



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:31 PM UTC

PDB ID : 4ZJL / pdb_00004zjl
Title : Crystal structure of AcrB in complex with antibiotic in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-29
Resolution : 3.47 Å(reported)

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

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

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:

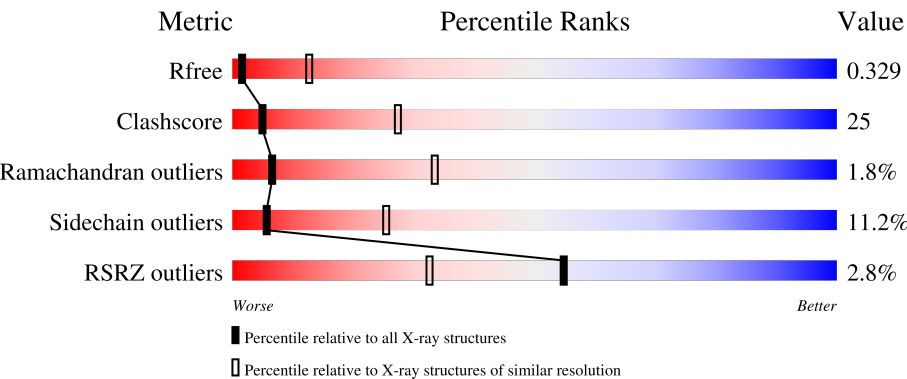
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 3.47 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	1049	3% 48% 44% 7%
1	B	1049	% 52% 41% 6%
1	C	1049	4% 47% 45% 7%
1	D	1049	2% 47% 45% 7%
1	E	1049	2% 48% 43% 7%

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Mol	Chain	Length	Quality of chain
1	F	1049	5% 47% 44% 8% ..

2 Entry composition [i](#)

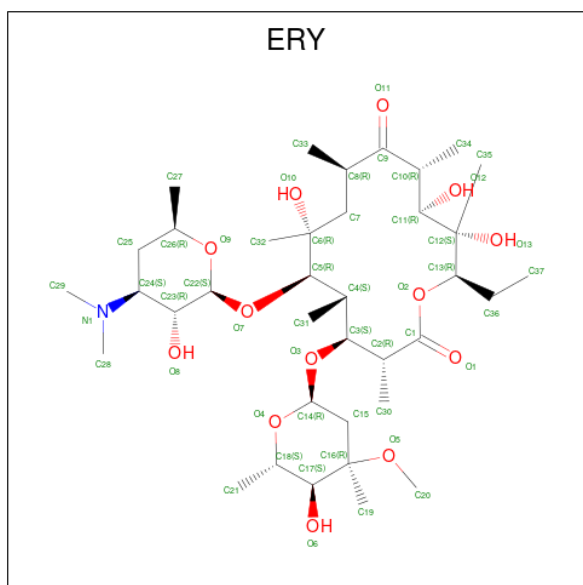
There are 4 unique types of molecules in this entry. The entry contains 47962 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

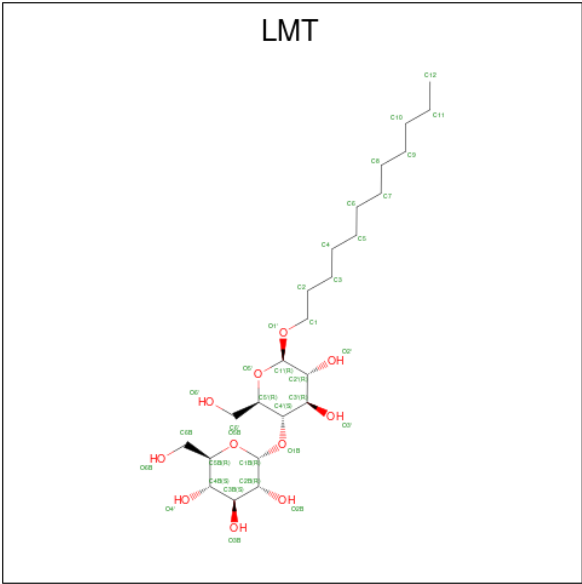
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7942	5105	1315	1479	43			
1	B	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	C	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	D	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	E	1042	Total	C	N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

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



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

- Molecule 3 is DODECYL-BETA-D-MALTOSE (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		

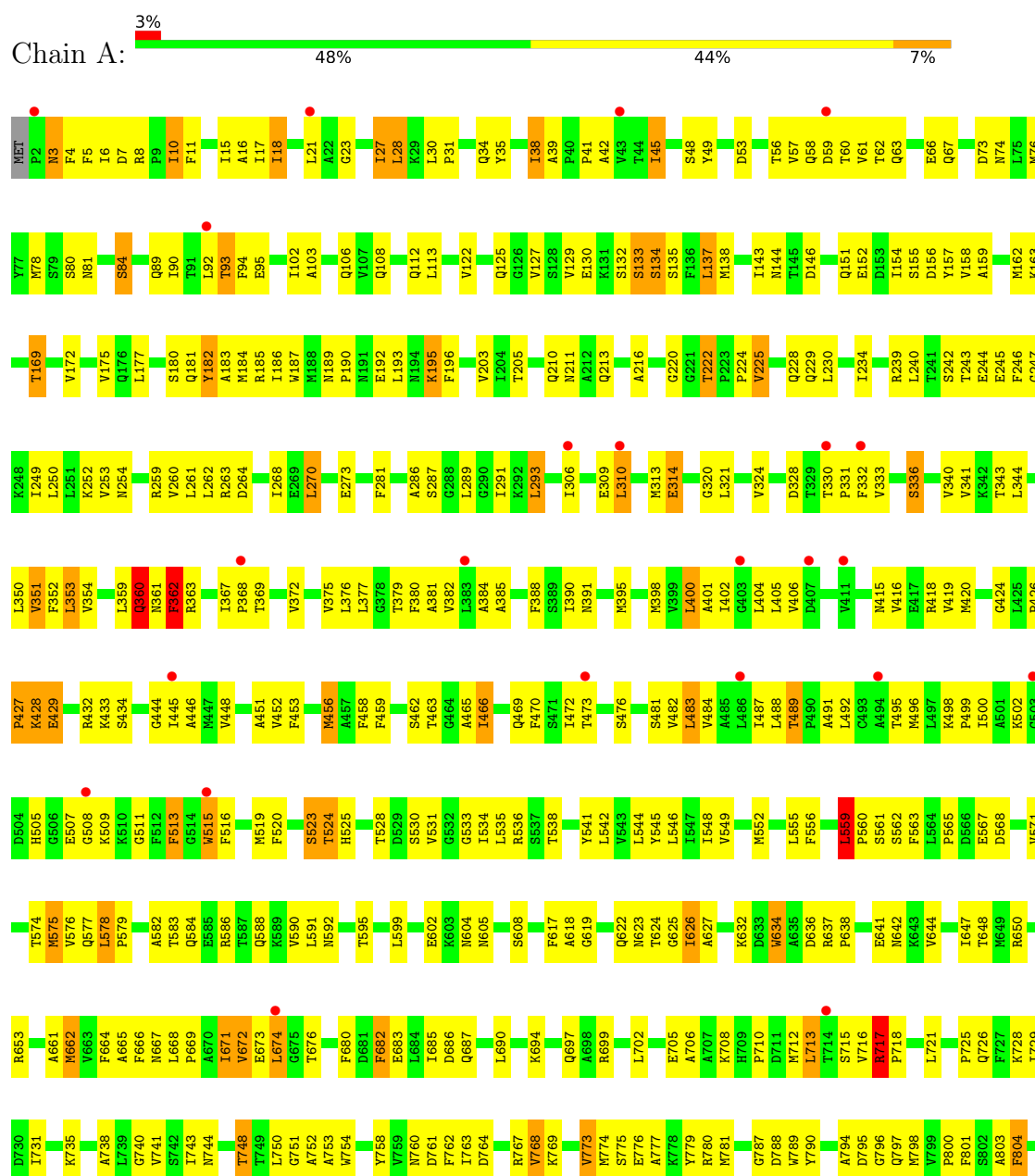
- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

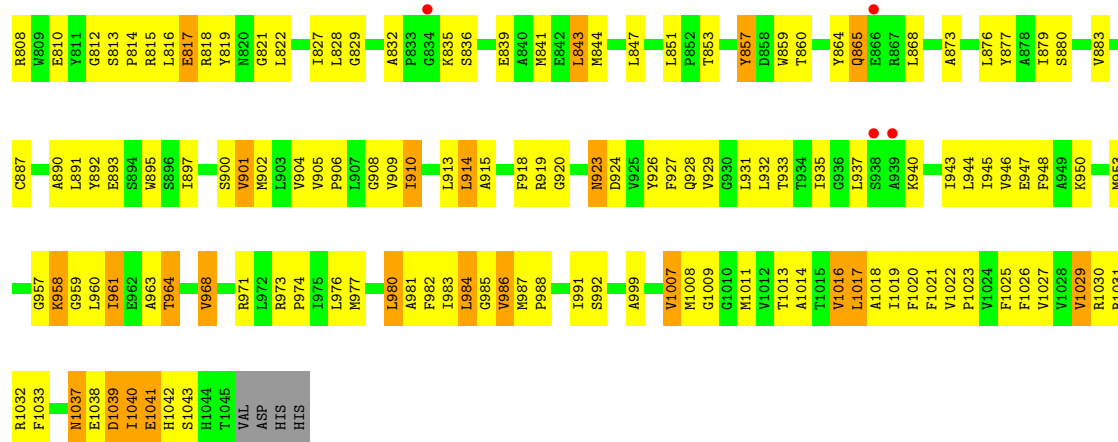
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ni 1	0	0
4	C	1	Total 1	Ni 1	0	0
4	E	1	Total 1	Ni 1	0	0

3 Residue-property plots

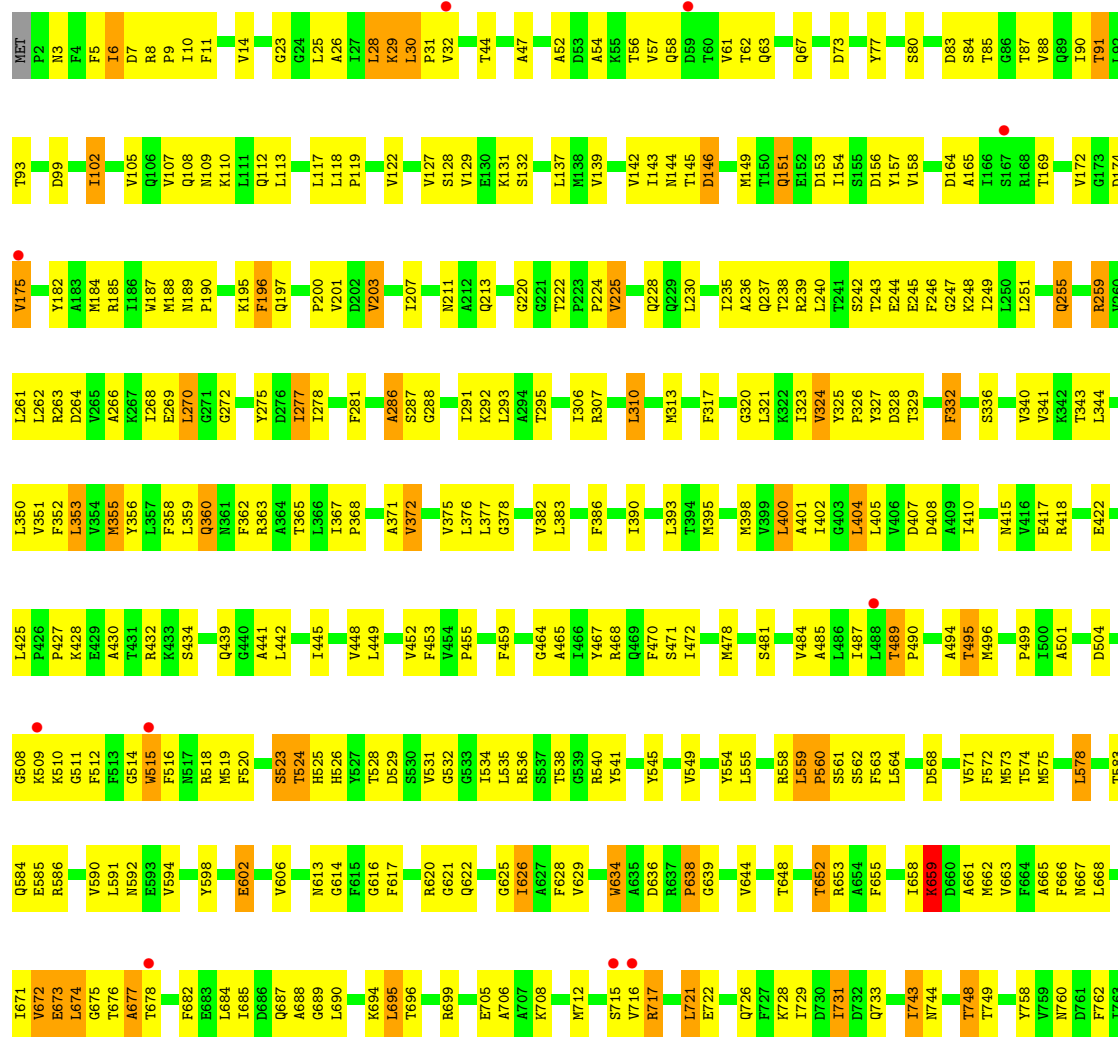
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

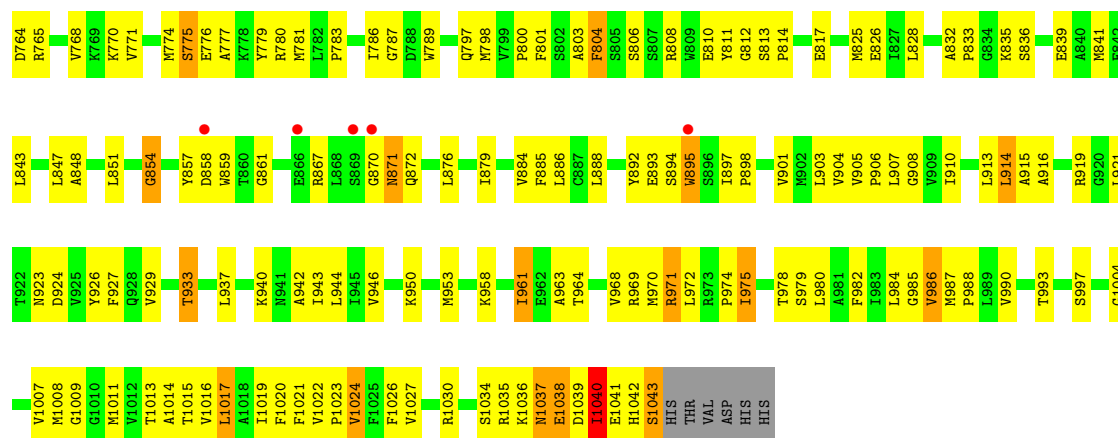
- Molecule 1: Multidrug efflux pump subunit AcrB



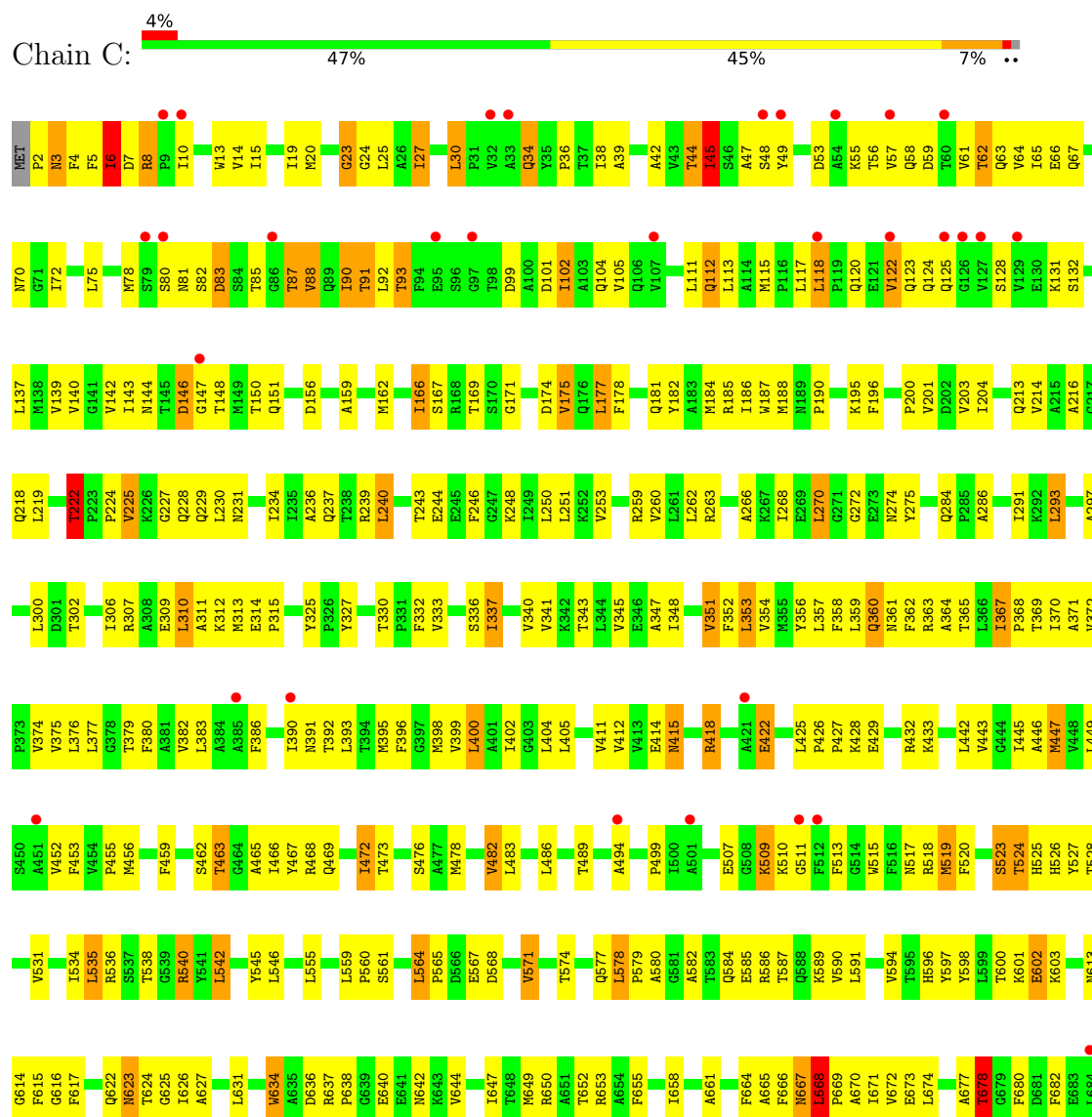


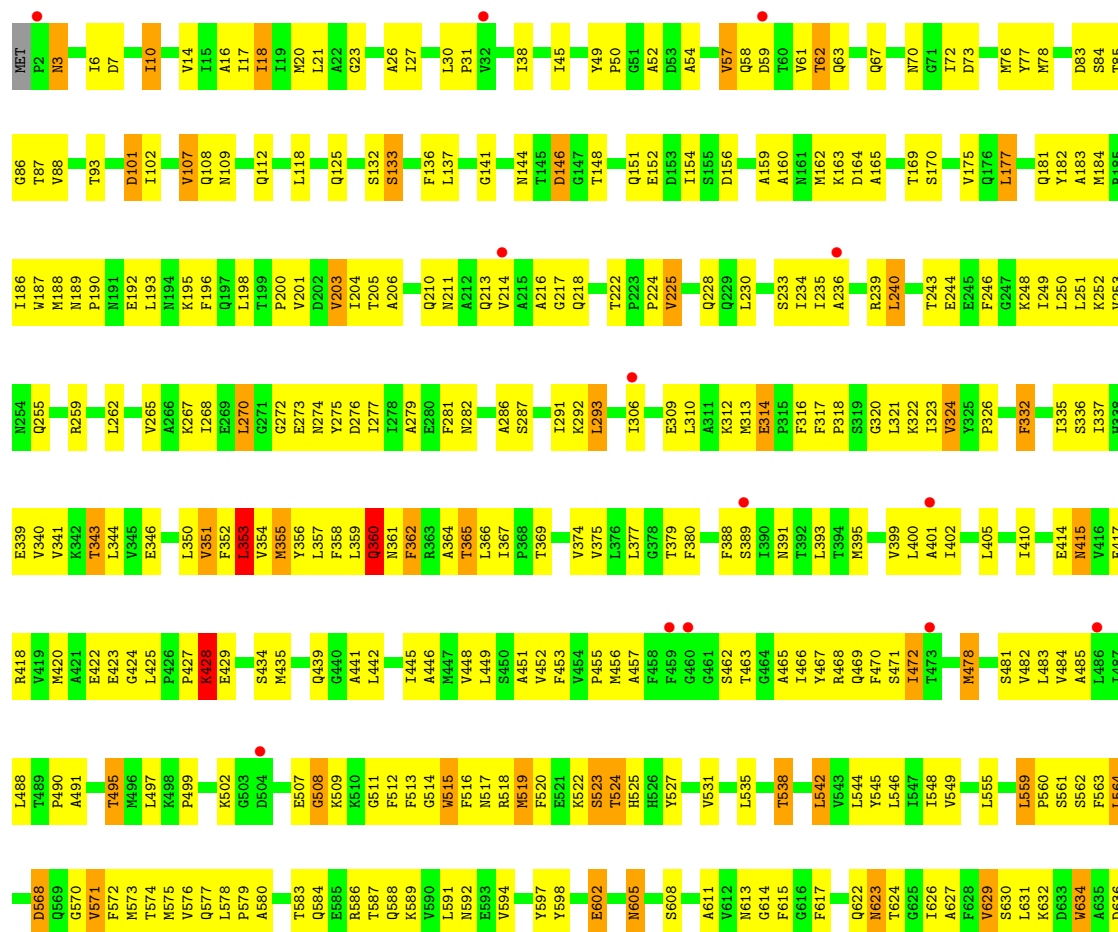
• Molecule 1: Multidrug efflux pump subunit AcrB

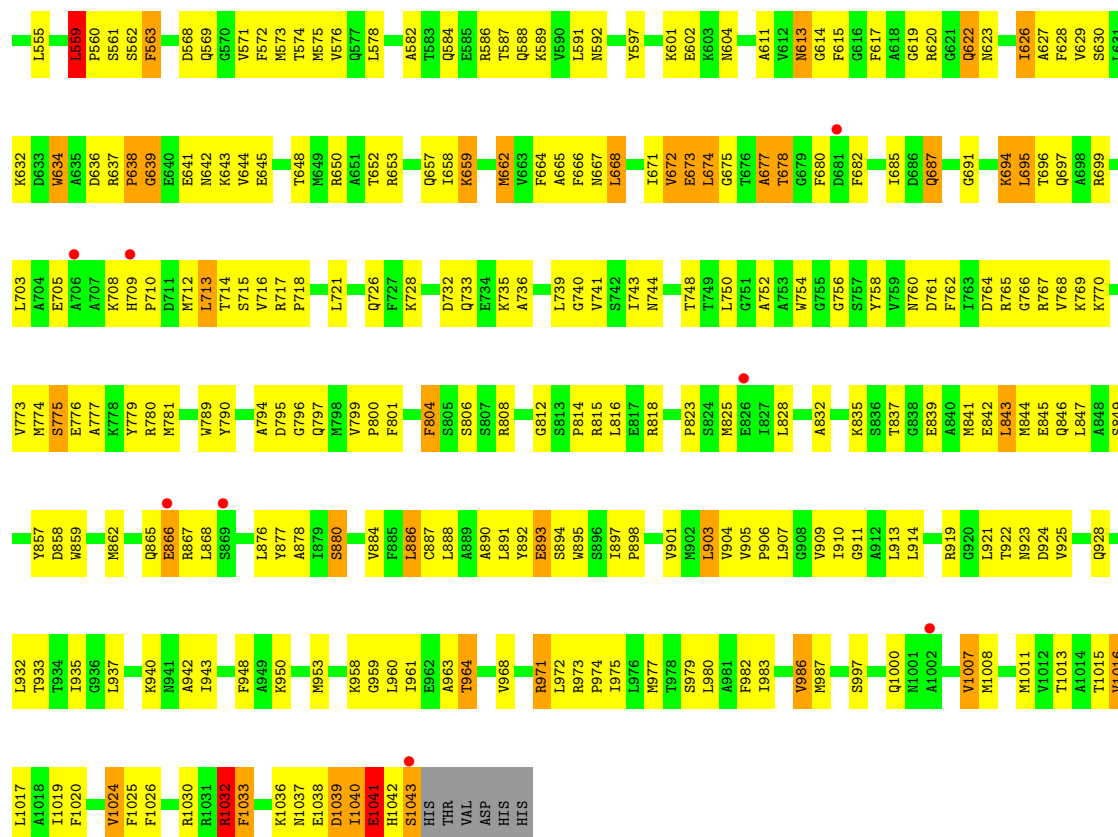




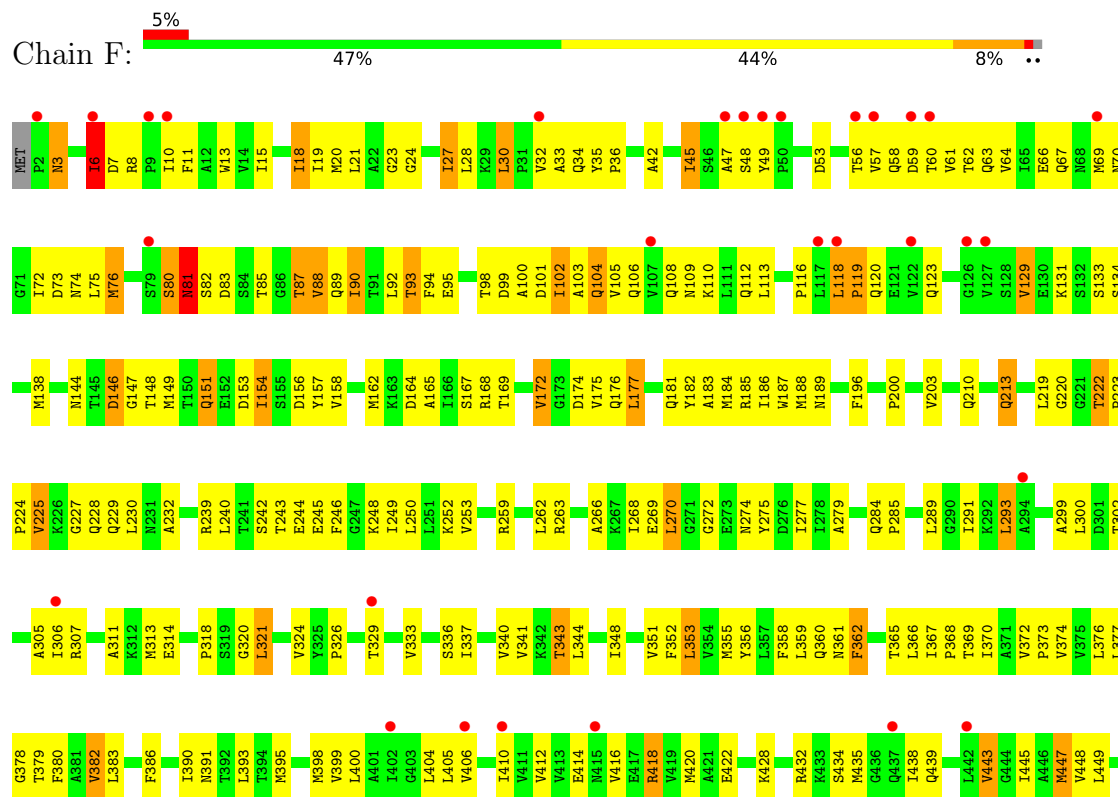
• Molecule 1: Multidrug efflux pump subunit AcrB

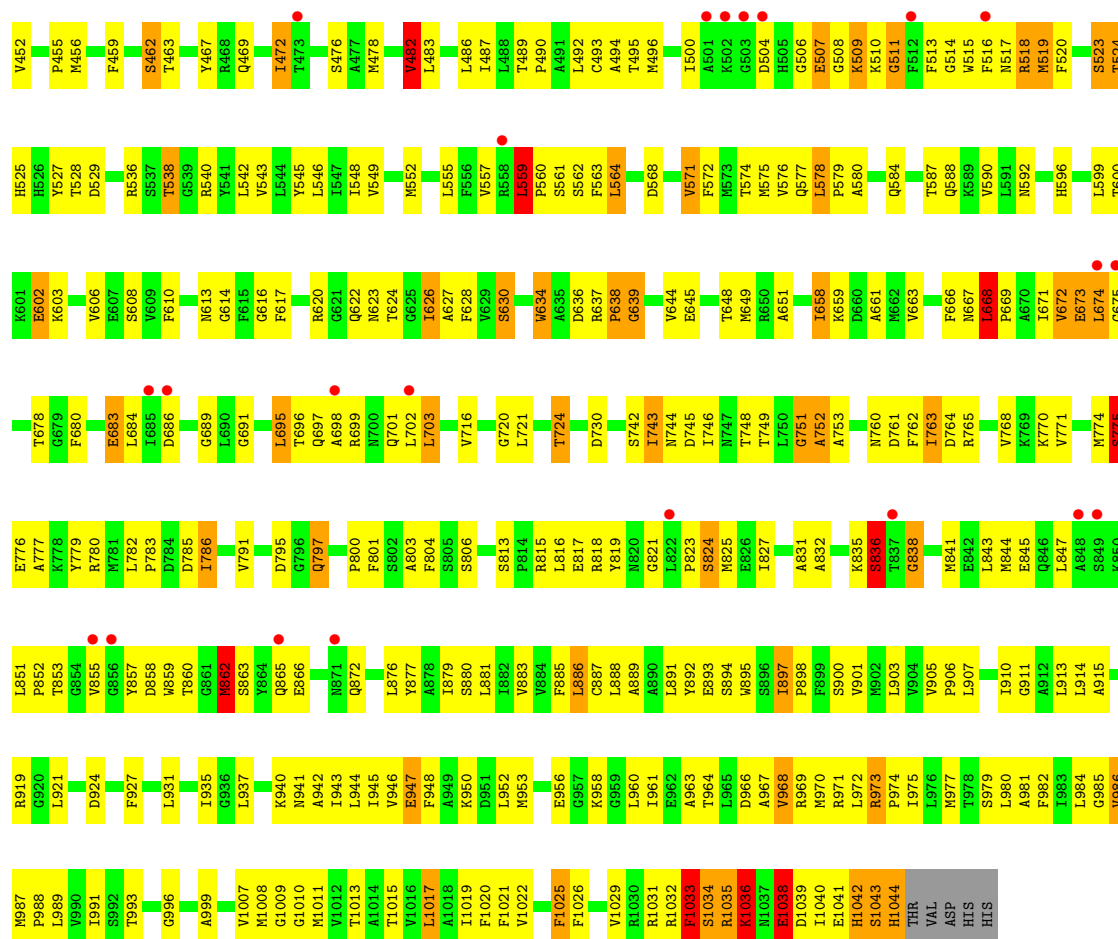






• Molecule 1: Multidrug efflux pump subunit AcrB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	150.95Å 155.66Å 217.01Å 90.00° 92.67° 90.00°	Depositor
Resolution (Å)	19.97 – 3.47 19.97 – 3.47	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.97-3.47) 92.4 (19.97-3.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.251 , 0.321 0.263 , 0.329	Depositor DCC
R_{free} test set	6376 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	91.0	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.056 for -k,-h,-l 0.066 for k,h,-l 0.060 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	47962	wwPDB-VP
Average B, all atoms (Å ²)	82.0	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 44.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5068e-04.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	1/8094 (0.0%)	1.23	37/10990 (0.3%)
1	B	0.78	1/8076 (0.0%)	1.21	37/10965 (0.3%)
1	C	0.79	2/8076 (0.0%)	1.25	57/10965 (0.5%)
1	D	0.74	0/8076	1.19	36/10965 (0.3%)
1	E	0.75	0/8076	1.22	36/10965 (0.3%)
1	F	0.77	0/8087	1.26	58/10980 (0.5%)
All	All	0.77	4/48485 (0.0%)	1.23	261/65830 (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	2
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	2
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	678	THR	CA-CB	6.33	1.60	1.53
1	C	122	VAL	CA-CB	6.01	1.61	1.54
1	C	687	GLN	CA-C	5.37	1.56	1.52
1	A	372	VAL	CA-C	5.13	1.57	1.52

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	559	LEU	CA-C-N	16.14	136.38	119.76
1	E	559	LEU	C-N-CA	16.14	136.38	119.76
1	B	559	LEU	CA-C-N	14.46	135.08	119.90
1	B	559	LEU	C-N-CA	14.46	135.08	119.90
1	A	35	TYR	CA-C-N	-12.49	108.22	120.21
1	A	35	TYR	C-N-CA	-12.49	108.22	120.21
1	A	39	ALA	CA-C-N	11.02	127.70	119.66
1	A	39	ALA	C-N-CA	11.02	127.70	119.66
1	F	118	LEU	CA-C-N	10.68	130.78	119.78
1	F	118	LEU	C-N-CA	10.68	130.78	119.78
1	E	30	LEU	CA-C-N	10.43	130.54	119.90
1	E	30	LEU	C-N-CA	10.43	130.54	119.90
1	C	118	LEU	CA-C-N	9.45	129.51	119.78
1	C	118	LEU	C-N-CA	9.45	129.51	119.78
1	C	83	ASP	N-CA-C	9.44	125.81	109.96
1	A	619	GLY	N-CA-C	9.22	124.52	111.42
1	F	559	LEU	CA-C-N	9.13	129.48	119.90
1	F	559	LEU	C-N-CA	9.13	129.48	119.90
1	C	7	ASP	CA-C-N	8.86	132.13	122.74
1	C	7	ASP	C-N-CA	8.86	132.13	122.74
1	D	559	LEU	CA-C-N	8.44	128.94	119.83
1	D	559	LEU	C-N-CA	8.44	128.94	119.83
1	C	616	GLY	N-CA-C	-8.27	99.03	111.10
1	C	668	LEU	CA-C-N	8.18	128.33	120.31
1	C	668	LEU	C-N-CA	8.18	128.33	120.31
1	F	1042	HIS	N-CA-C	8.08	122.31	110.59
1	D	515	TRP	N-CA-C	-8.05	103.35	113.01
1	E	709	HIS	CA-C-N	7.99	128.18	119.87
1	E	709	HIS	C-N-CA	7.99	128.18	119.87
1	E	498	LYS	CA-C-N	7.90	127.66	119.76
1	E	498	LYS	C-N-CA	7.90	127.66	119.76
1	B	1037	ASN	CA-C-N	7.81	135.75	121.70
1	B	1037	ASN	C-N-CA	7.81	135.75	121.70
1	A	254	ASN	N-CA-C	7.73	121.02	110.35
1	D	367	ILE	CA-C-N	-7.72	111.76	119.56
1	D	367	ILE	C-N-CA	-7.72	111.76	119.56
1	F	223	PRO	CA-C-N	-7.61	112.90	120.21
1	F	223	PRO	C-N-CA	-7.61	112.90	120.21
1	C	973	ARG	CA-C-N	-7.58	111.15	119.19
1	C	973	ARG	C-N-CA	-7.58	111.15	119.19
1	E	674	LEU	N-CA-C	7.53	121.92	109.95
1	E	288	GLY	N-CA-C	7.37	124.66	110.66
1	B	288	GLY	N-CA-C	7.35	124.87	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	THR	N-CA-C	7.22	119.84	110.53
1	E	243	THR	N-CA-C	-7.10	103.58	111.82
1	A	864	TYR	N-CA-C	-6.99	103.09	111.69
1	D	614	GLY	N-CA-C	-6.93	106.23	114.48
1	E	629	VAL	N-CA-C	6.92	117.84	107.80
1	E	532	GLY	N-CA-C	-6.81	104.61	112.50
1	E	177	LEU	N-CA-C	6.77	120.70	109.46
1	B	532	GLY	N-CA-C	-6.73	104.62	112.83
1	F	838	GLY	N-CA-C	6.70	120.77	112.73
1	E	866	GLU	N-CA-C	6.67	119.90	111.69
1	F	7	ASP	CA-C-N	6.67	129.81	122.74
1	F	7	ASP	C-N-CA	6.67	129.81	122.74
1	D	73	ASP	N-CA-C	6.65	119.93	109.96
1	C	640	GLU	N-CA-C	-6.62	105.02	113.23
1	C	677	ALA	N-CA-C	6.61	117.19	108.07
1	C	540	ARG	NE-CZ-NH2	6.59	125.14	119.20
1	D	851	LEU	CA-C-N	6.59	128.08	119.84
1	D	851	LEU	C-N-CA	6.59	128.08	119.84
1	F	60	THR	N-CA-C	-6.59	105.77	113.88
1	C	666	PHE	N-CA-C	6.59	118.22	108.60
1	F	1036	LYS	N-CA-C	6.56	124.77	110.80
1	F	172	VAL	N-CA-C	6.54	117.54	107.99
1	A	808	ARG	N-CA-C	6.53	117.09	107.88
1	A	865	GLN	N-CA-C	6.53	118.06	111.07
1	A	851	LEU	CA-C-N	6.50	127.97	119.84
1	A	851	LEU	C-N-CA	6.50	127.97	119.84
1	D	673	GLU	N-CA-C	6.45	120.07	111.30
1	B	685	ILE	N-CA-C	6.44	117.12	108.11
1	F	35	TYR	CA-C-N	6.41	126.87	120.52
1	F	35	TYR	C-N-CA	6.41	126.87	120.52
1	B	629	VAL	N-CA-C	6.37	117.04	107.80
1	C	85	THR	N-CA-C	-6.37	105.38	113.02
1	C	617	PHE	N-CA-C	-6.37	105.15	113.17
1	C	8	ARG	CA-C-N	6.34	126.25	119.28
1	C	8	ARG	C-N-CA	6.34	126.25	119.28
1	B	73	ASP	N-CA-C	6.29	119.40	109.96
1	E	964	THR	N-CA-C	-6.27	104.36	111.07
1	A	1017	LEU	N-CA-C	-6.24	106.64	114.56
1	F	919	ARG	N-CA-C	-6.22	100.22	109.86
1	F	824	SER	N-CA-C	6.17	118.34	109.14
1	F	518	ARG	N-CA-C	-6.14	104.50	111.07
1	A	28	LEU	N-CA-C	6.08	117.91	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	674	LEU	N-CA-C	6.08	118.19	109.14
1	D	214	VAL	N-CA-C	6.06	116.84	108.12
1	C	364	ALA	N-CA-C	-6.04	104.25	111.69
1	C	4	PHE	N-CA-C	-6.00	104.07	111.75
1	A	489	THR	CA-C-N	-5.99	112.40	119.05
1	A	489	THR	C-N-CA	-5.99	112.40	119.05
1	F	897	ILE	CA-C-N	-5.98	112.37	119.84
1	F	897	ILE	C-N-CA	-5.98	112.37	119.84
1	F	119	PRO	N-CA-C	5.98	120.71	111.21
1	D	896	SER	CA-C-N	5.96	123.99	120.24
1	D	896	SER	C-N-CA	5.96	123.99	120.24
1	F	1034	SER	CA-C-N	5.96	132.42	121.70
1	F	1034	SER	C-N-CA	5.96	132.42	121.70
1	B	563	PHE	N-CA-C	-5.94	105.12	112.72
1	D	49	TYR	CA-C-N	5.92	126.26	119.93
1	D	49	TYR	C-N-CA	5.92	126.26	119.93
1	A	559	LEU	CA-C-N	5.90	125.84	119.76
1	A	559	LEU	C-N-CA	5.90	125.84	119.76
1	F	973	ARG	CA-C-N	-5.89	112.94	119.19
1	F	973	ARG	C-N-CA	-5.89	112.94	119.19
1	A	134	SER	N-CA-C	-5.88	107.92	114.62
1	F	30	LEU	CA-C-N	5.83	126.13	119.83
1	F	30	LEU	C-N-CA	5.83	126.13	119.83
1	B	964	THR	N-CA-C	-5.82	104.84	111.07
1	F	921	LEU	N-CA-C	5.80	118.93	110.17
1	C	919	ARG	N-CA-C	-5.80	101.37	110.36
1	B	929	VAL	N-CA-C	-5.80	104.71	110.62
1	F	836	SER	N-CA-C	-5.79	98.46	110.80
1	B	797	GLN	N-CA-C	5.79	119.16	109.95
1	A	456	MET	CB-CG-SD	-5.78	95.35	112.70
1	C	515	TRP	CA-CB-CG	5.78	124.58	113.60
1	F	7	ASP	N-CA-C	-5.77	103.64	111.55
1	E	489	THR	CA-C-N	-5.76	112.66	119.05
1	E	489	THR	C-N-CA	-5.76	112.66	119.05
1	B	895	TRP	N-CA-C	-5.76	106.21	113.18
1	B	30	LEU	CA-C-N	5.74	125.75	119.90
1	B	30	LEU	C-N-CA	5.74	125.75	119.90
1	F	213	GLN	N-CA-C	-5.72	100.38	109.59
1	F	786	ILE	CA-C-N	5.67	126.24	120.00
1	F	786	ILE	C-N-CA	5.67	126.24	120.00
1	C	7	ASP	N-CA-C	-5.66	103.79	111.55
1	D	512	PHE	N-CA-C	-5.66	105.11	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	666	PHE	N-CA-C	5.65	116.85	108.60
1	C	724	THR	CA-C-N	5.65	125.83	119.90
1	C	724	THR	C-N-CA	5.65	125.83	119.90
1	F	80	SER	N-CA-C	5.65	117.37	108.96
1	C	80	SER	N-CA-C	5.64	117.65	109.07
1	B	659	LYS	N-CA-C	5.64	118.26	109.52
1	C	23	GLY	N-CA-C	5.63	119.97	112.77
1	C	768	VAL	N-CA-C	5.61	116.31	109.30
1	C	90	ILE	N-CA-C	5.61	115.93	107.80
1	D	640	GLU	N-CA-C	-5.59	106.30	113.23
1	D	428	LYS	N-CA-C	5.59	117.84	111.02
1	E	3	ASN	N-CA-C	-5.59	104.82	111.69
1	C	418	ARG	N-CA-C	-5.58	105.28	111.36
1	E	500	ILE	N-CA-C	5.58	115.98	108.17
1	E	808	ARG	N-CA-C	5.57	115.73	107.88
1	E	438	ILE	N-CA-C	5.57	118.34	112.83
1	F	85	THR	N-CA-C	-5.55	106.36	113.02
1	C	1036	LYS	N-CA-C	-5.53	105.68	113.20
1	C	702	LEU	N-CA-C	5.53	116.98	111.07
1	C	851	LEU	CA-C-N	5.52	126.75	119.84
1	C	851	LEU	C-N-CA	5.52	126.75	119.84
1	C	30	LEU	CA-C-N	5.52	125.53	119.90
1	C	30	LEU	C-N-CA	5.52	125.53	119.90
1	B	560	PRO	N-CA-C	5.51	119.12	110.80
1	C	998	GLY	N-CA-C	-5.50	106.12	112.50
1	C	91	THR	N-CA-C	5.49	117.67	108.73
1	F	763	ILE	N-CA-C	5.48	114.64	106.85
1	A	1029	VAL	N-CA-C	5.47	115.67	110.42
1	E	214	VAL	N-CA-C	5.47	115.77	108.11
1	D	864	TYR	N-CA-C	-5.46	104.73	111.40
1	C	685	ILE	N-CA-C	5.46	115.76	108.11
1	C	801	PHE	N-CA-C	-5.46	105.43	111.71
1	F	651	ALA	N-CA-C	-5.46	105.25	111.14
1	C	614	GLY	N-CA-C	-5.45	107.99	114.48
1	B	85	THR	N-CA-C	-5.45	106.48	113.02
1	D	240	LEU	N-CA-C	5.45	117.55	110.53
1	C	218	GLN	N-CA-C	5.44	117.35	108.76
1	B	854	GLY	N-CA-C	-5.42	107.06	114.64
1	E	878	ALA	N-CA-C	-5.42	105.28	111.07
1	B	568	ASP	N-CA-C	-5.41	101.90	109.96
1	B	549	VAL	N-CA-C	5.41	115.61	110.53
1	F	863	SER	N-CA-C	-5.38	107.73	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	724	THR	CA-C-N	5.37	125.54	119.90
1	F	724	THR	C-N-CA	5.37	125.54	119.90
1	D	973	ARG	CA-C-N	-5.32	113.55	119.19
1	D	973	ARG	C-N-CA	-5.32	113.55	119.19
1	D	478	MET	N-CA-C	5.32	116.76	111.07
1	D	580	ALA	N-CA-C	5.32	117.74	110.24
1	D	676	THR	N-CA-C	-5.31	103.02	110.35
1	E	868	LEU	N-CA-C	5.31	118.22	111.69
1	F	529	ASP	N-CA-C	-5.31	104.91	111.33
1	C	222	THR	N-CA-C	-5.30	103.39	110.07
1	F	81	ASN	N-CA-C	5.30	117.71	108.76
1	B	975	ILE	N-CA-C	-5.29	104.80	110.36
1	C	678	THR	N-CA-C	5.29	118.85	109.96
1	B	515	TRP	N-CA-C	-5.28	106.67	113.01
1	A	466	ILE	N-CA-C	5.27	115.48	110.42
1	B	372	VAL	O-C-N	5.27	123.79	120.42
1	D	365	THR	N-CA-C	-5.25	106.13	112.54
1	A	458	PHE	N-CA-C	5.24	118.80	112.93
1	C	367	ILE	CA-C-N	-5.24	114.27	119.56
1	C	367	ILE	C-N-CA	-5.24	114.27	119.56
1	F	813	SER	CA-C-N	-5.23	114.39	120.04
1	F	813	SER	C-N-CA	-5.23	114.39	120.04
1	E	1032	ARG	N-CA-C	5.23	118.71	107.67
1	B	1040	ILE	N-CA-C	5.23	120.21	109.34
1	B	3	ASN	N-CA-C	-5.22	105.27	111.69
1	C	240	LEU	N-CA-C	5.22	117.26	110.53
1	A	130	GLU	N-CA-C	5.21	117.31	109.23
1	A	125	GLN	N-CA-C	-5.21	106.43	112.89
1	A	717	ARG	CA-C-N	-5.20	114.37	119.99
1	A	717	ARG	C-N-CA	-5.20	114.37	119.99
1	F	668	LEU	CA-C-N	5.20	125.40	120.31
1	F	668	LEU	C-N-CA	5.20	125.40	120.31
1	C	778	LYS	N-CA-C	5.19	119.10	112.87
1	D	353	LEU	N-CA-C	5.19	117.02	111.36
1	E	450	SER	N-CA-C	-5.19	106.45	112.89
1	D	671	ILE	CB-CA-C	-5.19	102.78	111.29
1	A	515	TRP	N-CA-C	-5.18	106.65	112.87
1	C	813	SER	CA-C-N	5.18	126.02	120.47
1	C	813	SER	C-N-CA	5.18	126.02	120.47
1	F	154	ILE	N-CA-C	-5.18	105.28	110.30
1	D	495	THR	CB-CA-C	-5.18	101.59	110.24
1	E	321	LEU	N-CA-C	5.17	117.09	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	PHE	N-CA-C	5.17	117.31	111.11
1	C	132	SER	N-CA-C	5.17	117.39	109.07
1	E	416	VAL	N-CA-C	5.15	115.37	110.53
1	D	314	GLU	N-CA-C	5.15	121.18	109.81
1	D	77	TYR	N-CA-C	5.14	116.89	109.07
1	A	84	SER	N-CA-C	-5.13	106.85	113.01
1	A	314	GLU	CA-C-N	-5.13	114.38	119.56
1	A	314	GLU	C-N-CA	-5.13	114.38	119.56
1	D	964	THR	N-CA-C	-5.13	105.58	111.07
1	F	482	VAL	CB-CA-C	-5.13	105.22	112.14
1	A	662	MET	N-CA-C	5.12	118.57	109.96
1	B	832	ALA	CA-C-N	5.12	126.25	119.84
1	B	832	ALA	C-N-CA	5.12	126.25	119.84
1	B	560	PRO	CB-CA-C	-5.12	105.27	111.46
1	D	85	THR	N-CA-C	-5.12	106.88	113.02
1	E	576	VAL	N-CA-C	5.12	115.27	108.11
1	F	797	GLN	N-CA-C	5.10	118.38	110.17
1	D	379	THR	N-CA-C	-5.10	105.80	111.36
1	F	232	ALA	N-CA-C	5.10	116.59	108.79
1	F	857	TYR	N-CA-C	5.10	116.81	109.07
1	C	369	THR	N-CA-C	5.09	116.83	111.28
1	F	382	VAL	CB-CA-C	-5.09	105.27	112.14
1	C	667	ASN	N-CA-C	5.09	117.78	109.59
1	A	513	PHE	N-CA-C	-5.08	107.63	113.88
1	D	675	GLY	N-CA-C	5.08	125.22	113.18
1	A	38	ILE	CB-CA-C	-5.08	106.43	111.30
1	B	286	ALA	N-CA-C	5.07	117.43	108.75
1	C	45	ILE	N-CA-C	5.07	115.39	107.99
1	E	622	GLN	N-CA-C	-5.07	105.88	111.71
1	F	1022	VAL	CB-CA-C	-5.07	108.88	113.70
1	A	182	TYR	N-CA-C	5.07	117.65	110.50
1	B	371	ALA	N-CA-C	5.06	116.48	110.97
1	D	332	PHE	N-CA-C	5.06	116.48	111.07
1	C	330	THR	N-CA-C	5.05	120.98	109.81
1	E	604	ASN	N-CA-C	5.05	117.68	111.82
1	B	972	LEU	N-CA-C	-5.04	105.70	111.14
1	B	512	PHE	N-CA-C	5.04	118.58	112.23
1	F	832	ALA	CA-C-N	5.03	126.13	119.84
1	F	832	ALA	C-N-CA	5.03	126.13	119.84
1	E	972	LEU	N-CA-C	-5.03	105.71	111.14
1	F	89	GLN	N-CA-C	5.03	116.59	108.34
1	F	416	VAL	N-CA-C	5.03	115.25	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	667	ASN	CA-C-N	5.02	128.32	120.68
1	B	667	ASN	C-N-CA	5.02	128.32	120.68
1	A	813	SER	CA-C-N	5.02	125.84	120.47
1	A	813	SER	C-N-CA	5.02	125.84	120.47
1	E	1032	ARG	CA-C-N	5.01	130.72	121.70
1	E	1032	ARG	C-N-CA	5.01	130.72	121.70
1	C	824	SER	N-CA-C	5.00	116.59	109.14
1	F	1025	PHE	N-CA-C	-5.00	105.52	110.97

There are no chirality outliers.

All (8) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7942	0	8080	456	0
1	B	7925	0	8066	361	0
1	C	7925	0	8066	439	0
1	D	7925	0	8066	446	0
1	E	7925	0	8066	419	0
1	F	7935	0	8073	422	0
2	A	51	0	67	6	0
2	D	51	0	67	12	0
3	A	70	0	92	13	0
3	B	35	0	46	5	0
3	C	35	0	46	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	70	0	92	6	0
3	E	35	0	46	5	0
3	F	35	0	46	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	47962	0	48919	2436	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 25.

All (2436) 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:941:ASN:HD21	1:F:1015:THR:HG22	1.18	1.04
1:D:210:GLN:HE22	1:D:250:LEU:HB3	1.27	0.99
1:E:691:GLY:H	1:E:694:LYS:HE3	1.27	0.98
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.48	0.96
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.49	0.94
1:A:134:SER:OG	2:A:1101:ERY:H323	1.67	0.93
1:D:228:GLN:NE2	1:D:230:LEU:O	2.01	0.93
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.51	0.91
1:D:415:ASN:HD22	1:D:434:SER:HB2	1.34	0.91
1:B:775:SER:OG	1:B:776:GLU:O	1.88	0.91
1:D:225:VAL:HG12	1:E:777:ALA:HB1	1.50	0.90
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.53	0.89
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.54	0.88
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.56	0.87
1:B:901:VAL:HG21	1:B:943:ILE:HG13	1.57	0.87
1:A:644:VAL:HG11	1:A:667:ASN:HB2	1.54	0.87
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.56	0.87
1:C:894:SER:HB3	1:C:897:ILE:HG12	1.57	0.87
1:F:559:LEU:HD23	1:F:560:PRO:HD2	1.55	0.87
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.56	0.86
1:C:892:TYR:O	1:C:894:SER:N	2.07	0.86
1:A:424:GLY:HA3	1:A:502:LYS:HB3	1.58	0.86
1:E:516:PHE:HA	1:E:519:MET:HG3	1.57	0.86
1:B:696:THR:HG23	1:B:699:ARG:HH12	1.38	0.86
1:A:38:ILE:HD11	1:A:466:ILE:HD11	1.57	0.86
1:A:877:TYR:OH	1:A:928:GLN:NE2	2.09	0.85
1:B:350:LEU:HD13	1:B:984:LEU:HB3	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	1.58	0.85
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.59	0.85
1:F:937:LEU:HD13	1:F:1011:MET:HE2	1.59	0.84
1:B:525:HIS:CD2	1:B:529:ASP:OD2	2.31	0.84
1:B:634:TRP:H	1:B:634:TRP:CD1	1.94	0.84
1:F:3:ASN:HD22	1:F:435:MET:HG3	1.42	0.84
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.11	0.83
1:C:428:LYS:HG2	1:C:494:ALA:HB1	1.60	0.83
1:D:38:ILE:HG23	1:D:462:SER:HB2	1.60	0.83
1:F:356:TYR:HA	1:F:365:THR:HG21	1.60	0.83
1:C:740:GLY:O	1:C:794:ALA:N	2.12	0.83
1:F:901:VAL:HG23	1:F:942:ALA:HB3	1.58	0.83
1:C:465:ALA:HA	1:C:468:ARG:HH12	1.43	0.82
1:E:222:THR:HA	1:E:224:PRO:HD3	1.61	0.82
1:A:935:ILE:HD12	3:A:1103:LMT:H72	1.62	0.82
1:B:971:ARG:O	1:B:975:ILE:HG12	1.78	0.82
1:C:356:TYR:HA	1:C:365:THR:HG21	1.60	0.82
1:D:445:ILE:HD13	1:D:940:LYS:HE3	1.60	0.82
1:A:971:ARG:HG2	1:A:974:PRO:HG2	1.61	0.82
1:A:832:ALA:HB3	1:A:835:LYS:HD3	1.60	0.81
1:B:525:HIS:NE2	1:B:529:ASP:OD2	2.12	0.81
1:C:579:PRO:HD3	1:C:661:ALA:HB2	1.63	0.81
1:D:187:TRP:HB3	1:D:776:GLU:HA	1.63	0.81
1:A:137:LEU:HD22	1:A:293:LEU:HG	1.60	0.81
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.63	0.81
1:E:559:LEU:HD22	1:E:560:PRO:HD2	1.63	0.81
1:E:225:VAL:HG12	1:F:777:ALA:HB1	1.63	0.80
1:C:669:PRO:HB2	1:C:862:MET:HE2	1.62	0.80
1:C:3:ASN:N	1:C:3:ASN:OD1	2.14	0.80
1:A:562:SER:HB2	1:A:924:ASP:HB3	1.63	0.80
1:D:244:GLU:HG2	1:D:248:LYS:HE2	1.63	0.80
1:A:445:ILE:HD13	1:A:940:LYS:HE3	1.63	0.80
1:C:240:LEU:HB2	1:C:246:PHE:HE1	1.47	0.80
1:D:781:MET:HE3	1:F:228:GLN:HE21	1.47	0.79
1:A:690:LEU:HB3	1:A:694:LYS:HD3	1.64	0.79
1:D:181:GLN:OE1	1:D:767:ARG:NH2	2.15	0.79
1:D:740:GLY:O	1:D:794:ALA:N	2.14	0.79
1:E:530:SER:OG	3:E:1101:LMT:O2'	1.66	0.79
1:A:67:GLN:OE1	1:C:767:ARG:NH1	2.15	0.79
1:D:700:ASN:HA	1:D:703:LEU:HD12	1.63	0.79
1:A:427:PRO:HD3	1:A:499:PRO:HB3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:690:LEU:HB3	1:D:694:LYS:HD3	1.65	0.79
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.65	0.79
1:E:415:ASN:ND2	1:E:437:GLN:OE1	2.16	0.78
1:D:137:LEU:HD22	1:D:293:LEU:HG	1.65	0.78
1:A:181:GLN:OE1	1:A:767:ARG:NH2	2.16	0.78
1:B:516:PHE:HA	1:B:519:MET:HG3	1.65	0.78
1:E:959:GLY:HA2	1:E:1040:ILE:HB	1.65	0.78
1:A:222:THR:HA	1:A:224:PRO:HD3	1.64	0.77
1:B:508:GLY:O	1:B:510:LYS:N	2.16	0.77
1:A:1037:ASN:HA	1:A:1038:GLU:HB2	1.63	0.77
1:E:979:SER:OG	1:E:1015:THR:HG21	1.84	0.77
1:D:507:GLU:O	1:D:509:LYS:N	2.17	0.77
1:B:151:GLN:HE22	1:B:278:ILE:HA	1.48	0.77
1:D:196:PHE:O	1:D:252:LYS:NZ	2.18	0.77
1:A:579:PRO:HD3	1:A:661:ALA:HB2	1.66	0.77
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.66	0.77
1:C:664:PHE:HD2	1:C:717:ARG:HD2	1.50	0.77
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.67	0.77
1:E:832:ALA:HB3	1:E:835:LYS:HD3	1.67	0.77
1:D:775:SER:OG	1:D:776:GLU:O	2.02	0.76
1:B:14:VAL:HG22	1:C:886:LEU:HD12	1.64	0.76
1:B:228:GLN:NE2	1:C:781:MET:SD	2.59	0.76
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.17	0.76
1:E:196:PHE:O	1:E:252:LYS:NZ	2.17	0.76
1:C:971:ARG:HB3	1:C:971:ARG:CZ	2.15	0.76
1:B:668:LEU:HD23	1:B:668:LEU:H	1.50	0.76
1:E:971:ARG:O	1:E:975:ILE:HG12	1.85	0.76
1:A:901:VAL:HG21	1:A:943:ILE:HG13	1.68	0.76
1:D:236:ALA:O	1:E:728:LYS:NZ	2.19	0.76
1:D:986:VAL:HG12	1:D:1008:MET:HE3	1.67	0.76
1:E:652:THR:HG23	1:E:665:ALA:HB3	1.67	0.75
1:C:34:GLN:HE21	1:C:333:VAL:HG22	1.50	0.75
1:D:453:PHE:O	1:D:471:SER:OG	2.04	0.75
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.68	0.75
1:A:1039:ASP:HA	1:A:1040:ILE:HB	1.68	0.75
1:C:944:LEU:HB3	1:C:971:ARG:NE	2.01	0.75
1:D:448:VAL:HG22	1:D:887:CYS:HB3	1.67	0.75
1:C:382:VAL:HG21	1:C:476:SER:HB2	1.69	0.75
1:C:228:GLN:NE2	1:C:230:LEU:O	2.19	0.74
1:F:775:SER:OG	1:F:776:GLU:O	2.04	0.74
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:SER:OG	3:A:1102:LMT:O2'	1.93	0.74
1:A:758:TYR:OH	1:A:761:ASP:OD1	2.05	0.74
1:E:340:VAL:HG21	1:E:395:MET:HB3	1.69	0.74
1:D:491:ALA:O	1:D:495:THR:OG1	2.04	0.74
1:B:228:GLN:HE22	1:C:781:MET:HB3	1.52	0.74
1:F:634:TRP:CD1	1:F:634:TRP:H	2.06	0.74
1:A:350:LEU:HD22	1:A:984:LEU:HB3	1.69	0.74
1:A:986:VAL:HG21	1:A:1007:VAL:HG11	1.69	0.74
1:C:307:ARG:NH2	1:C:314:GLU:OE2	2.21	0.74
1:D:586:ARG:O	1:D:589:LYS:HB3	1.88	0.74
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.71	0.73
1:B:26:ALA:O	1:B:30:LEU:HB2	1.89	0.73
1:A:728:LYS:NZ	1:C:236:ALA:O	2.16	0.73
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.23	0.73
1:E:588:GLN:O	1:E:592:ASN:ND2	2.22	0.73
1:A:360:GLN:NE2	1:A:513:PHE:HB3	2.03	0.73
1:B:1035:ARG:HG3	1:B:1036:LYS:HG3	1.71	0.73
1:D:516:PHE:HA	1:D:519:MET:SD	2.29	0.73
1:E:775:SER:OG	1:E:776:GLU:O	2.06	0.73
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.17	0.73
1:B:1037:ASN:HA	1:B:1038:GLU:HB2	1.71	0.72
1:D:579:PRO:HD3	1:D:661:ALA:HB2	1.70	0.72
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.71	0.72
1:C:699:ARG:NH1	1:C:825:MET:SD	2.62	0.72
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.71	0.72
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.70	0.72
1:F:58:GLN:OE1	1:F:818:ARG:NH1	2.23	0.72
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.72	0.72
1:B:7:ASP:OD2	1:B:432:ARG:NH2	2.22	0.72
1:B:187:TRP:NE1	1:B:269:GLU:OE2	2.23	0.71
1:F:156:ASP:OD1	1:F:765:ARG:NH2	2.23	0.71
1:B:6:ILE:O	1:B:428:LYS:NZ	2.23	0.71
1:B:696:THR:HG23	1:B:699:ARG:NH1	2.04	0.71
1:B:1036:LYS:HA	1:B:1038:GLU:HG2	1.72	0.71
1:D:343:THR:HG21	1:D:989:LEU:HD21	1.71	0.71
1:E:428:LYS:HG2	1:E:494:ALA:HB1	1.72	0.71
1:F:83:ASP:HB2	1:F:87:THR:O	1.89	0.71
1:B:415:ASN:HD22	1:B:434:SER:HB2	1.56	0.71
1:D:156:ASP:OD2	1:D:769:LYS:NZ	2.23	0.71
1:F:892:TYR:O	1:F:894:SER:N	2.24	0.71
1:A:637:ARG:NH1	1:A:642:ASN:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.73	0.71
1:A:740:GLY:O	1:A:794:ALA:N	2.22	0.71
1:D:781:MET:HE3	1:F:228:GLN:NE2	2.05	0.71
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.72	0.70
1:D:888:LEU:HD13	1:D:901:VAL:HG13	1.70	0.70
1:D:712:MET:HE3	1:D:839:GLU:HB3	1.72	0.70
1:E:42:ALA:HB2	1:E:93:THR:HG23	1.73	0.70
1:F:667:ASN:O	1:F:678:THR:OG1	2.07	0.70
1:A:781:MET:HE1	1:C:225:VAL:H	1.55	0.70
1:C:53:ASP:OD1	1:C:56:THR:OG1	2.08	0.70
1:A:210:GLN:NE2	1:A:250:LEU:O	2.24	0.70
1:B:236:ALA:O	1:C:728:LYS:NZ	2.16	0.70
1:B:262:LEU:HG	1:B:268:ILE:HD11	1.71	0.70
1:B:508:GLY:HA2	1:B:518:ARG:HH21	1.55	0.70
1:F:449:LEU:HB2	1:F:478:MET:HE2	1.74	0.70
1:C:941:ASN:ND2	1:C:1015:THR:HG22	2.07	0.70
1:A:225:VAL:HG12	1:B:777:ALA:HB1	1.73	0.70
1:B:901:VAL:HG23	1:B:942:ALA:HB3	1.72	0.70
1:C:507:GLU:HG2	1:C:518:ARG:HG3	1.73	0.70
1:D:699:ARG:NH1	1:D:825:MET:SD	2.64	0.70
1:D:1034:SER:OG	1:D:1035:ARG:N	2.14	0.70
1:D:317:PHE:CD2	1:D:321:LEU:HD12	2.26	0.70
1:D:583:THR:HG21	1:F:229:GLN:HA	1.74	0.70
1:F:525:HIS:HA	1:F:528:THR:HG22	1.74	0.70
1:A:451:ALA:HB1	1:A:883:VAL:HG12	1.72	0.70
1:A:452:VAL:HG11	3:A:1103:LMT:H111	1.74	0.70
1:F:452:VAL:O	1:F:455:PRO:HD2	1.91	0.70
1:E:448:VAL:HG13	1:E:884:VAL:HG22	1.74	0.69
1:E:562:SER:HB3	1:E:924:ASP:HB3	1.74	0.69
1:B:452:VAL:HG23	1:B:453:PHE:CD2	2.27	0.69
1:F:262:LEU:HG	1:F:268:ILE:HD11	1.74	0.69
1:B:404:LEU:HD23	1:B:478:MET:HG3	1.73	0.69
1:A:605:ASN:HD22	1:A:647:ILE:HD11	1.56	0.69
1:A:775:SER:OG	1:A:776:GLU:O	2.10	0.69
1:A:945:ILE:HG13	1:A:971:ARG:HH22	1.56	0.69
1:F:153:ASP:OD2	1:F:182:TYR:OH	2.09	0.69
1:F:746:ILE:HG22	1:F:791:VAL:HG21	1.75	0.69
1:F:941:ASN:ND2	1:F:1015:THR:HG22	2.01	0.69
1:C:568:ASP:OD1	1:C:637:ARG:NH1	2.20	0.69
1:D:18:ILE:HG13	1:E:886:LEU:HD23	1.75	0.69
1:D:326:PRO:O	1:D:630:SER:OG	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ILE:HD13	1:C:25:LEU:HD21	1.74	0.69
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.73	0.69
1:A:426:PRO:HB2	1:A:429:GLU:OE2	1.93	0.69
1:A:637:ARG:HB3	1:A:642:ASN:HB3	1.74	0.69
1:C:580:ALA:HB1	1:C:724:THR:HG23	1.74	0.69
1:D:1037:ASN:HA	1:D:1038:GLU:HB2	1.75	0.69
1:B:531:VAL:O	1:B:534:ILE:HG13	1.93	0.69
1:C:356:TYR:C	1:C:358:PHE:H	2.01	0.69
1:D:355:MET:HB3	1:D:365:THR:OG1	1.92	0.69
1:F:196:PHE:O	1:F:252:LYS:NZ	2.25	0.69
1:C:519:MET:O	1:C:523:SER:OG	2.06	0.68
1:D:535:LEU:HD21	1:D:1027:VAL:HG21	1.75	0.68
1:C:520:PHE:O	1:C:524:THR:HG22	1.92	0.68
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.74	0.68
1:D:109:ASN:HD21	1:F:129:VAL:HG23	1.58	0.68
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.28	0.68
1:C:831:ALA:HB3	1:C:835:LYS:HG3	1.74	0.68
1:B:156:ASP:OD1	1:B:765:ARG:NH2	2.27	0.68
1:D:971:ARG:HG2	1:D:974:PRO:HG2	1.76	0.68
1:F:762:PHE:CE1	1:F:764:ASP:HB2	2.29	0.68
1:C:841:MET:O	1:C:845:GLU:HG2	1.94	0.68
1:D:228:GLN:OE1	1:E:781:MET:HE3	1.92	0.68
1:E:986:VAL:HG21	1:E:1007:VAL:HG11	1.74	0.68
1:A:957:GLY:O	1:A:1042:HIS:N	2.27	0.68
1:C:937:LEU:HD13	1:C:1011:MET:HE2	1.76	0.68
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.75	0.68
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.75	0.68
1:D:442:LEU:O	1:D:445:ILE:HG13	1.94	0.68
1:A:634:TRP:CD1	1:A:634:TRP:H	2.11	0.67
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.76	0.67
1:F:222:THR:HA	1:F:224:PRO:HD3	1.75	0.67
1:A:80:SER:HB3	1:A:90:ILE:HG12	1.76	0.67
1:D:350:LEU:HD13	1:D:984:LEU:HB3	1.77	0.67
1:E:242:SER:HB2	1:E:245:GLU:H	1.58	0.67
1:F:577:GLN:HG3	1:F:624:THR:HG22	1.76	0.67
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.77	0.67
1:D:516:PHE:O	1:D:519:MET:HG2	1.94	0.67
1:E:159:ALA:O	1:E:767:ARG:NH2	2.28	0.67
1:F:937:LEU:HD11	1:F:982:PHE:CE2	2.30	0.67
1:B:559:LEU:HD23	1:B:560:PRO:HD2	1.76	0.67
1:E:415:ASN:CG	1:E:418:ARG:HH12	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:PHE:CE1	1:C:857:TYR:HB2	2.29	0.67
1:E:680:PHE:CZ	1:E:844:MET:HG3	2.29	0.67
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.77	0.67
1:E:262:LEU:HG	1:E:268:ILE:HD11	1.76	0.67
1:B:146:ASP:OD2	1:B:146:ASP:N	2.23	0.67
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.77	0.67
1:A:332:PHE:O	1:A:336:SER:HB3	1.94	0.67
1:B:139:VAL:HB	1:B:327:TYR:HB3	1.76	0.67
1:C:775:SER:OG	1:C:776:GLU:O	2.12	0.67
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.77	0.67
1:E:441:ALA:O	1:E:445:ILE:HG23	1.95	0.67
1:F:404:LEU:HG	1:F:449:LEU:HD13	1.77	0.67
1:F:885:PHE:HD2	1:F:886:LEU:HD22	1.60	0.67
1:C:907:LEU:HG	1:C:1017:LEU:HD23	1.76	0.66
1:A:931:LEU:HB3	3:A:1103:LMT:H51	1.77	0.66
1:A:971:ARG:CZ	1:A:971:ARG:HB3	2.24	0.66
1:B:448:VAL:HG13	1:B:884:VAL:HG22	1.77	0.66
1:D:213:GLN:HG2	1:D:239:ARG:HG2	1.75	0.66
1:D:800:PRO:HG2	1:D:803:ALA:HB2	1.77	0.66
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.76	0.66
1:A:932:LEU:HA	3:A:1103:LMT:H71	1.78	0.66
1:A:465:ALA:O	1:A:469:GLN:HG2	1.96	0.66
1:C:578:LEU:HG	1:C:587:THR:HG22	1.77	0.66
1:E:705:GLU:HB3	1:E:847:LEU:HD22	1.78	0.66
1:F:894:SER:HB3	1:F:897:ILE:HG12	1.77	0.66
1:C:404:LEU:HG	1:C:449:LEU:HD13	1.77	0.66
1:E:986:VAL:HG11	1:E:1007:VAL:HG12	1.77	0.66
1:D:902:MET:O	1:D:905:VAL:HG23	1.96	0.66
1:E:901:VAL:HG21	1:E:943:ILE:HG13	1.77	0.66
1:F:966:ASP:OD1	1:F:969:ARG:NH1	2.29	0.66
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.75	0.66
1:D:415:ASN:HD22	1:D:434:SER:CB	2.07	0.66
1:D:1035:ARG:HH22	1:D:1036:LYS:HE3	1.61	0.66
1:F:610:PHE:HB3	1:F:628:PHE:HB2	1.78	0.66
1:B:555:LEU:HB3	1:B:913:LEU:HB3	1.78	0.66
1:B:971:ARG:HB3	1:B:971:ARG:CZ	2.24	0.66
1:C:668:LEU:HD23	1:C:668:LEU:H	1.61	0.65
1:E:983:ILE:HG23	1:E:1008:MET:HE2	1.76	0.65
1:C:120:GLN:HA	1:C:123:GLN:HB2	1.79	0.65
1:F:324:VAL:HG23	1:F:326:PRO:HD3	1.76	0.65
1:F:817:GLU:OE2	1:F:825:MET:HA	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.78	0.65
1:B:688:ALA:O	1:B:690:LEU:N	2.29	0.65
1:E:574:THR:HG23	1:E:627:ALA:HB3	1.79	0.65
1:E:801:PHE:HA	1:E:804:PHE:CE2	2.31	0.65
1:F:562:SER:HB2	1:F:924:ASP:HB3	1.77	0.65
1:D:465:ALA:O	1:D:469:GLN:HG2	1.97	0.65
1:E:324:VAL:HG13	1:E:326:PRO:HD3	1.79	0.65
1:E:696:THR:HG23	1:E:699:ARG:NH1	2.12	0.65
1:C:940:LYS:NZ	1:C:978:THR:HG21	2.11	0.65
1:C:1038:GLU:HA	1:C:1039:ASP:HB2	1.77	0.65
1:E:588:GLN:HE21	1:E:592:ASN:HD21	1.44	0.65
1:C:414:GLU:HG3	1:C:977:MET:HE1	1.79	0.65
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.78	0.65
2:D:1101:ERY:H18	2:D:1101:ERY:H5	1.77	0.65
1:F:953:MET:HE2	1:F:963:ALA:HB3	1.79	0.65
1:B:352:PHE:HD2	1:B:353:LEU:HD23	1.61	0.65
1:C:449:LEU:HB2	1:C:478:MET:HE2	1.78	0.65
1:F:831:ALA:HB3	1:F:835:LYS:HG3	1.78	0.65
1:F:943:ILE:O	1:F:947:GLU:HB3	1.96	0.65
1:B:540:ARG:NH2	3:B:1101:LMT:O6B	2.30	0.65
1:C:634:TRP:CD1	1:C:634:TRP:H	2.10	0.65
1:F:434:SER:O	1:F:438:ILE:HG12	1.97	0.65
1:F:587:THR:OG1	1:F:613:ASN:ND2	2.26	0.65
1:D:211:ASN:O	1:D:760:ASN:ND2	2.30	0.65
1:D:418:ARG:O	1:D:422:GLU:HB2	1.97	0.64
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.79	0.64
1:A:155:SER:HB3	1:A:180:SER:H	1.62	0.64
1:A:225:VAL:H	1:B:781:MET:CE	2.10	0.64
1:A:781:MET:CE	1:C:225:VAL:H	2.10	0.64
1:D:225:VAL:H	1:E:781:MET:CE	2.09	0.64
1:C:359:LEU:O	1:C:361:ASN:N	2.31	0.64
1:A:781:MET:HE3	1:C:228:GLN:OE1	1.97	0.64
1:F:482:VAL:O	1:F:486:LEU:HG	1.97	0.64
1:A:491:ALA:O	1:A:495:THR:OG1	2.13	0.64
1:A:563:PHE:HE2	1:A:671:ILE:HD13	1.62	0.64
1:E:508:GLY:O	1:E:510:LYS:N	2.30	0.64
1:F:695:LEU:HD22	1:F:855:VAL:HG22	1.79	0.64
1:E:907:LEU:HG	1:E:1017:LEU:HD23	1.78	0.64
1:A:6:ILE:HD11	1:A:432:ARG:HE	1.63	0.64
1:A:18:ILE:HG13	1:B:886:LEU:HD23	1.80	0.64
1:B:578:LEU:HD21	1:B:590:VAL:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:790:TYR:HB3	1:D:798:MET:HB3	1.79	0.64
1:E:14:VAL:HG22	1:F:886:LEU:HD12	1.79	0.64
1:A:565:PRO:HG2	1:A:567:GLU:OE2	1.98	0.64
1:F:399:VAL:HG11	1:F:989:LEU:HD21	1.80	0.64
1:D:470:PHE:CD2	1:D:929:VAL:HG11	2.33	0.64
1:A:507:GLU:O	1:A:509:LYS:N	2.30	0.64
1:B:445:ILE:HG21	1:B:940:LYS:HD2	1.79	0.64
1:A:516:PHE:HA	1:A:519:MET:HG3	1.78	0.63
1:C:482:VAL:O	1:C:486:LEU:HG	1.97	0.63
1:D:225:VAL:HG13	1:E:781:MET:HE2	1.78	0.63
1:B:1037:ASN:HA	1:B:1038:GLU:CB	2.29	0.63
1:D:418:ARG:NH2	1:D:948:PHE:HE2	1.95	0.63
1:D:987:MET:HA	1:D:1008:MET:HE1	1.80	0.63
1:B:536:ARG:NH1	3:B:1101:LMT:O3B	2.31	0.63
1:F:1038:GLU:HB2	1:F:1039:ASP:CG	2.23	0.63
1:B:146:ASP:OD2	1:B:320:GLY:HA3	1.98	0.63
1:A:987:MET:SD	1:A:1008:MET:HE1	2.38	0.63
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.29	0.63
1:C:272:GLY:N	1:C:275:TYR:OH	2.26	0.63
1:D:146:ASP:OD2	1:D:146:ASP:N	2.19	0.63
1:D:222:THR:OG1	1:E:275:TYR:O	2.16	0.63
1:E:80:SER:HB3	1:E:90:ILE:HG12	1.80	0.63
1:D:253:VAL:HG12	1:D:259:ARG:HG2	1.79	0.63
1:D:360:GLN:OE1	1:D:513:PHE:HB3	1.98	0.63
1:E:49:TYR:HE1	1:E:60:THR:HG21	1.62	0.63
1:C:597:TYR:HE1	1:C:601:LYS:HD2	1.64	0.63
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.63	0.63
1:E:634:TRP:H	1:E:634:TRP:CD1	2.12	0.63
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.79	0.63
1:A:588:GLN:NE2	1:A:592:ASN:OD1	2.31	0.63
1:A:575:MET:HE2	1:A:617:PHE:HD2	1.64	0.62
1:C:634:TRP:CD1	1:C:634:TRP:N	2.63	0.62
1:F:120:GLN:HA	1:F:123:GLN:HB2	1.79	0.62
1:A:928:GLN:OE1	3:A:1103:LMT:O6'	2.10	0.62
1:F:702:LEU:HD21	1:F:844:MET:HE1	1.81	0.62
1:B:658:ILE:O	1:B:659:LYS:HD2	1.99	0.62
1:D:726:GLN:NE2	1:D:812:GLY:HA3	2.14	0.62
1:E:139:VAL:O	1:E:326:PRO:HD2	1.99	0.62
1:E:559:LEU:HD11	1:E:922:THR:HA	1.82	0.62
1:F:456:MET:HA	1:F:876:LEU:HD21	1.80	0.62
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.81	0.62
1:B:87:THR:HG21	1:B:620:ARG:HH12	1.65	0.62
1:D:183:ALA:HB2	1:D:273:GLU:HG3	1.81	0.62
1:E:153:ASP:OD2	1:E:182:TYR:OH	2.18	0.62
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.34	0.62
1:F:636:ASP:O	1:F:638:PRO:HD3	1.99	0.62
1:A:359:LEU:O	1:A:361:ASN:N	2.33	0.62
1:B:1013:THR:O	1:B:1017:LEU:HB2	1.98	0.62
1:C:352:PHE:HD2	1:C:353:LEU:HD23	1.63	0.62
1:B:362:PHE:HA	1:B:365:THR:HG22	1.81	0.62
1:B:717:ARG:HD2	1:B:828:LEU:HB2	1.81	0.62
1:C:907:LEU:HD23	1:C:1017:LEU:HB3	1.81	0.62
1:D:617:PHE:HD2	2:D:1101:ERY:H361	1.63	0.62
1:B:764:ASP:OD1	1:B:765:ARG:HG3	2.00	0.62
1:E:272:GLY:N	1:E:275:TYR:OH	2.25	0.62
1:E:545:TYR:OH	1:E:903:LEU:O	2.18	0.62
1:E:568:ASP:O	1:E:634:TRP:HZ3	1.83	0.62
1:E:634:TRP:CD1	1:E:634:TRP:N	2.68	0.62
1:E:919:ARG:HB3	1:E:921:LEU:HD23	1.80	0.62
1:E:534:ILE:HG22	3:E:1101:LMT:H5'	1.81	0.61
1:D:318:PRO:HD2	1:D:321:LEU:HG	1.81	0.61
2:D:1101:ERY:H323	2:D:1101:ERY:H211	1.82	0.61
1:A:744:ASN:O	1:A:748:THR:HG23	2.00	0.61
1:C:185:ARG:HB3	1:C:187:TRP:NE1	2.15	0.61
1:D:945:ILE:HG13	1:D:971:ARG:HH22	1.65	0.61
1:E:43:VAL:HG22	1:E:131:LYS:HG3	1.80	0.61
1:F:753:ALA:O	1:F:775:SER:HB3	1.99	0.61
1:A:350:LEU:HD13	1:A:984:LEU:O	1.99	0.61
1:C:452:VAL:O	1:C:455:PRO:HD2	2.00	0.61
1:D:712:MET:SD	1:D:835:LYS:HE2	2.40	0.61
1:E:259:ARG:H	1:E:259:ARG:HD3	1.65	0.61
1:C:201:VAL:HG23	1:C:749:THR:HG23	1.82	0.61
1:A:45:ILE:HG23	1:A:129:VAL:HG22	1.83	0.61
1:E:435:MET:SD	1:E:490:PRO:HB3	2.41	0.61
1:F:352:PHE:HD2	1:F:353:LEU:HD23	1.64	0.61
1:A:452:VAL:HA	1:A:880:SER:OG	2.00	0.61
1:E:174:ASP:HB3	1:E:292:LYS:HB2	1.83	0.61
1:E:572:PHE:HA	1:E:668:LEU:HD21	1.83	0.61
1:F:600:THR:O	1:F:603:LYS:HG3	2.01	0.61
1:A:211:ASN:OD1	1:A:240:LEU:HG	2.01	0.61
1:A:225:VAL:HG13	1:B:781:MET:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:LEU:HD13	1:F:783:PRO:HG3	1.82	0.61
1:B:327:TYR:HB2	1:B:628:PHE:CZ	2.35	0.61
1:D:519:MET:O	1:D:523:SER:OG	2.10	0.61
1:D:781:MET:HE1	1:F:225:VAL:H	1.66	0.61
1:E:327:TYR:HB2	1:E:628:PHE:CZ	2.36	0.61
1:C:137:LEU:HD22	1:C:293:LEU:HD23	1.82	0.60
1:D:225:VAL:H	1:E:781:MET:HE2	1.64	0.60
1:D:634:TRP:CD1	1:D:634:TRP:H	2.17	0.60
1:A:108:GLN:NE2	1:B:109:ASN:O	2.34	0.60
1:A:134:SER:OG	2:A:1101:ERY:C32	2.48	0.60
1:B:225:VAL:HG12	1:C:777:ALA:HB1	1.84	0.60
1:B:744:ASN:O	1:B:748:THR:HG23	2.01	0.60
1:C:351:VAL:HG22	1:C:981:ALA:HB1	1.82	0.60
1:D:907:LEU:HD23	1:D:1017:LEU:HB3	1.83	0.60
1:F:185:ARG:HB3	1:F:187:TRP:NE1	2.16	0.60
1:F:672:VAL:O	1:F:674:LEU:N	2.32	0.60
1:F:961:ILE:HD12	1:F:961:ILE:H	1.65	0.60
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.82	0.60
1:B:452:VAL:HG23	1:B:453:PHE:HD2	1.65	0.60
1:C:222:THR:HA	1:C:224:PRO:HD3	1.83	0.60
1:F:291:ILE:HG21	1:F:306:ILE:HD11	1.81	0.60
1:F:576:VAL:HG22	1:F:663:VAL:HG13	1.82	0.60
1:F:744:ASN:O	1:F:748:THR:HG23	2.01	0.60
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.83	0.60
1:A:253:VAL:HG12	1:A:259:ARG:HG2	1.84	0.60
1:A:844:MET:HA	1:A:844:MET:HE2	1.84	0.60
1:D:1013:THR:O	1:D:1017:LEU:HB2	2.00	0.60
1:A:112:GLN:HG3	1:B:112:GLN:OE1	2.01	0.60
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.84	0.60
1:B:979:SER:OG	1:B:1015:THR:HG21	2.02	0.60
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.65	0.60
1:A:1019:ILE:HG13	1:A:1020:PHE:CD1	2.37	0.60
1:B:1016:VAL:HG22	3:B:1101:LMT:H112	1.83	0.60
1:B:1034:SER:OG	1:B:1035:ARG:N	2.28	0.60
1:C:789:TRP:HB2	1:C:801:PHE:CD2	2.37	0.60
1:C:1038:GLU:HA	1:C:1039:ASP:CB	2.31	0.60
1:F:580:ALA:HB1	1:F:724:THR:HG22	1.83	0.60
1:D:61:VAL:HG22	1:D:118:LEU:HD22	1.82	0.60
1:E:531:VAL:O	1:E:534:ILE:HG13	2.02	0.60
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.83	0.60
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:HB2	1:B:246:PHE:CE1	2.37	0.60
1:D:58:GLN:HE21	1:D:63:GLN:HE21	1.48	0.60
1:E:281:PHE:CZ	1:E:324:VAL:HG21	2.36	0.60
1:A:211:ASN:O	1:A:760:ASN:ND2	2.35	0.60
1:D:272:GLY:N	1:D:275:TYR:OH	2.29	0.60
1:E:695:LEU:HD22	1:E:825:MET:SD	2.41	0.60
1:F:462:SER:HB3	1:F:865:GLN:HG2	1.84	0.60
1:B:405:LEU:HD22	1:B:481:SER:HB3	1.84	0.60
1:A:196:PHE:O	1:A:252:LYS:NZ	2.35	0.59
1:A:1030:ARG:HH12	1:A:1033:PHE:HB2	1.67	0.59
1:B:200:PRO:HB2	1:B:749:THR:HG22	1.82	0.59
1:B:277:ILE:HA	1:B:613:ASN:O	2.01	0.59
1:E:717:ARG:HD2	1:E:828:LEU:HB2	1.83	0.59
1:F:242:SER:HB2	1:F:245:GLU:HG3	1.84	0.59
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.84	0.59
1:A:158:VAL:HA	1:A:162:MET:HE3	1.83	0.59
1:C:465:ALA:HA	1:C:468:ARG:NH1	2.13	0.59
1:C:744:ASN:O	1:C:748:THR:HG23	2.02	0.59
1:D:699:ARG:NH2	1:D:722:GLU:OE1	2.35	0.59
1:E:26:ALA:O	1:E:30:LEU:HB2	2.02	0.59
1:A:360:GLN:HE22	1:A:513:PHE:HB3	1.67	0.59
1:E:971:ARG:HB3	1:E:971:ARG:CZ	2.32	0.59
1:F:104:GLN:NE2	1:F:108:GLN:OE1	2.35	0.59
1:A:388:PHE:CZ	1:A:472:ILE:HG12	2.37	0.59
1:B:1037:ASN:HB3	1:B:1040:ILE:HG12	1.84	0.59
1:D:239:ARG:NH1	1:D:761:ASP:O	2.36	0.59
1:E:399:VAL:O	1:E:402:ILE:HG12	2.01	0.59
1:E:1013:THR:O	1:E:1017:LEU:HB2	2.02	0.59
1:F:684:LEU:HD22	1:F:827:ILE:HD11	1.84	0.59
1:B:11:PHE:CE1	1:C:890:ALA:HB1	2.38	0.59
1:B:652:THR:HG23	1:B:665:ALA:H	1.68	0.59
1:C:623:ASN:N	1:C:623:ASN:OD1	2.27	0.59
1:D:844:MET:HA	1:D:844:MET:HE2	1.84	0.59
1:D:873:ALA:HB2	3:D:1103:LMT:H51	1.84	0.59
1:E:144:ASN:ND2	1:E:149:MET:HE3	2.17	0.59
1:F:352:PHE:HA	1:F:355:MET:HE2	1.84	0.59
1:A:781:MET:HE2	1:C:225:VAL:HG13	1.85	0.59
1:C:789:TRP:HB2	1:C:801:PHE:HD2	1.67	0.59
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.85	0.59
1:A:1037:ASN:CA	1:A:1038:GLU:HB2	2.30	0.59
1:C:156:ASP:OD1	1:C:765:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:897:ILE:HD13	1:D:950:LYS:HE3	1.85	0.59
1:E:9:PRO:HB3	1:E:495:THR:HG21	1.84	0.59
1:E:250:LEU:HD21	1:E:253:VAL:HG23	1.84	0.59
1:E:261:LEU:N	1:E:264:ASP:OD2	2.35	0.59
1:E:332:PHE:HD1	1:E:634:TRP:HH2	1.50	0.59
1:A:62:THR:HG21	1:A:818:ARG:HD3	1.83	0.59
1:D:309:GLU:O	1:D:312:LYS:HB2	2.02	0.59
1:D:457:ALA:O	1:D:468:ARG:NE	2.35	0.59
1:D:781:MET:HB3	1:F:228:GLN:HE22	1.68	0.59
1:F:888:LEU:HD21	1:F:943:ILE:HD11	1.85	0.59
1:A:575:MET:HE2	1:A:617:PHE:CD2	2.37	0.59
1:B:415:ASN:CG	1:B:418:ARG:HH12	2.10	0.59
1:D:344:LEU:HD21	1:D:399:VAL:HG22	1.83	0.59
1:C:200:PRO:HB2	1:C:749:THR:HG22	1.85	0.59
1:D:344:LEU:HD22	1:D:402:ILE:HD12	1.83	0.59
1:F:157:TYR:HD2	1:F:162:MET:HE2	1.67	0.59
1:B:235:ILE:O	1:C:728:LYS:HD2	2.03	0.58
1:B:237:GLN:HG3	1:C:731:ILE:HD11	1.85	0.58
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.38	0.58
1:D:971:ARG:CZ	1:D:971:ARG:HB3	2.33	0.58
1:F:58:GLN:HA	1:F:62:THR:HB	1.85	0.58
1:F:698:ALA:O	1:F:701:GLN:HB3	2.03	0.58
1:B:441:ALA:O	1:B:445:ILE:HG23	2.02	0.58
1:B:455:PRO:O	1:B:876:LEU:HD13	2.02	0.58
1:C:310:LEU:O	1:C:314:GLU:HG3	2.03	0.58
1:D:251:LEU:HD11	1:D:262:LEU:HA	1.84	0.58
1:A:928:GLN:OE1	3:A:1103:LMT:C6'	2.51	0.58
1:D:108:GLN:HE21	1:D:112:GLN:HE21	1.50	0.58
1:D:637:ARG:HD2	1:D:642:ASN:O	2.03	0.58
1:D:919:ARG:NH1	1:D:1005:THR:OG1	2.35	0.58
1:D:1031:ARG:HH12	1:D:1038:GLU:HG3	1.68	0.58
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.85	0.58
1:E:675:GLY:HA2	1:E:862:MET:HG3	1.84	0.58
1:F:447:MET:HE3	1:F:888:LEU:HD23	1.84	0.58
1:A:456:MET:SD	1:A:932:LEU:HD11	2.44	0.58
1:A:1030:ARG:HH12	1:A:1033:PHE:CB	2.16	0.58
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.85	0.58
1:F:379:THR:HG23	1:F:476:SER:OG	2.03	0.58
1:C:945:ILE:HA	1:C:971:ARG:NH1	2.19	0.58
1:D:909:VAL:HG22	1:D:931:LEU:HD21	1.85	0.58
1:E:240:LEU:HB2	1:E:246:PHE:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:703:LEU:HD21	1:E:718:PRO:HD3	1.86	0.58
1:F:538:THR:HG23	1:F:542:LEU:HD13	1.86	0.58
1:F:910:ILE:O	1:F:914:LEU:HB2	2.03	0.58
1:F:947:GLU:HG3	1:F:948:PHE:HD1	1.69	0.58
1:B:80:SER:HB3	1:B:90:ILE:HG12	1.85	0.58
1:C:83:ASP:HB2	1:C:87:THR:O	2.03	0.58
1:D:617:PHE:HA	2:D:1101:ERY:H351	1.85	0.58
1:F:343:THR:HG21	1:F:989:LEU:CD2	2.34	0.58
1:A:836:SER:HB3	1:A:839:GLU:CD	2.28	0.58
1:C:36:PRO:O	1:C:38:ILE:HG13	2.03	0.58
1:E:151:GLN:HE22	1:E:278:ILE:HA	1.68	0.58
1:A:584:GLN:HB2	1:A:622:GLN:HG2	1.84	0.58
1:C:81:ASN:OD1	1:C:815:ARG:NH1	2.37	0.58
1:E:165:ALA:HB3	1:E:313:MET:CE	2.33	0.58
1:E:671:ILE:HB	1:E:674:LEU:HG	1.86	0.58
1:F:578:LEU:HG	1:F:587:THR:HG22	1.86	0.58
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.39	0.58
1:B:99:ASP:HB3	1:B:102:ILE:HB	1.86	0.58
1:B:188:MET:HA	1:B:266:ALA:HB2	1.84	0.58
1:D:222:THR:HA	1:D:224:PRO:HD3	1.86	0.58
1:D:768:VAL:HG12	1:E:63:GLN:OE1	2.03	0.58
1:A:225:VAL:H	1:B:781:MET:HE2	1.69	0.57
1:A:945:ILE:CG1	1:A:971:ARG:HH22	2.15	0.57
1:B:261:LEU:N	1:B:264:ASP:OD2	2.33	0.57
1:E:44:THR:HG1	1:E:91:THR:HG1	1.26	0.57
1:A:974:PRO:HA	1:A:977:MET:HE3	1.85	0.57
1:C:58:GLN:O	1:C:62:THR:HB	2.03	0.57
1:C:190:PRO:HB3	1:C:789:TRP:CZ3	2.39	0.57
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.87	0.57
1:C:915:ALA:HB2	1:C:1009:GLY:HA3	1.86	0.57
1:D:344:LEU:HD21	1:D:399:VAL:HA	1.86	0.57
1:F:520:PHE:O	1:F:524:THR:HG22	2.02	0.57
1:F:1021:PHE:HB3	1:F:1025:PHE:CE1	2.39	0.57
1:F:1043:SER:OG	1:F:1044:HIS:N	2.37	0.57
1:C:463:THR:HG23	1:C:467:TYR:CE1	2.40	0.57
1:E:396:PHE:O	1:E:400:LEU:HB2	2.04	0.57
1:E:442:LEU:O	1:E:445:ILE:HG13	2.03	0.57
1:E:713:LEU:HD21	1:E:843:LEU:HD12	1.86	0.57
1:F:1034:SER:OG	1:F:1035:ARG:HA	2.04	0.57
1:A:53:ASP:OD1	1:A:56:THR:OG1	2.16	0.57
1:A:544:LEU:O	1:A:548:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:LEU:HD23	1:B:560:PRO:CD	2.34	0.57
1:C:49:TYR:HD1	1:C:57:VAL:HG12	1.70	0.57
1:C:426:PRO:HD2	1:C:429:GLU:HB3	1.86	0.57
1:E:678:THR:HA	1:E:837:THR:OG1	2.03	0.57
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.86	0.57
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.85	0.57
1:A:242:SER:OG	1:A:245:GLU:HG3	2.04	0.57
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	1.87	0.57
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.39	0.57
1:C:201:VAL:HG22	1:C:748:THR:OG1	2.05	0.57
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.87	0.57
1:B:916:ALA:O	1:B:919:ARG:N	2.36	0.57
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.87	0.57
1:C:404:LEU:HB3	1:C:478:MET:SD	2.45	0.57
1:C:688:ALA:O	1:C:690:LEU:N	2.38	0.57
1:C:698:ALA:O	1:C:701:GLN:HB3	2.04	0.57
1:D:17:ILE:HG22	1:E:886:LEU:HD21	1.86	0.57
1:D:78:MET:O	1:D:820:ASN:N	2.26	0.57
1:F:358:PHE:CD2	1:F:977:MET:HG3	2.40	0.57
1:F:568:ASP:CG	1:F:637:ARG:HH12	2.12	0.57
1:B:340:VAL:HG11	1:B:395:MET:HE3	1.86	0.57
1:B:985:GLY:O	1:B:988:PRO:HD2	2.04	0.57
1:D:919:ARG:HG2	1:D:920:GLY:H	1.69	0.57
1:E:441:ALA:HA	1:E:891:LEU:HD21	1.87	0.57
1:F:3:ASN:HD22	1:F:435:MET:CG	2.16	0.57
1:A:577:GLN:OE1	1:A:624:THR:HG22	2.05	0.57
1:B:28:LEU:HB3	1:B:29:LYS:HD2	1.87	0.57
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.40	0.57
1:B:668:LEU:H	1:B:668:LEU:CD2	2.14	0.57
1:D:415:ASN:HB3	1:D:434:SER:HB2	1.87	0.57
1:D:928:GLN:HG2	3:D:1103:LMT:H82	1.86	0.57
1:B:987:MET:HA	1:B:1008:MET:HE1	1.87	0.57
1:C:795:ASP:OD2	1:C:797:GLN:HG2	2.05	0.57
1:E:591:LEU:HD13	1:E:611:ALA:HB1	1.86	0.57
1:F:372:VAL:HG22	1:F:405:LEU:HD11	1.86	0.57
1:B:652:THR:CG2	1:B:665:ALA:H	2.18	0.57
1:C:57:VAL:HG23	1:C:82:SER:HB3	1.87	0.57
1:C:650:ARG:O	1:C:653:ARG:HB3	2.05	0.57
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.05	0.57
1:D:876:LEU:HD23	1:D:879:ILE:HD12	1.86	0.57
1:D:986:VAL:HG21	1:D:1007:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.87	0.57
1:A:801:PHE:HA	1:A:804:PHE:CE2	2.40	0.56
1:A:958:LYS:C	1:A:1040:ILE:HG12	2.30	0.56
1:A:973:ARG:HG2	1:A:977:MET:HE2	1.87	0.56
1:B:142:VAL:HG21	1:B:158:VAL:HG22	1.87	0.56
1:B:224:PRO:HA	1:C:781:MET:HE1	1.87	0.56
1:E:532:GLY:O	1:E:535:LEU:N	2.37	0.56
1:A:225:VAL:HG22	1:B:781:MET:HE2	1.88	0.56
1:A:717:ARG:HE	1:A:828:LEU:HB2	1.69	0.56
1:A:777:ALA:HB1	1:C:225:VAL:HG12	1.86	0.56
1:B:695:LEU:HD22	1:B:825:MET:SD	2.45	0.56
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.86	0.56
1:C:228:GLN:NE2	1:C:230:LEU:H	2.02	0.56
1:D:815:ARG:HH21	2:D:1101:ERY:H291	1.70	0.56
1:F:113:LEU:O	1:F:116:PRO:HD2	2.05	0.56
1:A:154:ILE:O	1:A:157:TYR:N	2.38	0.56
1:A:644:VAL:CG1	1:A:667:ASN:HB2	2.32	0.56
1:A:728:LYS:HB2	1:A:810:GLU:OE1	2.05	0.56
1:C:990:VAL:HG13	1:C:1005:THR:OG1	2.05	0.56
1:D:59:ASP:HB3	1:F:763:ILE:HD11	1.87	0.56
1:E:733:GLN:HE22	1:E:743:ILE:HG21	1.69	0.56
1:F:64:VAL:HA	1:F:67:GLN:OE1	2.06	0.56
1:F:351:VAL:HG22	1:F:981:ALA:HB1	1.87	0.56
1:F:455:PRO:HG2	1:F:880:SER:HA	1.88	0.56
1:F:555:LEU:HB3	1:F:913:LEU:HB3	1.87	0.56
1:C:427:PRO:HD3	1:C:499:PRO:HB3	1.88	0.56
1:D:210:GLN:NE2	1:D:250:LEU:HB3	2.10	0.56
1:E:58:GLN:OE1	1:E:816:LEU:HD13	2.04	0.56
1:F:945:ILE:HA	1:F:971:ARG:NH1	2.20	0.56
1:A:49:TYR:HE1	1:A:60:THR:HG21	1.70	0.56
1:A:73:ASP:OD2	1:C:131:LYS:NZ	2.33	0.56
1:A:563:PHE:CE2	1:A:671:ILE:HD13	2.40	0.56
1:D:201:VAL:HA	1:D:204:ILE:HD12	1.86	0.56
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.88	0.56
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.86	0.56
1:B:545:TYR:HE2	1:B:907:LEU:HD11	1.70	0.56
1:C:47:ALA:HB3	1:C:88:VAL:HG13	1.88	0.56
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.71	0.56
1:C:959:GLY:HA2	1:C:1041:GLU:HA	1.87	0.56
1:D:317:PHE:HB3	1:D:321:LEU:HB3	1.87	0.56
1:E:901:VAL:HG23	1:E:942:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:587:THR:HG21	1:F:622:GLN:O	2.06	0.56
1:A:705:GLU:HB3	1:A:847:LEU:HD22	1.88	0.56
1:A:913:LEU:HD23	1:A:927:PHE:HZ	1.70	0.56
1:B:153:ASP:OD2	1:B:182:TYR:OH	2.23	0.56
1:C:356:TYR:C	1:C:358:PHE:N	2.63	0.56
1:C:380:PHE:CD2	1:C:383:LEU:HD12	2.40	0.56
1:D:3:ASN:HA	1:D:6:ILE:HG12	1.88	0.56
1:D:781:MET:HE2	1:F:225:VAL:HG13	1.87	0.56
1:F:971:ARG:HB3	1:F:971:ARG:NH1	2.21	0.56
1:D:235:ILE:O	1:E:728:LYS:HD2	2.06	0.56
1:E:575:MET:HA	1:E:626:ILE:HG13	1.87	0.56
1:D:276:ASP:OD1	1:F:222:THR:HG21	2.05	0.56
1:E:758:TYR:HE1	1:E:770:LYS:HG2	1.71	0.56
1:F:53:ASP:OD1	1:F:56:THR:OG1	2.17	0.56
1:A:530:SER:CB	3:A:1102:LMT:H2O2	2.18	0.56
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.31	0.56
1:C:987:MET:HG3	1:C:1008:MET:HE1	1.87	0.56
1:D:644:VAL:HG11	1:D:667:ASN:HB2	1.87	0.56
1:D:682:PHE:HD2	1:D:683:GLU:N	2.04	0.56
1:D:728:LYS:HB2	1:D:810:GLU:CD	2.31	0.56
1:E:380:PHE:HA	1:E:383:LEU:HD12	1.88	0.56
1:F:1035:ARG:NH1	1:F:1038:GLU:OE1	2.39	0.56
1:A:186:ILE:HB	1:A:773:VAL:HG22	1.88	0.55
1:C:746:ILE:HG13	1:C:747:ASN:N	2.21	0.55
1:C:966:ASP:OD1	1:C:969:ARG:NH2	2.39	0.55
1:F:187:TRP:HA	1:F:774:MET:O	2.06	0.55
1:F:579:PRO:HD3	1:F:661:ALA:HB2	1.87	0.55
1:C:898:PRO:HA	1:C:901:VAL:HG12	1.89	0.55
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.89	0.55
1:E:582:ALA:HA	1:E:586:ARG:HH21	1.71	0.55
1:E:710:PRO:HA	1:E:713:LEU:O	2.06	0.55
1:F:343:THR:HG21	1:F:989:LEU:HD21	1.87	0.55
1:A:549:VAL:O	1:A:552:MET:HE2	2.06	0.55
1:C:585:GLU:O	1:C:589:LYS:HG3	2.07	0.55
1:C:762:PHE:CE1	1:C:764:ASP:HB2	2.41	0.55
1:C:945:ILE:HG12	1:C:971:ARG:HH22	1.70	0.55
1:D:225:VAL:HG22	1:E:781:MET:HE2	1.88	0.55
1:E:156:ASP:OD1	1:E:765:ARG:NH2	2.39	0.55
1:E:216:ALA:HB1	1:E:234:ILE:HG22	1.87	0.55
1:E:516:PHE:CA	1:E:519:MET:HG3	2.34	0.55
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ALA:HB2	1:A:177:LEU:HD11	1.88	0.55
1:A:459:PHE:CZ	1:A:873:ALA:HA	2.40	0.55
1:B:400:LEU:HD12	1:B:933:THR:HG21	1.89	0.55
1:C:187:TRP:HA	1:C:774:MET:O	2.05	0.55
1:C:752:ALA:O	1:C:774:MET:HA	2.07	0.55
1:D:683:GLU:HG2	1:D:819:TYR:CG	2.41	0.55
1:F:382:VAL:HG21	1:F:476:SER:HB2	1.89	0.55
1:A:935:ILE:HG21	3:A:1103:LMT:H112	1.88	0.55
1:B:616:GLY:HA2	1:B:626:ILE:HB	1.87	0.55
1:C:764:ASP:OD1	1:C:765:ARG:HG3	2.07	0.55
1:E:632:LYS:O	1:E:637:ARG:NE	2.36	0.55
1:A:184:MET:HE3	1:A:184:MET:HA	1.87	0.55
1:A:535:LEU:HD21	1:A:1027:VAL:HG21	1.89	0.55
1:A:790:TYR:HB3	1:A:798:MET:HB3	1.88	0.55
1:B:355:MET:HE1	1:B:410:ILE:HG12	1.87	0.55
1:D:637:ARG:HB3	1:D:642:ASN:HB3	1.87	0.55
1:E:80:SER:CB	1:E:90:ILE:HG12	2.36	0.55
1:E:415:ASN:HD22	1:E:434:SER:CB	2.18	0.55
1:E:613:ASN:HD22	1:E:614:GLY:N	2.05	0.55
1:F:101:ASP:OD1	1:F:131:LYS:NZ	2.27	0.55
1:F:144:ASN:OD1	1:F:148:THR:HA	2.07	0.55
1:F:944:LEU:HB3	1:F:971:ARG:NE	2.22	0.55
1:F:1042:HIS:CG	1:F:1043:SER:N	2.75	0.55
1:A:897:ILE:HA	1:A:1029:VAL:CG1	2.37	0.55
1:B:344:LEU:HD23	1:B:402:ILE:HD11	1.88	0.55
1:B:184:MET:HA	1:B:184:MET:HE3	1.89	0.55
1:B:733:GLN:HE22	1:B:743:ILE:HG21	1.71	0.55
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.88	0.55
1:D:359:LEU:O	1:D:361:ASN:N	2.40	0.55
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.88	0.55
1:F:947:GLU:HG3	1:F:948:PHE:N	2.21	0.55
1:A:420:MET:HB3	1:A:500:ILE:HB	1.88	0.55
1:B:841:MET:HE1	1:B:867:ARG:HG3	1.88	0.55
1:F:877:TYR:O	1:F:881:LEU:HG	2.07	0.55
1:A:229:GLN:HE21	1:B:586:ARG:HD3	1.71	0.55
1:B:238:THR:OG1	1:C:728:LYS:NZ	2.39	0.55
1:B:415:ASN:OD1	1:B:418:ARG:NH1	2.36	0.55
1:C:187:TRP:HE3	1:C:775:SER:O	1.90	0.55
1:C:393:LEU:HD13	1:C:466:ILE:HG23	1.89	0.55
1:C:801:PHE:HA	1:C:804:PHE:CE2	2.42	0.55
1:C:961:ILE:HD12	1:C:961:ILE:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ASN:ND2	1:F:129:VAL:HG23	2.22	0.55
1:D:112:GLN:HG3	1:E:112:GLN:OE1	2.07	0.55
1:D:568:ASP:OD1	1:D:637:ARG:NH1	2.26	0.55
1:F:447:MET:HG2	1:F:891:LEU:HD22	1.89	0.55
1:C:948:PHE:HD2	1:C:970:MET:HE3	1.72	0.54
1:D:944:LEU:HB3	1:D:971:ARG:CZ	2.37	0.54
1:E:143:ILE:HG22	1:E:286:ALA:HB2	1.90	0.54
1:F:568:ASP:OD1	1:F:637:ARG:NH1	2.39	0.54
1:A:459:PHE:HZ	1:A:873:ALA:HA	1.72	0.54
1:A:535:LEU:CD2	1:A:1027:VAL:HG21	2.37	0.54
1:B:119:PRO:HG2	1:B:122:VAL:HB	1.87	0.54
1:D:658:ILE:HG13	1:D:659:LYS:NZ	2.23	0.54
1:E:343:THR:HG22	1:E:344:LEU:HD23	1.88	0.54
1:F:45:ILE:HB	1:F:90:ILE:HG12	1.89	0.54
1:F:99:ASP:HB3	1:F:102:ILE:HB	1.89	0.54
1:F:253:VAL:HG22	1:F:259:ARG:HG2	1.90	0.54
1:F:404:LEU:HB3	1:F:478:MET:SD	2.47	0.54
1:A:169:THR:HG21	1:A:306:ILE:HG13	1.89	0.54
1:A:453:PHE:CE2	1:A:932:LEU:HB3	2.42	0.54
1:A:622:GLN:HE21	1:C:222:THR:HG22	1.72	0.54
1:A:976:LEU:O	1:A:980:LEU:HB2	2.08	0.54
1:B:726:GLN:NE2	1:B:812:GLY:HA3	2.23	0.54
1:B:1042:HIS:CG	1:B:1043:SER:H	2.25	0.54
1:C:144:ASN:O	1:C:284:GLN:NE2	2.40	0.54
1:C:943:ILE:O	1:C:947:GLU:HB3	2.07	0.54
1:E:344:LEU:HD22	1:E:402:ILE:HG21	1.89	0.54
1:F:184:MET:HB2	1:F:762:PHE:CE2	2.42	0.54
1:F:751:GLY:O	1:F:753:ALA:N	2.41	0.54
1:C:418:ARG:O	1:C:422:GLU:HB2	2.07	0.54
1:C:586:ARG:O	1:C:589:LYS:HB2	2.08	0.54
1:D:441:ALA:O	1:D:445:ILE:HG23	2.07	0.54
1:F:277:ILE:HA	1:F:613:ASN:O	2.07	0.54
1:F:617:PHE:CE1	1:F:626:ILE:HD11	2.42	0.54
1:A:726:GLN:OE1	1:A:812:GLY:HA3	2.07	0.54
1:D:744:ASN:O	1:D:748:THR:HG23	2.07	0.54
1:D:834:GLY:O	1:D:835:LYS:HD2	2.07	0.54
1:F:699:ARG:HD3	1:F:825:MET:SD	2.48	0.54
1:F:948:PHE:HD2	1:F:970:MET:HE3	1.72	0.54
1:A:42:ALA:HB2	1:A:93:THR:HG23	1.89	0.54
1:C:674:LEU:HD22	1:C:861:GLY:HA2	1.90	0.54
1:C:703:LEU:HD11	1:C:718:PRO:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:941:ASN:HD21	1:C:1015:THR:HG22	1.72	0.54
1:F:519:MET:O	1:F:523:SER:OG	2.18	0.54
1:F:563:PHE:CE2	1:F:564:LEU:HD22	2.43	0.54
1:B:671:ILE:HB	1:B:674:LEU:HD12	1.89	0.54
1:C:360:GLN:OE1	1:C:517:ASN:ND2	2.33	0.54
1:D:946:VAL:HG13	1:D:1026:PHE:CE1	2.43	0.54
1:E:911:GLY:HA2	1:E:1013:THR:HG21	1.89	0.54
1:F:435:MET:HE3	1:F:490:PRO:HB3	1.89	0.54
1:B:706:ALA:CB	1:B:716:VAL:HG11	2.38	0.54
1:D:352:PHE:HD2	1:D:353:LEU:HD23	1.72	0.54
1:F:20:MET:HG2	1:F:374:VAL:HA	1.90	0.54
1:F:945:ILE:HA	1:F:971:ARG:HH12	1.72	0.54
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.88	0.54
1:B:575:MET:HA	1:B:626:ILE:HG13	1.89	0.54
1:B:919:ARG:HB3	1:B:921:LEU:HD23	1.89	0.54
1:C:571:VAL:N	1:C:631:LEU:HD12	2.22	0.54
1:C:579:PRO:HD3	1:C:661:ALA:CB	2.36	0.54
1:D:70:ASN:HB2	1:F:167:SER:HB2	1.90	0.54
1:E:32:VAL:HG21	1:E:300:LEU:HD13	1.89	0.54
1:E:54:ALA:HB2	1:E:84:SER:HB3	1.89	0.54
1:F:447:MET:HE1	1:F:887:CYS:HB3	1.89	0.54
1:F:563:PHE:HB2	1:F:866:GLU:HG3	1.89	0.54
1:F:1043:SER:HB2	1:F:1044:HIS:CE1	2.43	0.54
1:A:84:SER:HB3	1:A:814:PRO:HA	1.89	0.54
1:A:419:VAL:HG11	1:A:433:LYS:HG2	1.90	0.54
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.89	0.54
1:C:559:LEU:HD23	1:C:560:PRO:HD2	1.90	0.54
1:D:10:ILE:HG13	1:E:895:TRP:CE2	2.42	0.54
1:E:519:MET:O	1:E:523:SER:OG	2.23	0.54
1:F:599:LEU:O	1:F:603:LYS:HG2	2.08	0.54
1:A:330:THR:HB	1:A:331:PRO:HD3	1.90	0.53
1:A:1040:ILE:HG13	1:A:1041:GLU:N	2.22	0.53
1:C:801:PHE:HD1	1:C:804:PHE:HE2	1.55	0.53
1:D:274:ASN:ND2	1:D:276:ASP:OD2	2.30	0.53
1:D:391:ASN:O	1:D:395:MET:HG2	2.07	0.53
1:E:790:TYR:CE1	1:E:800:PRO:HB3	2.43	0.53
1:F:376:LEU:O	1:F:379:THR:N	2.41	0.53
1:F:549:VAL:O	1:F:552:MET:HB3	2.08	0.53
1:A:591:LEU:HD11	1:A:625:GLY:HA3	1.90	0.53
1:A:960:LEU:O	1:A:964:THR:HG23	2.09	0.53
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910:ILE:O	1:B:914:LEU:HB2	2.08	0.53
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.43	0.53
1:C:952:LEU:HD11	1:C:970:MET:HE1	1.90	0.53
1:F:616:GLY:HA2	1:F:626:ILE:HD12	1.89	0.53
1:F:800:PRO:HG2	1:F:803:ALA:HB2	1.90	0.53
1:F:817:GLU:HB2	1:F:824:SER:O	2.08	0.53
1:F:915:ALA:HB2	1:F:1009:GLY:HA3	1.89	0.53
1:F:952:LEU:O	1:F:956:GLU:HB2	2.08	0.53
1:F:967:ALA:HA	1:F:970:MET:HE2	1.90	0.53
1:A:932:LEU:HD23	3:A:1103:LMT:H71	1.89	0.53
1:B:44:THR:OG1	1:B:91:THR:OG1	2.24	0.53
1:B:775:SER:OG	1:B:780:ARG:HG2	2.07	0.53
1:E:453:PHE:O	1:E:471:SER:OG	2.14	0.53
1:F:507:GLU:HG2	1:F:518:ARG:HG3	1.90	0.53
1:A:1038:GLU:HB3	1:A:1039:ASP:C	2.33	0.53
1:C:244:GLU:HG2	1:C:248:LYS:HE3	1.89	0.53
1:E:196:PHE:N	1:E:196:PHE:HD1	2.06	0.53
1:C:178:PHE:HE2	1:C:615:PHE:CD1	2.25	0.53
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.89	0.53
1:C:531:VAL:HG21	1:C:968:VAL:HG11	1.90	0.53
1:E:160:ALA:HA	1:E:767:ARG:NH2	2.23	0.53
1:F:80:SER:HB3	1:F:90:ILE:HG22	1.91	0.53
1:A:146:ASP:OD2	1:A:146:ASP:N	2.39	0.53
1:B:272:GLY:N	1:B:275:TYR:OH	2.34	0.53
1:B:362:PHE:O	1:B:365:THR:HG22	2.08	0.53
1:C:682:PHE:HE1	1:C:857:TYR:HB2	1.70	0.53
1:E:987:MET:HG3	1:E:1008:MET:HE1	1.91	0.53
3:E:1101:LMT:H5B	3:E:1101:LMT:H6D	1.89	0.53
1:F:686:ASP:OD2	1:F:823:PRO:HD2	2.09	0.53
1:A:352:PHE:HD2	1:A:353:LEU:HD23	1.74	0.53
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.08	0.53
1:E:104:GLN:HE21	1:F:109:ASN:HD22	1.55	0.53
1:E:196:PHE:N	1:E:196:PHE:CD1	2.77	0.53
1:A:453:PHE:CD2	1:A:932:LEU:HD13	2.44	0.53
1:B:52:ALA:HB1	1:B:56:THR:HB	1.91	0.53
1:B:415:ASN:HD22	1:B:434:SER:CB	2.19	0.53
1:B:644:VAL:O	1:B:648:THR:HG23	2.08	0.53
1:E:511:GLY:HA2	1:E:515:TRP:HD1	1.73	0.53
1:E:1037:ASN:H	1:E:1038:GLU:HA	1.74	0.53
1:F:548:ILE:HD13	1:F:1017:LEU:HD21	1.91	0.53
1:F:555:LEU:HD11	1:F:914:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:GLY:HA2	1:A:536:ARG:HH11	1.73	0.53
1:B:11:PHE:HE1	1:C:890:ALA:HB1	1.74	0.53
1:C:5:PHE:HD2	1:C:6:ILE:HG12	1.74	0.53
1:C:253:VAL:HG22	1:C:259:ARG:HG2	1.90	0.53
1:D:316:PHE:CD1	1:E:687:GLN:HG2	2.43	0.53
1:B:363:ARG:HD3	1:B:496:MET:O	2.09	0.53
1:B:614:GLY:HA2	1:B:621:GLY:O	2.09	0.53
1:D:14:VAL:HG11	1:E:890:ALA:HB2	1.91	0.53
1:F:897:ILE:HG23	1:F:946:VAL:CG1	2.39	0.53
1:A:520:PHE:O	1:A:524:THR:HG22	2.09	0.52
1:B:508:GLY:CA	1:B:518:ARG:HH21	2.22	0.52
1:C:178:PHE:HE2	1:C:615:PHE:HD1	1.57	0.52
1:C:356:TYR:O	1:C:358:PHE:N	2.41	0.52
1:D:727:PHE:HD1	1:D:809:TRP:CE2	2.27	0.52
1:E:42:ALA:HB3	1:E:132:SER:HB3	1.91	0.52
1:E:415:ASN:OD1	1:E:418:ARG:NH1	2.40	0.52
1:E:888:LEU:HD21	1:E:943:ILE:HD11	1.92	0.52
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.44	0.52
1:A:34:GLN:HB2	1:A:333:VAL:HG22	1.90	0.52
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.27	0.52
1:A:448:VAL:O	1:A:451:ALA:HB3	2.09	0.52
1:B:545:TYR:OH	1:B:903:LEU:O	2.21	0.52
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.90	0.52
1:F:720:GLY:HA2	1:F:815:ARG:HH21	1.74	0.52
1:F:801:PHE:HA	1:F:804:PHE:CE2	2.45	0.52
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.44	0.52
1:B:378:GLY:O	1:B:382:VAL:HG23	2.09	0.52
1:B:894:SER:HB2	1:B:897:ILE:HD12	1.91	0.52
1:C:945:ILE:HA	1:C:971:ARG:HH12	1.75	0.52
1:D:72:ILE:HD13	1:D:107:VAL:HA	1.90	0.52
1:D:159:ALA:HB2	1:D:177:LEU:HD11	1.89	0.52
1:D:957:GLY:O	1:D:1040:ILE:HB	2.09	0.52
1:B:144:ASN:ND2	1:B:149:MET:HE3	2.25	0.52
1:C:250:LEU:HD21	1:C:253:VAL:HG23	1.91	0.52
1:C:352:PHE:CD2	1:C:353:LEU:HD23	2.44	0.52
1:C:414:GLU:OE1	1:C:973:ARG:HD3	2.09	0.52
1:C:971:ARG:HB3	1:C:971:ARG:NH1	2.24	0.52
1:D:17:ILE:CG2	1:E:886:LEU:HD21	2.40	0.52
1:E:228:GLN:NE2	1:E:230:LEU:O	2.39	0.52
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.39	0.52
1:A:715:SER:O	1:A:717:ARG:HD3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:940:LYS:HZ2	1:C:978:THR:HG21	1.74	0.52
1:D:563:PHE:CD1	3:D:1103:LMT:H5B	2.45	0.52
1:E:344:LEU:HD21	1:E:399:VAL:HA	1.91	0.52
1:E:484:VAL:HG13	1:E:488:LEU:HB3	1.91	0.52
1:E:682:PHE:CZ	1:E:857:TYR:HB2	2.45	0.52
1:F:876:LEU:O	1:F:880:SER:HB2	2.08	0.52
1:A:595:THR:O	1:A:599:LEU:HG	2.10	0.52
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.90	0.52
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.92	0.52
1:C:30:LEU:HD23	1:C:390:ILE:HD11	1.91	0.52
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.40	0.52
1:C:587:THR:HG21	1:C:622:GLN:O	2.09	0.52
1:D:400:LEU:HD23	1:D:929:VAL:HG12	1.91	0.52
1:D:418:ARG:HD3	1:D:422:GLU:OE1	2.10	0.52
1:D:945:ILE:HG13	1:D:971:ARG:NH2	2.24	0.52
1:E:42:ALA:O	1:E:132:SER:N	2.39	0.52
1:E:49:TYR:CE1	1:E:60:THR:HG21	2.43	0.52
1:F:352:PHE:CD2	1:F:353:LEU:HD23	2.45	0.52
1:A:361:ASN:HD21	1:A:498:LYS:HB2	1.74	0.52
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.90	0.52
1:C:455:PRO:HG2	1:C:880:SER:HA	1.92	0.52
1:C:885:PHE:HD2	1:C:886:LEU:HD22	1.75	0.52
1:F:244:GLU:HG2	1:F:248:LYS:HE3	1.92	0.52
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.38	0.52
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.91	0.52
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.92	0.52
1:D:362:PHE:O	1:D:366:LEU:HG	2.09	0.52
1:E:156:ASP:OD2	1:E:769:LYS:NZ	2.42	0.52
1:E:178:PHE:O	1:E:287:SER:OG	2.26	0.52
1:F:45:ILE:HD12	1:F:90:ILE:HG13	1.92	0.52
1:A:195:LYS:HG2	1:A:196:PHE:CE2	2.45	0.52
1:A:404:LEU:HD12	1:A:937:LEU:CD2	2.40	0.52
1:A:897:ILE:HD13	1:A:950:LYS:HE3	1.91	0.52
1:A:919:ARG:HG2	1:A:920:GLY:H	1.74	0.52
1:B:327:TYR:HD1	1:B:628:PHE:CZ	2.27	0.52
1:F:34:GLN:CB	1:F:333:VAL:HG22	2.36	0.52
1:F:82:SER:HB2	1:F:816:LEU:HB2	1.92	0.52
1:F:380:PHE:HD2	1:F:383:LEU:HD12	1.74	0.52
1:F:574:THR:HG23	1:F:627:ALA:HB3	1.92	0.52
1:F:987:MET:HG3	1:F:1008:MET:HE1	1.91	0.52
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:VAL:O	1:C:447:MET:HB3	2.10	0.52
1:C:664:PHE:CD2	1:C:717:ARG:HD2	2.38	0.52
1:D:449:LEU:HB3	1:D:478:MET:SD	2.50	0.52
1:D:708:LYS:C	1:D:710:PRO:HD3	2.35	0.52
1:F:469:GLN:O	1:F:472:ILE:HG22	2.10	0.52
1:F:945:ILE:CG1	1:F:971:ARG:HH22	2.23	0.52
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.43	0.51
1:B:501:ALA:O	1:B:504:ASP:HB2	2.10	0.51
1:C:78:MET:HG3	1:C:92:LEU:HD13	1.92	0.51
1:C:587:THR:HG21	1:C:623:ASN:HA	1.93	0.51
1:C:982:PHE:HD2	1:C:1011:MET:HG2	1.74	0.51
1:F:66:GLU:OE1	1:F:821:GLY:HA2	2.09	0.51
1:F:672:VAL:C	1:F:674:LEU:H	2.18	0.51
1:F:911:GLY:HA3	1:F:1010:GLY:HA2	1.92	0.51
1:A:775:SER:OG	1:A:780:ARG:HG2	2.10	0.51
1:A:971:ARG:C	1:A:974:PRO:HD2	2.35	0.51
1:B:139:VAL:O	1:B:326:PRO:HD2	2.09	0.51
1:B:953:MET:HE1	1:B:1026:PHE:HE2	1.75	0.51
1:C:23:GLY:HA3	1:C:377:LEU:O	2.10	0.51
1:D:58:GLN:HE21	1:D:63:GLN:NE2	2.07	0.51
1:D:712:MET:O	1:D:832:ALA:N	2.37	0.51
1:D:728:LYS:HB2	1:D:810:GLU:OE1	2.09	0.51
1:D:817:GLU:OE1	2:D:1101:ERY:H282	2.10	0.51
1:A:30:LEU:HD11	1:A:384:ALA:HA	1.91	0.51
1:C:727:PHE:HD1	1:C:809:TRP:CE2	2.28	0.51
1:D:31:PRO:O	1:D:389:SER:HB2	2.10	0.51
1:D:559:LEU:HD23	1:D:560:PRO:HD2	1.92	0.51
1:E:932:LEU:HD23	1:E:935:ILE:HD12	1.92	0.51
1:F:104:GLN:HG3	1:F:105:VAL:N	2.24	0.51
1:A:725:PRO:HA	1:A:810:GLU:O	2.10	0.51
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.46	0.51
1:B:1026:PHE:O	1:B:1030:ARG:HB2	2.09	0.51
1:D:573:MET:HB3	1:D:666:PHE:CE1	2.44	0.51
1:D:815:ARG:NH2	2:D:1101:ERY:H291	2.25	0.51
1:E:740:GLY:O	1:E:794:ALA:N	2.43	0.51
1:F:506:GLY:C	1:F:508:GLY:H	2.19	0.51
1:F:898:PRO:HA	1:F:901:VAL:HG12	1.93	0.51
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.91	0.51
1:C:2:PRO:O	1:C:5:PHE:HB3	2.09	0.51
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.92	0.51
1:C:188:MET:HA	1:C:266:ALA:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:694:LYS:HD3	1:C:694:LYS:N	2.23	0.51
1:C:897:ILE:HG23	1:C:946:VAL:CG1	2.41	0.51
1:C:971:ARG:C	1:C:974:PRO:HD2	2.36	0.51
1:D:246:PHE:HA	1:D:249:ILE:HG13	1.93	0.51
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.46	0.51
1:A:960:LEU:HD21	1:A:1027:VAL:HG13	1.92	0.51
1:B:54:ALA:HB2	1:B:84:SER:HB3	1.93	0.51
1:C:1034:SER:OG	1:C:1037:ASN:HB3	2.11	0.51
1:E:715:SER:O	1:E:717:ARG:HG3	2.11	0.51
1:F:352:PHE:HA	1:F:355:MET:CE	2.41	0.51
1:F:801:PHE:CD1	1:F:804:PHE:HE2	2.29	0.51
1:F:960:LEU:HD23	1:F:1031:ARG:HH21	1.76	0.51
1:A:190:PRO:HG3	1:A:779:TYR:HB3	1.92	0.51
1:A:228:GLN:OE1	1:B:781:MET:HE3	2.10	0.51
1:B:418:ARG:O	1:B:422:GLU:HB2	2.10	0.51
1:B:534:ILE:CD1	1:B:1024:VAL:HG22	2.41	0.51
1:C:743:ILE:H	1:C:743:ILE:HD12	1.76	0.51
1:D:246:PHE:O	1:D:262:LEU:HD23	2.11	0.51
1:D:415:ASN:ND2	1:D:434:SER:HB2	2.15	0.51
1:D:617:PHE:CD2	2:D:1101:ERY:H361	2.43	0.51
1:E:584:GLN:HB2	1:E:622:GLN:HG2	1.91	0.51
1:A:935:ILE:CG2	3:A:1103:LMT:H112	2.41	0.51
1:A:953:MET:HE2	1:A:963:ALA:HB3	1.91	0.51
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.92	0.51
1:C:841:MET:SD	1:C:863:SER:HB3	2.51	0.51
1:D:358:PHE:O	1:D:359:LEU:HD23	2.11	0.51
1:D:910:ILE:O	1:D:914:LEU:HB2	2.11	0.51
1:F:455:PRO:HB3	1:F:879:ILE:HG22	1.93	0.51
1:F:525:HIS:O	1:F:528:THR:HG22	2.11	0.51
1:F:545:TYR:OH	1:F:903:LEU:O	2.22	0.51
1:C:66:GLU:OE1	1:C:821:GLY:HA2	2.11	0.51
1:C:196:PHE:HD1	1:C:260:VAL:CG1	2.24	0.51
1:C:702:LEU:HD12	1:C:851:LEU:HD11	1.92	0.51
1:C:945:ILE:CG1	1:C:971:ARG:HH22	2.24	0.51
1:D:507:GLU:C	1:D:509:LYS:H	2.18	0.51
1:E:351:VAL:HG21	1:E:406:VAL:HG11	1.94	0.51
1:E:448:VAL:HG21	1:E:888:LEU:HD21	1.93	0.51
1:E:658:ILE:HG13	1:E:659:LYS:HD2	1.93	0.51
1:E:658:ILE:O	1:E:659:LYS:HD2	2.11	0.51
1:E:858:ASP:OD1	1:E:859:TRP:N	2.39	0.51
1:F:11:PHE:CE2	1:F:15:ILE:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:MET:HA	1:F:266:ALA:HB2	1.93	0.51
1:F:673:GLU:H	1:F:673:GLU:CD	2.19	0.51
1:A:61:VAL:HG21	1:A:122:VAL:HG21	1.92	0.50
1:A:225:VAL:HG12	1:B:777:ALA:CB	2.40	0.50
1:A:897:ILE:HA	1:A:1029:VAL:HG11	1.93	0.50
1:A:937:LEU:O	1:A:940:LYS:HB3	2.12	0.50
1:A:959:GLY:HA2	1:A:1040:ILE:HB	1.91	0.50
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.46	0.50
1:C:372:VAL:HG22	1:C:405:LEU:HD11	1.93	0.50
1:F:509:LYS:HE2	1:F:513:PHE:HD1	1.75	0.50
1:F:947:GLU:HG3	1:F:948:PHE:CD1	2.45	0.50
1:B:129:VAL:O	1:C:113:LEU:HD21	2.10	0.50
1:B:636:ASP:O	1:B:638:PRO:HD3	2.10	0.50
1:C:239:ARG:NH1	1:C:761:ASP:HB2	2.27	0.50
1:C:509:LYS:HE2	1:C:513:PHE:CD1	2.46	0.50
1:D:425:LEU:HD12	1:D:425:LEU:H	1.76	0.50
1:E:84:SER:HB3	1:E:814:PRO:HA	1.93	0.50
1:E:1019:ILE:HG13	1:E:1020:PHE:HD1	1.76	0.50
1:A:17:ILE:HG22	1:B:886:LEU:HD21	1.94	0.50
1:A:138:MET:HE2	1:A:328:ASP:OD1	2.11	0.50
1:A:545:TYR:HB2	1:A:1021:PHE:CE2	2.47	0.50
1:A:865:GLN:O	1:A:868:LEU:HB2	2.11	0.50
1:A:944:LEU:O	1:A:947:GLU:HB3	2.11	0.50
1:C:186:ILE:HG22	1:C:773:VAL:HG23	1.93	0.50
1:C:944:LEU:HD22	1:C:971:ARG:HD2	1.93	0.50
1:D:62:THR:OG1	1:D:88:VAL:HG21	2.11	0.50
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.47	0.50
1:F:572:PHE:HD1	1:F:666:PHE:O	1.95	0.50
1:F:686:ASP:HB3	1:F:823:PRO:O	2.11	0.50
1:F:841:MET:HG2	1:F:859:TRP:CH2	2.47	0.50
1:A:1031:ARG:O	1:A:1032:ARG:HG3	2.11	0.50
1:B:583:THR:HG22	1:B:585:GLU:H	1.76	0.50
1:C:61:VAL:HA	1:C:118:LEU:CD2	2.42	0.50
1:C:990:VAL:HG21	1:C:1008:MET:SD	2.51	0.50
1:D:623:ASN:OD1	1:D:623:ASN:N	2.27	0.50
1:E:104:GLN:OE1	1:E:131:LYS:HD3	2.11	0.50
1:E:317:PHE:CE2	1:E:323:ILE:HD13	2.46	0.50
1:F:13:TRP:CH2	1:F:370:ILE:HD13	2.46	0.50
1:F:418:ARG:HD3	1:F:422:GLU:OE2	2.10	0.50
1:F:584:GLN:HB2	1:F:622:GLN:HG2	1.92	0.50
1:A:4:PHE:HB3	1:A:8:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:HG22	1:B:287:SER:HB3	1.92	0.50
1:D:281:PHE:CE1	1:D:608:SER:HB2	2.47	0.50
1:D:900:SER:HB3	1:D:1029:VAL:HG21	1.94	0.50
1:E:144:ASN:HA	1:E:320:GLY:O	2.11	0.50
1:E:175:VAL:HG23	1:F:70:ASN:HD22	1.77	0.50
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.42	0.50
1:E:901:VAL:HG23	1:E:942:ALA:CB	2.41	0.50
1:A:401:ALA:O	1:A:405:LEU:HG	2.12	0.50
1:A:582:ALA:HA	1:A:586:ARG:HH21	1.77	0.50
1:B:61:VAL:HG21	1:B:122:VAL:HG21	1.94	0.50
1:C:195:LYS:HG2	1:C:196:PHE:CE2	2.47	0.50
1:D:282:ASN:HD21	1:D:608:SER:HA	1.75	0.50
1:D:351:VAL:HG22	1:D:981:ALA:HB1	1.94	0.50
1:F:210:GLN:HE22	1:F:250:LEU:H	1.59	0.50
1:B:848:ALA:HA	1:B:851:LEU:HG	1.93	0.50
1:D:10:ILE:HG13	1:E:895:TRP:CZ2	2.47	0.50
1:D:31:PRO:HB2	1:D:389:SER:CB	2.40	0.50
1:D:393:LEU:HD22	1:D:470:PHE:HE1	1.76	0.50
1:D:690:LEU:O	1:D:694:LYS:HB2	2.11	0.50
1:E:537:SER:OG	1:E:540:ARG:NH2	2.43	0.50
1:E:762:PHE:CE1	1:E:764:ASP:HB2	2.46	0.50
1:E:897:ILE:N	1:E:898:PRO:HD2	2.27	0.50
1:F:362:PHE:O	1:F:366:LEU:HG	2.11	0.50
1:F:435:MET:O	1:F:439:GLN:HG2	2.11	0.50
1:A:533:GLY:HA2	1:A:536:ARG:NH1	2.27	0.50
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.77	0.50
1:B:220:GLY:HA3	1:B:230:LEU:O	2.12	0.50
1:C:58:GLN:HA	1:C:62:THR:HB	1.93	0.50
1:C:376:LEU:O	1:C:379:THR:N	2.45	0.50
1:D:170:SER:OG	1:E:74:ASN:N	2.39	0.50
1:E:795:ASP:OD2	1:E:796:GLY:N	2.45	0.50
1:F:13:TRP:HH2	1:F:370:ILE:HD13	1.77	0.50
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.27	0.50
1:B:165:ALA:HB3	1:B:313:MET:CE	2.42	0.50
1:C:520:PHE:CZ	1:C:973:ARG:HG3	2.47	0.50
1:C:983:ILE:HG13	1:C:1011:MET:HG3	1.94	0.50
1:D:16:ALA:HB2	1:D:488:LEU:HD13	1.93	0.50
1:D:591:LEU:HD13	1:D:611:ALA:HB1	1.92	0.50
1:E:451:ALA:O	1:E:880:SER:OG	2.26	0.50
1:E:844:MET:HE2	1:E:844:MET:HA	1.94	0.50
1:E:888:LEU:HD13	1:E:901:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:PHE:CD1	1:A:804:PHE:HE2	2.30	0.49
1:B:108:GLN:OE1	1:C:112:GLN:HB3	2.12	0.49
1:B:801:PHE:CD1	1:B:804:PHE:HE2	2.30	0.49
1:C:34:GLN:HG3	1:C:333:VAL:HA	1.93	0.49
1:C:343:THR:HG21	1:C:989:LEU:HD23	1.94	0.49
1:C:678:THR:O	1:C:830:GLN:HG2	2.12	0.49
1:C:897:ILE:O	1:C:901:VAL:HG12	2.13	0.49
1:E:211:ASN:OD1	1:E:240:LEU:N	2.41	0.49
1:E:837:THR:HG22	1:E:841:MET:SD	2.52	0.49
1:A:415:ASN:HD22	1:A:434:SER:HB2	1.77	0.49
1:A:650:ARG:O	1:A:653:ARG:HB3	2.12	0.49
1:C:386:PHE:CD1	1:C:472:ILE:HD11	2.47	0.49
1:E:575:MET:HG3	1:E:664:PHE:HB2	1.93	0.49
1:F:23:GLY:HA3	1:F:377:LEU:HB3	1.95	0.49
1:A:220:GLY:HA3	1:A:230:LEU:O	2.13	0.49
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.47	0.49
1:B:244:GLU:HG2	1:B:248:LYS:HE3	1.94	0.49
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.94	0.49
1:B:520:PHE:O	1:B:524:THR:HG22	2.11	0.49
1:C:139:VAL:HB	1:C:327:TYR:HB3	1.93	0.49
1:C:668:LEU:H	1:C:668:LEU:CD2	2.23	0.49
1:D:31:PRO:HB2	1:D:389:SER:HB3	1.94	0.49
1:D:322:LYS:HG2	1:D:323:ILE:O	2.13	0.49
1:D:634:TRP:CD1	1:D:634:TRP:N	2.81	0.49
1:D:832:ALA:HB3	1:D:835:LYS:HD3	1.92	0.49
1:F:76:MET:HG3	1:F:95:GLU:CD	2.38	0.49
1:F:527:TYR:OH	1:F:968:VAL:HG13	2.13	0.49
1:A:224:PRO:HB2	1:B:781:MET:HE1	1.94	0.49
1:A:568:ASP:O	1:A:634:TRP:HZ3	1.96	0.49
1:C:20:MET:HG2	1:C:374:VAL:HA	1.94	0.49
1:C:228:GLN:HE21	1:C:230:LEU:H	1.59	0.49
1:E:636:ASP:O	1:E:638:PRO:HD3	2.12	0.49
1:F:76:MET:HE3	1:F:95:GLU:OE1	2.12	0.49
1:F:176:GLN:OE1	1:F:620:ARG:NH2	2.26	0.49
1:F:623:ASN:N	1:F:623:ASN:OD1	2.40	0.49
1:F:841:MET:HE3	1:F:859:TRP:CE2	2.47	0.49
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.19	0.49
1:A:685:ILE:HD11	1:A:819:TYR:CD2	2.48	0.49
1:A:893:GLU:OE2	1:C:8:ARG:HB3	2.11	0.49
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.78	0.49
1:C:352:PHE:HZ	1:C:362:PHE:CE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:530:SER:O	1:E:534:ILE:HG23	2.12	0.49
1:E:790:TYR:HE1	1:E:800:PRO:HB3	1.77	0.49
1:E:1038:GLU:C	1:E:1040:ILE:N	2.71	0.49
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.94	0.49
1:A:190:PRO:HB2	1:A:788:ASP:O	2.13	0.49
1:A:605:ASN:ND2	1:A:647:ILE:HD11	2.25	0.49
1:A:795:ASP:OD2	1:A:796:GLY:N	2.44	0.49
1:B:327:TYR:HB2	1:B:628:PHE:CE2	2.48	0.49
1:B:398:MET:HE3	1:B:398:MET:HB3	1.59	0.49
1:C:584:GLN:N	1:C:622:GLN:HB3	2.28	0.49
1:C:800:PRO:HG2	1:C:803:ALA:HB2	1.93	0.49
1:C:904:VAL:HG21	1:C:942:ALA:HB2	1.95	0.49
1:C:1038:GLU:CA	1:C:1039:ASP:HB2	2.43	0.49
1:D:344:LEU:HD22	1:D:402:ILE:CD1	2.41	0.49
1:D:699:ARG:O	1:D:703:LEU:HG	2.13	0.49
1:D:713:LEU:HD21	1:D:843:LEU:CD1	2.40	0.49
1:E:190:PRO:HG3	1:E:779:TYR:HB3	1.94	0.49
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.94	0.49
1:A:668:LEU:HD23	1:A:668:LEU:H	1.76	0.49
1:B:675:GLY:C	1:B:677:ALA:H	2.20	0.49
1:B:946:VAL:HG13	1:B:1026:PHE:CE1	2.47	0.49
1:D:1030:ARG:HA	1:D:1030:ARG:NH1	2.27	0.49
1:F:3:ASN:ND2	1:F:435:MET:HG3	2.18	0.49
1:A:860:THR:HG21	2:A:1101:ERY:H281	1.95	0.49
1:D:678:THR:HA	1:D:837:THR:OG1	2.12	0.49
1:D:982:PHE:HD2	1:D:1011:MET:HG3	1.78	0.49
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.94	0.49
1:E:525:HIS:O	1:E:526:HIS:C	2.55	0.49
3:B:1101:LMT:H6E	3:B:1101:LMT:O5B	2.13	0.49
1:C:860:THR:HA	1:C:864:TYR:HB2	1.95	0.49
1:D:309:GLU:HA	1:D:312:LYS:HD2	1.95	0.49
1:E:102:ILE:O	1:E:106:GLN:HG3	2.11	0.49
1:E:182:TYR:HB2	1:E:769:LYS:NZ	2.27	0.49
1:A:182:TYR:HB2	1:A:769:LYS:NZ	2.27	0.49
1:C:636:ASP:C	1:C:638:PRO:HD3	2.38	0.49
1:D:132:SER:OG	1:D:133:SER:N	2.46	0.49
1:D:141:GLY:HA3	1:D:324:VAL:HG12	1.95	0.49
1:E:327:TYR:HB2	1:E:628:PHE:CE2	2.48	0.49
1:E:375:VAL:HB	1:E:405:LEU:HD13	1.95	0.49
1:E:973:ARG:O	1:E:977:MET:HG3	2.13	0.49
1:F:514:GLY:C	1:F:516:PHE:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:GLY:CA	1:A:502:LYS:HB3	2.37	0.48
1:A:444:GLY:O	1:A:448:VAL:HG23	2.13	0.48
1:A:914:LEU:O	1:A:918:PHE:HB2	2.13	0.48
1:A:945:ILE:HG13	1:A:971:ARG:NH2	2.24	0.48
1:B:485:ALA:HA	1:B:489:THR:HG23	1.95	0.48
1:B:485:ALA:O	1:B:490:PRO:HD3	2.13	0.48
1:D:216:ALA:HB1	1:D:234:ILE:HG22	1.95	0.48
1:D:279:ALA:HB3	1:D:286:ALA:O	2.13	0.48
1:D:568:ASP:O	1:D:634:TRP:HZ3	1.96	0.48
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.95	0.48
1:E:142:VAL:HG13	1:E:323:ILE:HD12	1.95	0.48
1:E:584:GLN:N	1:E:622:GLN:HB3	2.28	0.48
1:F:510:LYS:HG2	1:F:511:GLY:N	2.28	0.48
1:F:563:PHE:HE2	1:F:564:LEU:HD22	1.78	0.48
1:A:261:LEU:N	1:A:264:ASP:OD2	2.44	0.48
1:A:426:PRO:O	1:A:429:GLU:HG2	2.13	0.48
1:C:55:LYS:HD2	1:C:55:LYS:O	2.13	0.48
1:C:545:TYR:OH	1:C:903:LEU:O	2.19	0.48
1:C:841:MET:HG2	1:C:859:TRP:CH2	2.48	0.48
1:C:940:LYS:HE2	1:C:941:ASN:OD1	2.13	0.48
1:E:132:SER:O	1:E:132:SER:OG	2.24	0.48
1:E:175:VAL:HG23	1:F:70:ASN:ND2	2.28	0.48
1:E:218:GLN:HG3	1:E:221:GLY:HA2	1.95	0.48
1:A:56:THR:O	1:A:60:THR:HG22	2.13	0.48
1:A:534:ILE:HG23	3:A:1102:LMT:HI'	1.95	0.48
1:A:706:ALA:HB2	1:A:844:MET:HE1	1.94	0.48
1:A:905:VAL:HG13	1:A:935:ILE:HD13	1.95	0.48
1:C:382:VAL:HG11	1:C:476:SER:HB3	1.95	0.48
1:E:587:THR:OG1	1:E:622:GLN:O	2.26	0.48
1:F:944:LEU:HD12	1:F:975:ILE:HG12	1.96	0.48
1:B:80:SER:CB	1:B:90:ILE:HG12	2.44	0.48
1:B:538:THR:O	1:B:541:TYR:HB2	2.13	0.48
1:B:774:MET:HG2	1:B:775:SER:N	2.27	0.48
1:B:897:ILE:N	1:B:898:PRO:HD2	2.29	0.48
1:C:34:GLN:HE21	1:C:333:VAL:CG2	2.21	0.48
1:C:414:GLU:HG2	1:C:973:ARG:NH1	2.28	0.48
1:C:636:ASP:O	1:C:638:PRO:HD3	2.12	0.48
1:C:947:GLU:HG3	1:C:948:PHE:N	2.27	0.48
1:D:146:ASP:HB2	1:D:148:THR:HG23	1.95	0.48
1:D:605:ASN:N	1:D:605:ASN:OD1	2.46	0.48
1:E:30:LEU:HD12	1:E:31:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:PHE:O	1:F:262:LEU:HD23	2.14	0.48
1:F:669:PRO:HB2	1:F:862:MET:SD	2.54	0.48
1:F:979:SER:CB	1:F:1015:THR:HG21	2.43	0.48
1:A:576:VAL:HG21	1:A:591:LEU:CD2	2.44	0.48
1:A:712:MET:O	1:A:832:ALA:N	2.45	0.48
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.47	0.48
1:A:982:PHE:O	1:A:985:GLY:N	2.46	0.48
1:A:1016:VAL:O	1:A:1016:VAL:HG12	2.12	0.48
1:B:404:LEU:HD21	1:B:449:LEU:HD22	1.96	0.48
1:C:694:LYS:HA	1:C:697:GLN:OE1	2.13	0.48
1:D:351:VAL:O	1:D:355:MET:HB2	2.13	0.48
1:D:602:GLU:HG3	1:D:605:ASN:ND2	2.28	0.48
1:E:24:GLY:O	1:E:28:LEU:HB2	2.13	0.48
1:E:744:ASN:O	1:E:748:THR:HG23	2.13	0.48
1:E:846:GLN:O	1:E:849:SER:OG	2.22	0.48
1:F:835:LYS:HG2	1:F:836:SER:N	2.28	0.48
1:A:5:PHE:HE2	1:A:11:PHE:CD1	2.31	0.48
1:A:893:GLU:CD	1:C:8:ARG:HB3	2.39	0.48
1:B:562:SER:HB3	1:B:924:ASP:HB3	1.96	0.48
1:C:201:VAL:HG23	1:C:749:THR:CG2	2.44	0.48
1:C:940:LYS:O	1:C:943:ILE:HB	2.14	0.48
1:D:750:LEU:HD12	1:D:754:TRP:CD1	2.48	0.48
1:D:913:LEU:HD23	1:D:927:PHE:HZ	1.78	0.48
3:D:1102:LMT:H5B	3:D:1102:LMT:H6E	1.94	0.48
1:E:732:ASP:OD1	1:E:735:LYS:HG3	2.13	0.48
1:E:909:VAL:HG12	1:E:913:LEU:HG	1.95	0.48
1:E:987:MET:HE2	1:E:987:MET:HB3	1.79	0.48
1:E:1037:ASN:HB2	1:E:1038:GLU:O	2.14	0.48
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.94	0.48
1:A:80:SER:CB	1:A:90:ILE:HG12	2.42	0.48
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.95	0.48
1:A:172:VAL:CG2	1:A:306:ILE:HD11	2.43	0.48
1:B:1020:PHE:O	1:B:1023:PRO:HG2	2.13	0.48
1:C:3:ASN:C	1:C:5:PHE:N	2.71	0.48
1:C:398:MET:HG2	1:C:473:THR:HG21	1.96	0.48
1:D:762:PHE:CE1	1:D:764:ASP:HB2	2.49	0.48
1:D:894:SER:HB2	1:D:897:ILE:HD12	1.94	0.48
1:A:575:MET:HE3	1:A:626:ILE:HD11	1.96	0.48
1:A:767:ARG:HH12	1:B:67:GLN:CD	2.22	0.48
1:A:891:LEU:HD23	1:A:892:TYR:CE1	2.48	0.48
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:ILE:HG13	1:A:1041:GLU:H	1.79	0.48
1:C:214:VAL:HB	1:C:236:ALA:HB3	1.95	0.48
1:E:186:ILE:HB	1:E:773:VAL:HG23	1.96	0.48
1:A:376:LEU:O	1:A:377:LEU:C	2.56	0.48
1:A:382:VAL:HG11	1:A:476:SER:HB2	1.96	0.48
1:A:519:MET:O	1:A:523:SER:OG	2.28	0.48
2:A:1101:ERY:H71	2:A:1101:ERY:H10	1.62	0.48
1:B:459:PHE:O	1:B:464:GLY:HA3	2.14	0.48
1:C:525:HIS:HA	1:C:528:THR:HG22	1.96	0.48
1:C:531:VAL:O	1:C:534:ILE:HG13	2.13	0.48
1:C:817:GLU:OE2	1:C:825:MET:HA	2.14	0.48
1:D:726:GLN:O	1:D:810:GLU:HG2	2.14	0.48
1:D:781:MET:CE	1:F:225:VAL:H	2.26	0.48
1:E:39:ALA:HA	1:E:462:SER:OG	2.14	0.48
1:E:675:GLY:C	1:E:677:ALA:H	2.22	0.48
1:E:1038:GLU:C	1:E:1040:ILE:H	2.21	0.48
1:F:761:ASP:OD1	1:F:770:LYS:HA	2.14	0.48
1:A:429:GLU:H	1:A:429:GLU:CD	2.21	0.48
1:A:683:GLU:HG2	1:A:819:TYR:CG	2.49	0.48
1:C:44:THR:OG1	1:C:91:THR:OG1	2.24	0.48
1:C:156:ASP:OD2	1:C:182:TYR:HB2	2.14	0.48
1:C:358:PHE:O	1:C:359:LEU:HD23	2.14	0.48
1:C:391:ASN:OD1	1:C:393:LEU:HB2	2.14	0.48
1:D:352:PHE:CD2	1:D:353:LEU:HD23	2.49	0.48
1:D:571:VAL:N	1:D:631:LEU:HD12	2.29	0.48
1:D:680:PHE:HD1	1:D:859:TRP:HZ3	1.61	0.48
1:D:801:PHE:HA	1:D:804:PHE:CE2	2.49	0.48
1:E:525:HIS:HA	1:E:528:THR:HG22	1.96	0.48
1:E:1016:VAL:O	1:E:1016:VAL:HG12	2.14	0.48
1:A:7:ASP:O	1:A:8:ARG:HG3	2.13	0.47
1:A:376:LEU:O	1:A:379:THR:N	2.47	0.47
1:A:559:LEU:HD22	1:A:923:ASN:H	1.79	0.47
1:A:702:LEU:HD22	1:A:827:ILE:HD13	1.96	0.47
1:A:832:ALA:CB	1:A:835:LYS:HD3	2.38	0.47
1:B:986:VAL:HG12	1:B:1008:MET:HE3	1.96	0.47
1:C:682:PHE:CZ	1:C:857:TYR:HB2	2.49	0.47
1:D:277:ILE:HA	1:D:613:ASN:O	2.13	0.47
1:E:169:THR:HG21	1:E:306:ILE:HG13	1.95	0.47
1:E:289:LEU:HA	1:E:289:LEU:HD23	1.66	0.47
1:E:507:GLU:HG2	1:E:518:ARG:HA	1.96	0.47
1:F:492:LEU:O	1:F:496:MET:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:911:GLY:HA2	1:F:1013:THR:HG21	1.96	0.47
1:A:902:MET:O	1:A:905:VAL:HG23	2.14	0.47
1:B:188:MET:HA	1:B:266:ALA:CB	2.44	0.47
1:B:332:PHE:C	1:B:332:PHE:CD2	2.93	0.47
1:C:527:TYR:OH	1:C:968:VAL:HG13	2.14	0.47
1:D:26:ALA:O	1:D:30:LEU:HB2	2.14	0.47
1:D:58:GLN:NE2	1:D:818:ARG:NH1	2.61	0.47
1:D:423:GLU:O	1:D:502:LYS:HB3	2.14	0.47
1:D:1030:ARG:HA	1:D:1030:ARG:HH11	1.79	0.47
1:E:196:PHE:HD2	1:E:260:VAL:HG22	1.77	0.47
1:E:462:SER:H	1:E:865:GLN:HE21	1.62	0.47
1:E:534:ILE:HD11	1:E:1024:VAL:HG22	1.95	0.47
1:E:658:ILE:C	1:E:659:LYS:HD2	2.39	0.47
1:F:42:ALA:HB2	1:F:93:THR:HG23	1.95	0.47
1:F:74:ASN:HB2	1:F:98:THR:HG21	1.96	0.47
1:F:146:ASP:O	1:F:148:THR:N	2.47	0.47
1:F:614:GLY:O	1:F:620:ARG:HA	2.14	0.47
1:F:775:SER:OG	1:F:780:ARG:HG2	2.14	0.47
1:A:63:GLN:OE1	1:C:768:VAL:HG12	2.14	0.47
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.95	0.47
1:C:75:LEU:HD11	1:C:92:LEU:HB3	1.96	0.47
1:C:348:ILE:HG13	1:C:402:ILE:CD1	2.42	0.47
1:C:586:ARG:HA	1:C:589:LYS:HD2	1.96	0.47
1:D:508:GLY:H	1:D:518:ARG:HG3	1.78	0.47
1:E:662:MET:HA	1:E:662:MET:HE3	1.95	0.47
1:A:648:THR:HB	1:A:665:ALA:O	2.13	0.47
1:A:909:VAL:HA	1:A:931:LEU:HD21	1.96	0.47
1:B:904:VAL:HG13	1:B:907:LEU:HD22	1.96	0.47
1:C:382:VAL:HG11	1:C:476:SER:CB	2.44	0.47
1:C:449:LEU:HD21	1:C:937:LEU:HD23	1.96	0.47
1:C:877:TYR:O	1:C:881:LEU:HG	2.14	0.47
1:D:198:LEU:HD11	1:D:252:LYS:HB2	1.97	0.47
1:E:255:GLN:OE1	1:E:256:ASP:N	2.47	0.47
1:E:659:LYS:HE3	1:E:659:LYS:HA	1.97	0.47
1:A:172:VAL:HG22	1:A:306:ILE:HD11	1.94	0.47
1:A:210:GLN:HE22	1:A:250:LEU:N	2.13	0.47
1:B:32:VAL:HG12	1:B:390:ILE:HD12	1.96	0.47
1:B:270:LEU:HA	1:B:270:LEU:HD12	1.63	0.47
1:B:317:PHE:CE2	1:B:323:ILE:HD13	2.50	0.47
1:B:344:LEU:HD13	1:B:376:LEU:HD13	1.96	0.47
1:B:583:THR:HB	1:B:586:ARG:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:GLU:CG	1:C:248:LYS:HE3	2.45	0.47
1:C:637:ARG:HD2	1:C:642:ASN:O	2.13	0.47
1:C:682:PHE:HE2	1:C:702:LEU:HD11	1.80	0.47
1:D:203:VAL:O	1:D:206:ALA:HB3	2.15	0.47
1:D:890:ALA:HB1	1:F:11:PHE:CD1	2.50	0.47
1:E:2:PRO:O	1:E:6:ILE:HD12	2.14	0.47
1:F:73:ASP:OD2	1:F:106:GLN:NE2	2.33	0.47
1:F:973:ARG:HG2	1:F:977:MET:HE2	1.96	0.47
1:A:379:THR:HA	1:A:382:VAL:HG23	1.96	0.47
1:B:9:PRO:HB3	1:B:495:THR:HG21	1.96	0.47
1:B:442:LEU:O	1:B:445:ILE:HG13	2.14	0.47
1:B:465:ALA:HA	1:B:468:ARG:NH1	2.30	0.47
1:D:535:LEU:CD2	1:D:1027:VAL:HG21	2.45	0.47
1:D:559:LEU:HD23	1:D:560:PRO:CD	2.45	0.47
1:D:1040:ILE:HG22	1:D:1041:GLU:N	2.29	0.47
1:F:227:GLY:O	1:F:229:GLN:HG3	2.14	0.47
1:F:996:GLY:O	1:F:999:ALA:N	2.48	0.47
1:B:534:ILE:HG22	3:B:1101:LMT:H5'	1.97	0.47
1:B:836:SER:OG	1:B:839:GLU:HG3	2.14	0.47
1:B:907:LEU:HG	1:B:1017:LEU:HD23	1.96	0.47
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.97	0.47
1:C:787:GLY:C	1:C:789:TRP:H	2.23	0.47
1:D:58:GLN:HA	1:D:62:THR:HB	1.97	0.47
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.49	0.47
1:D:417:GLU:OE1	1:D:497:LEU:HD21	2.14	0.47
1:D:562:SER:HB2	1:D:924:ASP:HB3	1.97	0.47
1:D:754:TRP:CZ3	1:F:219:LEU:HD23	2.49	0.47
1:D:888:LEU:HB2	1:D:898:PRO:HB3	1.97	0.47
1:D:1031:ARG:O	1:D:1032:ARG:HG3	2.14	0.47
1:D:1035:ARG:NH2	1:D:1036:LYS:HG3	2.30	0.47
1:E:652:THR:HG23	1:E:665:ALA:CB	2.42	0.47
1:E:904:VAL:HG21	1:E:942:ALA:CB	2.45	0.47
1:E:971:ARG:C	1:E:974:PRO:HD2	2.40	0.47
1:F:900:SER:HB3	1:F:1029:VAL:HG21	1.96	0.47
1:F:971:ARG:C	1:F:974:PRO:HD2	2.40	0.47
1:A:367:ILE:HG12	1:A:492:LEU:HB3	1.96	0.47
1:A:690:LEU:HD11	1:A:853:THR:O	2.15	0.47
1:A:751:GLY:O	1:A:753:ALA:N	2.48	0.47
1:B:222:THR:HA	1:B:224:PRO:HD3	1.96	0.47
1:C:142:VAL:HG21	1:C:162:MET:HE1	1.97	0.47
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:LEU:HD12	1:D:31:PRO:HD2	1.96	0.47
1:D:692:HIS:O	1:D:696:THR:OG1	2.29	0.47
1:D:944:LEU:O	1:D:947:GLU:HB3	2.14	0.47
1:E:187:TRP:NE1	1:E:269:GLU:OE2	2.48	0.47
1:F:220:GLY:HA3	1:F:230:LEU:O	2.15	0.47
1:A:375:VAL:HB	1:A:405:LEU:HD13	1.96	0.47
1:A:420:MET:HB2	1:A:500:ILE:HD12	1.96	0.47
1:C:63:GLN:O	1:C:67:GLN:HG3	2.15	0.47
1:C:801:PHE:CD1	1:C:804:PHE:HE2	2.31	0.47
1:C:1016:VAL:HG13	3:C:1101:LMT:H112	1.96	0.47
1:D:125:GLN:OE1	1:D:770:LYS:HE3	2.15	0.47
1:D:841:MET:HE1	1:D:867:ARG:HG3	1.97	0.47
1:E:213:GLN:HE21	1:E:239:ARG:HG3	1.80	0.47
1:E:764:ASP:OD1	1:E:765:ARG:HG3	2.14	0.47
1:F:185:ARG:HB3	1:F:187:TRP:HE1	1.79	0.47
1:F:311:ALA:O	1:F:314:GLU:HB2	2.14	0.47
1:F:514:GLY:HA2	1:F:517:ASN:OD1	2.14	0.47
1:F:696:THR:HG23	1:F:699:ARG:HH12	1.80	0.47
1:A:127:VAL:HB	1:B:113:LEU:HD22	1.96	0.47
1:A:602:GLU:OE2	1:A:650:ARG:NH1	2.48	0.47
1:A:937:LEU:HD23	1:A:937:LEU:HA	1.74	0.47
1:A:1039:ASP:H	1:A:1040:ILE:HD13	1.80	0.47
1:B:189:ASN:OD1	1:B:190:PRO:HD2	2.14	0.47
1:B:783:PRO:O	1:B:786:ILE:HG12	2.15	0.47
1:B:961:ILE:H	1:B:961:ILE:HG13	1.52	0.47
1:C:214:VAL:CG2	1:C:237:GLN:HB2	2.45	0.47
1:C:371:ALA:O	1:C:375:VAL:HG23	2.14	0.47
1:C:600:THR:O	1:C:603:LYS:HG3	2.15	0.47
1:C:922:THR:O	1:C:924:ASP:N	2.48	0.47
1:D:356:TYR:C	1:D:358:PHE:H	2.23	0.47
1:D:388:PHE:CE2	1:D:472:ILE:HD12	2.50	0.47
1:D:549:VAL:HG22	1:D:906:PRO:HG2	1.97	0.47
1:E:416:VAL:HG21	1:E:493:CYS:SG	2.55	0.47
1:E:508:GLY:H	1:E:518:ARG:HE	1.63	0.47
1:E:736:ALA:HB1	1:E:741:VAL:HG23	1.96	0.47
1:A:3:ASN:O	1:A:4:PHE:C	2.58	0.46
1:A:525:HIS:HA	1:A:528:THR:HG22	1.96	0.46
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.51	0.46
1:B:244:GLU:O	1:B:247:GLY:N	2.48	0.46
1:C:196:PHE:N	1:C:196:PHE:CD2	2.83	0.46
1:C:455:PRO:HG3	1:C:883:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:LEU:HD23	1:C:560:PRO:CD	2.46	0.46
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.79	0.46
1:E:32:VAL:HA	1:E:390:ILE:O	2.15	0.46
1:E:615:PHE:HD2	1:E:620:ARG:HG2	1.81	0.46
1:E:775:SER:HB3	1:E:780:ARG:HD3	1.98	0.46
1:E:841:MET:HE1	1:E:867:ARG:HB2	1.96	0.46
1:E:960:LEU:O	1:E:964:THR:HG23	2.15	0.46
1:E:982:PHE:HD2	1:E:1011:MET:HE2	1.79	0.46
1:F:184:MET:HA	1:F:184:MET:HE3	1.97	0.46
1:F:356:TYR:C	1:F:358:PHE:H	2.23	0.46
1:F:356:TYR:CA	1:F:365:THR:HG21	2.39	0.46
1:F:892:TYR:C	1:F:894:SER:H	2.22	0.46
1:A:574:THR:CG2	1:A:627:ALA:HB3	2.46	0.46
1:A:618:ALA:C	1:A:815:ARG:HH22	2.22	0.46
1:B:259:ARG:O	1:B:259:ARG:HG2	2.13	0.46
1:B:554:TYR:CZ	1:B:558:ARG:HG3	2.50	0.46
1:C:124:GLN:HG3	1:C:125:GLN:N	2.27	0.46
1:C:692:HIS:C	1:C:692:HIS:CD2	2.93	0.46
1:D:83:ASP:HB2	1:D:87:THR:O	2.15	0.46
1:D:189:ASN:HB3	1:D:192:GLU:HB2	1.96	0.46
1:D:350:LEU:HD23	1:D:350:LEU:HA	1.73	0.46
1:D:676:THR:OG1	1:D:679:GLY:HA3	2.15	0.46
1:D:682:PHE:CD2	1:D:683:GLU:N	2.83	0.46
1:E:795:ASP:OD2	1:E:797:GLN:N	2.47	0.46
1:E:818:ARG:HH12	1:E:823:PRO:HG3	1.80	0.46
1:F:391:ASN:OD1	1:F:393:LEU:HB2	2.15	0.46
1:F:671:ILE:CG2	1:F:674:LEU:HB2	2.45	0.46
1:F:743:ILE:H	1:F:743:ILE:HD12	1.81	0.46
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.60	0.46
1:A:34:GLN:HB2	1:A:333:VAL:CG2	2.45	0.46
1:A:244:GLU:O	1:A:247:GLY:N	2.48	0.46
1:A:531:VAL:HG12	1:A:535:LEU:HD12	1.96	0.46
1:A:781:MET:HE2	1:C:225:VAL:HG22	1.97	0.46
1:A:929:VAL:O	1:A:932:LEU:HB2	2.15	0.46
1:A:1007:VAL:HG12	1:A:1008:MET:N	2.28	0.46
1:B:184:MET:HB3	1:B:771:VAL:HG13	1.97	0.46
1:B:242:SER:HB2	1:B:245:GLU:HG3	1.98	0.46
1:B:525:HIS:HA	1:B:528:THR:HG22	1.96	0.46
1:B:801:PHE:HA	1:B:804:PHE:CE2	2.51	0.46
1:B:990:VAL:HG22	1:B:1004:GLY:C	2.40	0.46
1:D:198:LEU:HD23	1:D:792:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:623:ASN:O	1:E:623:ASN:ND2	2.48	0.46
1:E:726:GLN:NE2	1:E:812:GLY:HA3	2.30	0.46
1:F:412:VAL:CG1	1:F:435:MET:HE1	2.45	0.46
1:F:945:ILE:HG13	1:F:971:ARG:HH22	1.80	0.46
1:B:61:VAL:HG22	1:B:118:LEU:HD22	1.96	0.46
1:B:514:GLY:C	1:B:516:PHE:H	2.23	0.46
1:B:1015:THR:C	1:B:1017:LEU:H	2.24	0.46
1:C:39:ALA:CB	1:C:673:GLU:HG2	2.46	0.46
1:C:216:ALA:HB1	1:C:234:ILE:HG22	1.97	0.46
1:C:568:ASP:O	1:C:634:TRP:HZ3	1.99	0.46
1:C:649:MET:HE1	1:C:653:ARG:NH2	2.31	0.46
1:D:520:PHE:O	1:D:524:THR:HG22	2.16	0.46
1:E:177:LEU:HG	1:E:289:LEU:HD21	1.97	0.46
1:E:195:LYS:NZ	1:E:196:PHE:HE1	2.13	0.46
1:E:367:ILE:HB	1:E:368:PRO:HD3	1.98	0.46
1:E:892:TYR:O	1:E:893:GLU:HB2	2.15	0.46
1:F:449:LEU:HD23	1:F:449:LEU:HA	1.73	0.46
1:F:946:VAL:HG13	1:F:1026:PHE:CE1	2.51	0.46
1:A:222:THR:HG23	1:B:275:TYR:HB2	1.97	0.46
1:A:382:VAL:O	1:A:385:ALA:HB3	2.15	0.46
1:A:583:THR:HG21	1:C:228:GLN:HG3	1.97	0.46
1:B:185:ARG:HB3	1:B:187:TRP:NE1	2.31	0.46
1:B:662:MET:HA	1:B:662:MET:HE3	1.98	0.46
1:B:715:SER:O	1:B:717:ARG:HG3	2.15	0.46
1:C:45:ILE:HD12	1:C:90:ILE:HB	1.96	0.46
1:C:101:ASP:O	1:C:105:VAL:HG23	2.15	0.46
1:C:332:PHE:CD1	1:C:634:TRP:CH2	3.04	0.46
1:C:966:ASP:O	1:C:970:MET:HG2	2.15	0.46
1:D:435:MET:HE3	1:D:435:MET:HB3	1.73	0.46
1:D:781:MET:HB3	1:F:228:GLN:NE2	2.30	0.46
1:E:559:LEU:HD12	1:E:923:ASN:HB2	1.98	0.46
1:E:904:VAL:HG21	1:E:942:ALA:HB2	1.97	0.46
1:F:752:ALA:O	1:F:774:MET:HA	2.16	0.46
1:F:1038:GLU:HB2	1:F:1039:ASP:OD1	2.14	0.46
1:A:586:ARG:O	1:A:590:VAL:HG23	2.16	0.46
1:A:641:GLU:HB2	1:A:650:ARG:NH2	2.31	0.46
1:A:841:MET:HE3	1:A:859:TRP:CD2	2.51	0.46
1:B:535:LEU:HD22	1:B:1027:VAL:HG11	1.98	0.46
1:C:425:LEU:HD13	1:C:429:GLU:HG3	1.97	0.46
1:C:577:GLN:HG3	1:C:624:THR:HG22	1.98	0.46
1:C:671:ILE:HB	1:C:862:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:ALA:HB1	1:D:468:ARG:HG3	1.97	0.46
1:D:538:THR:HG21	1:D:1028:VAL:HG21	1.97	0.46
1:D:588:GLN:HE21	1:D:592:ASN:CG	2.24	0.46
1:E:104:GLN:NE2	1:F:109:ASN:HD22	2.14	0.46
1:E:149:MET:HB2	1:E:153:ASP:CB	2.45	0.46
1:E:203:VAL:O	1:E:207:ILE:HG13	2.16	0.46
1:E:242:SER:OG	1:E:245:GLU:HG3	2.16	0.46
1:E:355:MET:HB2	1:E:355:MET:HE3	1.53	0.46
1:E:415:ASN:HB3	1:E:434:SER:HB2	1.97	0.46
1:F:351:VAL:HG11	1:F:406:VAL:HG11	1.96	0.46
1:F:1025:PHE:O	1:F:1029:VAL:HG23	2.15	0.46
1:A:16:ALA:HB2	1:A:488:LEU:HD13	1.98	0.46
1:A:187:TRP:HE3	1:A:775:SER:O	1.97	0.46
1:A:768:VAL:HG12	1:B:63:GLN:OE1	2.15	0.46
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.96	0.46
1:B:356:TYR:C	1:B:358:PHE:H	2.24	0.46
1:C:354:VAL:HG23	1:C:984:LEU:HD12	1.98	0.46
1:C:456:MET:HA	1:C:459:PHE:CD1	2.51	0.46
1:C:525:HIS:C	1:C:525:HIS:CD2	2.92	0.46
1:C:743:ILE:HA	1:C:746:ILE:HG23	1.97	0.46
1:A:982:PHE:HD2	1:A:1011:MET:HE2	1.80	0.46
1:B:953:MET:HE2	1:B:963:ALA:HB3	1.98	0.46
1:C:898:PRO:O	1:C:901:VAL:N	2.49	0.46
1:E:57:VAL:HB	1:E:88:VAL:CG2	2.46	0.46
1:E:196:PHE:CD2	1:E:260:VAL:HG22	2.51	0.46
1:F:344:LEU:O	1:F:348:ILE:HG13	2.15	0.46
1:A:228:GLN:NE2	1:A:230:LEU:O	2.47	0.46
1:A:623:ASN:OD1	1:A:623:ASN:N	2.42	0.46
1:A:669:PRO:HG2	1:A:676:THR:HG22	1.97	0.46
1:B:61:VAL:CG2	1:B:122:VAL:HG21	2.45	0.46
1:B:888:LEU:HA	1:B:888:LEU:HD23	1.53	0.46
1:C:340:VAL:HG11	1:C:395:MET:CB	2.33	0.46
1:D:76:MET:HB2	1:D:93:THR:O	2.16	0.46
1:D:723:ASP:HA	1:D:812:GLY:O	2.15	0.46
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.98	0.46
1:F:183:ALA:O	1:F:270:LEU:HD12	2.16	0.46
1:F:418:ARG:O	1:F:422:GLU:HB2	2.16	0.46
1:F:483:LEU:HA	1:F:483:LEU:HD23	1.77	0.46
1:F:774:MET:HG2	1:F:775:SER:N	2.31	0.46
1:A:211:ASN:CG	1:A:240:LEU:HG	2.40	0.46
1:A:427:PRO:CD	1:A:499:PRO:HB3	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LEU:HD22	1:B:661:ALA:CB	2.45	0.46
1:B:774:MET:HG2	1:B:775:SER:H	1.81	0.46
1:C:555:LEU:HD11	1:C:914:LEU:HD12	1.98	0.46
1:C:973:ARG:HG2	1:C:977:MET:CE	2.46	0.46
1:E:142:VAL:HG12	1:E:321:LEU:HD11	1.98	0.46
1:E:447:MET:HB3	1:E:887:CYS:SG	2.56	0.46
1:E:1042:HIS:HB3	1:E:1043:SER:HB3	1.96	0.46
1:F:74:ASN:O	1:F:94:PHE:HD2	1.98	0.46
1:F:186:ILE:HG12	1:F:268:ILE:HG12	1.97	0.46
1:A:513:PHE:O	1:A:516:PHE:HB3	2.16	0.45
1:A:648:THR:HB	1:A:665:ALA:C	2.41	0.45
1:B:355:MET:HG2	1:B:365:THR:HA	1.97	0.45
1:C:188:MET:HA	1:C:266:ALA:CB	2.47	0.45
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.46	0.45
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.51	0.45
1:D:605:ASN:HD22	1:D:647:ILE:HD11	1.81	0.45
1:D:754:TRP:CH2	1:D:780:ARG:HA	2.51	0.45
1:D:953:MET:HE3	1:D:953:MET:HB2	1.73	0.45
1:E:712:MET:SD	1:E:835:LYS:HG2	2.56	0.45
1:F:75:LEU:HD11	1:F:92:LEU:HD12	1.97	0.45
1:F:420:MET:HB3	1:F:500:ILE:HB	1.98	0.45
1:A:1039:ASP:N	1:A:1040:ILE:HD13	2.32	0.45
1:B:407:ASP:OD1	1:B:978:THR:OG1	2.30	0.45
1:B:897:ILE:HD13	1:B:950:LYS:HE3	1.98	0.45
1:D:865:GLN:HE21	1:D:865:GLN:HA	1.82	0.45
1:E:65:ILE:O	1:E:69:MET:HG2	2.17	0.45
1:E:455:PRO:O	1:E:876:LEU:HD13	2.15	0.45
1:E:514:GLY:C	1:E:516:PHE:H	2.22	0.45
1:E:713:LEU:HD11	1:E:843:LEU:HD12	1.98	0.45
1:E:888:LEU:HD13	1:E:901:VAL:CG1	2.45	0.45
1:F:36:PRO:HD3	1:F:391:ASN:CG	2.42	0.45
1:F:668:LEU:H	1:F:668:LEU:HG	1.22	0.45
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.16	0.45
1:A:577:GLN:O	1:A:661:ALA:HB1	2.16	0.45
1:A:800:PRO:O	1:A:803:ALA:HB3	2.15	0.45
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.98	0.45
1:A:902:MET:C	1:A:904:VAL:H	2.25	0.45
1:B:858:ASP:OD1	1:B:859:TRP:N	2.48	0.45
1:D:576:VAL:HG21	1:D:591:LEU:HD23	1.98	0.45
1:D:674:LEU:HD22	1:D:675:GLY:H	1.80	0.45
1:E:637:ARG:HB3	1:E:642:ASN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:GLY:O	1:F:27:ILE:HG13	2.16	0.45
1:F:58:GLN:HG2	1:F:63:GLN:NE2	2.30	0.45
1:F:164:ASP:HB3	1:F:168:ARG:HH22	1.81	0.45
1:F:858:ASP:OD2	1:F:859:TRP:N	2.40	0.45
1:A:446:ALA:CB	1:A:482:VAL:HG21	2.45	0.45
1:B:453:PHE:O	1:B:471:SER:OG	2.27	0.45
1:C:429:GLU:O	1:C:433:LYS:HB2	2.16	0.45
1:C:940:LYS:HZ1	1:C:978:THR:HG21	1.77	0.45
1:D:678:THR:HG21	1:D:835:LYS:O	2.17	0.45
1:D:953:MET:HE1	1:D:960:LEU:HD12	1.97	0.45
1:E:953:MET:HE1	1:E:1026:PHE:HE2	1.82	0.45
1:F:158:VAL:HA	1:F:162:MET:HE3	1.98	0.45
1:F:680:PHE:CD2	1:F:859:TRP:HZ3	2.34	0.45
1:F:776:GLU:HB2	1:F:779:TYR:CE1	2.52	0.45
1:F:898:PRO:O	1:F:901:VAL:N	2.48	0.45
1:A:74:ASN:O	1:A:94:PHE:HD2	2.00	0.45
1:A:636:ASP:O	1:A:638:PRO:HD3	2.17	0.45
1:A:1039:ASP:CA	1:A:1040:ILE:HB	2.43	0.45
1:B:541:TYR:CD1	1:B:541:TYR:N	2.85	0.45
1:B:564:LEU:HD13	1:B:671:ILE:HD12	1.99	0.45
1:C:354:VAL:HG22	1:C:980:LEU:HD23	1.98	0.45
1:C:379:THR:HG23	1:C:476:SER:OG	2.16	0.45
1:D:159:ALA:HB2	1:D:177:LEU:CD1	2.47	0.45
1:D:522:LYS:O	1:D:525:HIS:HB3	2.17	0.45
1:D:876:LEU:HD23	1:D:876:LEU:HA	1.82	0.45
1:F:644:VAL:O	1:F:648:THR:HG23	2.16	0.45
1:A:80:SER:O	1:A:817:GLU:HA	2.17	0.45
1:A:340:VAL:HG12	1:A:395:MET:HE3	1.97	0.45
1:A:418:ARG:NH2	1:A:948:PHE:HE2	2.15	0.45
1:A:511:GLY:HA2	1:A:515:TRP:CD1	2.51	0.45
1:B:946:VAL:HG13	1:B:1026:PHE:CD1	2.52	0.45
1:C:53:ASP:O	1:C:56:THR:HB	2.17	0.45
1:C:567:GLU:OE1	1:C:996:GLY:HA2	2.17	0.45
1:D:112:GLN:OE1	1:D:112:GLN:HA	2.16	0.45
1:D:400:LEU:CD2	1:D:929:VAL:HG12	2.47	0.45
1:E:166:ILE:HD11	1:E:310:LEU:CD1	2.46	0.45
1:A:705:GLU:HA	1:A:708:LYS:HD3	1.99	0.45
1:A:876:LEU:HD23	1:A:876:LEU:HA	1.67	0.45
1:C:555:LEU:HD23	1:C:555:LEU:HA	1.62	0.45
1:C:730:ASP:OD1	1:C:808:ARG:NE	2.34	0.45
1:D:20:MET:HG2	1:D:374:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:888:LEU:HD22	1:D:901:VAL:HG11	1.99	0.45
1:D:907:LEU:O	1:D:1013:THR:OG1	2.30	0.45
1:E:184:MET:HA	1:E:184:MET:HE3	1.99	0.45
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.42	0.45
1:E:775:SER:OG	1:E:776:GLU:N	2.49	0.45
1:F:293:LEU:HD11	1:F:299:ALA:HA	1.97	0.45
1:F:578:LEU:HD22	1:F:661:ALA:CB	2.47	0.45
1:F:638:PRO:HB2	1:F:639:GLY:H	1.64	0.45
1:F:684:LEU:HD23	1:F:825:MET:HB2	1.98	0.45
1:F:841:MET:O	1:F:845:GLU:HG2	2.17	0.45
1:F:971:ARG:HH21	1:F:975:ILE:HD11	1.82	0.45
1:A:541:TYR:N	1:A:541:TYR:CD1	2.82	0.45
1:A:617:PHE:CZ	2:A:1101:ERY:H312	2.52	0.45
1:A:750:LEU:HD12	1:A:754:TRP:CD1	2.52	0.45
1:A:1030:ARG:HA	1:A:1030:ARG:NH1	2.30	0.45
1:B:149:MET:HG3	1:B:154:ILE:HG13	1.98	0.45
1:B:259:ARG:HG3	1:B:261:LEU:HG	1.97	0.45
1:B:407:ASP:OD2	1:B:940:LYS:NZ	2.46	0.45
1:B:584:GLN:HB2	1:B:622:GLN:HG2	1.99	0.45
1:B:634:TRP:CD1	1:B:634:TRP:N	2.72	0.45
1:D:240:LEU:HD12	1:D:246:PHE:CZ	2.52	0.45
1:D:598:TYR:CE2	1:D:629:VAL:HG21	2.52	0.45
1:D:674:LEU:HD22	1:D:862:MET:HB3	1.99	0.45
1:D:695:LEU:HD22	1:D:825:MET:SD	2.57	0.45
2:D:1101:ERY:H5	2:D:1101:ERY:C18	2.44	0.45
1:E:578:LEU:HB2	1:E:623:ASN:O	2.16	0.45
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.99	0.45
1:F:94:PHE:CE1	1:F:103:ALA:HB1	2.51	0.45
1:F:249:ILE:O	1:F:262:LEU:N	2.48	0.45
1:A:344:LEU:HD11	1:A:398:MET:CB	2.47	0.45
1:C:973:ARG:HG2	1:C:977:MET:HE2	1.98	0.45
1:D:162:MET:O	1:D:164:ASP:N	2.50	0.45
1:D:423:GLU:C	1:D:502:LYS:HB3	2.42	0.45
1:D:514:GLY:C	1:D:516:PHE:N	2.75	0.45
1:D:878:ALA:O	1:D:882:ILE:HG12	2.16	0.45
1:D:925:VAL:O	1:D:928:GLN:N	2.50	0.45
1:E:189:ASN:OD1	1:E:190:PRO:HD2	2.16	0.45
1:E:1041:GLU:OE1	1:E:1041:GLU:N	2.50	0.45
1:F:32:VAL:HG22	1:F:390:ILE:HB	1.99	0.45
1:F:318:PRO:HG2	1:F:321:LEU:HG	1.98	0.45
1:F:463:THR:HG22	1:F:467:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:561:SER:O	1:F:838:GLY:HA3	2.17	0.45
1:F:937:LEU:HD11	1:F:982:PHE:HE2	1.80	0.45
1:A:354:VAL:HG21	1:A:981:ALA:HA	1.99	0.45
1:A:584:GLN:N	1:A:622:GLN:HB3	2.32	0.45
1:B:58:GLN:HA	1:B:62:THR:HB	1.98	0.45
1:B:310:LEU:HD23	1:B:325:TYR:OH	2.17	0.45
1:C:196:PHE:HD1	1:C:260:VAL:HG13	1.82	0.45
1:C:399:VAL:HG11	1:C:989:LEU:HD21	1.98	0.45
1:C:960:LEU:HB3	1:C:1040:ILE:HG23	1.99	0.45
1:D:470:PHE:HD2	1:D:929:VAL:HG11	1.80	0.45
1:D:902:MET:C	1:D:904:VAL:H	2.25	0.45
1:D:1019:ILE:HG13	1:D:1020:PHE:CD1	2.51	0.45
1:D:1040:ILE:HG22	1:D:1041:GLU:H	1.81	0.45
1:E:187:TRP:HE3	1:E:775:SER:O	2.00	0.45
1:E:291:ILE:HG21	1:E:306:ILE:HD11	1.99	0.45
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.99	0.45
1:E:463:THR:OG1	1:E:464:GLY:N	2.50	0.45
1:E:563:PHE:HE1	1:E:866:GLU:OE2	2.00	0.45
1:A:4:PHE:O	1:A:8:ARG:HD2	2.17	0.44
1:A:680:PHE:CE2	1:A:829:GLY:HA3	2.53	0.44
1:A:841:MET:HE3	1:A:859:TRP:CE2	2.52	0.44
1:B:154:ILE:O	1:B:157:TYR:N	2.49	0.44
1:C:953:MET:HE1	1:C:1026:PHE:HE2	1.83	0.44
1:D:23:GLY:HA3	1:D:377:LEU:O	2.17	0.44
1:D:224:PRO:HB2	1:E:781:MET:HE1	1.99	0.44
1:D:456:MET:SD	1:D:932:LEU:HD11	2.56	0.44
1:D:886:LEU:HD13	1:F:18:ILE:HG13	1.99	0.44
1:D:948:PHE:O	1:D:952:LEU:HG	2.17	0.44
1:F:219:LEU:HD13	1:F:230:LEU:HD21	1.98	0.44
1:F:888:LEU:HD13	1:F:901:VAL:HG11	1.98	0.44
1:A:909:VAL:HG22	1:A:935:ILE:HD11	1.98	0.44
1:A:983:ILE:HG23	1:A:1008:MET:HE2	1.99	0.44
1:B:758:TYR:HE1	1:B:770:LYS:CG	2.30	0.44
1:C:167:SER:HB3	1:C:175:VAL:HG21	1.98	0.44
1:C:240:LEU:HD12	1:C:246:PHE:CD1	2.52	0.44
1:D:270:LEU:HD12	1:D:270:LEU:HA	1.57	0.44
1:D:658:ILE:O	1:D:659:LYS:HD3	2.17	0.44
1:D:922:THR:O	1:D:924:ASP:N	2.50	0.44
1:E:30:LEU:HG	1:E:31:PRO:HD2	1.99	0.44
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.98	0.44
1:E:438:ILE:HG22	1:E:948:PHE:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:619:GLY:HA2	1:E:815:ARG:NH1	2.31	0.44
1:E:937:LEU:HD23	1:E:937:LEU:HA	1.69	0.44
1:F:69:MET:SD	1:F:72:ILE:HD11	2.57	0.44
1:F:177:LEU:HD23	1:F:289:LEU:HD23	1.99	0.44
1:F:272:GLY:N	1:F:275:TYR:OH	2.35	0.44
1:F:508:GLY:O	1:F:509:LYS:HB2	2.16	0.44
1:F:683:GLU:HG2	1:F:819:TYR:CG	2.53	0.44
1:A:58:GLN:OE1	1:A:816:LEU:HD13	2.16	0.44
1:A:76:MET:HE3	1:A:95:GLU:CD	2.42	0.44
1:A:377:LEU:HA	1:A:377:LEU:HD23	1.77	0.44
1:A:671:ILE:HD12	1:A:674:LEU:O	2.18	0.44
1:A:781:MET:CE	1:C:228:GLN:HB2	2.47	0.44
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.32	0.44
1:D:335:ILE:O	1:D:339:GLU:HG2	2.18	0.44
1:E:40:PRO:HD3	1:E:462:SER:OG	2.16	0.44
1:E:412:VAL:HG22	1:E:438:ILE:HD11	1.99	0.44
1:E:1040:ILE:O	1:E:1041:GLU:HB3	2.17	0.44
1:F:81:ASN:HD21	1:F:815:ARG:NH1	2.15	0.44
1:F:302:THR:O	1:F:305:ALA:HB3	2.17	0.44
1:F:1034:SER:HB3	1:F:1035:ARG:HB3	1.99	0.44
1:A:775:SER:HG	1:A:780:ARG:HG2	1.81	0.44
1:B:699:ARG:NH2	1:B:722:GLU:OE1	2.50	0.44
1:B:728:LYS:HB2	1:B:810:GLU:CD	2.42	0.44
1:B:808:ARG:NH1	1:B:810:GLU:OE2	2.51	0.44
1:C:24:GLY:O	1:C:27:ILE:HG13	2.17	0.44
1:C:546:LEU:HD23	1:C:546:LEU:HA	1.83	0.44
1:D:572:PHE:CE1	1:D:648:THR:HG22	2.52	0.44
1:D:885:PHE:CE1	1:D:898:PRO:HB2	2.53	0.44
1:D:900:SER:HA	1:D:1025:PHE:HB3	2.00	0.44
1:D:904:VAL:CG1	1:D:938:SER:HB3	2.48	0.44
1:E:146:ASP:OD1	1:E:148:THR:OG1	2.35	0.44
1:F:378:GLY:O	1:F:382:VAL:HG23	2.17	0.44
1:A:185:ARG:HB3	1:A:187:TRP:NE1	2.32	0.44
1:A:224:PRO:CB	1:B:781:MET:HE1	2.47	0.44
1:A:391:ASN:O	1:A:395:MET:HG2	2.18	0.44
1:A:507:GLU:C	1:A:509:LYS:N	2.76	0.44
1:B:758:TYR:HE1	1:B:770:LYS:HG2	1.82	0.44
1:B:800:PRO:HG2	1:B:803:ALA:HB2	2.00	0.44
1:C:182:TYR:O	1:C:769:LYS:HD3	2.18	0.44
1:C:380:PHE:HA	1:C:383:LEU:HD12	1.99	0.44
1:C:1016:VAL:HG12	1:C:1016:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:ILE:CG2	1:D:287:SER:HB3	2.45	0.44
1:D:217:GLY:HA3	1:E:754:TRP:C	2.42	0.44
1:D:866:GLU:HB2	3:D:1103:LMT:O2B	2.17	0.44
1:E:375:VAL:HG13	1:E:480:LEU:HB3	1.99	0.44
1:A:239:ARG:HB2	1:A:763:ILE:HD12	1.99	0.44
1:A:363:ARG:O	1:A:496:MET:HE2	2.18	0.44
1:A:559:LEU:HD23	1:A:560:PRO:CD	2.45	0.44
1:B:190:PRO:HG3	1:B:779:TYR:HB3	1.99	0.44
1:C:293:LEU:HD11	1:C:297:ALA:O	2.17	0.44
1:C:363:ARG:H	1:C:363:ARG:HG2	1.66	0.44
1:C:888:LEU:HD23	1:C:888:LEU:HA	1.78	0.44
1:D:893:GLU:OE2	1:F:8:ARG:HB3	2.16	0.44
1:E:743:ILE:H	1:E:743:ILE:HD12	1.82	0.44
1:E:910:ILE:O	1:E:914:LEU:HB2	2.16	0.44
1:F:100:ALA:O	1:F:103:ALA:HB3	2.17	0.44
1:F:340:VAL:CG1	1:F:395:MET:HB3	2.47	0.44
1:A:187:TRP:HA	1:A:774:MET:O	2.17	0.44
1:A:309:GLU:HG3	1:A:313:MET:HE3	1.99	0.44
1:A:360:GLN:HE21	1:A:360:GLN:HB3	1.58	0.44
1:A:549:VAL:O	1:A:552:MET:HB3	2.18	0.44
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.99	0.44
1:C:568:ASP:OD1	1:C:644:VAL:HG23	2.18	0.44
1:C:597:TYR:HD2	1:C:598:TYR:CD1	2.35	0.44
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.99	0.44
1:D:357:LEU:HD23	1:D:357:LEU:O	2.16	0.44
1:D:795:ASP:OD2	1:D:796:GLY:N	2.50	0.44
1:D:893:GLU:CD	1:F:8:ARG:HB3	2.42	0.44
1:D:938:SER:OG	1:D:1014:ALA:HB1	2.17	0.44
1:E:894:SER:HB3	1:E:897:ILE:HB	1.99	0.44
1:F:447:MET:HE1	1:F:887:CYS:C	2.43	0.44
1:A:7:ASP:C	1:A:8:ARG:HG3	2.43	0.44
1:A:404:LEU:HD12	1:A:937:LEU:HD21	2.00	0.44
1:A:729:ILE:HG22	1:A:731:ILE:HD11	2.00	0.44
1:A:752:ALA:O	1:A:774:MET:HA	2.17	0.44
1:B:383:LEU:O	1:B:386:PHE:N	2.51	0.44
1:B:602:GLU:HB3	1:B:606:VAL:HG23	1.99	0.44
1:C:185:ARG:HD3	1:C:185:ARG:HA	1.71	0.44
1:C:680:PHE:CD2	1:C:859:TRP:HZ3	2.35	0.44
1:C:785:ASP:HA	1:C:788:ASP:OD2	2.18	0.44
1:C:905:VAL:HB	1:C:906:PRO:HD3	2.00	0.44
1:D:54:ALA:HB2	1:D:84:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ILE:HD12	1:F:101:ASP:HB3	2.00	0.44
1:D:218:GLN:HG2	1:D:233:SER:HA	1.98	0.44
1:D:893:GLU:OE2	1:F:11:PHE:HB2	2.18	0.44
1:D:984:LEU:HD23	1:D:984:LEU:HA	1.77	0.44
1:D:1016:VAL:O	1:D:1016:VAL:HG12	2.18	0.44
1:E:459:PHE:O	1:E:464:GLY:HA3	2.18	0.44
1:E:520:PHE:O	1:E:524:THR:HG22	2.17	0.44
1:E:739:LEU:HD13	1:E:799:VAL:HG11	1.99	0.44
1:F:669:PRO:HG2	1:F:675:GLY:HA3	2.00	0.44
1:F:898:PRO:O	1:F:901:VAL:HG12	2.18	0.44
1:F:953:MET:HE3	1:F:953:MET:HB2	1.68	0.44
1:A:30:LEU:HD12	1:A:31:PRO:HD2	2.00	0.44
1:A:80:SER:HA	1:A:89:GLN:O	2.18	0.44
1:A:672:VAL:HB	1:A:673:GLU:OE2	2.18	0.44
1:A:986:VAL:HG21	1:A:1007:VAL:CG1	2.45	0.44
1:B:249:ILE:HG12	1:B:262:LEU:HB2	1.99	0.44
1:B:484:VAL:O	1:B:489:THR:HG23	2.18	0.44
1:B:555:LEU:HA	1:B:555:LEU:HD23	1.75	0.44
1:C:542:LEU:HA	1:C:542:LEU:HD12	1.69	0.44
1:C:652:THR:OG1	1:C:665:ALA:N	2.46	0.44
1:D:165:ALA:HB3	1:D:313:MET:HE1	2.00	0.44
1:D:915:ALA:HB2	1:D:1009:GLY:HA3	1.99	0.44
1:E:314:GLU:N	1:E:315:PRO:HD2	2.32	0.44
1:E:568:ASP:O	1:E:634:TRP:CZ3	2.69	0.44
1:E:588:GLN:HE21	1:E:592:ASN:ND2	2.14	0.44
1:E:726:GLN:CD	1:E:812:GLY:HA3	2.43	0.44
1:E:775:SER:OG	1:E:780:ARG:HG2	2.17	0.44
1:E:1019:ILE:HG13	1:E:1020:PHE:CD1	2.53	0.44
1:F:33:ALA:O	1:F:391:ASN:HA	2.17	0.44
1:A:158:VAL:HA	1:A:162:MET:CE	2.47	0.43
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.74	0.43
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.52	0.43
1:B:376:LEU:HA	1:B:376:LEU:HD23	1.52	0.43
1:B:525:HIS:O	1:B:526:HIS:C	2.60	0.43
1:B:894:SER:HB3	1:B:897:ILE:H	1.83	0.43
1:C:159:ALA:HB2	1:C:177:LEU:HD11	1.99	0.43
1:C:706:ALA:HB1	1:C:713:LEU:HD22	1.99	0.43
1:C:723:ASP:OD1	1:C:813:SER:HB3	2.18	0.43
1:D:393:LEU:HD12	1:D:469:GLN:HG3	2.00	0.43
1:D:644:VAL:CG1	1:D:667:ASN:HB2	2.48	0.43
1:E:35:TYR:HE2	1:E:393:LEU:HD21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:575:MET:HE2	1:E:575:MET:HB2	1.78	0.43
1:E:789:TRP:HB2	1:E:801:PHE:CE2	2.53	0.43
1:E:1032:ARG:HA	1:E:1033:PHE:HB3	2.00	0.43
1:F:110:LYS:O	1:F:113:LEU:HB2	2.18	0.43
1:F:645:GLU:O	1:F:649:MET:HB2	2.17	0.43
1:A:602:GLU:CD	1:A:650:ARG:HH11	2.26	0.43
1:C:396:PHE:CD1	1:C:1003:VAL:HG21	2.53	0.43
1:C:483:LEU:HA	1:C:483:LEU:HD23	1.71	0.43
1:C:535:LEU:HD21	1:C:1027:VAL:HG21	2.00	0.43
1:D:182:TYR:HD1	1:D:182:TYR:HA	1.69	0.43
1:D:193:LEU:HD13	1:D:200:PRO:HD3	2.01	0.43
1:D:462:SER:O	1:D:466:ILE:HG12	2.18	0.43
1:D:514:GLY:HA2	1:D:517:ASN:ND2	2.33	0.43
1:D:563:PHE:O	1:D:564:LEU:HD12	2.18	0.43
1:E:55:LYS:HG2	1:E:59:ASP:OD2	2.18	0.43
1:E:588:GLN:HG3	1:E:592:ASN:HD21	1.82	0.43
1:E:644:VAL:HG11	1:E:667:ASN:ND2	2.33	0.43
1:E:717:ARG:HD2	1:E:717:ARG:O	2.18	0.43
1:E:877:TYR:HD2	1:E:877:TYR:HA	1.60	0.43
1:F:138:MET:HE3	1:F:138:MET:HB2	1.71	0.43
1:F:359:LEU:O	1:F:361:ASN:N	2.51	0.43
1:F:557:VAL:C	1:F:559:LEU:H	2.26	0.43
1:F:578:LEU:CG	1:F:587:THR:HG22	2.46	0.43
1:F:905:VAL:HB	1:F:906:PRO:HD3	1.99	0.43
1:F:1021:PHE:HB3	1:F:1025:PHE:CZ	2.53	0.43
1:A:27:ILE:HG12	1:A:380:PHE:CD2	2.53	0.43
1:A:216:ALA:HB1	1:A:234:ILE:HG22	1.98	0.43
1:A:699:ARG:HD2	1:A:718:PRO:HB3	2.00	0.43
1:A:857:TYR:HE2	1:C:312:LYS:NZ	2.17	0.43
1:B:174:ASP:HB3	1:B:292:LYS:HB2	1.99	0.43
1:B:520:PHE:O	1:B:523:SER:OG	2.28	0.43
1:B:682:PHE:CE2	1:B:857:TYR:HB2	2.53	0.43
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.99	0.43
1:C:201:VAL:O	1:C:204:ILE:HB	2.18	0.43
1:C:309:GLU:HG3	1:C:313:MET:HE3	2.00	0.43
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.53	0.43
1:D:555:LEU:HD11	1:D:914:LEU:HD12	2.00	0.43
1:D:752:ALA:O	1:D:774:MET:HA	2.19	0.43
1:D:937:LEU:HD12	1:D:1011:MET:SD	2.58	0.43
1:E:184:MET:HB2	1:E:762:PHE:CE2	2.53	0.43
1:E:545:TYR:CE2	1:E:1025:PHE:HZ	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:574:THR:CG2	1:E:627:ALA:HB3	2.47	0.43
1:F:445:ILE:HG12	1:F:940:LYS:HG3	2.00	0.43
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.52	0.43
1:A:344:LEU:HD11	1:A:398:MET:HB2	2.00	0.43
1:B:203:VAL:O	1:B:207:ILE:HG13	2.19	0.43
1:B:1042:HIS:CG	1:B:1043:SER:N	2.86	0.43
1:C:159:ALA:HB2	1:C:177:LEU:CD1	2.49	0.43
1:C:359:LEU:HB2	1:C:365:THR:HG23	2.00	0.43
1:C:602:GLU:OE2	1:C:650:ARG:NH1	2.51	0.43
1:C:931:LEU:O	1:C:934:THR:HB	2.18	0.43
1:D:332:PHE:HB2	1:D:634:TRP:HH2	1.82	0.43
1:D:712:MET:HB3	1:D:713:LEU:HD22	2.00	0.43
1:D:945:ILE:CG1	1:D:971:ARG:HH22	2.31	0.43
1:E:355:MET:CE	1:E:410:ILE:HG12	2.49	0.43
1:E:572:PHE:CE1	1:E:648:THR:HG22	2.53	0.43
1:F:200:PRO:HB2	1:F:749:THR:HG22	1.99	0.43
1:F:277:ILE:CD1	1:F:620:ARG:HH11	2.32	0.43
1:F:702:LEU:HB2	1:F:851:LEU:HD11	2.00	0.43
1:F:760:ASN:O	1:F:771:VAL:HB	2.19	0.43
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.99	0.43
1:B:83:ASP:HB2	1:B:87:THR:O	2.17	0.43
1:B:717:ARG:CD	1:B:828:LEU:HB2	2.46	0.43
1:B:721:LEU:HB3	1:B:814:PRO:HG2	1.99	0.43
1:C:227:GLY:O	1:C:229:GLN:HG3	2.19	0.43
1:C:446:ALA:HA	1:C:478:MET:HE3	2.00	0.43
1:D:182:TYR:O	1:D:769:LYS:HB3	2.17	0.43
1:D:354:VAL:HG12	1:D:355:MET:HE3	2.00	0.43
1:D:422:GLU:HB3	1:D:423:GLU:HG3	2.00	0.43
1:D:768:VAL:HG13	1:E:67:GLN:HE22	1.84	0.43
1:D:912:ALA:O	1:D:915:ALA:N	2.51	0.43
1:D:974:PRO:HA	1:D:977:MET:HE3	2.00	0.43
1:E:104:GLN:HE21	1:F:109:ASN:ND2	2.15	0.43
1:F:602:GLU:HB3	1:F:606:VAL:HG23	2.00	0.43
1:F:669:PRO:CG	1:F:675:GLY:HA3	2.49	0.43
1:A:483:LEU:HD13	1:A:487:ILE:HD12	2.01	0.43
1:A:946:VAL:HG13	1:A:1026:PHE:CD1	2.53	0.43
1:B:545:TYR:HE2	1:B:907:LEU:CD1	2.30	0.43
1:D:240:LEU:HD12	1:D:246:PHE:CE1	2.54	0.43
1:D:615:PHE:CZ	2:D:1101:ERY:H343	2.53	0.43
1:D:908:GLY:HA2	1:D:1014:ALA:HB2	1.98	0.43
1:E:512:PHE:HB3	1:E:513:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:TYR:HD1	1:F:57:VAL:HG12	1.81	0.43
1:F:782:LEU:O	1:F:785:ASP:HB2	2.18	0.43
1:F:960:LEU:O	1:F:964:THR:HG23	2.19	0.43
1:A:445:ILE:HD12	1:A:446:ALA:N	2.33	0.43
1:B:23:GLY:HA3	1:B:377:LEU:O	2.19	0.43
1:B:187:TRP:HE3	1:B:775:SER:O	2.02	0.43
1:B:470:PHE:HZ	1:B:926:TYR:HE2	1.67	0.43
1:B:1037:ASN:HA	1:B:1038:GLU:CG	2.48	0.43
1:C:181:GLN:OE1	1:C:767:ARG:NH2	2.49	0.43
1:D:800:PRO:O	1:D:803:ALA:HB3	2.19	0.43
1:E:959:GLY:O	1:E:963:ALA:N	2.41	0.43
1:F:284:GLN:CG	1:F:285:PRO:HD2	2.49	0.43
1:F:398:MET:HE3	1:F:398:MET:HB3	1.66	0.43
1:A:133:SER:OG	1:A:135:SER:O	2.36	0.43
1:A:712:MET:HG2	1:A:843:LEU:HG	2.01	0.43
1:A:961:ILE:H	1:A:961:ILE:HG13	1.38	0.43
1:B:5:PHE:CE1	1:B:487:ILE:HG12	2.54	0.43
1:B:175:VAL:HG23	1:C:70:ASN:HD22	1.83	0.43
1:B:196:PHE:N	1:B:196:PHE:CD1	2.87	0.43
1:B:356:TYR:HE1	1:B:362:PHE:HA	1.83	0.43
1:B:511:GLY:HA2	1:B:515:TRP:HE1	1.84	0.43
1:B:721:LEU:HD12	1:B:721:LEU:HA	1.91	0.43
1:B:870:GLY:C	1:B:872:GLN:H	2.27	0.43
1:B:1019:ILE:HG13	1:B:1020:PHE:CD1	2.53	0.43
1:C:146:ASP:O	1:C:148:THR:N	2.51	0.43
1:C:412:VAL:CG2	1:C:442:LEU:HD11	2.49	0.43
1:C:520:PHE:CE2	1:C:973:ARG:HG3	2.53	0.43
1:C:525:HIS:O	1:C:526:HIS:C	2.62	0.43
1:C:787:GLY:O	1:C:789:TRP:N	2.52	0.43
1:C:938:SER:HB3	1:C:1014:ALA:HB1	2.01	0.43
1:C:960:LEU:O	1:C:964:THR:HG23	2.19	0.43
1:D:63:GLN:O	1:D:67:GLN:HG3	2.17	0.43
1:E:213:GLN:HG2	1:E:239:ARG:HG3	2.00	0.43
1:E:508:GLY:HA2	1:E:518:ARG:NE	2.34	0.43
1:E:909:VAL:C	1:E:911:GLY:N	2.76	0.43
1:E:1042:HIS:HB3	1:E:1043:SER:CB	2.49	0.43
1:F:608:SER:OG	1:F:630:SER:HB3	2.18	0.43
1:A:66:GLU:OE1	1:A:821:GLY:HA2	2.18	0.43
1:A:132:SER:OG	1:A:133:SER:N	2.51	0.43
1:A:189:ASN:OD1	1:A:190:PRO:HD2	2.19	0.43
1:A:428:LYS:HG3	1:A:429:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:898:PRO:O	1:B:901:VAL:HG12	2.19	0.43
1:C:332:PHE:HD1	1:C:634:TRP:CH2	2.37	0.43
1:C:892:TYR:C	1:C:894:SER:H	2.23	0.43
1:C:991:ILE:C	1:C:991:ILE:HD13	2.43	0.43
1:D:50:PRO:C	1:D:52:ALA:H	2.27	0.43
1:D:101:ASP:OD1	1:D:101:ASP:N	2.48	0.43
1:D:137:LEU:HD23	1:D:291:ILE:HG22	2.01	0.43
1:D:897:ILE:HA	1:D:1029:VAL:HG11	2.01	0.43
1:E:244:GLU:O	1:E:247:GLY:N	2.51	0.43
1:E:894:SER:HB2	1:E:897:ILE:HD12	2.00	0.43
1:E:905:VAL:HB	1:E:906:PRO:HD3	2.01	0.43
1:F:34:GLN:HB2	1:F:333:VAL:HG13	1.99	0.43
1:F:158:VAL:HG22	1:F:162:MET:HE3	2.00	0.43
1:F:355:MET:HG2	1:F:410:ILE:HD11	1.99	0.43
1:F:578:LEU:HB3	1:F:579:PRO:HD2	2.01	0.43
1:F:889:ALA:HB2	1:F:898:PRO:HG2	2.00	0.43
1:A:81:ASN:OD1	2:A:1101:ERY:H272	2.19	0.43
1:A:177:LEU:HA	1:A:177:LEU:HD23	1.69	0.43
1:A:196:PHE:CD1	1:A:260:VAL:HG13	2.53	0.43
1:A:360:GLN:CD	1:A:513:PHE:HB3	2.44	0.43
1:A:420:MET:HE3	1:A:500:ILE:HD12	2.01	0.43
1:A:890:ALA:HB2	1:C:14:VAL:HG11	2.01	0.43
1:A:910:ILE:O	1:A:910:ILE:HG13	2.19	0.43
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.84	0.43
1:B:356:TYR:HD1	1:B:365:THR:HG21	1.84	0.43
1:B:376:LEU:O	1:B:377:LEU:C	2.62	0.43
1:B:393:LEU:HD22	1:B:470:PHE:HE1	1.84	0.43
1:C:166:ILE:O	1:C:169:THR:HB	2.19	0.43
1:C:445:ILE:HG12	1:C:940:LYS:CG	2.49	0.43
1:C:510:LYS:HG2	1:C:511:GLY:N	2.33	0.43
1:C:953:MET:HB2	1:C:953:MET:HE3	1.57	0.43
1:D:30:LEU:HD12	1:D:30:LEU:HA	1.80	0.43
1:D:38:ILE:CG2	1:D:462:SER:HB2	2.38	0.43
1:D:428:LYS:H	1:D:428:LYS:HG2	1.21	0.43
1:D:531:VAL:HG21	1:D:968:VAL:HG11	2.00	0.43
1:D:572:PHE:CD1	1:D:648:THR:HG22	2.53	0.43
1:D:897:ILE:HG12	1:D:1030:ARG:HD2	2.00	0.43
1:E:40:PRO:HA	1:E:41:PRO:HD3	1.75	0.43
1:E:459:PHE:CD2	1:E:876:LEU:HD12	2.53	0.43
1:E:539:GLY:O	1:E:542:LEU:HB2	2.19	0.43
1:F:187:TRP:NE1	1:F:269:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:382:VAL:HG11	1:F:476:SER:HB2	2.00	0.43
1:F:571:VAL:HG12	1:F:668:LEU:HD11	2.01	0.43
1:A:11:PHE:HE1	1:A:15:ILE:HD11	1.84	0.42
1:A:352:PHE:CD2	1:A:353:LEU:HD23	2.53	0.42
1:A:708:LYS:C	1:A:710:PRO:HD3	2.44	0.42
1:A:726:GLN:O	1:A:810:GLU:HG2	2.19	0.42
1:A:1018:ALA:O	1:A:1022:VAL:HG23	2.19	0.42
1:B:211:ASN:O	1:B:760:ASN:ND2	2.52	0.42
1:B:352:PHE:CD2	1:B:353:LEU:HD23	2.49	0.42
1:C:42:ALA:HB2	1:C:93:THR:HG23	2.01	0.42
1:C:686:ASP:HB3	1:C:823:PRO:HB2	2.01	0.42
1:D:484:VAL:HG13	1:D:488:LEU:HB3	2.01	0.42
1:D:702:LEU:HD22	1:D:827:ILE:HD13	2.01	0.42
1:D:971:ARG:C	1:D:974:PRO:HD2	2.44	0.42
1:E:239:ARG:NH1	1:E:761:ASP:HB2	2.34	0.42
1:F:382:VAL:HG11	1:F:476:SER:CB	2.48	0.42
1:F:504:ASP:C	1:F:506:GLY:N	2.77	0.42
1:F:984:LEU:HA	1:F:984:LEU:HD23	1.53	0.42
1:F:1015:THR:C	1:F:1017:LEU:H	2.27	0.42
1:A:155:SER:HB3	1:A:180:SER:N	2.28	0.42
1:A:362:PHE:CD2	1:A:362:PHE:N	2.85	0.42
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.57	0.42
1:B:401:ALA:O	1:B:405:LEU:HG	2.19	0.42
1:B:690:LEU:HD11	1:B:854:GLY:HA3	2.00	0.42
1:B:813:SER:HA	1:B:814:PRO:HD3	1.93	0.42
1:B:817:GLU:OE1	1:B:826:GLU:N	2.52	0.42
1:B:987:MET:HB3	1:B:987:MET:HE2	1.97	0.42
1:C:311:ALA:O	1:C:315:PRO:HD3	2.19	0.42
1:C:913:LEU:HD23	1:C:927:PHE:HZ	1.84	0.42
1:D:156:ASP:OD1	1:D:765:ARG:NH2	2.52	0.42
1:E:174:ASP:CB	1:E:292:LYS:HB2	2.46	0.42
1:F:144:ASN:HA	1:F:320:GLY:O	2.19	0.42
1:F:487:ILE:C	1:F:490:PRO:HD2	2.43	0.42
1:F:659:LYS:HD3	1:F:659:LYS:HA	1.82	0.42
1:F:776:GLU:HB2	1:F:779:TYR:CD1	2.54	0.42
1:A:210:GLN:HE22	1:A:250:LEU:H	1.66	0.42
1:B:7:ASP:C	1:B:8:ARG:HG3	2.44	0.42
1:B:144:ASN:HA	1:B:320:GLY:O	2.20	0.42
1:C:425:LEU:HD22	1:C:429:GLU:HG2	2.00	0.42
1:C:536:ARG:HD2	3:C:1101:LMT:O4'	2.19	0.42
1:D:441:ALA:HB2	1:D:947:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:467:TYR:CE2	1:D:925:VAL:HG22	2.54	0.42
1:E:766:GLY:O	1:F:59:ASP:HB2	2.20	0.42
1:E:801:PHE:CD1	1:E:804:PHE:HE2	2.38	0.42
1:E:1007:VAL:HG12	1:E:1008:MET:N	2.35	0.42
1:E:1037:ASN:HB2	1:E:1038:GLU:CA	2.50	0.42
1:F:181:GLN:HG2	1:F:182:TYR:N	2.34	0.42
1:F:452:VAL:C	1:F:455:PRO:HD2	2.44	0.42
1:F:546:LEU:HD23	1:F:546:LEU:HA	1.69	0.42
1:A:1026:PHE:CE2	1:A:1030:ARG:HG3	2.55	0.42
1:B:514:GLY:C	1:B:516:PHE:N	2.75	0.42
1:B:984:LEU:HD23	1:B:984:LEU:HA	1.63	0.42
1:C:453:PHE:HZ	1:C:933:THR:OG1	2.02	0.42
1:C:680:PHE:HA	1:C:863:SER:OG	2.20	0.42
1:D:997:SER:HA	1:D:1000:GLN:HB2	2.01	0.42
1:F:73:ASP:HB2	1:F:106:GLN:OE1	2.19	0.42
1:F:455:PRO:HG3	1:F:883:VAL:HG21	2.00	0.42
1:F:913:LEU:HD23	1:F:927:PHE:HZ	1.85	0.42
1:F:985:GLY:O	1:F:988:PRO:HD2	2.19	0.42
1:B:885:PHE:C	1:B:885:PHE:CD2	2.97	0.42
1:B:888:LEU:HD11	1:B:943:ILE:HD11	2.02	0.42
1:C:64:VAL:CG1	1:C:117:LEU:HB2	2.50	0.42
1:C:171:GLY:HA3	1:C:302:THR:OG1	2.19	0.42
1:C:246:PHE:O	1:C:262:LEU:HD23	2.19	0.42
1:D:108:GLN:NE2	1:E:109:ASN:O	2.53	0.42
1:D:190:PRO:HB3	1:D:789:TRP:CZ3	2.54	0.42
1:D:239:ARG:HH12	1:D:761:ASP:HB2	1.85	0.42
1:D:292:LYS:NZ	2:D:1101:ERY:O11	2.52	0.42
1:D:361:ASN:HB3	1:D:364:ALA:HB3	2.02	0.42
1:D:420:MET:HE1	1:D:497:LEU:HG	2.00	0.42
1:D:851:LEU:HB3	1:D:852:PRO:HD2	2.00	0.42
1:E:230:LEU:HG	1:E:231:ASN:N	2.33	0.42
1:E:355:MET:SD	1:E:365:THR:HA	2.60	0.42
1:E:519:MET:H	1:E:519:MET:HG2	1.59	0.42
1:E:549:VAL:O	1:E:552:MET:HB3	2.19	0.42
1:E:582:ALA:HA	1:E:586:ARG:NH2	2.33	0.42
1:F:277:ILE:HD11	1:F:620:ARG:HH11	1.84	0.42
1:F:340:VAL:HG11	1:F:395:MET:HB3	2.00	0.42
1:F:680:PHE:HB2	1:F:859:TRP:CZ3	2.54	0.42
1:A:375:VAL:HG22	1:A:484:VAL:HG21	2.02	0.42
1:A:604:ASN:O	1:A:632:LYS:HD2	2.20	0.42
1:A:953:MET:HE3	1:A:953:MET:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ALA:HB2	1:B:127:VAL:HG13	2.01	0.42
1:C:647:ILE:O	1:C:650:ARG:N	2.53	0.42
1:C:1030:ARG:C	1:C:1032:ARG:H	2.28	0.42
1:D:414:GLU:CD	1:D:974:PRO:HG3	2.45	0.42
1:D:452:VAL:C	1:D:455:PRO:HD2	2.45	0.42
1:D:577:GLN:OE1	1:D:624:THR:HG22	2.18	0.42
1:D:636:ASP:N	1:D:636:ASP:OD1	2.51	0.42
1:D:1011:MET:HE3	1:D:1011:MET:HB3	1.86	0.42
1:E:182:TYR:HB2	1:E:769:LYS:HZ2	1.84	0.42
1:F:6:ILE:C	1:F:8:ARG:H	2.26	0.42
1:F:509:LYS:O	1:F:518:ARG:NH1	2.52	0.42
1:F:617:PHE:CD1	1:F:626:ILE:HD11	2.55	0.42
1:F:1019:ILE:HG13	1:F:1020:PHE:CD1	2.54	0.42
1:A:30:LEU:HD23	1:A:390:ILE:HG13	2.01	0.42
1:A:578:LEU:HB2	1:A:623:ASN:O	2.19	0.42
1:A:787:GLY:O	1:A:789:TRP:N	2.52	0.42
1:A:857:TYR:N	1:A:857:TYR:CD2	2.88	0.42
1:B:201:VAL:HG23	1:B:749:THR:HG23	2.02	0.42
1:B:953:MET:HE3	1:B:953:MET:HB2	1.70	0.42
1:B:971:ARG:C	1:B:974:PRO:HD2	2.44	0.42
1:C:411:VAL:O	1:C:415:ASN:HB2	2.19	0.42
1:C:445:ILE:HG12	1:C:940:LYS:HG3	2.02	0.42
1:D:418:ARG:HH22	1:D:948:PHE:HE2	1.65	0.42
1:E:318:PRO:HG2	1:E:321:LEU:HB2	2.00	0.42
1:E:514:GLY:C	1:E:516:PHE:N	2.77	0.42
1:E:572:PHE:HA	1:E:668:LEU:CD2	2.47	0.42
1:E:678:THR:O	1:E:678:THR:OG1	2.27	0.42
1:E:925:VAL:O	1:E:928:GLN:N	2.53	0.42
1:F:15:ILE:O	1:F:19:ILE:HG13	2.20	0.42
1:F:443:VAL:HG12	1:F:891:LEU:HD21	2.01	0.42
1:F:540:ARG:O	1:F:543:VAL:HB	2.20	0.42
1:F:575:MET:HG2	1:F:666:PHE:HE1	1.85	0.42
1:A:102:ILE:HD13	1:A:102:ILE:HA	1.91	0.42
1:C:75:LEU:CD1	1:C:92:LEU:HB3	2.49	0.42
1:C:706:ALA:HB2	1:C:847:LEU:HD23	2.00	0.42
1:C:800:PRO:HB2	1:C:802:SER:OG	2.19	0.42
1:C:835:LYS:HG2	1:C:836:SER:N	2.35	0.42
1:D:546:LEU:HD23	1:D:546:LEU:HA	1.82	0.42
1:E:154:ILE:HG22	1:E:287:SER:HB3	2.02	0.42
1:E:789:TRP:HB2	1:E:801:PHE:HE2	1.83	0.42
1:E:818:ARG:NH1	1:E:823:PRO:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1026:PHE:O	1:E:1030:ARG:HB2	2.20	0.42
1:F:584:GLN:N	1:F:622:GLN:HB3	2.35	0.42
1:F:742:SER:O	1:F:745:ASP:HB2	2.20	0.42
1:F:987:MET:HE2	1:F:987:MET:HB3	1.93	0.42
1:A:94:PHE:CE1	1:A:103:ALA:HB1	2.55	0.42
1:A:634:TRP:CD1	1:A:634:TRP:N	2.85	0.42
1:B:57:VAL:HB	1:B:88:VAL:HG23	2.02	0.42
1:B:143:ILE:HG22	1:B:286:ALA:HB2	2.01	0.42
1:B:572:PHE:HD1	1:B:666:PHE:O	2.02	0.42
1:B:575:MET:HE2	1:B:575:MET:HB2	1.67	0.42
1:B:712:MET:CE	1:B:839:GLU:HB3	2.50	0.42
1:B:841:MET:HG2	1:B:859:TRP:CH2	2.55	0.42
1:B:913:LEU:HD23	1:B:927:PHE:HZ	1.85	0.42
1:C:270:LEU:HA	1:C:270:LEU:HD12	1.56	0.42
1:C:337:ILE:HG13	1:C:392:THR:HG23	2.02	0.42
1:C:456:MET:HB3	1:C:876:LEU:HD21	2.02	0.42
1:C:732:ASP:CG	1:C:735:LYS:HG3	2.44	0.42
1:C:886:LEU:HD13	1:C:886:LEU:HA	1.71	0.42
1:D:184:MET:HE2	1:D:268:ILE:HG23	2.01	0.42
1:D:224:PRO:CB	1:E:781:MET:HE1	2.49	0.42
1:D:343:THR:O	1:D:346:GLU:HB2	2.20	0.42
1:D:544:LEU:O	1:D:548:ILE:HG13	2.19	0.42
1:E:166:ILE:HD12	1:E:313:MET:HE1	2.01	0.42
1:E:589:LYS:O	1:E:592:ASN:HB2	2.20	0.42
1:A:456:MET:HB3	1:A:456:MET:HE2	1.50	0.42
1:E:185:ARG:HD3	1:E:185:ARG:HA	1.90	0.42
1:E:310:LEU:HA	1:E:310:LEU:HD12	1.84	0.42
1:E:685:ILE:HG22	1:E:687:GLN:OE1	2.20	0.42
1:F:931:LEU:O	1:F:935:ILE:HG13	2.19	0.42
1:A:472:ILE:HG22	1:A:473:THR:N	2.34	0.41
1:A:545:TYR:HB2	1:A:1021:PHE:HE2	1.85	0.41
1:A:644:VAL:O	1:A:648:THR:HG23	2.20	0.41
1:A:897:ILE:HG12	1:A:1030:ARG:HD2	2.01	0.41
1:B:787:GLY:C	1:B:789:TRP:H	2.28	0.41
1:C:230:LEU:HG	1:C:231:ASN:N	2.28	0.41
1:C:580:ALA:HB1	1:C:724:THR:CG2	2.48	0.41
1:C:587:THR:OG1	1:C:613:ASN:ND2	2.51	0.41
1:C:671:ILE:CG2	1:C:674:LEU:HB2	2.49	0.41
1:C:982:PHE:HB3	1:C:1011:MET:HE3	2.02	0.41
1:D:542:LEU:HD12	1:D:542:LEU:HA	1.82	0.41
1:D:583:THR:CG2	1:F:229:GLN:HA	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:675:GLY:H	1:D:862:MET:HB3	1.84	0.41
1:D:961:ILE:H	1:D:961:ILE:HD12	1.85	0.41
1:E:249:ILE:HD11	1:E:262:LEU:HD22	2.02	0.41
1:E:520:PHE:O	1:E:523:SER:OG	2.38	0.41
1:E:752:ALA:O	1:E:774:MET:HA	2.19	0.41
1:E:776:GLU:CG	1:E:777:ALA:H	2.32	0.41
1:E:844:MET:HE2	1:E:847:LEU:HB2	2.02	0.41
1:E:1019:ILE:C	1:E:1020:PHE:HD1	2.28	0.41
1:A:58:GLN:HG3	1:A:818:ARG:HD2	2.03	0.41
1:A:900:SER:HB3	1:A:1029:VAL:HG21	2.01	0.41
1:A:985:GLY:O	1:A:988:PRO:HD2	2.20	0.41
1:B:969:ARG:NH1	1:B:970:MET:HB3	2.34	0.41
1:C:39:ALA:HB3	1:C:673:GLU:HG2	2.01	0.41
1:C:356:TYR:CA	1:C:365:THR:HG21	2.41	0.41
1:C:564:LEU:HD23	1:C:670:ALA:HB3	2.01	0.41
1:D:190:PRO:HB3	1:D:789:TRP:CE3	2.54	0.41
1:D:262:LEU:HD12	1:D:265:VAL:CG2	2.50	0.41
1:D:587:THR:OG1	1:D:622:GLN:O	2.24	0.41
1:D:699:ARG:HD2	1:D:718:PRO:HB3	2.02	0.41
1:D:708:LYS:HE3	1:D:708:LYS:HB3	1.84	0.41
1:D:946:VAL:HG13	1:D:1026:PHE:CD1	2.55	0.41
1:E:754:TRP:CH2	1:E:780:ARG:HA	2.56	0.41
1:E:756:GLY:HA3	1:E:774:MET:HE2	2.02	0.41
1:F:894:SER:CB	1:F:897:ILE:HG12	2.48	0.41
1:F:944:LEU:HB3	1:F:971:ARG:HE	1.83	0.41
1:A:228:GLN:NE2	1:A:230:LEU:H	2.17	0.41
1:A:902:MET:C	1:A:904:VAL:N	2.77	0.41
1:B:5:PHE:HE2	1:B:11:PHE:HD2	1.68	0.41
1:B:197:GLN:HA	1:B:798:MET:HE2	2.03	0.41
1:B:425:LEU:HB2	1:B:430:ALA:HB2	2.02	0.41
1:B:459:PHE:CB	1:B:464:GLY:HA2	2.51	0.41
1:C:564:LEU:HG	1:C:565:PRO:HD2	2.01	0.41
1:D:6:ILE:HG13	1:D:7:ASP:N	2.34	0.41
1:D:375:VAL:HG21	1:D:481:SER:HA	2.02	0.41
1:D:401:ALA:O	1:D:405:LEU:HG	2.20	0.41
1:D:448:VAL:HG22	1:D:887:CYS:CB	2.44	0.41
1:D:764:ASP:OD1	1:D:765:ARG:HG3	2.20	0.41
1:D:961:ILE:H	1:D:961:ILE:CD1	2.31	0.41
1:E:94:PHE:CZ	1:E:103:ALA:HB1	2.55	0.41
1:E:119:PRO:HG2	1:E:122:VAL:HB	2.02	0.41
1:E:445:ILE:HG12	1:E:940:LYS:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:459:PHE:CE2	1:E:876:LEU:HD12	2.55	0.41
1:E:536:ARG:NE	3:E:1101:LMT:O3B	2.53	0.41
1:E:950:LYS:NZ	1:E:953:MET:SD	2.94	0.41
1:F:187:TRP:HE3	1:F:775:SER:O	2.03	0.41
1:F:352:PHE:HD1	1:F:369:THR:OG1	2.04	0.41
1:F:369:THR:O	1:F:373:PRO:HD2	2.20	0.41
1:A:78:MET:HG3	1:A:92:LEU:HG	2.01	0.41
1:A:183:ALA:HB2	1:A:273:GLU:HG3	2.01	0.41
1:A:832:ALA:HB3	1:A:835:LYS:CD	2.41	0.41
1:A:1040:ILE:HD11	1:A:1042:HIS:HB2	2.01	0.41
1:B:255:GLN:H	1:B:255:GLN:HG3	1.59	0.41
1:B:573:MET:HE3	1:B:628:PHE:HB2	2.01	0.41
1:C:591:LEU:HD11	1:C:625:GLY:HA3	2.01	0.41
1:D:160:ALA:HA	1:D:767:ARG:NE	2.35	0.41
1:D:452:VAL:HG12	1:D:880:SER:OG	2.20	0.41
1:D:568:ASP:CG	1:D:637:ARG:HH22	2.25	0.41
1:D:841:MET:O	1:D:845:GLU:HG3	2.20	0.41
1:D:1018:ALA:O	1:D:1022:VAL:HG23	2.20	0.41
1:E:273:GLU:OE1	1:E:770:LYS:HD2	2.21	0.41
1:E:534:ILE:HG22	3:E:1101:LMT:C5'	2.49	0.41
1:E:891:LEU:HA	1:E:891:LEU:HD12	1.68	0.41
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.76	0.41
1:B:14:VAL:HG22	1:C:886:LEU:CD1	2.42	0.41
1:B:185:ARG:HD3	1:B:185:ARG:HA	1.84	0.41
1:B:237:GLN:CG	1:C:731:ILE:HD11	2.50	0.41
1:B:359:LEU:HD13	1:B:417:GLU:HG3	2.01	0.41
1:B:684:LEU:HD12	1:B:684:LEU:HA	1.64	0.41
1:C:443:VAL:HG12	1:C:891:LEU:CD2	2.50	0.41
1:C:674:LEU:HD23	1:C:674:LEU:HA	1.91	0.41
1:C:713:LEU:HD21	1:C:844:MET:SD	2.60	0.41
1:D:57:VAL:HG21	1:D:86:GLY:HA2	2.02	0.41
1:E:362:PHE:O	1:E:366:LEU:HG	2.21	0.41
1:E:588:GLN:NE2	1:E:592:ASN:HD21	2.14	0.41
1:E:617:PHE:HD1	1:E:617:PHE:HA	1.75	0.41
1:F:34:GLN:HB2	1:F:333:VAL:CG2	2.35	0.41
1:F:149:MET:HG3	1:F:154:ILE:HG13	2.03	0.41
1:F:165:ALA:HB3	1:F:313:MET:HE1	2.02	0.41
1:F:751:GLY:C	1:F:753:ALA:N	2.78	0.41
1:F:795:ASP:OD2	1:F:797:GLN:HG2	2.21	0.41
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.84	0.41
1:A:416:VAL:HG12	1:A:420:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:LEU:HD23	1:A:847:LEU:HA	1.86	0.41
1:B:5:PHE:CE2	1:B:11:PHE:HD2	2.39	0.41
1:B:937:LEU:HD23	1:B:937:LEU:HA	1.73	0.41
1:C:61:VAL:HG21	1:C:122:VAL:HG21	2.03	0.41
1:C:574:THR:HG23	1:C:627:ALA:HB3	2.03	0.41
1:C:644:VAL:CG1	1:C:667:ASN:HB2	2.50	0.41
1:C:858:ASP:OD2	1:C:859:TRP:N	2.50	0.41
1:D:136:PHE:CD2	1:D:292:LYS:HG3	2.56	0.41
1:D:527:TYR:CE2	1:D:968:VAL:HG13	2.56	0.41
1:D:570:GLY:C	1:D:631:LEU:HD12	2.45	0.41
1:D:682:PHE:CE2	1:D:857:TYR:HB2	2.56	0.41
1:D:801:PHE:CD1	1:D:804:PHE:HE2	2.39	0.41
1:E:32:VAL:HG12	1:E:390:ILE:HB	2.01	0.41
1:E:189:ASN:HB3	1:E:192:GLU:HB2	2.02	0.41
1:E:537:SER:OG	1:E:540:ARG:NE	2.50	0.41
1:E:597:TYR:CD1	1:E:601:LYS:HD2	2.56	0.41
1:E:997:SER:HA	1:E:1000:GLN:HB2	2.03	0.41
1:F:356:TYR:C	1:F:358:PHE:N	2.79	0.41
1:F:897:ILE:HD11	1:F:950:LYS:HE2	2.02	0.41
1:F:1043:SER:HB2	1:F:1044:HIS:ND1	2.36	0.41
1:A:127:VAL:O	1:B:113:LEU:HD13	2.21	0.41
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.89	0.41
1:A:735:LYS:O	1:A:738:ALA:HB3	2.20	0.41
1:B:352:PHE:CZ	1:B:362:PHE:HE1	2.39	0.41
1:B:459:PHE:HB3	1:B:464:GLY:HA2	2.02	0.41
1:B:594:VAL:HG22	1:B:655:PHE:CZ	2.56	0.41
1:B:950:LYS:HE2	1:B:950:LYS:HB2	1.73	0.41
1:D:314:GLU:OE1	1:D:323:ILE:HD12	2.20	0.41
1:D:605:ASN:O	1:D:632:LYS:N	2.45	0.41
1:D:684:LEU:HD12	1:D:684:LEU:HA	1.93	0.41
1:A:10:ILE:HG13	1:B:895:TRP:CE2	2.56	0.41
1:A:706:ALA:HB1	1:A:713:LEU:HD23	2.03	0.41
1:A:944:LEU:HD23	1:A:944:LEU:HA	1.89	0.41
1:B:77:TYR:OH	1:B:861:GLY:HA2	2.20	0.41
1:B:847:LEU:HD23	1:B:847:LEU:HA	1.88	0.41
1:C:594:VAL:HG22	1:C:655:PHE:CE2	2.56	0.41
1:C:751:GLY:O	1:C:753:ALA:N	2.54	0.41
1:D:108:GLN:NE2	1:E:109:ASN:HB2	2.35	0.41
1:D:360:GLN:H	1:D:360:GLN:HG2	1.69	0.41
1:D:388:PHE:CZ	1:D:472:ILE:HD12	2.56	0.41
1:D:727:PHE:CD1	1:D:809:TRP:CE2	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:544:LEU:O	1:E:547:ILE:HB	2.21	0.41
1:F:514:GLY:C	1:F:516:PHE:N	2.79	0.41
1:F:578:LEU:HA	1:F:661:ALA:HB1	2.03	0.41
1:A:163:LYS:HD2	1:A:177:LEU:HG	2.03	0.41
1:A:245:GLU:O	1:A:249:ILE:HG13	2.20	0.41
1:A:310:LEU:O	1:A:314:GLU:HG3	2.21	0.41
1:A:530:SER:CB	3:A:1102:LMT:O2'	2.66	0.41
1:A:1041:GLU:H	1:A:1042:HIS:HA	1.86	0.41
1:B:164:ASP:OD2	1:C:67:GLN:HG2	2.21	0.41
1:B:291:ILE:HG21	1:B:306:ILE:HD11	2.02	0.41
1:B:574:THR:HG21	1:B:598:TYR:HE2	1.85	0.41
1:B:876:LEU:HD23	1:B:879:ILE:HD12	2.03	0.41
1:C:971:ARG:HH21	1:C:975:ILE:HD11	1.86	0.41
1:D:424:GLY:HA3	1:D:502:LYS:HB3	2.03	0.41
1:D:451:ALA:HB1	1:D:883:VAL:HG12	2.03	0.41
1:D:545:TYR:HB2	1:D:1021:PHE:CE2	2.56	0.41
1:D:584:GLN:HB2	1:D:622:GLN:HG2	2.03	0.41
1:D:597:TYR:CD2	1:D:598:TYR:CD1	3.09	0.41
1:D:641:GLU:HG2	1:D:642:ASN:N	2.36	0.41
1:D:682:PHE:O	1:D:826:GLU:HA	2.21	0.41
1:E:36:PRO:HG3	1:E:469:GLN:CD	2.46	0.41
1:E:354:VAL:O	1:E:358:PHE:HB2	2.20	0.41
1:E:675:GLY:HA2	1:E:862:MET:SD	2.61	0.41
1:E:699:ARG:HE	1:E:718:PRO:HG3	1.85	0.41
1:E:750:LEU:HD12	1:E:754:TRP:CD1	2.56	0.41
1:E:839:GLU:O	1:E:842:GLU:HB3	2.21	0.41
1:E:841:MET:O	1:E:845:GLU:HG3	2.21	0.41
1:E:887:CYS:O	1:E:890:ALA:HB3	2.21	0.41
1:E:922:THR:O	1:E:924:ASP:N	2.53	0.41
1:E:1033:PHE:C	1:E:1033:PHE:CD2	2.99	0.41
1:F:72:ILE:HD13	1:F:72:ILE:HG21	1.87	0.41
1:F:172:VAL:HG13	1:F:291:ILE:HG23	2.02	0.41
1:F:311:ALA:HA	1:F:314:GLU:CD	2.46	0.41
1:F:888:LEU:CD1	1:F:901:VAL:HG11	2.50	0.41
1:A:246:PHE:HA	1:A:249:ILE:HG13	2.02	0.41
1:A:682:PHE:CE2	1:A:857:TYR:HB2	2.56	0.41
1:B:993:THR:O	1:B:997:SER:HB3	2.21	0.41
1:B:1011:MET:HE3	1:B:1011:MET:HB3	1.87	0.41
1:C:671:ILE:HG21	1:C:674:LEU:HB2	2.01	0.41
1:D:201:VAL:HG23	1:D:749:THR:HG23	2.02	0.41
1:D:355:MET:HE1	1:D:410:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:VAL:HG11	1:D:405:LEU:HD22	2.03	0.41
1:D:538:THR:HG21	1:D:1028:VAL:CG2	2.51	0.41
1:D:636:ASP:O	1:D:638:PRO:HD3	2.21	0.41
1:D:1007:VAL:HG12	1:D:1008:MET:N	2.36	0.41
1:E:166:ILE:O	1:E:169:THR:HB	2.20	0.41
1:E:200:PRO:HA	1:E:203:VAL:HG23	2.03	0.41
1:E:680:PHE:CE1	1:E:682:PHE:HB2	2.56	0.41
1:F:49:TYR:HB3	1:F:57:VAL:HG12	2.02	0.41
1:F:151:GLN:NE2	1:F:279:ALA:O	2.54	0.41
1:F:382:VAL:O	1:F:386:PHE:HD2	2.04	0.41
1:A:67:GLN:HG2	1:C:767:ARG:HH12	1.85	0.40
1:A:525:HIS:O	1:A:528:THR:HG22	2.21	0.40
1:A:1030:ARG:HA	1:A:1030:ARG:HH11	1.86	0.40
1:B:242:SER:HB2	1:B:245:GLU:H	1.87	0.40
1:B:448:VAL:HG13	1:B:884:VAL:CG2	2.49	0.40
1:B:459:PHE:HD1	1:B:467:TYR:CD1	2.39	0.40
1:B:535:LEU:HA	1:B:535:LEU:HD23	1.78	0.40
1:B:982:PHE:CD2	1:B:1011:MET:HG3	2.56	0.40
1:C:13:TRP:HH2	1:C:370:ILE:HD13	1.86	0.40
1:C:307:ARG:NE	1:C:325:TYR:OH	2.54	0.40
1:C:365:THR:O	1:C:368:PRO:HD2	2.21	0.40
1:C:396:PHE:O	1:C:400:LEU:HB2	2.21	0.40
1:C:687:GLN:HG3	1:C:688:ALA:N	2.36	0.40
1:D:467:TYR:HE2	1:D:925:VAL:HG22	1.85	0.40
1:D:485:ALA:O	1:D:490:PRO:HD3	2.21	0.40
1:D:671:ILE:H	1:D:671:ILE:HG13	1.59	0.40
1:D:678:THR:HG22	1:D:837:THR:N	2.36	0.40
1:D:890:ALA:HB1	1:F:11:PHE:CE1	2.56	0.40
1:D:894:SER:HB3	1:D:897:ILE:HB	2.03	0.40
1:D:1034:SER:HG	1:D:1035:ARG:H	1.60	0.40
1:F:459:PHE:CE2	1:F:872:GLN:HB3	2.56	0.40
1:F:560:PRO:HB2	1:F:836:SER:OG	2.21	0.40
1:F:979:SER:OG	1:F:1015:THR:HG21	2.20	0.40
1:A:352:PHE:CD2	1:A:352:PHE:C	3.00	0.40
1:A:680:PHE:CZ	1:A:829:GLY:HA3	2.57	0.40
1:A:801:PHE:HA	1:A:804:PHE:HE2	1.84	0.40
1:C:950:LYS:HG3	1:C:951:ASP:N	2.36	0.40
1:D:144:ASN:HA	1:D:320:GLY:O	2.21	0.40
1:D:332:PHE:O	1:D:336:SER:HB2	2.21	0.40
1:D:574:THR:HG23	1:D:627:ALA:HB3	2.03	0.40
1:D:602:GLU:OE1	1:D:650:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:LYS:HG2	1:E:196:PHE:CE1	2.56	0.40
1:E:555:LEU:HD23	1:E:555:LEU:HA	1.82	0.40
1:E:573:MET:HE2	1:E:626:ILE:HG12	2.03	0.40
1:F:329:THR:O	1:F:333:VAL:HG23	2.21	0.40
1:F:414:GLU:HG2	1:F:973:ARG:NH1	2.36	0.40
1:F:931:LEU:HD23	1:F:931:LEU:HA	1.72	0.40
1:F:937:LEU:HD13	1:F:1011:MET:CE	2.40	0.40
1:A:144:ASN:HA	1:A:320:GLY:O	2.21	0.40
1:A:182:TYR:HB2	1:A:769:LYS:HZ2	1.86	0.40
1:A:344:LEU:HD22	1:A:402:ILE:CD1	2.52	0.40
1:B:172:VAL:HG13	1:B:291:ILE:HG23	2.02	0.40
1:B:729:ILE:HG22	1:B:731:ILE:HD13	2.03	0.40
1:B:915:ALA:CB	1:B:1009:GLY:HA3	2.41	0.40
1:C:263:ARG:O	1:C:263:ARG:HG2	2.22	0.40
1:C:445:ILE:HG23	1:C:940:LYS:HG3	2.03	0.40
1:C:594:VAL:O	1:C:597:TYR:N	2.55	0.40
1:D:188:MET:HE3	1:D:188:MET:HB2	1.85	0.40
1:D:377:LEU:O	1:D:380:PHE:HB2	2.21	0.40
1:D:710:PRO:HA	1:D:713:LEU:O	2.21	0.40
1:D:948:PHE:N	1:D:948:PHE:CD1	2.89	0.40
1:E:6:ILE:HD11	1:E:435:MET:HG3	2.02	0.40
1:E:30:LEU:CD1	1:E:31:PRO:HD2	2.50	0.40
1:E:267:LYS:HD3	1:E:776:GLU:OE2	2.21	0.40
1:E:294:ALA:HB3	1:E:297:ALA:HB2	2.02	0.40
1:E:416:VAL:HG11	1:E:497:LEU:HD23	2.04	0.40
1:E:639:GLY:O	1:E:643:LYS:HG3	2.21	0.40
1:F:58:GLN:CD	1:F:818:ARG:HD2	2.47	0.40
1:F:102:ILE:HD13	1:F:102:ILE:HA	1.84	0.40
1:F:321:LEU:HD23	1:F:321:LEU:HA	1.75	0.40
1:F:510:LYS:H	1:F:510:LYS:HD3	1.85	0.40
1:F:701:GLN:HE22	1:F:852:PRO:HD3	1.86	0.40
1:F:703:LEU:HD21	1:F:716:VAL:HG12	2.04	0.40
1:A:400:LEU:CD2	1:A:929:VAL:HG12	2.50	0.40
1:A:505:HIS:O	1:A:507:GLU:N	2.55	0.40
1:A:682:PHE:HD2	1:A:683:GLU:N	2.19	0.40
1:A:686:ASP:O	1:A:822:LEU:HD13	2.22	0.40
1:B:137:LEU:HD12	1:B:329:THR:HG22	2.03	0.40
1:B:195:LYS:HB3	1:B:196:PHE:HD1	1.86	0.40
1:B:655:PHE:HB3	1:B:663:VAL:HB	2.03	0.40
1:B:871:ASN:N	1:B:871:ASN:OD1	2.54	0.40
1:B:904:VAL:HG21	1:B:942:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:944:LEU:HD23	1:B:944:LEU:HA	1.78	0.40
1:C:398:MET:HE3	1:C:398:MET:HB3	1.87	0.40
1:C:459:PHE:CZ	1:C:876:LEU:HA	2.56	0.40
1:C:591:LEU:HD23	1:C:591:LEU:HA	1.92	0.40
1:C:735:LYS:O	1:C:738:ALA:HB3	2.21	0.40
1:D:70:ASN:OD1	1:D:70:ASN:N	2.54	0.40
1:D:414:GLU:CG	1:D:974:PRO:HG3	2.52	0.40
1:D:666:PHE:N	1:D:666:PHE:CD1	2.89	0.40
2:D:1101:ERY:H313	2:D:1101:ERY:C20	2.52	0.40
1:E:641:GLU:HB2	1:E:650:ARG:NH2	2.37	0.40
1:E:644:VAL:O	1:E:645:GLU:C	2.64	0.40
1:F:118:LEU:HA	1:F:119:PRO:HD3	1.94	0.40
1:F:783:PRO:O	1:F:786:ILE:HG12	2.21	0.40
1:A:453:PHE:HE2	1:A:932:LEU:HB3	1.83	0.40
1:A:895:TRP:CE2	1:C:10:ILE:HG12	2.56	0.40
1:A:926:TYR:HE1	1:A:999:ALA:HB1	1.86	0.40
1:A:953:MET:HG3	1:A:958:LYS:O	2.22	0.40
1:B:143:ILE:O	1:B:321:LEU:HA	2.21	0.40
1:B:591:LEU:HD11	1:B:625:GLY:HA3	2.04	0.40
1:B:987:MET:CA	1:B:1008:MET:HE1	2.51	0.40
1:B:1016:VAL:HG12	1:B:1016:VAL:O	2.21	0.40
1:C:15:ILE:O	1:C:19:ILE:HG13	2.22	0.40
1:C:65:ILE:HG23	1:C:111:LEU:HD23	2.03	0.40
1:D:201:VAL:O	1:D:204:ILE:HB	2.22	0.40
1:D:666:PHE:N	1:D:666:PHE:HD1	2.20	0.40
3:D:1103:LMT:H21	3:D:1103:LMT:H1'	1.78	0.40
1:E:31:PRO:HB2	1:E:389:SER:HB2	2.02	0.40
1:E:1033:PHE:C	1:E:1033:PHE:HD2	2.30	0.40
1:F:588:GLN:NE2	1:F:592:ASN:OD1	2.52	0.40
1:F:986:VAL:CG1	1:F:1008:MET:HB2	2.51	0.40
1:F:1032:ARG:O	1:F:1033:PHE:HB2	2.21	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	1042/1049 (99%)	943 (90%)	86 (8%)	13 (1%)	10	41
1	B	1040/1049 (99%)	955 (92%)	68 (6%)	17 (2%)	7	36
1	C	1040/1049 (99%)	934 (90%)	88 (8%)	18 (2%)	7	34
1	D	1040/1049 (99%)	943 (91%)	83 (8%)	14 (1%)	9	39
1	E	1040/1049 (99%)	947 (91%)	72 (7%)	21 (2%)	6	32
1	F	1041/1049 (99%)	932 (90%)	81 (8%)	28 (3%)	4	27
All	All	6243/6294 (99%)	5654 (91%)	478 (8%)	111 (2%)	6	33

All (111) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	F	836	SER
1	F	893	GLU
1	F	1033	PHE
1	F	1036	LYS
1	F	1038	GLU
1	F	1043	SER
1	A	991	ILE
1	A	1037	ASN
1	B	638	PRO
1	B	672	VAL
1	B	689	GLY
1	B	893	GLU
1	B	1040	ILE
1	C	146	ASP
1	C	147	GLY
1	C	509	LYS
1	C	689	GLY
1	C	836	SER
1	C	871	ASN
1	D	1036	LYS
1	D	1042	HIS
1	E	638	PRO
1	E	672	VAL
1	E	677	ALA
1	E	1040	ILE
1	F	133	SER
1	F	147	GLY
1	F	511	GLY
1	F	638	PRO
1	F	639	GLY
1	F	689	GLY
1	F	1040	ILE
1	A	133	SER
1	A	263	ARG
1	A	923	ASN
1	A	992	SER
1	A	1043	SER
1	B	263	ARG
1	B	833	PRO
1	C	775	SER
1	C	870	GLY
1	C	1035	ARG

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Mol	Chain	Res	Type
1	D	163	LYS
1	D	775	SER
1	E	511	GLY
1	E	775	SER
1	F	146	ASP
1	F	862	MET
1	B	775	SER
1	C	62	THR
1	D	1034	SER
1	E	134	SER
1	E	263	ARG
1	E	1036	LYS
1	F	263	ARG
1	F	775	SER
1	B	892	TYR
1	B	923	ASN
1	C	6	ILE
1	C	357	LEU
1	D	62	THR
1	D	960	LEU
1	D	1033	PHE
1	E	903	LEU
1	F	507	GLU
1	F	536	ARG
1	F	752	ALA
1	B	676	THR
1	D	133	SER
1	E	62	THR
1	A	1040	ILE
1	C	658	ILE
1	D	751	GLY
1	E	508	GLY
1	F	751	GLY
1	E	639	GLY
1	A	1016	VAL
1	B	639	GLY
1	C	751	GLY
1	E	1016	VAL
1	F	658	ILE
1	A	427	PRO
1	A	910	ILE
1	F	6	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	850/855 (99%)	763 (90%)	87 (10%)	7	28
1	B	848/855 (99%)	759 (90%)	89 (10%)	6	27
1	C	848/855 (99%)	758 (89%)	90 (11%)	6	27
1	D	848/855 (99%)	746 (88%)	102 (12%)	5	23
1	E	848/855 (99%)	748 (88%)	100 (12%)	5	23
1	F	849/855 (99%)	747 (88%)	102 (12%)	5	23
All	All	5091/5130 (99%)	4521 (89%)	570 (11%)	6	25

All (570) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	10	ILE
1	A	18	ILE
1	A	21	LEU
1	A	27	ILE
1	A	45	ILE
1	A	48	SER
1	A	57	VAL
1	A	93	THR
1	A	137	LEU
1	A	151	GLN
1	A	152	GLU
1	A	169	THR
1	A	175	VAL
1	A	195	LYS
1	A	203	VAL
1	A	205	THR
1	A	222	THR
1	A	225	VAL
1	A	243	THR
1	A	270	LEU
1	A	293	LEU

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Mol	Chain	Res	Type
1	A	310	LEU
1	A	321	LEU
1	A	324	VAL
1	A	336	SER
1	A	341	VAL
1	A	343	THR
1	A	351	VAL
1	A	353	LEU
1	A	360	GLN
1	A	362	PHE
1	A	369	THR
1	A	400	LEU
1	A	406	VAL
1	A	428	LYS
1	A	429	GLU
1	A	462	SER
1	A	463	THR
1	A	483	LEU
1	A	489	THR
1	A	523	SER
1	A	524	THR
1	A	538	THR
1	A	542	LEU
1	A	559	LEU
1	A	561	SER
1	A	571	VAL
1	A	575	MET
1	A	578	LEU
1	A	626	ILE
1	A	634	TRP
1	A	662	MET
1	A	664	PHE
1	A	666	PHE
1	A	671	ILE
1	A	672	VAL
1	A	674	LEU
1	A	682	PHE
1	A	687	GLN
1	A	697	GLN
1	A	713	LEU
1	A	716	VAL
1	A	717	ARG

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Mol	Chain	Res	Type
1	A	721	LEU
1	A	741	VAL
1	A	743	ILE
1	A	748	THR
1	A	768	VAL
1	A	773	VAL
1	A	797	GLN
1	A	804	PHE
1	A	817	GLU
1	A	843	LEU
1	A	857	TYR
1	A	901	VAL
1	A	914	LEU
1	A	933	THR
1	A	958	LYS
1	A	961	ILE
1	A	964	THR
1	A	968	VAL
1	A	980	LEU
1	A	984	LEU
1	A	986	VAL
1	A	1007	VAL
1	A	1041	GLU
1	B	6	ILE
1	B	10	ILE
1	B	25	LEU
1	B	28	LEU
1	B	29	LYS
1	B	91	THR
1	B	93	THR
1	B	102	ILE
1	B	105	VAL
1	B	107	VAL
1	B	117	LEU
1	B	128	SER
1	B	131	LYS
1	B	145	THR
1	B	146	ASP
1	B	151	GLN
1	B	169	THR
1	B	175	VAL
1	B	196	PHE

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Mol	Chain	Res	Type
1	B	203	VAL
1	B	225	VAL
1	B	243	THR
1	B	255	GLN
1	B	259	ARG
1	B	270	LEU
1	B	277	ILE
1	B	293	LEU
1	B	295	THR
1	B	310	LEU
1	B	324	VAL
1	B	332	PHE
1	B	336	SER
1	B	341	VAL
1	B	343	THR
1	B	351	VAL
1	B	353	LEU
1	B	355	MET
1	B	360	GLN
1	B	372	VAL
1	B	400	LEU
1	B	404	LEU
1	B	439	GLN
1	B	472	ILE
1	B	489	THR
1	B	495	THR
1	B	523	SER
1	B	524	THR
1	B	561	SER
1	B	571	VAL
1	B	578	LEU
1	B	592	ASN
1	B	602	GLU
1	B	617	PHE
1	B	626	ILE
1	B	634	TRP
1	B	652	THR
1	B	653	ARG
1	B	659	LYS
1	B	672	VAL
1	B	673	GLU
1	B	687	GLN

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Mol	Chain	Res	Type
1	B	694	LYS
1	B	695	LEU
1	B	708	LYS
1	B	717	ARG
1	B	721	LEU
1	B	731	ILE
1	B	743	ILE
1	B	748	THR
1	B	768	VAL
1	B	804	PHE
1	B	806	SER
1	B	811	TYR
1	B	835	LYS
1	B	843	LEU
1	B	871	ASN
1	B	914	LEU
1	B	933	THR
1	B	958	LYS
1	B	961	ILE
1	B	968	VAL
1	B	971	ARG
1	B	980	LEU
1	B	986	VAL
1	B	1007	VAL
1	B	1017	LEU
1	B	1024	VAL
1	B	1041	GLU
1	B	1043	SER
1	C	3	ASN
1	C	6	ILE
1	C	27	ILE
1	C	34	GLN
1	C	44	THR
1	C	45	ILE
1	C	48	SER
1	C	59	ASP
1	C	72	ILE
1	C	87	THR
1	C	88	VAL
1	C	93	THR
1	C	102	ILE
1	C	104	GLN

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Mol	Chain	Res	Type
1	C	112	GLN
1	C	115	MET
1	C	151	GLN
1	C	166	ILE
1	C	174	ASP
1	C	175	VAL
1	C	177	LEU
1	C	203	VAL
1	C	222	THR
1	C	225	VAL
1	C	243	THR
1	C	270	LEU
1	C	274	ASN
1	C	293	LEU
1	C	300	LEU
1	C	310	LEU
1	C	336	SER
1	C	337	ILE
1	C	341	VAL
1	C	345	VAL
1	C	351	VAL
1	C	353	LEU
1	C	400	LEU
1	C	415	ASN
1	C	422	GLU
1	C	432	ARG
1	C	447	MET
1	C	462	SER
1	C	463	THR
1	C	472	ILE
1	C	482	VAL
1	C	489	THR
1	C	519	MET
1	C	523	SER
1	C	524	THR
1	C	535	LEU
1	C	538	THR
1	C	540	ARG
1	C	542	LEU
1	C	561	SER
1	C	564	LEU
1	C	571	VAL

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Mol	Chain	Res	Type
1	C	578	LEU
1	C	596	HIS
1	C	602	GLU
1	C	623	ASN
1	C	626	ILE
1	C	634	TRP
1	C	668	LEU
1	C	672	VAL
1	C	678	THR
1	C	694	LYS
1	C	714	THR
1	C	716	VAL
1	C	721	LEU
1	C	724	THR
1	C	746	ILE
1	C	768	VAL
1	C	775	SER
1	C	804	PHE
1	C	807	SER
1	C	843	LEU
1	C	847	LEU
1	C	860	THR
1	C	876	LEU
1	C	886	LEU
1	C	895	TRP
1	C	947	GLU
1	C	950	LYS
1	C	958	LYS
1	C	968	VAL
1	C	980	LEU
1	C	986	VAL
1	C	991	ILE
1	C	1007	VAL
1	C	1032	ARG
1	D	3	ASN
1	D	10	ILE
1	D	18	ILE
1	D	21	LEU
1	D	27	ILE
1	D	45	ILE
1	D	57	VAL
1	D	101	ASP

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Mol	Chain	Res	Type
1	D	107	VAL
1	D	146	ASP
1	D	151	GLN
1	D	152	GLU
1	D	169	THR
1	D	175	VAL
1	D	177	LEU
1	D	195	LYS
1	D	203	VAL
1	D	205	THR
1	D	225	VAL
1	D	243	THR
1	D	255	GLN
1	D	267	LYS
1	D	270	LEU
1	D	293	LEU
1	D	310	LEU
1	D	324	VAL
1	D	337	ILE
1	D	341	VAL
1	D	343	THR
1	D	351	VAL
1	D	353	LEU
1	D	355	MET
1	D	360	GLN
1	D	362	PHE
1	D	369	THR
1	D	415	ASN
1	D	428	LYS
1	D	429	GLU
1	D	439	GLN
1	D	463	THR
1	D	472	ILE
1	D	483	LEU
1	D	519	MET
1	D	523	SER
1	D	524	THR
1	D	538	THR
1	D	542	LEU
1	D	561	SER
1	D	564	LEU
1	D	568	ASP

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Mol	Chain	Res	Type
1	D	571	VAL
1	D	575	MET
1	D	578	LEU
1	D	594	VAL
1	D	602	GLU
1	D	605	ASN
1	D	623	ASN
1	D	626	ILE
1	D	629	VAL
1	D	634	TRP
1	D	662	MET
1	D	666	PHE
1	D	668	LEU
1	D	671	ILE
1	D	672	VAL
1	D	674	LEU
1	D	682	PHE
1	D	687	GLN
1	D	697	GLN
1	D	713	LEU
1	D	714	THR
1	D	717	ARG
1	D	721	LEU
1	D	726	GLN
1	D	741	VAL
1	D	743	ILE
1	D	748	THR
1	D	757	SER
1	D	768	VAL
1	D	773	VAL
1	D	797	GLN
1	D	804	PHE
1	D	806	SER
1	D	815	ARG
1	D	843	LEU
1	D	857	TYR
1	D	862	MET
1	D	865	GLN
1	D	901	VAL
1	D	922	THR
1	D	931	LEU
1	D	933	THR

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Mol	Chain	Res	Type
1	D	943	ILE
1	D	958	LYS
1	D	961	ILE
1	D	968	VAL
1	D	978	THR
1	D	980	LEU
1	D	986	VAL
1	D	1007	VAL
1	D	1041	GLU
1	D	1042	HIS
1	E	3	ASN
1	E	6	ILE
1	E	10	ILE
1	E	18	ILE
1	E	25	LEU
1	E	28	LEU
1	E	44	THR
1	E	45	ILE
1	E	48	SER
1	E	60	THR
1	E	91	THR
1	E	93	THR
1	E	102	ILE
1	E	105	VAL
1	E	107	VAL
1	E	109	ASN
1	E	117	LEU
1	E	128	SER
1	E	145	THR
1	E	151	GLN
1	E	175	VAL
1	E	177	LEU
1	E	196	PHE
1	E	203	VAL
1	E	205	THR
1	E	225	VAL
1	E	230	LEU
1	E	255	GLN
1	E	259	ARG
1	E	270	LEU
1	E	277	ILE
1	E	293	LEU

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Mol	Chain	Res	Type
1	E	295	THR
1	E	310	LEU
1	E	324	VAL
1	E	329	THR
1	E	337	ILE
1	E	341	VAL
1	E	343	THR
1	E	351	VAL
1	E	353	LEU
1	E	355	MET
1	E	358	PHE
1	E	372	VAL
1	E	410	ILE
1	E	439	GLN
1	E	472	ILE
1	E	513	PHE
1	E	519	MET
1	E	523	SER
1	E	524	THR
1	E	526	HIS
1	E	540	ARG
1	E	559	LEU
1	E	561	SER
1	E	563	PHE
1	E	569	GLN
1	E	571	VAL
1	E	602	GLU
1	E	613	ASN
1	E	626	ILE
1	E	630	SER
1	E	634	TRP
1	E	653	ARG
1	E	657	GLN
1	E	659	LYS
1	E	662	MET
1	E	668	LEU
1	E	672	VAL
1	E	673	GLU
1	E	678	THR
1	E	687	GLN
1	E	694	LYS
1	E	695	LEU

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Mol	Chain	Res	Type
1	E	697	GLN
1	E	708	LYS
1	E	713	LEU
1	E	714	THR
1	E	716	VAL
1	E	721	LEU
1	E	760	ASN
1	E	768	VAL
1	E	804	PHE
1	E	806	SER
1	E	843	LEU
1	E	880	SER
1	E	886	LEU
1	E	933	THR
1	E	958	LYS
1	E	961	ILE
1	E	968	VAL
1	E	971	ARG
1	E	980	LEU
1	E	986	VAL
1	E	1007	VAL
1	E	1024	VAL
1	E	1032	ARG
1	E	1033	PHE
1	E	1041	GLU
1	E	1043	SER
1	F	3	ASN
1	F	6	ILE
1	F	10	ILE
1	F	18	ILE
1	F	21	LEU
1	F	27	ILE
1	F	28	LEU
1	F	45	ILE
1	F	48	SER
1	F	76	MET
1	F	81	ASN
1	F	87	THR
1	F	88	VAL
1	F	90	ILE
1	F	93	THR
1	F	102	ILE

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Mol	Chain	Res	Type
1	F	104	GLN
1	F	112	GLN
1	F	129	VAL
1	F	151	GLN
1	F	169	THR
1	F	174	ASP
1	F	175	VAL
1	F	177	LEU
1	F	189	ASN
1	F	203	VAL
1	F	222	THR
1	F	225	VAL
1	F	243	THR
1	F	270	LEU
1	F	274	ASN
1	F	293	LEU
1	F	300	LEU
1	F	307	ARG
1	F	321	LEU
1	F	336	SER
1	F	337	ILE
1	F	341	VAL
1	F	343	THR
1	F	353	LEU
1	F	362	PHE
1	F	400	LEU
1	F	418	ARG
1	F	432	ARG
1	F	443	VAL
1	F	447	MET
1	F	448	VAL
1	F	462	SER
1	F	472	ILE
1	F	482	VAL
1	F	489	THR
1	F	493	CYS
1	F	495	THR
1	F	515	TRP
1	F	519	MET
1	F	523	SER
1	F	524	THR
1	F	538	THR

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Mol	Chain	Res	Type
1	F	559	LEU
1	F	564	LEU
1	F	571	VAL
1	F	578	LEU
1	F	596	HIS
1	F	602	GLU
1	F	626	ILE
1	F	630	SER
1	F	634	TRP
1	F	658	ILE
1	F	668	LEU
1	F	672	VAL
1	F	674	LEU
1	F	683	GLU
1	F	695	LEU
1	F	697	GLN
1	F	703	LEU
1	F	721	LEU
1	F	730	ASP
1	F	743	ILE
1	F	768	VAL
1	F	775	SER
1	F	806	SER
1	F	843	LEU
1	F	847	LEU
1	F	853	THR
1	F	860	THR
1	F	862	MET
1	F	886	LEU
1	F	895	TRP
1	F	947	GLU
1	F	958	LYS
1	F	968	VAL
1	F	972	LEU
1	F	980	LEU
1	F	986	VAL
1	F	991	ILE
1	F	993	THR
1	F	1007	VAL
1	F	1017	LEU
1	F	1033	PHE
1	F	1035	ARG

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Mol	Chain	Res	Type
1	F	1038	GLU
1	F	1044	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	109	ASN
1	A	210	GLN
1	A	229	GLN
1	A	231	ASN
1	A	298	ASN
1	A	361	ASN
1	A	709	HIS
1	B	34	GLN
1	B	68	ASN
1	B	109	ASN
1	B	151	GLN
1	B	228	GLN
1	B	415	ASN
1	B	469	GLN
1	B	526	HIS
1	B	744	ASN
1	B	865	GLN
1	C	34	GLN
1	C	108	GLN
1	C	144	ASN
1	C	161	ASN
1	C	213	GLN
1	C	231	ASN
1	C	622	GLN
1	C	726	GLN
1	C	846	GLN
1	D	58	GLN
1	D	68	ASN
1	D	74	ASN
1	D	108	GLN
1	D	109	ASN
1	D	210	GLN
1	D	231	ASN
1	D	282	ASN
1	D	284	GLN

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Mol	Chain	Res	Type
1	D	415	ASN
1	D	517	ASN
1	D	588	GLN
1	D	605	ASN
1	D	709	HIS
1	D	719	ASN
1	D	737	GLN
1	D	865	GLN
1	D	1037	ASN
1	E	67	GLN
1	E	81	ASN
1	E	213	GLN
1	E	231	ASN
1	E	361	ASN
1	E	517	ASN
1	E	588	GLN
1	E	592	ASN
1	E	667	ASN
1	E	701	GLN
1	E	760	ASN
1	F	81	ASN
1	F	104	GLN
1	F	108	GLN
1	F	109	ASN
1	F	161	ASN
1	F	194	ASN
1	F	228	GLN
1	F	231	ASN
1	F	361	ASN
1	F	415	ASN
1	F	439	GLN
1	F	588	GLN
1	F	592	ASN
1	F	692	HIS
1	F	726	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMT	A	1103	-	36,36,36	1.79	8 (22%)	47,47,47	1.61	10 (21%)
3	LMT	B	1101	-	36,36,36	1.85	10 (27%)	47,47,47	1.59	10 (21%)
3	LMT	D	1103	-	36,36,36	1.86	10 (27%)	47,47,47	1.47	5 (10%)
3	LMT	C	1101	-	36,36,36	1.76	10 (27%)	47,47,47	1.11	4 (8%)
3	LMT	A	1102	-	36,36,36	1.76	8 (22%)	47,47,47	1.44	7 (14%)
2	ERY	D	1101	-	53,53,53	1.29	2 (3%)	82,82,82	1.99	20 (24%)
3	LMT	E	1101	-	36,36,36	1.81	11 (30%)	47,47,47	1.70	11 (23%)
3	LMT	D	1102	-	36,36,36	1.78	9 (25%)	47,47,47	1.07	3 (6%)
2	ERY	A	1101	-	53,53,53	1.24	3 (5%)	82,82,82	2.11	25 (30%)
3	LMT	F	1101	-	36,36,36	1.84	8 (22%)	47,47,47	1.17	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	1103	-	-	12/21/61/61	0/2/2/2
3	LMT	B	1101	-	-	12/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	D	1103	-	-	10/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	9/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	7/21/61/61	0/2/2/2
2	ERY	D	1101	-	-	24/72/107/107	1/3/3/3
3	LMT	E	1101	-	-	14/21/61/61	0/2/2/2
3	LMT	D	1102	-	-	11/21/61/61	0/2/2/2
2	ERY	A	1101	-	-	35/72/107/107	0/3/3/3
3	LMT	F	1101	-	-	8/21/61/61	0/2/2/2

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	ERY	O2-C1	6.10	1.48	1.34
2	A	1101	ERY	O2-C1	5.22	1.46	1.34
3	E	1101	LMT	O1'-C1'	4.83	1.48	1.40
3	B	1101	LMT	O1'-C1'	4.64	1.47	1.40
3	F	1101	LMT	O1'-C1'	4.40	1.47	1.40
3	D	1103	LMT	O1'-C1'	4.38	1.47	1.40
3	D	1102	LMT	O1'-C1'	4.22	1.47	1.40
3	A	1103	LMT	O5B-C1B	4.22	1.52	1.41
3	D	1103	LMT	O5'-C5'	4.19	1.54	1.44
3	D	1103	LMT	O5B-C1B	4.08	1.52	1.41
3	C	1101	LMT	O5'-C5'	3.98	1.54	1.44
3	A	1102	LMT	O5'-C5'	3.88	1.53	1.44
3	B	1101	LMT	O5B-C1B	3.85	1.51	1.41
3	D	1102	LMT	O5'-C5'	3.84	1.53	1.44
3	A	1103	LMT	O1'-C1'	3.82	1.46	1.40
3	F	1101	LMT	O5'-C5'	3.77	1.53	1.44
3	A	1102	LMT	O5B-C1B	3.67	1.51	1.41
3	A	1102	LMT	O1'-C1'	3.67	1.46	1.40
3	F	1101	LMT	O5B-C1B	3.66	1.51	1.41
3	C	1101	LMT	O1'-C1'	3.60	1.46	1.40
3	B	1101	LMT	O5'-C5'	3.49	1.52	1.44
3	D	1103	LMT	O5'-C1'	3.49	1.50	1.41
3	D	1102	LMT	O5B-C1B	3.40	1.50	1.41
3	E	1101	LMT	O5'-C5'	3.38	1.52	1.44
3	D	1102	LMT	C6'-C5'	-3.35	1.40	1.51
3	A	1103	LMT	C6'-C5'	-3.34	1.40	1.51
3	A	1103	LMT	O5'-C5'	3.32	1.52	1.44
3	D	1103	LMT	O3B-C3B	3.31	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1101	LMT	O5'-C1'	3.30	1.50	1.41
3	A	1103	LMT	O3B-C3B	3.24	1.51	1.43
3	E	1101	LMT	C6'-C5'	-3.22	1.41	1.51
3	C	1101	LMT	O5B-C1B	3.18	1.50	1.41
3	D	1102	LMT	O5'-C1'	3.11	1.49	1.41
3	E	1101	LMT	O5'-C1'	3.10	1.49	1.41
3	B	1101	LMT	O5'-C1'	3.09	1.49	1.41
3	B	1101	LMT	C6'-C5'	-3.07	1.41	1.51
3	E	1101	LMT	O5B-C1B	3.06	1.49	1.41
3	F	1101	LMT	O5'-C1'	3.05	1.49	1.41
3	C	1101	LMT	C6'-C5'	-3.04	1.41	1.51
3	A	1102	LMT	C6'-C5'	-3.01	1.41	1.51
3	F	1101	LMT	C6'-C5'	-3.00	1.41	1.51
3	A	1102	LMT	O5'-C1'	2.87	1.49	1.41
3	E	1101	LMT	O3B-C3B	2.81	1.49	1.43
3	D	1102	LMT	O3B-C3B	2.76	1.49	1.43
3	A	1102	LMT	O3B-C3B	2.71	1.49	1.43
3	D	1103	LMT	O2'-C2'	2.71	1.49	1.43
3	D	1103	LMT	C6'-C5'	-2.66	1.42	1.51
3	A	1103	LMT	O5'-C1'	2.61	1.48	1.41
3	B	1101	LMT	O2'-C2'	2.54	1.49	1.43
3	F	1101	LMT	O3B-C3B	2.53	1.49	1.43
3	A	1103	LMT	O2'-C2'	2.52	1.49	1.43
3	C	1101	LMT	O2'-C2'	2.49	1.49	1.43
2	D	1101	ERY	O9-C22	2.46	1.48	1.41
3	B	1101	LMT	O3B-C3B	2.32	1.48	1.43
3	B	1101	LMT	C5-C4	2.32	1.63	1.51
3	B	1101	LMT	O3'-C3'	2.32	1.48	1.43
3	C	1101	LMT	O3B-C3B	2.30	1.48	1.43
3	F	1101	LMT	C5-C4	2.29	1.63	1.51
3	D	1102	LMT	O2'-C2'	2.28	1.48	1.43
3	A	1102	LMT	O2'-C2'	2.27	1.48	1.43
3	C	1101	LMT	C3B-C2B	-2.25	1.46	1.52
3	D	1102	LMT	C5-C4	2.25	1.63	1.51
3	D	1103	LMT	C5-C4	2.25	1.63	1.51
3	A	1102	LMT	C5-C4	2.24	1.62	1.51
2	A	1101	ERY	C23-C24	2.23	1.58	1.53
3	E	1101	LMT	O2'-C2'	2.22	1.48	1.43
3	E	1101	LMT	C5-C4	2.19	1.62	1.51
3	E	1101	LMT	C3B-C2B	-2.18	1.46	1.52
3	B	1101	LMT	C3'-C2'	-2.17	1.46	1.52
3	C	1101	LMT	C3'-C2'	-2.17	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1101	LMT	C3'-C2'	-2.17	1.46	1.52
3	D	1102	LMT	O3'-C3'	2.15	1.48	1.43
3	C	1101	LMT	C5-C4	2.15	1.62	1.51
3	A	1103	LMT	O3'-C3'	2.12	1.48	1.43
2	A	1101	ERY	O6-C17	2.08	1.46	1.42
3	E	1101	LMT	O3'-C3'	2.08	1.48	1.43
3	D	1103	LMT	O3'-C3'	2.05	1.48	1.43
3	E	1101	LMT	C3'-C2'	-2.03	1.47	1.52
3	D	1103	LMT	C4'-C5'	2.02	1.58	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	ERY	C20-O5-C16	6.19	130.12	117.51
2	A	1101	ERY	O7-C5-C4	-6.17	102.66	111.58
2	D	1101	ERY	O12-C11-C10	5.69	118.84	110.77
2	D	1101	ERY	C22-O7-C5	5.39	125.44	116.26
2	D	1101	ERY	C29-N1-C24	5.15	128.00	113.15
2	A	1101	ERY	O2-C1-O1	-5.04	114.85	123.95
3	E	1101	LMT	C1'-C2'-C3'	4.77	120.04	110.01
2	D	1101	ERY	C33-C8-C7	-4.72	101.10	109.88
2	A	1101	ERY	C22-O7-C5	4.60	124.09	116.26
3	A	1103	LMT	C1'-O5'-C5'	-4.59	104.76	113.72
3	A	1102	LMT	C1'-C2'-C3'	4.52	119.52	110.01
2	A	1101	ERY	C13-O2-C1	-4.49	110.35	118.20
3	A	1102	LMT	C2'-C3'-C4'	4.43	119.73	109.68
2	A	1101	ERY	C19-C16-C15	-4.40	102.96	110.64
3	B	1101	LMT	O1'-C1'-C2'	4.40	114.95	108.27
2	D	1101	ERY	O2-C13-C36	4.20	115.17	107.36
3	F	1101	LMT	O5B-C5B-C4B	4.13	117.15	109.70
3	E	1101	LMT	O1'-C1'-C2'	4.07	114.45	108.27
2	D	1101	ERY	C20-O5-C16	4.02	125.70	117.51
3	E	1101	LMT	O5B-C5B-C4B	3.99	116.89	109.70
3	A	1103	LMT	C2'-C3'-C4'	3.93	118.59	109.68
3	B	1101	LMT	C1B-O1B-C4'	-3.86	108.83	117.98
2	D	1101	ERY	C25-C24-N1	-3.73	105.11	115.59
3	A	1103	LMT	C1'-C2'-C3'	3.61	117.61	110.01
3	A	1103	LMT	C3B-C4B-C5B	3.56	116.68	110.23
3	E	1101	LMT	O2'-C2'-C3'	-3.50	102.12	110.38
3	D	1103	LMT	C1'-C2'-C3'	3.46	117.30	110.01
2	A	1101	ERY	O2-C13-C12	3.44	112.70	107.28
3	B	1101	LMT	C3B-C4B-C5B	3.36	116.32	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1101	LMT	C1-O1'-C1'	3.35	119.40	113.68
3	D	1103	LMT	C1B-O1B-C4'	-3.34	110.06	117.98
2	A	1101	ERY	C29-N1-C24	3.33	122.73	113.15
3	D	1103	LMT	C3B-C4B-C5B	3.32	116.25	110.23
2	D	1101	ERY	C3-C4-C5	3.26	117.96	111.17
2	D	1101	ERY	O9-C26-C27	3.22	112.91	106.88
2	A	1101	ERY	C3-C4-C5	3.21	117.86	111.17
2	A	1101	ERY	O7-C22-C23	3.21	115.98	108.09
3	C	1101	LMT	C1B-O1B-C4'	-3.19	110.42	117.98
3	E	1101	LMT	C1B-C2B-C3B	-3.17	103.33	110.01
2	A	1101	ERY	O7-C5-C6	3.11	110.11	106.40
2	D	1101	ERY	C22-O9-C26	3.07	117.65	112.91
3	E	1101	LMT	C2'-C3'-C4'	3.06	116.63	109.68
3	C	1101	LMT	C6B-C5B-C4B	-3.06	105.51	113.02
3	D	1102	LMT	C1'-C2'-C3'	3.05	116.44	110.01
3	D	1103	LMT	C2'-C3'-C4'	3.00	116.50	109.68
2	D	1101	ERY	O7-C5-C4	-2.98	107.27	111.58
3	B	1101	LMT	O5B-C5B-C4B	2.96	115.04	109.70
3	A	1102	LMT	C1B-O1B-C4'	-2.90	111.10	117.98
3	C	1101	LMT	O5B-C5B-C4B	2.90	114.92	109.70
2	D	1101	ERY	C36-C13-C12	-2.85	109.99	115.20
3	B	1101	LMT	O3B-C3B-C2B	-2.83	103.71	110.38
3	B	1101	LMT	C4B-C3B-C2B	2.81	115.76	110.83
3	B	1101	LMT	C6B-C5B-C4B	-2.78	106.19	113.02
2	A	1101	ERY	O9-C26-C27	2.76	112.04	106.88
2	D	1101	ERY	C33-C8-C9	2.75	116.08	109.43
2	A	1101	ERY	O2-C1-C2	2.75	117.40	111.53
2	D	1101	ERY	C31-C4-C3	-2.74	106.57	111.40
2	D	1101	ERY	O4-C18-C21	2.70	112.73	106.74
2	A	1101	ERY	C31-C4-C3	-2.69	106.66	111.40
3	E	1101	LMT	C1B-O1B-C4'	-2.63	111.73	117.98
3	A	1103	LMT	O5B-C5B-C6B	2.63	112.95	106.44
3	A	1103	LMT	O1'-C1'-C2'	2.62	112.25	108.27
2	D	1101	ERY	O5-C16-C17	2.57	107.58	103.86
2	A	1101	ERY	O12-C11-C10	2.54	114.38	110.77
2	D	1101	ERY	C30-C2-C3	2.53	118.65	113.00
3	A	1103	LMT	O5B-C5B-C4B	2.52	114.24	109.70
2	A	1101	ERY	C15-C16-C17	2.52	111.95	107.64
3	D	1103	LMT	O1B-C1B-C2B	2.51	114.27	108.09
3	D	1102	LMT	O2B-C2B-C1B	-2.50	104.12	110.08
3	E	1101	LMT	O5B-C1B-C2B	-2.45	105.34	110.37
3	F	1101	LMT	C1'-C2'-C3'	2.45	115.16	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1101	LMT	O3B-C3B-C2B	-2.44	104.64	110.38
2	A	1101	ERY	O10-C6-C32	-2.42	102.89	108.48
3	E	1101	LMT	O5'-C5'-C6'	2.38	112.34	106.44
2	A	1101	ERY	O4-C18-C21	2.37	111.99	106.74
3	A	1102	LMT	O1'-C1'-C2'	2.35	111.85	108.27
3	B	1101	LMT	C1B-O5B-C5B	2.35	118.31	113.72
2	A	1101	ERY	C35-C12-C13	2.34	114.42	111.26
3	E	1101	LMT	O5'-C5'-C4'	-2.33	104.91	109.72
3	A	1102	LMT	O5B-C5B-C4B	2.32	113.88	109.70
2	A	1101	ERY	C7-C8-C9	-2.30	109.47	113.32
2	A	1101	ERY	O6-C17-C16	2.21	115.08	111.08
3	A	1102	LMT	O5'-C5'-C6'	2.19	111.86	106.44
3	A	1103	LMT	O5'-C5'-C4'	-2.18	105.23	109.72
2	D	1101	ERY	C16-C17-C18	-2.17	107.96	111.12
3	A	1103	LMT	C4B-C3B-C2B	2.17	114.64	110.83
2	D	1101	ERY	O13-C12-C13	-2.17	103.92	107.24
3	B	1101	LMT	O3B-C3B-C4B	-2.17	105.26	110.38
3	A	1102	LMT	O2'-C2'-C3'	-2.17	105.26	110.38
2	A	1101	ERY	C30-C2-C3	2.12	117.75	113.00
3	A	1103	LMT	C1B-O5B-C5B	2.12	117.85	113.72
3	F	1101	LMT	C6B-C5B-C4B	-2.11	107.83	113.02
2	A	1101	ERY	C25-C24-N1	-2.10	109.69	115.59
3	E	1101	LMT	O5'-C1'-C2'	2.10	114.67	110.37
3	B	1101	LMT	C3'-C4'-C5'	2.08	115.55	110.93
2	D	1101	ERY	O11-C9-C10	-2.07	117.76	120.64
2	A	1101	ERY	O13-C12-C11	2.06	112.88	108.88
2	A	1101	ERY	O4-C14-C15	2.04	115.90	112.08
3	D	1102	LMT	O5B-C5B-C4B	2.01	113.33	109.70

There are no chirality outliers.

All (142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	ERY	C9-C10-C11-C12
2	A	1101	ERY	C34-C10-C11-C12
2	A	1101	ERY	C10-C11-C12-C13
2	A	1101	ERY	C10-C11-C12-C35
2	A	1101	ERY	C10-C11-C12-O13
2	A	1101	ERY	O12-C11-C12-C13
2	A	1101	ERY	O12-C11-C12-C35
2	A	1101	ERY	O12-C11-C12-O13
2	A	1101	ERY	C11-C12-C13-O2

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Mol	Chain	Res	Type	Atoms
2	A	1101	ERY	C11-C12-C13-C36
2	A	1101	ERY	O13-C12-C13-O2
2	A	1101	ERY	C2-C1-O2-C13
2	A	1101	ERY	O1-C1-C2-C3
2	A	1101	ERY	C6-C5-O7-C22
2	A	1101	ERY	C32-C6-C7-C8
2	A	1101	ERY	O10-C6-C7-C8
2	A	1101	ERY	C23-C24-N1-C29
2	A	1101	ERY	C25-C24-N1-C29
2	D	1101	ERY	C9-C10-C11-C12
2	D	1101	ERY	C34-C10-C11-C12
2	D	1101	ERY	C10-C11-C12-C13
2	D	1101	ERY	C10-C11-C12-C35
2	D	1101	ERY	C10-C11-C12-O13
2	D	1101	ERY	O12-C11-C12-C35
2	D	1101	ERY	O12-C11-C12-O13
2	D	1101	ERY	O1-C1-O2-C13
2	D	1101	ERY	C33-C8-C9-C10
2	D	1101	ERY	C23-C24-N1-C29
2	D	1101	ERY	C25-C24-N1-C29
3	A	1103	LMT	C2'-C1'-O1'-C1
3	A	1103	LMT	O5'-C1'-O1'-C1
3	D	1102	LMT	C2'-C1'-O1'-C1
3	D	1103	LMT	O5B-C1B-O1B-C4'
3	E	1101	LMT	O5'-C5'-C6'-O6'
2	D	1101	ERY	C2-C1-O2-C13
3	A	1103	LMT	O5B-C1B-O1B-C4'
3	D	1103	LMT	C2-C3-C4-C5
3	E	1101	LMT	C4'-C5'-C6'-O6'
3	F	1101	LMT	C4B-C5B-C6B-O6B
3	D	1102	LMT	C3-C4-C5-C6
3	C	1101	LMT	O5'-C1'-O1'-C1
3	E	1101	LMT	O5'-C1'-O1'-C1
3	D	1102	LMT	C4B-C5B-C6B-O6B
3	E	1101	LMT	C3-C4-C5-C6
3	C	1101	LMT	O5'-C5'-C6'-O6'
3	C	1101	LMT	C2'-C1'-O1'-C1
3	E	1101	LMT	C2'-C1'-O1'-C1
3	E	1101	LMT	C4B-C5B-C6B-O6B
3	A	1103	LMT	C4B-C5B-C6B-O6B
3	B	1101	LMT	C4B-C5B-C6B-O6B
3	F	1101	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
3	C	1101	LMT	C4'-C5'-C6'-O6'
3	D	1102	LMT	O5'-C1'-O1'-C1
3	D	1102	LMT	O5B-C5B-C6B-O6B
3	E	1101	LMT	O1'-C1-C2-C3
3	A	1102	LMT	O1'-C1-C2-C3
2	A	1101	ERY	C25-C24-N1-C28
3	D	1103	LMT	C4-C5-C6-C7
2	A	1101	ERY	O1-C1-O2-C13
3	A	1102	LMT	C5-C6-C7-C8
3	B	1101	LMT	O5'-C5'-C6'-O6'
3	C	1101	LMT	C6-C7-C8-C9
3	A	1103	LMT	O5'-C5'-C6'-O6'
3	C	1101	LMT	O1'-C1-C2-C3
3	A	1102	LMT	C2'-C1'-O1'-C1
2	A	1101	ERY	O2-C13-C36-C37
3	B	1101	LMT	C4'-C5'-C6'-O6'
3	B	1101	LMT	C3-C4-C5-C6
2	A	1101	ERY	C4-C5-O7-C22
3	B	1101	LMT	C2-C3-C4-C5
3	A	1102	LMT	O5'-C1'-O1'-C1
3	D	1102	LMT	C11-C10-C9-C8
3	B	1101	LMT	O5B-C5B-C6B-O6B
3	A	1103	LMT	C2-C3-C4-C5
3	F	1101	LMT	O1'-C1-C2-C3
2	A	1101	ERY	C2-C3-C4-C31
2	A	1101	ERY	C35-C12-C13-C36
2	D	1101	ERY	C35-C12-C13-O2
2	A	1101	ERY	O3-C3-C4-C5
3	D	1103	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	C1-C2-C3-C4
3	E	1101	LMT	C5-C6-C7-C8
2	D	1101	ERY	C33-C8-C9-O11
3	D	1102	LMT	O1'-C1-C2-C3
3	A	1103	LMT	C4'-C5'-C6'-O6'
3	E	1101	LMT	C6-C7-C8-C9
2	D	1101	ERY	O12-C11-C12-C13
3	B	1101	LMT	C11-C10-C9-C8
3	B	1101	LMT	C4-C5-C6-C7
3	D	1102	LMT	C1-C2-C3-C4
3	E	1101	LMT	C9-C10-C11-C12
3	F	1101	LMT	C7-C8-C9-C10
3	B	1101	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	F	1101	LMT	C4-C5-C6-C7
3	D	1103	LMT	C2-C1-O1'-C1'
3	E	1101	LMT	C2-C1-O1'-C1'
2	A	1101	ERY	C7-C8-C9-C10
2	A	1101	ERY	O4-C14-O3-C3
2	A	1101	ERY	O3-C3-C4-C31
3	F	1101	LMT	C3-C4-C5-C6
3	F	1101	LMT	C1-C2-C3-C4
2	A	1101	ERY	C34-C10-C11-O12
3	D	1103	LMT	C6-C7-C8-C9
3	A	1103	LMT	O5B-C5B-C6B-O6B
3	A	1103	LMT	O1'-C1-C2-C3
3	D	1102	LMT	C6-C7-C8-C9
3	B	1101	LMT	C5-C6-C7-C8
2	D	1101	ERY	C11-C12-C13-O2
3	E	1101	LMT	O5B-C5B-C6B-O6B
3	A	1103	LMT	C4-C5-C6-C7
3	D	1103	LMT	C7-C8-C9-C10
3	D	1102	LMT	C5-C6-C7-C8
3	C	1101	LMT	C2-C1-O1'-C1'
2	A	1101	ERY	C2-C3-C4-C5
3	A	1103	LMT	C5-C6-C7-C8
2	D	1101	ERY	C4-C5-O7-C22
2	A	1101	ERY	C7-C8-C9-O11
2	D	1101	ERY	C6-C5-O7-C22
3	B	1101	LMT	C6-C7-C8-C9
2	A	1101	ERY	C6-C7-C8-C33
2	D	1101	ERY	O4-C14-O3-C3
3	A	1103	LMT	C6-C7-C8-C9
3	D	1103	LMT	C3-C4-C5-C6
2	D	1101	ERY	C7-C8-C9-C10
3	D	1103	LMT	C1-C2-C3-C4
2	A	1101	ERY	C12-C13-C36-C37
2	D	1101	ERY	C34-C10-C11-O12
2	D	1101	ERY	C32-C6-C7-C8
2	A	1101	ERY	C9-C10-C11-O12
2	D	1101	ERY	C9-C10-C11-O12
3	D	1102	LMT	C9-C10-C11-C12
3	E	1101	LMT	C11-C10-C9-C8
2	A	1101	ERY	C6-C7-C8-C9
3	A	1102	LMT	C11-C10-C9-C8
3	A	1102	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	E	1101	LMT	C4-C5-C6-C7
3	C	1101	LMT	C4-C5-C6-C7
3	F	1101	LMT	C4'-C5'-C6'-O6'
3	C	1101	LMT	C7-C8-C9-C10
2	D	1101	ERY	C7-C8-C9-O11
3	D	1103	LMT	C9-C10-C11-C12
3	A	1102	LMT	C3-C4-C5-C6

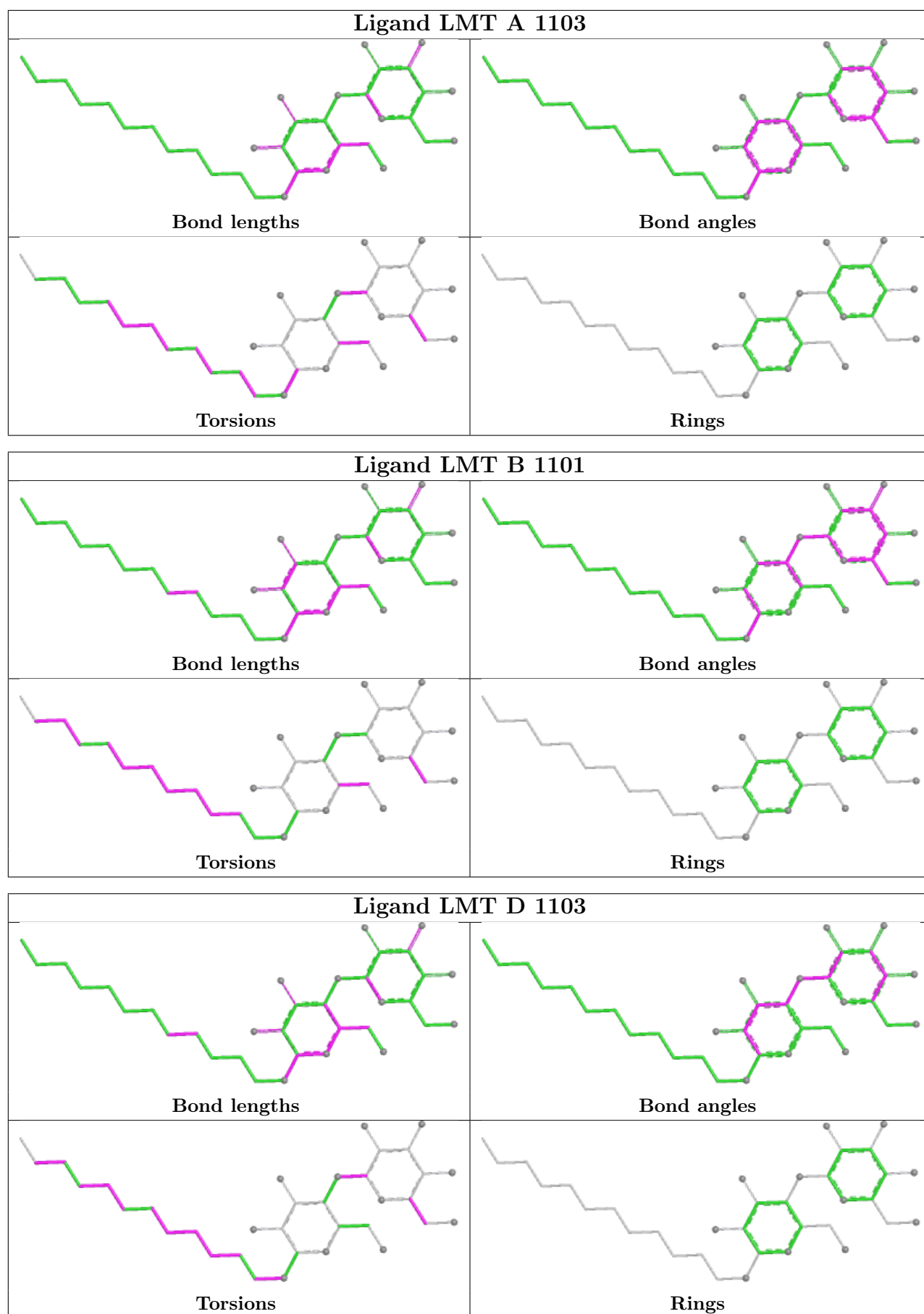
All (1) ring outliers are listed below:

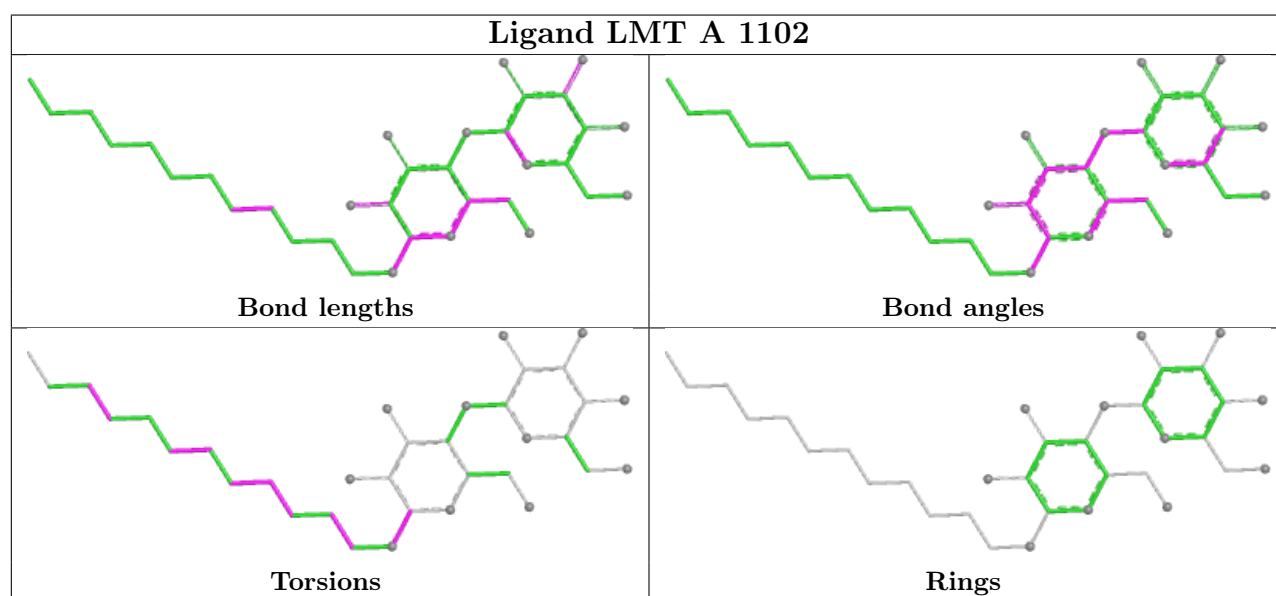
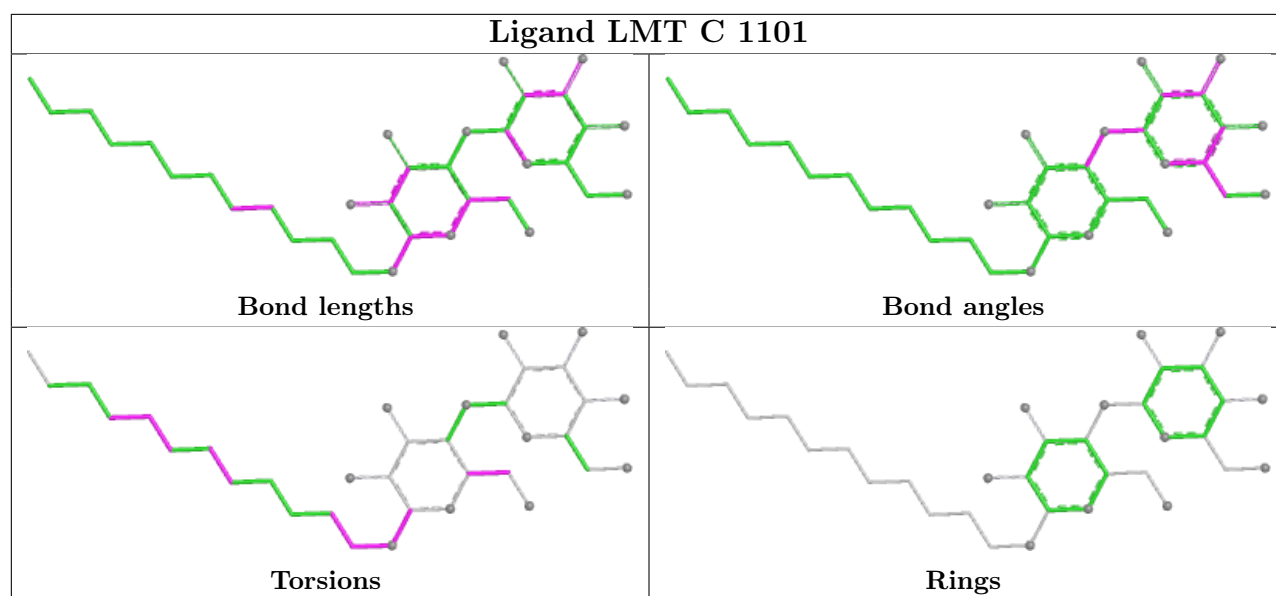
Mol	Chain	Res	Type	Atoms
2	D	1101	ERY	C22-C23-C24-C25-C26-O9

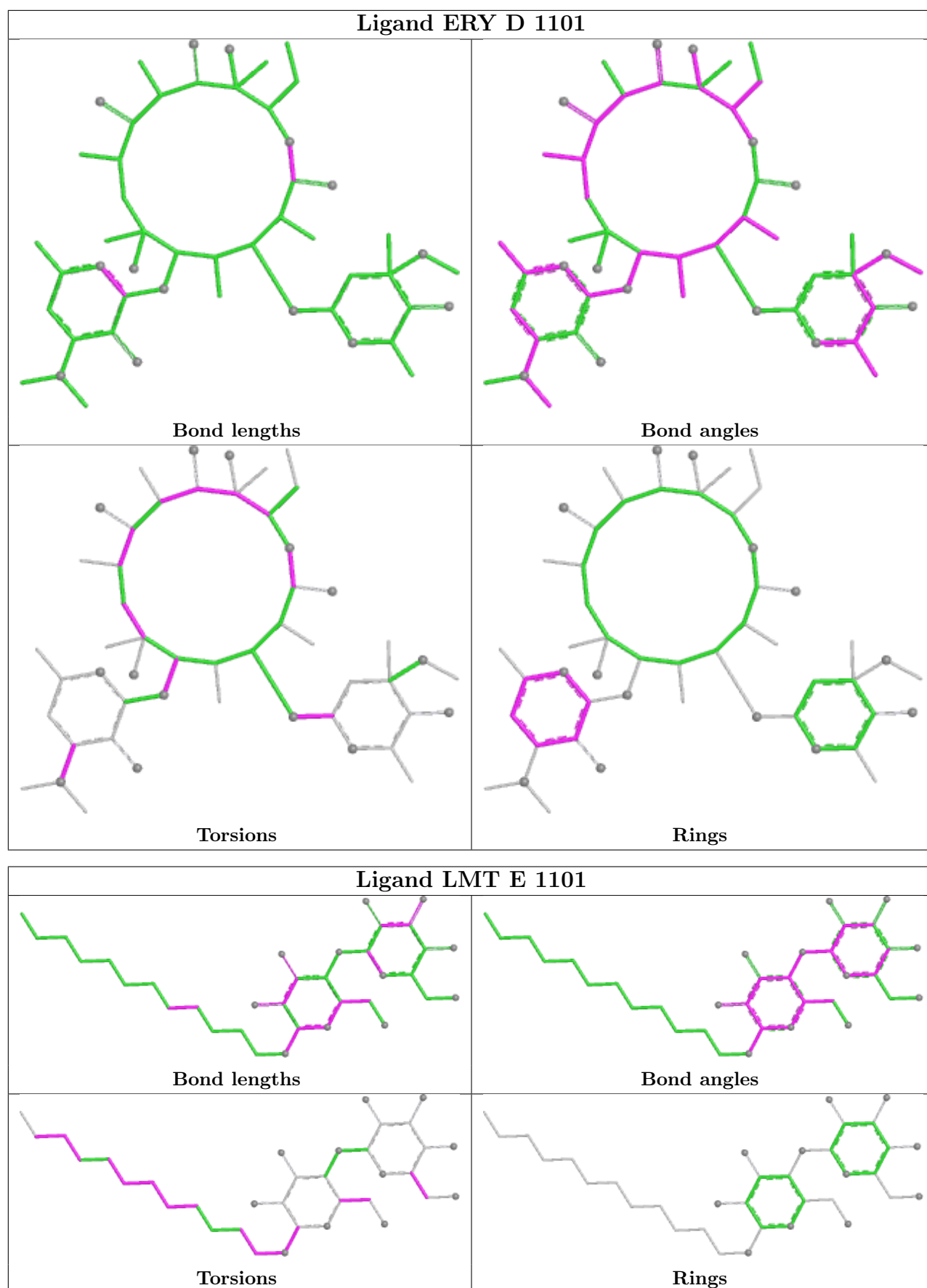
9 monomers are involved in 49 short contacts:

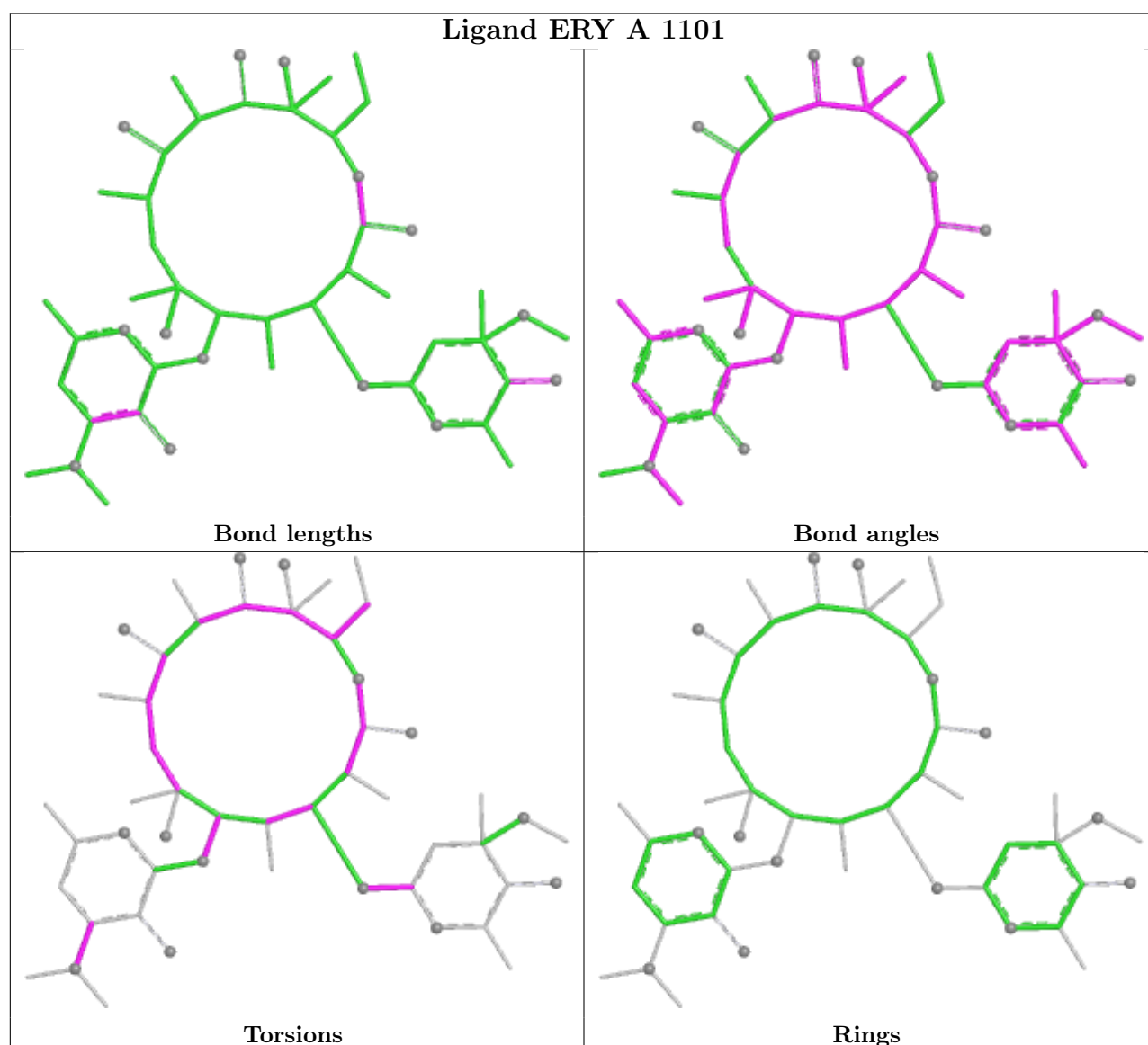
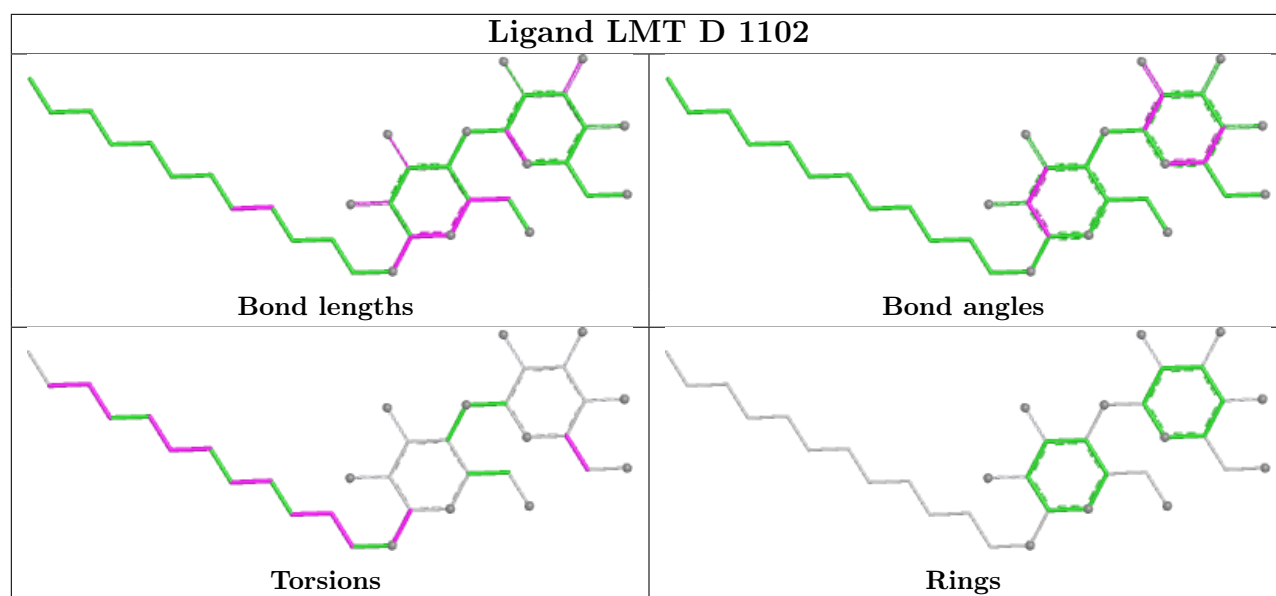
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1103	LMT	9	0
3	B	1101	LMT	5	0
3	D	1103	LMT	5	0
3	C	1101	LMT	2	0
3	A	1102	LMT	4	0
2	D	1101	ERY	12	0
3	E	1101	LMT	5	0
3	D	1102	LMT	1	0
2	A	1101	ERY	6	0

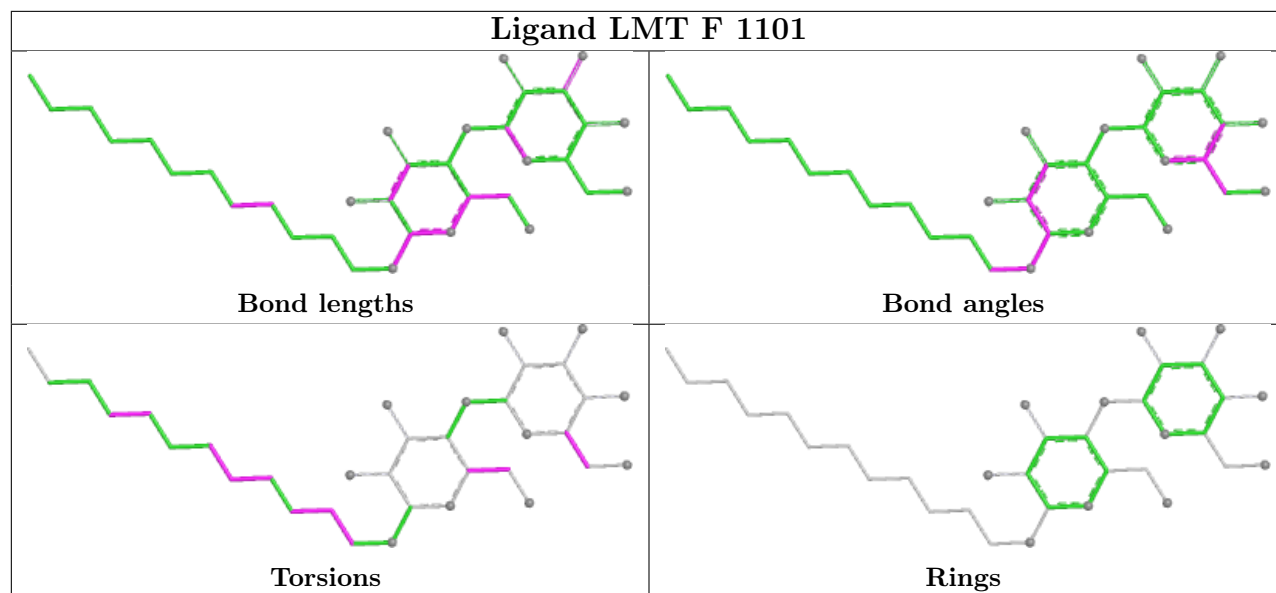
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	1044/1049 (99%)	0.13	27 (2%) 57 34	46, 78, 106, 147	0
1	B	1042/1049 (99%)	0.05	15 (1%) 73 49	50, 76, 102, 148	0
1	C	1042/1049 (99%)	0.17	43 (4%) 41 23	43, 77, 103, 155	0
1	D	1042/1049 (99%)	0.17	16 (1%) 72 48	45, 86, 112, 147	0
1	E	1042/1049 (99%)	0.18	23 (2%) 62 38	55, 86, 108, 147	0
1	F	1043/1049 (99%)	0.24	52 (4%) 34 19	52, 82, 106, 158	0
All	All	6255/6294 (99%)	0.16	176 (2%) 55 32	43, 81, 107, 158	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	291	ILE	7.5
1	F	503	GLY	6.0
1	F	48	SER	6.0
1	E	290	GLY	5.5
1	B	869	SER	5.0
1	C	122	VAL	4.9
1	D	59	ASP	4.8
1	C	127	VAL	4.8
1	D	389	SER	4.6
1	F	59	ASP	4.6
1	F	57	VAL	4.5
1	F	107	VAL	4.5
1	B	870	GLY	4.4
1	C	97	GLY	4.4
1	F	122	VAL	4.3
1	B	715	SER	4.3
1	C	871	ASN	4.2
1	C	57	VAL	4.1
1	A	494	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	33	ALA	3.7
1	B	858	ASP	3.7
1	F	47	ALA	3.6
1	F	306	ILE	3.6
1	F	406	VAL	3.6
1	C	54	ALA	3.6
1	F	855	VAL	3.6
1	F	118	LEU	3.6
1	C	822	LEU	3.5
1	D	681	ASP	3.5
1	C	719	ASN	3.5
1	F	49	TYR	3.4
1	F	685	ILE	3.4
1	C	872	GLN	3.4
1	E	869	SER	3.4
1	A	486	LEU	3.4
1	F	849	SER	3.3
1	D	460	GLY	3.3
1	B	488	LEU	3.3
1	F	127	VAL	3.3
1	F	865	GLN	3.3
1	C	385	ALA	3.3
1	F	126	GLY	3.3
1	D	306	ILE	3.2
1	C	9	PRO	3.2
1	B	59	ASP	3.2
1	F	410	ILE	3.1
1	C	501	ALA	3.1
1	C	826	GLU	3.1
1	F	856	GLY	3.0
1	C	79	SER	3.0
1	A	59	ASP	3.0
1	B	515	TRP	2.9
1	F	501	ALA	2.9
1	C	684	LEU	2.9
1	A	330	THR	2.9
1	A	938	SER	2.9
1	F	79	SER	2.9
1	A	407	ASP	2.8
1	E	293	LEU	2.8
1	A	43	VAL	2.8
1	F	2	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	509	LYS	2.8
1	F	60	THR	2.8
1	F	56	THR	2.7
1	F	504	ASP	2.7
1	D	2	PRO	2.7
1	D	870	GLY	2.7
1	C	855	VAL	2.7
1	A	332	PHE	2.7
1	D	504	ASP	2.7
1	E	6	ILE	2.6
1	A	834	GLY	2.6
1	E	826	GLU	2.6
1	E	508	GLY	2.6
1	F	848	ALA	2.6
1	C	118	LEU	2.6
1	E	488	LEU	2.6
1	D	486	LEU	2.6
1	C	107	VAL	2.6
1	D	459	PHE	2.5
1	E	681	ASP	2.5
1	F	686	ASP	2.5
1	C	86	GLY	2.5
1	C	49	TYR	2.5
1	C	32	VAL	2.5
1	A	473	THR	2.5
1	F	702	LEU	2.5
1	A	508	GLY	2.5
1	D	401	ALA	2.5
1	A	866	GLU	2.5
1	A	92	LEU	2.4
1	F	675	GLY	2.4
1	F	10	ILE	2.4
1	E	292	LYS	2.4
1	B	678	THR	2.4
1	E	706	ALA	2.4
1	A	310	LEU	2.4
1	F	9	PRO	2.4
1	C	10	ILE	2.4
1	F	402	ILE	2.4
1	E	866	GLU	2.4
1	C	1040	ILE	2.4
1	F	822	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	32	VAL	2.4
1	C	848	ALA	2.3
1	C	511	GLY	2.3
1	F	69	MET	2.3
1	E	709	HIS	2.3
1	F	442	LEU	2.3
1	A	714	THR	2.3
1	B	167	SER	2.3
1	F	837	THR	2.3
1	A	21	LEU	2.3
1	F	117	LEU	2.3
1	D	855	VAL	2.3
1	A	503	GLY	2.3
1	C	126	GLY	2.3
1	B	895	TRP	2.3
1	F	516	PHE	2.3
1	C	147	GLY	2.2
1	D	236	ALA	2.2
1	F	871	ASN	2.2
1	E	495	THR	2.2
1	C	48	SER	2.2
1	E	167	SER	2.2
1	E	1043	SER	2.2
1	B	716	VAL	2.2
1	C	95	GLU	2.2
1	A	674	LEU	2.2
1	F	698	ALA	2.2
1	C	512	PHE	2.2
1	F	415	ASN	2.2
1	A	403	GLY	2.2
1	E	285	PRO	2.2
1	F	558	ARG	2.2
1	F	473	THR	2.2
1	D	32	VAL	2.2
1	C	390	ILE	2.2
1	C	421	ALA	2.2
1	F	50	PRO	2.2
1	D	214	VAL	2.1
1	F	6	ILE	2.1
1	A	368	PRO	2.1
1	A	515	TRP	2.1
1	D	473	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	674	LEU	2.1
1	C	125	GLN	2.1
1	A	939	ALA	2.1
1	E	465	ALA	2.1
1	A	445	ILE	2.1
1	E	541	TYR	2.1
1	C	854	GLY	2.1
1	F	502	LYS	2.1
1	B	866	GLU	2.1
1	F	512	PHE	2.1
1	C	80	SER	2.1
1	B	32	VAL	2.1
1	E	405	LEU	2.1
1	F	329	THR	2.1
1	C	451	ALA	2.1
1	C	494	ALA	2.1
1	F	294	ALA	2.1
1	A	411	VAL	2.0
1	C	129	VAL	2.0
1	E	253	VAL	2.0
1	C	836	SER	2.0
1	E	1002	ALA	2.0
1	C	865	GLN	2.0
1	A	383	LEU	2.0
1	A	306	ILE	2.0
1	C	60	THR	2.0
1	E	114	ALA	2.0
1	A	2	PRO	2.0
1	F	437	GLN	2.0
1	B	175	VAL	2.0
1	C	868	LEU	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

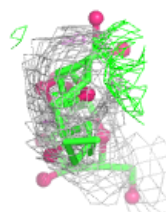
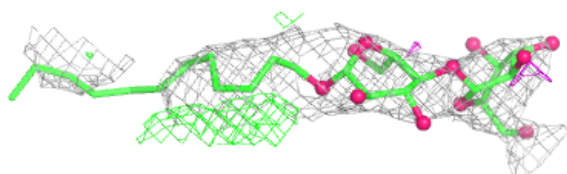
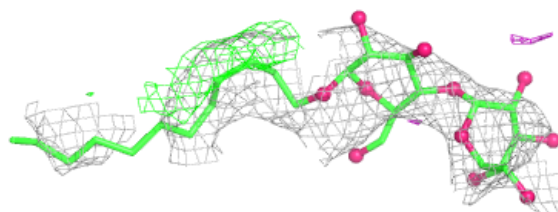
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	LMT	D	1103	35/35	0.57	0.21	79,95,103,110	0
2	ERY	D	1101	51/51	0.59	0.18	71,84,96,107	51
3	LMT	F	1101	35/35	0.68	0.13	48,88,105,110	0
2	ERY	A	1101	51/51	0.79	0.15	70,79,90,95	51
3	LMT	B	1101	35/35	0.79	0.12	53,82,105,107	0
3	LMT	A	1103	35/35	0.81	0.15	82,95,107,111	0
3	LMT	E	1101	35/35	0.84	0.10	45,79,97,125	0
3	LMT	A	1102	35/35	0.84	0.09	28,83,89,94	0
3	LMT	C	1101	35/35	0.87	0.10	64,84,95,96	0
3	LMT	D	1102	35/35	0.88	0.09	64,82,96,102	0
4	NI	A	1104	1/1	0.99	0.04	61,61,61,61	0
4	NI	C	1102	1/1	0.99	0.02	72,72,72,72	0
4	NI	E	1102	1/1	1.00	0.02	79,79,79,79	0

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

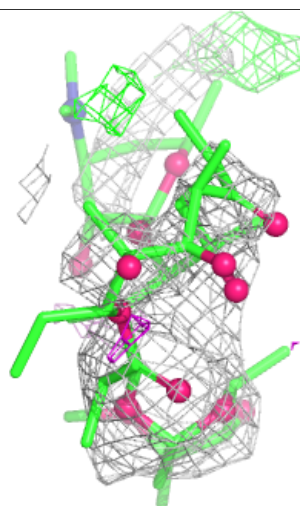
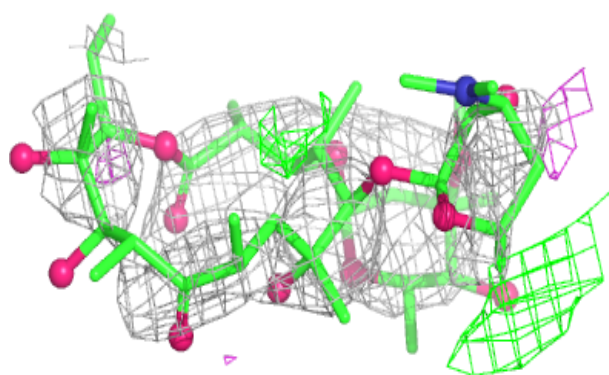
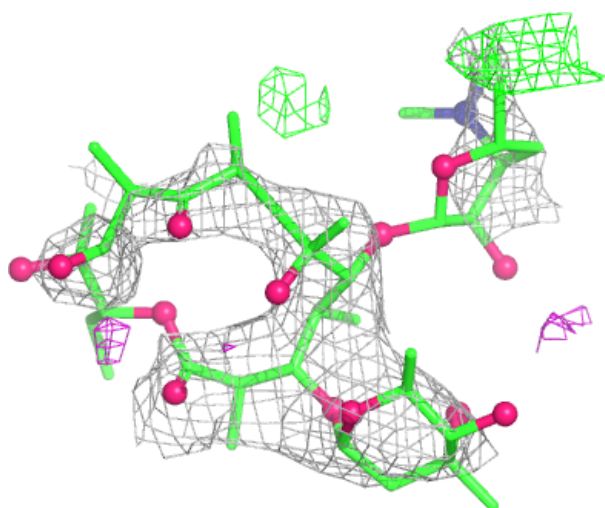
Electron density around LMT D 1103:

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



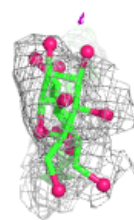
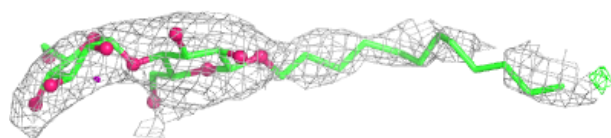
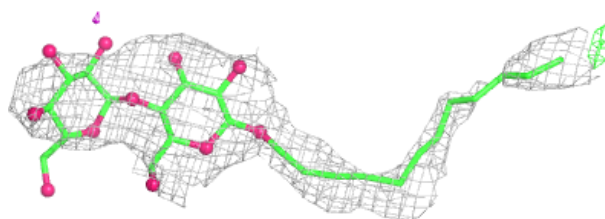
Electron density around ERY D 1101:

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



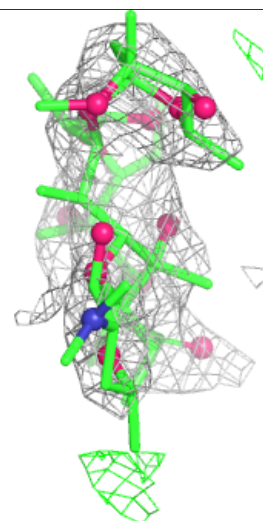
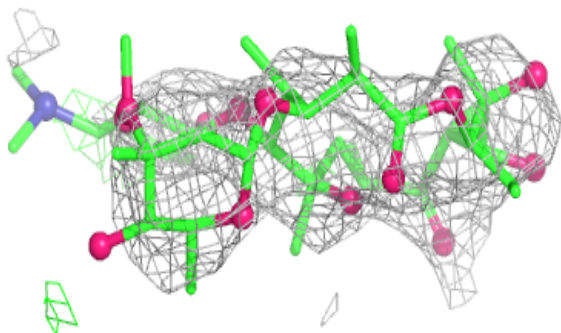
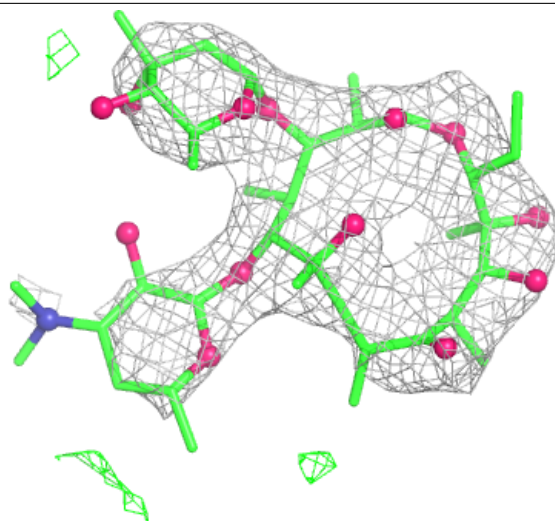
Electron density around LMT F 1101:

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



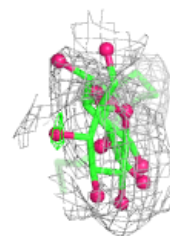
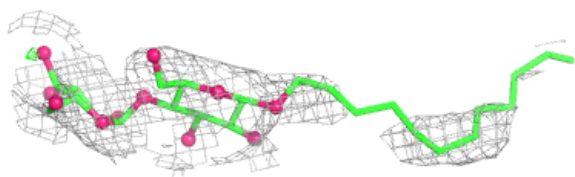
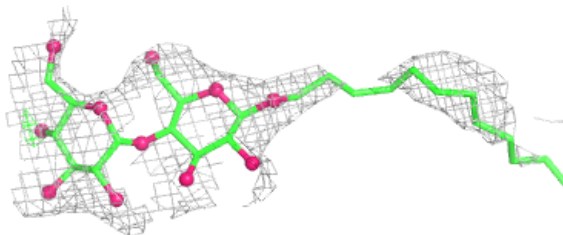
Electron density around ERY A 1101:

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

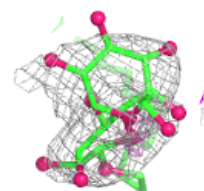
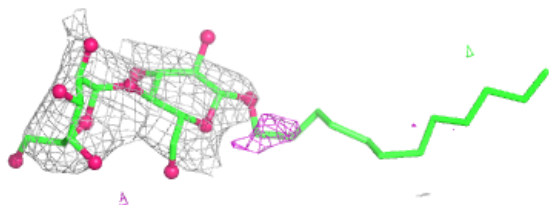
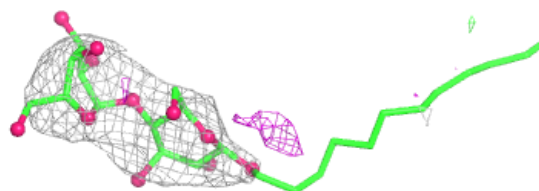


Electron density around LMT B 1101:

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

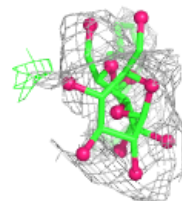
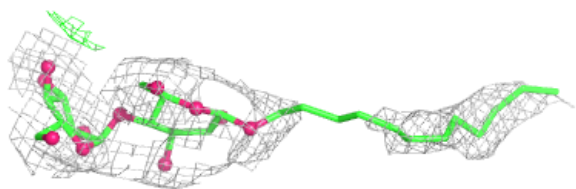
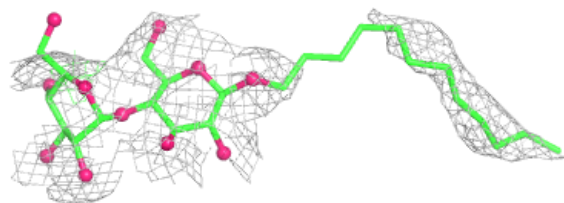
**Electron density around LMT A 1103:**

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

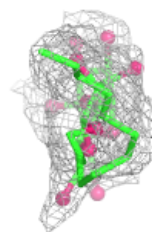
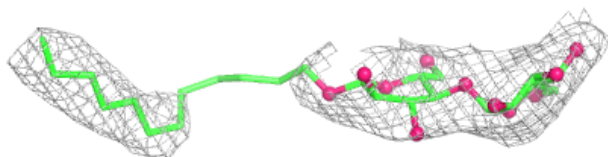
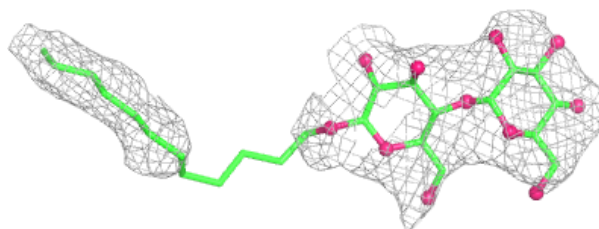


Electron density around LMT E 1101:

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

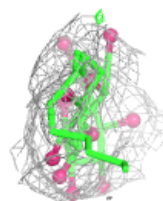
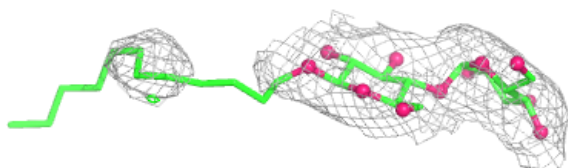
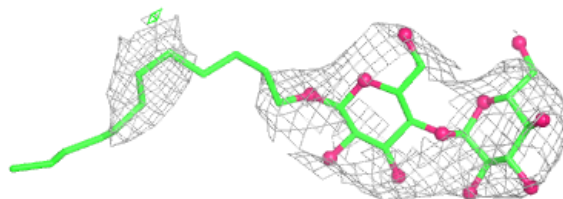
**Electron density around LMT A 1102:**

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

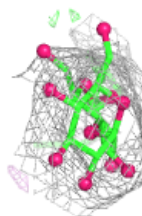
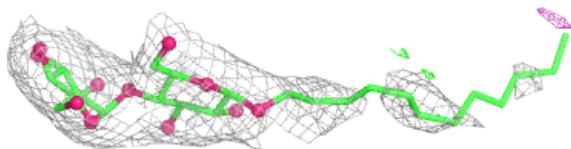
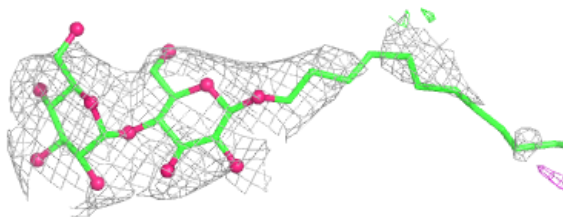


Electron density around LMT C 1101:

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

**Electron density around LMT 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.