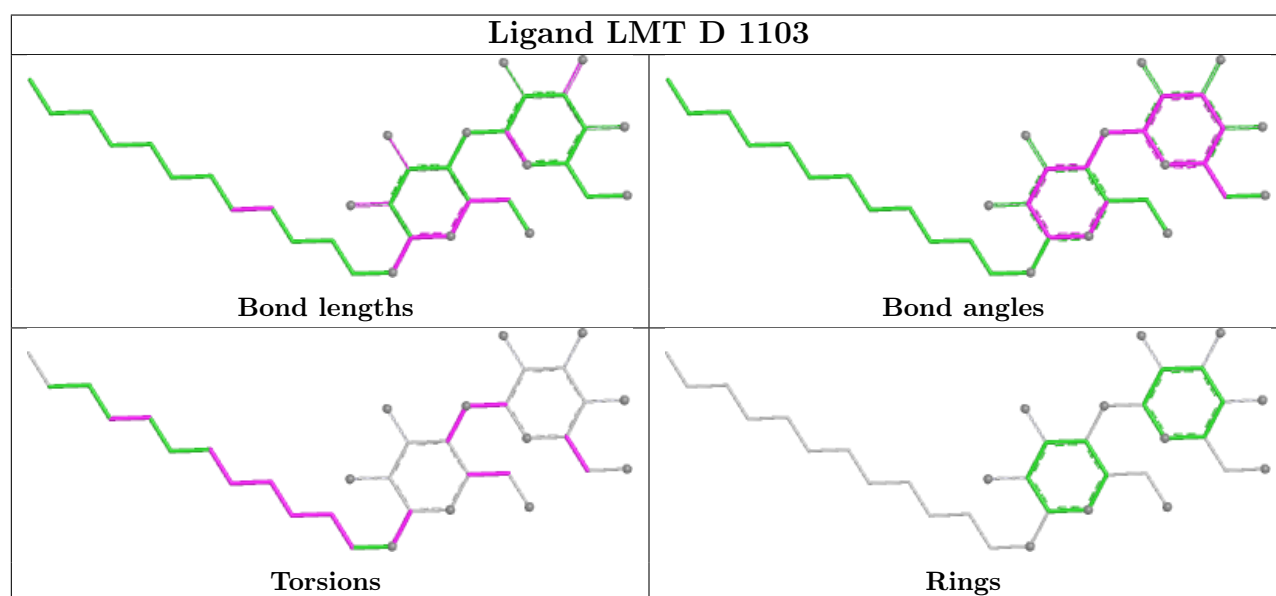
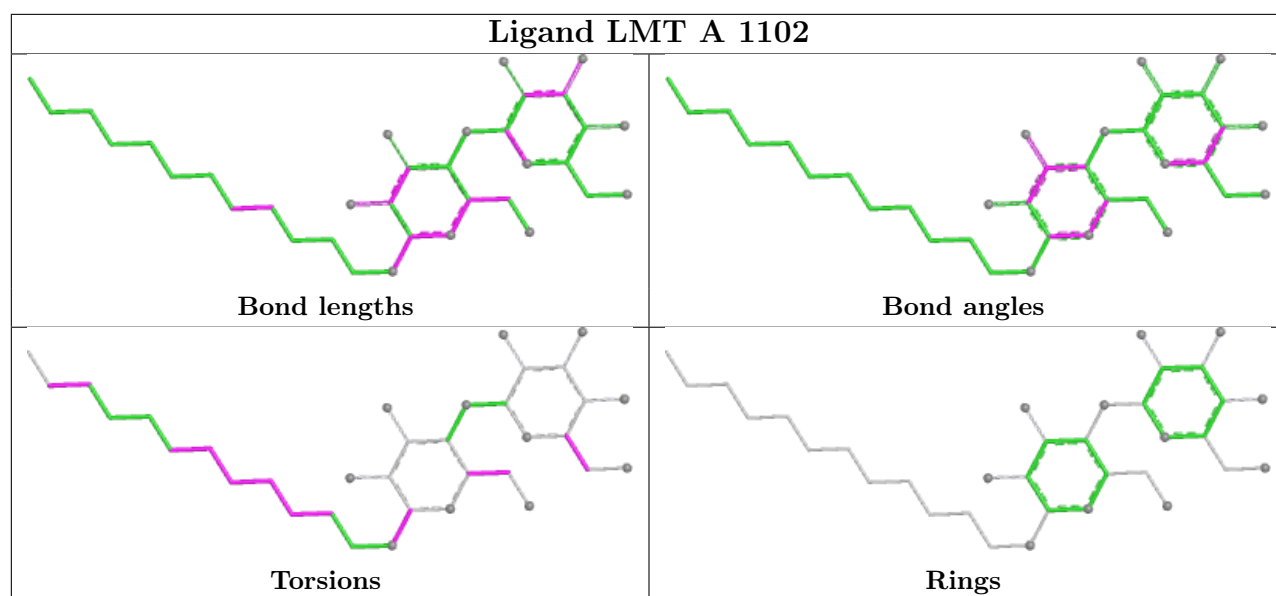
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1101	LMT	11	0
2	D	1101	ERY	4	0
3	C	1101	LMT	1	0
3	B	2100	LMT	7	0
3	F	2100	LMT	2	0
3	A	1102	LMT	5	0
3	D	1103	LMT	7	0
3	A	1103	LMT	2	0

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









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	1038/1044 (99%)	-0.19	12 (1%)	76 50	36, 75, 109, 154	0
1	B	1037/1044 (99%)	-0.28	5 (0%)	87 66	31, 73, 111, 150	0
1	C	1036/1044 (99%)	-0.13	19 (1%)	67 40	35, 76, 112, 139	0
1	D	1038/1044 (99%)	-0.20	12 (1%)	76 50	34, 84, 123, 154	0
1	E	1037/1044 (99%)	-0.14	13 (1%)	75 48	46, 87, 118, 148	0
1	F	1037/1044 (99%)	-0.01	32 (3%)	51 29	41, 85, 119, 143	0
All	All	6223/6264 (99%)	-0.16	93 (1%)	72 44	31, 81, 116, 154	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	501	ALA	5.7
1	E	291	ILE	5.5
1	C	851	GLY	4.7
1	D	59	ASP	4.6
1	C	122	VAL	4.5
1	F	48	SER	4.4
1	C	127	VAL	4.3
1	F	107	VAL	4.1
1	F	122	VAL	4.1
1	B	864	SER	4.0
1	A	494	ALA	4.0
1	E	864	SER	3.9
1	C	833	GLY	3.9
1	F	503	GLY	3.7
1	F	406	VAL	3.7
1	C	832	THR	3.6
1	C	97	GLY	3.6
1	F	851	GLY	3.6
1	B	59	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	864	SER	3.5
1	C	79	SER	3.4
1	C	866	ASN	3.4
1	F	57	VAL	3.3
1	A	400	LEU	3.3
1	C	33	ALA	3.3
1	F	49	TYR	3.2
1	E	299	ALA	3.2
1	C	817	LEU	3.1
1	F	843	ALA	3.1
1	E	290	GLY	3.1
1	D	306	ILE	3.1
1	A	473	THR	3.0
1	C	69	MET	3.0
1	F	473	THR	3.0
1	F	697	LEU	2.9
1	E	33	ALA	2.9
1	F	850	VAL	2.9
1	C	887	TYR	2.9
1	C	398	MET	2.9
1	E	293	LEU	2.8
1	E	488	LEU	2.8
1	A	407	ASP	2.8
1	C	390	ILE	2.8
1	F	849	GLY	2.8
1	F	441	ALA	2.7
1	A	486	LEU	2.7
1	B	514	GLY	2.7
1	A	310	LEU	2.7
1	D	486	LEU	2.7
1	C	59	ASP	2.6
1	B	710	SER	2.6
1	F	294	ALA	2.6
1	F	860	GLN	2.6
1	C	49	TYR	2.5
1	A	383	LEU	2.5
1	A	864	SER	2.5
1	C	844	SER	2.5
1	E	292	LYS	2.5
1	F	863	LEU	2.5
1	F	831	SER	2.4
1	E	164	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	121	GLU	2.3
1	F	118	LEU	2.3
1	F	410	ILE	2.3
1	F	864	SER	2.3
1	C	831	SER	2.3
1	A	59	ASP	2.2
1	D	423	GLU	2.2
1	D	383	LEU	2.2
1	D	37	THR	2.2
1	F	69	MET	2.2
1	F	822	ILE	2.1
1	D	460	GLY	2.1
1	E	300	LEU	2.1
1	A	35	TYR	2.1
1	F	494	ALA	2.1
1	F	95	GLU	2.1
1	A	445	ILE	2.1
1	D	860	GLN	2.1
1	E	541	TYR	2.1
1	F	50	PRO	2.1
1	B	890	TRP	2.0
1	D	832	THR	2.0
1	F	60	THR	2.0
1	F	474	ILE	2.0
1	E	233	SER	2.0
1	A	493	CYS	2.0
1	C	61	VAL	2.0
1	D	400	LEU	2.0
1	D	870	SER	2.0
1	F	844	SER	2.0
1	F	714	ASN	2.0
1	E	175	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

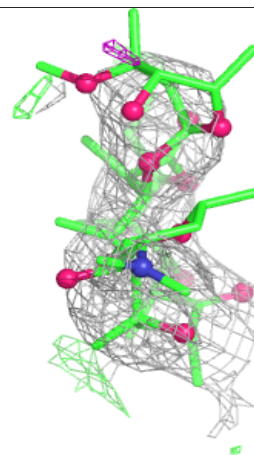
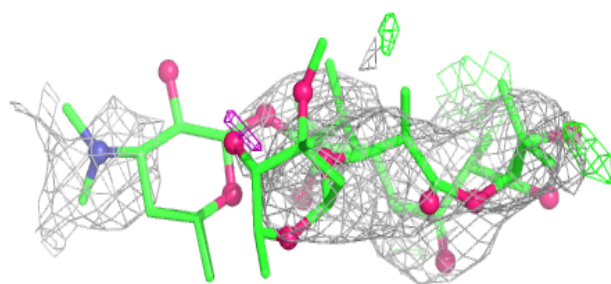
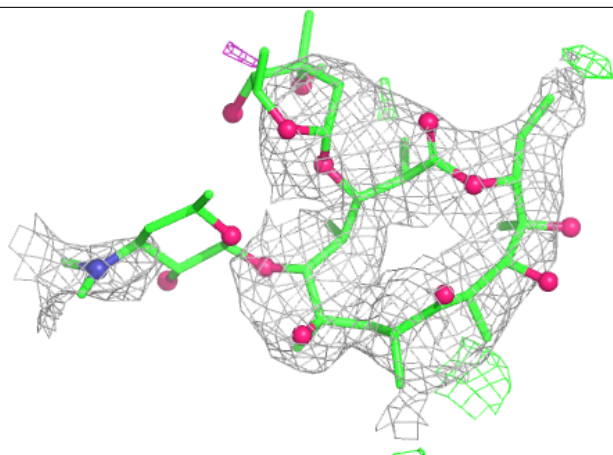
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ERY	D	1101	51/51	0.56	0.16	62,93,101,108	51
2	ERY	A	1101	51/51	0.70	0.15	81,93,101,104	51
3	LMT	D	1103	35/35	0.71	0.16	77,92,105,106	0
3	LMT	C	1101	35/35	0.86	0.09	62,75,83,87	0
3	LMT	F	2100	35/35	0.87	0.09	49,75,87,96	0
3	LMT	B	2100	35/35	0.88	0.09	34,66,78,87	0
3	LMT	A	1103	35/35	0.88	0.12	65,90,106,109	0
3	LMT	D	1102	35/35	0.89	0.08	38,74,82,84	0
3	LMT	E	1101	35/35	0.90	0.08	63,72,86,108	0
3	LMT	A	1102	35/35	0.93	0.07	49,70,79,82	0
4	NI	A	1104	1/1	0.99	0.02	67,67,67,67	0
4	NI	E	1102	1/1	0.99	0.04	73,73,73,73	0
4	NI	C	1102	1/1	1.00	0.02	77,77,77,77	0

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

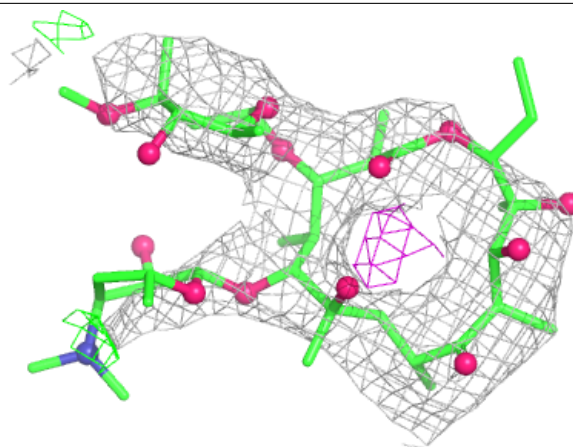
Electron density around ERY D 1101:

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

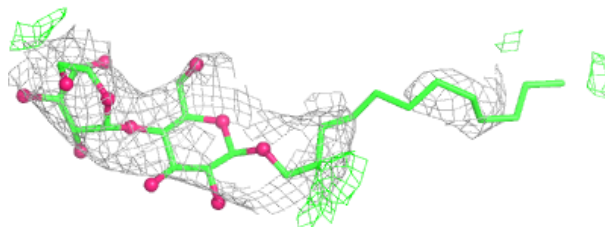


Electron density around ERY A 1101:

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

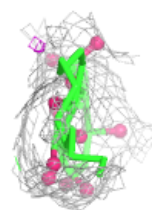
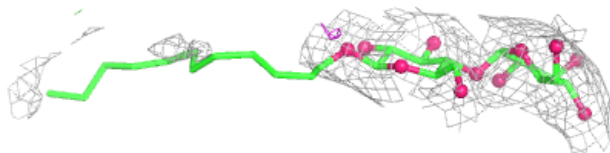
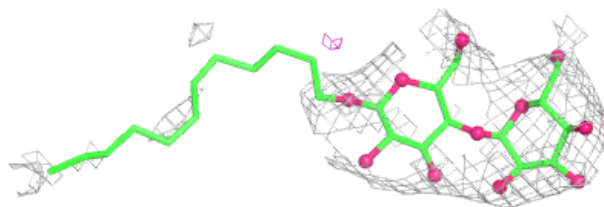
**Electron density around LMT D 1103:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

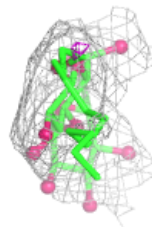
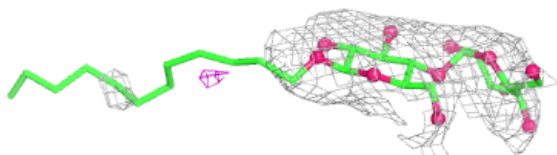
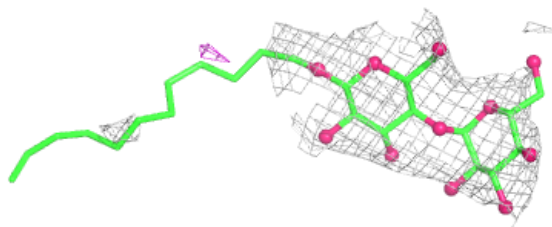


Electron density around LMT C 1101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

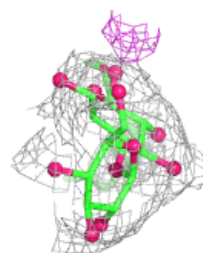
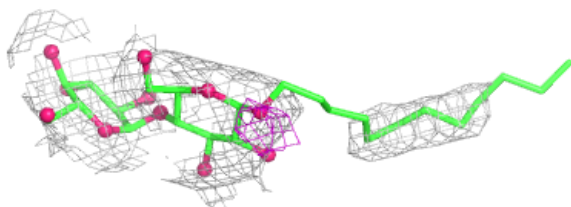
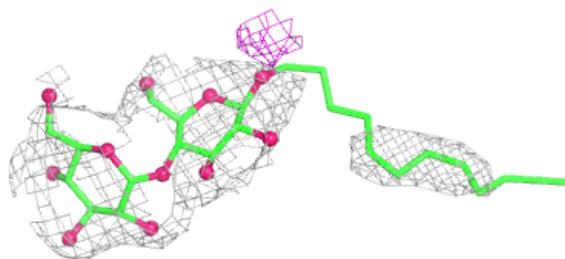
**Electron density around LMT F 2100:**

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

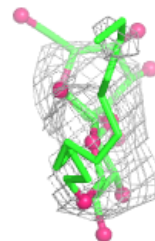
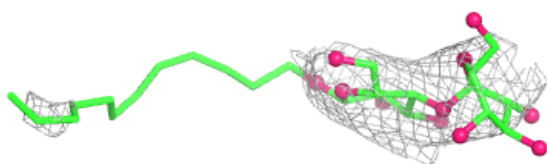
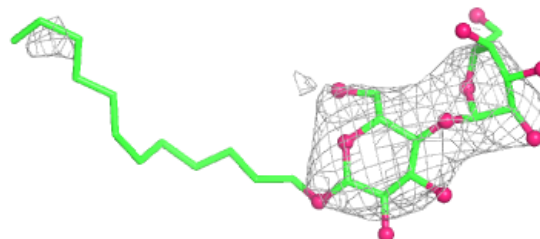


Electron density around LMT B 2100:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

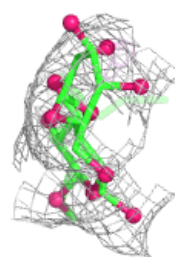
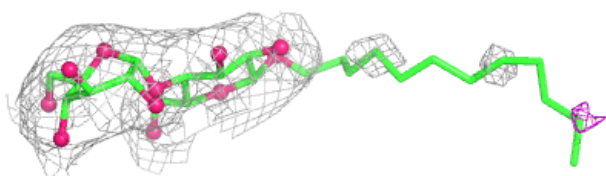
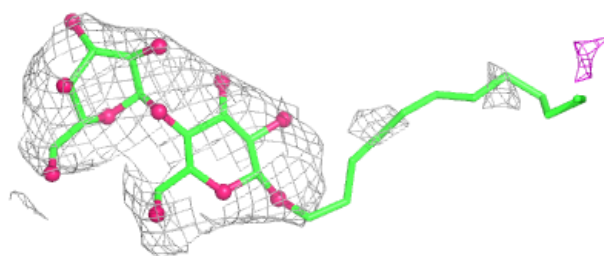
**Electron density around LMT A 1103:**

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

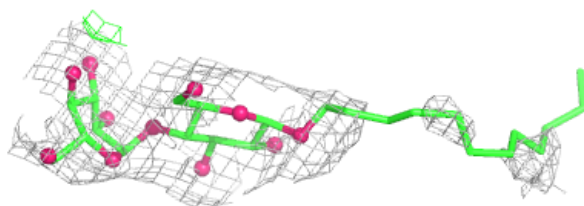
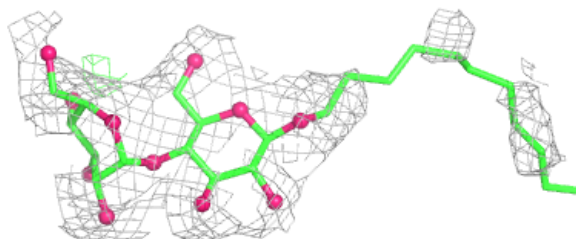


Electron density around LMT D 1102:

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

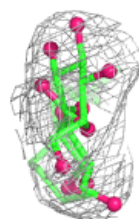
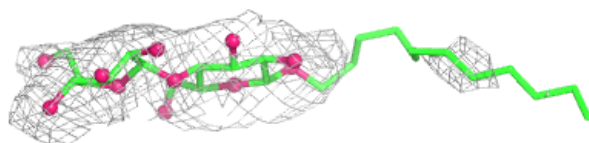
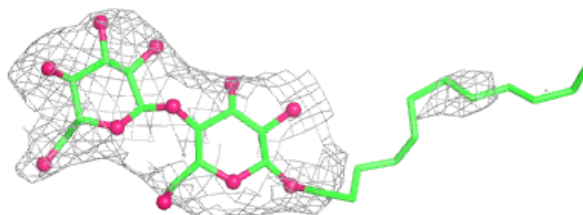
**Electron density around LMT E 1101:**

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



Electron density around LMT A 1102:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.