



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:44 AM UTC

PDB ID : 4ZIT / pdb_00004zit
Title : Crystal structure of AcrB in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-28
Resolution : 3.30 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

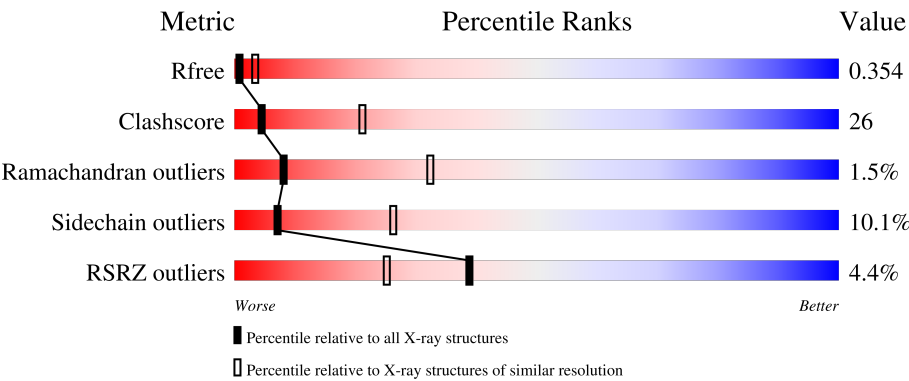
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	4% 46% 46% 7%
1	B	1049	2% 50% 43% 6%
1	C	1049	4% 45% 47% 6%
1	D	1049	3% 43% 49% 6%
1	E	1049	5% 45% 47% 7%

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Mol	Chain	Length	Quality of chain
1	F	1049	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	C	1101	X	-	-	-

2 Entry composition [i](#)

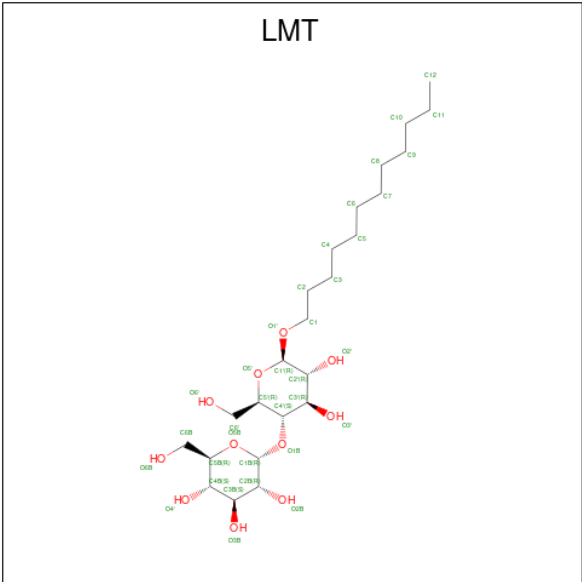
There are 3 unique types of molecules in this entry. The entry contains 47773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	B	1043	Total	C	N	O	S	0	0	0
			7935	5101	1314	1477	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	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

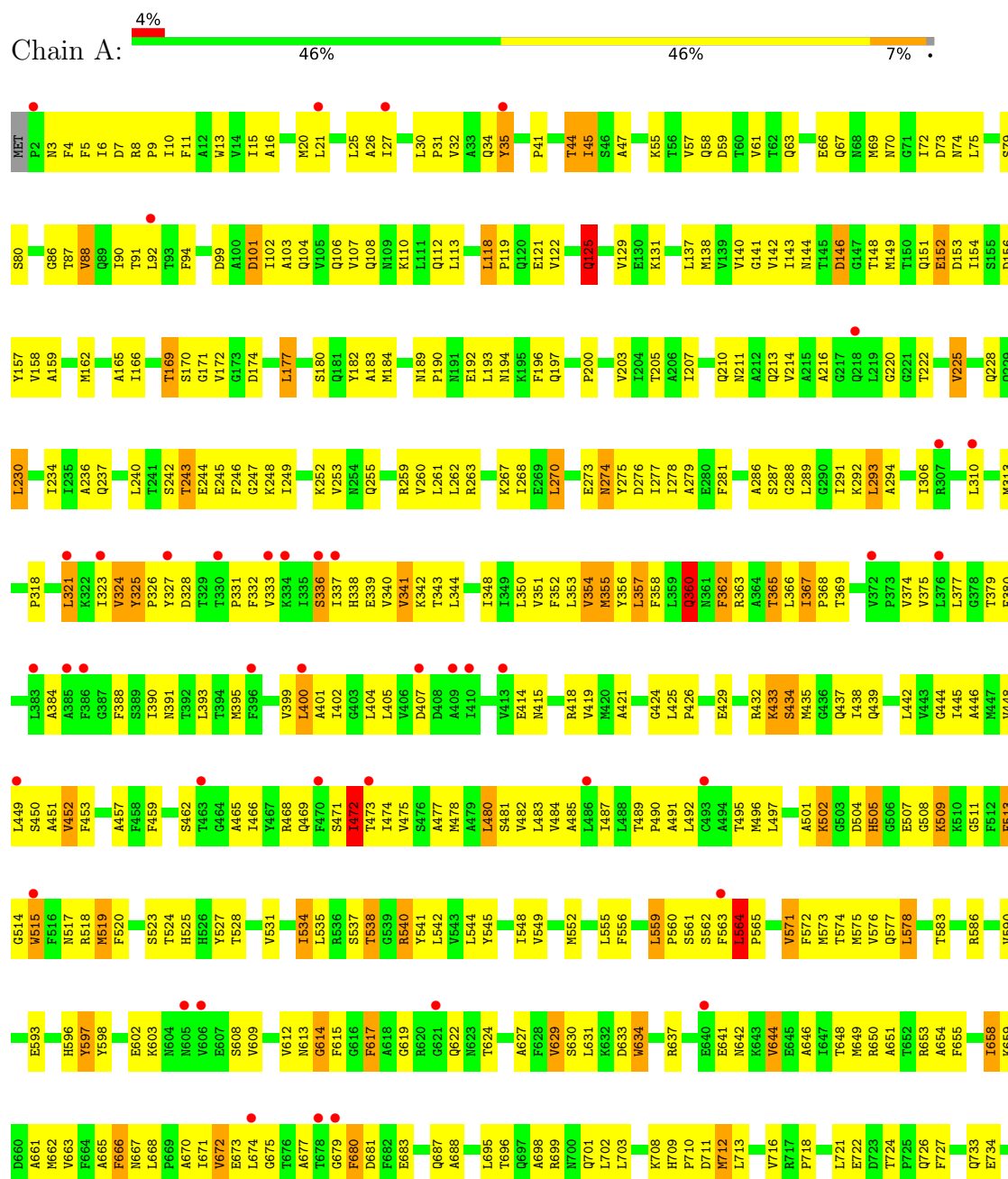
- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

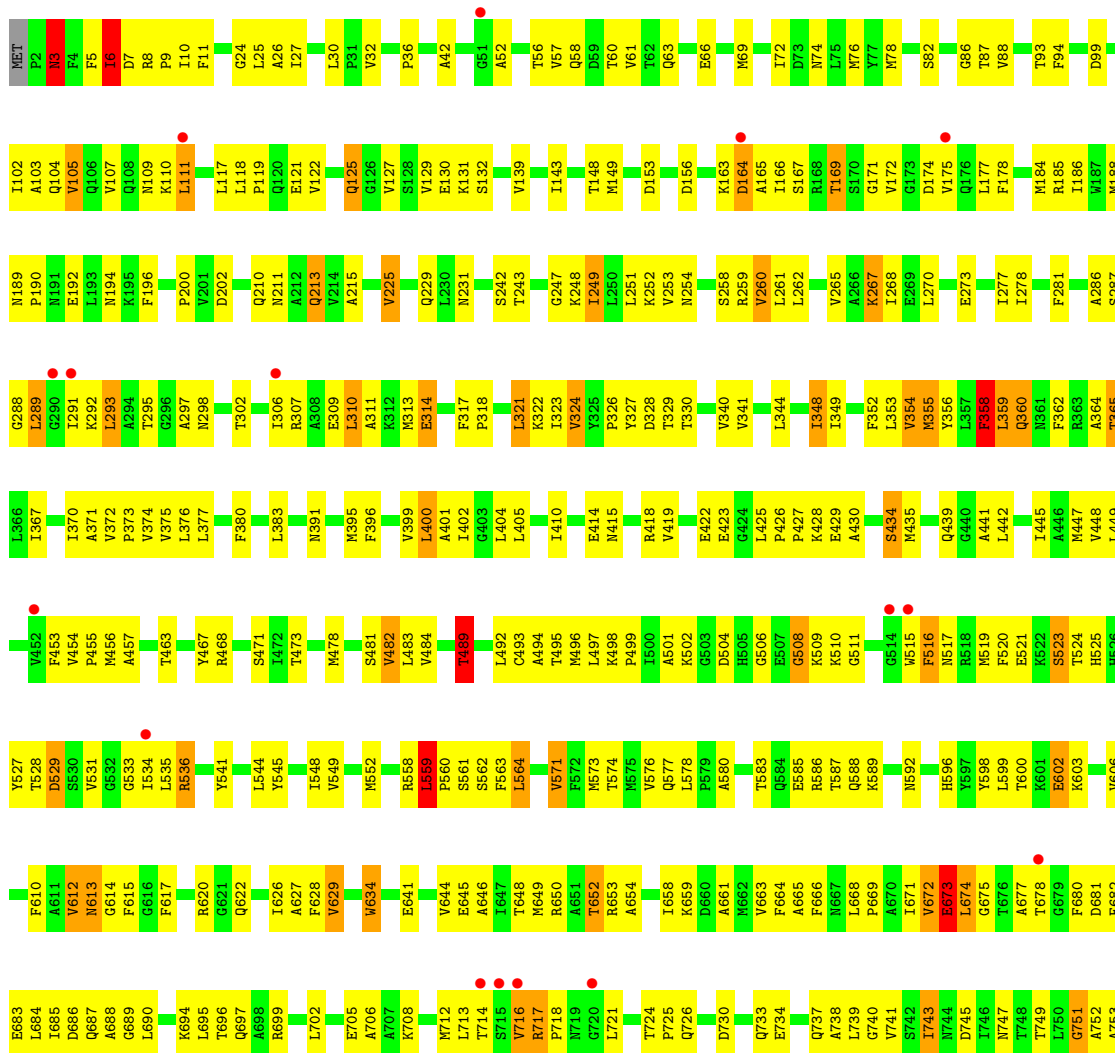
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0
3	C	1	Total Ni 1 1	0	0
3	E	1	Total Ni 1 1	0	0

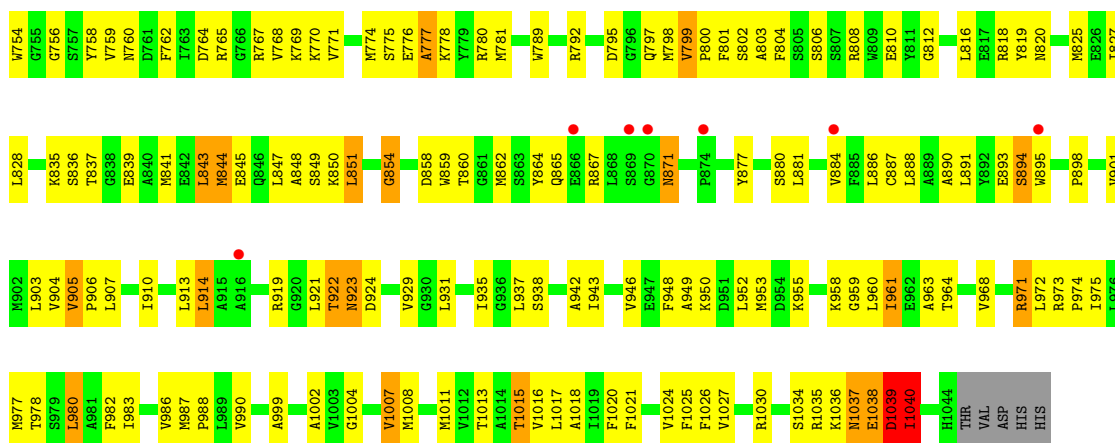
3 Residue-property plots

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.

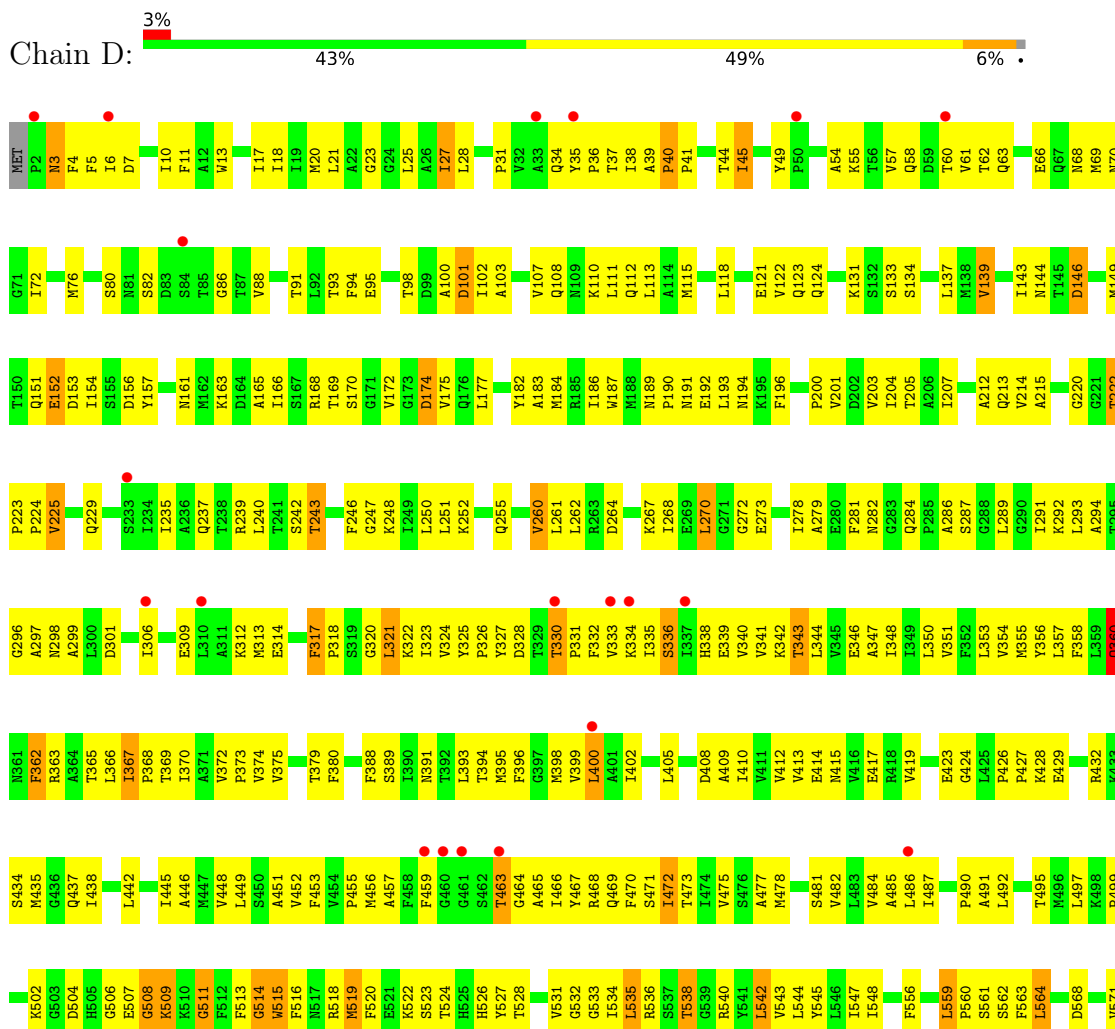
• Molecule 1: Multidrug efflux pump subunit AcrB

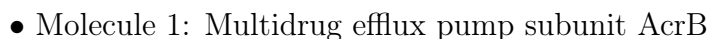


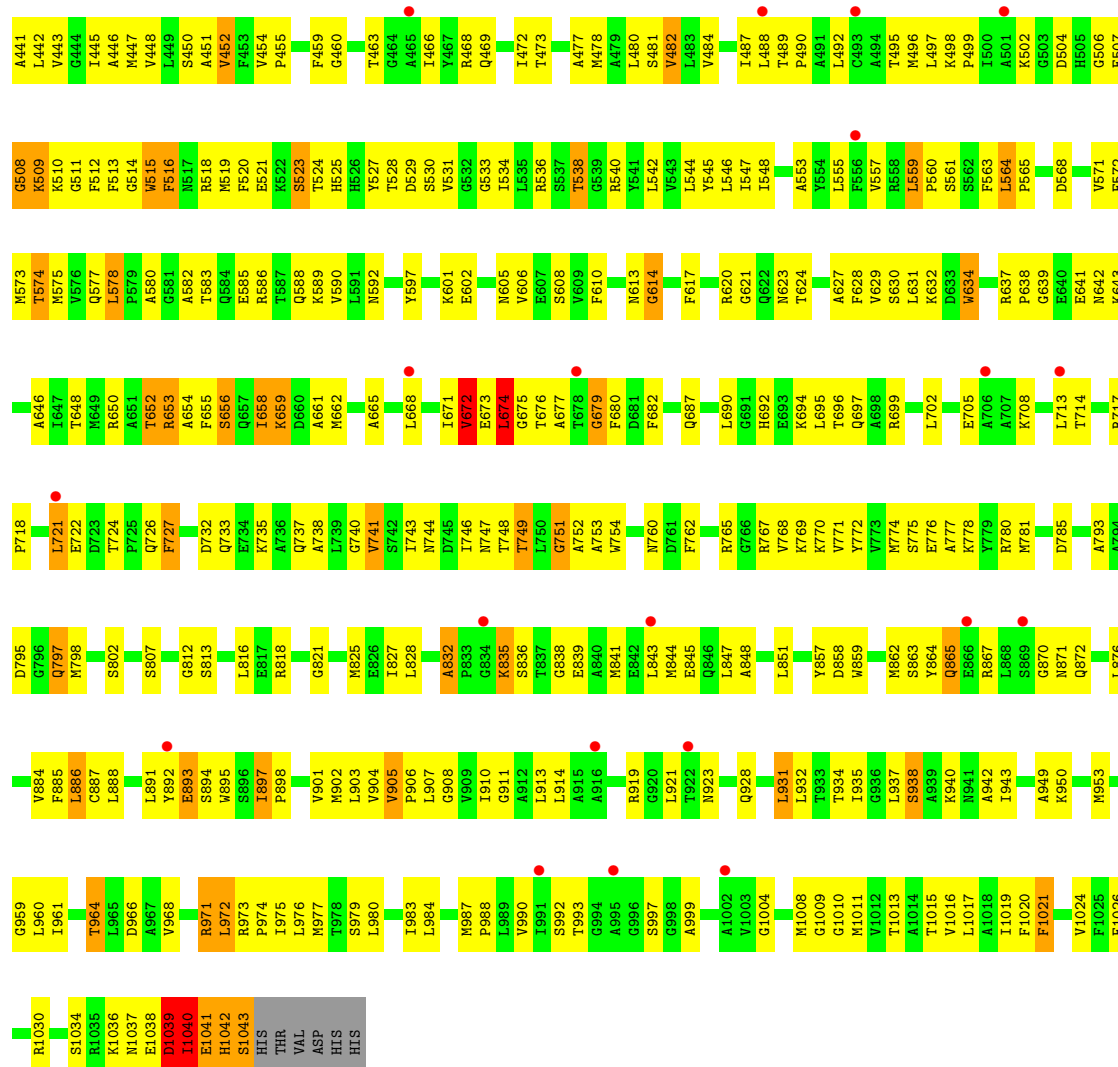




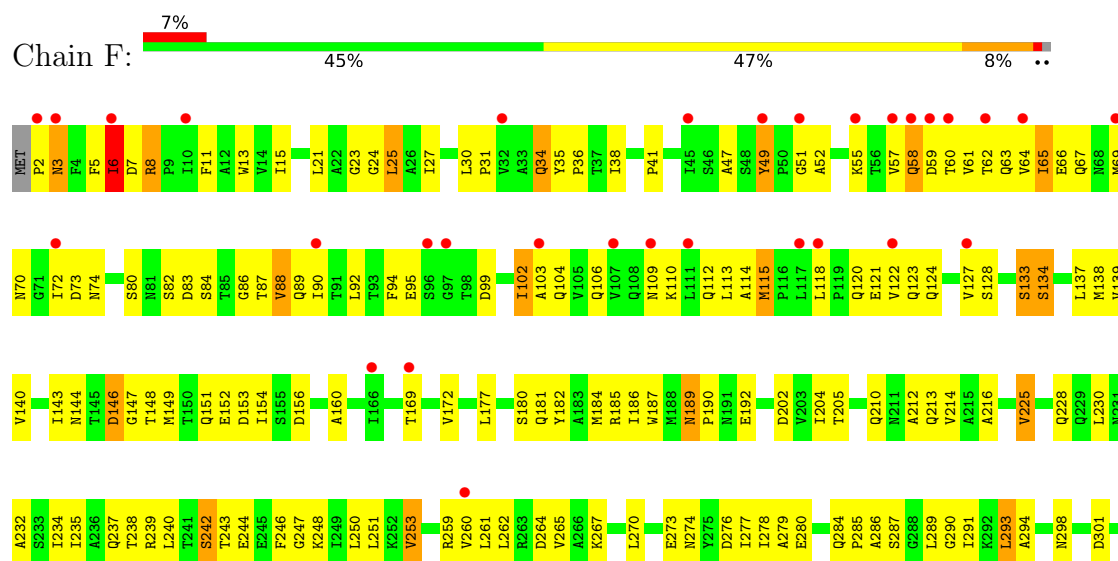
- Molecule 1: Multidrug efflux pump subunit AcrB







• Molecule 1: Multidrug efflux pump subunit AcrB





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.84Å 156.86Å 218.58Å 90.00° 92.70° 90.00°	Depositor
Resolution (Å)	19.95 – 3.30 19.95 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.95-3.30) 96.8 (19.95-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.268 , 0.339 0.281 , 0.354	Depositor DCC
R_{free} test set	7703 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	92.0	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.095 for -k,-h,-l 0.105 for k,h,-l 0.105 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47773	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 47.49 % 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 9.8479e-05.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	3/8076 (0.0%)	1.25	47/10965 (0.4%)
1	B	0.84	4/8087 (0.0%)	1.23	48/10980 (0.4%)
1	C	0.85	1/8076 (0.0%)	1.26	54/10965 (0.5%)
1	D	0.78	1/8076 (0.0%)	1.24	49/10965 (0.4%)
1	E	0.78	2/8076 (0.0%)	1.20	40/10965 (0.4%)
1	F	0.81	4/8076 (0.0%)	1.25	51/10965 (0.5%)
All	All	0.82	15/48467 (0.0%)	1.24	289/65805 (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	2
1	B	0	1
1	C	0	2
1	E	0	1
1	F	0	2
All	All	0	8

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	905	VAL	CA-CB	8.00	1.58	1.54
1	A	1022	VAL	CA-CB	7.75	1.58	1.54
1	F	426	PRO	CA-C	7.25	1.55	1.51
1	F	897	ILE	CA-CB	6.23	1.58	1.53
1	F	534	ILE	CA-CB	6.02	1.61	1.54
1	D	399	VAL	CA-CB	-5.56	1.48	1.54
1	B	534	ILE	CA-CB	5.48	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	905	VAL	CA-CB	5.43	1.56	1.54
1	F	676	THR	CA-CB	5.42	1.61	1.53
1	C	426	PRO	CA-C	5.38	1.54	1.51
1	A	505	HIS	ND1-CE1	-5.37	1.27	1.32
1	B	982	PHE	CA-C	-5.32	1.46	1.52
1	E	931	LEU	CA-C	-5.30	1.45	1.52
1	A	505	HIS	CG-ND1	5.15	1.44	1.38
1	B	105	VAL	CA-CB	5.07	1.60	1.54

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	673	GLU	N-CA-C	10.48	125.79	111.54
1	B	559	LEU	CA-C-N	10.44	130.20	119.76
1	B	559	LEU	C-N-CA	10.44	130.20	119.76
1	A	679	GLY	N-CA-C	10.04	124.04	110.69
1	D	515	TRP	N-CA-C	-9.94	100.41	112.54
1	D	509	LYS	N-CA-C	9.81	121.56	111.07
1	C	515	TRP	N-CA-C	-9.75	100.50	111.71
1	A	35	TYR	CA-C-N	-9.53	111.07	120.21
1	A	35	TYR	C-N-CA	-9.53	111.07	120.21
1	F	515	TRP	N-CA-C	-9.44	100.86	111.71
1	E	515	TRP	N-CA-C	-9.34	100.98	111.82
1	C	39	ALA	CA-C-N	9.33	126.47	119.66
1	C	39	ALA	C-N-CA	9.33	126.47	119.66
1	D	374	VAL	N-CA-C	8.89	118.89	110.53
1	B	489	THR	CA-C-N	-8.40	109.72	119.05
1	B	489	THR	C-N-CA	-8.40	109.72	119.05
1	E	498	LYS	CA-C-N	8.21	128.14	119.85
1	E	498	LYS	C-N-CA	8.21	128.14	119.85
1	F	668	LEU	CA-C-N	8.06	127.95	120.21
1	F	668	LEU	C-N-CA	8.06	127.95	120.21
1	B	367	ILE	CA-C-N	-7.76	111.72	119.56
1	B	367	ILE	C-N-CA	-7.76	111.72	119.56
1	D	367	ILE	CA-C-N	-7.74	111.75	119.56
1	D	367	ILE	C-N-CA	-7.74	111.75	119.56
1	C	8	ARG	CA-C-N	7.70	127.75	119.28
1	C	8	ARG	C-N-CA	7.70	127.75	119.28
1	A	515	TRP	N-CA-C	-7.58	103.13	112.38
1	B	617	PHE	N-CA-C	-7.55	103.65	113.17
1	F	7	ASP	CA-C-N	7.50	130.69	122.74
1	F	7	ASP	C-N-CA	7.50	130.69	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	564	LEU	CA-C-N	7.48	127.24	119.76
1	D	564	LEU	C-N-CA	7.48	127.24	119.76
1	A	426	PRO	CA-C-N	7.29	128.96	119.84
1	A	426	PRO	C-N-CA	7.29	128.96	119.84
1	E	964	THR	N-CA-C	-7.23	103.40	111.28
1	A	118	LEU	CA-C-N	7.20	127.63	119.92
1	A	118	LEU	C-N-CA	7.20	127.63	119.92
1	D	314	GLU	N-CA-C	7.13	123.42	113.57
1	F	404	LEU	N-CA-C	7.13	120.46	111.69
1	C	967	ALA	N-CA-C	-7.08	103.25	110.97
1	C	115	MET	N-CA-C	7.08	123.29	113.45
1	F	189	ASN	CA-C-N	7.05	126.66	119.19
1	F	189	ASN	C-N-CA	7.05	126.66	119.19
1	A	472	ILE	N-CA-C	6.96	117.08	110.53
1	D	813	SER	CA-C-N	6.96	127.92	120.47
1	D	813	SER	C-N-CA	6.96	127.92	120.47
1	A	434	SER	N-CA-C	-6.92	103.82	111.36
1	C	617	PHE	N-CA-C	-6.92	104.46	113.17
1	F	562	SER	N-CA-C	6.84	120.46	109.79
1	A	867	ARG	N-CA-C	6.83	119.74	111.82
1	C	531	VAL	N-CA-C	-6.81	103.68	110.62
1	B	851	LEU	CA-C-N	6.77	127.16	119.92
1	B	851	LEU	C-N-CA	6.77	127.16	119.92
1	B	854	GLY	N-CA-C	-6.74	106.45	115.21
1	F	812	GLY	N-CA-C	-6.71	99.72	110.18
1	B	894	SER	N-CA-C	6.71	120.09	109.50
1	A	513	PHE	N-CA-C	-6.69	104.25	112.88
1	B	1037	ASN	CA-C-N	6.68	133.73	121.70
1	B	1037	ASN	C-N-CA	6.68	133.73	121.70
1	B	674	LEU	N-CA-C	6.66	119.54	110.55
1	A	341	VAL	N-CA-C	6.65	116.78	110.53
1	D	1034	SER	N-CA-C	6.65	119.77	109.60
1	C	619	GLY	N-CA-C	-6.63	101.14	110.63
1	A	426	PRO	O-C-N	6.62	124.36	121.31
1	F	617	PHE	N-CA-C	-6.62	104.83	113.17
1	C	180	SER	N-CA-C	6.57	119.88	109.50
1	B	359	LEU	N-CA-C	-6.57	104.99	114.12
1	A	614	GLY	N-CA-C	-6.50	106.47	114.92
1	D	617	PHE	N-CA-C	-6.49	104.99	113.17
1	F	964	THR	N-CA-C	-6.49	104.20	111.28
1	F	60	THR	N-CA-C	-6.47	105.03	113.12
1	A	782	LEU	CA-C-N	6.42	126.10	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	782	LEU	C-N-CA	6.42	126.10	119.56
1	F	89	GLN	N-CA-C	6.41	118.89	107.80
1	F	122	VAL	N-CA-C	-6.38	104.53	110.53
1	A	673	GLU	N-CA-C	6.38	120.21	111.54
1	F	616	GLY	N-CA-C	-6.37	102.38	111.42
1	A	433	LYS	N-CA-C	6.34	117.85	111.07
1	A	680	PHE	N-CA-C	6.34	118.58	109.14
1	C	90	ILE	N-CA-C	6.33	116.98	107.80
1	B	3	ASN	N-CA-C	-6.32	104.48	111.36
1	D	992	SER	N-CA-C	6.31	124.23	110.80
1	D	666	PHE	N-CA-C	6.29	118.33	108.96
1	E	521	GLU	N-CA-C	6.26	117.80	110.97
1	C	946	VAL	N-CA-C	6.26	116.43	110.42
1	F	691	GLY	N-CA-C	6.25	120.56	112.18
1	E	323	ILE	N-CA-C	-6.23	100.74	109.21
1	C	945	ILE	N-CA-C	6.23	116.28	110.42
1	C	973	ARG	CA-C-N	-6.22	112.44	119.28
1	C	973	ARG	C-N-CA	-6.22	112.44	119.28
1	D	426	PRO	O-C-N	6.22	124.17	121.31
1	E	77	TYR	N-CA-C	6.16	117.59	108.60
1	C	278	ILE	N-CA-C	6.15	117.63	108.46
1	C	277	ILE	N-CA-C	6.14	116.71	107.75
1	C	172	VAL	N-CA-C	6.14	116.95	107.99
1	D	317	PHE	CA-C-N	6.13	126.09	120.21
1	D	317	PHE	C-N-CA	6.13	126.09	120.21
1	D	975	ILE	N-CA-C	-6.10	103.95	110.36
1	E	727	PHE	N-CA-C	6.09	119.63	107.62
1	A	365	THR	N-CA-C	-6.08	105.12	112.54
1	B	498	LYS	N-CA-C	6.07	117.46	109.93
1	B	1039	ASP	N-CA-C	-6.07	106.20	113.97
1	B	905	VAL	CB-CA-C	-6.06	107.94	113.70
1	C	85	THR	N-CA-C	-6.06	106.14	112.93
1	A	325	TYR	CA-C-N	6.04	127.38	119.84
1	A	325	TYR	C-N-CA	6.04	127.38	119.84
1	F	8	ARG	CA-C-N	6.03	125.91	119.28
1	F	8	ARG	C-N-CA	6.03	125.91	119.28
1	B	426	PRO	CA-C-N	6.01	127.36	119.84
1	B	426	PRO	C-N-CA	6.01	127.36	119.84
1	A	509	LYS	CA-C-N	-5.99	113.25	122.60
1	A	509	LYS	C-N-CA	-5.99	113.25	122.60
1	C	386	PHE	N-CA-C	-5.99	105.73	113.16
1	C	22	ALA	N-CA-C	-5.98	104.84	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	164	ASP	N-CA-C	5.96	119.03	111.69
1	A	1039	ASP	CA-C-N	5.94	132.39	121.70
1	A	1039	ASP	C-N-CA	5.94	132.39	121.70
1	D	618	ALA	N-CA-C	-5.93	104.89	111.36
1	C	668	LEU	CA-C-N	5.92	126.74	120.11
1	C	668	LEU	C-N-CA	5.92	126.74	120.11
1	F	65	ILE	N-CA-C	5.90	116.55	110.82
1	D	174	ASP	N-CA-C	5.89	119.25	109.46
1	F	922	THR	N-CA-C	5.89	118.24	108.99
1	F	243	THR	N-CA-C	-5.89	104.99	111.82
1	D	535	LEU	N-CA-C	-5.88	106.06	113.18
1	F	666	PHE	N-CA-C	5.88	117.19	108.60
1	F	399	VAL	N-CA-C	-5.87	103.92	110.62
1	B	288	GLY	N-CA-C	5.86	119.66	111.10
1	C	959	GLY	N-CA-C	-5.82	103.23	112.66
1	C	453	PHE	N-CA-C	-5.80	106.16	113.18
1	D	214	VAL	N-CA-C	5.80	117.03	108.45
1	D	896	SER	CA-C-N	5.79	123.89	120.24
1	D	896	SER	C-N-CA	5.79	123.89	120.24
1	F	49	TYR	CA-CB-CG	5.79	124.32	113.90
1	E	213	GLN	N-CA-C	-5.78	101.91	110.46
1	C	7	ASP	CA-C-N	5.77	128.86	122.74
1	C	7	ASP	C-N-CA	5.77	128.86	122.74
1	A	519	MET	CB-CG-SD	5.77	130.01	112.70
1	B	164	ASP	N-CA-C	5.77	120.45	112.90
1	F	945	ILE	N-CA-C	5.76	115.84	110.42
1	F	453	PHE	N-CA-C	-5.76	106.21	113.18
1	F	115	MET	CA-C-N	-5.76	113.75	119.56
1	F	115	MET	C-N-CA	-5.76	113.75	119.56
1	B	895	TRP	N-CA-C	-5.75	106.10	113.23
1	B	364	ALA	N-CA-C	-5.75	105.10	111.36
1	C	106	GLN	N-CA-C	5.73	117.53	111.28
1	B	287	SER	CA-C-N	-5.72	115.41	121.48
1	B	287	SER	C-N-CA	-5.72	115.41	121.48
1	C	330	THR	N-CA-C	5.72	120.54	112.75
1	B	435	MET	N-CA-C	-5.70	105.06	111.28
1	D	632	LYS	N-CA-C	-5.69	102.61	110.35
1	E	529	ASP	N-CA-C	-5.68	104.30	111.11
1	C	632	LYS	N-CA-C	-5.66	102.66	110.35
1	D	284	GLN	CA-C-N	5.65	125.58	119.76
1	D	284	GLN	C-N-CA	5.65	125.58	119.76
1	C	213	GLN	N-CA-C	-5.64	101.67	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	519	MET	CB-CG-SD	5.64	129.63	112.70
1	B	529	ASP	N-CA-C	-5.64	104.34	111.11
1	E	674	LEU	N-CA-C	5.63	122.80	110.80
1	A	450	SER	N-CA-C	-5.62	105.30	111.82
1	B	1040	ILE	N-CA-C	5.61	121.01	109.34
1	A	666	PHE	N-CA-C	5.61	117.59	109.07
1	F	58	GLN	N-CA-C	5.61	117.47	111.36
1	C	170	SER	N-CA-C	5.60	117.59	108.63
1	B	439	GLN	N-CA-C	5.60	117.85	111.02
1	D	139	VAL	N-CA-C	5.60	116.19	107.28
1	B	961	ILE	N-CA-C	5.59	116.32	110.62
1	A	125	GLN	N-CA-C	-5.58	105.20	112.23
1	E	895	TRP	N-CA-C	-5.54	106.01	112.89
1	D	272	GLY	N-CA-C	5.54	118.30	111.93
1	C	1005	THR	N-CA-C	5.53	117.76	111.02
1	F	232	ALA	N-CA-C	5.52	117.24	108.79
1	C	310	LEU	N-CA-C	5.52	116.98	111.07
1	C	561	SER	N-CA-C	5.51	118.47	107.62
1	E	287	SER	CA-C-N	-5.51	115.64	121.48
1	E	287	SER	C-N-CA	-5.51	115.64	121.48
1	B	534	ILE	N-CA-C	-5.49	105.61	113.07
1	F	489	THR	CA-C-N	-5.49	112.96	119.05
1	F	489	THR	C-N-CA	-5.49	112.96	119.05
1	F	7	ASP	N-CA-C	-5.46	103.08	110.68
1	B	777	ALA	N-CA-C	5.46	117.68	111.02
1	C	644	VAL	N-CA-C	5.45	120.68	109.34
1	D	229	GLN	N-CA-C	-5.45	106.36	114.64
1	E	897	ILE	CB-CA-C	-5.43	108.59	114.35
1	A	724	THR	CA-C-N	-5.43	114.20	119.90
1	A	724	THR	C-N-CA	-5.43	114.20	119.90
1	E	1009	GLY	N-CA-C	-5.43	106.21	112.83
1	E	402	ILE	CB-CA-C	-5.41	104.15	112.05
1	C	498	LYS	CA-C-N	-5.41	114.36	119.76
1	C	498	LYS	C-N-CA	-5.41	114.36	119.76
1	D	40	PRO	CA-C-N	-5.41	114.22	119.90
1	D	40	PRO	C-N-CA	-5.41	114.22	119.90
1	A	950	LYS	N-CA-C	-5.39	104.44	111.02
1	B	6	ILE	N-CA-C	-5.39	104.35	111.09
1	E	838	GLY	N-CA-C	5.39	119.20	112.73
1	B	483	LEU	CA-CB-CG	5.38	135.14	116.30
1	D	1022	VAL	CB-CA-C	-5.38	108.59	113.70
1	B	799	VAL	CA-C-N	-5.38	115.04	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	799	VAL	C-N-CA	-5.38	115.04	120.31
1	A	171	GLY	N-CA-C	-5.37	107.26	115.00
1	F	887	CYS	N-CA-C	-5.37	105.33	111.07
1	E	672	VAL	N-CA-C	5.37	120.50	109.34
1	E	614	GLY	N-CA-C	-5.35	108.32	114.69
1	F	813	SER	N-CA-C	-5.35	102.75	110.40
1	F	451	ALA	N-CA-C	5.33	117.84	111.71
1	D	428	LYS	N-CA-C	5.33	116.77	111.07
1	E	435	MET	N-CA-C	-5.32	105.48	111.28
1	D	1031	ARG	N-CA-C	-5.31	107.34	112.97
1	B	425	LEU	CA-C-N	-5.31	115.79	119.66
1	B	425	LEU	C-N-CA	-5.31	115.79	119.66
1	F	25	LEU	N-CA-C	-5.31	105.58	111.36
1	E	317	PHE	CA-C-N	5.30	125.29	120.21
1	E	317	PHE	C-N-CA	5.30	125.29	120.21
1	E	289	LEU	N-CA-C	5.29	117.05	108.26
1	A	596	HIS	N-CA-C	5.28	117.12	111.36
1	C	564	LEU	CA-C-N	-5.28	114.48	119.76
1	C	564	LEU	C-N-CA	-5.28	114.48	119.76
1	C	521	GLU	N-CA-C	-5.27	105.43	111.07
1	A	277	ILE	N-CA-C	5.27	115.44	107.75
1	A	1010	GLY	N-CA-C	-5.26	106.27	112.64
1	C	824	SER	N-CA-C	5.26	117.18	109.24
1	D	515	TRP	CA-C-N	5.26	127.64	120.54
1	D	515	TRP	C-N-CA	5.26	127.64	120.54
1	F	737	GLN	N-CA-C	-5.24	105.57	111.28
1	E	1041	GLU	N-CA-C	5.23	121.34	114.75
1	C	559	LEU	CA-C-N	5.23	124.99	119.76
1	C	559	LEU	C-N-CA	5.23	124.99	119.76
1	E	76	MET	N-CA-C	-5.22	104.50	111.24
1	E	679	GLY	N-CA-C	5.20	120.30	111.19
1	C	100	ALA	N-CA-C	5.20	116.64	110.97
1	B	454	VAL	CA-C-N	-5.20	113.57	119.28
1	B	454	VAL	C-N-CA	-5.20	113.57	119.28
1	D	4	PHE	CB-CA-C	-5.19	102.12	110.74
1	A	180	SER	N-CA-C	5.19	117.28	109.23
1	B	622	GLN	N-CA-C	-5.19	105.74	111.71
1	E	832	ALA	CA-C-N	5.19	126.33	119.84
1	E	832	ALA	C-N-CA	5.19	126.33	119.84
1	B	260	VAL	N-CA-C	5.19	115.05	107.37
1	D	668	LEU	CA-C-N	-5.18	114.38	119.92
1	D	668	LEU	C-N-CA	-5.18	114.38	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	276	ASP	N-CA-C	5.18	117.01	111.36
1	F	862	MET	N-CA-C	5.18	116.61	111.07
1	A	480	LEU	N-CA-C	5.17	116.91	111.28
1	E	134	SER	N-CA-C	-5.17	106.75	113.16
1	E	1040	ILE	N-CA-C	5.17	120.08	109.34
1	C	229	GLN	CA-C-N	-5.16	115.88	123.00
1	C	229	GLN	C-N-CA	-5.16	115.88	123.00
1	D	851	LEU	CA-C-N	5.15	126.28	119.84
1	D	851	LEU	C-N-CA	5.15	126.28	119.84
1	E	656	SER	N-CA-C	-5.15	104.62	112.04
1	F	897	ILE	CB-CA-C	-5.15	108.89	114.35
1	B	130	GLU	N-CA-C	5.14	117.00	109.24
1	D	548	ILE	CB-CA-C	-5.14	105.40	111.97
1	D	674	LEU	N-CA-C	5.13	116.86	108.55
1	C	778	LYS	N-CA-C	5.13	119.41	113.20
1	B	426	PRO	O-C-N	5.13	123.67	121.31
1	D	671	ILE	CB-CA-C	-5.10	102.92	111.29
1	A	538	THR	N-CA-C	5.09	116.91	111.36
1	F	561	SER	N-CA-C	5.09	117.69	107.41
1	C	132	SER	N-CA-C	5.08	117.02	108.73
1	A	564	LEU	N-CA-C	5.08	114.14	108.25
1	F	370	ILE	N-CA-C	-5.08	106.17	113.07
1	A	367	ILE	CA-C-N	-5.07	114.52	119.64
1	A	367	ILE	C-N-CA	-5.07	114.52	119.64
1	C	633	ASP	CA-C-N	5.07	127.78	120.38
1	C	633	ASP	C-N-CA	5.07	127.78	120.38
1	C	4	PHE	N-CA-C	-5.06	105.27	111.75
1	D	971	ARG	CB-CA-C	5.06	119.22	111.02
1	F	905	VAL	CB-CA-C	-5.05	108.90	113.70
1	B	289	LEU	N-CA-C	5.05	116.62	108.34
1	E	367	ILE	CA-C-N	-5.05	114.46	119.56
1	E	367	ILE	C-N-CA	-5.05	114.46	119.56
1	F	516	PHE	N-CA-C	5.05	116.64	111.03
1	E	426	PRO	O-C-N	5.05	123.63	121.31
1	F	804	PHE	N-CA-C	5.05	118.47	111.71
1	C	269	GLU	N-CA-C	5.04	117.05	109.23
1	D	317	PHE	N-CA-C	5.04	116.24	109.83
1	A	672	VAL	N-CA-C	-5.04	102.37	109.63
1	E	439	GLN	N-CA-C	5.03	117.16	111.02
1	E	352	PHE	N-CA-C	-5.03	105.80	111.28
1	F	580	ALA	N-CA-C	5.02	117.51	110.23
1	E	128	SER	N-CA-C	5.02	117.08	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	849	SER	N-CA-C	-5.02	107.11	113.18
1	F	567	GLU	N-CA-C	5.01	117.61	109.24
1	F	973	ARG	CA-C-N	-5.01	113.48	119.05
1	F	973	ARG	C-N-CA	-5.01	113.48	119.05
1	E	563	PHE	N-CA-C	-5.01	106.31	112.72
1	A	1041	GLU	CA-C-N	5.01	130.72	121.70
1	A	1041	GLU	C-N-CA	5.01	130.72	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1038	GLU	Peptide
1	A	540	ARG	Sidechain
1	B	1039	ASP	Peptide
1	C	540	ARG	Sidechain
1	C	6	ILE	Peptide
1	E	1039	ASP	Peptide
1	F	6	ILE	Peptide
1	F	812	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7925	0	8066	458	0
1	B	7935	0	8073	373	0
1	C	7925	0	8066	424	1
1	D	7925	0	8066	443	1
1	E	7925	0	8066	457	0
1	F	7925	0	8066	466	0
2	A	35	0	46	3	0
2	B	35	0	46	7	0
2	C	35	0	46	0	0
2	D	35	0	46	7	0
2	E	35	0	46	10	0
2	F	35	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	47773	0	48679	2541	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (2541) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:ARG:HG2	1:A:974:PRO:HG2	1.44	0.96
1:B:1035:ARG:HG3	1:B:1036:LYS:HG3	1.49	0.95
1:B:959:GLY:HA2	1:B:1040:ILE:HB	1.46	0.95
1:C:937:LEU:HD13	1:C:1011:MET:HE2	1.47	0.93
1:C:944:LEU:HB3	1:C:971:ARG:HD2	1.50	0.93
1:D:41:PRO:HG2	1:D:94:PHE:HB2	1.48	0.92
1:A:1034:SER:HB3	1:A:1035:ARG:HA	1.50	0.92
1:B:541:TYR:HH	2:B:1101:LMT:H6'	1.00	0.91
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.52	0.90
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.53	0.90
1:D:225:VAL:HG22	1:E:781:MET:HE2	1.51	0.90
1:B:225:VAL:HG12	1:C:777:ALA:HB1	1.52	0.89
2:E:1101:LMT:H5B	2:E:1101:LMT:H6D	1.54	0.89
1:F:559:LEU:HD22	1:F:560:PRO:HD2	1.53	0.89
1:A:619:GLY:HA3	1:A:815:ARG:HH22	1.36	0.88
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.37	0.88
1:C:634:TRP:CD1	1:C:634:TRP:H	1.92	0.87
1:F:731:ILE:HD13	1:F:746:ILE:HD11	1.54	0.87
1:E:733:GLN:HE22	1:E:743:ILE:HG21	1.39	0.87
1:E:699:ARG:NH2	1:E:722:GLU:OE2	2.08	0.86
1:B:562:SER:HB3	1:B:924:ASP:HB3	1.57	0.86
1:D:712:MET:HE1	1:D:835:LYS:HE2	1.56	0.86
1:C:919:ARG:O	1:C:921:LEU:N	2.09	0.86
1:D:57:VAL:HG21	1:D:86:GLY:HA2	1.55	0.86
1:E:146:ASP:OD2	1:E:146:ASP:N	2.07	0.86
1:D:696:THR:HG23	1:D:699:ARG:HH12	1.41	0.86
1:E:196:PHE:O	1:E:252:LYS:NZ	2.09	0.85
1:F:35:TYR:HB3	1:F:38:ILE:HD12	1.58	0.85
1:A:445:ILE:HD13	1:A:940:LYS:HE3	1.58	0.85
1:B:1037:ASN:HA	1:B:1038:GLU:HG2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.59	0.84
1:A:957:GLY:HA2	1:A:1042:HIS:HB3	1.59	0.84
1:C:892:TYR:O	1:C:894:SER:N	2.11	0.84
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.59	0.84
1:F:901:VAL:HG23	1:F:942:ALA:HB3	1.60	0.84
1:A:537:SER:OG	1:A:540:ARG:HD2	1.78	0.83
1:E:507:GLU:HG2	1:E:518:ARG:HA	1.61	0.82
1:D:360:GLN:NE2	1:D:513:PHE:O	2.12	0.82
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.60	0.82
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.15	0.81
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.62	0.81
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.62	0.81
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.62	0.81
1:C:137:LEU:HD22	1:C:293:LEU:HD23	1.61	0.81
1:E:634:TRP:H	1:E:634:TRP:CD1	1.99	0.81
1:B:652:THR:HG23	1:B:665:ALA:H	1.46	0.80
1:C:577:GLN:HG3	1:C:624:THR:HG22	1.63	0.80
1:C:151:GLN:NE2	1:C:279:ALA:O	2.13	0.80
1:D:400:LEU:HD23	1:D:929:VAL:HG12	1.64	0.80
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.61	0.80
1:B:422:GLU:O	1:B:502:LYS:NZ	2.15	0.80
1:D:781:MET:HE2	1:F:225:VAL:HG22	1.64	0.80
1:F:987:MET:HG3	1:F:1008:MET:HE1	1.63	0.80
1:E:441:ALA:HA	1:E:891:LEU:HD21	1.64	0.79
1:E:156:ASP:OD2	1:E:769:LYS:NZ	2.14	0.79
1:F:82:SER:HB2	1:F:816:LEU:HB2	1.65	0.79
1:D:596:HIS:O	1:D:600:THR:OG1	2.01	0.79
1:A:243:THR:HG23	1:A:268:ILE:HG22	1.64	0.78
1:D:564:LEU:HB2	1:D:671:ILE:HD11	1.65	0.78
1:A:196:PHE:O	1:A:252:LYS:NZ	2.17	0.78
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.17	0.78
1:C:641:GLU:HB2	1:C:650:ARG:HH22	1.49	0.78
1:A:703:LEU:HD21	1:A:718:PRO:HD3	1.66	0.77
1:B:668:LEU:HD23	1:B:668:LEU:H	1.48	0.77
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.63	0.77
1:A:129:VAL:O	1:B:110:LYS:NZ	2.17	0.77
1:A:973:ARG:HG2	1:A:977:MET:HE2	1.64	0.77
1:C:53:ASP:OD1	1:C:56:THR:OG1	2.01	0.77
1:F:358:PHE:HD1	1:F:977:MET:HG3	1.47	0.77
1:D:55:LYS:NZ	1:F:238:THR:OG1	2.16	0.77
1:E:530:SER:CB	2:E:1101:LMT:H2O2	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:699:ARG:HE	1:E:718:PRO:HG3	1.49	0.77
1:F:307:ARG:NH2	1:F:314:GLU:OE2	2.18	0.77
1:B:973:ARG:HG2	1:B:977:MET:HE2	1.66	0.76
1:C:578:LEU:HG	1:C:587:THR:HG22	1.66	0.76
1:F:248:LYS:HA	1:F:261:LEU:HD13	1.67	0.76
1:D:536:ARG:NH2	2:D:1101:LMT:O3B	2.18	0.76
1:E:641:GLU:HA	1:E:646:ALA:HB3	1.66	0.76
1:E:976:LEU:HD21	2:E:1101:LMT:H111	1.68	0.76
1:A:1041:GLU:HB3	1:A:1042:HIS:HA	1.67	0.76
1:B:9:PRO:HB3	1:B:495:THR:HG21	1.68	0.76
1:F:910:ILE:O	1:F:914:LEU:HB2	1.85	0.76
1:A:451:ALA:HB1	1:A:883:VAL:HG12	1.67	0.76
1:D:82:SER:HB2	1:D:816:LEU:HB2	1.67	0.76
1:F:596:HIS:O	1:F:600:THR:OG1	2.04	0.75
1:F:733:GLN:HE22	1:F:743:ILE:HG21	1.50	0.75
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.69	0.75
1:A:70:ASN:O	1:A:110:LYS:NZ	2.19	0.75
1:C:240:LEU:HB2	1:C:246:PHE:HE1	1.49	0.75
1:E:326:PRO:O	1:E:630:SER:OG	2.04	0.75
1:B:185:ARG:HH12	1:B:774:MET:HE3	1.52	0.75
1:A:146:ASP:HB2	1:A:148:THR:HG23	1.69	0.75
1:C:159:ALA:HB2	1:C:177:LEU:HD11	1.67	0.75
1:E:508:GLY:HA3	1:E:518:ARG:HE	1.52	0.75
1:A:400:LEU:HD21	1:A:930:GLY:HA2	1.69	0.74
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.67	0.74
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.69	0.74
1:C:587:THR:HG21	1:C:622:GLN:O	1.86	0.74
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.69	0.74
1:C:356:TYR:HA	1:C:365:THR:HG21	1.68	0.74
1:D:133:SER:OG	1:D:134:SER:N	2.20	0.74
1:D:156:ASP:OD2	1:D:769:LYS:NZ	2.20	0.74
1:E:174:ASP:HB3	1:E:292:LYS:HB2	1.69	0.74
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.67	0.74
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.70	0.74
1:F:343:THR:HG21	1:F:989:LEU:HD23	1.67	0.74
1:A:144:ASN:HD22	1:A:321:LEU:HD23	1.50	0.74
1:A:1040:ILE:HG13	1:A:1041:GLU:H	1.51	0.74
1:B:508:GLY:O	1:B:510:LYS:N	2.21	0.74
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.70	0.74
1:A:781:MET:HE2	1:C:225:VAL:HG22	1.68	0.74
1:F:664:PHE:HD2	1:F:717:ARG:HD3	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:298:ASN:ND2	1:F:301:ASP:OD2	2.21	0.74
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.21	0.73
1:C:3:ASN:N	1:C:3:ASN:OD1	2.21	0.73
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.70	0.73
1:E:559:LEU:HD23	1:E:560:PRO:HD2	1.71	0.73
1:F:61:VAL:HA	1:F:118:LEU:HD22	1.69	0.73
1:B:362:PHE:O	1:B:365:THR:HG22	1.89	0.73
1:F:979:SER:HA	1:F:1011:MET:HE3	1.71	0.73
1:A:634:TRP:CD1	1:A:634:TRP:H	2.07	0.73
1:D:137:LEU:HD13	1:D:293:LEU:HD12	1.71	0.73
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.71	0.72
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.71	0.72
1:B:213:GLN:HE22	1:C:52:ALA:HA	1.54	0.72
1:B:658:ILE:O	1:B:659:LYS:HD2	1.89	0.72
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.69	0.72
1:B:423:GLU:HA	1:B:502:LYS:HZ3	1.53	0.72
1:B:536:ARG:NH2	2:B:1101:LMT:O2B	2.20	0.72
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.71	0.72
1:D:777:ALA:HB1	1:F:225:VAL:HG12	1.70	0.72
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.72	0.72
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.71	0.72
1:A:655:PHE:HB3	1:A:663:VAL:HB	1.71	0.72
1:C:201:VAL:HA	1:C:204:ILE:HD12	1.71	0.72
1:D:712:MET:HB3	1:D:713:LEU:HD22	1.70	0.72
1:C:598:TYR:HB3	1:C:606:VAL:HG21	1.72	0.72
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.72	0.72
1:E:165:ALA:HB3	1:E:313:MET:HE3	1.71	0.72
1:F:58:GLN:OE1	1:F:818:ARG:NH1	2.23	0.72
1:F:537:SER:OG	1:F:540:ARG:NH2	2.23	0.72
1:F:668:LEU:HD23	1:F:668:LEU:H	1.54	0.72
1:E:156:ASP:OD1	1:E:765:ARG:NH2	2.22	0.71
1:E:508:GLY:O	1:E:510:LYS:N	2.23	0.71
1:B:24:GLY:O	1:B:27:ILE:HG22	1.89	0.71
1:E:7:ASP:OD1	1:E:432:ARG:NH2	2.23	0.71
1:C:450:SER:HB2	1:C:475:VAL:HG22	1.72	0.71
1:C:746:ILE:HG13	1:C:747:ASN:N	2.06	0.71
1:F:133:SER:OG	1:F:293:LEU:O	2.07	0.71
1:C:596:HIS:O	1:C:600:THR:OG1	2.08	0.71
1:C:588:GLN:O	1:C:592:ASN:ND2	2.23	0.71
1:D:982:PHE:O	1:D:985:GLY:N	2.24	0.71
1:E:971:ARG:O	1:E:975:ILE:HG12	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:GLN:NE2	1:F:513:PHE:O	2.16	0.71
1:E:743:ILE:HA	1:E:746:ILE:HD12	1.72	0.71
1:D:335:ILE:O	1:D:339:GLU:HG2	1.91	0.71
1:E:540:ARG:NH1	2:E:1101:LMT:O6B	2.19	0.71
1:F:510:LYS:HA	1:F:518:ARG:HH12	1.54	0.71
1:C:668:LEU:HD23	1:C:668:LEU:H	1.56	0.70
1:D:634:TRP:CD1	1:D:634:TRP:H	2.09	0.70
1:F:187:TRP:HB3	1:F:776:GLU:HG2	1.73	0.70
1:A:259:ARG:HH21	1:A:261:LEU:HD11	1.55	0.70
1:D:170:SER:HB2	1:E:75:LEU:H	1.56	0.70
1:E:983:ILE:HG23	1:E:1008:MET:HE2	1.71	0.70
1:E:1013:THR:O	1:E:1017:LEU:HB2	1.92	0.70
1:A:971:ARG:C	1:A:974:PRO:HD2	2.16	0.70
1:A:1016:VAL:HG13	2:A:1101:LMT:H112	1.74	0.70
1:C:564:LEU:HG	1:C:565:PRO:HD2	1.73	0.70
1:E:540:ARG:HH12	2:E:1101:LMT:H6B	1.39	0.70
1:B:172:VAL:HG13	1:B:291:ILE:HG23	1.72	0.70
1:D:540:ARG:NH2	2:D:1101:LMT:O6B	2.24	0.70
1:C:960:LEU:HB3	1:C:1040:ILE:HG23	1.74	0.70
1:D:6:ILE:HG13	1:D:7:ASP:N	2.06	0.70
1:F:634:TRP:CD1	1:F:634:TRP:H	2.09	0.70
1:D:66:GLU:OE2	1:D:80:SER:OG	2.07	0.69
1:F:340:VAL:HG11	1:F:395:MET:HB3	1.75	0.69
1:F:456:MET:HB3	1:F:876:LEU:HD21	1.73	0.69
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.73	0.69
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.74	0.69
1:E:637:ARG:HB3	1:E:642:ASN:HB3	1.74	0.69
1:A:400:LEU:HD11	1:A:1007:VAL:HG21	1.74	0.69
1:B:423:GLU:HA	1:B:502:LYS:NZ	2.07	0.69
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.74	0.69
1:E:589:LYS:HA	1:E:592:ASN:HD22	1.57	0.69
1:E:901:VAL:HG21	1:E:943:ILE:HG13	1.73	0.69
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.75	0.69
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.28	0.69
1:D:298:ASN:HB3	1:D:301:ASP:HB2	1.75	0.69
1:B:907:LEU:HG	1:B:1017:LEU:HD23	1.75	0.69
1:D:1040:ILE:HG12	1:D:1041:GLU:H	1.58	0.69
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.57	0.69
1:E:149:MET:HB2	1:E:153:ASP:HB3	1.74	0.69
1:C:982:PHE:O	1:C:985:GLY:N	2.25	0.69
1:D:491:ALA:O	1:D:495:THR:OG1	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:TYR:O	1:E:161:ASN:ND2	2.21	0.69
1:E:959:GLY:HA2	1:E:1040:ILE:HB	1.75	0.69
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.75	0.69
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.74	0.69
1:A:712:MET:HB3	1:A:713:LEU:HD22	1.73	0.69
1:C:904:VAL:HG21	1:C:942:ALA:HB2	1.73	0.69
1:D:196:PHE:HB3	1:D:252:LYS:NZ	2.07	0.69
1:E:57:VAL:HG11	1:E:86:GLY:HA2	1.74	0.69
1:E:588:GLN:O	1:E:592:ASN:ND2	2.26	0.69
1:A:654:ALA:O	1:A:658:ILE:HG12	1.92	0.69
1:E:169:THR:HG21	1:E:306:ILE:HG13	1.74	0.69
1:E:1037:ASN:H	1:E:1038:GLU:HA	1.58	0.69
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.73	0.69
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.74	0.69
1:A:747:ASN:ND2	1:C:237:GLN:OE1	2.25	0.69
1:B:196:PHE:O	1:B:252:LYS:NZ	2.24	0.69
1:D:70:ASN:O	1:D:110:LYS:NZ	2.25	0.69
1:D:598:TYR:HB3	1:D:606:VAL:HG21	1.74	0.69
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.74	0.68
1:E:362:PHE:O	1:E:365:THR:HG22	1.92	0.68
1:F:509:LYS:O	1:F:518:ARG:NH1	2.26	0.68
1:F:739:LEU:HD13	1:F:799:VAL:HG11	1.75	0.68
1:D:49:TYR:HB3	1:D:57:VAL:HG22	1.74	0.68
1:D:115:MET:O	1:D:123:GLN:NE2	2.26	0.68
1:F:702:LEU:HD12	1:F:851:LEU:HD11	1.76	0.68
1:F:3:ASN:OD1	1:F:3:ASN:N	2.26	0.68
1:F:73:ASP:OD2	1:F:106:GLN:NE2	2.24	0.68
1:F:667:ASN:O	1:F:678:THR:OG1	2.11	0.68
1:A:564:LEU:HD23	1:A:565:PRO:HD2	1.75	0.68
1:C:309:GLU:HG3	1:C:313:MET:HE3	1.73	0.68
1:E:146:ASP:OD2	1:E:320:GLY:HA3	1.94	0.68
1:F:577:GLN:HG3	1:F:624:THR:HG22	1.76	0.68
1:D:393:LEU:HD11	1:D:466:ILE:HD13	1.76	0.68
1:E:949:ALA:HB3	1:E:1026:PHE:HE1	1.59	0.68
1:A:768:VAL:HG12	1:B:63:GLN:HE21	1.58	0.68
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.74	0.68
1:C:363:ARG:HB3	1:C:363:ARG:HH11	1.59	0.68
1:D:170:SER:OG	1:E:74:ASN:N	2.22	0.68
1:F:452:VAL:HG12	1:F:880:SER:HB3	1.76	0.68
1:A:491:ALA:O	1:A:495:THR:OG1	2.06	0.67
1:E:675:GLY:HA2	1:E:862:MET:SD	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.76	0.67
1:B:26:ALA:O	1:B:30:LEU:HB2	1.94	0.67
1:C:115:MET:HE1	1:C:123:GLN:HG2	1.75	0.67
1:D:475:VAL:HA	1:D:478:MET:HE2	1.76	0.67
1:C:72:ILE:HD13	1:C:107:VAL:HG22	1.76	0.67
1:E:9:PRO:HB3	1:E:495:THR:HG21	1.76	0.67
1:F:24:GLY:O	1:F:27:ILE:HG12	1.94	0.67
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.28	0.67
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.77	0.67
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.29	0.67
1:F:527:TYR:HB2	2:F:1101:LMT:H101	1.77	0.67
1:A:350:LEU:HD22	1:A:984:LEU:HB3	1.76	0.67
1:D:562:SER:HB2	1:D:924:ASP:HB3	1.77	0.67
1:B:775:SER:OG	1:B:776:GLU:O	2.13	0.67
1:D:113:LEU:HD11	1:F:128:SER:HB3	1.77	0.67
1:E:376:LEU:O	1:E:379:THR:N	2.27	0.67
1:E:531:VAL:O	1:E:534:ILE:HG13	1.93	0.67
1:E:858:ASP:OD1	1:E:859:TRP:N	2.27	0.67
1:F:506:GLY:C	1:F:508:GLY:H	2.01	0.67
1:B:267:LYS:HD3	1:B:776:GLU:OE2	1.95	0.67
1:F:251:LEU:HD11	1:F:262:LEU:HA	1.74	0.67
1:A:531:VAL:O	1:A:534:ILE:HG13	1.94	0.67
1:E:213:GLN:HE22	1:F:52:ALA:HA	1.60	0.67
1:F:180:SER:OG	1:F:274:ASN:O	2.07	0.67
1:F:578:LEU:HG	1:F:587:THR:HG22	1.75	0.67
1:A:225:VAL:HG22	1:B:781:MET:HE2	1.75	0.67
1:C:889:ALA:HB1	1:C:895:TRP:HZ3	1.59	0.67
1:E:237:GLN:OE1	1:F:747:ASN:ND2	2.28	0.67
1:B:739:LEU:HD13	1:B:799:VAL:HG11	1.77	0.66
1:F:358:PHE:CD1	1:F:977:MET:HG3	2.30	0.66
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.77	0.66
1:B:167:SER:CB	1:B:175:VAL:HG21	2.25	0.66
1:F:808:ARG:NH1	1:F:810:GLU:OE2	2.28	0.66
1:A:957:GLY:CA	1:A:1042:HIS:HB3	2.25	0.66
1:D:330:THR:HG23	1:D:334:LYS:HD2	1.75	0.66
1:A:149:MET:HE3	1:A:153:ASP:HB3	1.77	0.66
1:D:448:VAL:HG22	1:D:887:CYS:HB3	1.76	0.66
1:D:904:VAL:HG21	1:D:942:ALA:HB2	1.77	0.66
1:F:885:PHE:HD2	1:F:886:LEU:HD22	1.60	0.66
1:D:641:GLU:HB2	1:D:650:ARG:HH22	1.60	0.66
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ALA:HB1	1:A:505:HIS:CE1	2.30	0.66
1:E:901:VAL:HG23	1:E:942:ALA:HB3	1.78	0.66
1:E:931:LEU:O	1:E:935:ILE:HG13	1.96	0.66
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.29	0.66
1:A:573:MET:HG3	1:A:666:PHE:CE2	2.31	0.66
1:B:58:GLN:O	1:B:63:GLN:HG3	1.95	0.66
1:B:559:LEU:HD22	1:B:560:PRO:HD2	1.78	0.66
1:A:571:VAL:HG22	1:A:630:SER:HA	1.77	0.65
1:D:897:ILE:HA	1:D:1029:VAL:HG11	1.78	0.65
1:F:365:THR:O	1:F:368:PRO:HD2	1.95	0.65
1:C:686:ASP:OD1	1:C:690:LEU:HB2	1.96	0.65
1:A:137:LEU:HB2	1:A:293:LEU:HB2	1.79	0.65
1:A:362:PHE:O	1:A:365:THR:HG22	1.96	0.65
1:A:540:ARG:HG3	1:A:541:TYR:HD1	1.62	0.65
1:A:540:ARG:HG3	1:A:541:TYR:CD1	2.31	0.65
1:B:359:LEU:C	1:B:360:GLN:HG2	2.21	0.65
1:D:184:MET:HB3	1:D:771:VAL:HG13	1.79	0.65
1:D:967:ALA:O	1:D:971:ARG:NH1	2.28	0.65
1:E:658:ILE:O	1:E:659:LYS:HD2	1.96	0.65
1:B:610:PHE:HB3	1:B:628:PHE:HB3	1.77	0.65
1:C:947:GLU:HG3	1:C:948:PHE:HD1	1.61	0.65
1:A:923:ASN:ND2	1:A:923:ASN:O	2.30	0.65
1:E:189:ASN:HB3	1:E:192:GLU:HB2	1.79	0.65
1:E:702:LEU:HD13	1:E:851:LEU:HD21	1.79	0.65
1:C:744:ASN:O	1:C:748:THR:HG23	1.97	0.65
1:B:139:VAL:O	1:B:326:PRO:HD2	1.96	0.64
1:D:174:ASP:HB3	1:D:292:LYS:HB2	1.79	0.64
1:B:511:GLY:HA2	1:B:515:TRP:CD1	2.32	0.64
1:B:971:ARG:O	1:B:975:ILE:HG12	1.98	0.64
1:D:453:PHE:O	1:D:471:SER:OG	2.12	0.64
1:D:655:PHE:HB3	1:D:663:VAL:HB	1.80	0.64
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.32	0.64
1:F:452:VAL:O	1:F:455:PRO:HD2	1.97	0.64
1:A:960:LEU:HD21	1:A:1027:VAL:HG13	1.78	0.64
1:B:1013:THR:O	1:B:1017:LEU:HB2	1.96	0.64
1:C:979:SER:HA	1:C:1011:MET:HE3	1.79	0.64
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.80	0.64
1:B:536:ARG:NE	2:B:1101:LMT:O3B	2.30	0.64
1:D:243:THR:HG23	1:D:268:ILE:HG22	1.80	0.64
1:D:516:PHE:HA	1:D:519:MET:HE2	1.79	0.64
1:D:568:ASP:O	1:D:634:TRP:HZ3	1.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:LEU:HD12	1:E:263:ARG:HH12	1.63	0.64
1:B:156:ASP:OD1	1:B:765:ARG:NH2	2.30	0.64
1:D:318:PRO:HD2	1:D:321:LEU:HD12	1.78	0.64
1:F:424:GLY:HA3	1:F:502:LYS:HB2	1.79	0.64
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.30	0.64
1:E:907:LEU:HG	1:E:1017:LEU:HD23	1.80	0.64
1:C:944:LEU:HB3	1:C:971:ARG:CD	2.27	0.64
1:E:844:MET:HE2	1:E:844:MET:HA	1.78	0.64
1:C:682:PHE:CE1	1:C:857:TYR:HB2	2.33	0.64
1:E:14:VAL:HG22	1:F:886:LEU:HD12	1.78	0.64
1:D:894:SER:HB3	1:D:897:ILE:HB	1.79	0.64
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.80	0.64
1:D:168:ARG:HB3	1:E:75:LEU:HD22	1.80	0.64
1:D:931:LEU:O	1:D:935:ILE:HG13	1.98	0.64
1:D:869:SER:OG	1:D:872:GLN:NE2	2.31	0.63
1:D:971:ARG:HB3	1:D:971:ARG:HH11	1.63	0.63
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.80	0.63
1:F:671:ILE:HD13	1:F:674:LEU:HD12	1.81	0.63
1:D:388:PHE:CE1	1:D:472:ILE:HG21	2.34	0.63
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.79	0.63
1:C:671:ILE:HD13	1:C:674:LEU:HD12	1.80	0.63
1:E:108:GLN:HE22	1:F:109:ASN:HA	1.64	0.63
1:F:379:THR:HG23	1:F:476:SER:OG	1.97	0.63
1:F:479:ALA:O	1:F:482:VAL:HG23	1.99	0.63
1:A:94:PHE:CE1	1:A:103:ALA:HB1	2.34	0.63
1:B:400:LEU:HG	1:B:929:VAL:HG12	1.80	0.63
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.80	0.63
1:D:507:GLU:O	1:D:509:LYS:N	2.29	0.63
1:E:318:PRO:HD2	1:E:321:LEU:HD22	1.80	0.63
1:E:445:ILE:HG21	1:E:940:LYS:HD2	1.81	0.63
1:B:919:ARG:HB3	1:B:921:LEU:HD23	1.80	0.63
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.80	0.63
1:C:559:LEU:HD23	1:C:560:PRO:HD2	1.79	0.63
1:D:358:PHE:CD1	1:D:977:MET:HG2	2.33	0.63
1:E:950:LYS:HA	1:E:953:MET:HE3	1.79	0.63
1:A:668:LEU:HD23	1:A:668:LEU:H	1.62	0.63
1:A:696:THR:HG23	1:A:699:ARG:HH12	1.64	0.63
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.80	0.63
1:E:776:GLU:HG2	1:E:777:ALA:H	1.63	0.63
1:A:457:ALA:HB1	1:A:468:ARG:HG3	1.81	0.63
1:C:435:MET:HE3	1:C:490:PRO:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:971:ARG:NH1	1:D:971:ARG:HB3	2.13	0.63
1:E:415:ASN:ND2	1:E:437:GLN:OE1	2.28	0.63
1:A:520:PHE:O	1:A:524:THR:HG23	1.98	0.63
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.81	0.63
1:F:971:ARG:NE	1:F:971:ARG:O	2.31	0.63
1:A:832:ALA:HB3	1:A:835:LYS:HD3	1.82	0.62
1:D:72:ILE:HD13	1:D:107:VAL:HG22	1.79	0.62
1:D:644:VAL:HG11	1:D:667:ASN:HB2	1.80	0.62
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.80	0.62
1:F:358:PHE:HE2	1:F:516:PHE:HZ	1.45	0.62
1:A:357:LEU:HD23	1:A:358:PHE:CD1	2.34	0.62
1:B:1011:MET:O	1:B:1015:THR:HG23	1.99	0.62
1:D:412:VAL:HG22	1:D:438:ILE:HD12	1.81	0.62
1:D:728:LYS:HG2	1:D:808:ARG:NH1	2.14	0.62
1:B:682:PHE:HE2	1:B:684:LEU:HB2	1.63	0.62
1:E:64:VAL:HG11	1:E:117:LEU:HB2	1.80	0.62
1:E:149:MET:HB2	1:E:153:ASP:CB	2.29	0.62
1:A:174:ASP:HB3	1:A:292:LYS:HB2	1.80	0.62
1:C:493:CYS:O	1:C:497:LEU:HB2	1.99	0.62
1:C:694:LYS:HE3	1:C:694:LYS:H	1.65	0.62
1:D:580:ALA:HB1	1:D:724:THR:HG22	1.80	0.62
1:F:146:ASP:O	1:F:148:THR:N	2.33	0.62
1:F:713:LEU:HD21	1:F:843:LEU:HD12	1.80	0.62
1:B:441:ALA:HA	1:B:891:LEU:HD21	1.79	0.62
1:C:261:LEU:N	1:C:264:ASP:OD2	2.32	0.62
1:C:597:TYR:HE1	1:C:601:LYS:HD2	1.63	0.62
1:C:960:LEU:O	1:C:964:THR:HG23	1.99	0.62
1:D:282:ASN:HD21	1:D:608:SER:HA	1.63	0.62
1:A:475:VAL:HA	1:A:478:MET:HE2	1.80	0.62
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.80	0.62
1:B:974:PRO:HA	1:B:977:MET:HE3	1.82	0.62
1:F:578:LEU:HB2	1:F:623:ASN:HB2	1.81	0.62
1:A:958:LYS:O	1:A:1040:ILE:HG12	2.00	0.62
1:C:171:GLY:HA3	1:C:302:THR:OG1	1.99	0.62
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.30	0.62
1:A:276:ASP:HA	1:C:222:THR:HG21	1.82	0.62
1:A:844:MET:HA	1:A:844:MET:HE2	1.81	0.62
1:A:983:ILE:HG23	1:A:1008:MET:HE2	1.81	0.62
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.82	0.62
1:E:165:ALA:HB3	1:E:313:MET:CE	2.29	0.62
1:F:154:ILE:HG22	1:F:287:SER:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:PHE:HA	1:F:355:MET:HE2	1.80	0.62
1:A:733:GLN:NE2	1:A:743:ILE:HG21	2.15	0.62
1:B:950:LYS:HZ1	1:B:1030:ARG:HH21	1.48	0.62
1:D:194:ASN:HA	1:D:798:MET:HE2	1.82	0.62
1:D:674:LEU:HD23	1:D:675:GLY:N	2.14	0.62
1:F:372:VAL:HG22	1:F:405:LEU:HD11	1.81	0.62
1:B:987:MET:HG3	1:B:1008:MET:HE1	1.82	0.61
1:C:101:ASP:OD1	1:C:131:LYS:NZ	2.33	0.61
1:C:520:PHE:O	1:C:524:THR:HG23	2.00	0.61
1:D:144:ASN:HA	1:D:320:GLY:O	2.00	0.61
1:D:700:ASN:HA	1:D:703:LEU:HD12	1.81	0.61
1:F:363:ARG:HG2	1:F:363:ARG:HH11	1.65	0.61
1:A:184:MET:HG2	1:A:246:PHE:CE2	2.36	0.61
1:B:759:VAL:HG12	1:B:760:ASN:HB2	1.81	0.61
1:F:674:LEU:HD22	1:F:861:GLY:HA2	1.83	0.61
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.65	0.61
1:E:680:PHE:HB2	1:E:863:SER:OG	2.00	0.61
1:F:120:GLN:HA	1:F:123:GLN:HB2	1.81	0.61
1:A:225:VAL:HG12	1:B:777:ALA:HB1	1.82	0.61
1:A:415:ASN:HD22	1:A:434:SER:HB2	1.66	0.61
1:B:484:VAL:O	1:B:489:THR:HG23	2.00	0.61
1:C:187:TRP:HA	1:C:774:MET:O	2.00	0.61
1:C:944:LEU:HD13	1:C:975:ILE:HG12	1.82	0.61
1:D:578:LEU:HD21	1:D:590:VAL:HG21	1.81	0.61
1:D:641:GLU:HA	1:D:646:ALA:HB3	1.82	0.61
1:F:139:VAL:HG22	1:F:290:GLY:HA2	1.81	0.61
1:F:429:GLU:O	1:F:433:LYS:HB2	2.01	0.61
1:F:610:PHE:HB3	1:F:628:PHE:HB2	1.82	0.61
1:D:149:MET:HE3	1:D:153:ASP:HB3	1.81	0.61
1:D:225:VAL:HG12	1:E:777:ALA:HB1	1.82	0.61
1:D:983:ILE:HG23	1:D:1008:MET:HE2	1.81	0.61
1:F:408:ASP:OD2	1:F:408:ASP:N	2.32	0.61
1:F:897:ILE:HG23	1:F:946:VAL:CG1	2.30	0.61
1:F:1021:PHE:HB3	1:F:1025:PHE:CE1	2.35	0.61
1:A:559:LEU:HD13	1:A:923:ASN:HB2	1.82	0.61
1:B:648:THR:O	1:B:652:THR:OG1	2.19	0.61
1:C:198:LEU:HD11	1:C:252:LYS:HB2	1.83	0.61
1:B:1037:ASN:HA	1:B:1038:GLU:CG	2.29	0.61
1:C:326:PRO:O	1:C:630:SER:HB2	2.00	0.61
1:E:795:ASP:OD2	1:E:797:GLN:HG3	2.00	0.61
1:F:455:PRO:HG3	1:F:883:VAL:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:O	1:A:247:GLY:N	2.34	0.60
1:A:768:VAL:HG12	1:B:63:GLN:NE2	2.16	0.60
1:A:795:ASP:OD2	1:A:797:GLN:HG3	2.00	0.60
1:B:82:SER:HB2	1:B:816:LEU:HB2	1.82	0.60
1:A:696:THR:OG1	1:A:825:MET:HE1	2.01	0.60
1:A:944:LEU:HB3	1:A:971:ARG:CZ	2.31	0.60
1:B:52:ALA:HB1	1:B:56:THR:HB	1.83	0.60
1:B:596:HIS:O	1:B:600:THR:OG1	2.09	0.60
1:C:479:ALA:O	1:C:482:VAL:HG23	2.02	0.60
1:D:368:PRO:HG3	1:D:413:VAL:HG21	1.82	0.60
1:E:583:THR:HG22	1:E:585:GLU:H	1.66	0.60
1:D:18:ILE:HG13	1:E:886:LEU:HD23	1.83	0.60
1:D:247:GLY:O	1:D:261:LEU:HB3	2.01	0.60
1:D:900:SER:HA	1:D:1025:PHE:HB3	1.83	0.60
1:A:514:GLY:HA2	1:A:517:ASN:HD22	1.66	0.60
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.82	0.60
1:C:576:VAL:HG21	1:C:591:LEU:HD23	1.83	0.60
1:C:889:ALA:HB1	1:C:895:TRP:CZ3	2.35	0.60
1:D:251:LEU:HD11	1:D:262:LEU:HA	1.83	0.60
1:A:184:MET:HE1	1:A:243:THR:OG1	2.01	0.60
1:A:326:PRO:HA	1:A:630:SER:OG	2.00	0.60
1:A:515:TRP:O	1:A:519:MET:HG3	2.01	0.60
1:A:959:GLY:HA2	1:A:1040:ILE:HB	1.84	0.60
1:D:514:GLY:HA2	1:D:516:PHE:HB3	1.83	0.60
1:D:605:ASN:HD21	1:D:642:ASN:CG	2.09	0.60
1:E:516:PHE:HA	1:E:519:MET:HE2	1.84	0.60
1:F:979:SER:CB	1:F:1015:THR:HG21	2.32	0.60
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.82	0.60
1:C:15:ILE:O	1:C:19:ILE:HG13	2.02	0.60
1:D:531:VAL:O	1:D:534:ILE:HG13	2.01	0.60
1:E:26:ALA:O	1:E:30:LEU:HB2	2.01	0.60
1:E:525:HIS:HA	1:E:528:THR:HG22	1.84	0.60
1:F:311:ALA:HA	1:F:314:GLU:CD	2.27	0.60
1:F:351:VAL:HG11	1:F:406:VAL:HG11	1.84	0.60
1:F:519:MET:O	1:F:523:SER:OG	2.18	0.60
1:A:6:ILE:HG13	1:A:7:ASP:N	2.16	0.60
1:A:549:VAL:O	1:A:552:MET:HB3	2.00	0.60
1:C:359:LEU:HB2	1:C:365:THR:HG22	1.84	0.60
1:C:556:PHE:HD1	1:C:913:LEU:HD21	1.66	0.60
1:D:429:GLU:OE1	1:D:432:ARG:NH1	2.34	0.60
1:E:1037:ASN:N	1:E:1038:GLU:HA	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.37	0.60
1:A:9:PRO:HG2	1:A:10:ILE:HD12	1.82	0.60
1:E:166:ILE:O	1:E:169:THR:HB	2.02	0.60
1:F:559:LEU:HD12	1:F:923:ASN:HB2	1.83	0.60
1:A:445:ILE:CD1	1:A:940:LYS:HE3	2.30	0.60
1:B:493:CYS:O	1:B:497:LEU:HB2	2.00	0.60
1:D:781:MET:CE	1:F:225:VAL:H	2.14	0.60
1:D:910:ILE:O	1:D:914:LEU:HB2	2.01	0.60
1:E:733:GLN:NE2	1:E:743:ILE:HG21	2.13	0.60
1:A:47:ALA:HB3	1:A:88:VAL:HG13	1.82	0.60
1:A:193:LEU:HD13	1:A:200:PRO:HD3	1.83	0.60
1:A:360:GLN:NE2	1:A:513:PHE:HB3	2.16	0.60
1:A:549:VAL:O	1:A:552:MET:HE2	2.02	0.60
1:B:699:ARG:HD3	1:B:825:MET:HE2	1.84	0.60
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.84	0.60
1:B:652:THR:HG22	1:B:664:PHE:HD1	1.66	0.59
1:E:154:ILE:HG22	1:E:287:SER:HB3	1.83	0.59
1:F:598:TYR:HB3	1:F:606:VAL:HG21	1.83	0.59
1:A:248:LYS:HA	1:A:261:LEU:HD13	1.83	0.59
1:B:990:VAL:HG22	1:B:1004:GLY:HA3	1.85	0.59
1:D:400:LEU:HD11	1:D:1007:VAL:HG21	1.84	0.59
1:D:578:LEU:HB2	1:D:623:ASN:HB2	1.85	0.59
1:E:544:LEU:O	1:E:548:ILE:HG13	2.01	0.59
1:F:762:PHE:CE1	1:F:764:ASP:HB2	2.37	0.59
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.85	0.59
1:D:157:TYR:O	1:D:161:ASN:ND2	2.26	0.59
1:D:375:VAL:HG11	1:D:405:LEU:HD22	1.85	0.59
1:B:60:THR:HG22	1:B:119:PRO:HD3	1.83	0.59
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.82	0.59
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.38	0.59
1:E:653:ARG:O	1:E:656:SER:OG	2.19	0.59
1:F:1035:ARG:HD3	1:F:1038:GLU:OE1	2.03	0.59
1:B:166:ILE:O	1:B:169:THR:HB	2.02	0.59
1:B:356:TYR:C	1:B:358:PHE:H	2.11	0.59
1:D:201:VAL:HA	1:D:204:ILE:HD12	1.84	0.59
1:E:520:PHE:O	1:E:523:SER:OG	2.20	0.59
1:A:699:ARG:NH2	1:A:722:GLU:OE2	2.35	0.59
1:D:60:THR:HG23	1:D:61:VAL:HG23	1.84	0.59
1:D:442:LEU:O	1:D:445:ILE:HG13	2.02	0.59
1:D:733:GLN:OE1	1:D:743:ILE:HG21	2.02	0.59
2:B:1101:LMT:H5B	2:B:1101:LMT:H6D	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:ALA:O	1:D:468:ARG:NE	2.30	0.59
1:F:671:ILE:HD12	1:F:862:MET:SD	2.43	0.59
1:C:945:ILE:HA	1:C:971:ARG:NH1	2.18	0.59
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.02	0.59
1:D:1013:THR:O	1:D:1017:LEU:HB2	2.03	0.59
1:E:76:MET:HB2	1:E:93:THR:O	2.03	0.59
1:E:142:VAL:HG21	1:E:158:VAL:HG21	1.84	0.59
1:C:733:GLN:OE1	1:C:743:ILE:HG21	2.03	0.59
1:D:699:ARG:NH2	1:D:722:GLU:OE2	2.36	0.59
1:E:43:VAL:HG22	1:E:131:LYS:HG3	1.85	0.59
1:E:200:PRO:HB2	1:E:749:THR:HG22	1.85	0.59
1:E:213:GLN:HA	1:E:237:GLN:O	2.02	0.59
1:E:702:LEU:HD11	1:E:847:LEU:HB3	1.84	0.59
1:A:142:VAL:HG21	1:A:162:MET:HE1	1.85	0.59
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.85	0.59
1:B:519:MET:O	1:B:523:SER:OG	2.21	0.59
1:B:910:ILE:O	1:B:914:LEU:HB2	2.03	0.59
1:D:366:LEU:HA	1:D:369:THR:HB	1.85	0.59
1:D:987:MET:SD	1:D:1008:MET:HE1	2.43	0.59
1:E:7:ASP:CG	1:E:432:ARG:HH21	2.09	0.59
1:E:932:LEU:HA	1:E:935:ILE:HD12	1.84	0.59
1:F:172:VAL:HG13	1:F:291:ILE:HG23	1.85	0.59
1:F:455:PRO:HG2	1:F:880:SER:HA	1.84	0.59
1:B:167:SER:HB2	1:B:175:VAL:HG21	1.84	0.58
1:B:184:MET:HB3	1:B:771:VAL:HG13	1.85	0.58
1:C:139:VAL:HG21	1:C:628:PHE:CE2	2.38	0.58
1:F:267:LYS:HB2	1:F:776:GLU:OE1	2.02	0.58
1:B:696:THR:HG23	1:B:699:ARG:HH12	1.67	0.58
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.84	0.58
1:C:743:ILE:H	1:C:743:ILE:HD12	1.69	0.58
1:D:154:ILE:O	1:D:157:TYR:N	2.37	0.58
1:E:960:LEU:O	1:E:964:THR:HG23	2.03	0.58
1:A:332:PHE:O	1:A:336:SER:HB3	2.03	0.58
1:E:158:VAL:HG22	1:E:162:MET:HE2	1.85	0.58
1:A:66:GLU:OE2	1:A:80:SER:OG	2.21	0.58
1:B:448:VAL:HG13	1:B:884:VAL:HG13	1.85	0.58
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.39	0.58
1:C:249:ILE:HB	1:C:262:LEU:HB2	1.85	0.58
1:C:941:ASN:ND2	1:C:1015:THR:HG22	2.18	0.58
1:D:932:LEU:HA	1:D:935:ILE:HD12	1.85	0.58
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:MET:CE	1:C:225:VAL:H	2.16	0.58
1:B:167:SER:HB2	1:C:70:ASN:ND2	2.18	0.58
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.69	0.58
1:D:223:PRO:O	1:E:780:ARG:NH2	2.36	0.58
1:A:646:ALA:HA	1:A:649:MET:HE3	1.86	0.58
1:A:1040:ILE:HG13	1:A:1041:GLU:N	2.18	0.58
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.84	0.58
1:F:527:TYR:CE2	1:F:968:VAL:HG13	2.39	0.58
1:A:953:MET:HE2	1:A:963:ALA:HB3	1.85	0.58
1:B:634:TRP:H	1:B:634:TRP:CD1	2.20	0.58
1:E:16:ALA:HB2	1:E:488:LEU:HD13	1.85	0.58
1:E:435:MET:SD	1:E:490:PRO:HB3	2.44	0.58
1:F:520:PHE:O	1:F:524:THR:HG22	2.03	0.58
1:F:664:PHE:CD2	1:F:717:ARG:HD3	2.35	0.58
1:A:69:MET:HE1	1:A:107:VAL:O	2.03	0.58
1:A:253:VAL:HG12	1:A:259:ARG:HG2	1.86	0.58
1:A:644:VAL:HG11	1:A:667:ASN:HB2	1.84	0.58
1:A:974:PRO:HA	1:A:977:MET:HE3	1.84	0.58
1:B:415:ASN:ND2	1:B:418:ARG:HH12	2.02	0.58
1:F:817:GLU:OE2	1:F:825:MET:HA	2.03	0.58
1:B:905:VAL:HG13	1:B:935:ILE:HG23	1.85	0.58
1:D:375:VAL:HB	1:D:405:LEU:HD13	1.85	0.58
1:D:721:LEU:HB2	1:D:814:PRO:HG2	1.86	0.58
1:F:465:ALA:HA	1:F:468:ARG:NH1	2.18	0.58
1:A:375:VAL:HG21	1:A:481:SER:HA	1.86	0.58
1:A:562:SER:HB2	1:A:924:ASP:HB3	1.85	0.58
1:B:511:GLY:HA2	1:B:515:TRP:NE1	2.19	0.58
1:B:535:LEU:HD13	1:B:1027:VAL:HG21	1.86	0.58
1:C:197:GLN:HA	1:C:798:MET:SD	2.43	0.58
1:D:776:GLU:HB3	1:D:779:TYR:CE1	2.39	0.58
1:E:210:GLN:HE22	1:E:250:LEU:HB3	1.69	0.58
1:F:278:ILE:HG13	1:F:613:ASN:HB3	1.84	0.58
1:F:462:SER:O	1:F:466:ILE:HG12	2.03	0.58
1:A:680:PHE:HB2	1:A:859:TRP:HZ3	1.68	0.57
1:C:363:ARG:NH1	1:C:363:ARG:H	2.01	0.57
1:E:1019:ILE:HG13	1:E:1020:PHE:CD1	2.39	0.57
1:F:11:PHE:O	1:F:15:ILE:HG13	2.03	0.57
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.86	0.57
1:B:688:ALA:O	1:B:690:LEU:HG	2.04	0.57
1:B:726:GLN:CD	1:B:812:GLY:HA3	2.29	0.57
1:C:971:ARG:HB3	1:C:971:ARG:CZ	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:LEU:HD23	1:E:325:TYR:OH	2.04	0.57
1:E:919:ARG:HB3	1:E:921:LEU:HD23	1.85	0.57
1:F:447:MET:HE1	1:F:891:LEU:HB2	1.86	0.57
1:F:937:LEU:HD13	1:F:1011:MET:SD	2.44	0.57
1:A:225:VAL:H	1:B:781:MET:HE2	1.68	0.57
1:C:971:ARG:NE	1:C:971:ARG:O	2.37	0.57
1:A:165:ALA:HB3	1:A:313:MET:HE1	1.85	0.57
1:B:72:ILE:HD13	1:B:107:VAL:HA	1.86	0.57
1:E:44:THR:OG1	1:E:91:THR:OG1	2.22	0.57
1:F:858:ASP:OD2	1:F:859:TRP:N	2.37	0.57
1:A:424:GLY:HA3	1:A:502:LYS:CG	2.35	0.57
1:C:452:VAL:HG12	1:C:880:SER:HB3	1.85	0.57
1:D:137:LEU:HB2	1:D:293:LEU:HB2	1.87	0.57
1:E:144:ASN:ND2	1:E:319:SER:O	2.37	0.57
1:E:318:PRO:HG2	1:E:321:LEU:HB2	1.86	0.57
1:E:405:LEU:HD21	1:E:477:ALA:HB1	1.87	0.57
1:F:239:ARG:HB2	1:F:763:ILE:HD12	1.85	0.57
1:C:66:GLU:OE2	1:C:80:SER:OG	2.09	0.57
1:E:573:MET:HE1	1:E:617:PHE:HE2	1.69	0.57
1:F:949:ALA:HB3	1:F:1026:PHE:HE2	1.70	0.57
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.87	0.57
1:C:492:LEU:O	1:C:496:MET:HG2	2.05	0.57
1:D:201:VAL:HG23	1:D:749:THR:HG23	1.86	0.57
1:D:398:MET:HE2	1:D:473:THR:HG23	1.87	0.57
1:F:888:LEU:HD21	1:F:943:ILE:HD11	1.87	0.57
1:F:915:ALA:HB2	1:F:1009:GLY:HA3	1.85	0.57
1:B:907:LEU:HD21	1:B:1021:PHE:HB2	1.87	0.57
1:E:932:LEU:HD23	1:E:935:ILE:HD12	1.86	0.57
1:F:380:PHE:HA	1:F:383:LEU:HD12	1.87	0.57
1:F:940:LYS:NZ	1:F:978:THR:HG21	2.18	0.57
1:F:979:SER:HB3	1:F:1015:THR:HG21	1.87	0.57
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.40	0.57
1:E:38:ILE:HD13	1:E:466:ILE:HG12	1.87	0.57
1:C:450:SER:O	1:C:454:VAL:HG23	2.04	0.57
1:F:507:GLU:HG2	1:F:518:ARG:HA	1.86	0.57
1:A:709:HIS:HB2	1:A:713:LEU:HD23	1.87	0.56
1:A:958:LYS:C	1:A:1040:ILE:HG12	2.30	0.56
1:B:57:VAL:HG11	1:B:86:GLY:O	2.05	0.56
1:B:66:GLU:OE2	1:B:818:ARG:HD3	2.04	0.56
1:D:242:SER:O	1:D:246:PHE:HD1	1.87	0.56
1:D:781:MET:HE1	1:F:225:VAL:H	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:PHE:CD1	1:F:977:MET:HE2	2.40	0.56
1:F:409:ALA:O	1:F:413:VAL:HG23	2.05	0.56
1:F:976:LEU:O	1:F:980:LEU:HB2	2.05	0.56
1:A:140:VAL:N	1:A:289:LEU:O	2.36	0.56
1:C:376:LEU:HD22	1:C:398:MET:HE3	1.87	0.56
1:C:393:LEU:HD13	1:C:466:ILE:HA	1.86	0.56
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.87	0.56
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.04	0.56
1:A:743:ILE:HA	1:A:746:ILE:HD12	1.87	0.56
1:B:186:ILE:HG12	1:B:268:ILE:HG12	1.86	0.56
1:B:189:ASN:OD1	1:B:190:PRO:HD2	2.06	0.56
1:B:696:THR:HG23	1:B:699:ARG:NH1	2.21	0.56
1:C:713:LEU:HD21	1:C:843:LEU:HD12	1.88	0.56
1:D:405:LEU:HD22	1:D:481:SER:HB3	1.88	0.56
1:D:412:VAL:HG22	1:D:438:ILE:CD1	2.35	0.56
1:E:76:MET:HE1	1:E:865:GLN:HE22	1.70	0.56
1:F:69:MET:HG3	1:F:92:LEU:HD11	1.86	0.56
1:F:144:ASN:HB3	1:F:148:THR:HG23	1.86	0.56
1:A:4:PHE:HB3	1:A:8:ARG:NH1	2.20	0.56
1:A:492:LEU:O	1:A:496:MET:HG2	2.06	0.56
1:A:519:MET:O	1:A:523:SER:OG	2.15	0.56
1:A:577:GLN:OE1	1:A:624:THR:HG22	2.05	0.56
1:A:597:TYR:HB3	1:A:655:PHE:HZ	1.71	0.56
1:B:535:LEU:HD21	1:B:1024:VAL:HA	1.87	0.56
1:C:3:ASN:O	1:C:6:ILE:N	2.38	0.56
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.87	0.56
1:D:934:THR:O	1:D:938:SER:OG	2.20	0.56
1:E:327:TYR:HB2	1:E:628:PHE:CZ	2.40	0.56
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.86	0.56
1:A:57:VAL:HG21	1:A:86:GLY:CA	2.35	0.56
1:A:157:TYR:CZ	1:A:318:PRO:HD3	2.41	0.56
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.86	0.56
1:C:380:PHE:HA	1:C:383:LEU:HD12	1.88	0.56
1:C:681:ASP:HB2	1:C:828:LEU:HD23	1.86	0.56
1:D:100:ALA:HB1	1:D:131:LYS:HD2	1.87	0.56
1:E:186:ILE:HG12	1:E:268:ILE:HG12	1.86	0.56
1:F:968:VAL:O	1:F:972:LEU:HB2	2.05	0.56
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.05	0.56
1:B:844:MET:HE2	1:B:844:MET:HA	1.87	0.56
1:A:841:MET:HE1	1:A:867:ARG:HG3	1.88	0.56
1:B:950:LYS:NZ	1:B:1030:ARG:HH21	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:LYS:HA	1:D:261:LEU:HD13	1.86	0.56
1:D:556:PHE:HD1	1:D:913:LEU:HD21	1.71	0.56
1:E:752:ALA:O	1:E:774:MET:HA	2.05	0.56
1:F:160:ALA:HA	1:F:767:ARG:HE	1.71	0.56
1:F:404:LEU:HB3	1:F:478:MET:SD	2.45	0.56
1:F:420:MET:HE3	1:F:500:ILE:HD12	1.87	0.56
1:A:259:ARG:NH1	1:B:734:GLU:OE1	2.36	0.56
1:A:344:LEU:HD21	1:A:399:VAL:HA	1.87	0.56
1:A:393:LEU:HD11	1:A:466:ILE:HD13	1.88	0.56
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.86	0.56
1:C:987:MET:HG3	1:C:1008:MET:HE1	1.88	0.56
1:E:175:VAL:HG23	1:F:70:ASN:ND2	2.20	0.56
1:E:911:GLY:HA3	1:E:1013:THR:OG1	2.05	0.56
1:B:455:PRO:HG2	1:B:880:SER:OG	2.04	0.56
1:D:751:GLY:O	1:D:753:ALA:N	2.39	0.56
1:A:35:TYR:CE2	1:A:564:LEU:HD21	2.41	0.56
1:C:688:ALA:O	1:C:690:LEU:N	2.39	0.56
1:D:239:ARG:NH1	1:D:761:ASP:O	2.38	0.56
1:E:415:ASN:O	1:E:419:VAL:HG23	2.06	0.56
1:F:298:ASN:HB3	1:F:301:ASP:HB2	1.87	0.56
1:C:11:PHE:O	1:C:11:PHE:HD2	1.88	0.55
1:E:979:SER:HB3	1:E:1015:THR:HG21	1.88	0.55
1:B:211:ASN:O	1:B:760:ASN:ND2	2.39	0.55
1:B:717:ARG:NE	1:B:828:LEU:HB2	2.22	0.55
1:B:745:ASP:O	1:B:749:THR:OG1	2.14	0.55
1:A:99:ASP:HB3	1:A:102:ILE:HB	1.88	0.55
1:B:888:LEU:HD21	1:B:943:ILE:HD11	1.89	0.55
1:C:407:ASP:OD2	1:C:940:LYS:HD2	2.06	0.55
1:C:1026:PHE:O	1:C:1030:ARG:HG2	2.06	0.55
1:D:559:LEU:HD23	1:D:560:PRO:HD2	1.89	0.55
1:D:989:LEU:HB3	1:D:1000:GLN:O	2.06	0.55
1:E:58:GLN:O	1:E:63:GLN:HG3	2.06	0.55
1:F:186:ILE:HD13	1:F:262:LEU:HD21	1.87	0.55
1:F:414:GLU:OE1	1:F:973:ARG:HD3	2.07	0.55
1:F:443:VAL:O	1:F:447:MET:HB3	2.06	0.55
1:F:945:ILE:HA	1:F:971:ARG:NH1	2.20	0.55
1:A:753:ALA:O	1:A:775:SER:HB3	2.06	0.55
1:D:261:LEU:N	1:D:264:ASP:OD2	2.40	0.55
1:F:187:TRP:HA	1:F:774:MET:O	2.06	0.55
1:D:733:GLN:NE2	1:F:210:GLN:HG2	2.21	0.55
1:E:241:THR:N	1:E:245:GLU:OE1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:261:LEU:HD12	1:E:263:ARG:NH1	2.21	0.55
1:E:261:LEU:N	1:E:264:ASP:OD2	2.38	0.55
1:F:506:GLY:O	1:F:508:GLY:N	2.32	0.55
1:A:1037:ASN:N	1:A:1038:GLU:HB2	2.22	0.55
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.87	0.55
1:C:501:ALA:O	1:C:504:ASP:HB2	2.06	0.55
1:C:762:PHE:CE1	1:C:764:ASP:HB2	2.42	0.55
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.88	0.55
1:D:971:ARG:C	1:D:974:PRO:HD2	2.32	0.55
1:E:934:THR:O	1:E:938:SER:OG	2.23	0.55
1:C:421:ALA:HB1	1:C:505:HIS:H	1.71	0.55
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.88	0.55
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.89	0.55
2:E:1101:LMT:H6D	2:E:1101:LMT:C5B	2.34	0.55
1:F:57:VAL:HG23	1:F:82:SER:HB3	1.89	0.55
1:A:58:GLN:NE2	1:A:59:ASP:OD1	2.36	0.55
1:D:58:GLN:OE1	1:D:818:ARG:NH1	2.38	0.55
1:E:524:THR:O	1:E:527:TYR:HB3	2.07	0.55
1:E:577:GLN:NE2	1:E:721:LEU:HD11	2.21	0.55
1:A:622:GLN:HE21	1:C:222:THR:HG22	1.72	0.55
1:B:699:ARG:HD2	1:B:718:PRO:HB3	1.89	0.55
1:D:1016:VAL:HG12	2:D:1101:LMT:H91	1.89	0.55
1:F:65:ILE:HB	1:F:90:ILE:HD12	1.88	0.55
1:A:154:ILE:O	1:A:157:TYR:N	2.40	0.55
1:A:424:GLY:HA3	1:A:502:LYS:CB	2.37	0.55
1:B:76:MET:SD	1:B:864:TYR:HE2	2.30	0.55
1:B:327:TYR:HB2	1:B:628:PHE:CE2	2.41	0.55
1:B:583:THR:HG22	1:B:585:GLU:H	1.71	0.55
1:B:752:ALA:O	1:B:774:MET:HA	2.07	0.55
1:C:343:THR:HA	1:C:346:GLU:OE1	2.07	0.55
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.88	0.55
1:E:184:MET:HE1	1:E:243:THR:HB	1.89	0.55
1:E:430:ALA:O	1:E:433:LYS:HB3	2.07	0.55
1:F:112:GLN:HA	1:F:115:MET:HB2	1.87	0.55
1:F:214:VAL:HG23	1:F:237:GLN:HB2	1.89	0.55
1:A:982:PHE:O	1:A:985:GLY:N	2.40	0.54
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.90	0.54
1:B:573:MET:HA	1:B:629:VAL:HG23	1.89	0.54
1:C:278:ILE:HG13	1:C:613:ASN:HB3	1.88	0.54
1:C:599:LEU:O	1:C:603:LYS:HG2	2.07	0.54
1:E:440:GLY:C	1:E:891:LEU:HD11	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:559:LEU:HD13	1:E:923:ASN:HB2	1.89	0.54
1:F:414:GLU:HG2	1:F:973:ARG:NH1	2.21	0.54
1:A:101:ASP:OD1	1:A:101:ASP:N	2.41	0.54
1:A:121:GLU:O	1:A:125:GLN:HB2	2.07	0.54
1:A:573:MET:HA	1:A:629:VAL:HG23	1.88	0.54
1:A:976:LEU:O	1:A:980:LEU:HB2	2.07	0.54
1:B:442:LEU:O	1:B:445:ILE:HG13	2.06	0.54
1:B:492:LEU:O	1:B:496:MET:HG2	2.07	0.54
1:E:355:MET:SD	1:E:365:THR:HA	2.47	0.54
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.89	0.54
1:E:910:ILE:O	1:E:914:LEU:HB2	2.07	0.54
1:F:776:GLU:HB2	1:F:779:TYR:CE1	2.43	0.54
1:F:923:ASN:HD22	1:F:923:ASN:C	2.14	0.54
1:F:960:LEU:HD21	1:F:1027:VAL:HA	1.89	0.54
1:F:982:PHE:O	1:F:985:GLY:N	2.41	0.54
1:E:415:ASN:CG	1:E:418:ARG:HH12	2.15	0.54
1:F:1042:HIS:CG	1:F:1043:SER:H	2.24	0.54
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.90	0.54
1:A:573:MET:HE1	1:A:617:PHE:CE2	2.41	0.54
1:C:210:GLN:OE1	1:C:249:ILE:HG23	2.08	0.54
1:D:267:LYS:HD2	1:D:776:GLU:CD	2.33	0.54
1:E:335:ILE:O	1:E:339:GLU:HG2	2.08	0.54
1:A:702:LEU:HD12	1:A:851:LEU:HD21	1.89	0.54
1:B:588:GLN:O	1:B:592:ASN:ND2	2.40	0.54
1:C:725:PRO:HG3	1:C:811:TYR:CE1	2.43	0.54
1:C:881:LEU:HD22	1:C:902:MET:HE1	1.89	0.54
1:D:139:VAL:HB	1:D:327:TYR:HB3	1.89	0.54
1:D:945:ILE:HG12	1:D:971:ARG:CZ	2.37	0.54
1:E:175:VAL:HG23	1:F:70:ASN:HD22	1.73	0.54
1:E:448:VAL:HG13	1:E:884:VAL:HG22	1.89	0.54
1:F:420:MET:HB3	1:F:500:ILE:HB	1.88	0.54
1:F:568:ASP:OD1	1:F:637:ARG:NH1	2.31	0.54
1:A:901:VAL:HG21	1:A:943:ILE:HG13	1.88	0.54
1:B:318:PRO:HD2	1:B:321:LEU:HD22	1.88	0.54
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.89	0.54
1:D:448:VAL:HG22	1:D:887:CYS:CB	2.37	0.54
1:E:157:TYR:CZ	1:E:318:PRO:HD3	2.42	0.54
1:F:422:GLU:HB3	1:F:423:GLU:HG3	1.90	0.54
1:F:775:SER:OG	1:F:776:GLU:O	2.25	0.54
1:B:986:VAL:HG21	1:B:1007:VAL:HG11	1.89	0.54
1:C:893:GLU:HG3	1:C:893:GLU:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:GLU:O	1:E:125:GLN:HB2	2.08	0.54
1:F:13:TRP:CH2	1:F:370:ILE:HD13	2.42	0.54
1:F:284:GLN:HG3	1:F:285:PRO:HD2	1.90	0.54
1:F:926:TYR:HD1	1:F:1002:ALA:HB3	1.73	0.54
1:B:194:ASN:HA	1:B:798:MET:HE2	1.90	0.54
1:C:193:LEU:HD13	1:C:200:PRO:HD3	1.89	0.54
1:C:248:LYS:HA	1:C:261:LEU:HD13	1.90	0.54
1:C:895:TRP:HA	1:C:895:TRP:CE3	2.42	0.54
1:C:941:ASN:HD21	1:C:1015:THR:HG22	1.72	0.54
1:A:11:PHE:CD2	1:B:890:ALA:HB1	2.43	0.54
1:A:27:ILE:HD11	1:A:380:PHE:CD1	2.43	0.54
1:B:415:ASN:OD1	1:B:434:SER:HB2	2.08	0.54
1:B:730:ASP:OD1	1:B:808:ARG:NH2	2.40	0.54
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.90	0.54
1:C:420:MET:HE3	1:C:500:ILE:HB	1.89	0.54
1:C:907:LEU:HD21	1:C:1021:PHE:CB	2.38	0.54
1:D:69:MET:HE1	1:D:111:LEU:HB2	1.90	0.54
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.90	0.54
1:E:785:ASP:N	1:E:785:ASP:OD1	2.41	0.54
1:B:901:VAL:HG21	1:B:943:ILE:HG13	1.89	0.54
1:C:44:THR:OG1	1:C:91:THR:OG1	2.25	0.54
1:C:894:SER:HB3	1:C:897:ILE:HG12	1.88	0.54
1:E:751:GLY:O	1:E:753:ALA:N	2.41	0.54
1:E:281:PHE:HD1	1:E:610:PHE:HD1	1.55	0.53
1:E:375:VAL:O	1:E:379:THR:OG1	2.24	0.53
1:E:460:GLY:O	1:E:463:THR:OG1	2.25	0.53
1:B:668:LEU:H	1:B:668:LEU:CD2	2.21	0.53
1:B:705:GLU:HA	1:B:708:LYS:HD3	1.91	0.53
1:C:76:MET:HE3	1:C:95:GLU:OE2	2.07	0.53
1:D:49:TYR:CD1	1:D:60:THR:HG21	2.44	0.53
1:D:584:GLN:N	1:D:622:GLN:HB3	2.24	0.53
1:D:699:ARG:NE	1:D:718:PRO:HB3	2.24	0.53
1:E:218:GLN:HG3	1:E:221:GLY:HA3	1.90	0.53
1:E:1040:ILE:O	1:E:1041:GLU:HG3	2.07	0.53
1:A:279:ALA:HB3	1:A:286:ALA:O	2.09	0.53
1:B:356:TYR:O	1:B:358:PHE:N	2.34	0.53
1:B:602:GLU:OE2	1:B:650:ARG:HD2	2.09	0.53
1:D:156:ASP:OD1	1:D:765:ARG:NH2	2.41	0.53
1:D:563:PHE:O	1:D:564:LEU:HD12	2.09	0.53
1:F:587:THR:HG21	1:F:622:GLN:O	2.07	0.53
1:F:686:ASP:OD1	1:F:687:GLN:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLN:HE21	1:B:733:GLN:HE21	1.56	0.53
1:C:34:GLN:O	1:C:392:THR:OG1	2.26	0.53
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.90	0.53
1:C:453:PHE:HB3	1:C:471:SER:HA	1.88	0.53
1:C:979:SER:HB3	1:C:1015:THR:HG21	1.90	0.53
1:D:72:ILE:HD13	1:D:107:VAL:HA	1.91	0.53
1:D:419:VAL:HG13	1:D:423:GLU:OE2	2.09	0.53
1:E:76:MET:HE2	1:E:864:TYR:HE2	1.73	0.53
1:E:262:LEU:HG	1:E:268:ILE:HD11	1.90	0.53
1:F:375:VAL:HB	1:F:405:LEU:HD22	1.89	0.53
1:F:376:LEU:O	1:F:379:THR:N	2.41	0.53
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.43	0.53
1:D:564:LEU:HD22	1:D:671:ILE:HG12	1.90	0.53
1:E:214:VAL:HG21	1:F:747:ASN:ND2	2.23	0.53
1:F:699:ARG:HE	1:F:718:PRO:HB3	1.72	0.53
1:A:108:GLN:NE2	1:B:109:ASN:O	2.41	0.53
1:A:465:ALA:O	1:A:469:GLN:HG2	2.09	0.53
1:C:654:ALA:O	1:C:658:ILE:HG12	2.08	0.53
1:C:731:ILE:HD13	1:C:746:ILE:HD11	1.90	0.53
1:D:68:ASN:O	1:D:110:LYS:HB3	2.08	0.53
1:D:151:GLN:HG3	1:D:152:GLU:N	2.24	0.53
1:E:240:LEU:HB2	1:E:246:PHE:CE1	2.44	0.53
1:E:448:VAL:HG13	1:E:884:VAL:HG13	1.90	0.53
1:E:492:LEU:O	1:E:496:MET:HG2	2.09	0.53
1:E:606:VAL:HA	1:E:631:LEU:HD23	1.89	0.53
1:F:462:SER:HB3	1:F:865:GLN:HG2	1.91	0.53
1:A:434:SER:O	1:A:438:ILE:HG12	2.09	0.53
1:B:174:ASP:HB3	1:B:292:LYS:HD2	1.90	0.53
1:E:172:VAL:HG22	1:E:306:ILE:HD11	1.90	0.53
1:E:327:TYR:C	1:E:327:TYR:CD2	2.87	0.53
1:E:506:GLY:HA2	1:E:509:LYS:HD2	1.91	0.53
1:E:555:LEU:HD11	1:E:914:LEU:HD12	1.89	0.53
1:E:578:LEU:HD13	1:E:661:ALA:HB2	1.91	0.53
1:A:448:VAL:O	1:A:451:ALA:HB3	2.08	0.53
1:B:789:TRP:O	1:B:801:PHE:HD2	1.92	0.53
1:C:57:VAL:HG23	1:C:82:SER:HB3	1.90	0.53
1:C:882:ILE:O	1:C:886:LEU:HD22	2.08	0.53
1:E:632:LYS:O	1:E:637:ARG:NE	2.42	0.53
1:E:753:ALA:O	1:E:775:SER:HB3	2.08	0.53
1:F:396:PHE:O	1:F:400:LEU:HB2	2.09	0.53
1:A:242:SER:OG	1:A:245:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:PRO:HD3	1:B:391:ASN:CG	2.34	0.53
1:B:139:VAL:HG13	1:B:178:PHE:HE1	1.73	0.53
1:B:340:VAL:HG11	1:B:395:MET:HB3	1.91	0.53
1:B:396:PHE:O	1:B:400:LEU:HB2	2.08	0.53
1:C:363:ARG:HH11	1:C:363:ARG:CB	2.21	0.53
1:C:686:ASP:HB3	1:C:823:PRO:O	2.09	0.53
1:D:58:GLN:O	1:D:62:THR:HB	2.08	0.53
1:D:582:ALA:HB3	1:D:623:ASN:HB3	1.91	0.53
2:D:1101:LMT:H5B	2:D:1101:LMT:H6D	1.91	0.53
1:E:705:GLU:HB3	1:E:847:LEU:HD22	1.89	0.53
1:F:120:GLN:HG3	1:F:123:GLN:CD	2.34	0.53
1:F:212:ALA:HA	1:F:239:ARG:HG2	1.90	0.53
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.91	0.53
1:A:453:PHE:O	1:A:471:SER:OG	2.20	0.53
1:B:169:THR:HG21	1:B:306:ILE:HG13	1.90	0.53
1:D:298:ASN:OD1	1:D:301:ASP:N	2.40	0.53
1:E:189:ASN:ND2	1:E:190:PRO:HD2	2.24	0.53
1:E:445:ILE:HG12	1:E:940:LYS:HE3	1.90	0.53
1:A:744:ASN:O	1:A:748:THR:HG23	2.09	0.52
1:A:952:LEU:O	1:A:956:GLU:HB2	2.08	0.52
1:B:281:PHE:CZ	1:B:324:VAL:HG11	2.44	0.52
1:C:953:MET:HE2	1:C:963:ALA:HB3	1.91	0.52
1:D:95:GLU:HB2	1:D:98:THR:OG1	2.09	0.52
1:D:166:ILE:HD12	1:D:306:ILE:HG23	1.91	0.52
1:D:587:THR:HB	1:D:613:ASN:HD21	1.74	0.52
1:E:57:VAL:HG11	1:E:86:GLY:CA	2.39	0.52
1:E:60:THR:HG22	1:E:119:PRO:HD3	1.92	0.52
1:F:137:LEU:HB2	1:F:293:LEU:HB2	1.91	0.52
1:F:143:ILE:HG22	1:F:286:ALA:HB2	1.90	0.52
1:A:26:ALA:O	1:A:30:LEU:HB2	2.09	0.52
1:B:3:ASN:HA	1:B:6:ILE:HD12	1.90	0.52
1:B:800:PRO:HG2	1:B:803:ALA:HB2	1.91	0.52
1:C:525:HIS:HA	1:C:528:THR:HG22	1.91	0.52
1:D:196:PHE:HB3	1:D:252:LYS:HZ3	1.74	0.52
1:D:235:ILE:HD11	1:E:726:GLN:NE2	2.24	0.52
1:D:344:LEU:CD2	1:D:402:ILE:HD11	2.34	0.52
1:D:775:SER:HB2	1:D:789:TRP:HZ2	1.74	0.52
1:E:327:TYR:C	1:E:327:TYR:HD2	2.16	0.52
1:F:753:ALA:O	1:F:775:SER:HB3	2.09	0.52
1:B:354:VAL:O	1:B:358:PHE:HB2	2.10	0.52
1:B:456:MET:O	1:B:467:TYR:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ALA:HB2	1:B:471:SER:OG	2.10	0.52
1:E:544:LEU:HA	1:E:547:ILE:HD12	1.90	0.52
1:F:247:GLY:O	1:F:261:LEU:HB3	2.09	0.52
1:F:352:PHE:HA	1:F:355:MET:CE	2.39	0.52
1:A:401:ALA:O	1:A:405:LEU:HG	2.10	0.52
1:A:573:MET:HE1	1:A:617:PHE:HE2	1.75	0.52
1:A:902:MET:O	1:A:905:VAL:HG23	2.09	0.52
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.91	0.52
1:C:452:VAL:O	1:C:455:PRO:HD2	2.08	0.52
1:C:916:ALA:HB2	1:C:927:PHE:CE1	2.43	0.52
1:E:447:MET:HB3	1:E:887:CYS:SG	2.49	0.52
1:E:1039:ASP:N	1:E:1040:ILE:HG13	2.24	0.52
1:F:580:ALA:HB1	1:F:724:THR:HG22	1.91	0.52
1:F:986:VAL:HG21	1:F:1007:VAL:HG11	1.90	0.52
1:A:776:GLU:HG2	1:A:777:ALA:H	1.75	0.52
1:C:940:LYS:NZ	1:C:978:THR:HG21	2.25	0.52
1:D:456:MET:HG3	1:D:471:SER:HB2	1.92	0.52
1:F:451:ALA:HB1	1:F:883:VAL:HG12	1.90	0.52
1:A:650:ARG:O	1:A:653:ARG:HB3	2.08	0.52
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.40	0.52
1:F:187:TRP:CB	1:F:776:GLU:HG2	2.40	0.52
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.45	0.52
1:F:985:GLY:O	1:F:988:PRO:HD2	2.09	0.52
1:A:971:ARG:O	1:A:974:PRO:HD2	2.10	0.52
1:B:87:THR:HG21	1:B:620:ARG:NH2	2.25	0.52
1:B:586:ARG:O	1:B:589:LYS:HB3	2.09	0.52
1:C:188:MET:HB3	1:C:193:LEU:HD11	1.92	0.52
1:D:375:VAL:HG22	1:D:484:VAL:HG21	1.92	0.52
1:D:678:THR:HA	1:D:837:THR:OG1	2.10	0.52
1:D:781:MET:HE3	1:F:228:GLN:OE1	2.09	0.52
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.91	0.52
1:E:80:SER:HB3	1:E:90:ILE:HG12	1.91	0.52
1:E:533:GLY:HA2	1:E:536:ARG:HD3	1.92	0.52
1:F:778:LYS:HG3	1:F:779:TYR:CZ	2.45	0.52
1:F:971:ARG:HH21	1:F:975:ILE:HD11	1.75	0.52
1:A:407:ASP:HB3	1:A:940:LYS:HZ3	1.74	0.52
1:A:574:THR:HG21	1:A:598:TYR:CE2	2.44	0.52
1:C:901:VAL:HG23	1:C:942:ALA:CB	2.36	0.52
1:D:892:TYR:CD2	1:D:897:ILE:HG22	2.45	0.52
1:E:225:VAL:HG12	1:F:777:ALA:HB1	1.90	0.52
1:F:698:ALA:O	1:F:701:GLN:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ALA:O	1:A:490:PRO:HD3	2.10	0.52
1:B:267:LYS:N	1:B:267:LYS:HD2	2.24	0.52
1:B:669:PRO:HB3	1:B:674:LEU:HD12	1.91	0.52
1:C:82:SER:HB2	1:C:816:LEU:HB2	1.92	0.52
1:E:42:ALA:HB2	1:E:93:THR:HG23	1.91	0.52
1:F:250:LEU:HD11	1:F:259:ARG:HB3	1.92	0.52
1:F:682:PHE:CE1	1:F:857:TYR:HB2	2.44	0.52
1:F:780:ARG:O	1:F:781:MET:HE2	2.09	0.52
1:A:11:PHE:HE1	1:A:15:ILE:HD11	1.75	0.52
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.35	0.52
1:A:836:SER:HB3	1:A:839:GLU:HG3	1.92	0.52
1:A:841:MET:HG2	1:A:859:TRP:CH2	2.45	0.52
1:E:59:ASP:OD1	1:E:63:GLN:NE2	2.43	0.52
1:E:194:ASN:HA	1:E:798:MET:HE2	1.92	0.52
1:E:904:VAL:HG21	1:E:942:ALA:HB2	1.92	0.52
1:A:216:ALA:HB2	1:A:236:ALA:HB2	1.92	0.51
1:A:711:ASP:O	1:A:835:LYS:NZ	2.36	0.51
1:A:1020:PHE:CZ	2:A:1101:LMT:H32	2.46	0.51
1:B:273:GLU:CD	1:B:770:LYS:HD2	2.35	0.51
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.92	0.51
1:C:336:SER:O	1:C:340:VAL:HG23	2.09	0.51
1:C:453:PHE:O	1:C:471:SER:OG	2.25	0.51
1:D:332:PHE:O	1:D:336:SER:HB3	2.10	0.51
1:E:184:MET:HB2	1:E:762:PHE:CE2	2.46	0.51
1:E:339:GLU:OE1	1:E:342:LYS:HD3	2.11	0.51
1:E:1038:GLU:OE1	1:E:1040:ILE:HG12	2.10	0.51
1:F:521:GLU:O	1:F:524:THR:HG23	2.10	0.51
1:F:841:MET:HG2	1:F:859:TRP:CH2	2.45	0.51
2:A:1101:LMT:H6D	2:A:1101:LMT:O5B	2.09	0.51
1:B:82:SER:HA	1:B:88:VAL:HG22	1.92	0.51
1:B:172:VAL:HG22	1:B:306:ILE:HD11	1.92	0.51
1:C:247:GLY:O	1:C:261:LEU:HB3	2.11	0.51
1:C:940:LYS:HE2	1:C:941:ASN:OD1	2.10	0.51
1:D:163:LYS:HD2	1:D:289:LEU:HD21	1.91	0.51
1:D:362:PHE:HE2	1:D:363:ARG:HH21	1.59	0.51
1:D:435:MET:HE1	1:D:486:LEU:HD23	1.91	0.51
1:D:775:SER:OG	1:D:780:ARG:HG2	2.10	0.51
1:D:971:ARG:O	1:D:975:ILE:HG12	2.11	0.51
1:E:527:TYR:CE2	1:E:972:LEU:HG	2.45	0.51
1:E:897:ILE:N	1:E:898:PRO:HD2	2.25	0.51
1:F:83:ASP:HB2	1:F:87:THR:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:754:TRP:CH2	1:F:780:ARG:HA	2.45	0.51
1:F:760:ASN:O	1:F:771:VAL:HB	2.11	0.51
1:C:149:MET:HG3	1:C:154:ILE:HG13	1.92	0.51
1:C:1038:GLU:HA	1:C:1039:ASP:CB	2.40	0.51
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.93	0.51
1:D:637:ARG:HB3	1:D:642:ASN:HB3	1.92	0.51
1:D:776:GLU:HB3	1:D:779:TYR:CD1	2.45	0.51
1:F:733:GLN:NE2	1:F:743:ILE:HG21	2.22	0.51
1:A:3:ASN:O	1:A:6:ILE:HG12	2.10	0.51
1:A:11:PHE:CE1	1:A:15:ILE:HD11	2.45	0.51
1:A:790:TYR:HB3	1:A:798:MET:HB3	1.92	0.51
1:D:182:TYR:HD2	1:D:765:ARG:HH22	1.59	0.51
1:D:586:ARG:O	1:D:590:VAL:HG23	2.11	0.51
1:F:340:VAL:HG22	1:F:396:PHE:CE2	2.46	0.51
1:F:905:VAL:HB	1:F:906:PRO:HD3	1.93	0.51
1:A:992:SER:OG	1:A:1000:GLN:OE1	2.26	0.51
1:B:61:VAL:HG22	1:B:118:LEU:HD22	1.91	0.51
1:C:504:ASP:C	1:C:506:GLY:H	2.18	0.51
1:C:739:LEU:HD13	1:C:799:VAL:HG11	1.92	0.51
1:C:751:GLY:O	1:C:753:ALA:N	2.43	0.51
1:D:212:ALA:HA	1:D:239:ARG:HD3	1.92	0.51
1:D:690:LEU:HD21	1:D:853:THR:O	2.09	0.51
1:E:441:ALA:O	1:E:445:ILE:HG23	2.10	0.51
1:E:578:LEU:HD21	1:E:590:VAL:HG21	1.93	0.51
1:F:431:THR:HG21	1:F:490:PRO:O	2.11	0.51
1:F:650:ARG:O	1:F:653:ARG:HB3	2.10	0.51
1:A:905:VAL:HG13	1:A:935:ILE:HD13	1.93	0.51
1:B:415:ASN:O	1:B:419:VAL:HG23	2.10	0.51
1:B:654:ALA:O	1:B:658:ILE:HG12	2.11	0.51
1:C:686:ASP:OD2	1:C:823:PRO:HD2	2.11	0.51
1:D:728:LYS:HA	1:F:235:ILE:HB	1.92	0.51
1:E:102:ILE:O	1:E:106:GLN:HG3	2.10	0.51
1:E:139:VAL:O	1:E:326:PRO:HD2	2.10	0.51
1:E:904:VAL:HG21	1:E:942:ALA:CB	2.40	0.51
1:E:973:ARG:HG2	1:E:977:MET:HE2	1.92	0.51
1:F:261:LEU:N	1:F:264:ASP:OD2	2.43	0.51
1:F:340:VAL:CG1	1:F:395:MET:HB3	2.40	0.51
1:F:524:THR:O	1:F:528:THR:HG22	2.11	0.51
1:F:937:LEU:HD11	1:F:982:PHE:HE2	1.76	0.51
1:F:944:LEU:HD13	1:F:975:ILE:HG12	1.91	0.51
1:A:158:VAL:HA	1:A:162:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:VAL:HG12	1:A:615:PHE:HB3	1.93	0.51
1:A:885:PHE:CE1	1:A:899:PHE:CE2	2.98	0.51
1:D:165:ALA:HB3	1:D:313:MET:HE1	1.92	0.51
1:D:169:THR:HG21	1:D:306:ILE:HG13	1.92	0.51
1:D:953:MET:HE2	1:D:963:ALA:HB3	1.93	0.51
1:E:184:MET:HG2	1:E:246:PHE:CD2	2.46	0.51
1:E:597:TYR:CD2	1:E:655:PHE:HZ	2.29	0.51
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.93	0.51
1:A:424:GLY:HA3	1:A:502:LYS:HB3	1.93	0.51
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.91	0.51
1:A:459:PHE:CE2	1:A:876:LEU:HD12	2.45	0.51
1:C:693:GLU:HB3	1:C:694:LYS:HE2	1.93	0.51
1:D:800:PRO:HG2	1:D:803:ALA:HB2	1.93	0.51
1:F:1015:THR:OG1	1:F:1016:VAL:N	2.43	0.51
1:A:213:GLN:HA	1:A:237:GLN:O	2.11	0.51
1:C:396:PHE:O	1:C:400:LEU:HB2	2.11	0.51
1:C:400:LEU:O	1:C:404:LEU:HD13	2.10	0.51
1:D:328:ASP:O	1:D:331:PRO:HD2	2.11	0.51
1:D:728:LYS:HG2	1:D:808:ARG:CZ	2.41	0.51
1:D:844:MET:HA	1:D:844:MET:HE2	1.91	0.51
1:D:953:MET:SD	1:D:960:LEU:HA	2.51	0.51
1:E:165:ALA:HA	1:E:168:ARG:HB2	1.93	0.51
1:E:251:LEU:HD11	1:E:262:LEU:HA	1.91	0.51
1:E:643:LYS:NZ	1:E:993:THR:HG23	2.26	0.51
1:F:63:GLN:OE1	1:F:818:ARG:NH2	2.44	0.51
1:A:971:ARG:CZ	1:A:971:ARG:HB3	2.41	0.51
1:B:3:ASN:O	1:B:6:ILE:HB	2.11	0.51
1:B:69:MET:HE1	1:B:107:VAL:HG13	1.93	0.51
1:B:254:ASN:HB2	1:B:258:SER:O	2.11	0.51
1:C:156:ASP:OD2	1:C:769:LYS:NZ	2.41	0.51
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.93	0.51
1:E:58:GLN:HE21	1:E:816:LEU:HD13	1.76	0.51
1:F:23:GLY:O	1:F:27:ILE:HG23	2.11	0.51
1:F:404:LEU:HG	1:F:449:LEU:HD13	1.92	0.51
1:F:971:ARG:C	1:F:974:PRO:HD2	2.36	0.51
1:A:151:GLN:HE22	1:A:278:ILE:HG22	1.76	0.50
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.41	0.50
1:C:49:TYR:HD1	1:C:57:VAL:HG12	1.76	0.50
1:C:531:VAL:O	1:C:534:ILE:HG13	2.11	0.50
1:D:23:GLY:O	1:D:27:ILE:HB	2.11	0.50
1:D:58:GLN:O	1:D:63:GLN:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:SER:O	1:D:340:VAL:HG23	2.11	0.50
1:D:544:LEU:O	1:D:547:ILE:HB	2.11	0.50
1:F:380:PHE:HD2	1:F:383:LEU:HD12	1.75	0.50
1:F:901:VAL:HG23	1:F:942:ALA:CB	2.37	0.50
1:B:5:PHE:HE2	1:B:11:PHE:CD2	2.29	0.50
1:C:222:THR:HA	1:C:224:PRO:HD3	1.93	0.50
1:C:602:GLU:HG3	1:C:605:ASN:HD22	1.77	0.50
1:D:112:GLN:HG3	1:E:112:GLN:OE1	2.10	0.50
1:D:393:LEU:HB3	1:D:470:PHE:CE1	2.46	0.50
1:D:602:GLU:HB3	1:D:606:VAL:HG23	1.93	0.50
1:D:730:ASP:HB2	1:D:808:ARG:NH2	2.26	0.50
1:E:166:ILE:HG23	1:E:306:ILE:HG12	1.92	0.50
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.75	0.50
1:A:151:GLN:HG3	1:A:152:GLU:N	2.27	0.50
1:B:712:MET:HE1	1:B:839:GLU:HB3	1.93	0.50
1:C:343:THR:HG21	1:C:989:LEU:HD21	1.92	0.50
1:E:357:LEU:O	1:E:358:PHE:HD1	1.94	0.50
1:F:73:ASP:CG	1:F:106:GLN:HE22	2.19	0.50
1:F:694:LYS:H	1:F:694:LYS:HD2	1.77	0.50
1:F:898:PRO:O	1:F:902:MET:HG2	2.10	0.50
1:B:57:VAL:HG23	1:B:82:SER:HB3	1.92	0.50
1:C:578:LEU:HD12	1:C:582:ALA:HB1	1.92	0.50
1:C:934:THR:O	1:C:938:SER:OG	2.28	0.50
1:E:6:ILE:HD11	1:E:431:THR:HG22	1.92	0.50
1:E:82:SER:HB2	1:E:816:LEU:HB2	1.94	0.50
1:E:442:LEU:O	1:E:445:ILE:HG13	2.11	0.50
1:E:901:VAL:HG23	1:E:942:ALA:CB	2.42	0.50
1:F:310:LEU:O	1:F:314:GLU:HG3	2.12	0.50
1:F:428:LYS:O	1:F:432:ARG:HG3	2.11	0.50
1:F:923:ASN:O	1:F:923:ASN:ND2	2.36	0.50
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.93	0.50
1:A:293:LEU:HD22	1:A:294:ALA:H	1.76	0.50
1:A:360:GLN:HE22	1:A:513:PHE:HB3	1.76	0.50
1:D:379:THR:HG21	1:D:477:ALA:HB2	1.93	0.50
1:E:216:ALA:HB1	1:E:234:ILE:HG22	1.92	0.50
1:A:572:PHE:HB2	1:A:666:PHE:O	2.11	0.50
1:A:971:ARG:O	1:A:975:ILE:HG12	2.11	0.50
1:B:210:GLN:HG2	1:C:733:GLN:NE2	2.27	0.50
1:B:588:GLN:HG3	1:B:592:ASN:HD21	1.76	0.50
1:C:952:LEU:HD23	1:C:956:GLU:HG3	1.93	0.50
1:D:400:LEU:HD21	1:D:930:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:915:ALA:HB2	1:D:1009:GLY:HA3	1.93	0.50
1:E:46:SER:OG	1:E:89:GLN:HG2	2.11	0.50
1:E:222:THR:HA	1:E:224:PRO:HD3	1.93	0.50
1:E:340:VAL:HG22	1:E:396:PHE:CE2	2.47	0.50
1:E:379:THR:HA	1:E:480:LEU:HD12	1.94	0.50
1:A:734:GLU:HG2	1:C:250:LEU:HD22	1.93	0.50
1:A:907:LEU:HD21	1:A:1021:PHE:CD1	2.47	0.50
1:A:909:VAL:HG22	1:A:931:LEU:HD21	1.92	0.50
1:B:177:LEU:HD23	1:B:178:PHE:N	2.26	0.50
1:B:401:ALA:O	1:B:405:LEU:HG	2.11	0.50
1:B:894:SER:HB3	1:B:898:PRO:HD3	1.92	0.50
1:C:634:TRP:CD1	1:C:634:TRP:N	2.72	0.50
1:E:177:LEU:HG	1:E:289:LEU:HD21	1.93	0.50
1:E:396:PHE:O	1:E:400:LEU:HB2	2.12	0.50
1:E:564:LEU:HD13	1:E:674:LEU:HD21	1.94	0.50
1:E:892:TYR:O	1:E:893:GLU:HB2	2.11	0.50
1:F:66:GLU:OE1	1:F:821:GLY:HA2	2.11	0.50
1:F:431:THR:HG22	1:F:435:MET:CE	2.41	0.50
1:F:445:ILE:HG12	1:F:940:LYS:HG3	1.94	0.50
1:A:13:TRP:NE1	1:A:492:LEU:HD21	2.27	0.50
1:A:197:GLN:HA	1:A:798:MET:SD	2.52	0.50
1:C:658:ILE:O	1:C:659:LYS:NZ	2.37	0.50
1:D:408:ASP:OD2	1:D:940:LYS:NZ	2.28	0.50
1:D:609:VAL:HG22	1:D:629:VAL:HG13	1.94	0.50
1:D:781:MET:HE3	1:F:228:GLN:CD	2.37	0.50
1:D:909:VAL:HG22	1:D:931:LEU:HD21	1.94	0.50
1:E:184:MET:HG2	1:E:246:PHE:CE2	2.46	0.50
1:F:69:MET:SD	1:F:72:ILE:HD11	2.52	0.50
1:F:189:ASN:OD1	1:F:190:PRO:HD2	2.12	0.50
1:F:527:TYR:O	1:F:531:VAL:HG23	2.11	0.50
1:F:590:VAL:O	1:F:593:GLU:HB2	2.11	0.50
1:F:723:ASP:HA	1:F:813:SER:HA	1.94	0.50
1:A:140:VAL:HG11	1:A:310:LEU:HD21	1.93	0.50
1:A:350:LEU:HD13	1:A:985:GLY:HA2	1.93	0.50
1:C:144:ASN:O	1:C:148:THR:HG23	2.11	0.50
1:C:612:VAL:HG12	1:C:615:PHE:HB3	1.94	0.50
1:C:946:VAL:HG13	1:C:1026:PHE:CE1	2.47	0.50
1:D:222:THR:HA	1:D:224:PRO:HD3	1.93	0.50
1:D:451:ALA:O	1:D:880:SER:OG	2.22	0.50
1:D:668:LEU:H	1:D:668:LEU:HD23	1.77	0.50
1:E:580:ALA:HB1	1:E:724:THR:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:GLU:O	1:F:124:GLN:HG2	2.11	0.50
1:F:413:VAL:O	1:F:417:GLU:HG2	2.12	0.50
1:F:485:ALA:O	1:F:490:PRO:HD3	2.11	0.50
1:F:764:ASP:OD2	1:F:765:ARG:NH2	2.45	0.50
1:A:352:PHE:HD1	1:A:369:THR:HG21	1.77	0.49
1:B:249:ILE:HG12	1:B:262:LEU:HB2	1.94	0.49
1:B:527:TYR:O	1:B:531:VAL:HG23	2.12	0.49
1:B:871:ASN:OD1	1:B:871:ASN:N	2.30	0.49
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.93	0.49
1:C:379:THR:HG23	1:C:476:SER:OG	2.11	0.49
1:D:415:ASN:HB3	1:D:434:SER:HB2	1.94	0.49
1:D:778:LYS:HG3	1:D:779:TYR:CE2	2.47	0.49
1:E:58:GLN:OE1	1:E:818:ARG:NH1	2.45	0.49
1:E:602:GLU:HG3	1:E:605:ASN:HB2	1.94	0.49
1:F:64:VAL:HG12	1:F:114:ALA:HB1	1.93	0.49
1:F:332:PHE:HD1	1:F:634:TRP:CH2	2.30	0.49
1:F:587:THR:OG1	1:F:588:GLN:N	2.45	0.49
1:A:577:GLN:O	1:A:661:ALA:HB1	2.12	0.49
1:A:887:CYS:O	1:A:890:ALA:HB3	2.12	0.49
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	1.94	0.49
1:C:817:GLU:HB2	1:C:824:SER:O	2.12	0.49
1:D:957:GLY:O	1:D:1040:ILE:HG21	2.11	0.49
1:E:358:PHE:CD2	1:E:977:MET:HG3	2.47	0.49
1:E:574:THR:HG23	1:E:627:ALA:HB3	1.94	0.49
1:E:671:ILE:HB	1:E:674:LEU:HG	1.94	0.49
1:F:426:PRO:O	1:F:430:ALA:N	2.42	0.49
1:F:457:ALA:HB1	1:F:468:ARG:HG3	1.94	0.49
1:A:444:GLY:O	1:A:448:VAL:HG23	2.12	0.49
1:B:354:VAL:HG21	1:B:980:LEU:HB3	1.93	0.49
1:B:478:MET:O	1:B:482:VAL:HG12	2.12	0.49
1:B:563:PHE:O	1:B:564:LEU:HD12	2.11	0.49
1:D:196:PHE:HB3	1:D:252:LYS:HZ1	1.74	0.49
1:E:339:GLU:O	1:E:342:LYS:HB3	2.13	0.49
1:E:415:ASN:HD22	1:E:434:SER:CB	2.17	0.49
1:E:583:THR:H	1:E:586:ARG:HG3	1.77	0.49
1:F:746:ILE:HG13	1:F:747:ASN:N	2.26	0.49
1:B:139:VAL:HG13	1:B:178:PHE:CE1	2.47	0.49
1:B:525:HIS:HA	1:B:528:THR:HG22	1.93	0.49
1:B:877:TYR:HA	1:B:880:SER:HB2	1.93	0.49
1:B:1020:PHE:HZ	2:B:1101:LMT:H62	1.76	0.49
1:C:393:LEU:HD11	1:C:466:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:ILE:HG12	1:D:940:LYS:HE3	1.94	0.49
1:F:184:MET:HB3	1:F:771:VAL:HG13	1.95	0.49
1:F:904:VAL:O	1:F:907:LEU:N	2.45	0.49
1:A:177:LEU:HD23	1:A:288:GLY:O	2.13	0.49
1:A:501:ALA:O	1:A:504:ASP:HB2	2.13	0.49
1:B:671:ILE:O	1:B:673:GLU:N	2.40	0.49
1:C:455:PRO:HG2	1:C:880:SER:HA	1.94	0.49
1:C:600:THR:O	1:C:603:LYS:HG3	2.11	0.49
1:D:5:PHE:HE2	1:D:11:PHE:HD1	1.59	0.49
1:D:175:VAL:HG12	1:D:289:LEU:HD22	1.94	0.49
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.92	0.49
1:D:575:MET:HA	1:D:626:ILE:HD12	1.93	0.49
1:D:626:ILE:HG13	1:D:627:ALA:N	2.28	0.49
1:D:678:THR:HB	1:D:831:ALA:HB3	1.95	0.49
1:E:162:MET:HA	1:E:313:MET:CE	2.43	0.49
1:B:559:LEU:HD12	1:B:923:ASN:HB2	1.95	0.49
1:C:201:VAL:O	1:C:204:ILE:HB	2.13	0.49
1:C:668:LEU:HB2	1:C:669:PRO:HD2	1.93	0.49
1:D:449:LEU:HB3	1:D:478:MET:SD	2.53	0.49
1:D:459:PHE:CB	1:D:464:GLY:HA2	2.43	0.49
1:D:1034:SER:OG	1:D:1035:ARG:N	2.46	0.49
1:E:46:SER:HA	1:E:88:VAL:O	2.13	0.49
1:E:154:ILE:CG2	1:E:287:SER:HB3	2.42	0.49
1:F:506:GLY:C	1:F:508:GLY:N	2.71	0.49
1:F:587:THR:HG21	1:F:623:ASN:HA	1.94	0.49
1:A:228:GLN:OE1	1:B:781:MET:HE3	2.12	0.49
1:A:544:LEU:O	1:A:548:ILE:HG13	2.13	0.49
1:B:87:THR:HG21	1:B:620:ARG:HH22	1.78	0.49
1:B:405:LEU:HD22	1:B:481:SER:HB3	1.93	0.49
1:F:344:LEU:HD13	1:F:402:ILE:HD11	1.95	0.49
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.94	0.49
1:A:987:MET:SD	1:A:1008:MET:HE1	2.53	0.49
1:B:504:ASP:C	1:B:506:GLY:H	2.21	0.49
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.94	0.49
1:D:520:PHE:O	1:D:524:THR:HG23	2.13	0.49
1:F:65:ILE:HD11	1:F:118:LEU:HD11	1.95	0.49
1:A:442:LEU:O	1:A:445:ILE:HG13	2.12	0.49
1:A:831:ALA:HB2	1:A:840:ALA:HB2	1.93	0.49
1:A:900:SER:HB3	1:A:1029:VAL:HG21	1.93	0.49
1:B:577:GLN:O	1:B:661:ALA:HB1	2.13	0.49
1:C:150:THR:HG23	1:C:153:ASP:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:LEU:HD12	1:C:406:VAL:N	2.27	0.49
1:C:544:LEU:O	1:C:547:ILE:HB	2.13	0.49
1:C:578:LEU:CG	1:C:587:THR:HG22	2.39	0.49
1:D:262:LEU:HG	1:D:268:ILE:HD11	1.95	0.49
1:D:394:THR:HG23	1:D:469:GLN:HB3	1.95	0.49
1:E:177:LEU:HA	1:E:289:LEU:HD23	1.95	0.49
1:E:362:PHE:HA	1:E:365:THR:HG22	1.94	0.49
1:F:415:ASN:OD1	1:F:434:SER:HB2	2.13	0.49
1:C:567:GLU:OE1	1:C:996:GLY:HA2	2.12	0.49
1:C:623:ASN:N	1:C:623:ASN:OD1	2.46	0.49
1:C:907:LEU:HD21	1:C:1021:PHE:HB2	1.95	0.49
1:D:108:GLN:NE2	1:E:109:ASN:O	2.46	0.49
1:E:530:SER:OG	2:E:1101:LMT:H1'	2.12	0.49
1:E:658:ILE:C	1:E:659:LYS:HD2	2.37	0.49
1:E:717:ARG:HD2	1:E:828:LEU:HB2	1.94	0.49
1:F:507:GLU:HG2	1:F:518:ARG:HG3	1.94	0.49
1:B:463:THR:HG22	1:B:563:PHE:HE2	1.78	0.48
1:B:516:PHE:O	1:B:520:PHE:N	2.37	0.48
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.43	0.48
1:C:742:SER:O	1:C:746:ILE:HG23	2.13	0.48
1:D:455:PRO:HG2	1:D:880:SER:OG	2.13	0.48
1:D:527:TYR:O	1:D:531:VAL:HG23	2.13	0.48
1:F:427:PRO:O	1:F:431:THR:OG1	2.26	0.48
1:F:451:ALA:O	1:F:883:VAL:HG11	2.13	0.48
1:A:583:THR:H	1:A:586:ARG:HG3	1.78	0.48
1:B:251:LEU:HD21	1:B:262:LEU:HB2	1.95	0.48
1:C:332:PHE:O	1:C:336:SER:HB3	2.13	0.48
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.94	0.48
1:D:452:VAL:HA	1:D:880:SER:OG	2.12	0.48
1:D:532:GLY:O	1:D:536:ARG:HG3	2.13	0.48
1:D:744:ASN:O	1:D:748:THR:HG23	2.12	0.48
1:F:80:SER:OG	1:F:818:ARG:HB2	2.13	0.48
1:F:971:ARG:HB3	1:F:971:ARG:NH1	2.28	0.48
1:A:354:VAL:HG12	1:A:355:MET:HE3	1.95	0.48
1:B:166:ILE:HD12	1:B:309:GLU:HG3	1.95	0.48
1:C:13:TRP:HH2	1:C:370:ILE:HD13	1.78	0.48
1:E:602:GLU:OE2	1:E:650:ARG:NH1	2.46	0.48
1:F:562:SER:HB2	1:F:924:ASP:HB3	1.95	0.48
1:A:391:ASN:O	1:A:395:MET:HG2	2.12	0.48
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.94	0.48
1:A:1037:ASN:CA	1:A:1038:GLU:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:PRO:CD	1:B:499:PRO:HB3	2.41	0.48
1:C:590:VAL:HA	1:C:593:GLU:OE1	2.14	0.48
1:D:889:ALA:HA	1:D:894:SER:O	2.14	0.48
1:E:324:VAL:O	1:E:326:PRO:HD3	2.14	0.48
1:E:399:VAL:O	1:E:402:ILE:HG13	2.13	0.48
1:F:49:TYR:CD1	1:F:57:VAL:HA	2.48	0.48
1:A:79:SER:HA	1:A:818:ARG:O	2.14	0.48
1:A:138:MET:O	1:A:291:ILE:N	2.41	0.48
1:A:909:VAL:HA	1:A:931:LEU:HD21	1.95	0.48
1:B:121:GLU:O	1:B:125:GLN:HB2	2.14	0.48
1:B:371:ALA:O	1:B:375:VAL:HG23	2.13	0.48
1:E:36:PRO:HD3	1:E:391:ASN:CG	2.38	0.48
1:E:36:PRO:HG3	1:E:469:GLN:HG3	1.95	0.48
1:F:363:ARG:HH11	1:F:363:ARG:CG	2.26	0.48
1:B:383:LEU:HD11	1:B:473:THR:HG23	1.96	0.48
1:B:682:PHE:HB3	1:B:827:ILE:O	2.14	0.48
1:B:987:MET:HB3	1:B:987:MET:HE2	1.82	0.48
1:B:1020:PHE:CZ	2:B:1101:LMT:H62	2.48	0.48
1:D:838:GLY:O	1:D:841:MET:HB2	2.14	0.48
1:E:520:PHE:O	1:E:524:THR:HG23	2.13	0.48
1:E:832:ALA:HB3	1:E:835:LYS:HD2	1.95	0.48
1:F:343:THR:HG21	1:F:989:LEU:CD2	2.39	0.48
1:F:776:GLU:HB2	1:F:779:TYR:HE1	1.78	0.48
1:A:593:GLU:OE2	1:A:659:LYS:NZ	2.36	0.48
1:B:327:TYR:CD1	1:B:571:VAL:HG11	2.48	0.48
1:C:504:ASP:C	1:C:506:GLY:N	2.72	0.48
1:D:967:ALA:C	1:D:971:ARG:HH12	2.21	0.48
1:F:11:PHE:CE2	1:F:15:ILE:HD11	2.49	0.48
1:F:133:SER:O	1:F:134:SER:HB2	2.14	0.48
1:F:340:VAL:HG11	1:F:395:MET:CB	2.43	0.48
1:F:602:GLU:HB3	1:F:606:VAL:HG23	1.96	0.48
1:A:58:GLN:O	1:A:63:GLN:HG3	2.13	0.48
1:A:108:GLN:O	1:A:112:GLN:HG2	2.14	0.48
1:B:327:TYR:HD1	1:B:571:VAL:HG11	1.79	0.48
1:C:443:VAL:HG11	1:C:891:LEU:HD11	1.95	0.48
1:D:281:PHE:CZ	1:D:608:SER:HB2	2.49	0.48
1:D:901:VAL:HG21	1:D:943:ILE:HG13	1.95	0.48
1:F:2:PRO:O	1:F:5:PHE:HB3	2.14	0.48
1:F:242:SER:HB2	1:F:244:GLU:HB3	1.95	0.48
1:F:412:VAL:HA	1:F:438:ILE:CD1	2.43	0.48
1:A:421:ALA:HB1	1:A:505:HIS:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:SER:CB	1:A:1015:THR:HG21	2.44	0.48
1:B:717:ARG:CD	1:B:828:LEU:HB2	2.44	0.48
1:B:960:LEU:HD13	1:B:1030:ARG:HG2	1.96	0.48
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.96	0.48
1:D:193:LEU:HD13	1:D:200:PRO:HD3	1.96	0.48
1:D:293:LEU:HD11	1:D:299:ALA:HA	1.94	0.48
1:D:343:THR:O	1:D:344:LEU:C	2.55	0.48
1:D:960:LEU:O	1:D:964:THR:HG23	2.13	0.48
1:E:351:VAL:HG21	1:E:406:VAL:HG22	1.96	0.48
1:E:676:THR:O	1:E:679:GLY:N	2.47	0.48
1:E:699:ARG:HE	1:E:718:PRO:CG	2.24	0.48
1:E:903:LEU:O	1:E:906:PRO:HD2	2.13	0.48
1:F:949:ALA:HB3	1:F:1026:PHE:CE2	2.49	0.48
1:A:16:ALA:O	1:A:20:MET:HG3	2.14	0.48
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.95	0.48
1:B:904:VAL:HG21	1:B:942:ALA:CB	2.43	0.48
1:D:27:ILE:HD11	1:D:380:PHE:CE1	2.48	0.48
1:D:705:GLU:HB3	1:D:847:LEU:HD22	1.96	0.48
1:D:719:ASN:HB3	1:D:826:GLU:HG2	1.95	0.48
1:E:680:PHE:HB2	1:E:863:SER:HG	1.77	0.48
1:F:383:LEU:HD23	1:F:472:ILE:HD13	1.96	0.48
1:C:66:GLU:OE1	1:C:821:GLY:HA2	2.14	0.47
1:C:527:TYR:O	1:C:531:VAL:HG23	2.14	0.47
1:D:740:GLY:O	1:D:794:ALA:N	2.40	0.47
1:D:985:GLY:O	1:D:988:PRO:HD2	2.14	0.47
1:A:63:GLN:O	1:A:67:GLN:HG3	2.15	0.47
1:A:152:GLU:HB2	1:A:182:TYR:HE1	1.79	0.47
1:A:267:LYS:HD2	1:A:776:GLU:CD	2.39	0.47
1:A:425:LEU:HB3	1:A:429:GLU:HB2	1.96	0.47
1:A:757:SER:O	1:A:772:TYR:HA	2.14	0.47
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.96	0.47
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.48	0.47
1:B:743:ILE:HD12	1:B:743:ILE:H	1.78	0.47
1:C:690:LEU:HD11	1:C:854:GLY:O	2.14	0.47
1:C:982:PHE:O	1:C:983:ILE:C	2.57	0.47
1:D:391:ASN:O	1:D:395:MET:HG2	2.14	0.47
1:E:440:GLY:O	1:E:891:LEU:HD11	2.15	0.47
1:E:776:GLU:HG2	1:E:777:ALA:N	2.29	0.47
1:F:350:LEU:HD23	1:F:984:LEU:HB3	1.96	0.47
1:A:511:GLY:HA2	1:A:515:TRP:CD1	2.49	0.47
1:B:717:ARG:HE	1:B:828:LEU:HB2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ALA:HA	1:C:40:PRO:HD2	1.67	0.47
1:D:34:GLN:HB2	1:D:333:VAL:HG22	1.94	0.47
1:E:281:PHE:CE1	1:E:608:SER:HB2	2.49	0.47
1:E:504:ASP:C	1:E:506:GLY:H	2.23	0.47
1:F:84:SER:C	1:F:86:GLY:H	2.22	0.47
1:F:138:MET:HE2	1:F:140:VAL:HG22	1.96	0.47
1:F:149:MET:HG3	1:F:154:ILE:HG13	1.97	0.47
1:F:746:ILE:HG13	1:F:747:ASN:H	1.78	0.47
1:A:960:LEU:O	1:A:964:THR:HG23	2.15	0.47
1:B:225:VAL:HG13	1:C:781:MET:SD	2.54	0.47
1:B:678:THR:HA	1:B:837:THR:OG1	2.15	0.47
1:B:877:TYR:O	1:B:881:LEU:HG	2.13	0.47
1:C:351:VAL:HG12	1:C:355:MET:HE2	1.96	0.47
1:D:455:PRO:HG2	1:D:880:SER:CB	2.44	0.47
1:E:214:VAL:HG21	1:F:747:ASN:CG	2.39	0.47
1:E:572:PHE:CD1	1:E:648:THR:HG22	2.49	0.47
1:E:992:SER:O	1:E:997:SER:HB2	2.14	0.47
1:E:1037:ASN:HB2	1:E:1038:GLU:O	2.15	0.47
1:F:202:ASP:OD1	1:F:792:ARG:NH2	2.47	0.47
1:F:368:PRO:O	1:F:371:ALA:HB3	2.13	0.47
1:F:885:PHE:HE1	1:F:899:PHE:CE2	2.32	0.47
1:A:67:GLN:NE2	1:C:768:VAL:HG13	2.29	0.47
1:B:32:VAL:HG22	1:B:298:ASN:ND2	2.29	0.47
1:B:1038:GLU:C	1:B:1040:ILE:HG13	2.40	0.47
1:C:146:ASP:O	1:C:148:THR:N	2.47	0.47
1:C:418:ARG:HH11	1:C:422:GLU:CD	2.23	0.47
1:D:343:THR:O	1:D:346:GLU:N	2.47	0.47
1:D:634:TRP:CD1	1:D:634:TRP:N	2.82	0.47
1:E:61:VAL:HG21	1:E:122:VAL:HG21	1.96	0.47
1:E:246:PHE:HA	1:E:249:ILE:HG23	1.97	0.47
1:F:361:ASN:HB3	1:F:364:ALA:HB3	1.95	0.47
1:F:405:LEU:HD12	1:F:406:VAL:N	2.29	0.47
1:F:504:ASP:C	1:F:506:GLY:H	2.22	0.47
1:A:72:ILE:HD13	1:A:107:VAL:HG22	1.95	0.47
1:A:184:MET:HE3	1:A:184:MET:HA	1.97	0.47
1:A:535:LEU:HD23	1:A:535:LEU:HA	1.65	0.47
1:A:637:ARG:HB3	1:A:642:ASN:HB3	1.96	0.47
1:A:937:LEU:O	1:A:940:LYS:HB3	2.15	0.47
1:B:574:THR:HA	1:B:665:ALA:HA	1.96	0.47
1:B:685:ILE:HD11	1:B:819:TYR:CD2	2.49	0.47
1:D:610:PHE:HB3	1:D:628:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:VAL:HA	1:E:118:LEU:HD22	1.97	0.47
1:E:158:VAL:HB	1:E:177:LEU:HD11	1.96	0.47
1:F:345:VAL:O	1:F:348:ILE:HB	2.14	0.47
1:A:220:GLY:HA3	1:A:230:LEU:O	2.14	0.47
1:A:641:GLU:HA	1:A:646:ALA:HB3	1.96	0.47
1:A:671:ILE:HG21	1:A:674:LEU:HB3	1.95	0.47
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.80	0.47
1:A:1038:GLU:HB3	1:A:1039:ASP:C	2.39	0.47
1:B:164:ASP:OD2	1:C:67:GLN:HG2	2.15	0.47
1:B:501:ALA:O	1:B:504:ASP:HB2	2.15	0.47
1:B:645:GLU:O	1:B:649:MET:HB2	2.15	0.47
1:C:133:SER:OG	1:C:293:LEU:O	2.31	0.47
1:C:139:VAL:HA	1:C:289:LEU:O	2.14	0.47
1:C:375:VAL:HA	1:C:480:LEU:HD13	1.96	0.47
1:C:383:LEU:HD23	1:C:472:ILE:HD12	1.97	0.47
1:C:778:LYS:HG3	1:C:779:TYR:CZ	2.50	0.47
1:D:191:ASN:O	1:D:194:ASN:N	2.48	0.47
1:D:559:LEU:CD2	1:D:922:THR:HA	2.44	0.47
1:D:574:THR:HG23	1:D:627:ALA:HB3	1.96	0.47
1:E:238:THR:HG22	1:E:239:ARG:O	2.13	0.47
1:E:525:HIS:HA	1:E:528:THR:CG2	2.44	0.47
1:E:538:THR:HG22	1:E:1024:VAL:HG13	1.97	0.47
1:E:987:MET:HB3	1:E:988:PRO:HD3	1.96	0.47
1:F:253:VAL:HG13	1:F:259:ARG:HG2	1.96	0.47
1:F:588:GLN:O	1:F:592:ASN:ND2	2.48	0.47
1:F:941:ASN:CG	1:F:975:ILE:HG23	2.40	0.47
1:A:44:THR:HA	1:A:90:ILE:O	2.13	0.47
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.63	0.47
1:A:514:GLY:HA2	1:A:517:ASN:ND2	2.29	0.47
1:C:30:LEU:HD23	1:C:390:ILE:HD11	1.97	0.47
1:C:831:ALA:HB3	1:C:835:LYS:HG2	1.97	0.47
1:D:21:LEU:HD13	1:D:21:LEU:HA	1.63	0.47
1:D:183:ALA:HB2	1:D:273:GLU:HG3	1.97	0.47
1:D:573:MET:HG3	1:D:666:PHE:HE2	1.80	0.47
1:D:888:LEU:HD11	1:D:901:VAL:HG22	1.96	0.47
1:E:621:GLY:O	1:E:624:THR:HG22	2.14	0.47
1:F:453:PHE:HE1	1:F:474:ILE:HG21	1.80	0.47
1:F:982:PHE:HD2	1:F:1011:MET:HE2	1.79	0.47
1:A:69:MET:SD	1:A:72:ILE:HD11	2.55	0.47
1:A:75:LEU:HD23	1:C:168:ARG:HD3	1.97	0.47
1:A:578:LEU:CD2	1:A:590:VAL:HG21	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ASN:HB2	1:C:583:THR:HG22	1.97	0.47
1:B:725:PRO:HA	1:B:810:GLU:O	2.15	0.47
1:B:795:ASP:OD2	1:B:797:GLN:HG2	2.15	0.47
1:B:888:LEU:HA	1:B:888:LEU:HD23	1.65	0.47
1:D:121:GLU:O	1:D:124:GLN:HG2	2.15	0.47
1:D:538:THR:HG21	1:D:1028:VAL:HG22	1.97	0.47
1:D:907:LEU:HD21	1:D:1021:PHE:HB2	1.96	0.47
1:D:907:LEU:HD21	1:D:1021:PHE:CB	2.45	0.47
1:E:371:ALA:O	1:E:375:VAL:HG23	2.15	0.47
1:E:751:GLY:O	1:E:754:TRP:N	2.48	0.47
1:E:888:LEU:HA	1:E:888:LEU:HD23	1.49	0.47
1:A:214:VAL:HG21	1:B:747:ASN:CG	2.39	0.47
1:A:613:ASN:OD1	1:A:614:GLY:N	2.48	0.47
1:A:793:ALA:HB3	1:A:795:ASP:OD2	2.14	0.47
1:C:457:ALA:HB2	1:C:471:SER:OG	2.15	0.47
1:C:895:TRP:HA	1:C:895:TRP:HE3	1.78	0.47
1:D:888:LEU:HD12	1:D:902:MET:HG3	1.97	0.47
1:D:948:PHE:O	1:D:952:LEU:HG	2.15	0.47
1:E:732:ASP:OD1	1:E:735:LYS:HG3	2.14	0.47
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.97	0.47
1:F:382:VAL:HG11	1:F:476:SER:CB	2.45	0.47
1:F:736:ALA:O	1:F:741:VAL:HG23	2.15	0.47
1:A:146:ASP:OD2	1:A:146:ASP:N	2.29	0.46
1:A:169:THR:HG22	1:A:172:VAL:HG23	1.97	0.46
1:A:563:PHE:CD2	1:A:671:ILE:HD11	2.50	0.46
1:B:399:VAL:O	1:B:402:ILE:HG13	2.15	0.46
1:B:404:LEU:HD21	1:B:449:LEU:HD22	1.97	0.46
1:C:154:ILE:HG22	1:C:287:SER:HB3	1.96	0.46
1:C:641:GLU:HA	1:C:646:ALA:HB3	1.96	0.46
1:E:249:ILE:CG1	1:E:262:LEU:HB2	2.45	0.46
1:E:568:ASP:O	1:E:634:TRP:HZ3	1.98	0.46
1:E:841:MET:O	1:E:845:GLU:HG3	2.14	0.46
1:F:602:GLU:OE2	1:F:650:ARG:HD2	2.16	0.46
1:F:682:PHE:HE1	1:F:857:TYR:HB2	1.80	0.46
1:A:327:TYR:C	1:A:327:TYR:CD2	2.93	0.46
1:A:648:THR:HB	1:A:665:ALA:O	2.15	0.46
1:B:42:ALA:HB3	1:B:132:SER:HB3	1.96	0.46
1:B:213:GLN:NE2	1:C:52:ALA:HA	2.28	0.46
1:B:447:MET:HB3	1:B:887:CYS:SG	2.56	0.46
1:C:371:ALA:O	1:C:375:VAL:HG23	2.15	0.46
1:C:524:THR:O	1:C:528:THR:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:LEU:CD1	1:C:901:VAL:HG11	2.45	0.46
1:D:163:LYS:HE3	1:D:177:LEU:HB2	1.97	0.46
1:D:776:GLU:HG2	1:D:777:ALA:H	1.81	0.46
1:E:330:THR:HG22	1:E:334:LYS:HE2	1.97	0.46
1:E:332:PHE:O	1:E:336:SER:HB2	2.15	0.46
1:F:36:PRO:HD3	1:F:391:ASN:ND2	2.30	0.46
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.97	0.46
1:F:743:ILE:H	1:F:743:ILE:HD12	1.80	0.46
1:F:835:LYS:HG2	1:F:836:SER:H	1.80	0.46
1:A:681:ASP:HB2	1:A:862:MET:HE3	1.97	0.46
1:B:706:ALA:HB1	1:B:713:LEU:HD13	1.97	0.46
1:C:375:VAL:HB	1:C:405:LEU:HD22	1.97	0.46
1:C:725:PRO:HG3	1:C:811:TYR:HE1	1.81	0.46
1:C:944:LEU:CD1	1:C:975:ILE:HG12	2.45	0.46
1:D:347:ALA:O	1:D:351:VAL:HG23	2.16	0.46
1:D:540:ARG:O	1:D:543:VAL:HB	2.16	0.46
1:E:527:TYR:O	1:E:530:SER:HB3	2.14	0.46
1:F:566:ASP:OD1	1:F:678:THR:HG23	2.16	0.46
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.80	0.46
1:A:583:THR:HA	1:A:622:GLN:OE1	2.15	0.46
1:B:143:ILE:HG12	1:B:322:LYS:O	2.16	0.46
1:B:578:LEU:HD21	1:B:587:THR:HA	1.97	0.46
1:B:753:ALA:O	1:B:775:SER:HB3	2.16	0.46
1:C:562:SER:HB2	1:C:924:ASP:HB3	1.96	0.46
1:C:735:LYS:O	1:C:738:ALA:HB3	2.15	0.46
1:D:184:MET:HB3	1:D:771:VAL:HG22	1.98	0.46
1:D:485:ALA:O	1:D:490:PRO:HD3	2.15	0.46
1:D:545:TYR:HB2	1:D:1021:PHE:HE2	1.81	0.46
1:E:450:SER:HB2	1:E:454:VAL:HG23	1.97	0.46
1:E:508:GLY:HA3	1:E:518:ARG:NE	2.25	0.46
1:E:652:THR:OG1	1:E:665:ALA:HB3	2.15	0.46
1:F:151:GLN:NE2	1:F:279:ALA:H	2.14	0.46
1:B:310:LEU:HG	1:B:323:ILE:HG13	1.98	0.46
1:B:713:LEU:HD11	1:B:843:LEU:HD12	1.97	0.46
1:C:76:MET:N	1:C:93:THR:O	2.46	0.46
1:C:170:SER:O	1:C:302:THR:HA	2.14	0.46
1:C:841:MET:HG2	1:C:859:TRP:CH2	2.51	0.46
1:D:55:LYS:HZ1	1:F:238:THR:HG1	1.56	0.46
1:D:250:LEU:HD23	1:E:737:GLN:NE2	2.30	0.46
1:D:417:GLU:OE1	1:D:497:LEU:HD11	2.16	0.46
1:E:13:TRP:HA	1:E:13:TRP:CE3	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:GLU:HB3	1:F:182:TYR:HE1	1.80	0.46
1:F:278:ILE:CG1	1:F:613:ASN:HB3	2.45	0.46
1:F:368:PRO:HG3	1:F:413:VAL:HG21	1.97	0.46
1:F:382:VAL:HG21	1:F:476:SER:HB2	1.96	0.46
1:F:549:VAL:O	1:F:552:MET:HB3	2.15	0.46
1:F:623:ASN:OD1	1:F:623:ASN:N	2.45	0.46
1:F:873:ALA:HB2	1:F:928:GLN:NE2	2.29	0.46
1:A:659:LYS:HA	1:A:659:LYS:HD3	1.67	0.46
1:B:104:GLN:HG3	1:B:129:VAL:HG12	1.98	0.46
1:B:758:TYR:CE1	1:B:770:LYS:HD3	2.50	0.46
1:C:121:GLU:O	1:C:124:GLN:HG2	2.15	0.46
1:C:144:ASN:HA	1:C:320:GLY:O	2.16	0.46
1:C:366:LEU:O	1:C:370:ILE:HG13	2.16	0.46
1:D:449:LEU:HD13	1:D:478:MET:SD	2.55	0.46
1:D:507:GLU:C	1:D:509:LYS:H	2.22	0.46
1:D:974:PRO:O	1:D:975:ILE:C	2.59	0.46
1:E:162:MET:O	1:E:164:ASP:N	2.48	0.46
1:E:255:GLN:H	1:E:255:GLN:HG3	1.21	0.46
1:E:310:LEU:CD2	1:E:323:ILE:HG21	2.45	0.46
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.96	0.46
1:F:895:TRP:HA	1:F:895:TRP:CE3	2.50	0.46
1:A:449:LEU:HB3	1:A:478:MET:SD	2.56	0.46
1:A:457:ALA:HB2	1:A:471:SER:CB	2.46	0.46
1:A:597:TYR:CG	1:A:655:PHE:CZ	3.04	0.46
1:A:1039:ASP:H	1:A:1040:ILE:HB	1.80	0.46
1:B:600:THR:O	1:B:603:LYS:HB2	2.15	0.46
1:B:683:GLU:HG2	1:B:819:TYR:CG	2.50	0.46
1:C:427:PRO:O	1:C:431:THR:OG1	2.30	0.46
1:C:611:ALA:HA	1:C:627:ALA:HA	1.97	0.46
1:C:947:GLU:HG3	1:C:948:PHE:CD1	2.47	0.46
1:D:189:ASN:HB3	1:D:192:GLU:HB2	1.97	0.46
1:D:423:GLU:O	1:D:502:LYS:HB3	2.16	0.46
1:D:562:SER:OG	1:D:922:THR:HG21	2.16	0.46
1:D:957:GLY:O	1:D:1040:ILE:HD13	2.16	0.46
1:E:727:PHE:CE1	1:E:807:SER:HB2	2.51	0.46
1:F:566:ASP:CG	1:F:678:THR:HG23	2.40	0.46
1:F:574:THR:HG23	1:F:627:ALA:HB3	1.97	0.46
1:A:363:ARG:O	1:A:496:MET:HE2	2.16	0.46
1:A:375:VAL:HG13	1:A:480:LEU:HB3	1.98	0.46
1:B:166:ILE:HG12	1:B:310:LEU:HD13	1.97	0.46
1:B:517:ASN:O	1:B:521:GLU:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:LEU:HD22	1:B:851:LEU:HD11	1.97	0.46
1:C:2:PRO:O	1:C:5:PHE:HB3	2.16	0.46
1:D:57:VAL:HG21	1:D:86:GLY:CA	2.36	0.46
1:D:463:THR:HG23	1:D:467:TYR:CD1	2.51	0.46
1:D:897:ILE:HA	1:D:1029:VAL:CG1	2.43	0.46
1:D:987:MET:HB3	1:D:988:PRO:HD3	1.98	0.46
1:E:32:VAL:HG12	1:E:390:ILE:HB	1.97	0.46
1:E:478:MET:O	1:E:482:VAL:HG12	2.15	0.46
1:E:741:VAL:HB	1:E:746:ILE:HD11	1.97	0.46
1:F:366:LEU:HA	1:F:369:THR:HB	1.97	0.46
1:F:449:LEU:HD23	1:F:936:GLY:HA3	1.96	0.46
1:F:534:ILE:HB	1:F:541:TYR:CZ	2.51	0.46
1:F:652:THR:HG23	1:F:664:PHE:HD1	1.80	0.46
1:F:885:PHE:CD2	1:F:886:LEU:HD22	2.47	0.46
1:A:781:MET:HE1	1:C:225:VAL:H	1.81	0.46
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.61	0.46
1:B:641:GLU:HA	1:B:646:ALA:HB3	1.98	0.46
1:C:238:THR:HG22	1:C:239:ARG:O	2.16	0.46
1:C:445:ILE:HG12	1:C:940:LYS:HG3	1.98	0.46
1:C:641:GLU:OE2	1:C:641:GLU:N	2.37	0.46
1:C:972:LEU:O	1:C:975:ILE:HB	2.16	0.46
1:D:139:VAL:HA	1:D:289:LEU:O	2.15	0.46
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.98	0.46
1:E:344:LEU:HD23	1:E:402:ILE:HD11	1.98	0.46
1:F:447:MET:SD	1:F:891:LEU:HD22	2.56	0.46
1:A:375:VAL:HG22	1:A:484:VAL:HG21	1.98	0.46
1:B:613:ASN:HD22	1:B:613:ASN:C	2.24	0.46
1:B:903:LEU:HB3	1:B:1025:PHE:CE2	2.51	0.46
1:C:48:SER:C	1:C:50:PRO:HD3	2.41	0.46
1:C:211:ASN:OD1	1:C:240:LEU:HG	2.16	0.46
1:C:698:ALA:O	1:C:701:GLN:HB3	2.16	0.46
1:C:785:ASP:O	1:C:789:TRP:HD1	1.98	0.46
1:C:987:MET:HB3	1:C:987:MET:HE2	1.71	0.46
1:D:252:LYS:HE2	1:D:260:VAL:HG21	1.98	0.46
1:D:346:GLU:O	1:D:350:LEU:HD12	2.16	0.46
1:D:424:GLY:HA3	1:D:502:LYS:HB3	1.97	0.46
1:D:459:PHE:CE2	1:D:876:LEU:HD12	2.51	0.46
1:D:515:TRP:O	1:D:519:MET:HG3	2.16	0.46
1:D:752:ALA:O	1:D:774:MET:HA	2.15	0.46
1:E:184:MET:HB3	1:E:771:VAL:HG13	1.98	0.46
1:E:188:MET:HE1	1:E:200:PRO:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:564:LEU:HD12	1:F:564:LEU:HA	1.85	0.46
1:B:149:MET:HB2	1:B:153:ASP:CB	2.45	0.45
1:B:247:GLY:O	1:B:261:LEU:HB3	2.16	0.45
1:B:310:LEU:CD2	1:B:323:ILE:HG21	2.46	0.45
1:B:702:LEU:HD13	1:B:848:ALA:HA	1.97	0.45
1:C:447:MET:HE3	1:C:887:CYS:SG	2.57	0.45
1:C:562:SER:OG	1:C:922:THR:HG21	2.16	0.45
1:C:584:GLN:N	1:C:622:GLN:HB3	2.31	0.45
1:D:445:ILE:O	1:D:449:LEU:HB2	2.16	0.45
1:E:193:LEU:HD13	1:E:200:PRO:HD3	1.97	0.45
1:E:224:PRO:HA	1:F:781:MET:HE1	1.98	0.45
1:E:597:TYR:CD1	1:E:601:LYS:HD2	2.51	0.45
1:E:680:PHE:CE1	1:E:682:PHE:HB2	2.50	0.45
1:E:682:PHE:CE1	1:E:857:TYR:HB2	2.52	0.45
1:E:738:ALA:C	1:E:740:GLY:H	2.23	0.45
1:A:5:PHE:HE2	1:A:11:PHE:CD1	2.33	0.45
1:A:110:LYS:O	1:A:113:LEU:N	2.45	0.45
1:A:225:VAL:H	1:B:781:MET:CE	2.29	0.45
1:A:377:LEU:O	1:A:380:PHE:HB2	2.16	0.45
1:A:404:LEU:HD23	1:A:449:LEU:HD13	1.98	0.45
1:A:758:TYR:CD1	1:A:770:LYS:HD3	2.51	0.45
1:B:558:ARG:HD3	1:B:558:ARG:HA	1.77	0.45
1:B:847:LEU:O	1:B:850:LYS:HB2	2.15	0.45
1:C:48:SER:O	1:C:50:PRO:HD3	2.17	0.45
1:D:172:VAL:HG13	1:D:291:ILE:HG23	1.98	0.45
1:D:400:LEU:HA	1:D:400:LEU:HD12	1.53	0.45
1:D:456:MET:HE3	1:D:471:SER:N	2.31	0.45
1:D:535:LEU:HD22	1:D:1027:VAL:HG21	1.98	0.45
1:D:713:LEU:CD2	1:D:843:LEU:HD12	2.46	0.45
1:E:414:GLU:HG3	1:E:974:PRO:HB3	1.98	0.45
1:E:468:ARG:HG2	1:E:472:ILE:HD13	1.98	0.45
1:F:953:MET:HE2	1:F:963:ALA:HB3	1.99	0.45
1:A:293:LEU:HD22	1:A:294:ALA:N	2.32	0.45
1:A:819:TYR:N	1:A:822:LEU:O	2.48	0.45
1:C:346:GLU:O	1:C:350:LEU:HD13	2.17	0.45
1:C:817:GLU:OE2	1:C:825:MET:HA	2.16	0.45
1:C:818:ARG:NH2	1:C:821:GLY:O	2.49	0.45
1:C:947:GLU:HG3	1:C:948:PHE:N	2.30	0.45
1:D:17:ILE:HA	1:D:20:MET:HE2	1.99	0.45
1:E:445:ILE:CG2	1:E:940:LYS:HD2	2.46	0.45
1:E:972:LEU:HD22	1:E:972:LEU:HA	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:460:GLY:O	1:F:868:LEU:HD21	2.16	0.45
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.97	0.45
1:A:597:TYR:CB	1:A:655:PHE:HZ	2.30	0.45
1:A:964:THR:HG21	1:A:1027:VAL:HG23	1.99	0.45
1:B:310:LEU:HD23	1:B:323:ILE:HG21	1.98	0.45
1:C:434:SER:O	1:C:437:GLN:N	2.45	0.45
1:D:237:GLN:OE1	1:E:747:ASN:ND2	2.40	0.45
1:D:293:LEU:HD23	1:D:294:ALA:N	2.30	0.45
1:D:933:THR:O	1:D:936:GLY:N	2.49	0.45
1:E:545:TYR:O	1:E:548:ILE:N	2.50	0.45
1:E:597:TYR:HD1	1:E:601:LYS:HD2	1.81	0.45
1:E:987:MET:HB2	1:E:1008:MET:HE1	1.97	0.45
1:F:69:MET:HA	1:F:72:ILE:HD11	1.98	0.45
1:A:325:TYR:HA	1:A:326:PRO:HD2	1.85	0.45
1:A:910:ILE:O	1:A:914:LEU:HB2	2.17	0.45
1:B:355:MET:HE1	1:B:410:ILE:HG12	1.97	0.45
1:C:400:LEU:HD23	1:C:474:ILE:HD11	1.99	0.45
1:C:408:ASP:HB3	1:C:485:ALA:HB2	1.99	0.45
1:C:644:VAL:HG12	1:C:645:GLU:N	2.31	0.45
1:D:514:GLY:C	1:D:516:PHE:N	2.72	0.45
1:D:609:VAL:HG13	1:D:629:VAL:HG22	1.99	0.45
1:D:654:ALA:O	1:D:658:ILE:HG12	2.16	0.45
1:D:781:MET:SD	1:F:225:VAL:HG13	2.56	0.45
1:E:443:VAL:O	1:E:446:ALA:HB3	2.16	0.45
1:F:291:ILE:HD13	1:F:306:ILE:HD13	1.99	0.45
1:F:447:MET:HE2	1:F:888:LEU:HD23	1.98	0.45
1:F:527:TYR:CZ	1:F:968:VAL:HG13	2.51	0.45
1:A:156:ASP:OD2	1:A:182:TYR:HB2	2.16	0.45
1:B:7:ASP:C	1:B:8:ARG:HG3	2.41	0.45
1:B:419:VAL:HG13	1:B:423:GLU:OE1	2.16	0.45
1:B:544:LEU:O	1:B:548:ILE:HG13	2.16	0.45
1:C:142:VAL:HG21	1:C:158:VAL:HG22	1.99	0.45
1:C:356:TYR:C	1:C:358:PHE:H	2.23	0.45
1:C:443:VAL:O	1:C:447:MET:HB3	2.16	0.45
1:D:644:VAL:CG1	1:D:667:ASN:HB2	2.45	0.45
1:D:713:LEU:HG	1:D:844:MET:HE3	1.98	0.45
1:E:512:PHE:HB3	1:E:513:PHE:CD1	2.51	0.45
1:E:572:PHE:CE1	1:E:648:THR:HG22	2.51	0.45
1:F:228:GLN:NE2	1:F:230:LEU:O	2.41	0.45
1:A:848:ALA:HA	1:A:851:LEU:HG	1.99	0.45
1:B:545:TYR:CE2	1:B:1025:PHE:HZ	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:GLY:HA2	1:C:27:ILE:HG23	1.98	0.45
1:C:637:ARG:HD2	1:C:642:ASN:O	2.16	0.45
1:C:682:PHE:CZ	1:C:857:TYR:HB2	2.52	0.45
1:D:362:PHE:O	1:D:365:THR:HG22	2.16	0.45
1:D:434:SER:O	1:D:438:ILE:HG12	2.17	0.45
1:D:587:THR:OG1	1:D:622:GLN:O	2.23	0.45
1:D:982:PHE:O	1:D:983:ILE:C	2.59	0.45
1:E:516:PHE:HA	1:E:519:MET:HG3	1.98	0.45
1:E:564:LEU:CD1	1:E:671:ILE:HD12	2.47	0.45
1:E:680:PHE:HE1	1:E:682:PHE:HB2	1.81	0.45
1:E:836:SER:OG	1:E:839:GLU:HG3	2.16	0.45
1:E:894:SER:HB3	1:E:897:ILE:H	1.82	0.45
1:F:466:ILE:HG21	1:F:925:VAL:HG11	1.98	0.45
1:F:705:GLU:HA	1:F:708:LYS:HE3	1.99	0.45
1:F:960:LEU:O	1:F:963:ALA:N	2.49	0.45
1:A:727:PHE:CZ	1:A:807:SER:HB2	2.52	0.45
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.47	0.45
1:D:182:TYR:O	1:D:769:LYS:HD3	2.17	0.45
1:D:325:TYR:HA	1:D:326:PRO:HD2	1.93	0.45
1:D:591:LEU:HD12	1:D:613:ASN:HB2	1.99	0.45
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.47	0.45
1:E:949:ALA:HB3	1:E:1026:PHE:CE1	2.45	0.45
1:E:1011:MET:O	1:E:1015:THR:HG23	2.17	0.45
1:F:336:SER:O	1:F:340:VAL:HG23	2.17	0.45
1:F:1035:ARG:HH11	1:F:1038:GLU:CD	2.24	0.45
1:A:45:ILE:HD12	1:A:90:ILE:HB	1.98	0.45
1:A:575:MET:O	1:A:575:MET:HG3	2.17	0.45
1:B:999:ALA:O	1:B:1002:ALA:N	2.50	0.45
1:C:800:PRO:HG2	1:C:803:ALA:HB2	1.99	0.45
1:D:101:ASP:OD1	1:D:101:ASP:N	2.49	0.45
1:D:775:SER:HB2	1:D:789:TRP:CZ2	2.51	0.45
1:D:979:SER:CB	1:D:1015:THR:HG21	2.46	0.45
1:D:1030:ARG:HA	1:D:1030:ARG:HD2	1.63	0.45
1:E:240:LEU:HB2	1:E:246:PHE:HE1	1.82	0.45
1:E:280:GLU:HG2	1:E:284:GLN:O	2.17	0.45
1:E:466:ILE:HD13	1:E:564:LEU:HD11	1.99	0.45
1:F:94:PHE:CE1	1:F:103:ALA:HB1	2.52	0.45
1:F:307:ARG:NH1	1:F:325:TYR:OH	2.48	0.45
1:F:659:LYS:HG3	1:F:661:ALA:H	1.81	0.45
1:F:977:MET:HE3	1:F:977:MET:HB2	1.82	0.45
1:A:544:LEU:O	1:A:544:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:983:ILE:HG23	1:B:1008:MET:HE2	1.97	0.45
1:C:378:GLY:O	1:C:382:VAL:HG23	2.16	0.45
1:D:309:GLU:O	1:D:312:LYS:HB2	2.17	0.45
1:D:508:GLY:H	1:D:518:ARG:HG3	1.82	0.45
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.99	0.45
1:E:186:ILE:HD13	1:E:262:LEU:HD21	1.99	0.45
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.99	0.45
1:F:251:LEU:HD21	1:F:262:LEU:HB2	1.98	0.45
1:F:497:LEU:HA	1:F:497:LEU:HD12	1.56	0.45
1:F:641:GLU:HA	1:F:646:ALA:HB3	1.99	0.45
1:F:841:MET:HE3	1:F:859:TRP:CE2	2.52	0.45
1:A:259:ARG:NH2	1:A:261:LEU:HD11	2.27	0.44
1:A:350:LEU:HD13	1:A:984:LEU:O	2.17	0.44
1:B:377:LEU:O	1:B:380:PHE:HB2	2.17	0.44
1:B:1039:ASP:C	1:B:1040:ILE:HG13	2.43	0.44
1:C:150:THR:N	1:C:153:ASP:HB2	2.32	0.44
1:C:574:THR:HG21	1:C:598:TYR:HE2	1.81	0.44
1:D:13:TRP:CZ2	1:D:492:LEU:HD21	2.52	0.44
1:D:751:GLY:O	1:D:754:TRP:N	2.49	0.44
1:D:759:VAL:HG12	1:D:760:ASN:HB2	1.99	0.44
2:D:1101:LMT:H72	2:D:1101:LMT:H102	1.66	0.44
1:E:291:ILE:HD13	1:E:306:ILE:HD13	1.99	0.44
1:E:423:GLU:C	1:E:502:LYS:HB2	2.42	0.44
1:A:203:VAL:HG12	1:A:207:ILE:HD11	1.97	0.44
1:B:102:ILE:O	1:B:105:VAL:HG12	2.18	0.44
1:B:171:GLY:HA3	1:B:302:THR:OG1	2.17	0.44
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.53	0.44
1:D:3:ASN:O	1:D:6:ILE:HG12	2.16	0.44
1:D:891:LEU:HD12	1:D:891:LEU:HA	1.82	0.44
1:E:6:ILE:HD13	1:E:432:ARG:HG2	1.98	0.44
1:E:68:ASN:HB2	1:E:114:ALA:HB2	1.99	0.44
1:E:159:ALA:O	1:E:767:ARG:NH2	2.50	0.44
1:E:399:VAL:HA	1:E:402:ILE:HG13	1.98	0.44
1:E:455:PRO:O	1:E:876:LEU:HD13	2.16	0.44
1:E:1038:GLU:C	1:E:1040:ILE:N	2.75	0.44
1:F:563:PHE:HB2	1:F:866:GLU:HB2	1.99	0.44
1:F:982:PHE:CD2	1:F:1011:MET:HE2	2.52	0.44
1:A:32:VAL:HG13	1:A:390:ILE:O	2.17	0.44
1:A:261:LEU:HD12	1:A:263:ARG:NH1	2.31	0.44
1:A:680:PHE:CZ	1:A:844:MET:HG3	2.53	0.44
1:A:753:ALA:HB3	1:A:754:TRP:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ILE:HD13	1:C:25:LEU:HD21	1.99	0.44
1:B:27:ILE:HD13	1:B:380:PHE:CD1	2.53	0.44
1:C:356:TYR:CD1	1:C:365:THR:HG21	2.52	0.44
1:D:742:SER:HG	1:D:744:ASN:HD22	1.62	0.44
1:F:5:PHE:CE2	1:F:8:ARG:HD2	2.52	0.44
1:F:144:ASN:O	1:F:148:THR:HG23	2.17	0.44
1:F:730:ASP:OD1	1:F:808:ARG:NH2	2.51	0.44
1:A:21:LEU:HA	1:A:21:LEU:HD13	1.76	0.44
1:A:58:GLN:OE1	1:A:818:ARG:NH1	2.49	0.44
1:A:211:ASN:OD1	1:A:240:LEU:HG	2.16	0.44
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.86	0.44
1:A:774:MET:HG2	1:A:775:SER:N	2.33	0.44
1:B:99:ASP:HB3	1:B:102:ILE:HB	1.99	0.44
1:B:682:PHE:CD2	1:B:827:ILE:HD12	2.52	0.44
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.52	0.44
1:C:242:SER:HB2	1:C:245:GLU:H	1.81	0.44
1:C:699:ARG:HD3	1:C:825:MET:SD	2.56	0.44
1:D:220:GLY:O	1:D:224:PRO:HB3	2.18	0.44
1:E:80:SER:CB	1:E:90:ILE:HG12	2.48	0.44
1:A:183:ALA:HB2	1:A:273:GLU:HG3	1.99	0.44
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.77	0.44
1:B:524:THR:O	1:B:527:TYR:HB3	2.18	0.44
1:B:901:VAL:HG23	1:B:942:ALA:HB3	1.99	0.44
1:D:703:LEU:HD21	1:D:718:PRO:HD3	1.98	0.44
1:E:68:ASN:CB	1:E:114:ALA:HB2	2.48	0.44
1:E:448:VAL:O	1:E:452:VAL:HG13	2.17	0.44
1:E:744:ASN:O	1:E:748:THR:HG23	2.17	0.44
1:F:65:ILE:O	1:F:69:MET:HG2	2.18	0.44
1:F:185:ARG:HB3	1:F:187:TRP:NE1	2.33	0.44
1:F:587:THR:CG2	1:F:623:ASN:HA	2.46	0.44
1:F:990:VAL:HG22	1:F:1004:GLY:HA3	2.00	0.44
1:A:159:ALA:HB2	1:A:177:LEU:HD11	1.98	0.44
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.52	0.44
1:A:452:VAL:HG12	1:A:884:VAL:CG2	2.48	0.44
1:A:743:ILE:H	1:A:743:ILE:HD12	1.82	0.44
1:A:781:MET:SD	1:C:225:VAL:HG13	2.58	0.44
1:A:961:ILE:H	1:A:961:ILE:HG13	1.33	0.44
1:B:78:MET:N	1:B:820:ASN:OD1	2.49	0.44
1:B:767:ARG:HH22	1:C:67:GLN:NE2	2.15	0.44
1:C:192:GLU:HA	1:C:195:LYS:HE3	1.99	0.44
1:C:508:GLY:O	1:C:509:LYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.98	0.44
1:C:952:LEU:HB2	1:C:963:ALA:HB1	1.99	0.44
1:C:987:MET:O	1:C:991:ILE:HG22	2.18	0.44
1:D:34:GLN:HG3	1:D:332:PHE:HE2	1.82	0.44
1:D:270:LEU:HD12	1:D:270:LEU:HA	1.89	0.44
1:D:465:ALA:O	1:D:469:GLN:HG2	2.17	0.44
1:E:105:VAL:HG23	1:F:109:ASN:OD1	2.18	0.44
1:E:280:GLU:HG2	1:E:284:GLN:C	2.42	0.44
1:F:149:MET:HB2	1:F:153:ASP:CB	2.47	0.44
1:F:859:TRP:O	1:F:864:TYR:HD1	2.01	0.44
1:A:20:MET:SD	1:A:374:VAL:HG22	2.58	0.44
1:A:74:ASN:O	1:A:94:PHE:HD2	2.00	0.44
1:A:275:TYR:CD1	1:C:223:PRO:HD3	2.53	0.44
1:A:400:LEU:CD2	1:A:929:VAL:HG12	2.48	0.44
1:A:562:SER:OG	1:A:922:THR:HG21	2.17	0.44
1:A:726:GLN:O	1:A:810:GLU:HG2	2.18	0.44
1:B:156:ASP:OD2	1:B:769:LYS:NZ	2.31	0.44
1:B:937:LEU:HD23	1:B:937:LEU:HA	1.80	0.44
1:C:84:SER:C	1:C:86:GLY:H	2.25	0.44
1:C:587:THR:HG21	1:C:623:ASN:HA	2.00	0.44
1:E:359:LEU:C	1:E:360:GLN:HG2	2.43	0.44
1:E:990:VAL:HG22	1:E:1004:GLY:HA3	2.00	0.44
1:F:151:GLN:HB3	1:F:152:GLU:OE2	2.17	0.44
1:F:727:PHE:CZ	1:F:807:SER:HB2	2.52	0.44
1:F:889:ALA:HB1	1:F:895:TRP:CZ3	2.51	0.44
1:A:435:MET:HE3	1:A:439:GLN:HB2	1.99	0.44
1:A:508:GLY:N	1:A:518:ARG:HG3	2.32	0.44
1:C:194:ASN:HA	1:C:798:MET:HE2	1.99	0.44
1:C:587:THR:HA	1:C:590:VAL:HG23	2.00	0.44
1:C:889:ALA:HB2	1:C:898:PRO:HG2	2.00	0.44
1:D:680:PHE:CZ	1:D:829:GLY:HA3	2.53	0.44
1:E:72:ILE:HG23	1:E:106:GLN:OE1	2.18	0.44
1:E:544:LEU:O	1:E:547:ILE:HB	2.17	0.44
1:F:544:LEU:O	1:F:547:ILE:HB	2.18	0.44
1:F:564:LEU:HD12	1:F:565:PRO:HD2	2.00	0.44
1:A:644:VAL:HG11	1:A:667:ASN:CB	2.48	0.44
1:B:289:LEU:HD23	1:B:289:LEU:HA	1.79	0.44
1:B:549:VAL:O	1:B:552:MET:HB3	2.18	0.44
1:C:904:VAL:O	1:C:907:LEU:HB2	2.17	0.44
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.53	0.44
1:D:239:ARG:HD2	1:D:761:ASP:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:695:LEU:HB3	1:E:825:MET:SD	2.58	0.44
1:E:984:LEU:HD23	1:E:984:LEU:HA	1.76	0.44
1:F:63:GLN:O	1:F:67:GLN:HG3	2.18	0.44
1:F:84:SER:HB3	1:F:814:PRO:O	2.18	0.44
1:F:156:ASP:OD2	1:F:769:LYS:NZ	2.50	0.44
1:F:507:GLU:HG2	1:F:518:ARG:CG	2.47	0.44
1:A:30:LEU:HD11	1:A:384:ALA:HA	2.00	0.43
1:A:339:GLU:HB2	1:A:1000:GLN:HE22	1.83	0.43
1:A:726:GLN:OE1	1:C:235:ILE:HD11	2.18	0.43
1:A:992:SER:O	1:A:997:SER:HB2	2.18	0.43
1:B:61:VAL:HG21	1:B:122:VAL:HG21	2.00	0.43
1:B:706:ALA:HB2	1:B:844:MET:HE3	2.00	0.43
1:C:368:PRO:HA	1:C:409:ALA:HB1	2.00	0.43
1:C:727:PHE:HZ	1:C:807:SER:HB2	1.76	0.43
1:D:402:ILE:HD13	1:D:402:ILE:HG21	1.77	0.43
1:D:563:PHE:C	1:D:564:LEU:HD12	2.43	0.43
1:E:32:VAL:HG22	1:E:298:ASN:ND2	2.33	0.43
1:E:100:ALA:HB1	1:E:131:LYS:HE3	2.00	0.43
1:F:937:LEU:HD11	1:F:982:PHE:CE2	2.53	0.43
1:A:646:ALA:O	1:A:650:ARG:HG2	2.18	0.43
1:B:185:ARG:NH1	1:B:774:MET:HE3	2.27	0.43
1:B:352:PHE:C	1:B:352:PHE:CD2	2.96	0.43
1:B:427:PRO:O	1:B:430:ALA:HB3	2.18	0.43
1:B:613:ASN:HD22	1:B:614:GLY:N	2.15	0.43
1:C:1038:GLU:HA	1:C:1039:ASP:HB2	2.00	0.43
1:D:61:VAL:HA	1:D:118:LEU:HD22	1.99	0.43
2:D:1101:LMT:H31	2:D:1101:LMT:H62	1.59	0.43
1:E:166:ILE:HD12	1:E:309:GLU:HG3	2.00	0.43
1:E:200:PRO:HA	1:E:203:VAL:HG23	1.99	0.43
1:E:459:PHE:CE1	1:E:876:LEU:HD12	2.53	0.43
1:E:754:TRP:CH2	1:E:780:ARG:HA	2.53	0.43
1:F:692:HIS:NE2	1:F:723:ASP:OD1	2.49	0.43
1:A:158:VAL:HG22	1:A:162:MET:HE2	2.00	0.43
1:B:610:PHE:O	1:B:628:PHE:N	2.45	0.43
1:B:901:VAL:HG23	1:B:942:ALA:CB	2.49	0.43
1:C:56:THR:O	1:C:60:THR:OG1	2.24	0.43
1:C:465:ALA:O	1:C:469:GLN:HG2	2.18	0.43
1:C:509:LYS:HD2	1:C:509:LYS:HA	1.77	0.43
1:C:883:VAL:O	1:C:887:CYS:HB2	2.19	0.43
1:D:31:PRO:O	1:D:389:SER:HB2	2.18	0.43
1:D:470:PHE:CD2	1:D:929:VAL:HG21	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:761:ASP:OD1	1:D:770:LYS:HA	2.17	0.43
1:E:352:PHE:HE1	1:E:366:LEU:HD23	1.83	0.43
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.48	0.43
1:E:542:LEU:O	1:E:546:LEU:HG	2.17	0.43
1:E:652:THR:HG23	1:E:665:ALA:H	1.82	0.43
1:E:931:LEU:HD23	1:E:931:LEU:HA	1.84	0.43
1:E:1020:PHE:CZ	2:E:1101:LMT:H41	2.54	0.43
1:F:398:MET:HB3	1:F:398:MET:HE3	1.60	0.43
1:F:647:ILE:O	1:F:650:ARG:HG2	2.18	0.43
1:A:47:ALA:O	1:A:87:THR:HA	2.19	0.43
1:A:225:VAL:HG11	1:B:778:LYS:HA	2.00	0.43
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.53	0.43
1:A:379:THR:HG21	1:A:477:ALA:HB2	2.00	0.43
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.50	0.43
1:B:36:PRO:HD3	1:B:391:ASN:OD1	2.18	0.43
1:B:847:LEU:HA	1:B:847:LEU:HD23	1.83	0.43
1:B:913:LEU:HD23	1:B:913:LEU:HA	1.85	0.43
1:B:953:MET:HB2	1:B:953:MET:HE3	1.50	0.43
1:C:27:ILE:HG13	1:C:28:LEU:N	2.27	0.43
1:C:355:MET:HB2	1:C:355:MET:HE3	1.61	0.43
1:C:751:GLY:O	1:C:754:TRP:N	2.51	0.43
1:D:396:PHE:HE1	1:D:999:ALA:HB1	1.81	0.43
1:D:790:TYR:HB3	1:D:798:MET:HB3	1.99	0.43
1:E:588:GLN:HG3	1:E:592:ASN:HD21	1.83	0.43
1:E:908:GLY:O	1:E:1010:GLY:HA2	2.18	0.43
1:F:340:VAL:HG22	1:F:396:PHE:HE2	1.82	0.43
1:F:560:PRO:HB2	1:F:836:SER:OG	2.18	0.43
1:F:1015:THR:O	1:F:1017:LEU:N	2.51	0.43
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.98	0.43
1:A:893:GLU:OE1	1:C:11:PHE:HB2	2.18	0.43
1:B:149:MET:HB2	1:B:153:ASP:HB3	2.01	0.43
1:B:192:GLU:HB3	1:B:265:VAL:HA	2.01	0.43
1:C:21:LEU:HD23	1:C:21:LEU:HA	1.80	0.43
1:C:139:VAL:O	1:C:326:PRO:HD2	2.18	0.43
1:C:144:ASN:ND2	1:C:149:MET:SD	2.92	0.43
1:C:187:TRP:HZ3	1:C:774:MET:CE	2.32	0.43
1:C:509:LYS:HG2	1:C:513:PHE:HB2	1.99	0.43
1:D:165:ALA:HA	1:D:168:ARG:NH1	2.34	0.43
1:D:619:GLY:HA3	1:D:815:ARG:HH22	1.82	0.43
1:D:659:LYS:HD3	1:D:659:LYS:HA	1.71	0.43
1:E:182:TYR:HD1	1:E:182:TYR:HA	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:VAL:HG11	1:F:747:ASN:HB3	2.00	0.43
1:E:238:THR:OG1	1:F:728:LYS:NZ	2.51	0.43
1:E:654:ALA:C	1:E:656:SER:H	2.26	0.43
1:F:356:TYR:C	1:F:358:PHE:H	2.26	0.43
1:F:412:VAL:HA	1:F:438:ILE:HD12	2.00	0.43
1:A:61:VAL:HG21	1:A:122:VAL:HG21	2.01	0.43
1:A:104:GLN:OE1	1:A:131:LYS:HD3	2.19	0.43
1:A:118:LEU:HA	1:A:119:PRO:HD3	1.78	0.43
1:A:449:LEU:O	1:A:452:VAL:HG22	2.19	0.43
1:A:944:LEU:CB	1:A:971:ARG:NH2	2.81	0.43
1:B:682:PHE:HB3	1:B:827:ILE:HB	2.00	0.43
1:C:189:ASN:OD1	1:C:190:PRO:HD2	2.18	0.43
1:C:775:SER:HB2	1:C:789:TRP:CZ2	2.53	0.43
1:D:394:THR:HG22	1:D:473:THR:OG1	2.18	0.43
1:D:457:ALA:HB1	1:D:468:ARG:HG3	1.99	0.43
1:D:887:CYS:O	1:D:890:ALA:HB3	2.19	0.43
1:E:180:SER:HB3	1:E:273:GLU:H	1.83	0.43
1:E:778:LYS:H	1:E:778:LYS:HG2	1.64	0.43
1:F:893:GLU:O	1:F:893:GLU:HG3	2.18	0.43
1:F:984:LEU:HA	1:F:984:LEU:HD23	1.69	0.43
1:A:34:GLN:HB2	1:A:333:VAL:HG22	2.01	0.43
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.73	0.43
1:A:379:THR:OG1	1:A:477:ALA:HA	2.19	0.43
1:A:400:LEU:HD23	1:A:929:VAL:HG12	2.01	0.43
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.78	0.43
1:A:683:GLU:HG2	1:A:819:TYR:CG	2.53	0.43
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.54	0.43
1:B:754:TRP:CH2	1:B:780:ARG:HA	2.54	0.43
1:B:952:LEU:HA	1:B:952:LEU:HD23	1.78	0.43
1:C:182:TYR:O	1:C:769:LYS:HD3	2.19	0.43
1:C:187:TRP:HZ3	1:C:774:MET:HE2	1.83	0.43
1:C:519:MET:O	1:C:523:SER:OG	2.30	0.43
1:C:674:LEU:HD23	1:C:674:LEU:HA	1.84	0.43
1:D:58:GLN:HA	1:D:62:THR:HB	2.00	0.43
1:D:393:LEU:CD1	1:D:466:ILE:HA	2.49	0.43
1:D:559:LEU:HD23	1:D:560:PRO:CD	2.49	0.43
1:E:668:LEU:HD23	1:E:668:LEU:H	1.83	0.43
1:E:905:VAL:HG13	1:E:935:ILE:HG23	2.00	0.43
1:F:932:LEU:O	1:F:933:THR:C	2.61	0.43
1:A:246:PHE:HB3	1:A:268:ILE:HD13	2.00	0.43
1:A:781:MET:HE2	1:C:225:VAL:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:O	1:B:428:LYS:NZ	2.49	0.43
1:B:9:PRO:CB	1:B:495:THR:HG21	2.45	0.43
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.79	0.43
1:B:858:ASP:OD1	1:B:859:TRP:N	2.44	0.43
1:B:972:LEU:HD13	1:B:972:LEU:C	2.44	0.43
1:C:328:ASP:O	1:C:331:PRO:HD2	2.19	0.43
1:C:415:ASN:O	1:C:419:VAL:HG23	2.18	0.43
1:D:194:ASN:OD1	1:D:798:MET:HG3	2.18	0.43
1:D:370:ILE:C	1:D:373:PRO:HD2	2.44	0.43
1:D:414:GLU:HG3	1:D:974:PRO:HG3	2.01	0.43
1:D:706:ALA:HB3	1:D:716:VAL:HG21	2.00	0.43
1:E:185:ARG:HH12	1:E:774:MET:CE	2.32	0.43
1:E:230:LEU:HG	1:E:231:ASN:N	2.33	0.43
1:E:564:LEU:HD23	1:E:565:PRO:HD2	2.00	0.43
1:F:11:PHE:HE2	1:F:15:ILE:HD11	1.84	0.43
1:F:309:GLU:HG3	1:F:313:MET:HE3	1.99	0.43
1:F:380:PHE:O	1:F:383:LEU:HB2	2.19	0.43
1:F:1038:GLU:HA	1:F:1039:ASP:HA	1.81	0.43
1:A:708:LYS:C	1:A:710:PRO:HD3	2.44	0.43
1:B:578:LEU:HD13	1:B:661:ALA:HB2	2.01	0.43
1:B:950:LYS:HZ1	1:B:1030:ARG:NH2	2.14	0.43
2:B:1101:LMT:H6D	2:B:1101:LMT:C5B	2.48	0.43
1:D:278:ILE:HG13	1:D:613:ASN:HB3	2.00	0.43
1:D:858:ASP:OD2	1:D:859:TRP:N	2.49	0.43
1:E:589:LYS:O	1:E:592:ASN:HB2	2.19	0.43
1:E:682:PHE:CD2	1:E:827:ILE:HD12	2.53	0.43
1:F:192:GLU:HB3	1:F:265:VAL:HA	2.00	0.43
1:F:1035:ARG:HD3	1:F:1038:GLU:CD	2.43	0.43
1:A:75:LEU:HD11	1:A:92:LEU:HB3	2.01	0.43
1:A:228:GLN:NE2	1:A:230:LEU:O	2.43	0.43
1:A:344:LEU:CD2	1:A:399:VAL:HG22	2.49	0.43
1:B:510:LYS:O	1:B:515:TRP:HD1	2.02	0.43
1:C:757:SER:O	1:C:772:TYR:HA	2.18	0.43
1:C:898:PRO:HA	1:C:901:VAL:HG12	2.01	0.43
1:C:945:ILE:HG12	1:C:971:ARG:NH2	2.34	0.43
1:D:35:TYR:HB3	1:D:36:PRO:HD2	2.01	0.43
1:D:37:THR:OG1	1:D:296:GLY:HA2	2.18	0.43
1:D:54:ALA:HB1	1:D:816:LEU:HG	2.00	0.43
1:D:415:ASN:O	1:D:419:VAL:HG23	2.19	0.43
1:D:973:ARG:HB3	1:D:974:PRO:HD3	2.01	0.43
1:E:555:LEU:HB3	1:E:913:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1021:PHE:O	1:E:1024:VAL:HB	2.19	0.43
1:F:216:ALA:HB1	1:F:234:ILE:CG2	2.49	0.43
1:F:733:GLN:O	1:F:737:GLN:HG3	2.18	0.43
1:F:934:THR:O	1:F:935:ILE:C	2.57	0.43
1:A:216:ALA:HB1	1:A:234:ILE:HG22	2.01	0.42
1:A:400:LEU:HD11	1:A:1007:VAL:CG2	2.46	0.42
1:A:572:PHE:HD1	1:A:666:PHE:O	2.02	0.42
1:A:847:LEU:HD23	1:A:847:LEU:HA	1.83	0.42
1:B:348:ILE:HG22	1:B:349:ILE:N	2.34	0.42
1:B:801:PHE:HA	1:B:804:PHE:CZ	2.53	0.42
1:B:1026:PHE:CD2	1:B:1026:PHE:C	2.96	0.42
1:C:44:THR:HA	1:C:90:ILE:O	2.17	0.42
1:C:143:ILE:HG22	1:C:286:ALA:CB	2.46	0.42
1:C:510:LYS:HG2	1:C:511:GLY:N	2.34	0.42
1:C:610:PHE:HB3	1:C:628:PHE:HB2	2.00	0.42
1:C:659:LYS:HD3	1:C:659:LYS:HA	1.64	0.42
1:D:187:TRP:HA	1:D:774:MET:O	2.19	0.42
1:E:578:LEU:HB2	1:E:623:ASN:OD1	2.19	0.42
1:F:139:VAL:HA	1:F:289:LEU:O	2.19	0.42
1:F:293:LEU:HD22	1:F:294:ALA:H	1.84	0.42
1:F:828:LEU:HD23	1:F:828:LEU:HA	1.84	0.42
1:A:194:ASN:HA	1:A:798:MET:HE2	2.00	0.42
1:A:542:LEU:HD12	1:A:542:LEU:HA	1.78	0.42
1:A:703:LEU:CD2	1:A:718:PRO:HD3	2.44	0.42
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	2.01	0.42
1:B:317:PHE:HE2	1:B:323:ILE:HG12	1.84	0.42
1:B:453:PHE:O	1:B:456:MET:HG2	2.19	0.42
1:B:497:LEU:HD12	1:B:497:LEU:HA	1.77	0.42
1:B:612:VAL:HG12	1:B:615:PHE:HB3	2.01	0.42
1:D:252:LYS:HE2	1:D:252:LYS:HB3	1.72	0.42
1:D:357:LEU:HD23	1:D:357:LEU:O	2.18	0.42
1:D:984:LEU:HD23	1:D:984:LEU:HA	1.81	0.42
1:E:553:ALA:O	1:E:557:VAL:HG23	2.19	0.42
1:E:793:ALA:HB3	1:E:795:ASP:OD2	2.19	0.42
1:F:277:ILE:HD11	1:F:620:ARG:NH1	2.34	0.42
1:F:425:LEU:HD22	1:F:429:GLU:HG2	2.01	0.42
1:F:897:ILE:HD11	1:F:950:LYS:HE2	2.01	0.42
1:F:953:MET:SD	1:F:960:LEU:HA	2.59	0.42
1:A:69:MET:HE3	1:A:107:VAL:HG13	2.01	0.42
1:A:80:SER:HB3	1:A:90:ILE:HA	2.01	0.42
1:A:166:ILE:HA	1:A:166:ILE:HD13	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:TYR:O	1:A:548:ILE:N	2.53	0.42
1:B:602:GLU:OE2	1:B:650:ARG:NH1	2.52	0.42
1:B:958:LYS:HB3	1:B:963:ALA:HB2	2.01	0.42
1:C:5:PHE:C	1:C:5:PHE:CD2	2.97	0.42
1:C:376:LEU:HD22	1:C:398:MET:CE	2.49	0.42
1:C:393:LEU:CD1	1:C:466:ILE:HD13	2.49	0.42
1:C:404:LEU:HB3	1:C:478:MET:SD	2.59	0.42
1:C:931:LEU:O	1:C:935:ILE:HG13	2.19	0.42
1:D:414:GLU:CG	1:D:974:PRO:HG3	2.48	0.42
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.84	0.42
1:E:162:MET:HA	1:E:313:MET:HE1	2.01	0.42
1:E:162:MET:C	1:E:164:ASP:N	2.76	0.42
1:E:194:ASN:OD1	1:E:798:MET:HG3	2.18	0.42
1:E:330:THR:O	1:E:334:LYS:HG3	2.20	0.42
1:E:412:VAL:O	1:E:416:VAL:HG23	2.19	0.42
1:E:564:LEU:CD1	1:E:674:LEU:HD21	2.49	0.42
1:E:575:MET:HE2	1:E:575:MET:HB2	1.75	0.42
1:F:34:GLN:HB2	1:F:333:VAL:HG22	2.00	0.42
1:F:58:GLN:O	1:F:62:THR:HB	2.19	0.42
1:F:181:GLN:HG2	1:F:182:TYR:N	2.34	0.42
1:F:534:ILE:HG22	2:F:1101:LMT:H5'	2.00	0.42
1:F:536:ARG:HD2	2:F:1101:LMT:O4'	2.19	0.42
1:F:557:VAL:C	1:F:559:LEU:H	2.27	0.42
1:F:898:PRO:HA	1:F:901:VAL:HG12	2.01	0.42
1:A:375:VAL:CG2	1:A:481:SER:HA	2.49	0.42
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.54	0.42
1:A:948:PHE:CE2	1:A:971:ARG:HD3	2.55	0.42
1:B:511:GLY:HA2	1:B:515:TRP:HE1	1.82	0.42
1:B:733:GLN:O	1:B:737:GLN:HG3	2.18	0.42
1:C:640:GLU:O	1:C:643:LYS:HB3	2.20	0.42
1:C:655:PHE:HB3	1:C:663:VAL:HB	2.02	0.42
1:C:847:LEU:HD12	1:C:847:LEU:HA	1.90	0.42
1:D:39:ALA:HA	1:D:40:PRO:HD2	1.90	0.42
1:D:504:ASP:C	1:D:506:GLY:H	2.26	0.42
1:D:684:LEU:O	1:D:824:SER:HB2	2.20	0.42
1:E:57:VAL:HG11	1:E:86:GLY:O	2.19	0.42
1:E:78:MET:HE3	1:E:821:GLY:N	2.33	0.42
1:E:578:LEU:HA	1:E:661:ALA:HB1	2.00	0.42
1:E:682:PHE:CZ	1:E:857:TYR:HB2	2.54	0.42
1:E:902:MET:O	1:E:905:VAL:HG23	2.19	0.42
1:F:941:ASN:HD21	1:F:1015:THR:HG22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:HD11	1:A:432:ARG:HE	1.85	0.42
1:A:462:SER:O	1:A:466:ILE:HG12	2.19	0.42
1:A:572:PHE:HE2	1:A:631:LEU:HD21	1.83	0.42
1:A:835:LYS:HG3	1:A:839:GLU:OE2	2.20	0.42
1:B:76:MET:HB2	1:B:93:THR:O	2.20	0.42
1:B:143:ILE:HG22	1:B:286:ALA:HB2	2.02	0.42
1:B:167:SER:HB3	1:B:175:VAL:HG21	2.00	0.42
1:B:528:THR:O	1:B:529:ASP:C	2.60	0.42
1:B:887:CYS:O	1:B:890:ALA:HB3	2.18	0.42
1:C:69:MET:HE1	1:C:111:LEU:N	2.35	0.42
1:C:356:TYR:HA	1:C:365:THR:CG2	2.43	0.42
1:C:559:LEU:HA	1:C:560:PRO:HD2	1.84	0.42
1:D:137:LEU:HD22	1:D:293:LEU:HG	2.01	0.42
1:D:365:THR:O	1:D:368:PRO:HD2	2.18	0.42
1:D:578:LEU:HG	1:D:623:ASN:O	2.19	0.42
1:E:58:GLN:NE2	1:E:816:LEU:HD13	2.34	0.42
1:E:281:PHE:CD1	1:E:610:PHE:HD1	2.36	0.42
1:F:273:GLU:CD	1:F:770:LYS:HD2	2.44	0.42
1:F:563:PHE:CD2	1:F:564:LEU:HB2	2.54	0.42
1:F:576:VAL:HG13	1:F:663:VAL:HG22	2.01	0.42
1:F:957:GLY:HA3	1:F:1043:SER:HB2	2.01	0.42
1:A:55:LYS:HE2	1:A:55:LYS:HB3	1.92	0.42
1:A:57:VAL:HG21	1:A:86:GLY:O	2.19	0.42
1:A:207:ILE:O	1:A:211:ASN:HB3	2.19	0.42
1:A:583:THR:HG21	1:C:228:GLN:HG3	2.02	0.42
1:A:878:ALA:O	1:A:882:ILE:HG12	2.19	0.42
1:B:165:ALA:HB3	1:B:313:MET:HE1	2.01	0.42
1:B:344:LEU:HD23	1:B:402:ILE:HD11	2.02	0.42
1:B:1018:ALA:C	1:B:1020:PHE:N	2.77	0.42
1:B:1037:ASN:HA	1:B:1038:GLU:CB	2.49	0.42
1:D:445:ILE:HG21	1:D:940:LYS:HD2	2.01	0.42
1:D:753:ALA:O	1:D:775:SER:HB3	2.18	0.42
1:D:946:VAL:HG13	1:D:1026:PHE:CD1	2.55	0.42
1:D:1030:ARG:C	1:D:1032:ARG:H	2.26	0.42
1:E:43:VAL:HG22	1:E:131:LYS:HD2	2.02	0.42
1:E:602:GLU:OE1	1:E:650:ARG:HD2	2.20	0.42
1:E:726:GLN:NE2	1:E:812:GLY:HA3	2.35	0.42
1:E:870:GLY:C	1:E:872:GLN:H	2.27	0.42
1:E:923:ASN:OD1	1:E:928:GLN:NE2	2.49	0.42
1:F:30:LEU:HD12	1:F:30:LEU:HA	1.93	0.42
1:F:931:LEU:HD23	1:F:931:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:VAL:HG11	1:A:433:LYS:HG2	2.02	0.42
1:A:576:VAL:HG22	1:A:663:VAL:HG22	2.02	0.42
1:A:633:ASP:OD2	1:A:634:TRP:HD1	2.02	0.42
1:A:1030:ARG:HD2	1:A:1030:ARG:HA	1.64	0.42
1:B:599:LEU:HD23	1:B:599:LEU:HA	1.86	0.42
1:C:752:ALA:O	1:C:774:MET:HA	2.20	0.42
1:D:213:GLN:HA	1:D:237:GLN:O	2.19	0.42
1:D:338:HIS:NE2	1:D:342:LYS:HE3	2.35	0.42
1:E:891:LEU:HD12	1:E:891:LEU:HA	1.80	0.42
1:E:972:LEU:HD13	1:E:976:LEU:HD13	2.01	0.42
1:E:1030:ARG:HA	1:E:1030:ARG:HD2	1.77	0.42
1:F:881:LEU:HD23	1:F:935:ILE:HG21	2.01	0.42
1:A:138:MET:HE2	1:A:328:ASP:OD1	2.20	0.42
1:A:525:HIS:HA	1:A:528:THR:HG22	2.01	0.42
1:B:370:ILE:O	1:B:374:VAL:HG23	2.19	0.42
1:B:510:LYS:O	1:B:515:TRP:CD1	2.72	0.42
1:B:516:PHE:HA	1:B:519:MET:HE2	2.00	0.42
1:C:102:ILE:HD13	1:C:102:ILE:HA	1.87	0.42
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.74	0.42
1:C:441:ALA:HB2	1:C:948:PHE:HE1	1.85	0.42
1:C:464:GLY:O	1:C:468:ARG:HB2	2.20	0.42
1:C:716:VAL:HA	1:C:829:GLY:HA2	2.02	0.42
1:D:317:PHE:HA	1:D:318:PRO:HD3	1.83	0.42
1:D:533:GLY:O	1:D:536:ARG:HB2	2.19	0.42
1:D:865:GLN:HA	1:D:868:LEU:HD12	2.01	0.42
1:E:760:ASN:O	1:E:771:VAL:HB	2.20	0.42
1:E:919:ARG:HB3	1:E:921:LEU:CD2	2.50	0.42
1:F:110:LYS:O	1:F:113:LEU:HB2	2.19	0.42
1:F:328:ASP:O	1:F:331:PRO:HD2	2.19	0.42
1:F:895:TRP:HA	1:F:895:TRP:HE3	1.85	0.42
1:F:987:MET:HE2	1:F:987:MET:HB3	1.59	0.42
1:A:247:GLY:O	1:A:261:LEU:HB3	2.20	0.42
1:A:375:VAL:HG11	1:A:481:SER:HB3	2.01	0.42
1:B:175:VAL:HG23	1:C:70:ASN:HD21	1.85	0.42
1:B:415:ASN:HD21	1:B:948:PHE:HZ	1.67	0.42
1:C:61:VAL:HG13	1:C:118:LEU:HD13	2.02	0.42
1:C:507:GLU:HG2	1:C:518:ARG:HG3	2.01	0.42
1:C:591:LEU:HD12	1:C:613:ASN:HB2	2.02	0.42
1:C:979:SER:CB	1:C:1015:THR:HG21	2.50	0.42
1:D:5:PHE:CD2	1:D:487:ILE:HG23	2.54	0.42
1:D:49:TYR:CB	1:D:57:VAL:HG22	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:PHE:HB3	1:D:464:GLY:HA2	2.01	0.42
1:D:885:PHE:CE1	1:D:898:PRO:HB2	2.55	0.42
1:E:143:ILE:HG22	1:E:286:ALA:HB2	2.01	0.42
1:E:215:ALA:HA	1:F:51:GLY:HA3	2.02	0.42
1:E:235:ILE:HB	1:F:728:LYS:HA	2.02	0.42
1:E:347:ALA:CB	1:E:402:ILE:HG21	2.49	0.42
1:E:613:ASN:OD1	1:E:614:GLY:N	2.53	0.42
1:F:356:TYR:C	1:F:358:PHE:N	2.77	0.42
1:F:382:VAL:HG11	1:F:476:SER:HB3	2.02	0.42
1:F:775:SER:OG	1:F:780:ARG:HG2	2.20	0.42
1:F:907:LEU:CD2	1:F:1017:LEU:HB3	2.50	0.42
1:A:989:LEU:HD22	1:A:1000:GLN:HB3	2.01	0.42
1:B:706:ALA:HB1	1:B:716:VAL:HG11	2.01	0.42
1:C:68:ASN:OD1	1:C:114:ALA:HB2	2.19	0.42
1:C:252:LYS:HB3	1:C:260:VAL:CG2	2.50	0.42
1:C:355:MET:SD	1:C:368:PRO:HB2	2.60	0.42
1:D:61:VAL:CG2	1:D:122:VAL:HG21	2.49	0.42
1:D:76:MET:HB2	1:D:93:THR:O	2.19	0.42
1:D:322:LYS:HG2	1:D:323:ILE:O	2.20	0.42
1:D:867:ARG:HA	1:D:867:ARG:HD3	1.87	0.42
1:E:530:SER:OG	2:E:1101:LMT:C1'	2.68	0.42
1:E:582:ALA:HA	1:E:586:ARG:HH21	1.85	0.42
1:F:367:ILE:HD11	1:F:497:LEU:HD13	2.01	0.42
1:F:555:LEU:HB3	1:F:913:LEU:HB3	2.02	0.42
1:A:41:PRO:HG2	1:A:94:PHE:CB	2.40	0.41
1:A:511:GLY:HA2	1:A:515:TRP:HD1	1.85	0.41
1:A:562:SER:CB	1:A:924:ASP:HB3	2.50	0.41
1:A:698:ALA:O	1:A:701:GLN:HB3	2.20	0.41
1:A:712:MET:HG3	1:A:835:LYS:HE2	2.02	0.41
1:B:188:MET:HE1	1:B:200:PRO:HG3	2.02	0.41
1:B:652:THR:HG22	1:B:664:PHE:CD1	2.52	0.41
1:B:686:ASP:HA	1:B:854:GLY:O	2.20	0.41
1:C:144:ASN:HB3	1:C:148:THR:HG23	2.02	0.41
1:C:273:GLU:CD	1:C:770:LYS:HD2	2.44	0.41
1:D:45:ILE:HD11	1:D:69:MET:HE3	2.00	0.41
1:D:94:PHE:CE2	1:D:103:ALA:HB1	2.56	0.41
1:D:523:SER:O	1:D:526:HIS:HB2	2.20	0.41
1:D:909:VAL:HG22	1:D:931:LEU:CD2	2.50	0.41
1:D:925:VAL:HA	1:D:928:GLN:OE1	2.20	0.41
1:E:15:ILE:HD12	1:E:487:ILE:HG21	2.01	0.41
1:E:359:LEU:O	1:E:360:GLN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:TYR:CE1	1:F:57:VAL:HA	2.55	0.41
1:F:99:ASP:HB3	1:F:102:ILE:HB	2.02	0.41
1:F:400:LEU:HD11	1:F:1007:VAL:HG21	2.02	0.41
1:F:407:ASP:OD1	1:F:978:THR:HG23	2.20	0.41
1:F:693:GLU:HB3	1:F:694:LYS:HD2	2.02	0.41
1:F:1038:GLU:O	1:F:1038:GLU:HG2	2.19	0.41
1:A:971:ARG:CZ	1:A:971:ARG:CB	2.98	0.41
1:B:165:ALA:HB3	1:B:313:MET:CE	2.50	0.41
1:B:751:GLY:O	1:B:753:ALA:N	2.53	0.41
1:B:1018:ALA:C	1:B:1020:PHE:H	2.28	0.41
1:C:244:GLU:O	1:C:247:GLY:N	2.53	0.41
1:C:252:LYS:HB3	1:C:260:VAL:HG21	2.02	0.41
1:C:563:PHE:CD2	1:C:564:LEU:HB2	2.56	0.41
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.20	0.41
1:D:415:ASN:OD1	1:D:434:SER:HB2	2.21	0.41
1:E:352:PHE:HE1	1:E:366:LEU:CD2	2.33	0.41
1:F:213:GLN:HA	1:F:237:GLN:O	2.19	0.41
1:F:375:VAL:HG13	1:F:480:LEU:HB2	2.02	0.41
1:F:395:MET:HB3	1:F:395:MET:HE3	1.78	0.41
1:F:841:MET:SD	1:F:863:SER:HB2	2.60	0.41
1:F:934:THR:O	1:F:938:SER:OG	2.38	0.41
1:A:34:GLN:NE2	1:A:35:TYR:HE1	2.19	0.41
1:A:200:PRO:HB2	1:A:749:THR:HG22	2.01	0.41
1:A:355:MET:HE3	1:A:355:MET:HA	2.02	0.41
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.73	0.41
1:A:597:TYR:CZ	1:A:651:ALA:HA	2.54	0.41
1:B:311:ALA:O	1:B:314:GLU:HB2	2.21	0.41
1:B:468:ARG:CZ	1:B:468:ARG:HB2	2.51	0.41
1:B:681:ASP:O	1:B:860:THR:HG22	2.20	0.41
1:B:738:ALA:O	1:B:740:GLY:N	2.54	0.41
1:C:250:LEU:HD11	1:C:259:ARG:HB3	2.01	0.41
1:C:412:VAL:CG1	1:C:435:MET:HE1	2.50	0.41
1:C:578:LEU:HB3	1:C:579:PRO:HD2	2.02	0.41
1:C:910:ILE:O	1:C:914:LEU:HB2	2.20	0.41
1:D:58:GLN:HA	1:D:62:THR:OG1	2.20	0.41
1:D:293:LEU:CD2	1:D:297:ALA:HB3	2.50	0.41
1:D:372:VAL:O	1:D:373:PRO:C	2.64	0.41
1:D:544:LEU:HA	1:D:547:ILE:HD12	2.02	0.41
1:E:277:ILE:HG23	1:E:620:ARG:HH21	1.84	0.41
1:E:602:GLU:HB3	1:E:606:VAL:HG23	2.02	0.41
1:E:987:MET:HB3	1:E:987:MET:HE2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:PHE:HD1	1:F:977:MET:CG	2.26	0.41
1:F:531:VAL:HG11	1:F:968:VAL:HG11	2.03	0.41
1:A:565:PRO:O	1:A:670:ALA:HB2	2.20	0.41
1:B:562:SER:HB2	1:B:922:THR:CG2	2.51	0.41
1:B:717:ARG:HD2	1:B:828:LEU:HB2	2.01	0.41
1:C:184:MET:HG2	1:C:246:PHE:CD2	2.55	0.41
1:C:340:VAL:HG11	1:C:395:MET:HB3	2.02	0.41
1:C:413:VAL:O	1:C:417:GLU:HG2	2.21	0.41
1:C:519:MET:HE3	1:C:519:MET:HB3	1.91	0.41
1:C:586:ARG:O	1:C:590:VAL:HG23	2.20	0.41
1:C:693:GLU:HB3	1:C:694:LYS:CE	2.50	0.41
1:C:1016:VAL:HG12	1:C:1016:VAL:O	2.20	0.41
1:D:27:ILE:HD11	1:D:380:PHE:CD1	2.55	0.41
1:D:695:LEU:HD13	1:D:825:MET:SD	2.61	0.41
1:E:166:ILE:HD12	1:E:309:GLU:CG	2.49	0.41
1:E:252:LYS:HB3	1:E:252:LYS:HE2	1.61	0.41
1:E:508:GLY:CA	1:E:518:ARG:HE	2.26	0.41
1:F:49:TYR:N	1:F:86:GLY:O	2.42	0.41
1:F:559:LEU:HA	1:F:560:PRO:HD2	1.81	0.41
1:A:75:LEU:CD2	1:C:168:ARG:HD3	2.50	0.41
1:A:140:VAL:O	1:A:289:LEU:N	2.44	0.41
1:A:328:ASP:O	1:A:331:PRO:HD2	2.20	0.41
1:A:524:THR:O	1:A:527:TYR:HB3	2.20	0.41
1:B:680:PHE:HB2	1:B:859:TRP:CZ3	2.55	0.41
1:B:904:VAL:HA	1:B:1025:PHE:HE1	1.86	0.41
1:C:23:GLY:O	1:C:27:ILE:HG23	2.20	0.41
1:C:713:LEU:CD2	1:C:843:LEU:HD12	2.50	0.41
1:C:881:LEU:HB3	1:C:902:MET:HE1	2.03	0.41
1:D:34:GLN:NE2	1:D:35:TYR:HE1	2.18	0.41
1:D:409:ALA:O	1:D:413:VAL:HG23	2.19	0.41
1:E:24:GLY:O	1:E:27:ILE:HG22	2.21	0.41
1:E:347:ALA:HB1	1:E:402:ILE:HG21	2.02	0.41
1:E:726:GLN:CD	1:E:812:GLY:HA3	2.46	0.41
1:E:937:LEU:HD23	1:E:937:LEU:HA	1.88	0.41
1:E:987:MET:CB	1:E:1008:MET:HE1	2.50	0.41
1:E:1039:ASP:C	1:E:1040:ILE:HG13	2.45	0.41
1:F:684:LEU:C	1:F:685:ILE:HD12	2.45	0.41
1:F:878:ALA:O	1:F:882:ILE:HG13	2.21	0.41
1:F:885:PHE:CD2	1:F:885:PHE:C	2.98	0.41
1:F:940:LYS:HZ1	1:F:978:THR:HG21	1.84	0.41
1:A:141:GLY:O	1:A:323:ILE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.84	0.41
1:A:492:LEU:HD22	1:A:496:MET:SD	2.60	0.41
1:A:904:VAL:HG12	1:A:938:SER:HB3	2.03	0.41
1:C:154:ILE:O	1:C:157:TYR:N	2.54	0.41
1:C:181:GLN:O	1:C:272:GLY:HA2	2.20	0.41
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.50	0.41
1:C:422:GLU:HB3	1:C:423:GLU:HG3	2.01	0.41
1:C:703:LEU:CD1	1:C:718:PRO:HD3	2.51	0.41
1:C:1040:ILE:HG22	1:C:1040:ILE:O	2.20	0.41
1:D:38:ILE:HD11	1:D:466:ILE:HD11	2.02	0.41
1:D:113:LEU:HD21	1:F:128:SER:HB3	2.02	0.41
1:D:137:LEU:HD23	1:D:291:ILE:HG22	2.02	0.41
1:E:7:ASP:C	1:E:8:ARG:HG3	2.46	0.41
1:E:273:GLU:CD	1:E:770:LYS:HZ3	2.28	0.41
1:F:459:PHE:CE1	1:F:876:LEU:HG	2.56	0.41
1:A:27:ILE:HD11	1:A:380:PHE:CE1	2.56	0.41
1:A:252:LYS:HB3	1:A:252:LYS:HE2	1.75	0.41
1:A:274:ASN:OD1	1:A:276:ASP:HB2	2.20	0.41
1:A:472:ILE:HG22	1:A:473:THR:N	2.35	0.41
1:A:480:LEU:HA	1:A:480:LEU:HD23	1.87	0.41
1:A:507:GLU:HG3	1:A:518:ARG:HA	2.03	0.41
1:A:1035:ARG:HG2	1:A:1036:LYS:H	1.85	0.41
1:A:1040:ILE:HG13	1:A:1042:HIS:HB2	2.02	0.41
1:B:278:ILE:CG1	1:B:613:ASN:HB3	2.49	0.41
1:B:1015:THR:O	1:B:1017:LEU:N	2.54	0.41
1:C:365:THR:O	1:C:368:PRO:HD2	2.20	0.41
1:C:586:ARG:O	1:C:589:LYS:HB2	2.21	0.41
1:D:203:VAL:O	1:D:207:ILE:HG13	2.20	0.41
1:D:524:THR:O	1:D:528:THR:HG22	2.19	0.41
1:D:888:LEU:HD13	1:D:901:VAL:HG13	2.02	0.41
1:D:944:LEU:HD23	1:D:944:LEU:HA	1.78	0.41
1:E:5:PHE:HE2	1:E:11:PHE:CD2	2.39	0.41
1:E:185:ARG:CD	1:E:772:TYR:HB2	2.51	0.41
1:F:149:MET:HE3	1:F:153:ASP:HB3	2.02	0.41
1:F:327:TYR:C	1:F:327:TYR:CD2	2.99	0.41
1:F:392:THR:O	1:F:395:MET:HB2	2.20	0.41
1:F:504:ASP:C	1:F:506:GLY:N	2.76	0.41
1:F:684:LEU:HB3	1:F:825:MET:O	2.20	0.41
1:F:971:ARG:NH2	1:F:975:ILE:HD11	2.36	0.41
1:A:170:SER:HG	1:B:74:ASN:H	1.61	0.41
1:A:351:VAL:HG22	1:A:981:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:ARG:HE	1:A:718:PRO:HG3	1.85	0.41
1:B:675:GLY:HA2	1:B:862:MET:SD	2.61	0.41
1:B:716:VAL:HG23	1:B:827:ILE:CG2	2.51	0.41
1:B:836:SER:OG	1:B:839:GLU:HG3	2.21	0.41
1:C:80:SER:OG	1:C:818:ARG:HD3	2.20	0.41
1:D:72:ILE:HG21	1:D:107:VAL:HG23	2.03	0.41
1:D:597:TYR:CD2	1:D:655:PHE:CZ	3.09	0.41
1:D:648:THR:HB	1:D:665:ALA:O	2.20	0.41
1:E:310:LEU:HD21	1:E:323:ILE:HG21	2.03	0.41
1:E:565:PRO:HG2	1:E:999:ALA:HA	2.02	0.41
1:E:639:GLY:O	1:E:643:LYS:HG3	2.20	0.41
1:E:987:MET:CA	1:E:1008:MET:HE1	2.50	0.41
1:F:356:TYR:CE1	1:F:362:PHE:HD1	2.38	0.41
1:F:1018:ALA:O	1:F:1022:VAL:HG23	2.21	0.41
1:A:11:PHE:CE2	1:B:890:ALA:HB1	2.56	0.41
1:A:30:LEU:HA	1:A:31:PRO:HD3	1.92	0.41
1:A:154:ILE:HG22	1:A:287:SER:HB3	2.02	0.41
1:A:172:VAL:HG22	1:A:306:ILE:HD11	2.03	0.41
1:A:216:ALA:HB3	1:A:234:ILE:O	2.21	0.41
1:A:278:ILE:HG13	1:A:613:ASN:HB3	2.02	0.41
1:A:366:LEU:HA	1:A:366:LEU:HD23	1.62	0.41
1:A:985:GLY:O	1:A:988:PRO:HD2	2.20	0.41
1:A:1035:ARG:O	1:A:1036:LYS:C	2.63	0.41
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.56	0.41
1:B:355:MET:HE2	1:B:977:MET:SD	2.61	0.41
1:B:356:TYR:C	1:B:358:PHE:N	2.76	0.41
1:B:552:MET:HB3	1:B:552:MET:HE2	1.98	0.41
1:B:576:VAL:HG22	1:B:663:VAL:HG13	2.03	0.41
1:B:949:ALA:HB3	1:B:1026:PHE:CE1	2.55	0.41
1:C:77:TYR:CZ	1:C:93:THR:HG21	2.56	0.41
1:C:150:THR:H	1:C:153:ASP:HB2	1.85	0.41
1:C:151:GLN:NE2	1:C:286:ALA:O	2.54	0.41
1:C:926:TYR:HE1	1:C:999:ALA:HB1	1.86	0.41
1:C:1034:SER:OG	1:C:1037:ASN:HB3	2.21	0.41
1:D:143:ILE:O	1:D:321:LEU:HA	2.21	0.41
1:D:172:VAL:CG2	1:D:306:ILE:HD11	2.51	0.41
1:D:278:ILE:HD13	1:D:584:GLN:HE21	1.85	0.41
1:D:588:GLN:N	1:D:613:ASN:ND2	2.69	0.41
1:D:671:ILE:H	1:D:671:ILE:HG13	1.70	0.41
1:D:687:GLN:OE1	1:D:856:GLY:HA3	2.21	0.41
1:D:698:ALA:O	1:D:701:GLN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:726:GLN:CD	1:D:812:GLY:HA3	2.46	0.41
1:D:1018:ALA:C	1:D:1020:PHE:N	2.79	0.41
1:E:187:TRP:HA	1:E:774:MET:O	2.21	0.41
1:E:511:GLY:HA2	1:E:515:TRP:HD1	1.82	0.41
1:E:538:THR:CG2	1:E:1024:VAL:HG13	2.51	0.41
1:E:545:TYR:OH	1:E:906:PRO:HG2	2.20	0.41
1:E:643:LYS:HZ1	1:E:993:THR:HG23	1.85	0.41
1:E:699:ARG:HH22	1:E:722:GLU:CD	2.18	0.41
1:E:885:PHE:HD2	1:E:886:LEU:HD13	1.85	0.41
1:F:465:ALA:HA	1:F:468:ARG:CZ	2.51	0.41
1:F:542:LEU:O	1:F:545:TYR:HB3	2.21	0.41
1:F:578:LEU:HB2	1:F:623:ASN:CB	2.51	0.41
1:F:1032:ARG:O	1:F:1033:PHE:HB2	2.21	0.41
1:B:177:LEU:HA	1:B:289:LEU:HD23	2.03	0.41
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.54	0.41
1:B:376:LEU:O	1:B:377:LEU:C	2.63	0.41
1:B:533:GLY:HA2	1:B:536:ARG:HB2	2.03	0.41
1:B:888:LEU:HD13	1:B:901:VAL:HG11	2.03	0.41
1:B:946:VAL:HG22	1:B:1026:PHE:HD1	1.86	0.41
1:B:960:LEU:O	1:B:964:THR:HG23	2.21	0.41
1:B:1026:PHE:O	1:B:1030:ARG:HB2	2.21	0.41
1:C:104:GLN:HG3	1:C:105:VAL:N	2.35	0.41
1:D:542:LEU:HD12	1:D:542:LEU:HA	1.71	0.41
1:D:662:MET:HG2	1:D:664:PHE:CZ	2.56	0.41
1:D:937:LEU:O	1:D:938:SER:C	2.63	0.41
1:E:692:HIS:NE2	1:E:813:SER:HB2	2.35	0.41
1:F:907:LEU:HG	1:F:1017:LEU:HD23	2.03	0.41
1:F:926:TYR:HE1	1:F:999:ALA:HB1	1.86	0.41
1:A:453:PHE:CE2	1:A:474:ILE:HG21	2.56	0.40
1:A:870:GLY:O	1:A:872:GLN:HG3	2.21	0.40
1:A:897:ILE:HG12	1:A:1030:ARG:HD3	2.03	0.40
1:A:1040:ILE:CG1	1:A:1041:GLU:H	2.26	0.40
1:B:352:PHE:HD2	1:B:353:LEU:HD23	1.86	0.40
1:B:841:MET:O	1:B:845:GLU:HG3	2.22	0.40
1:C:3:ASN:C	1:C:5:PHE:N	2.79	0.40
1:D:393:LEU:HD12	1:D:469:GLN:HG3	2.03	0.40
1:D:414:GLU:CD	1:D:974:PRO:HG3	2.46	0.40
1:E:448:VAL:HA	1:E:451:ALA:HB3	2.03	0.40
1:E:586:ARG:O	1:E:589:LYS:HB3	2.21	0.40
1:F:6:ILE:H	1:F:6:ILE:HG12	1.41	0.40
1:F:47:ALA:HB2	1:F:127:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:LYS:HA	1:F:816:LEU:CD1	2.51	0.40
1:F:160:ALA:HA	1:F:767:ARG:NE	2.34	0.40
1:F:563:PHE:CE2	1:F:564:LEU:HD22	2.56	0.40
1:F:565:PRO:HG2	1:F:567:GLU:OE2	2.21	0.40
1:F:572:PHE:HB2	1:F:666:PHE:O	2.22	0.40
1:A:210:GLN:OE1	1:A:249:ILE:HG23	2.22	0.40
1:A:338:HIS:NE2	1:A:342:LYS:HD2	2.37	0.40
1:A:344:LEU:HD21	1:A:399:VAL:HG22	2.04	0.40
1:A:356:TYR:HE2	1:A:513:PHE:HE2	1.68	0.40
1:B:442:LEU:HA	1:B:442:LEU:HD23	1.79	0.40
1:B:760:ASN:O	1:B:771:VAL:HB	2.21	0.40
1:B:971:ARG:C	1:B:974:PRO:HD2	2.46	0.40
1:C:182:TYR:HD2	1:C:765:ARG:HH22	1.68	0.40
1:C:1018:ALA:O	1:C:1022:VAL:HG23	2.21	0.40
1:D:146:ASP:OD2	1:D:146:ASP:N	2.44	0.40
1:D:151:GLN:CG	1:D:152:GLU:N	2.84	0.40
1:D:189:ASN:HA	1:D:190:PRO:HD3	1.91	0.40
1:D:251:LEU:HD21	1:D:262:LEU:HD13	2.02	0.40
1:D:279:ALA:HB3	1:D:286:ALA:O	2.20	0.40
1:E:203:VAL:O	1:E:207:ILE:HG13	2.21	0.40
1:E:383:LEU:HD23	1:E:383:LEU:HA	1.92	0.40
1:E:1042:HIS:HB3	1:E:1043:SER:H	1.59	0.40
1:F:752:ALA:O	1:F:774:MET:HA	2.21	0.40
1:F:790:TYR:HB3	1:F:798:MET:HB3	2.01	0.40
1:A:507:GLU:C	1:A:509:LYS:H	2.29	0.40
1:A:577:GLN:HE22	1:A:624:THR:HG22	1.86	0.40
1:A:752:ALA:O	1:A:774:MET:HA	2.22	0.40
1:A:894:SER:HB3	1:A:897:ILE:HB	2.03	0.40
1:B:448:VAL:HG13	1:B:884:VAL:HG22	2.03	0.40
1:B:756:GLY:CA	1:B:774:MET:HG3	2.52	0.40
1:B:931:LEU:O	1:B:935:ILE:HG13	2.21	0.40
1:B:1015:THR:OG1	1:B:1016:VAL:N	2.53	0.40
1:C:466:ILE:H	1:C:466:ILE:HG12	1.77	0.40
1:C:668:LEU:H	1:C:668:LEU:CD2	2.30	0.40
1:C:701:GLN:HG2	1:C:705:GLU:OE2	2.20	0.40
1:C:940:LYS:O	1:C:943:ILE:HB	2.21	0.40
1:C:940:LYS:HZ2	1:C:978:THR:HG21	1.86	0.40
1:C:953:MET:HE1	1:C:960:LEU:HD12	2.04	0.40
1:D:356:TYR:O	1:D:360:GLN:N	2.48	0.40
1:D:846:GLN:O	1:D:850:LYS:HD3	2.21	0.40
1:E:2:PRO:HB2	1:E:439:GLN:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:713:LEU:HD11	1:E:844:MET:HE3	2.03	0.40
1:F:238:THR:HG22	1:F:239:ARG:O	2.21	0.40
1:F:453:PHE:CE1	1:F:474:ILE:HG21	2.57	0.40
1:F:666:PHE:N	1:F:666:PHE:CD1	2.88	0.40
1:A:152:GLU:HB2	1:A:182:TYR:CE1	2.56	0.40
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.56	0.40
1:B:163:LYS:HD2	1:B:177:LEU:HD12	2.03	0.40
1:B:348:ILE:HD13	1:B:348:ILE:HG21	1.80	0.40
1:B:650:ARG:O	1:B:653:ARG:HB3	2.21	0.40
1:C:187:TRP:CZ3	1:C:774:MET:HE2	2.56	0.40
1:C:344:LEU:HA	1:C:399:VAL:HG22	2.03	0.40
1:C:368:PRO:O	1:C:371:ALA:HB3	2.21	0.40
1:C:699:ARG:HE	1:C:718:PRO:HB3	1.87	0.40
1:C:937:LEU:O	1:C:938:SER:C	2.63	0.40
1:C:1037:ASN:HB3	1:C:1038:GLU:H	1.81	0.40
1:D:112:GLN:OE1	1:D:115:MET:HG3	2.22	0.40
1:D:225:VAL:H	1:E:781:MET:CE	2.35	0.40
1:D:706:ALA:HB1	1:D:716:VAL:HG11	2.03	0.40
1:D:777:ALA:CB	1:F:225:VAL:HG12	2.44	0.40
1:D:971:ARG:C	1:D:971:ARG:CZ	2.95	0.40
2:D:1101:LMT:H6D	2:D:1101:LMT:C5B	2.52	0.40
1:E:167:SER:CB	1:E:175:VAL:HG21	2.52	0.40
1:E:216:ALA:HB2	1:E:236:ALA:HB2	2.04	0.40
1:E:291:ILE:HG21	1:E:306:ILE:HD11	2.02	0.40
1:E:328:ASP:O	1:E:331:PRO:HD2	2.21	0.40
1:E:398:MET:HG2	1:E:473:THR:CG2	2.52	0.40
1:F:30:LEU:HA	1:F:31:PRO:HD3	1.89	0.40
1:F:149:MET:HB2	1:F:153:ASP:HB3	2.03	0.40
1:F:355:MET:HG2	1:F:410:ILE:HD11	2.04	0.40
1:F:636:ASP:O	1:F:638:PRO:HD3	2.22	0.40
1:F:778:LYS:H	1:F:778:LYS:HG2	1.58	0.40
1:F:923:ASN:C	1:F:923:ASN:ND2	2.79	0.40
1:F:964:THR:O	1:F:968:VAL:HB	2.21	0.40
1:A:110:LYS:HE2	1:C:130:GLU:OE2	2.21	0.40
1:A:261:LEU:HD12	1:A:263:ARG:CZ	2.51	0.40
1:A:483:LEU:HD13	1:A:487:ILE:HD12	2.04	0.40
1:A:781:MET:HE3	1:C:228:GLN:CD	2.46	0.40
1:A:944:LEU:HB3	1:A:971:ARG:NH2	2.37	0.40
1:C:520:PHE:HE1	1:C:976:LEU:HD22	1.87	0.40
1:C:525:HIS:O	1:C:526:HIS:C	2.64	0.40
1:C:931:LEU:HD23	1:C:931:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:586:ARG:HH11	1:D:586:ARG:HD2	1.78	0.40
1:D:644:VAL:HG12	1:D:645:GLU:N	2.33	0.40
1:E:157:TYR:CE1	1:E:318:PRO:HD3	2.57	0.40
1:E:158:VAL:HG11	1:E:289:LEU:HD11	2.03	0.40
1:E:189:ASN:HD22	1:E:190:PRO:HD2	1.85	0.40
1:E:527:TYR:HB2	2:E:1101:LMT:H82	2.04	0.40
1:E:848:ALA:HA	1:E:851:LEU:HG	2.04	0.40
1:F:462:SER:HB3	1:F:865:GLN:CG	2.50	0.40
1:F:785:ASP:N	1:F:785:ASP:OD1	2.55	0.40
1:F:932:LEU:O	1:F:935:ILE:N	2.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:GLU:OE2	1:D:522:LYS:NZ[1_556]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1040/1049 (99%)	940 (90%)	89 (9%)	11 (1%)	11	39
1	B	1041/1049 (99%)	950 (91%)	75 (7%)	16 (2%)	8	32
1	C	1040/1049 (99%)	946 (91%)	77 (7%)	17 (2%)	7	31
1	D	1040/1049 (99%)	954 (92%)	70 (7%)	16 (2%)	8	32
1	E	1040/1049 (99%)	946 (91%)	77 (7%)	17 (2%)	7	31
1	F	1040/1049 (99%)	946 (91%)	76 (7%)	18 (2%)	7	30
All	All	6241/6294 (99%)	5682 (91%)	464 (7%)	95 (2%)	8	32

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	677	ALA
1	A	991	ILE
1	A	1037	ASN
1	A	1040	ILE
1	B	509	LYS
1	B	516	PHE
1	B	673	GLU
1	B	677	ALA
1	B	689	GLY
1	B	1038	GLU
1	C	133	SER
1	C	360	GLN
1	C	509	LYS
1	C	689	GLY
1	C	836	SER
1	C	893	GLU
1	C	920	GLY
1	C	1037	ASN
1	D	508	GLY
1	D	511	GLY
1	D	992	SER
1	E	509	LYS
1	E	893	GLU
1	E	1042	HIS
1	F	133	SER
1	F	134	SER
1	F	146	ASP
1	F	360	GLN
1	F	836	SER
1	F	1035	ARG
1	F	1040	ILE
1	A	360	GLN
1	A	675	GLY
1	A	688	ALA
1	A	992	SER
1	A	1039	ASP
1	B	672	VAL
1	B	751	GLY
1	C	134	SER
1	C	146	ASP
1	C	147	GLY
1	C	751	GLY
1	C	871	ASN

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Mol	Chain	Res	Type
1	D	360	GLN
1	D	675	GLY
1	D	751	GLY
1	D	991	ILE
1	D	1033	PHE
1	E	508	GLY
1	E	672	VAL
1	E	674	LEU
1	E	677	ALA
1	E	1039	ASP
1	F	147	GLY
1	F	507	GLU
1	F	1033	PHE
1	A	751	GLY
1	B	1034	SER
1	B	1040	ILE
1	C	514	GLY
1	C	752	ALA
1	C	1042	HIS
1	D	215	ALA
1	D	752	ALA
1	E	516	PHE
1	E	751	GLY
1	F	514	GLY
1	F	1038	GLU
1	D	514	GLY
1	D	677	ALA
1	D	1034	SER
1	E	163	LYS
1	E	514	GLY
1	E	1034	SER
1	F	689	GLY
1	F	751	GLY
1	F	923	ASN
1	B	358	PHE
1	B	923	ASN
1	C	215	ALA
1	D	923	ASN
1	D	960	LEU
1	E	638	PRO
1	E	1040	ILE
1	B	215	ALA

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Mol	Chain	Res	Type
1	B	893	GLU
1	E	74	ASN
1	F	638	PRO
1	A	658	ILE
1	B	508	GLY
1	B	644	VAL
1	D	638	PRO
1	E	658	ILE
1	F	204	ILE
1	F	644	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	848/855 (99%)	768 (91%)	80 (9%)	8	30
1	B	849/855 (99%)	760 (90%)	89 (10%)	6	25
1	C	848/855 (99%)	762 (90%)	86 (10%)	7	26
1	D	848/855 (99%)	770 (91%)	78 (9%)	8	30
1	E	848/855 (99%)	759 (90%)	89 (10%)	6	25
1	F	848/855 (99%)	758 (89%)	90 (11%)	6	24
All	All	5089/5130 (99%)	4577 (90%)	512 (10%)	7	26

All (512) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	44	THR
1	A	45	ILE
1	A	88	VAL
1	A	91	THR
1	A	101	ASP
1	A	125	GLN
1	A	146	ASP

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Mol	Chain	Res	Type
1	A	152	GLU
1	A	169	THR
1	A	177	LEU
1	A	205	THR
1	A	222	THR
1	A	225	VAL
1	A	230	LEU
1	A	243	THR
1	A	255	GLN
1	A	260	VAL
1	A	270	LEU
1	A	274	ASN
1	A	293	LEU
1	A	321	LEU
1	A	324	VAL
1	A	336	SER
1	A	337	ILE
1	A	341	VAL
1	A	343	THR
1	A	348	ILE
1	A	353	LEU
1	A	354	VAL
1	A	355	MET
1	A	357	LEU
1	A	360	GLN
1	A	362	PHE
1	A	400	LEU
1	A	437	GLN
1	A	452	VAL
1	A	472	ILE
1	A	489	THR
1	A	502	LYS
1	A	534	ILE
1	A	538	THR
1	A	559	LEU
1	A	561	SER
1	A	564	LEU
1	A	571	VAL
1	A	578	LEU
1	A	597	TYR
1	A	602	GLU
1	A	603	LYS

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Mol	Chain	Res	Type
1	A	609	VAL
1	A	617	PHE
1	A	629	VAL
1	A	634	TRP
1	A	644	VAL
1	A	662	MET
1	A	672	VAL
1	A	687	GLN
1	A	695	LEU
1	A	712	MET
1	A	716	VAL
1	A	721	LEU
1	A	741	VAL
1	A	768	VAL
1	A	797	GLN
1	A	802	SER
1	A	806	SER
1	A	843	LEU
1	A	857	TYR
1	A	866	GLU
1	A	901	VAL
1	A	922	THR
1	A	931	LEU
1	A	938	SER
1	A	961	ILE
1	A	964	THR
1	A	971	ARG
1	A	980	LEU
1	A	990	VAL
1	A	1035	ARG
1	B	3	ASN
1	B	6	ILE
1	B	10	ILE
1	B	25	LEU
1	B	111	LEU
1	B	117	LEU
1	B	125	GLN
1	B	131	LYS
1	B	148	THR
1	B	169	THR
1	B	213	GLN
1	B	225	VAL

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Mol	Chain	Res	Type
1	B	229	GLN
1	B	242	SER
1	B	243	THR
1	B	249	ILE
1	B	253	VAL
1	B	259	ARG
1	B	260	VAL
1	B	267	LYS
1	B	270	LEU
1	B	277	ILE
1	B	293	LEU
1	B	295	THR
1	B	310	LEU
1	B	314	GLU
1	B	321	LEU
1	B	324	VAL
1	B	329	THR
1	B	330	THR
1	B	341	VAL
1	B	348	ILE
1	B	354	VAL
1	B	355	MET
1	B	358	PHE
1	B	360	GLN
1	B	365	THR
1	B	400	LEU
1	B	429	GLU
1	B	434	SER
1	B	482	VAL
1	B	489	THR
1	B	523	SER
1	B	536	ARG
1	B	559	LEU
1	B	561	SER
1	B	564	LEU
1	B	571	VAL
1	B	602	GLU
1	B	612	VAL
1	B	613	ASN
1	B	626	ILE
1	B	629	VAL
1	B	634	TRP

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Mol	Chain	Res	Type
1	B	652	THR
1	B	666	PHE
1	B	672	VAL
1	B	673	GLU
1	B	687	GLN
1	B	694	LYS
1	B	695	LEU
1	B	697	GLN
1	B	714	THR
1	B	716	VAL
1	B	717	ARG
1	B	721	LEU
1	B	741	VAL
1	B	743	ILE
1	B	768	VAL
1	B	802	SER
1	B	806	SER
1	B	835	LYS
1	B	843	LEU
1	B	844	MET
1	B	865	GLN
1	B	867	ARG
1	B	871	ASN
1	B	886	LEU
1	B	914	LEU
1	B	922	THR
1	B	938	SER
1	B	955	LYS
1	B	961	ILE
1	B	968	VAL
1	B	971	ARG
1	B	978	THR
1	B	980	LEU
1	B	1007	VAL
1	B	1015	THR
1	C	3	ASN
1	C	6	ILE
1	C	25	LEU
1	C	27	ILE
1	C	58	GLN
1	C	88	VAL
1	C	91	THR

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Mol	Chain	Res	Type
1	C	102	ILE
1	C	104	GLN
1	C	112	GLN
1	C	145	THR
1	C	148	THR
1	C	169	THR
1	C	177	LEU
1	C	242	SER
1	C	243	THR
1	C	253	VAL
1	C	255	GLN
1	C	260	VAL
1	C	270	LEU
1	C	280	GLU
1	C	293	LEU
1	C	330	THR
1	C	336	SER
1	C	337	ILE
1	C	341	VAL
1	C	342	LYS
1	C	354	VAL
1	C	362	PHE
1	C	363	ARG
1	C	392	THR
1	C	429	GLU
1	C	439	GLN
1	C	447	MET
1	C	448	VAL
1	C	452	VAL
1	C	463	THR
1	C	472	ILE
1	C	482	VAL
1	C	489	THR
1	C	510	LYS
1	C	526	HIS
1	C	530	SER
1	C	542	LEU
1	C	543	VAL
1	C	559	LEU
1	C	561	SER
1	C	571	VAL
1	C	578	LEU

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Mol	Chain	Res	Type
1	C	590	VAL
1	C	634	TRP
1	C	662	MET
1	C	666	PHE
1	C	672	VAL
1	C	678	THR
1	C	686	ASP
1	C	694	LYS
1	C	721	LEU
1	C	731	ILE
1	C	741	VAL
1	C	746	ILE
1	C	748	THR
1	C	749	THR
1	C	768	VAL
1	C	797	GLN
1	C	802	SER
1	C	843	LEU
1	C	847	LEU
1	C	860	THR
1	C	865	GLN
1	C	868	LEU
1	C	876	LEU
1	C	886	LEU
1	C	887	CYS
1	C	895	TRP
1	C	938	SER
1	C	947	GLU
1	C	953	MET
1	C	961	ILE
1	C	971	ARG
1	C	980	LEU
1	C	991	ILE
1	C	1011	MET
1	C	1035	ARG
1	C	1038	GLU
1	C	1041	GLU
1	D	3	ASN
1	D	10	ILE
1	D	25	LEU
1	D	27	ILE
1	D	28	LEU

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Mol	Chain	Res	Type
1	D	44	THR
1	D	45	ILE
1	D	88	VAL
1	D	91	THR
1	D	101	ASP
1	D	102	ILE
1	D	146	ASP
1	D	152	GLU
1	D	205	THR
1	D	222	THR
1	D	225	VAL
1	D	243	THR
1	D	255	GLN
1	D	260	VAL
1	D	270	LEU
1	D	321	LEU
1	D	324	VAL
1	D	330	THR
1	D	336	SER
1	D	341	VAL
1	D	343	THR
1	D	348	ILE
1	D	353	LEU
1	D	354	VAL
1	D	355	MET
1	D	360	GLN
1	D	362	PHE
1	D	400	LEU
1	D	410	ILE
1	D	437	GLN
1	D	463	THR
1	D	472	ILE
1	D	538	THR
1	D	542	LEU
1	D	559	LEU
1	D	561	SER
1	D	571	VAL
1	D	578	LEU
1	D	590	VAL
1	D	602	GLU
1	D	603	LYS
1	D	629	VAL

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Mol	Chain	Res	Type
1	D	634	TRP
1	D	657	GLN
1	D	662	MET
1	D	666	PHE
1	D	671	ILE
1	D	672	VAL
1	D	687	GLN
1	D	695	LEU
1	D	721	LEU
1	D	741	VAL
1	D	743	ILE
1	D	802	SER
1	D	806	SER
1	D	843	LEU
1	D	866	GLU
1	D	867	ARG
1	D	901	VAL
1	D	918	PHE
1	D	922	THR
1	D	931	LEU
1	D	938	SER
1	D	943	ILE
1	D	961	ILE
1	D	966	ASP
1	D	968	VAL
1	D	971	ARG
1	D	978	THR
1	D	980	LEU
1	D	990	VAL
1	D	1016	VAL
1	D	1040	ILE
1	E	3	ASN
1	E	6	ILE
1	E	17	ILE
1	E	25	LEU
1	E	28	LEU
1	E	29	LYS
1	E	58	GLN
1	E	91	THR
1	E	102	ILE
1	E	131	LYS
1	E	146	ASP

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Mol	Chain	Res	Type
1	E	177	LEU
1	E	182	TYR
1	E	189	ASN
1	E	203	VAL
1	E	205	THR
1	E	229	GLN
1	E	243	THR
1	E	249	ILE
1	E	253	VAL
1	E	255	GLN
1	E	259	ARG
1	E	260	VAL
1	E	270	LEU
1	E	291	ILE
1	E	293	LEU
1	E	295	THR
1	E	310	LEU
1	E	314	GLU
1	E	324	VAL
1	E	327	TYR
1	E	329	THR
1	E	330	THR
1	E	336	SER
1	E	337	ILE
1	E	353	LEU
1	E	354	VAL
1	E	365	THR
1	E	372	VAL
1	E	398	MET
1	E	400	LEU
1	E	439	GLN
1	E	452	VAL
1	E	482	VAL
1	E	523	SER
1	E	538	THR
1	E	559	LEU
1	E	561	SER
1	E	564	LEU
1	E	571	VAL
1	E	574	THR
1	E	578	LEU
1	E	629	VAL

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Mol	Chain	Res	Type
1	E	634	TRP
1	E	652	THR
1	E	653	ARG
1	E	659	LYS
1	E	662	MET
1	E	672	VAL
1	E	673	GLU
1	E	687	GLN
1	E	690	LEU
1	E	694	LYS
1	E	697	GLN
1	E	708	LYS
1	E	714	THR
1	E	721	LEU
1	E	741	VAL
1	E	749	THR
1	E	768	VAL
1	E	797	GLN
1	E	802	SER
1	E	835	LYS
1	E	843	LEU
1	E	865	GLN
1	E	867	ARG
1	E	871	ASN
1	E	886	LEU
1	E	938	SER
1	E	961	ILE
1	E	966	ASP
1	E	968	VAL
1	E	971	ARG
1	E	972	LEU
1	E	980	LEU
1	E	1016	VAL
1	E	1021	PHE
1	E	1036	LYS
1	E	1043	SER
1	F	3	ASN
1	F	6	ILE
1	F	21	LEU
1	F	25	LEU
1	F	34	GLN
1	F	59	ASP

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Mol	Chain	Res	Type
1	F	88	VAL
1	F	102	ILE
1	F	104	GLN
1	F	169	THR
1	F	177	LEU
1	F	205	THR
1	F	225	VAL
1	F	242	SER
1	F	253	VAL
1	F	260	VAL
1	F	270	LEU
1	F	280	GLU
1	F	293	LEU
1	F	327	TYR
1	F	335	ILE
1	F	337	ILE
1	F	341	VAL
1	F	354	VAL
1	F	357	LEU
1	F	358	PHE
1	F	363	ARG
1	F	408	ASP
1	F	447	MET
1	F	448	VAL
1	F	452	VAL
1	F	472	ILE
1	F	482	VAL
1	F	489	THR
1	F	510	LYS
1	F	515	TRP
1	F	523	SER
1	F	524	THR
1	F	526	HIS
1	F	534	ILE
1	F	538	THR
1	F	540	ARG
1	F	542	LEU
1	F	559	LEU
1	F	564	LEU
1	F	571	VAL
1	F	578	LEU
1	F	587	THR

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Mol	Chain	Res	Type
1	F	602	GLU
1	F	603	LYS
1	F	626	ILE
1	F	629	VAL
1	F	634	TRP
1	F	649	MET
1	F	658	ILE
1	F	666	PHE
1	F	672	VAL
1	F	681	ASP
1	F	685	ILE
1	F	695	LEU
1	F	697	GLN
1	F	703	LEU
1	F	713	LEU
1	F	721	LEU
1	F	731	ILE
1	F	741	VAL
1	F	746	ILE
1	F	775	SER
1	F	797	GLN
1	F	806	SER
1	F	843	LEU
1	F	847	LEU
1	F	860	THR
1	F	865	GLN
1	F	868	LEU
1	F	876	LEU
1	F	923	ASN
1	F	938	SER
1	F	947	GLU
1	F	953	MET
1	F	961	ILE
1	F	964	THR
1	F	968	VAL
1	F	971	ARG
1	F	972	LEU
1	F	980	LEU
1	F	990	VAL
1	F	991	ILE
1	F	1034	SER
1	F	1038	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	34	GLN
1	A	74	ASN
1	A	109	ASN
1	A	144	ASN
1	A	151	GLN
1	A	181	GLN
1	A	231	ASN
1	A	437	GLN
1	A	517	ASN
1	A	592	ASN
1	A	605	ASN
1	A	667	ASN
1	A	928	GLN
1	A	1001	ASN
1	B	63	GLN
1	B	144	ASN
1	B	189	ASN
1	B	231	ASN
1	B	391	ASN
1	B	588	GLN
1	B	592	ASN
1	B	613	ASN
1	B	733	GLN
1	B	744	ASN
1	B	1037	ASN
1	C	104	GLN
1	C	112	GLN
1	C	439	GLN
1	C	577	GLN
1	C	588	GLN
1	C	592	ASN
1	C	613	ASN
1	C	846	GLN
1	C	923	ASN
1	C	1001	ASN
1	D	68	ASN
1	D	74	ASN
1	D	125	GLN
1	D	391	ASN
1	D	517	ASN

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Mol	Chain	Res	Type
1	D	605	ASN
1	D	719	ASN
1	D	744	ASN
1	D	760	ASN
1	E	67	GLN
1	E	108	GLN
1	E	189	ASN
1	E	588	GLN
1	E	592	ASN
1	E	733	GLN
1	E	737	GLN
1	E	744	ASN
1	E	865	GLN
1	F	89	GLN
1	F	112	GLN
1	F	123	GLN
1	F	181	GLN
1	F	197	GLN
1	F	588	GLN
1	F	592	ASN
1	F	605	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	LMT	B	1101	-	36,36,36	1.75	10 (27%)	47,47,47	1.44	8 (17%)
2	LMT	A	1101	-	36,36,36	1.78	11 (30%)	47,47,47	1.11	3 (6%)
2	LMT	F	1101	-	36,36,36	1.76	8 (22%)	47,47,47	1.03	1 (2%)
2	LMT	D	1101	-	36,36,36	1.76	8 (22%)	47,47,47	1.28	7 (14%)
2	LMT	C	1101	-	36,36,36	1.92	10 (27%)	47,47,47	1.62	10 (21%)
2	LMT	E	1101	-	36,36,36	1.83	10 (27%)	47,47,47	1.14	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	B	1101	-	-	10/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	11/21/61/61	0/2/2/2
2	LMT	F	1101	-	-	8/21/61/61	0/2/2/2
2	LMT	D	1101	-	-	13/21/61/61	0/2/2/2
2	LMT	C	1101	-	1/1/10/10	13/21/61/61	0/2/2/2
2	LMT	E	1101	-	-	14/21/61/61	0/2/2/2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	LMT	O5'-C5'	4.62	1.55	1.44
2	E	1101	LMT	O1'-C1'	4.24	1.47	1.40
2	C	1101	LMT	O1'-C1'	4.24	1.47	1.40
2	A	1101	LMT	O5'-C5'	3.96	1.54	1.44
2	B	1101	LMT	O5B-C1B	3.92	1.51	1.41
2	D	1101	LMT	O5'-C5'	3.83	1.53	1.44
2	A	1101	LMT	O5B-C1B	3.79	1.51	1.41
2	E	1101	LMT	O5'-C5'	3.79	1.53	1.44
2	D	1101	LMT	O1'-C1'	3.77	1.46	1.40
2	E	1101	LMT	O5B-C1B	3.73	1.51	1.41
2	F	1101	LMT	O1'-C1'	3.72	1.46	1.40
2	C	1101	LMT	O5'-C1'	3.71	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1101	LMT	O5'-C5'	3.61	1.53	1.44
2	C	1101	LMT	O5B-C1B	3.60	1.51	1.41
2	F	1101	LMT	O5B-C1B	3.54	1.50	1.41
2	F	1101	LMT	C6'-C5'	-3.49	1.40	1.51
2	D	1101	LMT	O5B-C1B	3.47	1.50	1.41
2	B	1101	LMT	O1'-C1'	3.47	1.46	1.40
2	E	1101	LMT	C6'-C5'	-3.31	1.40	1.51
2	B	1101	LMT	O5'-C5'	3.30	1.52	1.44
2	F	1101	LMT	O5'-C1'	3.24	1.50	1.41
2	B	1101	LMT	C6'-C5'	-3.23	1.41	1.51
2	A	1101	LMT	O1'-C1'	3.15	1.45	1.40
2	A	1101	LMT	O5'-C1'	3.15	1.49	1.41
2	D	1101	LMT	O5'-C1'	3.13	1.49	1.41
2	D	1101	LMT	C6'-C5'	-3.10	1.41	1.51
2	A	1101	LMT	C6'-C5'	-3.10	1.41	1.51
2	E	1101	LMT	O5'-C1'	3.09	1.49	1.41
2	D	1101	LMT	O3B-C3B	2.99	1.50	1.43
2	C	1101	LMT	C6'-C5'	-2.90	1.42	1.51
2	F	1101	LMT	C3'-C2'	-2.81	1.45	1.52
2	F	1101	LMT	O3B-C3B	2.71	1.49	1.43
2	B	1101	LMT	O3B-C3B	2.64	1.49	1.43
2	C	1101	LMT	C3'-C2'	-2.62	1.45	1.52
2	B	1101	LMT	O5'-C1'	2.53	1.48	1.41
2	C	1101	LMT	O3B-C3B	2.52	1.49	1.43
2	A	1101	LMT	O3B-C3B	2.51	1.49	1.43
2	A	1101	LMT	C3'-C2'	-2.46	1.45	1.52
2	C	1101	LMT	O2'-C2'	2.45	1.49	1.43
2	E	1101	LMT	O2'-C2'	2.33	1.48	1.43
2	B	1101	LMT	C3B-C2B	-2.31	1.46	1.52
2	B	1101	LMT	C5-C4	2.25	1.63	1.51
2	D	1101	LMT	O2'-C2'	2.25	1.48	1.43
2	E	1101	LMT	C5-C4	2.24	1.62	1.51
2	C	1101	LMT	C5-C4	2.23	1.62	1.51
2	B	1101	LMT	O3'-C3'	2.22	1.48	1.43
2	E	1101	LMT	O3B-C3B	2.22	1.48	1.43
2	A	1101	LMT	O2'-C2'	2.20	1.48	1.43
2	B	1101	LMT	C3'-C2'	-2.17	1.46	1.52
2	A	1101	LMT	C3B-C2B	-2.17	1.46	1.52
2	E	1101	LMT	O3'-C3'	2.14	1.48	1.43
2	E	1101	LMT	C3B-C2B	-2.14	1.46	1.52
2	A	1101	LMT	O3'-C3'	2.10	1.48	1.43
2	F	1101	LMT	C5-C4	2.08	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	LMT	C5-C4	2.05	1.62	1.51
2	D	1101	LMT	C5-C4	2.04	1.61	1.51
2	C	1101	LMT	C2-C1	2.02	1.59	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	LMT	C4B-C3B-C2B	4.11	118.05	110.83
2	B	1101	LMT	C1'-O5'-C5'	-4.04	105.82	113.72
2	C	1101	LMT	C3B-C4B-C5B	3.85	117.21	110.23
2	B	1101	LMT	O5B-C5B-C4B	3.53	116.06	109.70
2	E	1101	LMT	C3B-C4B-C5B	-3.52	103.84	110.23
2	B	1101	LMT	C1B-O5B-C5B	3.52	120.59	113.72
2	A	1101	LMT	C1B-O1B-C4'	-3.44	109.83	117.98
2	C	1101	LMT	C1-O1'-C1'	3.41	119.51	113.68
2	C	1101	LMT	C1B-O1B-C4'	-3.35	110.03	117.98
2	C	1101	LMT	C1B-C2B-C3B	3.01	116.34	110.01
2	B	1101	LMT	O1'-C1'-C2'	2.89	112.66	108.27
2	A	1101	LMT	O5'-C5'-C6'	2.88	113.56	106.44
2	D	1101	LMT	C2'-C3'-C4'	2.80	116.03	109.68
2	C	1101	LMT	O3B-C3B-C4B	-2.77	103.86	110.38
2	D	1101	LMT	O1B-C1B-C2B	2.64	114.60	108.09
2	E	1101	LMT	O1'-C1'-C2'	2.55	112.14	108.27
2	D	1101	LMT	C1B-O1B-C4'	-2.47	112.11	117.98
2	B	1101	LMT	C1'-C2'-C3'	2.39	115.04	110.01
2	C	1101	LMT	O5'-C5'-C6'	2.37	112.31	106.44
2	D	1101	LMT	C1B-C2B-C3B	2.36	114.97	110.01
2	E	1101	LMT	C1-O1'-C1'	2.32	117.64	113.68
2	B	1101	LMT	O5'-C5'-C6'	2.29	112.11	106.44
2	E	1101	LMT	C1B-O1B-C4'	-2.25	112.65	117.98
2	F	1101	LMT	O4'-C4B-C3B	-2.23	105.12	110.38
2	C	1101	LMT	O1B-C1B-C2B	2.23	113.57	108.09
2	E	1101	LMT	C4B-C3B-C2B	-2.18	107.00	110.83
2	B	1101	LMT	O5'-C5'-C4'	-2.18	105.21	109.72
2	D	1101	LMT	O5B-C5B-C6B	2.16	111.79	106.44
2	D	1101	LMT	C1'-C2'-C3'	2.16	114.55	110.01
2	B	1101	LMT	O2'-C2'-C3'	-2.11	105.41	110.38
2	C	1101	LMT	O4'-C4B-C3B	-2.05	105.55	110.38
2	A	1101	LMT	C1'-C2'-C3'	-2.03	105.74	110.01
2	D	1101	LMT	O3'-C3'-C2'	-2.01	105.64	110.38
2	C	1101	LMT	O3B-C3B-C2B	-2.00	105.65	110.38

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1101	LMT	C3B

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	LMT	O5'-C5'-C6'-O6'
2	A	1101	LMT	O5'-C5'-C6'-O6'
2	F	1101	LMT	O5B-C5B-C6B-O6B
2	A	1101	LMT	O5B-C5B-C6B-O6B
2	C	1101	LMT	O5'-C5'-C6'-O6'
2	D	1101	LMT	C4B-C5B-C6B-O6B
2	D	1101	LMT	O5B-C5B-C6B-O6B
2	B	1101	LMT	C4'-C5'-C6'-O6'
2	A	1101	LMT	C4'-C5'-C6'-O6'
2	B	1101	LMT	O5'-C1'-O1'-C1
2	C	1101	LMT	O5'-C1'-O1'-C1
2	F	1101	LMT	C4B-C5B-C6B-O6B
2	E	1101	LMT	O5'-C5'-C6'-O6'
2	B	1101	LMT	O5B-C1B-O1B-C4'
2	E	1101	LMT	C4'-C5'-C6'-O6'
2	C	1101	LMT	C4'-C5'-C6'-O6'
2	F	1101	LMT	C4'-C5'-C6'-O6'
2	B	1101	LMT	C2'-C1'-O1'-C1
2	C	1101	LMT	C2'-C1'-O1'-C1
2	A	1101	LMT	C3-C4-C5-C6
2	E	1101	LMT	C4B-C5B-C6B-O6B
2	F	1101	LMT	O5'-C5'-C6'-O6'
2	D	1101	LMT	C3-C4-C5-C6
2	B	1101	LMT	O1'-C1-C2-C3
2	D	1101	LMT	O5'-C5'-C6'-O6'
2	D	1101	LMT	O1'-C1-C2-C3
2	D	1101	LMT	C7-C8-C9-C10
2	D	1101	LMT	C4'-C5'-C6'-O6'
2	B	1101	LMT	C3-C4-C5-C6
2	A	1101	LMT	C4B-C5B-C6B-O6B
2	C	1101	LMT	O1'-C1-C2-C3
2	F	1101	LMT	C1-C2-C3-C4
2	D	1101	LMT	C2-C3-C4-C5
2	D	1101	LMT	C4-C5-C6-C7
2	E	1101	LMT	C3-C4-C5-C6
2	B	1101	LMT	C7-C8-C9-C10
2	F	1101	LMT	C3-C4-C5-C6

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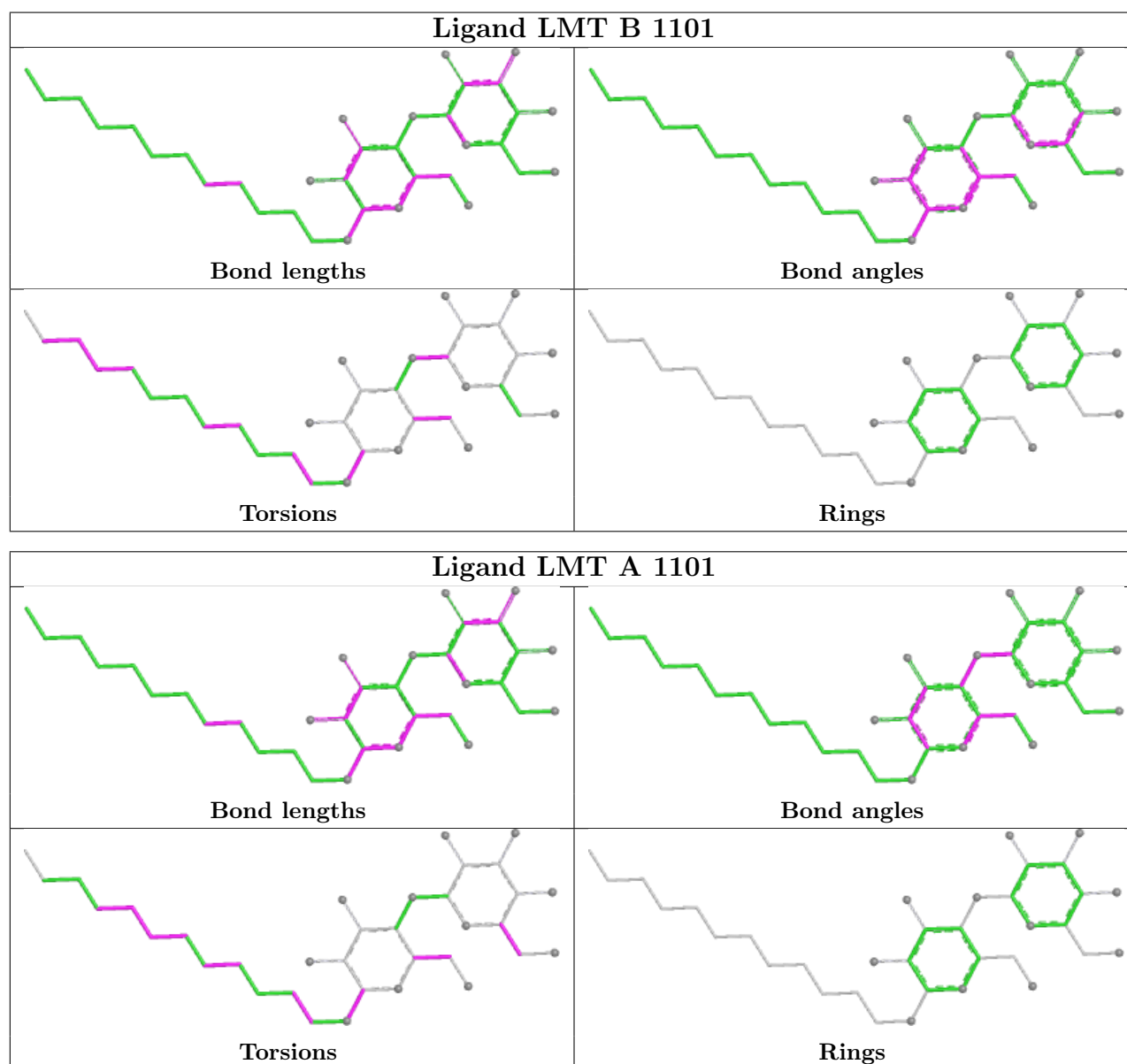
Mol	Chain	Res	Type	Atoms
2	E	1101	LMT	C5-C6-C7-C8
2	C	1101	LMT	C5-C6-C7-C8
2	C	1101	LMT	C4B-C5B-C6B-O6B
2	E	1101	LMT	C6-C7-C8-C9
2	E	1101	LMT	C4-C5-C6-C7
2	C	1101	LMT	C6-C7-C8-C9
2	E	1101	LMT	C1-C2-C3-C4
2	E	1101	LMT	C7-C8-C9-C10
2	D	1101	LMT	C11-C10-C9-C8
2	E	1101	LMT	O5B-C5B-C6B-O6B
2	F	1101	LMT	C5-C6-C7-C8
2	A	1101	LMT	O1'-C1-C2-C3
2	B	1101	LMT	C11-C10-C9-C8
2	D	1101	LMT	C2'-C1'-O1'-C1
2	A	1101	LMT	C5-C6-C7-C8
2	A	1101	LMT	C7-C8-C9-C10
2	D	1101	LMT	C2-C1-O1'-C1'
2	E	1101	LMT	O5B-C1B-O1B-C4'
2	A	1101	LMT	C2'-C1'-O1'-C1
2	E	1101	LMT	O1'-C1-C2-C3
2	C	1101	LMT	C7-C8-C9-C10
2	C	1101	LMT	C1-C2-C3-C4
2	E	1101	LMT	C2B-C1B-O1B-C4'
2	C	1101	LMT	O5B-C5B-C6B-O6B
2	C	1101	LMT	C2-C1-O1'-C1'
2	B	1101	LMT	C9-C10-C11-C12
2	D	1101	LMT	O5'-C1'-O1'-C1
2	A	1101	LMT	O5'-C1'-O1'-C1
2	F	1101	LMT	C6-C7-C8-C9
2	A	1101	LMT	C6-C7-C8-C9
2	C	1101	LMT	C2-C3-C4-C5
2	E	1101	LMT	C11-C10-C9-C8

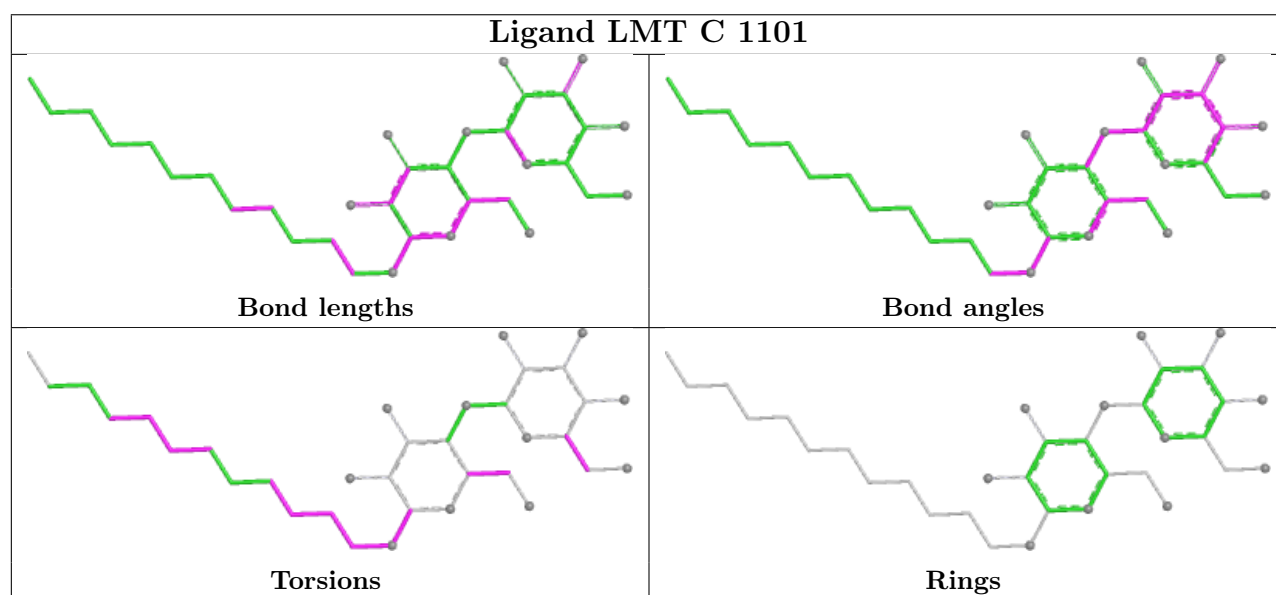
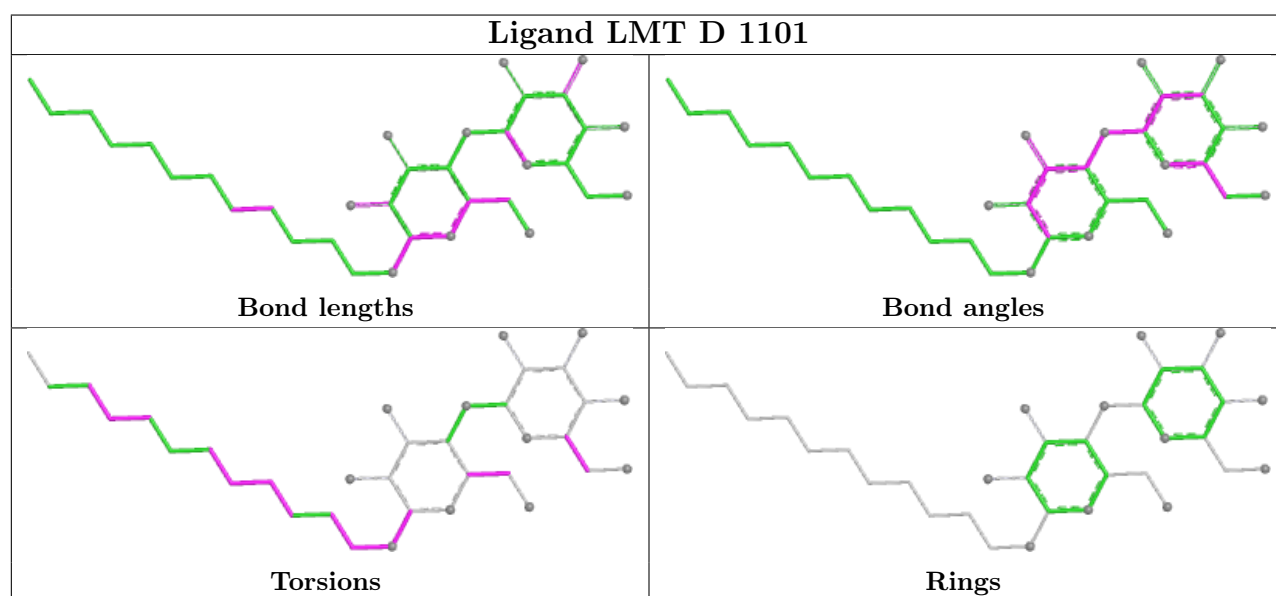
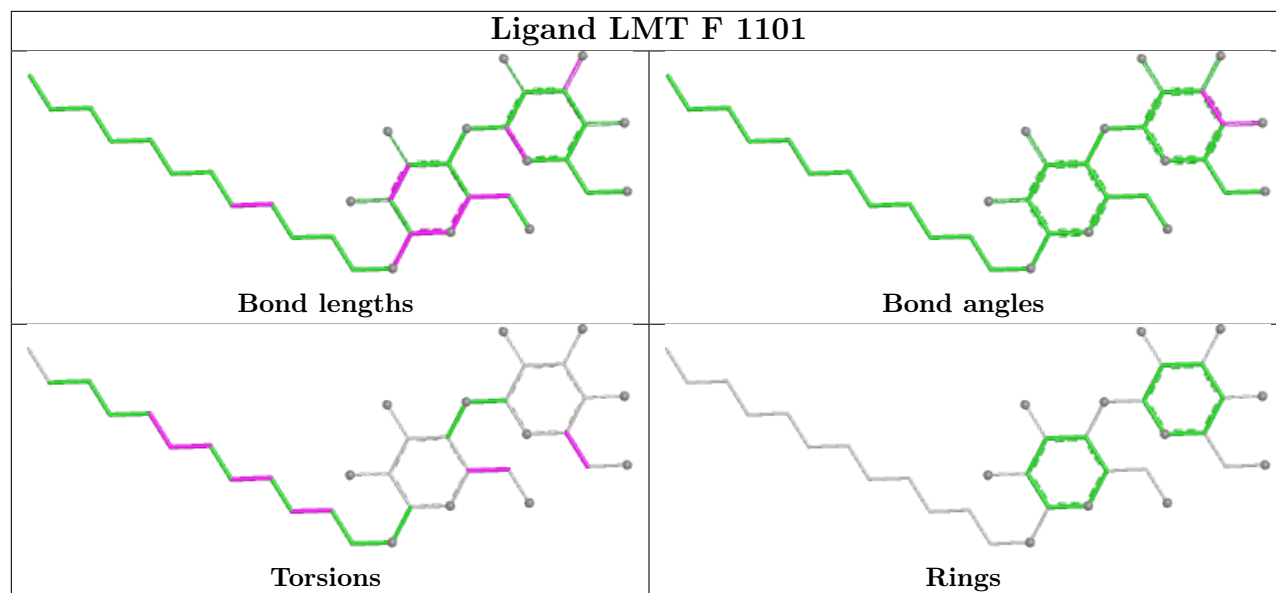
There are no ring outliers.

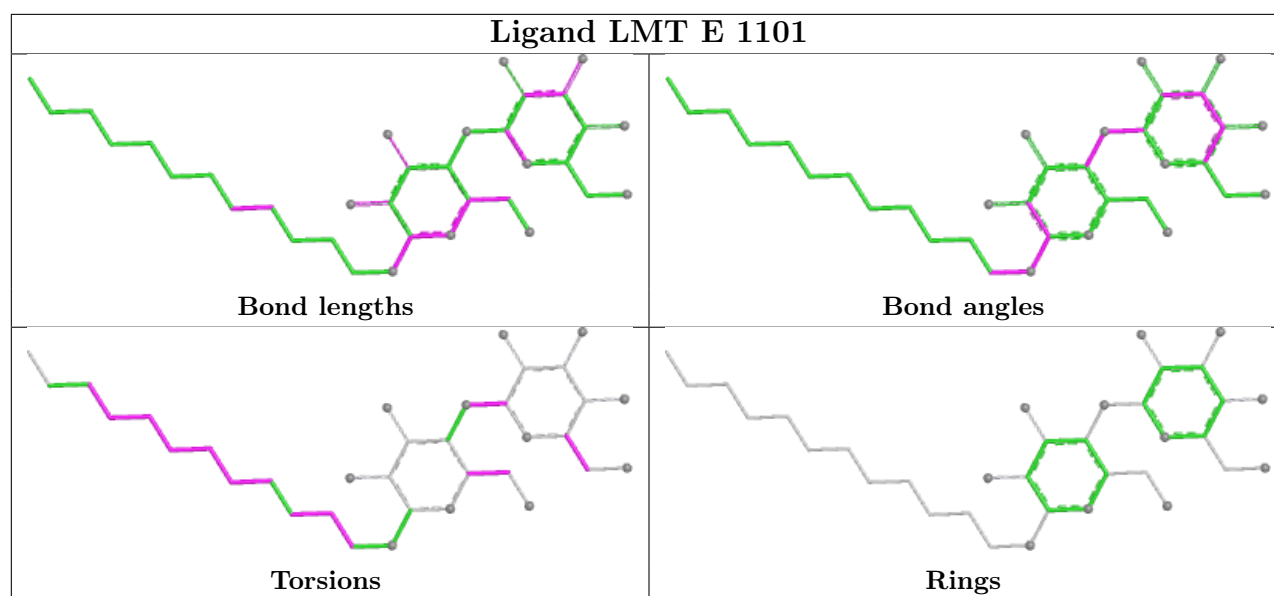
5 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	LMT	7	0
2	A	1101	LMT	3	0
2	F	1101	LMT	3	0
2	D	1101	LMT	7	0
2	E	1101	LMT	10	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	1042/1049 (99%)	0.29	46 (4%)	39	25	48, 78, 110, 142	0
1	B	1043/1049 (99%)	0.05	23 (2%)	62	43	36, 72, 102, 149	0
1	C	1042/1049 (99%)	0.15	45 (4%)	40	25	34, 72, 100, 155	0
1	D	1042/1049 (99%)	0.29	36 (3%)	47	31	40, 89, 116, 145	0
1	E	1042/1049 (99%)	0.39	53 (5%)	33	22	57, 90, 113, 158	0
1	F	1042/1049 (99%)	0.41	73 (7%)	22	15	51, 86, 112, 144	0
All	All	6253/6294 (99%)	0.26	276 (4%)	39	25	34, 82, 111, 158	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	869	SER	10.0
1	B	869	SER	9.9
1	E	291	ILE	8.4
1	F	856	GLY	8.3
1	C	69	MET	7.9
1	B	715	SER	7.3
1	F	501	ALA	6.1
1	C	822	LEU	6.0
1	E	164	ASP	5.4
1	F	836	SER	5.1
1	F	442	LEU	5.1
1	C	856	GLY	5.0
1	F	69	MET	4.9
1	E	290	GLY	4.9
1	C	871	ASN	4.7
1	A	383	LEU	4.5
1	F	837	THR	4.2
1	D	337	ILE	4.2
1	E	33	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	888	LEU	4.1
1	D	875	SER	4.1
1	E	366	LEU	4.1
1	F	441	ALA	4.0
1	E	105	VAL	4.0
1	A	385	ALA	4.0
1	A	376	LEU	4.0
1	F	873	ALA	4.0
1	D	869	SER	3.9
1	C	501	ALA	3.9
1	C	122	VAL	3.8
1	C	838	GLY	3.8
1	F	10	ILE	3.8
1	C	166	ILE	3.7
1	E	488	LEU	3.7
1	D	719	ASN	3.7
1	E	292	LYS	3.5
1	D	306	ILE	3.5
1	F	127	VAL	3.5
1	B	164	ASP	3.5
1	A	679	GLY	3.4
1	F	59	ASP	3.4
1	C	79	SER	3.4
1	F	675	GLY	3.4
1	D	714	THR	3.4
1	D	715	SER	3.3
1	A	334	LYS	3.3
1	D	460	GLY	3.2
1	F	49	TYR	3.2
1	F	481	SER	3.2
1	A	396	PHE	3.2
1	D	330	THR	3.2
1	D	50	PRO	3.2
1	F	122	VAL	3.2
1	A	678	THR	3.2
1	F	410	ILE	3.2
1	F	306	ILE	3.2
1	C	837	THR	3.2
1	E	174	ASP	3.1
1	F	503	GLY	3.1
1	F	117	LEU	3.1
1	C	403	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	605	ASN	3.1
1	A	400	LEU	3.1
1	B	870	GLY	3.1
1	A	372	VAL	3.1
1	F	3	ASN	3.1
1	E	137	LEU	3.1
1	D	866	GLU	3.1
1	C	9	PRO	3.0
1	D	677	ALA	3.0
1	B	884	VAL	3.0
1	B	678	THR	3.0
1	C	107	VAL	3.0
1	D	461	GLY	3.0
1	F	502	LYS	2.9
1	C	33	ALA	2.9
1	E	296	GLY	2.9
1	F	403	GLY	2.9
1	B	291	ILE	2.9
1	E	465	ALA	2.9
1	A	899	PHE	2.9
1	C	835	LYS	2.9
1	F	706	ALA	2.8
1	F	874	PRO	2.8
1	A	621	GLY	2.8
1	D	886	LEU	2.8
1	A	493	CYS	2.8
1	F	417	GLU	2.8
1	D	400	LEU	2.8
1	A	337	ILE	2.8
1	A	327	TYR	2.8
1	F	698	ALA	2.8
1	F	848	ALA	2.8
1	D	84	SER	2.8
1	E	713	LEU	2.7
1	B	866	GLU	2.7
1	A	407	ASP	2.7
1	F	415	ASN	2.7
1	A	321	LEU	2.7
1	F	51	GLY	2.7
1	C	868	LEU	2.7
1	D	865	GLN	2.7
1	E	2	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	92	LEU	2.7
1	C	127	VAL	2.7
1	C	402	ILE	2.6
1	B	714	THR	2.6
1	B	916	ALA	2.6
1	C	888	LEU	2.6
1	C	3	ASN	2.6
1	B	514	GLY	2.6
1	A	640	GLU	2.6
1	A	413	VAL	2.6
1	E	409	ALA	2.6
1	B	720	GLY	2.6
1	E	293	LEU	2.6
1	E	306	ILE	2.6
1	E	428	LYS	2.6
1	F	166	ILE	2.6
1	D	459	PHE	2.6
1	A	310	LEU	2.6
1	A	486	LEU	2.6
1	A	463	THR	2.6
1	B	515	TRP	2.6
1	D	463	THR	2.6
1	E	678	THR	2.6
1	D	334	LYS	2.6
1	A	2	PRO	2.6
1	E	177	LEU	2.6
1	E	922	THR	2.6
1	F	402	ILE	2.5
1	D	486	LEU	2.5
1	D	333	VAL	2.5
1	C	836	SER	2.5
1	E	843	LEU	2.5
1	C	855	VAL	2.5
1	C	494	ALA	2.5
1	E	706	ALA	2.5
1	C	65	ILE	2.5
1	E	6	ILE	2.5
1	F	169	THR	2.5
1	E	892	TYR	2.5
1	F	892	TYR	2.5
1	C	847	LEU	2.5
1	F	868	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	290	GLY	2.5
1	A	410	ILE	2.5
1	F	109	ASN	2.5
1	F	107	VAL	2.5
1	C	6	ILE	2.5
1	A	563	PHE	2.5
1	F	60	THR	2.5
1	A	470	PHE	2.4
1	F	676	THR	2.4
1	F	561	SER	2.4
1	A	307	ARG	2.4
1	F	118	LEU	2.4
1	D	716	VAL	2.4
1	B	534	ILE	2.4
1	E	866	GLU	2.4
1	F	96	SER	2.4
1	F	434	SER	2.4
1	F	57	VAL	2.4
1	F	103	ALA	2.4
1	A	386	PHE	2.4
1	D	60	THR	2.4
1	E	406	VAL	2.4
1	E	411	VAL	2.4
1	A	35	TYR	2.4
1	E	556	PHE	2.4
1	E	405	LEU	2.4
1	B	874	PRO	2.4
1	F	406	VAL	2.4
1	A	473	THR	2.3
1	E	834	GLY	2.3
1	C	72	ILE	2.3
1	E	390	ILE	2.3
1	F	500	ILE	2.3
1	F	827	ILE	2.3
1	F	1040	ILE	2.3
1	C	686	ASP	2.3
1	C	123	GLN	2.3
1	F	542	LEU	2.3
1	C	417	GLU	2.3
1	A	938	SER	2.3
1	C	421	ALA	2.3
1	F	864	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	895	TRP	2.3
1	F	819	TYR	2.3
1	C	8	ARG	2.3
1	E	315	PRO	2.3
1	A	847	LEU	2.3
1	F	702	LEU	2.3
1	F	32	VAL	2.3
1	F	6	ILE	2.3
1	D	33	ALA	2.3
1	D	859	TRP	2.3
1	D	816	LEU	2.3
1	C	514	GLY	2.2
1	E	303	ALA	2.2
1	D	676	THR	2.2
1	D	233	SER	2.2
1	A	606	VAL	2.2
1	F	475	VAL	2.2
1	F	45	ILE	2.2
1	A	21	LEU	2.2
1	A	409	ALA	2.2
1	A	674	LEU	2.2
1	C	97	GLY	2.2
1	C	851	LEU	2.2
1	D	678	THR	2.2
1	A	27	ILE	2.2
1	E	78	MET	2.2
1	E	995	ALA	2.2
1	A	330	THR	2.2
1	D	35	TYR	2.2
1	F	97	GLY	2.2
1	C	867	ARG	2.2
1	A	449	LEU	2.2
1	E	668	LEU	2.2
1	F	371	ALA	2.2
1	B	51	GLY	2.2
1	C	503	GLY	2.2
1	C	59	ASP	2.2
1	A	515	TRP	2.2
1	C	32	VAL	2.1
1	F	64	VAL	2.1
1	F	72	ILE	2.1
1	C	80	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	838	GLY	2.1
1	F	90	ILE	2.1
1	F	111	LEU	2.1
1	F	851	LEU	2.1
1	F	58	GLN	2.1
1	E	114	ALA	2.1
1	E	916	ALA	2.1
1	E	434	SER	2.1
1	F	849	SER	2.1
1	C	406	VAL	2.1
1	F	448	VAL	2.1
1	E	25	LEU	2.1
1	E	37	THR	2.1
1	B	111	LEU	2.1
1	E	493	CYS	2.1
1	F	2	PRO	2.1
1	A	336	SER	2.1
1	B	452	VAL	2.1
1	C	791	VAL	2.1
1	D	1040	ILE	2.1
1	E	166	ILE	2.1
1	D	840	ALA	2.1
1	E	501	ALA	2.1
1	E	1002	ALA	2.1
1	A	218	GLN	2.1
1	F	514	GLY	2.1
1	A	333	VAL	2.0
1	F	55	LYS	2.0
1	F	260	VAL	2.0
1	A	921	LEU	2.0
1	E	65	ILE	2.0
1	E	991	ILE	2.0
1	C	16	ALA	2.0
1	F	62	THR	2.0
1	C	458	PHE	2.0
1	B	175	VAL	2.0
1	E	61	VAL	2.0
1	E	158	VAL	2.0
1	B	306	ILE	2.0
1	D	6	ILE	2.0
1	E	72	ILE	2.0
1	C	789	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	2	PRO	2.0
1	B	716	VAL	2.0
1	D	310	LEU	2.0
1	E	721	LEU	2.0
1	A	323	ILE	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 [i](#)

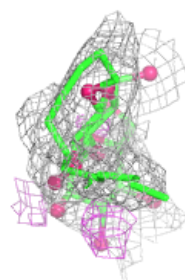
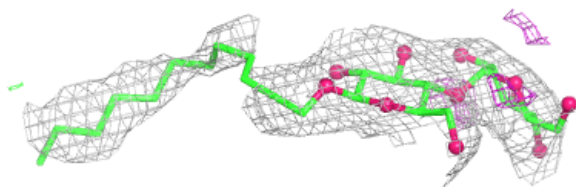
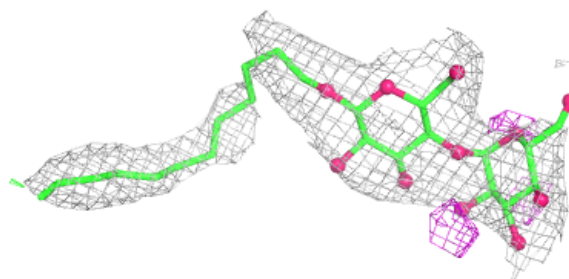
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LMT	F	1101	35/35	0.74	0.14	35,82,93,99	0
2	LMT	E	1101	35/35	0.80	0.13	54,94,105,108	0
2	LMT	B	1101	35/35	0.84	0.13	58,82,95,98	0
2	LMT	C	1101	35/35	0.86	0.10	30,75,84,93	0
2	LMT	A	1101	35/35	0.88	0.09	62,71,84,86	0
2	LMT	D	1101	35/35	0.88	0.09	38,77,87,92	0
3	NI	A	1102	1/1	0.98	0.05	79,79,79,79	0
3	NI	E	1102	1/1	0.98	0.05	96,96,96,96	0
3	NI	C	1102	1/1	0.99	0.04	80,80,80,80	0

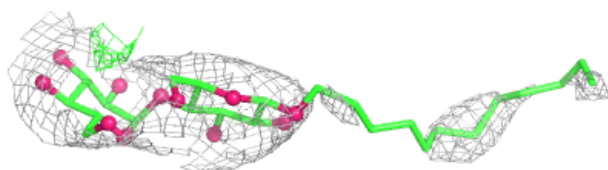
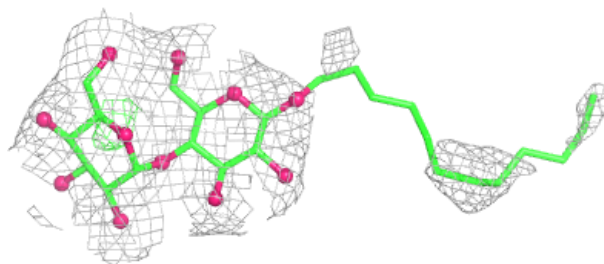
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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)

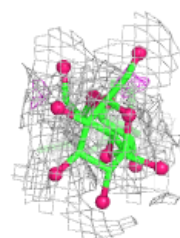
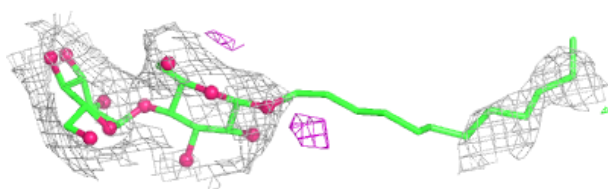
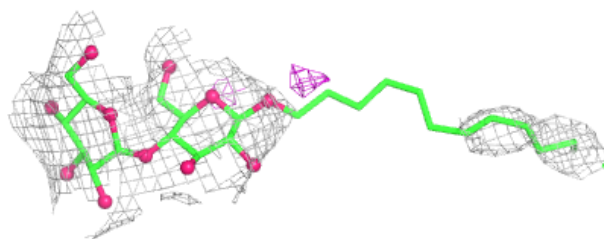
**Electron density around LMT E 1101:**

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

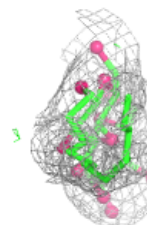
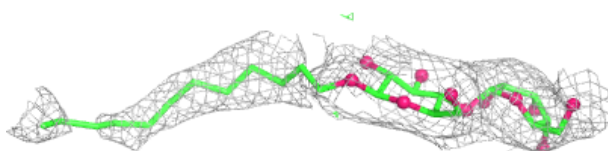
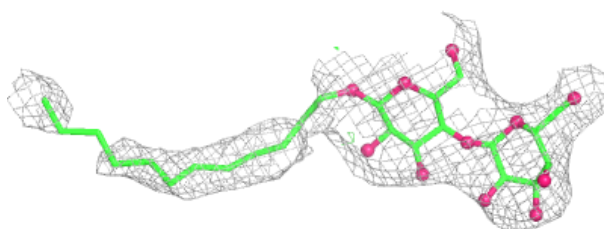


Electron density around LMT B 1101:

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

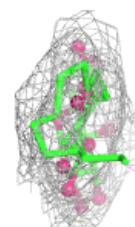
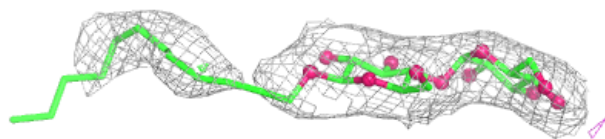
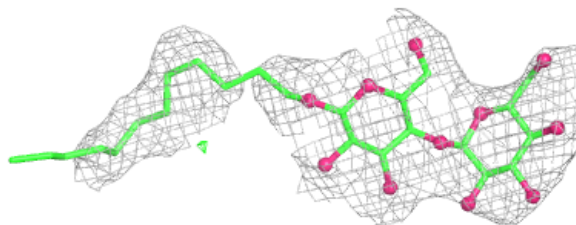
**Electron density around LMT C 1101:**

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

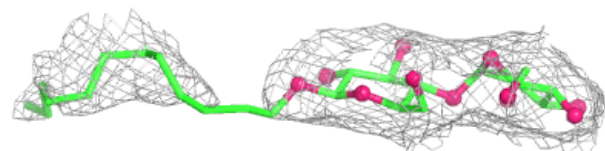
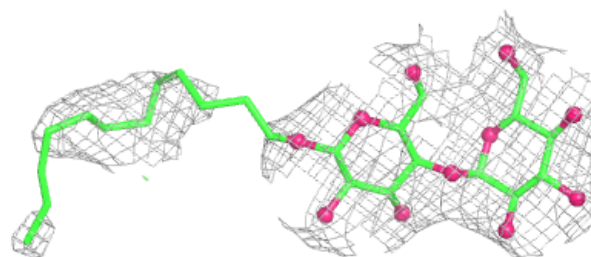


Electron density around LMT A 1101:

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

**Electron density around LMT D 1101:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.