



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:39 PM UTC

PDB ID : 7WLV / pdb_00007wlv
Title : Crystal Structure of the Multidrug efflux transporter BpeF from Burkholderia pseudomallei.
Authors : Kato, T.; Hung, L.-W.; Yamashita, E.; Okada, U.; Terwilliger, T.C.; Murakami, S.
Deposited on : 2022-01-13
Resolution : 3.00 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:

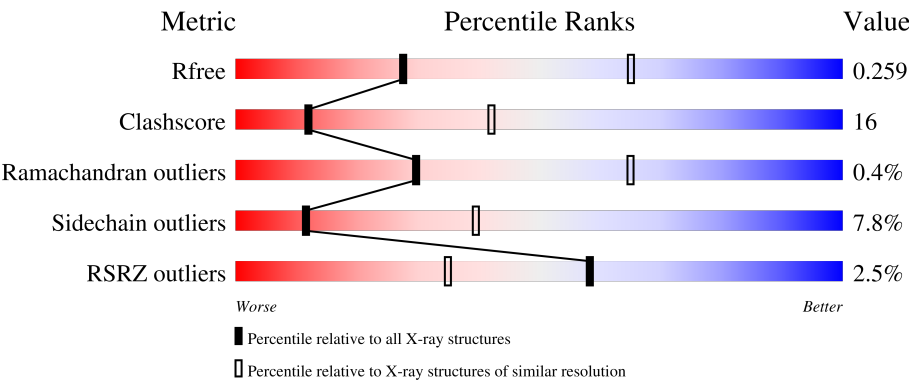
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1067	3% 61% 33% ..
1	B	1067	2% 63% 31% ..
1	C	1067	3% 66% 29% ..
1	D	1067	2% 64% 32% ..

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Mol	Chain	Length	Quality of chain
1	E	1067	2% 65% 28%
1	F	1067	2% 62% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47825 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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	0	0
			7920	5106	1341	1442	31			
1	B	1042	Total	C	N	O	S	0	0	0
			7920	5106	1341	1442	31			
1	C	1043	Total	C	N	O	S	0	0	0
			7929	5112	1343	1443	31			
1	D	1042	Total	C	N	O	S	0	0	0
			7920	5106	1341	1442	31			
1	E	1042	Total	C	N	O	S	0	0	0
			7921	5107	1342	1442	30			
1	F	1043	Total	C	N	O	S	0	0	0
			7929	5112	1343	1443	31			

There are 36 discrepancies between the modelled and reference sequences:

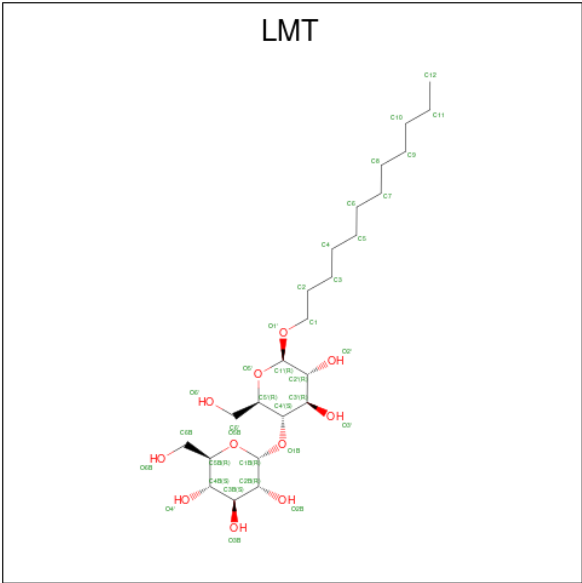
Chain	Residue	Modelled	Actual	Comment	Reference
A	1062	HIS	-	expression tag	UNP Q63NK6
A	1063	HIS	-	expression tag	UNP Q63NK6
A	1064	HIS	-	expression tag	UNP Q63NK6
A	1065	HIS	-	expression tag	UNP Q63NK6
A	1066	HIS	-	expression tag	UNP Q63NK6
A	1067	HIS	-	expression tag	UNP Q63NK6
B	1062	HIS	-	expression tag	UNP Q63NK6
B	1063	HIS	-	expression tag	UNP Q63NK6
B	1064	HIS	-	expression tag	UNP Q63NK6
B	1065	HIS	-	expression tag	UNP Q63NK6
B	1066	HIS	-	expression tag	UNP Q63NK6
B	1067	HIS	-	expression tag	UNP Q63NK6
C	1062	HIS	-	expression tag	UNP Q63NK6
C	1063	HIS	-	expression tag	UNP Q63NK6
C	1064	HIS	-	expression tag	UNP Q63NK6
C	1065	HIS	-	expression tag	UNP Q63NK6
C	1066	HIS	-	expression tag	UNP Q63NK6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1067	HIS	-	expression tag	UNP Q63NK6
D	1062	HIS	-	expression tag	UNP Q63NK6
D	1063	HIS	-	expression tag	UNP Q63NK6
D	1064	HIS	-	expression tag	UNP Q63NK6
D	1065	HIS	-	expression tag	UNP Q63NK6
D	1066	HIS	-	expression tag	UNP Q63NK6
D	1067	HIS	-	expression tag	UNP Q63NK6
E	1062	HIS	-	expression tag	UNP Q63NK6
E	1063	HIS	-	expression tag	UNP Q63NK6
E	1064	HIS	-	expression tag	UNP Q63NK6
E	1065	HIS	-	expression tag	UNP Q63NK6
E	1066	HIS	-	expression tag	UNP Q63NK6
E	1067	HIS	-	expression tag	UNP Q63NK6
F	1062	HIS	-	expression tag	UNP Q63NK6
F	1063	HIS	-	expression tag	UNP Q63NK6
F	1064	HIS	-	expression tag	UNP Q63NK6
F	1065	HIS	-	expression tag	UNP Q63NK6
F	1066	HIS	-	expression tag	UNP Q63NK6
F	1067	HIS	-	expression tag	UNP Q63NK6

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



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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

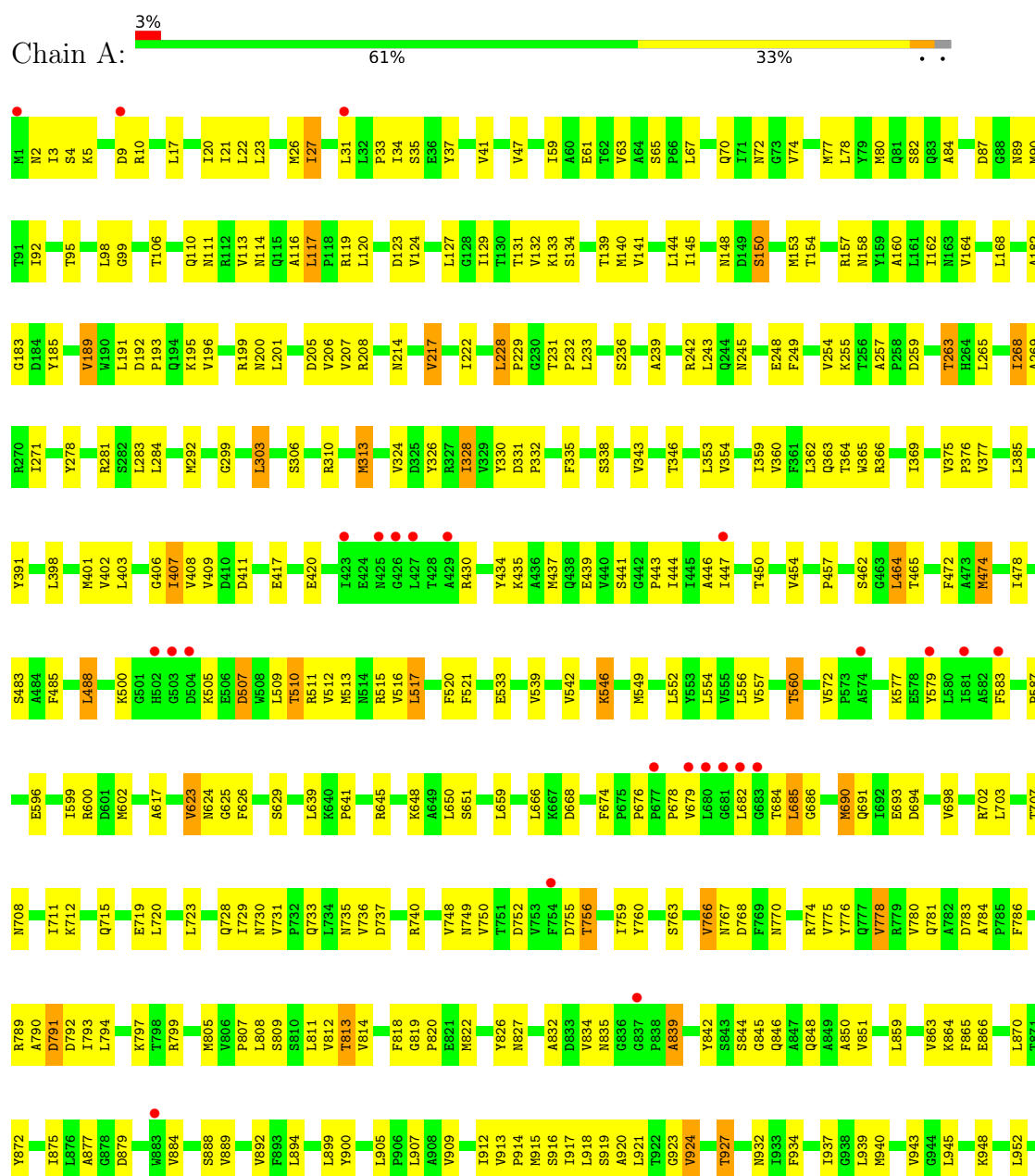
- Molecule 3 is water.

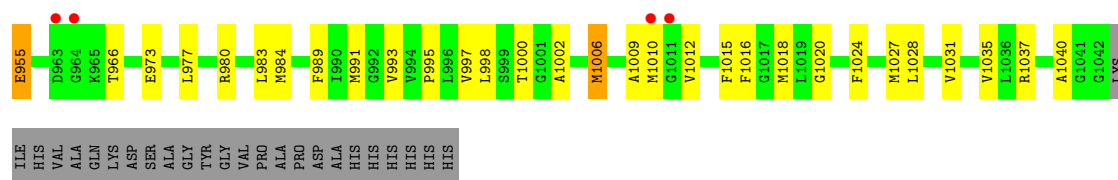
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	10	Total O 10 10	0	0
3	C	8	Total O 8 8	0	0
3	D	7	Total O 7 7	0	0
3	E	5	Total O 5 5	0	0
3	F	6	Total O 6 6	0	0

3 Residue-property plots

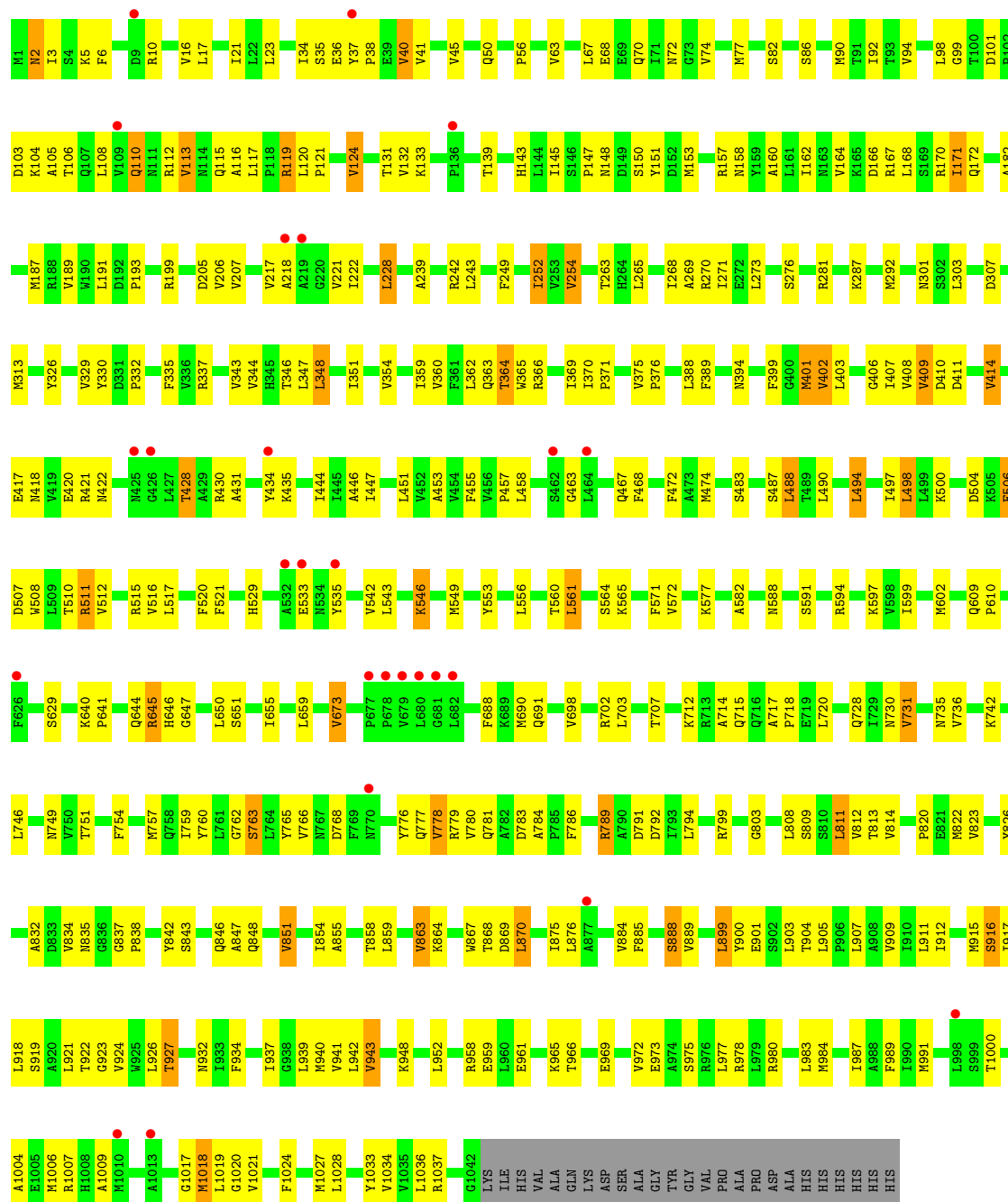
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Efflux pump membrane transporter

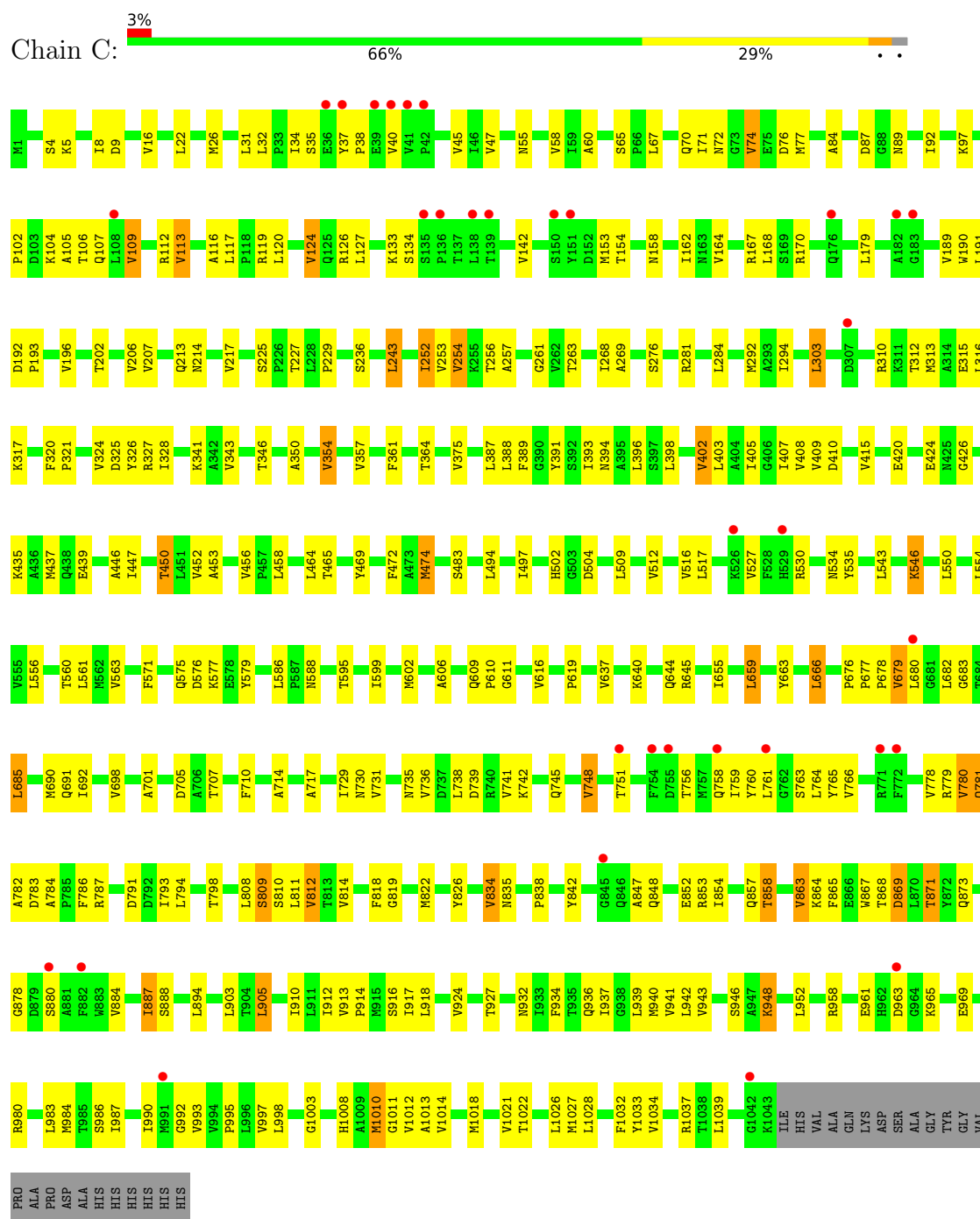




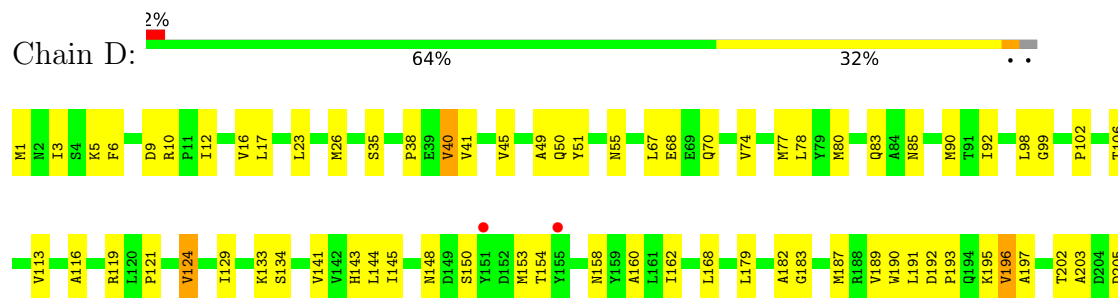
• Molecule 1: Efflux pump membrane transporter

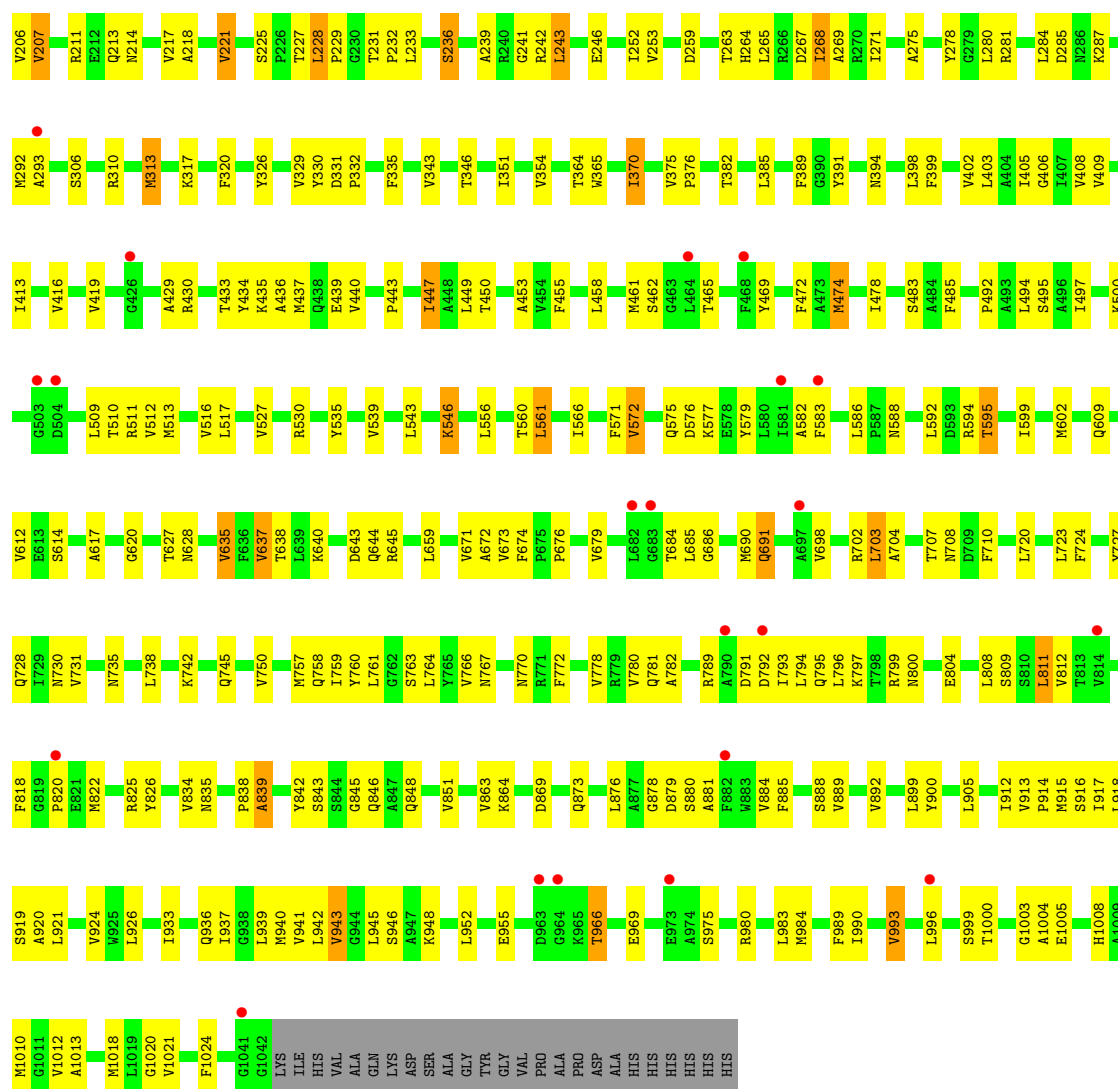


• Molecule 1: Efflux pump membrane transporter



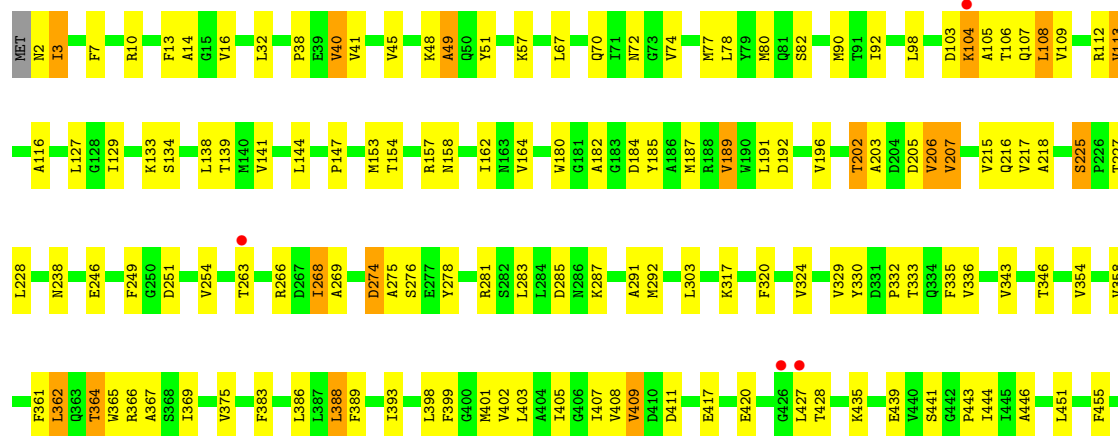
- Molecule 1: Efflux pump membrane transporter

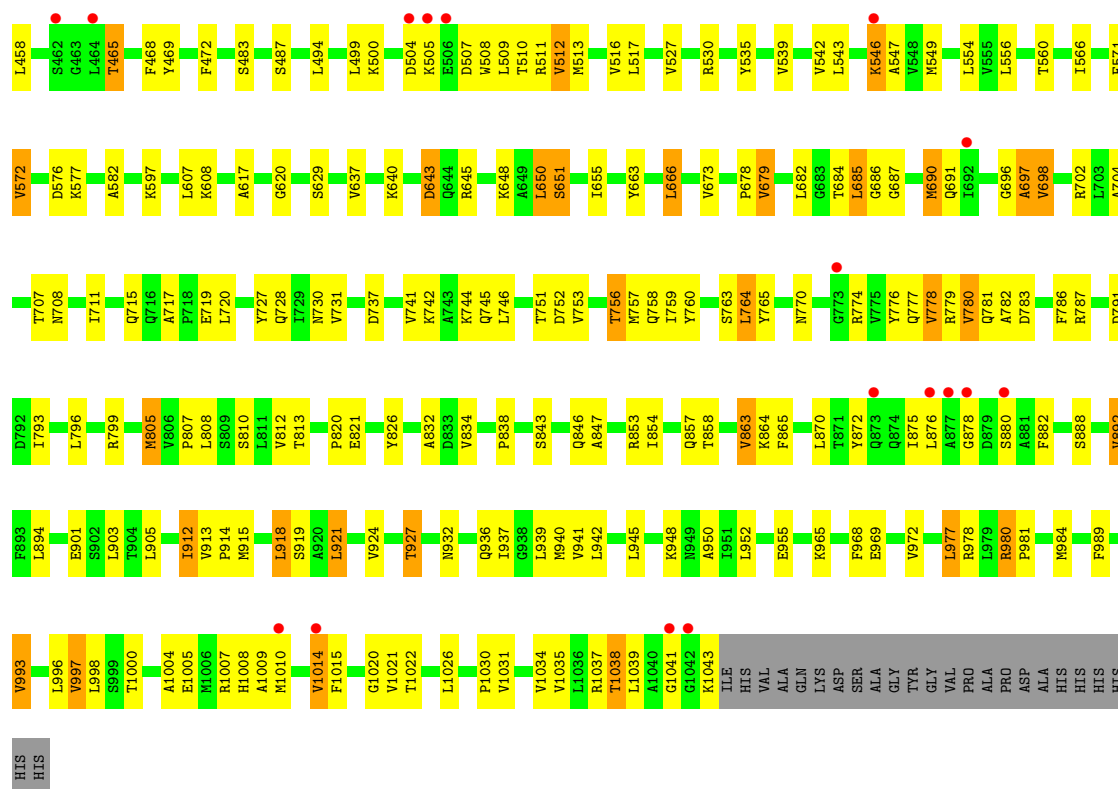




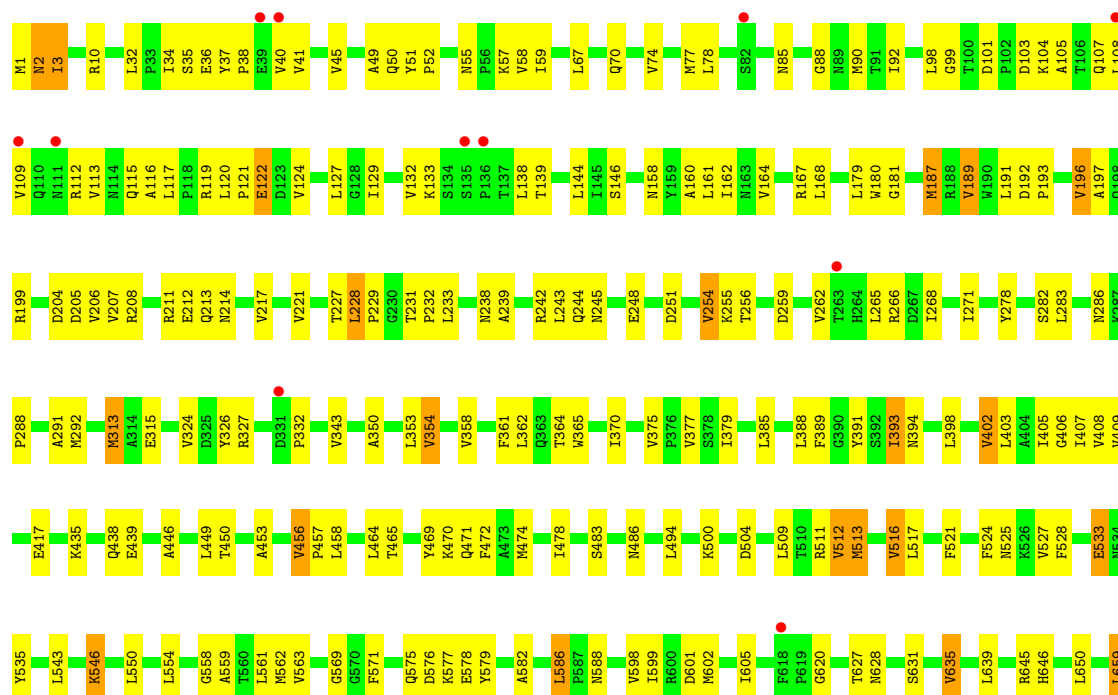
• Molecule 1: Efflux pump membrane transporter

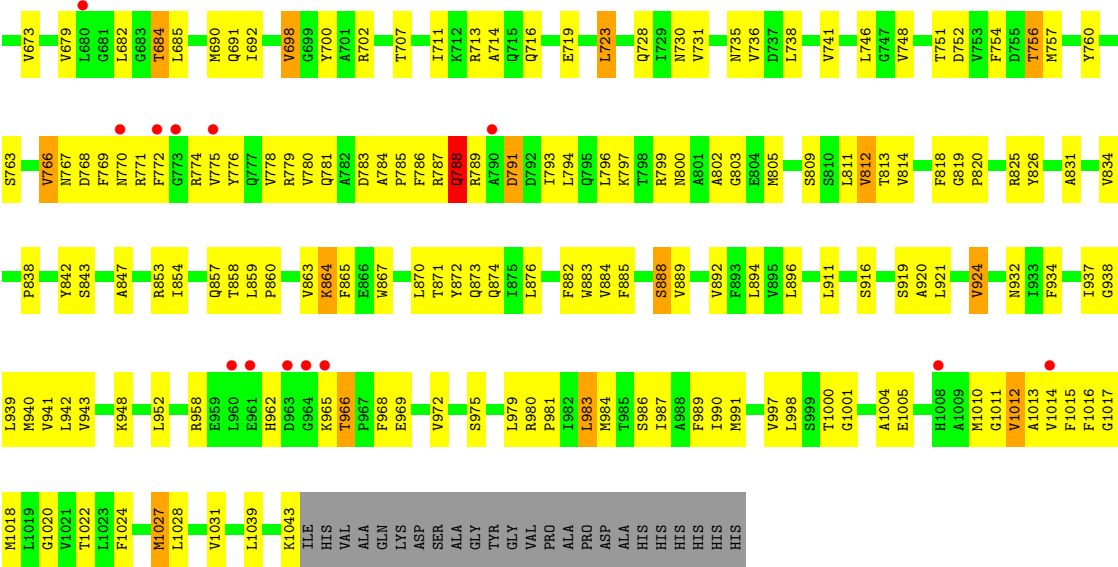
Chain E: 2% 65% 28%





• Molecule 1: Efflux pump membrane transporter





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	119.88Å 121.14Å 159.75Å 97.39° 111.19° 100.60°	Depositor
Resolution (Å)	49.02 – 3.00 49.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.02-3.00) 99.7 (49.02-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.211 , 0.259 0.211 , 0.259	Depositor DCC
R_{free} test set	7880 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	104.0	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 93.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	47825	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	0.43	0/8072	0.72	0/10990
1	B	0.43	0/8072	0.72	2/10990 (0.0%)
1	C	0.42	0/8081	0.69	0/11001
1	D	0.41	0/8072	0.68	0/10990
1	E	0.41	0/8073	0.70	0/10991
1	F	0.45	0/8081	0.73	0/11001
All	All	0.42	0/48451	0.71	2/65963 (0.0%)

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	B	0	1
1	E	0	2
1	F	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	763	SER	N-CA-C	5.71	117.60	110.91
1	B	789	ARG	CB-CG-CD	-5.24	99.24	111.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	506	GLU	Peptide
1	E	650	LEU	Peptide
1	E	696	GLY	Peptide
1	F	788	GLN	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	7920	0	8168	261	0
1	B	7920	0	8168	281	1
1	C	7929	0	8181	231	0
1	D	7920	0	8168	255	0
1	E	7921	0	8169	242	0
1	F	7929	0	8181	287	1
2	A	35	0	46	1	0
2	B	70	0	91	9	0
2	C	35	0	46	3	0
2	D	35	0	46	6	0
2	E	35	0	46	3	0
2	F	35	0	46	5	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	8	0	0	1	0
3	D	7	0	0	0	0
3	E	5	0	0	0	0
3	F	6	0	0	0	0
All	All	47825	0	49356	1521	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 16.

All (1521) 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:B:301:ASN:HD21	2:B:1102:LMT:H2'	1.32	0.93
1:A:114:ASN:HA	1:A:117:LEU:HD22	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:586:LEU:HD21	1:F:598:VAL:HG21	1.52	0.92
1:D:106:THR:HG21	1:D:133:LYS:HB3	1.54	0.90
1:F:70:GLN:HG3	1:F:116:ALA:HB2	1.53	0.90
1:F:698:VAL:HG13	1:F:702:ARG:HB2	1.54	0.90
1:F:115:GLN:O	1:F:119:ARG:NH2	2.05	0.88
1:B:497:ILE:HG23	1:B:498:LEU:HD13	1.55	0.88
1:F:791:ASP:HA	1:F:793:ILE:HG22	1.54	0.88
1:F:838:PRO:HB3	1:F:847:ALA:HB2	1.54	0.87
1:D:794:LEU:HD22	1:D:809:SER:HA	1.57	0.87
1:F:599:ILE:HA	1:F:602:MET:HE3	1.55	0.87
1:D:10:ARG:HH12	2:E:1101:LMT:H5'	1.39	0.86
1:E:678:PRO:HG2	1:E:682:LEU:HD21	1.58	0.86
1:B:728:GLN:NE2	1:B:730:ASN:OD1	2.08	0.85
1:D:586:LEU:HD13	1:D:595:THR:HG22	1.58	0.85
1:F:791:ASP:HB2	1:F:794:LEU:HD12	1.59	0.85
1:D:583:PHE:CE1	1:D:672:ALA:HB3	2.12	0.84
1:F:736:VAL:HG11	1:F:757:MET:HE1	1.57	0.84
1:E:698:VAL:HG13	1:E:702:ARG:HB3	1.58	0.84
1:F:189:VAL:HB	1:F:780:VAL:HG23	1.60	0.83
1:F:167:ARG:NH2	1:F:315:GLU:OE2	2.12	0.83
1:E:640:LYS:O	1:E:645:ARG:NH1	2.11	0.83
1:E:728:GLN:NE2	1:E:730:ASN:OD1	2.11	0.83
1:F:32:LEU:HD13	1:F:393:ILE:HD11	1.60	0.82
1:A:791:ASP:HB2	1:A:794:LEU:HD12	1.61	0.82
1:C:281:ARG:HB2	1:C:619:PRO:HG2	1.61	0.82
1:F:864:LYS:HD2	1:F:865:PHE:H	1.46	0.81
1:F:598:VAL:HG12	1:F:602:MET:HE2	1.62	0.81
1:F:793:ILE:HG21	1:F:814:VAL:HG21	1.63	0.80
1:C:1010:MET:HB3	1:C:1014:VAL:HG13	1.63	0.80
1:F:101:ASP:H	1:F:104:LYS:HZ3	1.26	0.80
1:F:41:VAL:HA	1:F:682:LEU:HD23	1.63	0.80
1:F:1001:GLY:H	1:F:1004:ALA:HB3	1.47	0.80
1:B:644:GLN:HG3	1:B:645:ARG:H	1.47	0.80
1:C:873:GLN:OE1	1:C:873:GLN:N	2.12	0.80
1:F:458:LEU:HD11	1:F:940:MET:HG3	1.64	0.80
1:A:728:GLN:NE2	1:A:730:ASN:OD1	2.12	0.79
1:B:542:VAL:HG12	1:B:549:MET:HE3	1.64	0.79
1:D:516:VAL:HG13	1:D:517:LEU:HG	1.62	0.79
1:A:507:ASP:OD1	1:A:510:THR:OG1	2.01	0.79
1:C:586:LEU:HD13	1:C:595:THR:HG22	1.63	0.79
1:C:678:PRO:HD2	1:C:682:LEU:HD11	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1010:MET:O	1:C:1014:VAL:N	2.15	0.78
1:C:458:LEU:HD21	1:C:940:MET:HG3	1.66	0.78
1:A:645:ARG:HB2	1:A:650:LEU:HD22	1.65	0.78
1:C:276:SER:O	1:C:779:ARG:NH1	2.17	0.78
1:E:153:MET:HE3	1:E:182:ALA:HB2	1.64	0.78
1:A:599:ILE:HA	1:A:602:MET:HE2	1.64	0.78
1:E:70:GLN:HG3	1:E:116:ALA:HB2	1.64	0.78
1:B:101:ASP:H	1:B:104:LYS:HE2	1.49	0.77
1:E:576:ASP:OD2	1:E:645:ARG:NH2	2.17	0.77
1:A:546:LYS:H	1:A:546:LYS:HD3	1.48	0.77
1:B:646:HIS:HA	1:B:650:LEU:HD22	1.67	0.76
1:F:122:GLU:H	1:F:122:GLU:CD	1.94	0.76
1:B:789:ARG:NH1	1:B:791:ASP:H	1.83	0.76
1:E:67:LEU:HD22	1:E:113:VAL:HG22	1.66	0.76
1:C:164:VAL:HG13	1:C:313:MET:HE1	1.67	0.76
1:B:167:ARG:HD2	1:B:170:ARG:HH21	1.50	0.76
1:C:760:TYR:HD1	1:C:782:ALA:HB2	1.50	0.76
1:D:583:PHE:CZ	1:D:672:ALA:HB3	2.22	0.75
1:B:45:VAL:HG13	1:B:106:THR:HG22	1.67	0.75
1:A:141:VAL:HG22	1:A:330:TYR:HB3	1.65	0.75
1:A:283:LEU:HB2	1:A:617:ALA:HB3	1.69	0.75
1:B:366:ARG:NH1	1:B:507:ASP:OD2	2.21	0.74
1:E:283:LEU:HB2	1:E:617:ALA:HB3	1.70	0.74
1:C:67:LEU:HD22	1:C:113:VAL:HG22	1.67	0.74
1:C:965:LYS:HB3	1:C:969:GLU:HG3	1.69	0.74
1:C:446:ALA:O	1:C:450:THR:HG23	1.87	0.74
1:D:187:MET:HE1	1:D:246:GLU:HG3	1.70	0.74
1:A:797:LYS:HE2	1:A:807:PRO:HG3	1.70	0.74
1:D:594:ARG:NH2	1:F:232:PRO:O	2.19	0.74
1:E:228:LEU:HD11	1:F:785:PRO:HA	1.70	0.74
1:C:714:ALA:HA	1:C:854:ILE:HD13	1.71	0.73
1:B:789:ARG:NH2	1:B:791:ASP:HB2	2.03	0.73
1:A:737:ASP:HB3	1:A:813:THR:HG23	1.68	0.73
1:B:265:LEU:HG	1:B:271:ILE:HD11	1.67	0.73
1:F:446:ALA:O	1:F:450:THR:HG23	1.89	0.73
1:D:842:TYR:HB3	1:D:846:GLN:HE21	1.53	0.73
1:B:571:PHE:HD1	1:B:572:VAL:HG12	1.54	0.72
1:F:464:LEU:HD23	1:F:571:PHE:CZ	2.24	0.72
1:D:154:THR:HG23	1:D:183:GLY:O	1.90	0.72
1:A:154:THR:HG23	1:A:183:GLY:O	1.89	0.72
1:D:102:PRO:O	1:D:106:THR:HG23	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:LEU:HG	1:D:271:ILE:HD11	1.72	0.71
1:F:799:ARG:HE	1:F:805:MET:HE1	1.55	0.71
1:A:265:LEU:HG	1:A:271:ILE:HD11	1.70	0.71
1:F:711:ILE:HG12	1:F:723:LEU:HD23	1.73	0.71
1:F:980:ARG:HG2	1:F:984:MET:HE2	1.72	0.71
1:D:375:VAL:HG22	1:D:408:VAL:HG12	1.72	0.71
1:C:45:VAL:HG13	1:C:106:THR:HG22	1.73	0.71
1:F:57:LYS:HE2	1:F:700:TYR:CZ	2.26	0.71
1:F:103:ASP:OD1	1:F:133:LYS:NZ	2.22	0.71
1:D:843:SER:N	1:D:846:GLN:HE22	1.88	0.71
1:F:645:ARG:HB2	1:F:650:LEU:HB3	1.73	0.71
1:C:405:ILE:O	1:C:409:VAL:HG12	1.91	0.70
1:F:997:VAL:HG23	1:F:1011:GLY:HA3	1.72	0.70
1:A:22:LEU:HD13	1:A:377:VAL:HG22	1.73	0.70
1:A:560:THR:HG22	1:A:918:LEU:HB2	1.72	0.70
1:E:945:LEU:HD11	1:E:989:PHE:HE2	1.56	0.70
1:B:707:THR:HG21	1:B:832:ALA:HB3	1.74	0.70
1:E:571:PHE:HD2	1:E:572:VAL:HG12	1.56	0.69
1:A:678:PRO:HG2	1:A:682:LEU:HD21	1.72	0.69
1:D:205:ASP:OD2	1:D:799:ARG:NH2	2.24	0.69
1:A:242:ARG:NH1	1:A:770:ASN:OD1	2.25	0.69
1:A:766:VAL:HG13	1:A:778:VAL:HG23	1.73	0.69
1:C:426:GLY:HA2	1:C:502:HIS:HD2	1.57	0.69
1:F:766:VAL:HG13	1:F:778:VAL:HG23	1.75	0.69
1:C:191:LEU:HD23	1:C:269:ALA:HB2	1.74	0.69
1:B:5:LYS:HD3	1:B:434:TYR:CE1	2.28	0.68
1:C:408:VAL:HG22	1:C:483:SER:HB2	1.75	0.68
1:E:446:ALA:HB2	2:E:1101:LMT:H41	1.75	0.68
1:E:678:PRO:HD2	1:E:682:LEU:HD11	1.74	0.68
1:A:794:LEU:HD22	1:A:809:SER:HA	1.75	0.68
1:C:153:MET:HE1	1:C:281:ARG:HB3	1.74	0.68
1:B:808:LEU:HD22	1:B:811:LEU:HD11	1.74	0.68
1:C:167:ARG:NH2	1:C:315:GLU:OE2	2.26	0.68
1:C:207:VAL:HG21	1:C:759:ILE:HD13	1.75	0.68
1:C:852:GLU:HG2	1:C:865:PHE:HZ	1.58	0.68
1:B:789:ARG:CZ	1:B:791:ASP:HB2	2.23	0.68
1:C:168:LEU:HD21	1:C:313:MET:HE3	1.74	0.68
1:E:217:VAL:HG11	1:F:754:PHE:CD2	2.28	0.68
1:F:417:GLU:HG3	1:F:984:MET:HE1	1.76	0.68
1:C:760:TYR:CD1	1:C:782:ALA:HB2	2.28	0.68
1:D:845:GLY:O	1:D:848:GLN:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:469:TYR:OH	1:D:936:GLN:OE1	2.13	0.67
1:F:405:ILE:O	1:F:409:VAL:HG12	1.94	0.67
1:E:196:VAL:HG22	1:E:268:ILE:HG13	1.76	0.67
1:A:900:TYR:HE1	1:A:955:GLU:HG2	1.57	0.67
1:B:191:LEU:HD23	1:B:269:ALA:HB2	1.76	0.67
1:B:698:VAL:HG12	1:B:702:ARG:HB2	1.75	0.67
1:E:205:ASP:OD2	1:E:799:ARG:NH2	2.27	0.67
1:F:217:VAL:HG21	1:F:239:ALA:HB3	1.74	0.67
1:C:257:ALA:N	1:C:261:GLY:O	2.19	0.67
1:A:346:THR:HG21	1:A:402:VAL:HG13	1.76	0.67
1:E:978:ARG:O	1:E:981:PRO:HD2	1.94	0.67
1:A:201:LEU:HD21	1:A:255:LYS:HB2	1.76	0.67
1:A:310:ARG:NH1	1:A:331:ASP:OD2	2.27	0.67
1:E:49:ALA:HB2	1:E:129:ILE:HD12	1.76	0.67
1:D:189:VAL:HB	1:D:780:VAL:HG23	1.76	0.67
1:B:765:TYR:CE1	1:B:777:GLN:HG2	2.30	0.67
1:C:761:LEU:HD11	1:C:793:ILE:HG13	1.77	0.67
1:D:141:VAL:HG23	1:D:329:VAL:HG23	1.77	0.67
1:F:164:VAL:HG13	1:F:313:MET:HE1	1.77	0.67
1:F:464:LEU:HD23	1:F:571:PHE:HZ	1.59	0.67
1:A:362:LEU:HG	1:A:420:GLU:HG2	1.76	0.67
1:A:411:ASP:OD1	1:A:948:LYS:NZ	2.25	0.67
1:C:102:PRO:O	1:C:106:THR:HG23	1.94	0.66
1:D:242:ARG:NH1	1:D:770:ASN:OD1	2.28	0.66
1:A:917:ILE:HD13	1:A:939:LEU:HD12	1.76	0.66
1:F:408:VAL:HG22	1:F:483:SER:HB2	1.76	0.66
1:D:698:VAL:HG12	1:D:702:ARG:HB2	1.77	0.66
1:F:70:GLN:O	1:F:112:ARG:NH1	2.26	0.66
1:F:958:ARG:HH22	2:F:1101:LMT:H6D	1.61	0.66
1:B:783:ASP:HB3	1:B:786:PHE:HD1	1.58	0.66
1:D:582:ALA:HB3	1:D:635:VAL:HG13	1.77	0.66
1:B:799:ARG:HD3	1:B:803:GLY:HA2	1.77	0.66
1:A:940:MET:HA	1:A:940:MET:HE2	1.77	0.66
1:B:2:ASN:HB2	1:B:5:LYS:HB2	1.78	0.66
1:D:546:LYS:H	1:D:546:LYS:HD3	1.59	0.66
1:E:375:VAL:HG22	1:E:408:VAL:HG12	1.78	0.66
1:F:146:SER:HB3	1:F:288:PRO:HG2	1.77	0.66
1:B:101:ASP:HB3	1:B:104:LYS:HG2	1.77	0.66
1:C:284:LEU:HD21	1:C:327:ARG:HD2	1.78	0.66
1:D:599:ILE:HA	1:D:602:MET:HE2	1.76	0.66
1:F:794:LEU:HD22	1:F:809:SER:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ILE:HD13	1:A:948:LYS:HZ3	1.62	0.65
1:A:736:VAL:HG22	1:A:814:VAL:HG22	1.77	0.65
1:A:359:ILE:HG23	1:A:513:MET:HE3	1.77	0.65
1:F:1001:GLY:H	1:F:1004:ALA:CB	2.09	0.65
1:A:973:GLU:O	1:A:977:LEU:HD23	1.96	0.65
1:B:167:ARG:HD2	1:B:170:ARG:NH2	2.11	0.65
1:C:682:LEU:HD13	1:C:685:LEU:HG	1.77	0.65
1:D:443:PRO:HG3	1:D:955:GLU:HG2	1.77	0.65
1:F:70:GLN:OE1	1:F:115:GLN:NE2	2.27	0.65
1:F:771:ARG:O	1:F:774:ARG:HB2	1.97	0.65
1:E:643:ASP:OD1	1:E:643:ASP:N	2.30	0.65
1:A:472:PHE:HB3	1:A:937:ILE:HG12	1.79	0.64
1:D:843:SER:H	1:D:846:GLN:HE22	1.45	0.64
1:F:197:ALA:HB1	1:F:797:LYS:HD2	1.79	0.64
1:F:453:ALA:O	1:F:888:SER:HB2	1.97	0.64
1:E:74:VAL:CG2	1:E:108:LEU:HD13	2.28	0.64
1:F:860:PRO:O	1:F:863:VAL:HG12	1.97	0.64
1:E:571:PHE:CD2	1:E:572:VAL:HG12	2.32	0.64
1:A:707:THR:HG21	1:A:832:ALA:HB3	1.79	0.64
1:B:205:ASP:OD2	1:B:799:ARG:NH2	2.30	0.64
1:C:546:LYS:HD3	1:C:546:LYS:H	1.63	0.64
1:E:698:VAL:HG22	1:E:702:ARG:NE	2.12	0.64
1:F:326:TYR:O	1:F:327:ARG:HD2	1.98	0.64
1:F:521:PHE:O	1:F:525:ASN:ND2	2.31	0.64
1:B:67:LEU:HD22	1:B:113:VAL:HG22	1.80	0.64
1:E:362:LEU:HG	1:E:420:GLU:HG2	1.79	0.64
1:E:411:ASP:OD1	1:E:948:LYS:NZ	2.22	0.64
1:F:576:ASP:OD2	1:F:645:ARG:NH2	2.31	0.64
1:B:987:ILE:HG22	1:B:991:MET:HE2	1.79	0.64
1:C:731:VAL:HG12	1:C:819:GLY:O	1.97	0.64
1:A:645:ARG:HB2	1:A:650:LEU:CD2	2.28	0.63
1:E:942:LEU:HD12	1:E:1021:VAL:HG21	1.80	0.63
1:D:196:VAL:HB	1:D:268:ILE:HD11	1.80	0.63
1:F:728:GLN:NE2	1:F:730:ASN:OD1	2.31	0.63
1:F:1018:MET:O	1:F:1022:THR:HG23	1.98	0.63
1:C:106:THR:HG21	1:C:133:LYS:HB3	1.80	0.63
1:E:157:ARG:HD2	1:E:182:ALA:O	1.97	0.63
1:A:189:VAL:CG2	1:A:780:VAL:HG22	2.28	0.63
1:B:417:GLU:OE2	1:B:980:ARG:NH1	2.31	0.63
1:F:588:ASN:HB3	1:F:731:VAL:HG23	1.80	0.63
1:B:958:ARG:NH1	1:B:959:GLU:OE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:VAL:O	1:F:113:VAL:HG23	1.99	0.63
1:B:794:LEU:HD22	1:B:809:SER:HA	1.80	0.63
1:C:534:ASN:OD1	1:C:535:TYR:N	2.32	0.63
1:D:148:ASN:OD1	1:D:150:SER:OG	2.13	0.63
1:A:923:GLY:O	1:A:927:THR:HG23	1.99	0.62
1:C:32:LEU:HD13	1:C:393:ILE:HD11	1.81	0.62
1:E:465:THR:HG23	1:E:571:PHE:HE1	1.63	0.62
1:F:768:ASP:HA	1:F:776:TYR:O	1.99	0.62
1:A:763:SER:HA	1:A:780:VAL:O	1.99	0.62
1:D:5:LYS:HG3	1:D:434:TYR:CE1	2.34	0.62
1:A:719:GLU:OE1	1:A:850:ALA:HB2	1.99	0.62
1:C:868:THR:HG23	1:C:869:ASP:HB2	1.81	0.62
1:D:575:GLN:HE22	1:D:1005:GLU:HB3	1.65	0.62
1:A:106:THR:OG1	1:A:133:LYS:HB2	1.99	0.62
1:F:713:ARG:HG3	1:F:854:ILE:HD12	1.82	0.62
1:F:772:PHE:O	1:F:774:ARG:HG2	1.99	0.62
1:A:228:LEU:HG	1:A:229:PRO:HD3	1.81	0.62
1:B:117:LEU:HA	1:B:120:LEU:HD23	1.82	0.62
1:D:203:ALA:O	1:D:206:VAL:HG12	1.99	0.62
1:E:707:THR:HG21	1:E:832:ALA:HB3	1.80	0.62
1:D:842:TYR:HB3	1:D:846:GLN:NE2	2.15	0.62
1:E:153:MET:HE1	1:E:281:ARG:HG2	1.82	0.62
1:F:199:ARG:HG2	1:F:199:ARG:HH11	1.65	0.62
1:A:599:ILE:HD13	1:A:602:MET:HE1	1.81	0.61
1:B:776:TYR:O	1:B:777:GLN:HB2	1.97	0.61
1:B:907:LEU:HB3	1:B:911:LEU:HD23	1.82	0.61
1:D:191:LEU:HD23	1:D:269:ALA:HB2	1.82	0.61
1:D:472:PHE:HB3	1:D:937:ILE:HG12	1.81	0.61
1:E:864:LYS:HG3	1:E:865:PHE:H	1.64	0.61
1:A:72:ASN:HA	1:A:77:MET:HE1	1.83	0.61
1:D:999:SER:HB2	1:D:1004:ALA:HB2	1.82	0.61
1:A:690:MET:HE2	1:A:865:PHE:CD2	2.35	0.61
1:A:790:ALA:O	1:A:793:ILE:HB	2.00	0.61
1:E:32:LEU:HD13	1:E:393:ILE:HD11	1.83	0.61
1:F:187:MET:HE3	1:F:187:MET:HA	1.82	0.61
1:B:715:GLN:OE1	1:B:715:GLN:N	2.33	0.61
1:E:737:ASP:O	1:E:812:VAL:HA	2.00	0.61
1:A:437:MET:HA	1:A:437:MET:HE3	1.83	0.61
1:B:307:ASP:OD2	2:B:1102:LMT:H4B	2.01	0.61
1:A:205:ASP:OD2	1:A:799:ARG:NH2	2.32	0.61
1:A:366:ARG:HA	1:A:369:ILE:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:715:GLN:N	1:E:715:GLN:OE1	2.33	0.61
1:F:228:LEU:HG	1:F:229:PRO:HD3	1.83	0.60
1:B:166:ASP:HB3	1:B:170:ARG:NH1	2.16	0.60
1:C:730:ASN:HA	1:C:818:PHE:HB3	1.82	0.60
1:C:854:ILE:O	1:C:858:THR:HG23	2.01	0.60
1:D:193:PRO:HA	1:D:196:VAL:HG13	1.84	0.60
1:D:213:GLN:NE2	1:D:252:ILE:HA	2.16	0.60
1:B:301:ASN:ND2	2:B:1102:LMT:H2'	2.09	0.60
1:B:388:LEU:HD23	1:B:389:PHE:CE1	2.36	0.60
1:C:738:LEU:HA	1:C:812:VAL:HG12	1.82	0.60
1:E:107:GLN:CD	1:F:107:GLN:HG3	2.26	0.60
1:E:527:VAL:O	1:E:530:ARG:HB3	2.01	0.60
1:A:84:ALA:O	1:A:822:MET:HA	2.02	0.60
1:D:213:GLN:HE22	1:D:252:ILE:HA	1.66	0.60
1:F:228:LEU:HD23	1:F:228:LEU:H	1.65	0.60
1:F:358:VAL:HG13	1:F:362:LEU:HD22	1.83	0.60
2:B:1101:LMT:H1B	2:B:1101:LMT:H6E	1.83	0.60
1:C:516:VAL:HG13	1:C:517:LEU:HG	1.83	0.60
1:D:763:SER:HB3	1:D:781:GLN:CD	2.25	0.60
1:A:444:ILE:HG21	1:A:488:LEU:HD13	1.84	0.60
1:A:980:ARG:O	1:A:984:MET:HG3	2.01	0.60
1:B:969:GLU:HA	1:B:972:VAL:HG22	1.84	0.60
1:A:67:LEU:HD22	1:A:113:VAL:HG23	1.83	0.60
1:A:844:SER:N	1:A:846:GLN:HE22	2.00	0.60
1:B:143:HIS:CD2	1:B:329:VAL:HG21	2.36	0.60
1:B:980:ARG:O	1:B:984:MET:HG3	2.01	0.60
1:D:453:ALA:O	1:D:888:SER:HB2	2.01	0.60
1:F:981:PRO:HA	1:F:984:MET:HE3	1.84	0.60
1:B:10:ARG:NH1	2:C:1101:LMT:O6'	2.35	0.59
1:C:599:ILE:HA	1:C:602:MET:HE2	1.82	0.59
1:D:738:LEU:HD13	1:D:812:VAL:HG12	1.84	0.59
1:B:599:ILE:HA	1:B:602:MET:HE2	1.83	0.59
1:B:884:VAL:HG12	1:B:885:PHE:HD1	1.66	0.59
1:D:12:ILE:HD13	1:E:903:LEU:HG	1.84	0.59
1:F:730:ASN:HA	1:F:818:PHE:HB3	1.84	0.59
1:B:965:LYS:HB3	1:B:969:GLU:HG3	1.84	0.59
1:C:116:ALA:HA	1:C:119:ARG:NH2	2.16	0.59
1:F:256:THR:HG22	1:F:262:VAL:HG12	1.84	0.59
1:B:511:ARG:HD2	1:B:515:ARG:NH2	2.17	0.59
1:F:500:LYS:HD3	1:F:504:ASP:HB3	1.83	0.59
1:A:430:ARG:HG2	1:A:434:TYR:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:LYS:H	1:B:546:LYS:HD3	1.66	0.59
1:E:760:TYR:HD1	1:E:782:ALA:HB2	1.66	0.59
1:B:217:VAL:HG21	1:B:239:ALA:HB3	1.84	0.59
1:B:783:ASP:HB3	1:B:786:PHE:CD1	2.37	0.59
1:A:117:LEU:HA	1:A:120:LEU:HD23	1.85	0.59
1:D:447:ILE:HD13	1:D:948:LYS:HG2	1.84	0.59
1:D:576:ASP:OD2	1:D:645:ARG:NH2	2.35	0.59
1:C:310:ARG:HG2	1:C:328:ILE:HD13	1.84	0.59
1:D:458:LEU:HD21	1:D:940:MET:HG3	1.85	0.59
1:B:108:LEU:O	1:B:112:ARG:HG2	2.03	0.59
1:B:168:LEU:HD11	1:B:313:MET:HE1	1.85	0.59
1:B:207:VAL:HG21	1:B:759:ILE:HD13	1.84	0.59
1:F:350:ALA:HA	1:F:353:LEU:HD12	1.84	0.59
1:E:691:GLN:HG3	1:E:826:TYR:CG	2.38	0.58
1:D:68:GLU:OE2	1:D:825:ARG:NE	2.31	0.58
1:E:1004:ALA:HB1	1:E:1007:ARG:HD2	1.85	0.58
1:F:179:LEU:HD21	1:F:292:MET:HE3	1.85	0.58
1:F:763:SER:HB3	1:F:781:GLN:CD	2.28	0.58
1:D:789:ARG:HD2	1:D:791:ASP:OD1	2.02	0.58
1:F:456:VAL:HG22	1:F:457:PRO:HD3	1.86	0.58
1:E:921:LEU:HD13	1:E:939:LEU:HD21	1.86	0.58
1:A:9:ASP:OD1	1:A:434:TYR:OH	2.17	0.58
1:E:405:ILE:O	1:E:409:VAL:HG13	2.03	0.58
1:F:251:ASP:OD1	1:F:266:ARG:NH2	2.35	0.58
1:C:71:ILE:O	1:C:74:VAL:HG22	2.04	0.58
1:D:145:ILE:HD12	1:D:284:LEU:HD23	1.86	0.58
1:F:244:GLN:HG3	1:F:245:ASN:HD22	1.67	0.58
1:B:23:LEU:HD11	1:C:887:ILE:HD13	1.85	0.58
1:C:588:ASN:HB3	1:C:731:VAL:HG23	1.85	0.58
1:D:141:VAL:HG22	1:D:330:TYR:HB3	1.85	0.58
1:D:919:SER:OG	1:D:1020:GLY:HA3	2.04	0.58
1:E:343:VAL:HG21	1:E:398:LEU:HB3	1.86	0.58
1:E:546:LYS:HE2	1:E:547:ALA:H	1.69	0.58
1:E:864:LYS:HG3	1:E:865:PHE:N	2.18	0.58
1:C:126:ARG:NH2	1:C:766:VAL:O	2.36	0.58
1:C:453:ALA:O	1:C:888:SER:HB2	2.04	0.58
1:E:516:VAL:HG13	1:E:517:LEU:HG	1.84	0.58
1:B:529:HIS:O	1:B:533:GLU:OE1	2.22	0.58
1:A:641:PRO:O	1:A:645:ARG:HG2	2.03	0.57
1:B:72:ASN:HA	1:B:77:MET:HE1	1.86	0.57
1:B:939:LEU:O	1:B:943:VAL:HG13	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:500:LYS:NZ	1:E:505:LYS:HD3	2.19	0.57
1:A:707:THR:O	1:A:711:ILE:HG13	2.04	0.57
1:B:344:VAL:O	1:B:348:LEU:HD22	2.05	0.57
1:D:38:PRO:O	1:D:40:VAL:HG22	2.04	0.57
1:A:157:ARG:HD2	1:A:182:ALA:O	2.03	0.57
1:A:217:VAL:HG21	1:A:239:ALA:HB3	1.86	0.57
1:B:749:ASN:CG	1:B:751:THR:HG22	2.29	0.57
1:C:736:VAL:HG22	1:C:814:VAL:HG22	1.87	0.57
1:D:207:VAL:HG11	1:D:759:ILE:HD13	1.85	0.57
1:E:105:ALA:O	1:E:109:VAL:HG12	2.04	0.57
1:A:229:PRO:HD2	1:A:231:THR:OG1	2.03	0.57
1:D:939:LEU:O	1:D:943:VAL:HG12	2.04	0.57
1:A:123:ASP:N	1:A:123:ASP:OD1	2.36	0.57
1:A:921:LEU:HA	1:A:924:VAL:HG13	1.87	0.57
1:E:16:VAL:HG13	1:F:894:LEU:HB3	1.87	0.57
1:E:40:VAL:HG11	1:E:468:PHE:CE1	2.40	0.57
1:F:968:PHE:O	1:F:972:VAL:HG23	2.04	0.57
1:A:313:MET:HB3	1:A:326:TYR:CE2	2.40	0.57
1:A:338:SER:HB3	1:A:1002:ALA:HB2	1.86	0.57
1:B:651:SER:O	1:B:655:ILE:HG12	2.04	0.57
1:C:1028:LEU:HD22	1:C:1032:PHE:CE2	2.40	0.57
1:F:35:SER:O	1:F:394:ASN:HA	2.04	0.57
1:F:942:LEU:CD1	1:F:1017:GLY:HA3	2.35	0.57
1:A:720:LEU:O	1:A:839:ALA:HB2	2.05	0.57
1:B:56:PRO:HB2	1:B:823:VAL:HG23	1.87	0.57
1:E:719:GLU:HG2	1:E:720:LEU:HD22	1.86	0.57
1:F:698:VAL:HG22	1:F:702:ARG:CZ	2.34	0.57
1:B:343:VAL:O	1:B:346:THR:HG22	2.04	0.57
1:B:408:VAL:HG22	1:B:483:SER:HB2	1.85	0.57
1:B:1004:ALA:HA	1:B:1007:ARG:HD3	1.86	0.57
1:C:158:ASN:O	1:C:162:ILE:HG12	2.04	0.57
1:C:509:LEU:HA	1:C:512:VAL:HG12	1.86	0.57
1:E:888:SER:O	1:E:892:VAL:HG13	2.05	0.57
1:E:1037:ARG:HH12	1:E:1041:GLY:HA3	1.70	0.57
1:F:211:ARG:HG3	1:F:766:VAL:HG23	1.86	0.57
1:F:791:ASP:C	1:F:793:ILE:N	2.62	0.57
1:C:403:LEU:HB3	1:C:941:VAL:HG21	1.87	0.56
1:E:742:LYS:HA	1:E:745:GLN:NE2	2.20	0.56
1:B:843:SER:O	1:B:846:GLN:NE2	2.38	0.56
1:E:72:ASN:HA	1:E:77:MET:HE1	1.86	0.56
1:E:180:TRP:HB2	1:E:291:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:692:ILE:HD12	1:F:707:THR:HG23	1.87	0.56
1:F:966:THR:HG23	1:F:968:PHE:H	1.69	0.56
1:D:535:TYR:OH	1:D:975:SER:HB2	2.05	0.56
1:F:738:LEU:HD23	1:F:812:VAL:HG12	1.87	0.56
1:A:343:VAL:HG21	1:A:398:LEU:HB3	1.88	0.56
1:F:370:ILE:HD12	1:F:494:LEU:HB3	1.86	0.56
1:A:189:VAL:HG22	1:A:780:VAL:HG22	1.86	0.56
1:B:228:LEU:H	1:B:228:LEU:HD22	1.70	0.56
1:C:958:ARG:NH2	2:C:1101:LMT:O5B	2.36	0.56
1:D:917:ILE:HD12	1:D:939:LEU:HD23	1.87	0.56
1:A:729:ILE:HG22	1:A:820:PRO:HB3	1.86	0.56
1:C:321:PRO:O	1:C:324:VAL:HG12	2.06	0.56
1:C:853:ARG:O	1:C:857:GLN:HG2	2.06	0.56
1:B:763:SER:HB3	1:B:781:GLN:CD	2.31	0.56
1:B:868:THR:HG23	1:B:868:THR:O	2.04	0.56
1:D:153:MET:HE1	1:D:281:ARG:HG2	1.87	0.56
1:D:915:MET:HB3	1:D:1024:PHE:CD2	2.41	0.56
1:E:45:VAL:HG11	1:E:109:VAL:HG11	1.87	0.56
1:F:350:ALA:O	1:F:354:VAL:HG13	2.06	0.56
1:A:513:MET:HE2	1:A:521:PHE:CE2	2.41	0.56
1:D:70:GLN:HG3	1:D:116:ALA:HB2	1.88	0.56
1:B:472:PHE:HB3	1:B:937:ILE:HG12	1.88	0.56
1:E:40:VAL:HG11	1:E:468:PHE:HE1	1.70	0.56
1:E:763:SER:HB3	1:E:781:GLN:CD	2.30	0.56
1:B:375:VAL:HG22	1:B:408:VAL:HG12	1.87	0.55
1:A:763:SER:HB3	1:A:781:GLN:CD	2.32	0.55
1:B:640:LYS:O	1:B:646:HIS:NE2	2.39	0.55
1:D:838:PRO:O	1:D:842:TYR:HB2	2.06	0.55
1:E:7:PHE:HB3	1:E:14:ALA:HB2	1.87	0.55
2:A:1101:LMT:H91	1:B:457:PRO:HG3	1.87	0.55
1:B:335:PHE:CE2	1:B:577:LYS:HE2	2.42	0.55
1:B:838:PRO:HB2	1:B:842:TYR:HB2	1.89	0.55
1:C:838:PRO:HB3	1:C:847:ALA:HB2	1.87	0.55
1:A:446:ALA:O	1:A:450:THR:HG23	2.07	0.55
1:C:663:TYR:HA	1:C:666:LEU:HD22	1.87	0.55
1:A:791:ASP:O	1:A:794:LEU:N	2.40	0.55
1:C:940:MET:O	1:C:943:VAL:HG22	2.06	0.55
1:D:811:LEU:HD12	1:D:812:VAL:HG13	1.88	0.55
1:A:444:ILE:O	1:A:447:ILE:HG13	2.06	0.55
1:A:5:LYS:HD3	1:A:434:TYR:CD1	2.42	0.55
1:D:599:ILE:HD13	1:D:602:MET:HE1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:VAL:HG22	1:E:268:ILE:CG1	2.36	0.55
1:B:106:THR:HG21	1:B:133:LYS:HB3	1.88	0.55
1:B:516:VAL:HG13	1:B:517:LEU:HG	1.87	0.55
1:D:310:ARG:NH1	1:D:331:ASP:OD2	2.40	0.55
1:E:192:ASP:O	1:E:196:VAL:HG23	2.07	0.55
1:A:596:GLU:OE2	1:A:600:ARG:NE	2.33	0.55
1:A:859:LEU:HB3	1:A:863:VAL:O	2.07	0.55
1:B:70:GLN:HB2	1:B:116:ALA:HB2	1.88	0.55
1:D:9:ASP:OD1	1:D:434:TYR:OH	2.20	0.55
1:E:189:VAL:HG22	1:E:780:VAL:HG12	1.89	0.55
1:E:472:PHE:HB3	1:E:937:ILE:HG12	1.88	0.55
1:A:691:GLN:HG3	1:A:826:TYR:CG	2.42	0.54
1:C:22:LEU:HG	1:C:26:MET:HE2	1.89	0.54
1:C:640:LYS:HD3	1:C:644:GLN:HG2	1.89	0.54
1:D:205:ASP:CG	1:D:799:ARG:HH22	2.15	0.54
1:D:946:SER:HB3	1:D:1021:VAL:HG22	1.88	0.54
1:F:207:VAL:HG23	1:F:766:VAL:HB	1.89	0.54
1:B:762:GLY:O	1:B:763:SER:OG	2.24	0.54
1:D:429:ALA:HB2	1:D:500:LYS:HA	1.88	0.54
1:E:154:THR:HG21	1:E:275:ALA:HB2	1.88	0.54
1:F:863:VAL:O	1:F:863:VAL:HG13	2.07	0.54
1:A:185:TYR:HB2	1:A:776:TYR:CE2	2.42	0.54
1:B:556:LEU:HB2	1:B:915:MET:HE1	1.90	0.54
1:D:191:LEU:HD11	1:D:206:VAL:HG11	1.89	0.54
1:D:389:PHE:CD2	1:D:474:MET:HE3	2.42	0.54
1:E:74:VAL:HG12	1:E:77:MET:HE3	1.90	0.54
1:E:650:LEU:O	1:E:655:ILE:HG13	2.06	0.54
1:B:276:SER:O	1:B:779:ARG:NH1	2.41	0.54
1:B:912:ILE:HD11	1:B:1028:LEU:HB3	1.88	0.54
1:F:229:PRO:HD2	1:F:231:THR:OG1	2.08	0.54
1:F:990:ILE:HD11	1:F:1018:MET:HB3	1.89	0.54
1:A:645:ARG:HH12	1:A:651:SER:HA	1.73	0.54
1:C:105:ALA:O	1:C:109:VAL:HG13	2.07	0.54
1:C:179:LEU:HD21	1:C:292:MET:HE3	1.90	0.54
1:D:437:MET:SD	1:D:492:PRO:HB3	2.48	0.54
1:E:704:ALA:HB2	1:E:727:TYR:HE2	1.73	0.54
1:F:772:PHE:HD2	1:F:774:ARG:HG3	1.73	0.54
1:A:72:ASN:HD21	1:C:170:ARG:HH21	1.55	0.54
1:C:997:VAL:HG12	1:C:998:LEU:HD12	1.90	0.54
1:D:144:LEU:HD12	1:D:160:ALA:HB2	1.90	0.54
1:D:217:VAL:HG21	1:D:239:ALA:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:ASN:HB3	1:F:58:VAL:HG23	1.90	0.54
1:F:966:THR:HG22	1:F:969:GLU:HG2	1.88	0.54
1:A:731:VAL:HG12	1:A:819:GLY:O	2.07	0.54
1:B:855:ALA:HA	1:B:858:THR:HG22	1.90	0.54
1:C:530:ARG:NH2	3:C:1201:HOH:O	2.39	0.54
1:F:45:VAL:HG11	1:F:109:VAL:HG21	1.90	0.54
1:F:353:LEU:HD22	1:F:991:MET:HE3	1.90	0.54
1:A:579:TYR:CZ	1:A:676:PRO:HB3	2.43	0.53
1:D:141:VAL:HG23	1:D:329:VAL:CG2	2.38	0.53
1:F:403:LEU:HD13	1:F:941:VAL:HG21	1.90	0.53
1:A:913:VAL:HG22	1:A:914:PRO:HD3	1.90	0.53
1:B:640:LYS:HE3	1:B:645:ARG:HH12	1.73	0.53
1:B:966:THR:HG22	1:B:969:GLU:HG2	1.89	0.53
1:C:838:PRO:HB2	1:C:842:TYR:HB2	1.89	0.53
1:C:932:ASN:OD1	1:C:934:PHE:HB2	2.09	0.53
1:D:789:ARG:HD3	1:D:791:ASP:H	1.73	0.53
1:E:776:TYR:O	1:E:777:GLN:HB2	2.07	0.53
1:F:760:TYR:CD2	1:F:796:LEU:HD22	2.44	0.53
1:A:690:MET:SD	1:A:834:VAL:HB	2.49	0.53
1:B:932:ASN:OD1	1:B:934:PHE:HB2	2.08	0.53
1:C:472:PHE:HB3	1:C:937:ILE:HG12	1.90	0.53
1:C:878:GLY:O	1:C:880:SER:N	2.41	0.53
1:D:449:LEU:HD12	2:D:1101:LMT:H61	1.90	0.53
1:A:842:TYR:HD2	1:A:846:GLN:HG3	1.73	0.53
1:B:359:ILE:CD1	1:B:365:TRP:HA	2.38	0.53
1:E:48:LYS:O	1:E:90:MET:O	2.26	0.53
1:F:942:LEU:HD11	1:F:1017:GLY:HA3	1.90	0.53
1:B:736:VAL:HG13	1:B:812:VAL:HG13	1.91	0.53
1:C:317:LYS:HA	1:C:320:PHE:CG	2.43	0.53
1:C:742:LYS:HG3	1:C:745:GLN:HE21	1.72	0.53
1:D:724:PHE:CE1	1:D:835:ASN:HB2	2.43	0.53
1:F:398:LEU:O	1:F:402:VAL:HG13	2.08	0.53
1:A:513:MET:HE2	1:A:521:PHE:CZ	2.44	0.53
1:C:55:ASN:HB3	1:C:58:VAL:HG23	1.91	0.53
1:E:799:ARG:HB2	1:E:805:MET:HE3	1.91	0.53
1:F:691:GLN:HG3	1:F:831:ALA:HB1	1.90	0.53
1:F:1024:PHE:O	1:F:1028:LEU:HB2	2.08	0.53
1:A:74:VAL:HG12	1:A:77:MET:HE3	1.90	0.53
1:B:591:SER:OG	1:B:594:ARG:HG3	2.08	0.53
1:C:72:ASN:HA	1:C:77:MET:HE1	1.90	0.53
1:A:98:LEU:HD12	1:A:99:GLY:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:LEU:O	1:B:565:LYS:HG2	2.09	0.53
1:B:942:LEU:HD21	1:B:1017:GLY:HA3	1.91	0.53
1:E:645:ARG:HD2	1:E:650:LEU:HD21	1.90	0.53
1:A:516:VAL:HG13	1:A:517:LEU:HD13	1.90	0.53
1:C:677:PRO:HG2	1:C:680:LEU:HD23	1.91	0.53
1:D:704:ALA:O	1:D:708:ASN:ND2	2.39	0.53
1:E:74:VAL:HG22	1:E:108:LEU:HD13	1.90	0.53
1:A:587:PRO:HD3	1:A:668:ASP:O	2.09	0.53
1:C:763:SER:CB	1:C:781:GLN:HB2	2.38	0.53
1:E:455:PHE:O	1:E:458:LEU:HB2	2.09	0.53
1:E:783:ASP:O	1:E:787:ARG:HG2	2.08	0.53
1:F:375:VAL:HG22	1:F:408:VAL:HG12	1.91	0.53
1:B:843:SER:N	1:B:846:GLN:HE22	2.06	0.52
1:D:85:ASN:ND2	1:D:627:THR:HB	2.23	0.52
1:E:203:ALA:O	1:E:206:VAL:HG13	2.09	0.52
1:F:582:ALA:HB3	1:F:635:VAL:HG13	1.90	0.52
1:F:599:ILE:HD13	1:F:602:MET:HE1	1.90	0.52
1:A:113:VAL:O	1:A:117:LEU:HD13	2.09	0.52
1:D:659:LEU:HB3	1:D:673:VAL:HG21	1.91	0.52
1:D:989:PHE:HD2	1:D:1018:MET:HE3	1.74	0.52
1:B:808:LEU:CD2	1:B:811:LEU:HD11	2.40	0.52
1:C:535:TYR:CE1	1:C:1026:LEU:HB3	2.44	0.52
1:D:839:ALA:O	1:D:842:TYR:HD1	1.92	0.52
1:F:799:ARG:NE	1:F:805:MET:HE1	2.24	0.52
1:A:59:ILE:HB	1:A:84:ALA:HB1	1.91	0.52
1:A:703:LEU:O	1:A:707:THR:HG23	2.10	0.52
1:B:40:VAL:HG11	1:B:468:PHE:CE1	2.44	0.52
1:C:739:ASP:HB3	1:C:742:LYS:HB3	1.92	0.52
1:F:67:LEU:HD22	1:F:113:VAL:HG13	1.92	0.52
1:A:191:LEU:HD11	1:A:206:VAL:HG11	1.90	0.52
1:B:560:THR:OG1	1:B:918:LEU:HB2	2.09	0.52
1:C:599:ILE:HG21	1:C:619:PRO:HD3	1.91	0.52
1:D:730:ASN:HA	1:D:818:PHE:HB3	1.90	0.52
1:E:191:LEU:HD23	1:E:269:ALA:HB2	1.91	0.52
1:E:207:VAL:HG11	1:E:759:ILE:HD13	1.91	0.52
1:B:189:VAL:HB	1:B:780:VAL:HG12	1.91	0.52
1:C:70:GLN:HG3	1:C:116:ALA:HB2	1.91	0.52
1:C:527:VAL:O	1:C:530:ARG:HB3	2.10	0.52
1:D:723:LEU:HA	1:D:835:ASN:O	2.10	0.52
1:E:107:GLN:OE1	1:F:107:GLN:HG3	2.10	0.52
1:C:4:SER:O	1:C:8:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:SER:O	1:C:394:ASN:HA	2.10	0.52
1:C:343:VAL:HG21	1:C:398:LEU:HB3	1.91	0.52
1:C:391:TYR:CZ	1:C:474:MET:HG2	2.45	0.52
1:D:370:ILE:HD13	1:D:416:VAL:HG23	1.92	0.52
1:D:399:PHE:O	1:D:402:VAL:HG12	2.09	0.52
1:D:579:TYR:CZ	1:D:676:PRO:HB3	2.45	0.52
1:E:645:ARG:HB2	1:E:650:LEU:CD2	2.40	0.52
1:E:945:LEU:HD11	1:E:989:PHE:CE2	2.41	0.52
1:F:244:GLN:HG2	1:F:248:GLU:OE1	2.09	0.52
1:A:733:GLN:HB3	1:C:236:SER:O	2.10	0.52
1:C:980:ARG:O	1:C:984:MET:HG3	2.10	0.52
1:F:962:HIS:CE1	2:F:1101:LMT:H4B	2.44	0.52
1:C:38:PRO:CD	1:C:396:LEU:HD23	2.40	0.52
1:E:217:VAL:HG11	1:F:754:PHE:CG	2.45	0.52
1:E:417:GLU:OE2	1:E:980:ARG:NH1	2.36	0.52
1:E:510:THR:HA	1:E:513:MET:HE2	1.91	0.52
1:E:880:SER:C	1:E:882:PHE:H	2.17	0.52
1:F:528:PHE:CE2	1:F:980:ARG:HG3	2.45	0.52
1:A:755:ASP:O	1:A:759:ILE:HG13	2.09	0.51
1:B:242:ARG:NH1	1:B:768:ASP:O	2.43	0.51
1:D:275:ALA:HB3	1:D:278:TYR:CZ	2.45	0.51
1:E:650:LEU:C	1:E:650:LEU:HD23	2.34	0.51
1:A:191:LEU:HD23	1:A:269:ALA:HB2	1.92	0.51
1:A:335:PHE:CE2	1:A:577:LYS:HD2	2.44	0.51
1:B:766:VAL:HB	1:B:778:VAL:HG23	1.92	0.51
1:D:691:GLN:HG2	1:D:826:TYR:HB3	1.91	0.51
1:E:760:TYR:CD1	1:E:782:ALA:HB2	2.46	0.51
1:E:764:LEU:HD22	1:E:765:TYR:H	1.75	0.51
1:F:265:LEU:HG	1:F:271:ILE:HD11	1.92	0.51
1:F:888:SER:O	1:F:892:VAL:HG23	2.11	0.51
1:C:74:VAL:HG13	1:C:112:ARG:NE	2.24	0.51
1:C:76:ASP:O	1:C:97:LYS:HG3	2.10	0.51
1:E:354:VAL:HG11	1:E:409:VAL:HB	1.93	0.51
1:F:74:VAL:HG12	1:F:77:MET:HE3	1.92	0.51
1:A:511:ARG:HD3	1:A:515:ARG:CZ	2.40	0.51
1:B:507:ASP:OD1	1:B:508:TRP:N	2.38	0.51
1:B:533:GLU:OE1	1:B:533:GLU:N	2.43	0.51
1:E:225:SER:HB2	1:F:278:TYR:HB3	1.93	0.51
1:E:753:VAL:HG12	1:E:757:MET:HE2	1.92	0.51
1:E:921:LEU:HA	1:E:924:VAL:HG22	1.93	0.51
1:E:927:THR:HG21	1:E:1009:ALA:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:385:LEU:HD12	1:F:478:ILE:HG23	1.92	0.51
1:F:388:LEU:HD23	1:F:389:PHE:CE1	2.45	0.51
1:A:557:VAL:HA	1:A:560:THR:HG23	1.93	0.51
1:B:370:ILE:HB	1:B:371:PRO:HD3	1.93	0.51
1:B:714:ALA:HA	1:B:854:ILE:HD13	1.93	0.51
1:B:961:GLU:OE2	1:B:1037:ARG:NH1	2.43	0.51
1:C:946:SER:HB3	1:C:1021:VAL:HG22	1.92	0.51
1:E:330:TYR:CD2	1:E:332:PRO:HD3	2.46	0.51
1:F:3:ILE:HD12	1:F:3:ILE:H	1.75	0.51
1:A:730:ASN:HA	1:A:818:PHE:HB3	1.92	0.51
1:B:848:GLN:HB2	1:B:867:TRP:CZ2	2.46	0.51
1:D:158:ASN:O	1:D:162:ILE:HG12	2.09	0.51
1:E:408:VAL:HG22	1:E:483:SER:HB2	1.93	0.51
1:E:774:ARG:HB2	1:E:776:TYR:HE1	1.76	0.51
1:A:153:MET:HE1	1:A:281:ARG:HG2	1.93	0.51
1:A:752:ASP:O	1:A:756:THR:OG1	2.29	0.51
1:F:728:GLN:O	1:F:820:PRO:HA	2.11	0.51
1:A:140:MET:HE2	1:A:328:ILE:HG23	1.92	0.51
1:C:74:VAL:HG13	1:C:112:ARG:HD2	1.93	0.51
1:C:793:ILE:O	1:C:808:LEU:HD21	2.11	0.51
1:E:184:ASP:OD1	1:E:185:TYR:N	2.41	0.51
1:E:543:LEU:HD22	1:E:1034:VAL:HG21	1.93	0.51
1:A:82:SER:HB3	1:A:92:ILE:HG12	1.93	0.51
1:A:153:MET:HE3	1:A:182:ALA:HB2	1.93	0.51
1:A:749:ASN:HB3	1:A:752:ASP:CG	2.36	0.51
1:B:989:PHE:CG	1:B:1018:MET:HE2	2.46	0.51
1:C:679:VAL:HG13	1:C:682:LEU:HD23	1.91	0.51
1:D:1010:MET:HA	1:D:1013:ALA:HB3	1.93	0.51
1:E:770:ASN:HA	1:E:774:ARG:O	2.11	0.51
1:E:843:SER:H	1:E:846:GLN:NE2	2.09	0.51
1:F:121:PRO:O	1:F:124:VAL:HG22	2.11	0.51
1:F:189:VAL:HG13	1:F:271:ILE:HG12	1.93	0.51
1:B:885:PHE:O	1:B:889:VAL:HG12	2.11	0.51
1:D:599:ILE:HD13	1:D:602:MET:CE	2.40	0.51
1:F:244:GLN:HG3	1:F:245:ASN:ND2	2.26	0.51
1:F:997:VAL:HG12	1:F:998:LEU:HD12	1.91	0.51
1:D:742:LYS:HG3	1:D:745:GLN:NE2	2.25	0.50
1:A:715:GLN:OE1	1:A:715:GLN:N	2.32	0.50
1:C:70:GLN:O	1:C:112:ARG:HD3	2.11	0.50
1:B:359:ILE:HD11	1:B:365:TRP:HA	1.92	0.50
1:E:435:LYS:O	1:E:439:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:HIS:O	1:D:326:TYR:HA	2.11	0.50
1:A:583:PHE:HE2	1:A:674:PHE:HD2	1.59	0.50
1:B:688:PHE:HB2	1:B:867:TRP:HZ3	1.77	0.50
1:B:1033:TYR:O	1:B:1037:ARG:HB2	2.11	0.50
1:D:772:PHE:CG	1:D:772:PHE:O	2.63	0.50
1:D:793:ILE:O	1:D:808:LEU:HD21	2.11	0.50
1:E:913:VAL:HG22	1:E:914:PRO:HD3	1.93	0.50
1:F:872:TYR:CZ	1:F:876:LEU:HD21	2.46	0.50
1:A:698:VAL:HG12	1:A:702:ARG:HB3	1.94	0.50
1:C:763:SER:HA	1:C:781:GLN:HB2	1.94	0.50
1:D:720:LEU:O	1:D:839:ALA:HB2	2.12	0.50
1:E:854:ILE:O	1:E:858:THR:HG23	2.12	0.50
1:F:682:LEU:HD12	1:F:682:LEU:O	2.11	0.50
1:F:731:VAL:HG12	1:F:819:GLY:O	2.10	0.50
1:B:193:PRO:HB3	1:B:760:TYR:CE1	2.47	0.50
1:D:265:LEU:HD12	1:D:268:ILE:HG23	1.94	0.50
1:D:990:ILE:HA	1:D:993:VAL:HG13	1.94	0.50
1:E:238:ASN:OD1	1:F:55:ASN:ND2	2.45	0.50
1:F:313:MET:HB3	1:F:326:TYR:CE2	2.47	0.50
1:F:736:VAL:HG22	1:F:814:VAL:HG22	1.93	0.50
1:A:740:ARG:NH1	1:A:750:VAL:HG21	2.27	0.50
1:B:543:LEU:HD22	1:B:1034:VAL:HG21	1.94	0.50
1:E:367:ALA:HA	1:E:499:LEU:HD21	1.93	0.50
1:E:560:THR:OG1	1:E:918:LEU:HG	2.12	0.50
1:E:1037:ARG:NH1	1:E:1041:GLY:HA3	2.26	0.50
1:F:343:VAL:HG21	1:F:398:LEU:HB3	1.93	0.50
1:F:882:PHE:HD2	1:F:883:TRP:CZ3	2.30	0.50
1:A:546:LYS:HD3	1:A:546:LYS:N	2.21	0.50
1:C:780:VAL:HG23	1:C:781:GLN:H	1.77	0.50
1:D:6:PHE:O	1:D:10:ARG:HD2	2.10	0.50
1:F:714:ALA:HB3	1:F:723:LEU:HD22	1.94	0.50
1:A:712:LYS:HA	1:A:715:GLN:HE22	1.77	0.49
1:B:157:ARG:HD2	1:B:182:ALA:O	2.11	0.49
1:B:644:GLN:HE22	1:E:608:LYS:HD3	1.77	0.49
1:D:225:SER:HB3	1:E:278:TYR:HB3	1.94	0.49
1:E:403:LEU:HB3	1:E:941:VAL:HG21	1.93	0.49
1:F:757:MET:HE2	1:F:793:ILE:HD11	1.92	0.49
1:A:1024:PHE:O	1:A:1028:LEU:HB2	2.12	0.49
1:B:742:LYS:O	1:B:746:LEU:HD23	2.12	0.49
1:D:35:SER:O	1:D:394:ASN:HA	2.11	0.49
1:D:800:ASN:OD1	1:D:804:GLU:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1010:MET:O	1:E:1014:VAL:HG22	2.11	0.49
1:B:121:PRO:HB2	1:B:124:VAL:HG23	1.93	0.49
1:A:193:PRO:HB3	1:A:760:TYR:CE1	2.47	0.49
1:B:35:SER:O	1:B:394:ASN:HA	2.12	0.49
1:C:504:ASP:OD1	1:C:504:ASP:N	2.40	0.49
1:C:692:ILE:HD12	1:C:707:THR:HG22	1.94	0.49
1:E:690:MET:HE3	1:E:865:PHE:CD2	2.46	0.49
1:E:872:TYR:O	1:E:875:ILE:HG22	2.13	0.49
1:F:59:ILE:HD11	1:F:88:GLY:HA2	1.94	0.49
1:A:61:GLU:O	1:A:65:SER:OG	2.31	0.49
1:A:228:LEU:H	1:A:228:LEU:HD23	1.77	0.49
1:A:330:TYR:CD2	1:A:332:PRO:HD3	2.47	0.49
1:B:444:ILE:O	1:B:447:ILE:HG13	2.12	0.49
1:C:5:LYS:NZ	1:C:9:ASP:OD2	2.46	0.49
1:D:560:THR:OG1	1:D:918:LEU:HB2	2.13	0.49
1:D:1004:ALA:HB1	1:D:1008:HIS:NE2	2.27	0.49
1:E:366:ARG:NH2	1:E:500:LYS:HE2	2.27	0.49
1:E:968:PHE:O	1:E:972:VAL:HG13	2.12	0.49
1:F:199:ARG:O	1:F:255:LYS:NZ	2.29	0.49
1:A:148:ASN:OD1	1:A:150:SER:OG	2.30	0.49
1:A:917:ILE:CD1	1:A:939:LEU:HD12	2.41	0.49
1:B:82:SER:HB3	1:B:92:ILE:HG12	1.93	0.49
1:B:249:PHE:O	1:B:252:ILE:HG13	2.12	0.49
1:B:691:GLN:HG2	1:B:868:THR:HG21	1.94	0.49
1:B:966:THR:HG22	1:B:969:GLU:CD	2.38	0.49
1:C:214:ASN:HB2	1:C:243:LEU:HD22	1.94	0.49
1:D:698:VAL:HG21	1:D:863:VAL:HG23	1.93	0.49
1:A:306:SER:O	1:A:310:ARG:HG3	2.12	0.49
1:B:599:ILE:HD13	1:B:602:MET:CE	2.43	0.49
1:C:410:ASP:CG	1:C:948:LYS:HZ1	2.20	0.49
1:C:852:GLU:HG2	1:C:865:PHE:CZ	2.44	0.49
1:D:83:GLN:NE2	1:D:822:MET:SD	2.86	0.49
1:D:592:LEU:HA	1:D:595:THR:OG1	2.13	0.49
1:F:259:ASP:N	1:F:259:ASP:OD1	2.43	0.49
1:F:919:SER:HB3	1:F:1020:GLY:HA3	1.95	0.49
1:A:90:MET:SD	1:A:92:ILE:HG13	2.53	0.49
1:C:546:LYS:O	1:C:550:LEU:HD13	2.13	0.49
1:D:509:LEU:HA	1:D:512:VAL:HG22	1.94	0.49
1:D:643:ASP:OD1	1:D:644:GLN:N	2.46	0.49
1:D:940:MET:HE2	1:D:940:MET:HA	1.94	0.49
1:F:391:TYR:CZ	1:F:474:MET:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ILE:HD13	1:B:451:LEU:HD13	1.95	0.49
1:D:419:VAL:HG22	1:D:433:THR:HA	1.95	0.49
1:E:49:ALA:HB3	1:E:90:MET:HE3	1.95	0.49
1:F:105:ALA:HA	1:F:108:LEU:HD12	1.93	0.49
1:F:860:PRO:HD2	1:F:863:VAL:HG11	1.93	0.49
1:B:68:GLU:O	1:B:72:ASN:HB2	2.13	0.49
1:B:919:SER:OG	1:B:1020:GLY:HA3	2.13	0.49
1:D:190:TRP:HA	1:D:781:GLN:O	2.12	0.49
1:D:306:SER:O	1:D:310:ARG:HG3	2.13	0.49
1:E:70:GLN:CG	1:E:116:ALA:HB2	2.40	0.49
1:E:704:ALA:HB2	1:E:727:TYR:CE2	2.48	0.49
1:F:558:GLY:O	1:F:562:MET:HG3	2.12	0.49
1:A:398:LEU:O	1:A:402:VAL:HG23	2.12	0.48
1:C:361:PHE:HB2	1:C:984:MET:HE3	1.94	0.48
1:D:571:PHE:HB2	1:D:685:LEU:HD13	1.94	0.48
1:F:577:LYS:O	1:F:578:GLU:HB2	2.13	0.48
1:A:47:VAL:HG22	1:A:131:THR:HG23	1.94	0.48
1:D:792:ASP:HA	1:D:795:GLN:HG2	1.94	0.48
1:D:913:VAL:N	1:D:914:PRO:HD2	2.28	0.48
1:E:760:TYR:O	1:E:782:ALA:HB3	2.13	0.48
1:A:35:SER:OG	1:A:37:TYR:O	2.31	0.48
1:A:78:LEU:N	1:A:95:THR:O	2.45	0.48
1:A:919:SER:OG	1:A:1020:GLY:HA3	2.12	0.48
1:B:103:ASP:HB3	1:C:104:LYS:HE3	1.95	0.48
1:B:313:MET:HG3	1:B:326:TYR:CG	2.48	0.48
1:D:253:VAL:HB	1:E:744:LYS:HD3	1.94	0.48
1:A:385:LEU:HD12	1:A:478:ILE:HG23	1.94	0.48
1:B:139:THR:O	1:B:332:PRO:HD2	2.13	0.48
1:B:351:ILE:HD11	1:B:376:PRO:HG3	1.95	0.48
1:C:990:ILE:O	1:C:993:VAL:HG22	2.13	0.48
1:E:103:ASP:OD1	1:E:133:LYS:HD2	2.14	0.48
1:F:458:LEU:HD21	1:F:940:MET:HE2	1.95	0.48
1:F:535:TYR:OH	1:F:975:SER:HB2	2.12	0.48
1:F:793:ILE:HG23	1:F:794:LEU:HG	1.95	0.48
1:A:74:VAL:HG12	1:A:77:MET:CE	2.44	0.48
1:B:917:ILE:HD13	1:B:939:LEU:HD22	1.96	0.48
1:D:116:ALA:HA	1:D:119:ARG:NH2	2.29	0.48
1:D:940:MET:O	1:D:943:VAL:HG13	2.13	0.48
1:E:74:VAL:HG21	1:E:108:LEU:HD13	1.96	0.48
1:E:764:LEU:HD22	1:E:765:TYR:N	2.28	0.48
1:F:528:PHE:HE2	1:F:980:ARG:HG3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ALA:HA	1:B:108:LEU:HD12	1.95	0.48
1:B:588:ASN:HB3	1:B:731:VAL:HG23	1.96	0.48
1:B:973:GLU:O	1:B:977:LEU:HD23	2.13	0.48
1:D:179:LEU:HD21	1:D:292:MET:HE3	1.94	0.48
1:D:704:ALA:HA	1:D:707:THR:HG22	1.96	0.48
1:A:257:ALA:O	1:A:259:ASP:N	2.46	0.48
1:A:359:ILE:CD1	1:A:365:TRP:HA	2.44	0.48
1:C:934:PHE:HB3	1:C:1010:MET:HE1	1.94	0.48
1:E:3:ILE:HD12	1:E:441:SER:HB3	1.95	0.48
1:E:49:ALA:HB2	1:E:129:ILE:CD1	2.44	0.48
1:E:70:GLN:O	1:E:112:ARG:HD3	2.12	0.48
1:F:403:LEU:CD2	1:F:1010:MET:HE1	2.44	0.48
1:A:723:LEU:HA	1:A:835:ASN:O	2.14	0.48
1:A:997:VAL:HG12	1:A:998:LEU:HD12	1.95	0.48
1:B:644:GLN:OE1	1:E:608:LYS:HD3	2.13	0.48
1:C:691:GLN:O	1:C:865:PHE:HA	2.14	0.48
1:D:16:VAL:HG13	1:E:894:LEU:HB3	1.96	0.48
1:D:313:MET:HB3	1:D:326:TYR:CE2	2.48	0.48
1:D:583:PHE:HE1	1:D:674:PHE:CE2	2.32	0.48
1:E:366:ARG:NH1	1:E:507:ASP:OD2	2.47	0.48
1:F:38:PRO:O	1:F:40:VAL:HG13	2.13	0.48
1:F:920:ALA:HB3	1:F:939:LEU:HD21	1.94	0.48
1:B:362:LEU:O	1:B:364:THR:HG22	2.14	0.48
1:C:913:VAL:CG2	1:C:914:PRO:HD3	2.44	0.48
1:D:121:PRO:HB2	1:D:124:VAL:HG23	1.95	0.48
1:D:406:GLY:HA2	1:D:989:PHE:HZ	1.79	0.48
1:A:70:GLN:HG3	1:A:116:ALA:HB2	1.95	0.48
1:A:119:ARG:NH2	1:C:126:ARG:O	2.47	0.48
1:A:249:PHE:O	1:A:265:LEU:HD23	2.14	0.48
1:D:202:THR:HG22	1:D:799:ARG:NH2	2.29	0.48
1:E:203:ALA:O	1:E:207:VAL:HG13	2.13	0.48
1:F:958:ARG:NH2	2:F:1101:LMT:H6D	2.27	0.48
1:B:50:GLN:O	1:B:124:VAL:HG13	2.14	0.47
1:C:793:ILE:HG21	1:C:814:VAL:HG21	1.95	0.47
1:E:863:VAL:HG12	1:E:863:VAL:O	2.14	0.47
1:A:363:GLN:HB3	1:A:521:PHE:CE2	2.49	0.47
1:B:411:ASP:OD1	1:B:948:LYS:NZ	2.43	0.47
1:B:640:LYS:HB3	1:B:644:GLN:HG2	1.95	0.47
1:C:168:LEU:HD13	1:C:294:ILE:HD11	1.97	0.47
1:D:228:LEU:H	1:D:228:LEU:HD22	1.79	0.47
1:D:691:GLN:HG2	1:D:826:TYR:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:663:TYR:HA	1:E:666:LEU:HD22	1.97	0.47
1:E:765:TYR:CE1	1:E:777:GLN:HG2	2.49	0.47
1:F:197:ALA:CB	1:F:797:LYS:HD2	2.42	0.47
1:F:228:LEU:HG	1:F:229:PRO:CD	2.43	0.47
1:F:791:ASP:C	1:F:791:ASP:OD1	2.57	0.47
1:A:110:GLN:HA	1:A:113:VAL:HG12	1.96	0.47
1:A:417:GLU:OE2	1:A:980:ARG:NE	2.46	0.47
1:A:599:ILE:HD13	1:A:602:MET:CE	2.44	0.47
1:B:765:TYR:HA	1:B:779:ARG:HG2	1.97	0.47
1:C:690:MET:HG2	1:C:691:GLN:H	1.78	0.47
1:D:49:ALA:HB2	1:D:129:ILE:HD12	1.95	0.47
1:D:391:TYR:CZ	1:D:474:MET:HG2	2.49	0.47
1:D:766:VAL:HB	1:D:778:VAL:HG23	1.96	0.47
1:E:1031:VAL:O	1:E:1035:VAL:HG23	2.13	0.47
1:F:361:PHE:CD1	1:F:984:MET:HG2	2.49	0.47
1:F:997:VAL:HG21	1:F:1012:VAL:HG22	1.95	0.47
1:A:17:LEU:HD13	1:A:485:PHE:HZ	1.80	0.47
1:A:158:ASN:O	1:A:162:ILE:HG12	2.14	0.47
1:A:164:VAL:HG13	1:A:313:MET:HE1	1.96	0.47
1:B:148:ASN:OD1	1:B:150:SER:OG	2.22	0.47
1:B:564:SER:HA	1:B:921:LEU:HD13	1.95	0.47
1:B:917:ILE:CD1	1:B:939:LEU:HD22	2.44	0.47
1:D:1:MET:HB2	2:D:1101:LMT:O2'	2.15	0.47
1:E:980:ARG:O	1:E:984:MET:HG3	2.13	0.47
1:B:410:ASP:OD2	1:B:948:LYS:HE3	2.14	0.47
1:B:640:LYS:HE3	1:B:645:ARG:NH1	2.29	0.47
1:B:691:GLN:HG3	1:B:826:TYR:CG	2.50	0.47
1:B:899:LEU:HD13	1:B:900:TYR:CD1	2.49	0.47
1:C:766:VAL:HB	1:C:778:VAL:HG23	1.97	0.47
1:E:164:VAL:HG11	1:E:292:MET:HE1	1.97	0.47
1:F:783:ASP:O	1:F:787:ARG:HG3	2.15	0.47
1:F:932:ASN:OD1	1:F:934:PHE:HB2	2.15	0.47
1:A:328:ILE:HG22	1:A:328:ILE:O	2.15	0.47
1:B:940:MET:O	1:B:943:VAL:HG22	2.14	0.47
1:D:187:MET:HE3	1:D:187:MET:HA	1.97	0.47
1:D:437:MET:HE3	1:D:437:MET:HA	1.96	0.47
1:E:45:VAL:HG11	1:E:109:VAL:CG1	2.45	0.47
1:F:1:MET:SD	1:F:3:ILE:HD11	2.54	0.47
1:A:63:VAL:HG13	1:A:120:LEU:HD12	1.95	0.47
1:B:243:LEU:HB2	1:B:249:PHE:CE1	2.49	0.47
1:B:458:LEU:HD21	1:B:885:PHE:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:789:ARG:C	1:B:789:ARG:HD3	2.39	0.47
1:C:691:GLN:HG2	1:C:826:TYR:CD2	2.50	0.47
1:C:1008:HIS:O	1:C:1011:GLY:N	2.36	0.47
1:E:202:THR:HG23	1:E:799:ARG:NH2	2.30	0.47
1:E:679:VAL:HG13	1:E:682:LEU:HD23	1.97	0.47
1:F:161:LEU:HD21	1:F:774:ARG:HH22	1.80	0.47
1:A:5:LYS:HB2	1:A:5:LYS:HE2	1.73	0.47
1:A:583:PHE:CE1	1:A:623:VAL:HG13	2.50	0.47
1:C:213:GLN:HE22	1:C:253:VAL:H	1.63	0.47
1:D:720:LEU:C	1:D:839:ALA:HB2	2.39	0.47
1:E:542:VAL:HA	1:E:549:MET:HE3	1.96	0.47
1:E:645:ARG:HB2	1:E:650:LEU:HD22	1.97	0.47
1:E:921:LEU:O	1:E:924:VAL:HG22	2.14	0.47
1:A:509:LEU:HA	1:A:512:VAL:HG22	1.97	0.47
1:A:894:LEU:HB3	1:C:16:VAL:HG13	1.96	0.47
1:C:189:VAL:HG23	1:C:189:VAL:O	2.15	0.47
1:C:986:SER:HA	1:C:1018:MET:HE2	1.96	0.47
1:D:317:LYS:HA	1:D:320:PHE:CD2	2.50	0.47
1:D:761:LEU:HD11	1:D:793:ILE:HG12	1.97	0.47
1:A:199:ARG:HG3	1:A:263:THR:HG21	1.97	0.47
1:C:38:PRO:HD2	1:C:396:LEU:HD23	1.96	0.47
1:C:783:ASP:OD1	1:C:784:ALA:N	2.47	0.47
1:C:939:LEU:O	1:C:943:VAL:HG13	2.15	0.47
1:D:259:ASP:OD1	1:D:259:ASP:N	2.48	0.47
1:D:588:ASN:ND2	1:D:730:ASN:O	2.44	0.47
1:B:38:PRO:O	1:B:40:VAL:HG22	2.15	0.46
1:B:899:LEU:HD13	1:B:900:TYR:CE1	2.51	0.46
1:C:848:GLN:HB2	1:C:867:TRP:CZ2	2.49	0.46
1:D:449:LEU:CD1	2:D:1101:LMT:H82	2.45	0.46
1:D:462:SER:OG	1:D:880:SER:HB2	2.15	0.46
1:F:417:GLU:HG3	1:F:984:MET:CE	2.43	0.46
1:A:464:LEU:HD13	1:A:464:LEU:H	1.78	0.46
1:B:270:ARG:NH1	1:B:783:ASP:OD2	2.49	0.46
1:B:582:ALA:HA	1:B:673:VAL:HA	1.96	0.46
1:C:120:LEU:HB3	1:C:124:VAL:CG2	2.44	0.46
1:F:586:LEU:HB2	1:F:631:SER:O	2.15	0.46
1:F:884:VAL:HG12	1:F:885:PHE:HD1	1.79	0.46
1:F:987:ILE:HG22	1:F:991:MET:HE2	1.96	0.46
1:A:983:LEU:HA	1:A:983:LEU:HD23	1.64	0.46
1:B:199:ARG:HE	1:B:263:THR:HG21	1.80	0.46
1:B:923:GLY:O	1:B:927:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:THR:HG22	1:B:969:GLU:CG	2.45	0.46
1:C:447:ILE:HG21	1:C:948:LYS:HG2	1.96	0.46
1:C:579:TYR:CZ	1:C:676:PRO:HB3	2.50	0.46
1:E:535:TYR:O	1:E:539:VAL:HG23	2.15	0.46
1:E:872:TYR:O	1:E:876:LEU:HD23	2.16	0.46
1:E:1005:GLU:O	1:E:1008:HIS:HB3	2.16	0.46
1:B:546:LYS:HD3	1:B:546:LYS:N	2.30	0.46
1:C:193:PRO:HD2	1:C:786:PHE:CD2	2.50	0.46
1:C:560:THR:OG1	1:C:918:LEU:HB2	2.15	0.46
1:E:48:LYS:O	1:E:49:ALA:HB3	2.16	0.46
1:F:559:ALA:O	1:F:563:VAL:HG23	2.15	0.46
1:F:791:ASP:C	1:F:793:ILE:H	2.23	0.46
1:A:783:ASP:OD1	1:A:784:ALA:N	2.48	0.46
1:A:945:LEU:HD22	1:A:1018:MET:HE1	1.98	0.46
1:B:254:VAL:HG21	1:B:268:ILE:HD11	1.98	0.46
1:B:905:LEU:HD23	1:B:905:LEU:HA	1.63	0.46
1:C:863:VAL:O	1:C:863:VAL:HG12	2.15	0.46
1:E:147:PRO:O	1:E:287:LYS:NZ	2.30	0.46
1:E:1030:PRO:O	1:E:1034:VAL:HG13	2.16	0.46
1:F:139:THR:O	1:F:332:PRO:HD2	2.15	0.46
1:A:694:ASP:HB2	1:A:703:LEU:HD13	1.98	0.46
1:B:90:MET:HE3	1:B:90:MET:HB3	1.85	0.46
1:B:989:PHE:CD2	1:B:1018:MET:HE2	2.51	0.46
1:D:280:LEU:HB2	1:D:628:ASN:OD1	2.16	0.46
1:E:494:LEU:HD23	1:E:494:LEU:HA	1.81	0.46
1:E:977:LEU:HD12	1:E:977:LEU:HA	1.64	0.46
1:F:736:VAL:HG21	1:F:757:MET:HE1	1.97	0.46
1:A:5:LYS:HD3	1:A:434:TYR:HD1	1.78	0.46
1:B:414:VAL:HG22	1:B:978:ARG:HH22	1.80	0.46
1:B:508:TRP:CD1	1:B:508:TRP:C	2.94	0.46
1:D:465:THR:HG23	1:D:571:PHE:HE2	1.80	0.46
1:E:246:GLU:OE1	1:E:246:GLU:N	2.36	0.46
1:F:45:VAL:HG11	1:F:109:VAL:CG2	2.46	0.46
1:F:682:LEU:CD1	1:F:870:LEU:HD13	2.45	0.46
1:F:1012:VAL:O	1:F:1016:PHE:HD2	1.99	0.46
1:A:17:LEU:O	1:A:21:ILE:HG13	2.14	0.46
1:B:644:GLN:O	1:B:646:HIS:N	2.48	0.46
1:C:192:ASP:O	1:C:196:VAL:HG23	2.16	0.46
1:C:924:VAL:HA	1:C:927:THR:HG22	1.98	0.46
1:C:990:ILE:HD11	1:C:1018:MET:HB2	1.97	0.46
1:D:808:LEU:HA	1:D:811:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:926:LEU:HD23	1:D:926:LEU:HA	1.82	0.46
1:E:444:ILE:HD13	1:E:487:SER:HB3	1.97	0.46
1:F:370:ILE:CD1	1:F:494:LEU:HB3	2.46	0.46
1:F:772:PHE:HD2	1:F:774:ARG:CG	2.29	0.46
1:D:197:ALA:HB1	1:D:797:LYS:HD2	1.97	0.46
1:E:965:LYS:HB3	1:E:969:GLU:HG3	1.98	0.46
1:F:770:ASN:HA	1:F:774:ARG:O	2.16	0.46
1:A:932:ASN:OD1	1:A:934:PHE:HB2	2.16	0.46
1:B:365:TRP:CZ3	1:B:369:ILE:HD11	2.51	0.46
1:B:915:MET:HE3	1:B:1024:PHE:CE2	2.51	0.46
1:C:494:LEU:O	1:C:497:ILE:HG22	2.16	0.46
1:C:905:LEU:HD13	1:C:905:LEU:HA	1.69	0.46
1:E:383:PHE:HA	1:E:386:LEU:HD12	1.98	0.46
1:E:978:ARG:C	1:E:981:PRO:HD2	2.41	0.46
1:A:168:LEU:HD21	1:A:313:MET:HE3	1.97	0.45
1:A:222:ILE:HG23	1:B:789:ARG:N	2.31	0.45
1:A:1037:ARG:NH2	1:A:1040:ALA:HB3	2.31	0.45
1:B:74:VAL:HG12	1:B:77:MET:HE3	1.98	0.45
1:B:343:VAL:HG22	1:B:402:VAL:CG1	2.46	0.45
1:B:641:PRO:O	1:B:644:GLN:HB3	2.15	0.45
1:D:285:ASP:O	1:D:287:LYS:HG3	2.16	0.45
1:D:703:LEU:O	1:D:707:THR:HG22	2.16	0.45
1:D:876:LEU:O	1:D:878:GLY:N	2.49	0.45
1:E:184:ASP:O	1:E:275:ALA:HA	2.16	0.45
1:E:997:VAL:CG1	1:E:998:LEU:HD12	2.45	0.45
1:A:245:ASN:ND2	1:A:248:GLU:HG3	2.31	0.45
1:B:644:GLN:HG3	1:B:645:ARG:N	2.24	0.45
1:C:560:THR:HA	1:C:918:LEU:HD13	1.98	0.45
1:D:214:ASN:O	1:D:767:ASN:ND2	2.49	0.45
1:D:758:GLN:NE2	1:D:764:LEU:HD12	2.31	0.45
1:E:276:SER:O	1:E:779:ARG:NH1	2.50	0.45
1:E:469:TYR:OH	1:E:936:GLN:OE1	2.34	0.45
1:F:90:MET:HE3	1:F:90:MET:HB3	1.77	0.45
1:F:599:ILE:HD13	1:F:602:MET:CE	2.47	0.45
1:A:4:SER:HB3	1:A:488:LEU:O	2.16	0.45
1:A:200:ASN:C	1:A:805:MET:HE3	2.41	0.45
1:A:205:ASP:OD1	1:A:208:ARG:NH2	2.49	0.45
1:A:406:GLY:HA2	1:A:989:PHE:CZ	2.52	0.45
1:A:720:LEU:HD11	1:A:851:VAL:HG23	1.98	0.45
1:A:808:LEU:HA	1:A:811:LEU:HB2	1.98	0.45
1:A:845:GLY:O	1:A:848:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLN:HG2	1:B:131:THR:HB	1.98	0.45
1:B:191:LEU:O	1:B:783:ASP:HB2	2.17	0.45
1:C:5:LYS:HA	1:C:8:ILE:HD12	1.99	0.45
1:C:678:PRO:HD2	1:C:682:LEU:HD21	1.98	0.45
1:F:127:LEU:HD11	1:F:779:ARG:HH22	1.82	0.45
1:A:940:MET:O	1:A:943:VAL:HG22	2.16	0.45
1:A:1015:PHE:HD1	1:A:1016:PHE:HD1	1.65	0.45
1:B:158:ASN:O	1:B:162:ILE:HG12	2.17	0.45
1:C:679:VAL:H	1:C:682:LEU:CD2	2.29	0.45
1:D:435:LYS:O	1:D:439:GLU:HG3	2.16	0.45
1:D:899:LEU:HD23	1:D:900:TYR:CE1	2.51	0.45
1:B:597:LYS:HD2	1:B:597:LYS:N	2.29	0.45
1:B:921:LEU:O	1:B:924:VAL:HG22	2.17	0.45
1:C:74:VAL:HG13	1:C:112:ARG:CD	2.47	0.45
1:D:579:TYR:CE1	1:D:676:PRO:HB3	2.51	0.45
1:D:710:PHE:HZ	1:D:851:VAL:HG13	1.81	0.45
1:F:187:MET:HB3	1:F:778:VAL:HG12	1.98	0.45
1:F:388:LEU:O	1:F:388:LEU:HG	2.14	0.45
1:A:915:MET:HB3	1:A:1024:PHE:CD2	2.52	0.45
1:D:203:ALA:O	1:D:207:VAL:HG13	2.17	0.45
1:D:406:GLY:HA2	1:D:989:PHE:CZ	2.52	0.45
1:D:571:PHE:CD1	1:D:572:VAL:HG23	2.52	0.45
1:D:952:LEU:HD23	1:D:952:LEU:HA	1.82	0.45
1:E:72:ASN:ND2	1:E:80:MET:HE2	2.32	0.45
1:E:361:PHE:HB2	1:E:984:MET:HE3	1.99	0.45
1:F:713:ARG:O	1:F:716:GLN:HB2	2.17	0.45
1:A:991:MET:O	1:A:995:PRO:HD2	2.17	0.45
1:B:70:GLN:HG2	1:B:112:ARG:O	2.17	0.45
1:B:166:ASP:HB3	1:B:170:ARG:HH12	1.80	0.45
1:B:375:VAL:HG21	1:B:409:VAL:HG23	1.98	0.45
1:C:748:VAL:HG21	1:C:811:LEU:HD21	1.98	0.45
1:E:708:ASN:HA	1:E:711:ILE:HG22	1.98	0.45
1:F:168:LEU:HD11	1:F:313:MET:HE3	1.98	0.45
1:F:569:GLY:O	1:F:843:SER:HB2	2.17	0.45
1:F:698:VAL:O	1:F:702:ARG:HD3	2.17	0.45
1:A:556:LEU:CD1	1:A:915:MET:HE1	2.47	0.45
1:B:36:GLU:OE2	1:B:37:TYR:HE1	1.99	0.45
1:B:254:VAL:HG11	1:B:268:ILE:HD13	1.99	0.45
1:B:446:ALA:HB2	2:B:1101:LMT:H32	1.99	0.45
1:B:919:SER:CB	1:B:1020:GLY:HA3	2.47	0.45
1:C:609:GLN:CD	1:C:610:PRO:HD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:VAL:HG12	1:D:293:ALA:HA	1.99	0.45
1:D:365:TRP:CD1	1:D:510:THR:HG1	2.35	0.45
1:F:232:PRO:O	1:F:233:LEU:HD23	2.16	0.45
1:A:10:ARG:NH2	2:B:1101:LMT:H3'	2.32	0.45
1:A:774:ARG:HB2	1:A:776:TYR:HE1	1.82	0.45
1:B:422:ASN:OD1	1:B:435:LYS:HD3	2.17	0.45
1:C:375:VAL:HG22	1:C:408:VAL:HG12	1.98	0.45
1:C:575:GLN:NE2	1:C:1003:GLY:HA2	2.32	0.45
1:D:232:PRO:HB2	1:D:233:LEU:HD22	1.99	0.45
1:E:57:LYS:HE3	1:E:820:PRO:HD2	1.98	0.45
1:F:719:GLU:HG3	1:F:842:TYR:CE2	2.52	0.45
1:A:693:GLU:OE1	1:A:866:GLU:HG3	2.17	0.45
1:B:360:VAL:HG22	1:B:520:PHE:HE2	1.81	0.45
1:B:644:GLN:NE2	1:E:608:LYS:HD3	2.32	0.45
1:B:736:VAL:HG13	1:B:812:VAL:CG1	2.47	0.45
1:B:952:LEU:HD23	1:B:952:LEU:HA	1.72	0.45
1:C:191:LEU:CD2	1:C:269:ALA:HB2	2.46	0.45
1:C:415:VAL:HG13	1:C:437:MET:CE	2.47	0.45
1:C:469:TYR:OH	1:C:936:GLN:OE1	2.34	0.45
1:C:794:LEU:HD12	1:C:809:SER:HA	1.99	0.45
1:D:217:VAL:HG13	1:D:241:GLY:HA3	1.99	0.45
1:D:335:PHE:CE2	1:D:577:LYS:HD2	2.52	0.45
1:D:443:PRO:CG	1:D:955:GLU:HG2	2.43	0.45
1:D:966:THR:HG23	1:D:969:GLU:CD	2.42	0.45
1:F:90:MET:SD	1:F:92:ILE:HG13	2.57	0.45
1:F:546:LYS:H	1:F:546:LYS:HD3	1.81	0.45
1:F:620:GLY:O	1:F:628:ASN:HA	2.16	0.45
1:F:752:ASP:O	1:F:756:THR:OG1	2.35	0.45
1:F:800:ASN:HD21	1:F:802:ALA:HB3	1.82	0.45
1:A:768:ASP:HB3	1:A:775:VAL:HG13	1.98	0.44
1:A:789:ARG:HB3	1:A:792:ASP:OD2	2.17	0.44
1:B:863:VAL:O	1:B:863:VAL:HG12	2.17	0.44
1:C:47:VAL:HB	1:C:92:ILE:HB	1.98	0.44
1:D:211:ARG:HG3	1:D:766:VAL:HG13	1.99	0.44
2:D:1101:LMT:H6E	1:F:10:ARG:HH12	1.81	0.44
1:E:458:LEU:HD11	1:E:940:MET:HG3	2.00	0.44
1:F:406:GLY:HA3	1:F:989:PHE:CZ	2.52	0.44
1:F:472:PHE:HB3	1:F:937:ILE:HG12	1.99	0.44
1:F:962:HIS:HE2	2:F:1101:LMT:H6'2	1.82	0.44
1:F:989:PHE:CD2	1:F:1018:MET:HE3	2.52	0.44
1:A:391:TYR:CZ	1:A:474:MET:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:HD13	1:A:407:ILE:N	2.33	0.44
1:A:708:ASN:O	1:A:712:LYS:HB2	2.17	0.44
1:C:213:GLN:HE22	1:C:253:VAL:N	2.15	0.44
1:D:10:ARG:HH12	2:E:1101:LMT:C5'	2.20	0.44
1:D:408:VAL:HG22	1:D:483:SER:HB2	1.98	0.44
1:D:609:GLN:HB3	1:D:612:VAL:HG21	1.99	0.44
1:F:588:ASN:OD1	1:F:588:ASN:N	2.50	0.44
1:A:23:LEU:O	1:A:27:ILE:HD13	2.17	0.44
1:A:679:VAL:HB	1:A:682:LEU:HD23	1.99	0.44
1:B:34:ILE:HG21	1:B:303:LEU:HG	1.99	0.44
1:B:82:SER:CB	1:B:92:ILE:HG12	2.47	0.44
1:B:330:TYR:CD2	1:B:332:PRO:HD3	2.52	0.44
1:B:707:THR:HG21	1:B:832:ALA:CB	2.45	0.44
1:B:915:MET:HE3	1:B:1024:PHE:CD2	2.52	0.44
1:C:1033:TYR:CE2	1:C:1037:ARG:HG3	2.51	0.44
1:E:317:LYS:HA	1:E:320:PHE:CG	2.52	0.44
1:E:648:LYS:HD2	1:E:648:LYS:HA	1.73	0.44
1:E:1039:LEU:HD13	1:E:1039:LEU:HA	1.86	0.44
1:A:1031:VAL:O	1:A:1035:VAL:HG23	2.18	0.44
1:B:1006:MET:HA	1:B:1009:ALA:HB3	1.99	0.44
1:B:1020:GLY:O	1:B:1024:PHE:HD1	2.00	0.44
1:F:377:VAL:HG12	1:F:486:ASN:HD21	1.82	0.44
1:F:450:THR:HB	1:F:892:VAL:HG13	1.99	0.44
1:F:691:GLN:HG2	1:F:826:TYR:CG	2.52	0.44
1:F:896:LEU:HD23	1:F:896:LEU:HA	1.72	0.44
1:A:195:LYS:O	1:A:268:ILE:HD11	2.17	0.44
1:A:556:LEU:HB3	1:A:915:MET:HE1	1.99	0.44
1:B:417:GLU:CD	1:B:980:ARG:HH11	2.24	0.44
1:B:736:VAL:HG22	1:B:814:VAL:HG22	1.99	0.44
1:C:420:GLU:O	1:C:424:GLU:HG3	2.17	0.44
1:D:728:GLN:O	1:D:820:PRO:HA	2.17	0.44
1:D:1003:GLY:C	1:D:1005:GLU:H	2.25	0.44
1:E:10:ARG:HH12	2:F:1101:LMT:H1'	1.83	0.44
1:E:144:LEU:HG	1:E:292:MET:HE2	2.00	0.44
1:E:679:VAL:O	1:E:682:LEU:HG	2.17	0.44
1:A:33:PRO:HB3	1:A:299:GLY:HA2	2.00	0.44
1:A:707:THR:HG21	1:A:832:ALA:CB	2.45	0.44
1:A:827:ASN:ND2	1:A:866:GLU:OE1	2.48	0.44
1:A:939:LEU:O	1:A:943:VAL:HG13	2.18	0.44
1:B:403:LEU:HB3	1:B:941:VAL:HG21	1.99	0.44
1:B:847:ALA:O	1:B:851:VAL:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:SER:OG	1:C:437:MET:HB3	2.18	0.44
1:C:435:LYS:O	1:C:439:GLU:HG3	2.18	0.44
1:C:763:SER:HB3	1:C:781:GLN:CD	2.42	0.44
1:D:375:VAL:HG21	1:D:409:VAL:HG12	1.99	0.44
1:D:933:ILE:HA	1:D:936:GLN:HB2	2.00	0.44
1:E:791:ASP:OD1	1:E:791:ASP:N	2.45	0.44
1:E:912:ILE:HD13	1:E:950:ALA:HB2	1.98	0.44
1:F:242:ARG:HD3	1:F:769:PHE:HA	1.98	0.44
1:F:543:LEU:HD21	1:F:1031:VAL:HA	2.00	0.44
1:F:919:SER:CB	1:F:1020:GLY:HA3	2.48	0.44
1:A:408:VAL:HG22	1:A:483:SER:HB2	1.99	0.44
1:A:446:ALA:HB2	1:A:899:LEU:HD13	1.98	0.44
1:B:351:ILE:O	1:B:354:VAL:HG12	2.17	0.44
1:D:189:VAL:HG13	1:D:271:ILE:HG12	2.00	0.44
1:D:720:LEU:HD21	1:D:851:VAL:HG23	2.00	0.44
1:E:582:ALA:HA	1:E:673:VAL:HA	2.00	0.44
1:E:996:LEU:O	1:E:1008:HIS:HA	2.17	0.44
1:A:37:TYR:CZ	1:A:679:VAL:HG22	2.53	0.44
1:B:17:LEU:O	1:B:21:ILE:HG12	2.17	0.44
1:B:646:HIS:HA	1:B:650:LEU:CD2	2.44	0.44
1:C:38:PRO:O	1:C:40:VAL:HG13	2.17	0.44
1:D:12:ILE:N	1:E:901:GLU:OE2	2.41	0.44
1:D:791:ASP:OD1	1:D:792:ASP:N	2.51	0.44
1:E:566:ILE:HD13	1:E:566:ILE:HA	1.84	0.44
1:E:853:ARG:HD3	1:E:857:GLN:NE2	2.33	0.44
1:F:57:LYS:HE2	1:F:700:TYR:CE1	2.52	0.44
1:F:98:LEU:HD12	1:F:99:GLY:H	1.83	0.44
1:A:98:LEU:HD12	1:A:99:GLY:N	2.32	0.44
1:B:218:ALA:HB3	1:C:758:GLN:CD	2.43	0.44
1:B:406:GLY:HA3	1:B:989:PHE:HZ	1.82	0.44
1:B:647:GLY:H	1:B:650:LEU:HB3	1.82	0.44
1:B:703:LEU:O	1:B:707:THR:HG23	2.17	0.44
1:D:561:LEU:HD13	1:D:561:LEU:HA	1.85	0.44
1:D:757:MET:O	1:D:761:LEU:HB2	2.17	0.44
1:D:772:PHE:HD1	1:E:697:ALA:H	1.64	0.44
1:E:45:VAL:HG13	1:E:106:THR:HG23	2.00	0.44
1:E:509:LEU:HA	1:E:512:VAL:HG13	1.99	0.44
1:F:571:PHE:CD1	1:F:874:GLN:OE1	2.71	0.44
1:A:375:VAL:HG22	1:A:408:VAL:HG12	1.99	0.43
1:A:539:VAL:HA	1:A:542:VAL:HG22	2.00	0.43
1:B:147:PRO:HA	1:B:287:LYS:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:MET:HE1	1:B:281:ARG:HB3	2.00	0.43
1:B:171:ILE:HG22	1:B:172:GLN:N	2.33	0.43
1:B:446:ALA:CB	1:B:899:LEU:HG	2.48	0.43
1:B:712:LYS:HA	1:B:715:GLN:HE22	1.81	0.43
1:C:191:LEU:HD21	1:C:206:VAL:HG11	2.00	0.43
1:C:701:ALA:HA	1:C:729:ILE:HD13	2.00	0.43
1:D:742:LYS:O	1:D:745:GLN:HG2	2.17	0.43
1:D:864:LYS:HA	1:D:864:LYS:HD3	1.70	0.43
1:E:1038:THR:O	1:E:1043:LYS:HB2	2.17	0.43
1:A:141:VAL:HA	1:A:292:MET:O	2.17	0.43
1:A:624:ASN:O	1:A:626:PHE:N	2.51	0.43
1:B:754:PHE:HD1	1:B:757:MET:HE3	1.83	0.43
1:D:78:LEU:HD21	1:D:873:GLN:HG2	2.00	0.43
1:E:38:PRO:O	1:E:40:VAL:HG22	2.19	0.43
1:E:158:ASN:O	1:E:162:ILE:HG12	2.17	0.43
1:F:365:TRP:HD1	1:F:513:MET:HE2	1.83	0.43
1:F:435:LYS:O	1:F:439:GLU:HG3	2.18	0.43
1:A:2:ASN:HB3	1:A:441:SER:OG	2.18	0.43
1:B:629:SER:HB2	1:B:822:MET:HE3	1.99	0.43
1:B:712:LYS:HA	1:B:715:GLN:NE2	2.34	0.43
1:C:84:ALA:O	1:C:822:MET:HA	2.19	0.43
1:C:766:VAL:HB	1:C:778:VAL:CG2	2.47	0.43
1:D:494:LEU:O	1:D:497:ILE:HG22	2.18	0.43
1:F:180:TRP:HB2	1:F:291:ALA:HB3	1.99	0.43
1:F:403:LEU:HD21	1:F:1010:MET:HE1	2.00	0.43
1:F:853:ARG:O	1:F:857:GLN:HG3	2.17	0.43
1:F:979:LEU:HG	1:F:983:LEU:HD22	2.00	0.43
1:A:72:ASN:ND2	1:C:170:ARG:HH21	2.16	0.43
1:B:691:GLN:HG2	1:B:868:THR:CG2	2.49	0.43
1:C:35:SER:OG	1:C:37:TYR:O	2.35	0.43
1:C:576:ASP:OD2	1:C:645:ARG:NH2	2.45	0.43
1:C:937:ILE:HD12	1:C:937:ILE:HA	1.75	0.43
1:D:382:THR:HG23	1:D:478:ILE:CG2	2.48	0.43
1:E:7:PHE:HE1	1:E:13:PHE:CD1	2.36	0.43
1:E:731:VAL:HG21	1:E:821:GLU:HB2	2.00	0.43
1:F:859:LEU:HB3	1:F:863:VAL:HG13	2.00	0.43
1:A:791:ASP:C	1:A:793:ILE:N	2.73	0.43
1:B:418:ASN:OD1	1:B:421:ARG:NH1	2.50	0.43
1:C:659:LEU:HD12	1:C:663:TYR:CZ	2.54	0.43
2:C:1101:LMT:H41	2:C:1101:LMT:H71	1.69	0.43
1:D:566:ILE:HD13	1:D:566:ILE:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:921:LEU:HA	1:D:924:VAL:HG12	2.00	0.43
1:E:215:VAL:HG22	1:E:216:GLN:O	2.17	0.43
1:E:451:LEU:HA	1:E:451:LEU:HD23	1.61	0.43
1:E:781:GLN:HG2	1:E:782:ALA:O	2.19	0.43
1:E:993:VAL:HG11	1:E:1015:PHE:HB2	2.00	0.43
1:F:997:VAL:CG2	1:F:1012:VAL:HG22	2.48	0.43
1:A:20:ILE:HD13	2:B:1101:LMT:H112	2.01	0.43
1:A:435:LYS:O	1:A:439:GLU:HG3	2.18	0.43
1:A:629:SER:HB2	1:A:822:MET:CE	2.48	0.43
1:B:34:ILE:HD13	1:B:301:ASN:CG	2.44	0.43
1:B:783:ASP:OD1	1:B:784:ALA:N	2.50	0.43
1:C:509:LEU:HA	1:C:512:VAL:CG1	2.47	0.43
1:C:934:PHE:O	1:C:937:ILE:HG22	2.19	0.43
1:E:285:ASP:OD1	1:E:607:LEU:HD21	2.19	0.43
1:E:685:LEU:HD12	1:E:686:GLY:H	1.84	0.43
1:F:50:GLN:HG2	1:F:52:PRO:HD3	1.99	0.43
1:B:428:THR:HG23	1:B:431:ALA:HB3	2.00	0.43
1:D:45:VAL:HG22	1:D:106:THR:HG22	1.99	0.43
1:D:685:LEU:HG	1:D:686:GLY:N	2.32	0.43
1:E:139:THR:O	1:E:332:PRO:HD2	2.19	0.43
1:E:218:ALA:HB2	1:F:51:TYR:CE1	2.54	0.43
1:E:335:PHE:CE2	1:E:577:LYS:HE2	2.53	0.43
1:E:808:LEU:O	1:E:812:VAL:HG22	2.19	0.43
1:E:905:LEU:HD23	1:E:905:LEU:HA	1.70	0.43
1:A:133:LYS:HE2	1:A:133:LYS:HB3	1.85	0.43
1:A:556:LEU:CB	1:A:915:MET:HE1	2.49	0.43
1:A:579:TYR:HA	1:A:639:LEU:HD12	2.01	0.43
1:B:553:TYR:HD1	1:B:915:MET:HE2	1.83	0.43
1:B:712:LYS:O	1:B:712:LYS:HG2	2.18	0.43
1:C:917:ILE:HA	1:C:939:LEU:CD2	2.49	0.43
1:C:983:LEU:O	1:C:987:ILE:HG12	2.18	0.43
1:C:983:LEU:HD23	1:C:983:LEU:HA	1.76	0.43
1:D:920:ALA:HB2	1:D:942:LEU:HD12	2.00	0.43
1:E:365:TRP:CZ3	1:E:369:ILE:HD11	2.54	0.43
1:E:465:THR:HG22	1:E:469:TYR:CE1	2.54	0.43
1:E:783:ASP:HB3	1:E:786:PHE:CD2	2.54	0.43
1:E:952:LEU:HA	1:E:952:LEU:HD23	1.63	0.43
1:F:228:LEU:CG	1:F:229:PRO:HD3	2.49	0.43
1:F:283:LEU:HD13	1:F:286:ASN:HA	2.01	0.43
1:F:924:VAL:HG23	1:F:1013:ALA:HB2	2.01	0.43
1:F:1010:MET:HE3	1:F:1014:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:HG21	1:A:303:LEU:CD2	2.48	0.43
1:A:353:LEU:CD2	1:A:991:MET:HE2	2.49	0.43
1:A:443:PRO:O	1:A:447:ILE:HG23	2.19	0.43
1:B:67:LEU:HD23	1:B:116:ALA:HB3	2.01	0.43
1:B:70:GLN:HG2	1:B:115:GLN:HB2	2.01	0.43
1:B:453:ALA:O	1:B:888:SER:HB2	2.19	0.43
1:C:764:LEU:HG	1:C:765:TYR:N	2.33	0.43
1:D:351:ILE:HD11	1:D:376:PRO:HG3	2.01	0.43
1:D:370:ILE:HD11	1:D:495:SER:HA	2.01	0.43
1:F:1010:MET:HE2	1:F:1010:MET:HB3	1.88	0.43
1:A:1006:MET:O	1:A:1009:ALA:HB3	2.19	0.43
1:B:101:ASP:O	1:B:104:LYS:HG2	2.19	0.43
1:B:859:LEU:HD23	1:B:859:LEU:HA	1.82	0.43
1:C:350:ALA:O	1:C:354:VAL:HG13	2.18	0.43
1:C:609:GLN:NE2	1:C:610:PRO:HD2	2.34	0.43
1:D:74:VAL:HG12	1:D:77:MET:HE3	2.00	0.43
1:D:494:LEU:HA	1:D:497:ILE:HG22	2.01	0.43
1:D:527:VAL:O	1:D:530:ARG:HB3	2.18	0.43
1:D:742:LYS:HG3	1:D:745:GLN:HE21	1.82	0.43
1:D:750:VAL:HG11	1:F:213:GLN:HG2	2.00	0.43
1:E:597:LYS:N	1:E:597:LYS:HD2	2.34	0.43
1:E:684:THR:OG1	1:E:687:GLY:N	2.50	0.43
1:F:535:TYR:CE1	1:F:1027:MET:HE1	2.54	0.43
1:A:462:SER:OG	1:A:877:ALA:HB1	2.18	0.42
1:A:546:LYS:O	1:A:549:MET:HB2	2.19	0.42
1:B:629:SER:HB2	1:B:822:MET:CE	2.49	0.42
1:D:1:MET:HE3	2:D:1101:LMT:O2'	2.18	0.42
1:D:980:ARG:O	1:D:984:MET:HG3	2.18	0.42
1:E:752:ASP:O	1:E:756:THR:OG1	2.37	0.42
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.90	0.42
1:B:937:ILE:HD12	1:B:937:ILE:HA	1.93	0.42
1:C:810:SER:C	1:C:811:LEU:HD12	2.44	0.42
1:C:1008:HIS:O	1:C:1010:MET:N	2.52	0.42
1:D:354:VAL:HG23	1:D:413:ILE:HD11	2.01	0.42
1:D:535:TYR:O	1:D:539:VAL:HG23	2.18	0.42
1:D:599:ILE:CG2	1:D:617:ALA:HB1	2.49	0.42
1:D:704:ALA:HB2	1:D:727:TYR:HE2	1.84	0.42
1:E:707:THR:O	1:E:711:ILE:HG22	2.19	0.42
1:F:67:LEU:HD23	1:F:116:ALA:HB3	2.00	0.42
1:B:307:ASP:OD2	2:B:1102:LMT:H2B	2.19	0.42
1:B:406:GLY:HA3	1:B:989:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:ASN:OD1	1:B:751:THR:HG22	2.19	0.42
1:C:611:GLY:HA3	1:C:655:ILE:CD1	2.49	0.42
1:C:1010:MET:HA	1:C:1013:ALA:HB3	2.01	0.42
1:D:192:ASP:O	1:D:195:LYS:N	2.52	0.42
1:D:264:HIS:N	1:D:267:ASP:OD2	2.45	0.42
1:D:760:TYR:HD1	1:D:782:ALA:HB2	1.85	0.42
1:E:937:ILE:HD12	1:E:937:ILE:HA	1.82	0.42
1:F:78:LEU:HD12	1:F:78:LEU:HA	1.70	0.42
1:F:205:ASP:OD1	1:F:208:ARG:NH2	2.53	0.42
1:A:74:VAL:CG1	1:A:77:MET:HB2	2.50	0.42
1:A:360:VAL:HG22	1:A:520:PHE:HE2	1.84	0.42
1:A:450:THR:O	1:A:454:VAL:HG23	2.19	0.42
1:C:87:ASP:CG	1:C:89:ASN:HD22	2.28	0.42
1:C:189:VAL:O	1:C:780:VAL:O	2.37	0.42
1:C:284:LEU:CD2	1:C:327:ARG:HD2	2.49	0.42
1:C:682:LEU:HD22	1:C:685:LEU:HD21	2.01	0.42
1:D:879:ASP:N	1:D:879:ASP:OD1	2.52	0.42
1:E:51:TYR:C	1:E:51:TYR:CD1	2.98	0.42
1:E:187:MET:O	1:E:778:VAL:HA	2.19	0.42
1:E:399:PHE:O	1:E:402:VAL:HG22	2.19	0.42
1:F:393:ILE:HG23	1:F:398:LEU:HD21	2.01	0.42
1:F:601:ASP:O	1:F:605:ILE:HG12	2.18	0.42
1:A:488:LEU:HA	1:A:488:LEU:HD12	1.84	0.42
1:C:402:VAL:O	1:C:405:ILE:HB	2.20	0.42
1:C:579:TYR:CE2	1:C:676:PRO:HB3	2.54	0.42
1:C:992:GLY:C	1:C:995:PRO:HD2	2.45	0.42
1:D:70:GLN:CG	1:D:116:ALA:HB2	2.49	0.42
1:D:458:LEU:HD11	1:D:885:PHE:HE1	1.85	0.42
1:D:461:MET:HG2	1:D:880:SER:OG	2.19	0.42
1:E:362:LEU:O	1:E:364:THR:HG22	2.19	0.42
1:E:698:VAL:O	1:E:702:ARG:HD3	2.19	0.42
1:F:38:PRO:HG3	1:F:471:GLN:CG	2.50	0.42
1:F:509:LEU:HA	1:F:512:VAL:HG12	2.02	0.42
1:F:575:GLN:HG3	1:F:1005:GLU:HB2	2.01	0.42
1:F:788:GLN:O	1:F:789:ARG:O	2.38	0.42
1:A:691:GLN:HG3	1:A:826:TYR:CD2	2.54	0.42
1:B:16:VAL:HG13	1:C:894:LEU:HB3	2.02	0.42
1:B:455:PHE:O	1:B:458:LEU:HB2	2.19	0.42
1:C:388:LEU:HD23	1:C:389:PHE:CE1	2.55	0.42
1:C:868:THR:O	1:C:871:THR:HG23	2.20	0.42
1:C:961:GLU:OE2	1:C:1037:ARG:NE	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:TYR:CD2	1:D:332:PRO:HD3	2.54	0.42
1:E:1004:ALA:CB	1:E:1007:ARG:HD2	2.49	0.42
1:F:2:ASN:OD1	1:F:438:GLN:NE2	2.47	0.42
1:A:168:LEU:HD11	1:A:313:MET:HE3	2.02	0.42
1:A:666:LEU:HA	1:A:666:LEU:HD23	1.76	0.42
1:A:684:THR:O	1:A:686:GLY:N	2.53	0.42
1:B:90:MET:SD	1:B:92:ILE:HG13	2.59	0.42
1:D:50:GLN:O	1:D:124:VAL:HG13	2.20	0.42
1:D:227:THR:HG22	1:D:229:PRO:HD2	2.02	0.42
1:D:455:PHE:CE1	1:D:940:MET:HB3	2.55	0.42
1:E:70:GLN:HG3	1:E:116:ALA:CB	2.43	0.42
1:E:251:ASP:OD1	1:E:266:ARG:NH1	2.46	0.42
1:F:85:ASN:ND2	1:F:627:THR:HB	2.35	0.42
1:F:516:VAL:HG12	1:F:517:LEU:HG	2.01	0.42
1:F:691:GLN:HG2	1:F:826:TYR:CB	2.50	0.42
1:A:952:LEU:HD23	1:A:952:LEU:HA	1.67	0.42
1:B:343:VAL:HG11	1:B:401:MET:HE3	2.02	0.42
1:B:363:GLN:HB3	1:B:521:PHE:CE2	2.55	0.42
1:B:543:LEU:HD23	1:B:543:LEU:HA	1.75	0.42
1:C:202:THR:HG22	1:C:798:THR:HA	2.02	0.42
1:C:986:SER:O	1:C:990:ILE:HG12	2.19	0.42
1:D:17:LEU:HD13	1:D:485:PHE:HZ	1.84	0.42
1:D:218:ALA:HB3	1:E:758:GLN:CD	2.45	0.42
1:D:704:ALA:HB2	1:D:727:TYR:CE2	2.54	0.42
1:E:333:THR:O	1:E:336:VAL:HG12	2.20	0.42
1:E:620:GLY:HA2	1:E:629:SER:O	2.20	0.42
1:F:34:ILE:HG12	1:F:393:ILE:HB	2.02	0.42
1:F:191:LEU:HD21	1:F:206:VAL:HG11	2.01	0.42
1:F:417:GLU:CG	1:F:984:MET:HE1	2.48	0.42
1:F:577:LYS:HD2	1:F:577:LYS:HA	1.73	0.42
1:F:921:LEU:HD23	1:F:921:LEU:HA	1.79	0.42
1:F:1012:VAL:HG12	1:F:1016:PHE:CE2	2.55	0.42
1:A:82:SER:CB	1:A:92:ILE:HG12	2.49	0.42
1:A:144:LEU:HA	1:A:144:LEU:HD23	1.82	0.42
1:A:145:ILE:HD12	1:A:284:LEU:HD23	2.01	0.42
1:B:370:ILE:CD1	1:B:494:LEU:HB3	2.49	0.42
1:C:1039:LEU:HD13	1:C:1039:LEU:HA	1.89	0.42
1:D:659:LEU:HD23	1:D:659:LEU:HA	1.82	0.42
1:F:579:TYR:HA	1:F:639:LEU:HD12	2.02	0.42
1:F:772:PHE:O	1:F:772:PHE:CG	2.71	0.42
1:A:268:ILE:HD12	1:A:268:ILE:HA	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:LEU:HD23	1:A:659:LEU:HA	1.83	0.42
1:B:599:ILE:HD13	1:B:602:MET:HE2	2.02	0.42
1:C:196:VAL:HG22	1:C:268:ILE:HB	2.01	0.42
1:C:738:LEU:HD23	1:C:812:VAL:HG13	2.02	0.42
1:C:742:LYS:HA	1:C:745:GLN:HG2	2.02	0.42
1:D:385:LEU:HD23	1:D:385:LEU:HA	1.82	0.42
1:D:588:ASN:HB3	1:D:731:VAL:HA	2.02	0.42
1:E:78:LEU:HA	1:E:78:LEU:HD23	1.65	0.42
1:E:838:PRO:HB3	1:E:847:ALA:HB2	2.01	0.42
1:F:800:ASN:OD1	1:F:803:GLY:N	2.53	0.42
1:A:192:ASP:O	1:A:196:VAL:HG23	2.20	0.41
1:A:195:LYS:HB3	1:A:268:ILE:HD12	2.01	0.41
1:B:463:GLY:O	1:B:467:GLN:HG2	2.20	0.41
1:B:728:GLN:O	1:B:820:PRO:HA	2.20	0.41
1:B:904:THR:HB	1:B:1036:LEU:HD12	2.00	0.41
1:C:808:LEU:HB2	1:C:812:VAL:HG22	2.02	0.41
1:D:187:MET:HB3	1:D:778:VAL:HG12	2.02	0.41
1:D:766:VAL:HB	1:D:778:VAL:CG2	2.49	0.41
1:E:303:LEU:HD21	1:E:336:VAL:CG1	2.50	0.41
1:E:443:PRO:HG3	1:E:955:GLU:HG2	2.01	0.41
1:E:500:LYS:HA	1:E:504:ASP:OD2	2.19	0.41
1:F:938:GLY:HA2	1:F:1010:MET:HE3	2.02	0.41
1:F:1039:LEU:HD23	1:F:1039:LEU:HA	1.89	0.41
1:B:187:MET:O	1:B:778:VAL:HA	2.20	0.41
1:B:430:ARG:HG2	1:B:434:TYR:CE2	2.55	0.41
1:B:766:VAL:HB	1:B:778:VAL:CG2	2.50	0.41
1:B:909:VAL:O	1:B:912:ILE:HG22	2.20	0.41
1:E:104:LYS:HA	1:E:104:LYS:HD3	1.90	0.41
1:F:375:VAL:O	1:F:379:ILE:HG12	2.19	0.41
1:F:934:PHE:O	1:F:937:ILE:HG22	2.19	0.41
1:F:986:SER:OG	1:F:1022:THR:HG22	2.20	0.41
1:A:144:LEU:HD12	1:A:160:ALA:HB2	2.02	0.41
1:B:63:VAL:HG13	1:B:120:LEU:HD12	2.02	0.41
1:D:391:TYR:OH	1:D:474:MET:HG2	2.21	0.41
1:D:465:THR:O	1:D:469:TYR:HD1	2.04	0.41
1:E:202:THR:HG22	1:E:805:MET:HE1	2.03	0.41
1:E:358:VAL:HG13	1:E:362:LEU:HD22	2.02	0.41
1:F:40:VAL:HB	1:F:464:LEU:HD11	2.01	0.41
1:F:104:LYS:O	1:F:107:GLN:HB3	2.20	0.41
1:F:120:LEU:HB3	1:F:124:VAL:CG2	2.51	0.41
1:B:222:ILE:HG23	1:C:787:ARG:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:ILE:O	1:C:781:GLN:HA	2.21	0.41
1:C:1028:LEU:HD22	1:C:1032:PHE:CZ	2.56	0.41
1:D:405:ILE:O	1:D:409:VAL:HG22	2.20	0.41
2:D:1101:LMT:H6E	1:F:10:ARG:NH1	2.35	0.41
1:E:82:SER:HB3	1:E:92:ILE:HG12	2.03	0.41
1:F:204:ASP:HA	1:F:207:VAL:HG12	2.03	0.41
1:F:867:TRP:CE3	1:F:871:THR:HG21	2.55	0.41
1:A:214:ASN:O	1:A:767:ASN:ND2	2.54	0.41
1:B:98:LEU:HD22	1:B:99:GLY:H	1.85	0.41
1:C:254:VAL:HG11	1:C:268:ILE:HD11	2.02	0.41
1:C:808:LEU:HD12	1:C:812:VAL:HG21	2.03	0.41
1:D:403:LEU:HB3	1:D:941:VAL:HG21	2.03	0.41
1:D:999:SER:CB	1:D:1004:ALA:HB2	2.47	0.41
1:F:682:LEU:HD11	1:F:870:LEU:HD13	2.02	0.41
1:F:870:LEU:O	1:F:873:GLN:HB2	2.21	0.41
1:F:1012:VAL:HG12	1:F:1016:PHE:HE2	1.84	0.41
1:B:369:ILE:HD12	1:B:369:ILE:H	1.86	0.41
1:B:444:ILE:HG21	1:B:488:LEU:HD13	2.02	0.41
1:B:500:LYS:HD2	1:B:504:ASP:O	2.19	0.41
1:B:688:PHE:HB2	1:B:867:TRP:CZ3	2.53	0.41
1:B:718:PRO:C	1:B:720:LEU:H	2.28	0.41
1:B:907:LEU:HB3	1:B:911:LEU:CD2	2.47	0.41
1:C:748:VAL:HG21	1:C:811:LEU:CD2	2.51	0.41
1:C:903:LEU:HD23	1:C:903:LEU:HA	1.79	0.41
1:C:942:LEU:HD23	1:C:942:LEU:HA	1.87	0.41
1:D:55:ASN:ND2	1:F:238:ASN:OD1	2.54	0.41
1:D:583:PHE:O	1:D:671:VAL:HA	2.21	0.41
1:E:645:ARG:CD	1:E:650:LEU:HD21	2.50	0.41
1:F:49:ALA:HB2	1:F:129:ILE:HD12	2.02	0.41
1:A:111:ASN:OD1	1:C:107:GLN:HG3	2.19	0.41
1:A:232:PRO:O	1:A:233:LEU:HD23	2.21	0.41
1:A:583:PHE:CD1	1:A:623:VAL:HG22	2.55	0.41
1:A:737:ASP:HB3	1:A:813:THR:CG2	2.45	0.41
1:A:905:LEU:HA	1:A:905:LEU:HD12	1.68	0.41
1:A:920:ALA:HB3	1:A:939:LEU:HD11	2.02	0.41
1:B:160:ALA:HA	1:B:164:VAL:HB	2.03	0.41
1:B:399:PHE:O	1:B:402:VAL:HG22	2.21	0.41
1:C:213:GLN:OE1	1:C:252:ILE:HA	2.21	0.41
1:D:614:SER:HB2	1:D:638:THR:OG1	2.21	0.41
1:D:794:LEU:HB3	1:D:809:SER:HB3	2.02	0.41
1:F:36:GLU:HG2	1:F:37:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:ASN:O	1:F:162:ILE:HG12	2.19	0.41
1:F:942:LEU:HD13	1:F:1017:GLY:HA3	2.02	0.41
1:A:34:ILE:HG21	1:A:303:LEU:HD22	2.03	0.41
1:A:690:MET:HE3	1:A:851:VAL:CG1	2.51	0.41
1:A:1015:PHE:HD1	1:A:1016:PHE:CD1	2.39	0.41
1:B:101:ASP:N	1:B:104:LYS:HE2	2.25	0.41
1:B:362:LEU:HG	1:B:420:GLU:HG2	2.02	0.41
1:B:417:GLU:OE2	1:B:980:ARG:HD2	2.21	0.41
1:B:609:GLN:CD	1:B:610:PRO:HD2	2.46	0.41
1:C:325:ASP:OD1	1:C:326:TYR:N	2.52	0.41
1:C:464:LEU:HD22	1:C:571:PHE:CZ	2.56	0.41
1:D:98:LEU:HD12	1:D:99:GLY:H	1.84	0.41
1:F:38:PRO:HD3	1:F:394:ASN:CG	2.46	0.41
1:A:87:ASP:OD2	1:A:89:ASN:ND2	2.51	0.41
1:A:124:VAL:HG12	1:A:129:ILE:HD11	2.02	0.41
1:A:512:VAL:O	1:A:516:VAL:HG12	2.20	0.41
1:A:759:ILE:HD13	1:A:759:ILE:HG21	1.88	0.41
1:A:768:ASP:OD2	1:B:119:ARG:HG3	2.20	0.41
1:A:872:TYR:O	1:A:875:ILE:HG22	2.21	0.41
1:B:444:ILE:HD13	1:B:487:SER:HB3	2.03	0.41
1:B:659:LEU:HD23	1:B:659:LEU:HA	1.92	0.41
1:B:901:GLU:O	1:B:901:GLU:HG3	2.21	0.41
1:C:34:ILE:HG21	1:C:303:LEU:CD2	2.51	0.41
1:C:611:GLY:HA3	1:C:655:ILE:HD11	2.03	0.41
1:C:677:PRO:HA	1:C:678:PRO:HD3	1.94	0.41
1:C:717:ALA:HB3	1:C:854:ILE:HD11	2.02	0.41
1:C:763:SER:CA	1:C:781:GLN:HB2	2.51	0.41
1:D:51:TYR:CD1	1:D:51:TYR:C	2.99	0.41
1:D:78:LEU:HD12	1:D:78:LEU:HA	1.75	0.41
1:D:90:MET:SD	1:D:92:ILE:HG13	2.61	0.41
1:D:221:VAL:HG12	1:D:236:SER:HA	2.03	0.41
1:D:612:VAL:HG13	1:D:637:VAL:HG12	2.03	0.41
1:D:704:ALA:HA	1:D:707:THR:CG2	2.50	0.41
1:E:571:PHE:O	1:E:932:ASN:HB2	2.21	0.41
1:E:1026:LEU:HD23	1:E:1026:LEU:HA	1.91	0.41
1:F:127:LEU:HD23	1:F:127:LEU:HA	1.90	0.41
1:F:192:ASP:O	1:F:196:VAL:HG12	2.21	0.41
1:F:543:LEU:HA	1:F:543:LEU:HD23	1.53	0.41
1:F:659:LEU:HB3	1:F:673:VAL:HG21	2.02	0.41
1:F:871:THR:O	1:F:874:GLN:HB2	2.20	0.41
1:A:500:LYS:HE3	1:A:505:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:VAL:O	1:A:912:ILE:HG22	2.21	0.41
1:B:6:PHE:O	1:B:10:ARG:HD2	2.21	0.41
1:B:150:SER:HB2	1:B:151:TYR:HD1	1.86	0.41
1:C:142:VAL:HG11	1:C:313:MET:SD	2.61	0.41
1:C:934:PHE:C	1:C:1010:MET:HE2	2.46	0.41
1:D:343:VAL:HG21	1:D:398:LEU:HB3	2.02	0.41
1:E:388:LEU:HD23	1:E:389:PHE:CE1	2.56	0.41
1:E:717:ALA:HB3	1:E:720:LEU:HD23	2.03	0.41
1:E:807:PRO:O	1:E:810:SER:OG	2.38	0.41
1:E:878:GLY:O	1:E:880:SER:N	2.51	0.41
1:F:193:PRO:HD2	1:F:786:PHE:CG	2.56	0.41
1:F:254:VAL:HG11	1:F:268:ILE:HD11	2.01	0.41
1:F:524:PHE:HA	1:F:527:VAL:HG12	2.03	0.41
1:F:783:ASP:OD1	1:F:784:ALA:N	2.52	0.41
1:A:139:THR:O	1:A:332:PRO:HD2	2.21	0.40
1:B:359:ILE:O	1:B:363:GLN:HA	2.20	0.40
1:B:916:SER:HB3	1:B:1021:VAL:HG22	2.02	0.40
1:C:341:LYS:HA	1:C:341:LYS:HD3	1.45	0.40
1:C:682:LEU:HD12	1:C:683:GLY:N	2.36	0.40
1:E:919:SER:HB3	1:E:1020:GLY:HA3	2.02	0.40
1:F:952:LEU:HD23	1:F:952:LEU:HA	1.92	0.40
1:F:1000:THR:HG22	1:F:1004:ALA:HB1	2.02	0.40
1:A:375:VAL:N	1:A:376:PRO:HD2	2.36	0.40
1:A:648:LYS:C	1:A:650:LEU:N	2.79	0.40
1:A:842:TYR:HB3	1:A:846:GLN:CD	2.45	0.40
1:B:903:LEU:HD23	1:B:903:LEU:HA	1.89	0.40
1:C:190:TRP:HB3	1:C:783:ASP:HA	2.03	0.40
1:C:710:PHE:CE2	1:C:834:VAL:HG21	2.56	0.40
1:C:910:ILE:O	1:C:913:VAL:HG22	2.21	0.40
1:D:168:LEU:HD11	1:D:313:MET:HE3	2.04	0.40
1:D:225:SER:HB3	1:E:278:TYR:CB	2.51	0.40
1:D:436:ALA:O	1:D:440:VAL:HG22	2.20	0.40
1:E:249:PHE:CZ	1:E:778:VAL:HG11	2.56	0.40
1:F:32:LEU:HD13	1:F:393:ILE:CD1	2.41	0.40
1:F:407:ILE:HD11	1:F:941:VAL:HG13	2.03	0.40
1:F:449:LEU:HA	1:F:449:LEU:HD23	1.65	0.40
1:F:533:GLU:OE1	1:F:533:GLU:N	2.55	0.40
1:A:80:MET:HE3	1:A:80:MET:HB2	1.86	0.40
1:A:403:LEU:HA	1:A:403:LEU:HD23	1.89	0.40
1:A:457:PRO:HG2	1:A:888:SER:HB2	2.02	0.40
1:A:786:PHE:O	1:A:792:ASP:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ILE:HG23	1:B:147:PRO:HG3	2.03	0.40
1:C:31:LEU:HB2	1:C:387:LEU:CD1	2.51	0.40
1:C:312:THR:O	1:C:316:LEU:HG	2.21	0.40
1:C:452:VAL:HG13	1:C:456:VAL:HG21	2.02	0.40
1:C:543:LEU:HD23	1:C:543:LEU:HA	1.77	0.40
1:D:144:LEU:HD23	1:D:144:LEU:HA	1.87	0.40
1:D:214:ASN:HB2	1:D:243:LEU:HD22	2.04	0.40
1:D:218:ALA:HB2	1:E:51:TYR:CE1	2.56	0.40
1:D:229:PRO:HD2	1:D:231:THR:OG1	2.22	0.40
1:D:640:LYS:O	1:D:645:ARG:HD3	2.21	0.40
1:D:942:LEU:HD23	1:D:942:LEU:HA	1.91	0.40
1:F:181:GLY:HA2	1:F:282:SER:HB2	2.02	0.40
1:F:469:TYR:O	1:F:470:LYS:C	2.64	0.40
1:F:965:LYS:HB3	1:F:969:GLU:HG3	2.03	0.40
1:F:1015:PHE:CD1	1:F:1015:PHE:C	2.99	0.40
1:A:698:VAL:CG1	1:A:702:ARG:HB3	2.50	0.40
1:B:56:PRO:HD3	1:B:86:SER:HA	2.02	0.40
1:B:347:LEU:HD22	2:B:1102:LMT:H123	2.04	0.40
1:B:421:ARG:HE	1:B:977:LEU:CD1	2.34	0.40
1:B:535:TYR:OH	1:B:975:SER:HB2	2.21	0.40
1:B:688:PHE:CE2	1:B:837:GLY:HA2	2.57	0.40
1:B:876:LEU:HD23	1:B:876:LEU:HA	1.83	0.40
1:C:60:ALA:O	1:C:65:SER:OG	2.40	0.40
1:C:1008:HIS:C	1:C:1010:MET:N	2.80	0.40
1:D:68:GLU:HA	1:D:80:MET:HE1	2.02	0.40
1:E:191:LEU:HD21	1:E:206:VAL:HG21	2.03	0.40
1:E:191:LEU:CD2	1:E:269:ALA:HB2	2.51	0.40
1:E:417:GLU:OE2	1:E:980:ARG:HD2	2.22	0.40
1:E:650:LEU:O	1:E:651:SER:C	2.63	0.40
1:F:144:LEU:HD12	1:F:160:ALA:HB2	2.02	0.40
1:F:214:ASN:O	1:F:767:ASN:ND2	2.55	0.40
1:F:736:VAL:CG1	1:F:757:MET:HE1	2.39	0.40
1:A:278:TYR:HB3	1:C:225:SER:HB3	2.02	0.40
1:A:556:LEU:O	1:A:560:THR:HG23	2.22	0.40
1:B:365:TRP:CE3	1:B:369:ILE:HD11	2.57	0.40
1:B:922:THR:O	1:B:926:LEU:N	2.50	0.40
1:C:577:LYS:HD2	1:C:577:LYS:HA	1.91	0.40
1:C:606:ALA:HA	1:C:659:LEU:HD11	2.04	0.40
1:C:952:LEU:HD23	1:C:952:LEU:HA	1.61	0.40
1:D:49:ALA:CB	1:D:129:ILE:HD12	2.51	0.40
1:D:406:GLY:CA	1:D:989:PHE:HZ	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:ARG:HG2	1:D:434:TYR:CE2	2.56	0.40
1:D:620:GLY:O	1:D:628:ASN:HA	2.21	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:B:792:ASP:OD1	1:F:789:ARG:NH2[1_565]	2.00	0.20

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1040/1067 (98%)	983 (94%)	51 (5%)	6 (1%)	21	56
1	B	1040/1067 (98%)	985 (95%)	50 (5%)	5 (0%)	24	60
1	C	1041/1067 (98%)	984 (94%)	55 (5%)	2 (0%)	43	76
1	D	1040/1067 (98%)	989 (95%)	47 (4%)	4 (0%)	30	65
1	E	1040/1067 (98%)	989 (95%)	47 (4%)	4 (0%)	30	65
1	F	1041/1067 (98%)	993 (95%)	46 (4%)	2 (0%)	43	76
All	All	6242/6402 (98%)	5923 (95%)	296 (5%)	23 (0%)	30	65

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	685	LEU
1	B	869	ASP
1	B	645	ARG
1	B	870	LEU
1	C	229	PRO
1	C	781	GLN

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Mol	Chain	Res	Type
1	D	881	ALA
1	E	651	SER
1	A	507	ASP
1	B	171	ILE
1	D	182	ALA
1	A	879	ASP
1	D	869	ASP
1	E	274	ASP
1	E	697	ALA
1	D	839	ALA
1	E	49	ALA
1	F	684	THR
1	A	328	ILE
1	A	839	ALA
1	F	393	ILE
1	B	717	ALA
1	A	625	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	849/868 (98%)	783 (92%)	66 (8%)	11	39
1	B	849/868 (98%)	789 (93%)	60 (7%)	13	43
1	C	850/868 (98%)	784 (92%)	66 (8%)	11	39
1	D	849/868 (98%)	792 (93%)	57 (7%)	15	46
1	E	849/868 (98%)	773 (91%)	76 (9%)	9	34
1	F	850/868 (98%)	780 (92%)	70 (8%)	10	37
All	All	5096/5208 (98%)	4701 (92%)	395 (8%)	11	39

All (395) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE

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Mol	Chain	Res	Type
1	A	26	MET
1	A	27	ILE
1	A	31	LEU
1	A	41	VAL
1	A	117	LEU
1	A	132	VAL
1	A	134	SER
1	A	150	SER
1	A	189	VAL
1	A	207	VAL
1	A	217	VAL
1	A	228	LEU
1	A	236	SER
1	A	243	LEU
1	A	254	VAL
1	A	263	THR
1	A	268	ILE
1	A	303	LEU
1	A	313	MET
1	A	324	VAL
1	A	354	VAL
1	A	364	THR
1	A	401	MET
1	A	407	ILE
1	A	409	VAL
1	A	464	LEU
1	A	465	THR
1	A	474	MET
1	A	488	LEU
1	A	510	THR
1	A	517	LEU
1	A	533	GLU
1	A	546	LYS
1	A	552	LEU
1	A	554	LEU
1	A	560	THR
1	A	572	VAL
1	A	623	VAL
1	A	685	LEU
1	A	690	MET
1	A	735	ASN
1	A	748	VAL

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Mol	Chain	Res	Type
1	A	756	THR
1	A	766	VAL
1	A	778	VAL
1	A	791	ASP
1	A	812	VAL
1	A	813	THR
1	A	864	LYS
1	A	870	LEU
1	A	884	VAL
1	A	889	VAL
1	A	892	VAL
1	A	907	LEU
1	A	916	SER
1	A	924	VAL
1	A	927	THR
1	A	955	GLU
1	A	966	THR
1	A	993	VAL
1	A	1000	THR
1	A	1006	MET
1	A	1010	MET
1	A	1012	VAL
1	A	1027	MET
1	B	2	ASN
1	B	3	ILE
1	B	40	VAL
1	B	41	VAL
1	B	94	VAL
1	B	110	GLN
1	B	113	VAL
1	B	119	ARG
1	B	124	VAL
1	B	132	VAL
1	B	206	VAL
1	B	221	VAL
1	B	228	LEU
1	B	252	ILE
1	B	254	VAL
1	B	273	LEU
1	B	292	MET
1	B	337	ARG
1	B	348	LEU

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Mol	Chain	Res	Type
1	B	364	THR
1	B	401	MET
1	B	402	VAL
1	B	409	VAL
1	B	414	VAL
1	B	428	THR
1	B	474	MET
1	B	488	LEU
1	B	490	LEU
1	B	494	LEU
1	B	498	LEU
1	B	506	GLU
1	B	510	THR
1	B	511	ARG
1	B	512	VAL
1	B	546	LYS
1	B	561	LEU
1	B	673	VAL
1	B	690	MET
1	B	731	VAL
1	B	735	ASN
1	B	778	VAL
1	B	811	LEU
1	B	813	THR
1	B	834	VAL
1	B	835	ASN
1	B	851	VAL
1	B	863	VAL
1	B	864	LYS
1	B	870	LEU
1	B	875	ILE
1	B	888	SER
1	B	899	LEU
1	B	916	SER
1	B	927	THR
1	B	943	VAL
1	B	983	LEU
1	B	1000	THR
1	B	1018	MET
1	B	1019	LEU
1	B	1027	MET
1	C	74	VAL

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Mol	Chain	Res	Type
1	C	109	VAL
1	C	113	VAL
1	C	117	LEU
1	C	124	VAL
1	C	127	LEU
1	C	134	SER
1	C	154	THR
1	C	217	VAL
1	C	227	THR
1	C	243	LEU
1	C	252	ILE
1	C	254	VAL
1	C	256	THR
1	C	263	THR
1	C	303	LEU
1	C	346	THR
1	C	354	VAL
1	C	357	VAL
1	C	364	THR
1	C	402	VAL
1	C	407	ILE
1	C	450	THR
1	C	465	THR
1	C	474	MET
1	C	546	LYS
1	C	554	LEU
1	C	556	LEU
1	C	561	LEU
1	C	563	VAL
1	C	616	VAL
1	C	637	VAL
1	C	659	LEU
1	C	666	LEU
1	C	679	VAL
1	C	685	LEU
1	C	698	VAL
1	C	705	ASP
1	C	735	ASN
1	C	741	VAL
1	C	748	VAL
1	C	751	THR
1	C	756	THR

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Mol	Chain	Res	Type
1	C	780	VAL
1	C	791	ASP
1	C	809	SER
1	C	812	VAL
1	C	834	VAL
1	C	835	ASN
1	C	858	THR
1	C	863	VAL
1	C	864	LYS
1	C	869	ASP
1	C	871	THR
1	C	884	VAL
1	C	887	ILE
1	C	905	LEU
1	C	912	ILE
1	C	916	SER
1	C	948	LYS
1	C	963	ASP
1	C	1010	MET
1	C	1012	VAL
1	C	1022	THR
1	C	1027	MET
1	C	1034	VAL
1	D	3	ILE
1	D	23	LEU
1	D	26	MET
1	D	40	VAL
1	D	41	VAL
1	D	67	LEU
1	D	113	VAL
1	D	124	VAL
1	D	134	SER
1	D	196	VAL
1	D	207	VAL
1	D	221	VAL
1	D	228	LEU
1	D	236	SER
1	D	243	LEU
1	D	263	THR
1	D	268	ILE
1	D	313	MET
1	D	346	THR

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Mol	Chain	Res	Type
1	D	364	THR
1	D	370	ILE
1	D	447	ILE
1	D	450	THR
1	D	474	MET
1	D	511	ARG
1	D	513	MET
1	D	543	LEU
1	D	546	LYS
1	D	556	LEU
1	D	561	LEU
1	D	572	VAL
1	D	595	THR
1	D	635	VAL
1	D	637	VAL
1	D	679	VAL
1	D	684	THR
1	D	690	MET
1	D	691	GLN
1	D	703	LEU
1	D	735	ASN
1	D	796	LEU
1	D	811	LEU
1	D	834	VAL
1	D	884	VAL
1	D	889	VAL
1	D	892	VAL
1	D	905	LEU
1	D	912	ILE
1	D	916	SER
1	D	943	VAL
1	D	945	LEU
1	D	966	THR
1	D	983	LEU
1	D	993	VAL
1	D	996	LEU
1	D	1000	THR
1	D	1012	VAL
1	E	2	ASN
1	E	3	ILE
1	E	40	VAL
1	E	41	VAL

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Mol	Chain	Res	Type
1	E	98	LEU
1	E	104	LYS
1	E	108	LEU
1	E	113	VAL
1	E	127	LEU
1	E	134	SER
1	E	138	LEU
1	E	141	VAL
1	E	189	VAL
1	E	202	THR
1	E	206	VAL
1	E	207	VAL
1	E	225	SER
1	E	227	THR
1	E	254	VAL
1	E	263	THR
1	E	268	ILE
1	E	274	ASP
1	E	324	VAL
1	E	329	VAL
1	E	346	THR
1	E	362	LEU
1	E	364	THR
1	E	388	LEU
1	E	401	MET
1	E	407	ILE
1	E	409	VAL
1	E	427	LEU
1	E	428	THR
1	E	465	THR
1	E	508	TRP
1	E	511	ARG
1	E	512	VAL
1	E	546	LYS
1	E	554	LEU
1	E	556	LEU
1	E	572	VAL
1	E	637	VAL
1	E	643	ASP
1	E	666	LEU
1	E	679	VAL
1	E	685	LEU

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Mol	Chain	Res	Type
1	E	690	MET
1	E	698	VAL
1	E	741	VAL
1	E	746	LEU
1	E	751	THR
1	E	756	THR
1	E	764	LEU
1	E	778	VAL
1	E	780	VAL
1	E	793	ILE
1	E	796	LEU
1	E	805	MET
1	E	813	THR
1	E	834	VAL
1	E	863	VAL
1	E	870	LEU
1	E	892	VAL
1	E	912	ILE
1	E	915	MET
1	E	918	LEU
1	E	921	LEU
1	E	927	THR
1	E	977	LEU
1	E	980	ARG
1	E	993	VAL
1	E	997	VAL
1	E	1000	THR
1	E	1014	VAL
1	E	1022	THR
1	E	1038	THR
1	F	2	ASN
1	F	3	ILE
1	F	117	LEU
1	F	122	GLU
1	F	132	VAL
1	F	138	LEU
1	F	187	MET
1	F	189	VAL
1	F	196	VAL
1	F	212	GLU
1	F	221	VAL
1	F	227	THR

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Mol	Chain	Res	Type
1	F	228	LEU
1	F	243	LEU
1	F	254	VAL
1	F	313	MET
1	F	324	VAL
1	F	354	VAL
1	F	364	THR
1	F	402	VAL
1	F	456	VAL
1	F	465	THR
1	F	511	ARG
1	F	512	VAL
1	F	513	MET
1	F	516	VAL
1	F	533	GLU
1	F	546	LYS
1	F	550	LEU
1	F	554	LEU
1	F	561	LEU
1	F	586	LEU
1	F	635	VAL
1	F	646	HIS
1	F	659	LEU
1	F	679	VAL
1	F	684	THR
1	F	685	LEU
1	F	690	MET
1	F	698	VAL
1	F	723	LEU
1	F	735	ASN
1	F	741	VAL
1	F	746	LEU
1	F	748	VAL
1	F	751	THR
1	F	756	THR
1	F	766	VAL
1	F	775	VAL
1	F	788	GLN
1	F	791	ASP
1	F	811	LEU
1	F	812	VAL
1	F	813	THR

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Mol	Chain	Res	Type
1	F	825	ARG
1	F	834	VAL
1	F	858	THR
1	F	864	LYS
1	F	888	SER
1	F	889	VAL
1	F	911	LEU
1	F	916	SER
1	F	924	VAL
1	F	943	VAL
1	F	948	LYS
1	F	966	THR
1	F	983	LEU
1	F	1012	VAL
1	F	1027	MET
1	F	1043	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	158	ASN
1	A	422	ASN
1	A	514	ASN
1	A	534	ASN
1	A	585	GLN
1	A	735	ASN
1	A	788	GLN
1	A	846	GLN
1	B	83	GLN
1	B	125	GLN
1	B	244	GLN
1	B	363	GLN
1	B	529	HIS
1	B	534	ASN
1	B	644	GLN
1	B	733	GLN
1	B	781	GLN
1	B	857	GLN
1	C	85	ASN
1	C	158	ASN
1	C	176	GLN

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Mol	Chain	Res	Type
1	C	502	HIS
1	C	525	ASN
1	C	575	GLN
1	C	691	GLN
1	C	745	GLN
1	D	2	ASN
1	D	111	ASN
1	D	264	HIS
1	D	363	GLN
1	D	525	ASN
1	D	575	GLN
1	D	691	GLN
1	D	745	GLN
1	D	758	GLN
1	D	846	GLN
1	E	115	GLN
1	E	394	ASN
1	E	502	HIS
1	E	514	ASN
1	E	788	GLN
1	E	857	GLN
1	F	55	ASN
1	F	83	GLN
1	F	158	ASN
1	F	176	GLN
1	F	525	ASN
1	F	585	GLN
1	F	609	GLN
1	F	733	GLN
1	F	788	GLN
1	F	1008	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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	F	1101	-	36,36,36	1.16	3 (8%)	47,47,47	1.50	7 (14%)
2	LMT	B	1102	-	36,36,36	1.17	2 (5%)	47,47,47	1.27	3 (6%)
2	LMT	B	1101	-	36,36,36	1.07	3 (8%)	47,47,47	1.14	6 (12%)
2	LMT	C	1101	-	36,36,36	1.08	1 (2%)	47,47,47	1.26	4 (8%)
2	LMT	E	1101	-	36,36,36	1.05	3 (8%)	47,47,47	1.26	5 (10%)
2	LMT	A	1101	-	36,36,36	1.01	2 (5%)	47,47,47	1.15	4 (8%)
2	LMT	D	1101	-	36,36,36	1.06	2 (5%)	47,47,47	1.06	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	F	1101	-	-	11/21/61/61	0/2/2/2
2	LMT	B	1102	-	-	6/21/61/61	0/2/2/2
2	LMT	B	1101	-	-	8/21/61/61	0/2/2/2
2	LMT	C	1101	-	-	12/21/61/61	0/2/2/2
2	LMT	E	1101	-	-	7/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	6/21/61/61	0/2/2/2
2	LMT	D	1101	-	-	14/21/61/61	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	LMT	C3'-C2'	2.64	1.59	1.52
2	B	1102	LMT	O3'-C3'	-2.55	1.36	1.43
2	B	1101	LMT	C3B-C2B	2.43	1.58	1.52
2	F	1101	LMT	O2'-C2'	-2.36	1.37	1.43
2	F	1101	LMT	C3'-C2'	2.33	1.58	1.52
2	B	1101	LMT	C1B-C2B	2.28	1.59	1.52
2	F	1101	LMT	O2B-C2B	-2.23	1.37	1.43
2	C	1101	LMT	C4B-C3B	2.21	1.58	1.52
2	D	1101	LMT	C1B-C2B	2.19	1.58	1.52
2	B	1102	LMT	O1B-C4'	-2.17	1.38	1.43
2	B	1101	LMT	O2'-C2'	-2.15	1.37	1.43
2	E	1101	LMT	C3B-C2B	2.14	1.57	1.52
2	A	1101	LMT	C3'-C2'	2.12	1.57	1.52
2	A	1101	LMT	O4'-C4B	-2.09	1.37	1.43
2	D	1101	LMT	C4B-C3B	2.05	1.57	1.52
2	E	1101	LMT	O4'-C4B	-2.03	1.37	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1102	LMT	C3'-C4'-C5'	-3.94	102.19	110.93
2	E	1101	LMT	C1'-C2'-C3'	3.61	117.60	110.01
2	F	1101	LMT	C1'-O5'-C5'	-3.55	106.78	113.72
2	F	1101	LMT	C3'-C4'-C5'	-3.53	103.10	110.93
2	C	1101	LMT	C1'-O5'-C5'	-3.28	107.31	113.72
2	A	1101	LMT	O5'-C1'-C2'	-3.11	103.97	110.37
2	C	1101	LMT	C3'-C4'-C5'	-3.08	104.09	110.93
2	A	1101	LMT	O5'-C5'-C4'	3.06	116.05	109.72
2	B	1101	LMT	O1B-C1B-C2B	2.91	115.24	108.09
2	F	1101	LMT	O1'-C1'-C2'	2.66	112.31	108.27
2	E	1101	LMT	C3'-C4'-C5'	-2.63	105.09	110.93
2	E	1101	LMT	O5B-C5B-C6B	2.63	112.96	106.44
2	B	1102	LMT	O5B-C5B-C4B	2.58	114.35	109.70
2	D	1101	LMT	O5'-C1'-O1'	-2.54	104.05	110.04
2	C	1101	LMT	O5B-C5B-C6B	2.51	112.67	106.44
2	D	1101	LMT	O5B-C5B-C4B	2.50	114.20	109.70
2	F	1101	LMT	O5B-C5B-C6B	2.50	112.63	106.44
2	F	1101	LMT	C1B-C2B-C3B	2.44	115.14	110.01
2	D	1101	LMT	C3'-C4'-C5'	-2.42	105.56	110.93
2	C	1101	LMT	O1'-C1-C2	-2.40	101.23	109.37
2	B	1101	LMT	O5B-C5B-C6B	2.40	112.38	106.44
2	B	1101	LMT	C3B-C4B-C5B	-2.38	105.92	110.23
2	E	1101	LMT	C2'-C3'-C4'	2.37	115.07	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	LMT	C1B-C2B-C3B	2.29	114.82	110.01
2	E	1101	LMT	O5'-C1'-C2'	2.27	115.03	110.37
2	B	1102	LMT	C1'-O5'-C5'	-2.25	109.33	113.72
2	B	1101	LMT	O5'-C1'-C2'	-2.24	105.77	110.37
2	F	1101	LMT	C4B-C3B-C2B	2.15	114.60	110.83
2	F	1101	LMT	C6'-C5'-C4'	2.12	119.34	113.38
2	A	1101	LMT	O5B-C1B-C2B	2.06	114.59	110.37
2	A	1101	LMT	O5B-C5B-C6B	2.05	111.51	106.44
2	B	1101	LMT	O5B-C1B-C2B	2.04	114.56	110.37
2	D	1101	LMT	O1B-C1B-C2B	2.03	113.08	108.09

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	LMT	C2-C1-O1'-C1'
2	D	1101	LMT	O5'-C1'-O1'-C1
2	B	1101	LMT	C2B-C1B-O1B-C4'
2	B	1101	LMT	O5'-C5'-C6'-O6'
2	A	1101	LMT	C4'-C5'-C6'-O6'
2	A	1101	LMT	O5'-C5'-C6'-O6'
2	B	1101	LMT	O5B-C5B-C6B-O6B
2	B	1101	LMT	C4'-C5'-C6'-O6'
2	C	1101	LMT	O5'-C1'-O1'-C1
2	E	1101	LMT	O5'-C1'-O1'-C1
2	F	1101	LMT	O5B-C5B-C6B-O6B
2	E	1101	LMT	C2'-C1'-O1'-C1
2	D	1101	LMT	O5'-C5'-C6'-O6'
2	E	1101	LMT	O5'-C5'-C6'-O6'
2	B	1101	LMT	C4B-C5B-C6B-O6B
2	C	1101	LMT	C4'-C5'-C6'-O6'
2	B	1101	LMT	O5B-C1B-O1B-C4'
2	C	1101	LMT	O1'-C1-C2-C3
2	E	1101	LMT	O1'-C1-C2-C3
2	D	1101	LMT	C4-C5-C6-C7
2	B	1102	LMT	O5B-C5B-C6B-O6B
2	D	1101	LMT	C11-C10-C9-C8
2	F	1101	LMT	C5-C6-C7-C8
2	D	1101	LMT	C6-C7-C8-C9
2	F	1101	LMT	C4-C5-C6-C7
2	A	1101	LMT	O5B-C5B-C6B-O6B
2	E	1101	LMT	C11-C10-C9-C8

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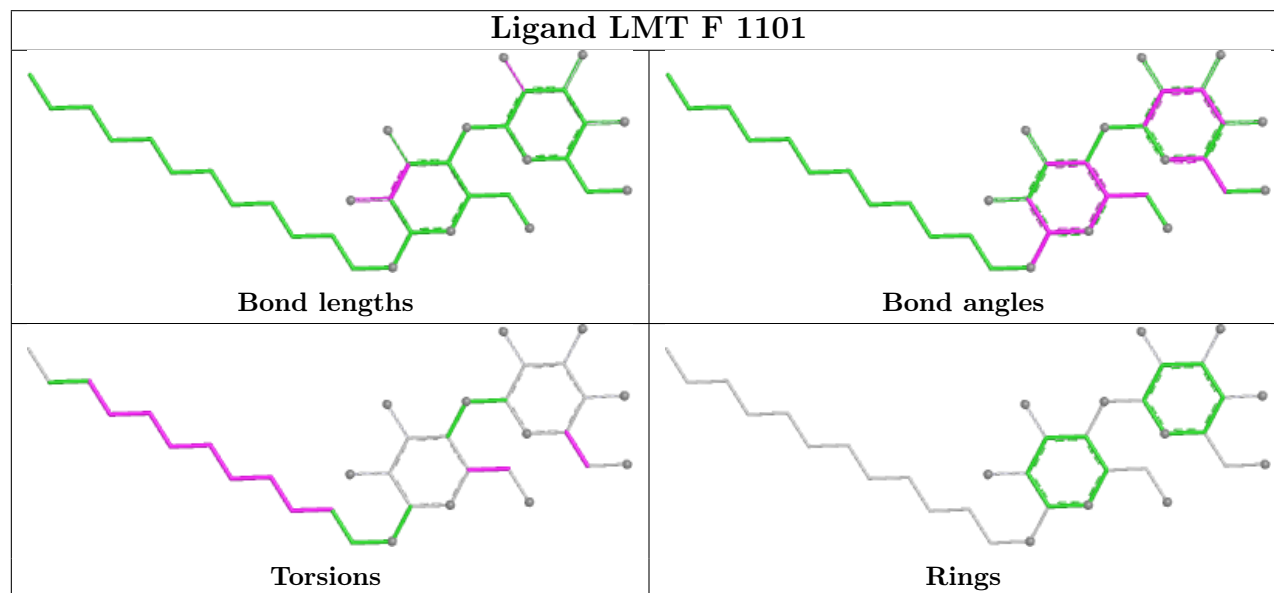
Mol	Chain	Res	Type	Atoms
2	C	1101	LMT	C2-C3-C4-C5
2	C	1101	LMT	C6-C7-C8-C9
2	F	1101	LMT	C4B-C5B-C6B-O6B
2	D	1101	LMT	C5-C6-C7-C8
2	C	1101	LMT	C4B-C5B-C6B-O6B
2	C	1101	LMT	C3-C4-C5-C6
2	D	1101	LMT	C2'-C1'-O1'-C1
2	F	1101	LMT	C1-C2-C3-C4
2	B	1102	LMT	C1-C2-C3-C4
2	C	1101	LMT	C7-C8-C9-C10
2	B	1102	LMT	C2-C1-O1'-C1'
2	D	1101	LMT	C4'-C5'-C6'-O6'
2	D	1101	LMT	C3-C4-C5-C6
2	F	1101	LMT	C7-C8-C9-C10
2	F	1101	LMT	C3-C4-C5-C6
2	D	1101	LMT	C1-C2-C3-C4
2	E	1101	LMT	C4B-C5B-C6B-O6B
2	F	1101	LMT	C11-C10-C9-C8
2	C	1101	LMT	C4-C5-C6-C7
2	B	1101	LMT	C5-C6-C7-C8
2	D	1101	LMT	C9-C10-C11-C12
2	F	1101	LMT	C6-C7-C8-C9
2	A	1101	LMT	C1-C2-C3-C4
2	C	1101	LMT	C2-C1-O1'-C1'
2	B	1102	LMT	C2-C3-C4-C5
2	A	1101	LMT	C11-C10-C9-C8
2	B	1102	LMT	O5'-C5'-C6'-O6'
2	B	1102	LMT	C3-C4-C5-C6
2	D	1101	LMT	O1'-C1-C2-C3
2	C	1101	LMT	C1-C2-C3-C4
2	D	1101	LMT	C7-C8-C9-C10
2	C	1101	LMT	O5'-C5'-C6'-O6'
2	B	1101	LMT	C3'-C4'-O1B-C1B
2	E	1101	LMT	C2B-C1B-O1B-C4'
2	D	1101	LMT	O5B-C5B-C6B-O6B
2	F	1101	LMT	C2-C3-C4-C5
2	F	1101	LMT	O5'-C5'-C6'-O6'

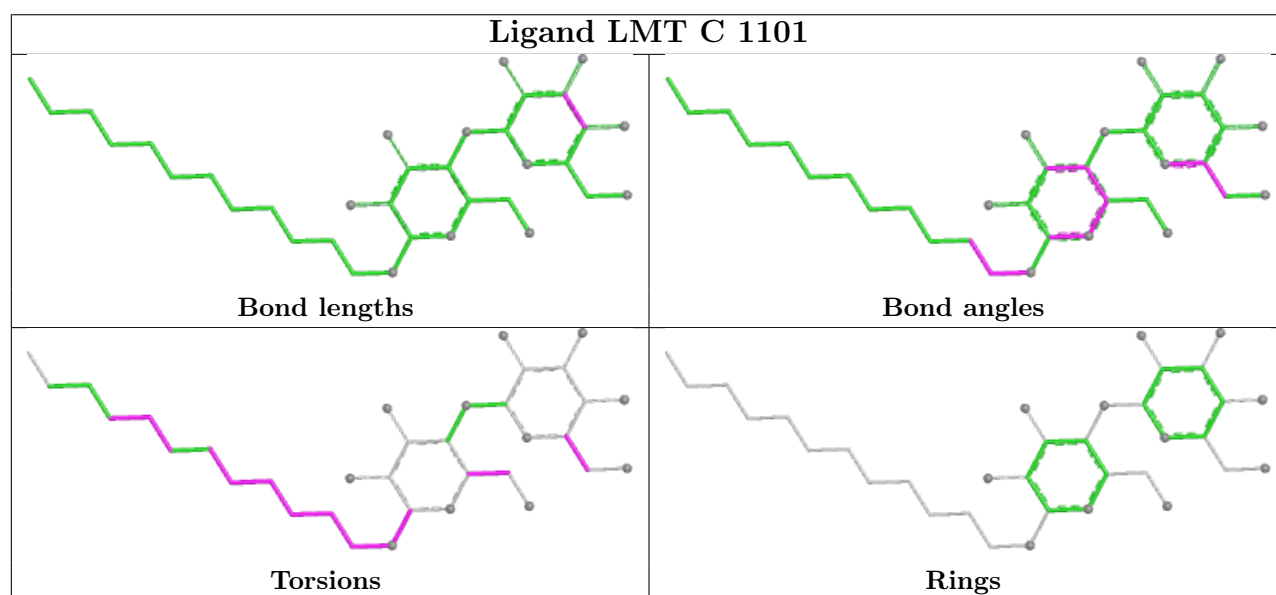
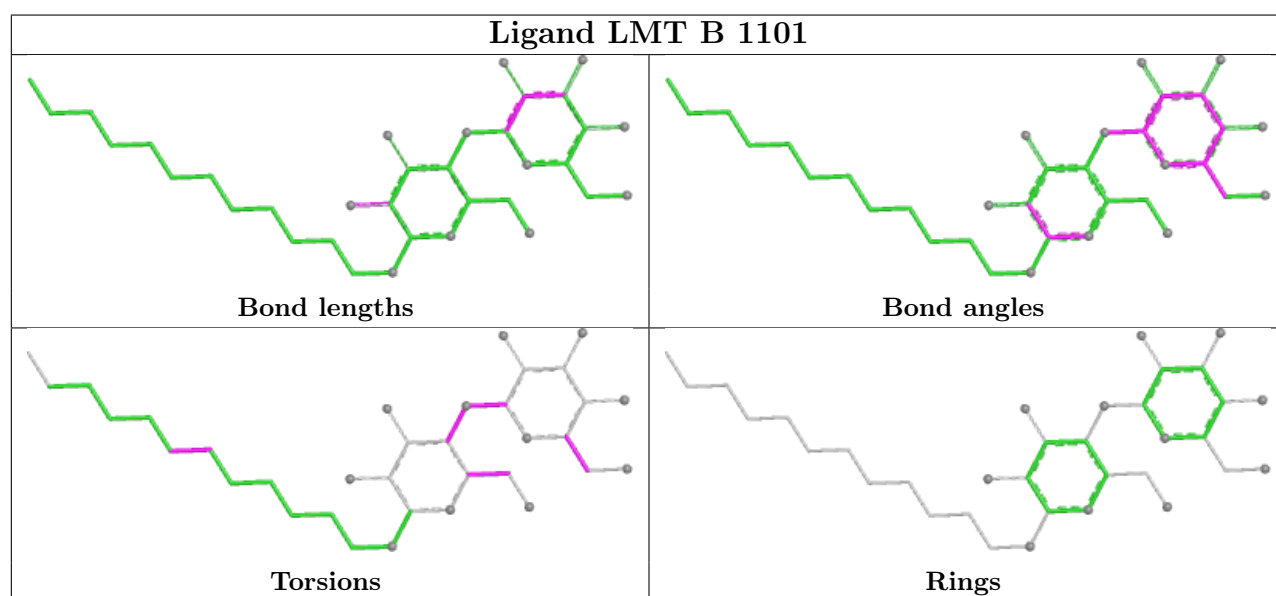
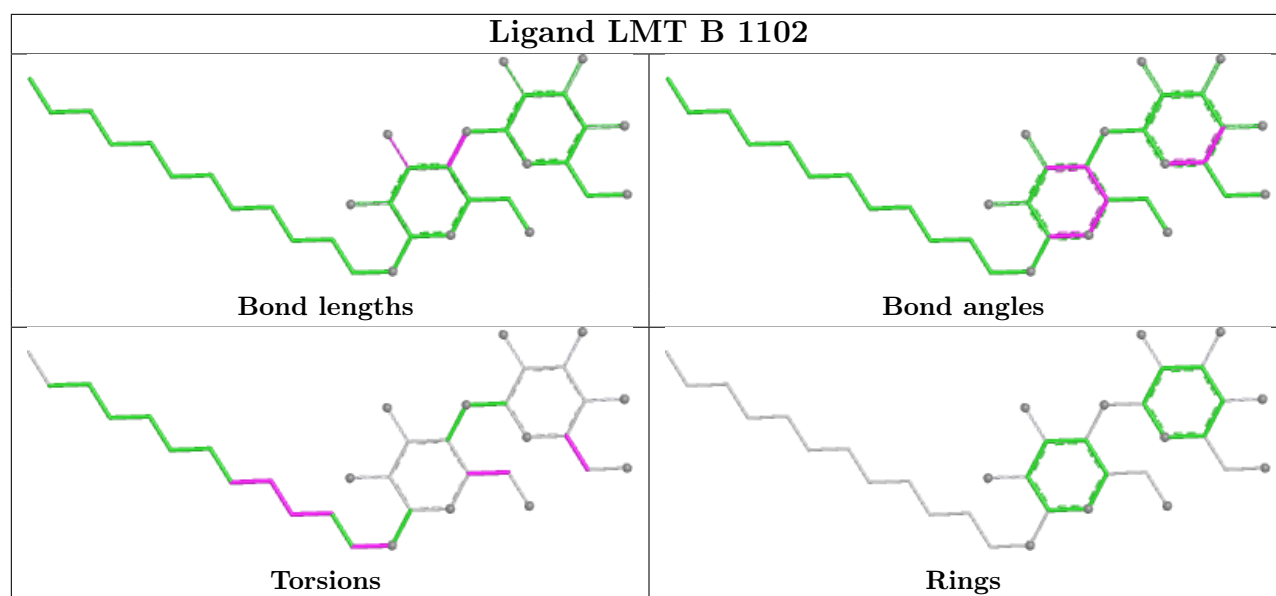
There are no ring outliers.

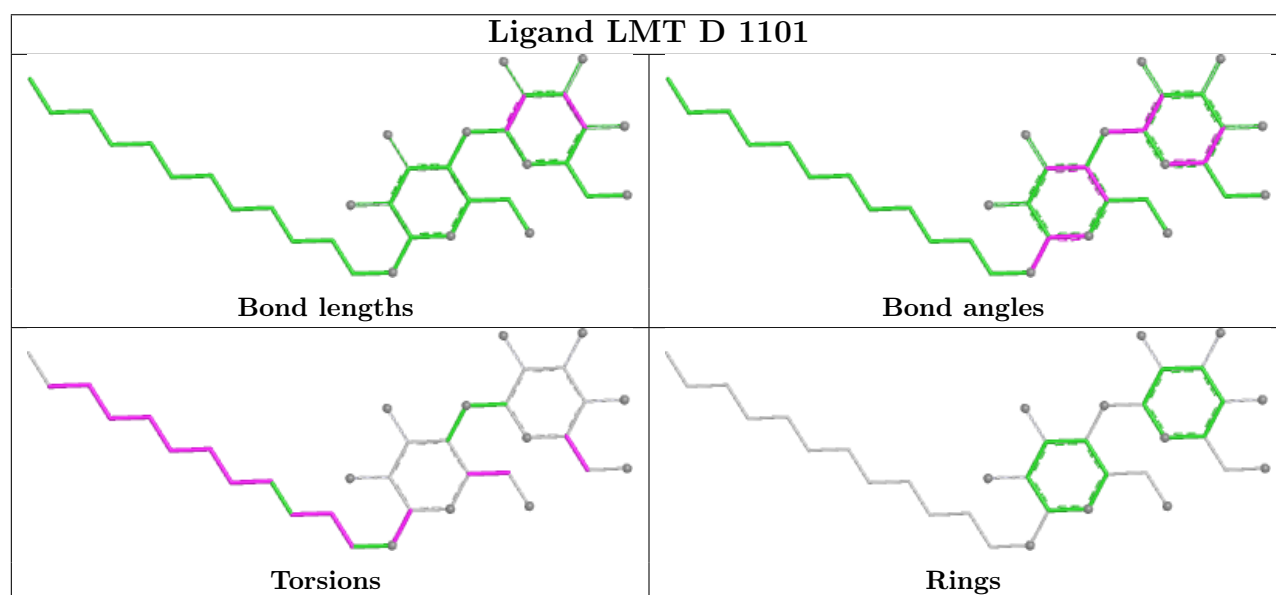
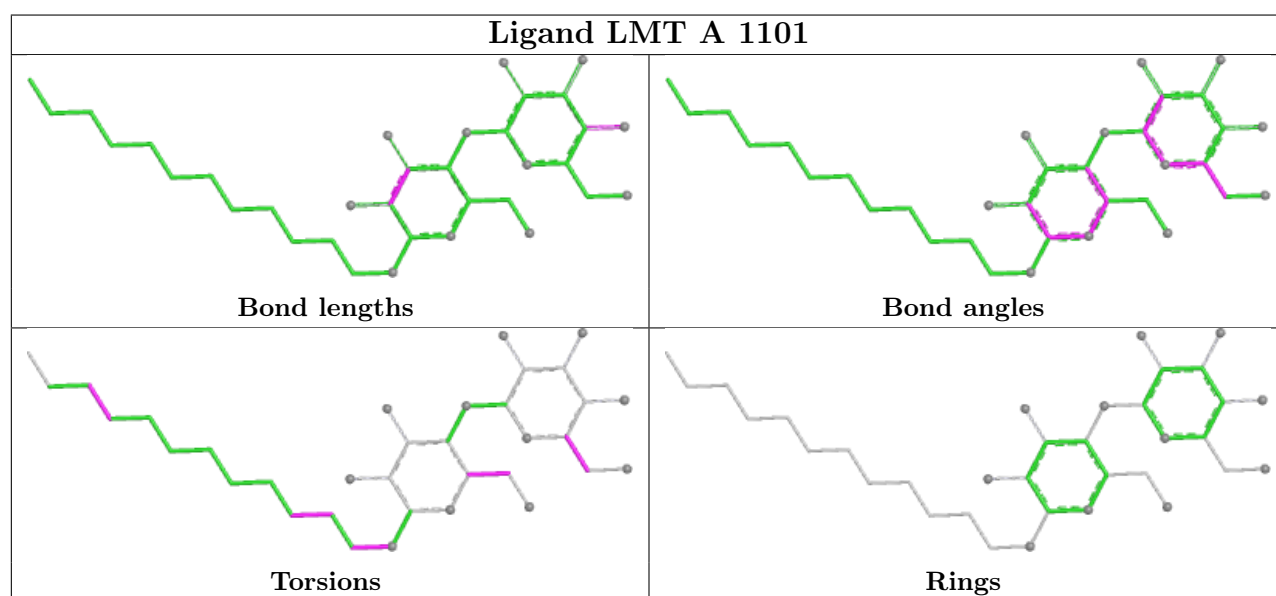
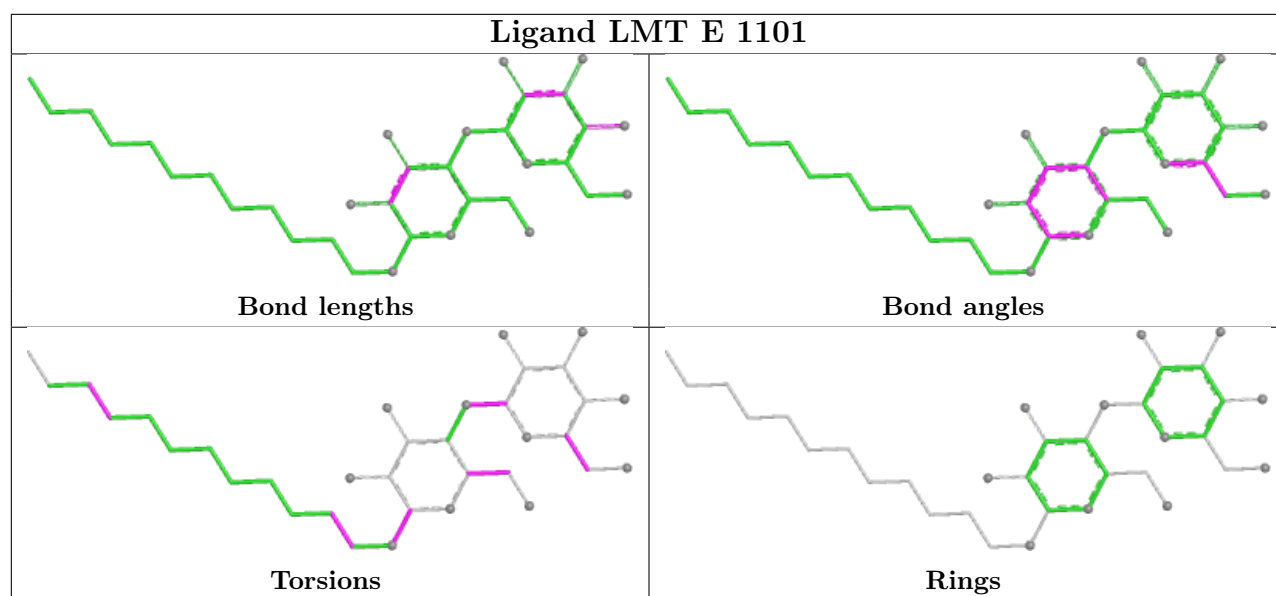
7 monomers are involved in 27 short contacts:

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

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1042/1067 (97%)	-0.19	29 (2%)	55	32	72, 110, 172, 249	0
1	B	1042/1067 (97%)	-0.15	26 (2%)	58	35	76, 107, 168, 296	0
1	C	1043/1067 (97%)	-0.09	33 (3%)	50	29	76, 115, 178, 298	0
1	D	1042/1067 (97%)	-0.16	23 (2%)	62	39	75, 108, 165, 312	0
1	E	1042/1067 (97%)	-0.24	21 (2%)	65	41	70, 112, 162, 320	0
1	F	1043/1067 (97%)	-0.12	24 (2%)	61	38	65, 107, 156, 317	0
All	All	6254/6402 (97%)	-0.16	156 (2%)	58	35	65, 110, 169, 320	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	683	GLY	7.1
1	A	502	HIS	6.4
1	B	680	LEU	5.8
1	B	682	LEU	5.4
1	A	426	GLY	5.3
1	F	773	GLY	5.2
1	B	877	ALA	5.1
1	C	991	MET	4.6
1	B	681	GLY	4.5
1	A	682	LEU	4.5
1	A	423	ILE	4.5
1	B	218	ALA	4.4
1	F	965	LYS	4.3
1	F	964	GLY	4.2
1	A	427	LEU	4.1
1	B	462	SER	4.0
1	A	583	PHE	4.0
1	D	155	TYR	4.0
1	D	503	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	754	PHE	4.0
1	A	504	ASP	3.9
1	D	151	TYR	3.9
1	D	682	LEU	3.9
1	E	877	ALA	3.8
1	B	425	ASN	3.8
1	F	963	ASP	3.8
1	D	790	ALA	3.7
1	B	678	PRO	3.7
1	C	182	ALA	3.7
1	C	41	VAL	3.7
1	D	814	VAL	3.7
1	B	1010	MET	3.7
1	B	533	GLU	3.6
1	D	973	GLU	3.6
1	B	679	VAL	3.5
1	F	770	ASN	3.5
1	F	40	VAL	3.4
1	F	111	ASN	3.4
1	C	136	PRO	3.4
1	B	532	ALA	3.4
1	E	426	GLY	3.3
1	E	427	LEU	3.2
1	D	583	PHE	3.2
1	D	964	GLY	3.2
1	D	697	ALA	3.2
1	F	1014	VAL	3.2
1	C	150	SER	3.2
1	F	82	SER	3.2
1	D	792	ASP	3.1
1	A	429	ALA	3.1
1	B	37	TYR	3.1
1	E	1042	GLY	3.0
1	E	464	LEU	3.0
1	C	1042	GLY	3.0
1	C	680	LEU	3.0
1	C	772	PHE	3.0
1	D	581	ILE	3.0
1	A	579	TYR	3.0
1	D	504	ASP	3.0
1	C	39	GLU	2.9
1	C	37	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	880	SER	2.9
1	E	876	LEU	2.9
1	D	464	LEU	2.9
1	E	1010	MET	2.9
1	C	42	PRO	2.8
1	C	751	THR	2.8
1	B	426	GLY	2.8
1	B	677	PRO	2.8
1	A	581	ILE	2.8
1	C	183	GLY	2.8
1	C	758	GLN	2.8
1	F	39	GLU	2.7
1	A	883	TRP	2.7
1	E	873	GLN	2.7
1	D	426	GLY	2.7
1	A	964	GLY	2.6
1	F	135	SER	2.6
1	E	462	SER	2.6
1	C	176	GLN	2.6
1	A	31	LEU	2.6
1	C	138	LEU	2.6
1	C	882	PHE	2.6
1	A	1011	GLY	2.6
1	F	108	LEU	2.6
1	B	219	ALA	2.6
1	B	9	ASP	2.5
1	B	770	ASN	2.5
1	E	504	ASP	2.5
1	C	151	TYR	2.5
1	C	845	GLY	2.5
1	C	771	ARG	2.5
1	A	447	ILE	2.5
1	A	1	MET	2.5
1	B	434	TYR	2.5
1	C	755	ASP	2.5
1	D	293	ALA	2.4
1	E	878	GLY	2.4
1	A	425	ASN	2.4
1	C	40	VAL	2.4
1	F	961	GLU	2.4
1	F	331	ASP	2.4
1	F	136	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	837	GLY	2.4
1	A	681	GLY	2.3
1	C	36	GLU	2.3
1	E	1041	GLY	2.3
1	A	9	ASP	2.3
1	F	772	PHE	2.3
1	C	526	LYS	2.3
1	A	574	ALA	2.3
1	B	998	LEU	2.3
1	B	626	PHE	2.3
1	A	680	LEU	2.3
1	C	529	HIS	2.3
1	C	135	SER	2.3
1	A	963	ASP	2.3
1	E	506	GLU	2.2
1	A	677	PRO	2.2
1	B	535	TYR	2.2
1	F	775	VAL	2.2
1	D	820	PRO	2.2
1	F	680	LEU	2.2
1	E	505	LYS	2.2
1	F	263	THR	2.2
1	E	1014	VAL	2.2
1	B	136	PRO	2.2
1	B	1013	ALA	2.2
1	E	263	THR	2.2
1	D	996	LEU	2.2
1	B	109	VAL	2.1
1	E	546	LYS	2.1
1	F	790	ALA	2.1
1	C	880	SER	2.1
1	F	618	PHE	2.1
1	E	692	ILE	2.1
1	D	468	PHE	2.1
1	B	464	LEU	2.1
1	C	963	ASP	2.1
1	D	963	ASP	2.1
1	F	960	LEU	2.1
1	E	773	GLY	2.1
1	F	109	VAL	2.1
1	C	108	LEU	2.1
1	F	1008	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1010	MET	2.1
1	C	139	THR	2.1
1	D	1041	GLY	2.1
1	E	104	LYS	2.0
1	A	503	GLY	2.0
1	A	683	GLY	2.0
1	A	754	PHE	2.0
1	A	679	VAL	2.0
1	C	307	ASP	2.0
1	D	882	PHE	2.0
1	C	761	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

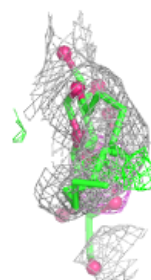
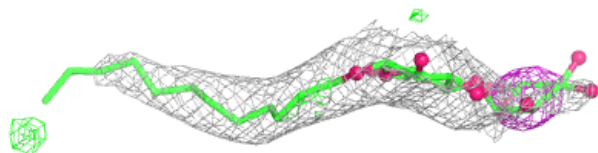
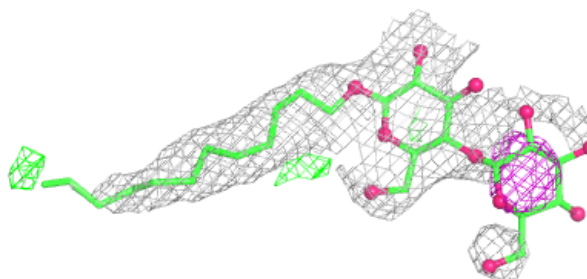
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	D	1101	35/35	0.78	0.16	82,132,147,148	0
2	LMT	A	1101	35/35	0.79	0.14	88,129,148,154	0
2	LMT	F	1101	35/35	0.82	0.13	85,126,134,138	0
2	LMT	E	1101	35/35	0.84	0.13	83,126,137,138	0
2	LMT	B	1101	35/35	0.84	0.14	83,122,135,137	0
2	LMT	C	1101	35/35	0.86	0.13	86,131,141,145	0
2	LMT	B	1102	35/35	0.90	0.11	96,108,121,125	0

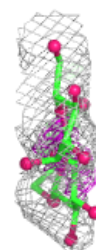
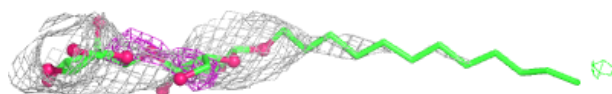
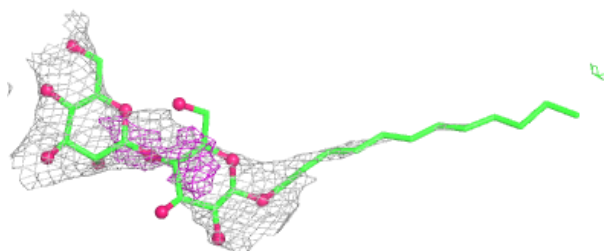
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT D 1101:

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

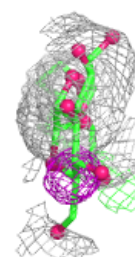
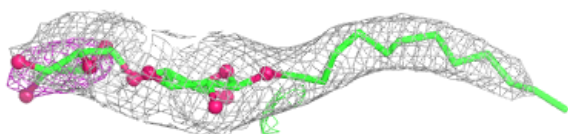
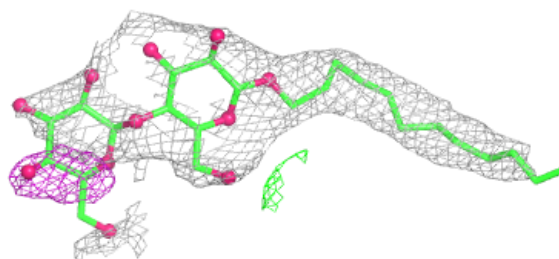
**Electron density around LMT A 1101:**

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

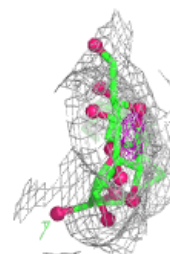
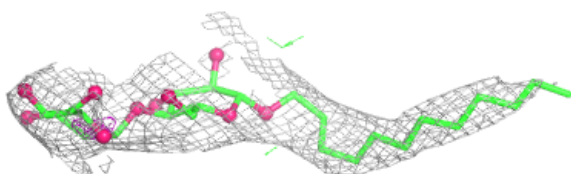
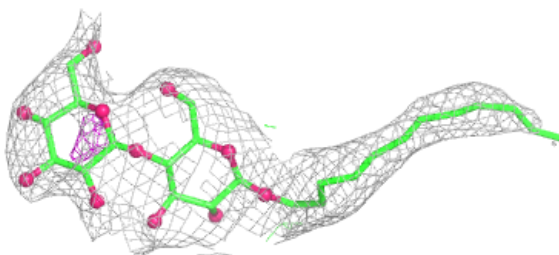


Electron density around LMT F 1101:

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

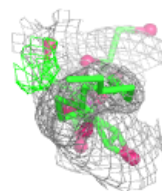
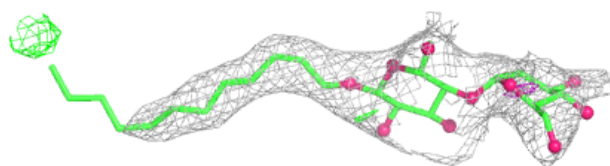
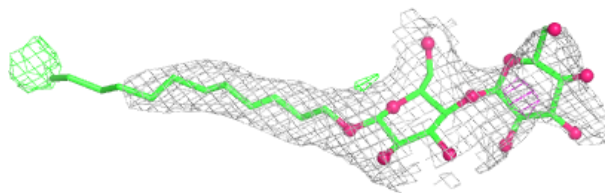
**Electron density around LMT E 1101:**

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

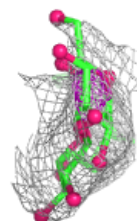
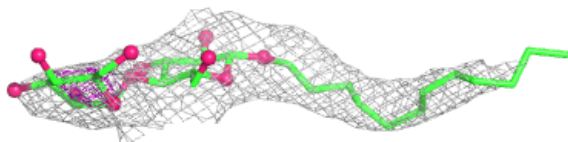
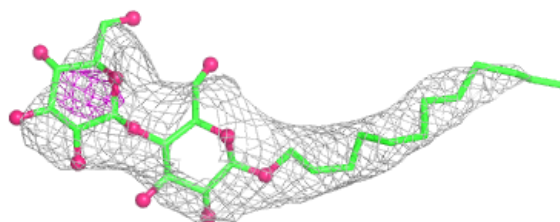


Electron density around LMT B 1101:

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

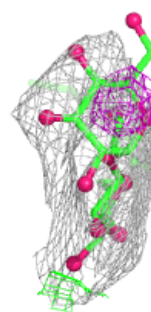
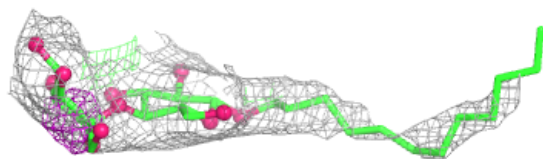
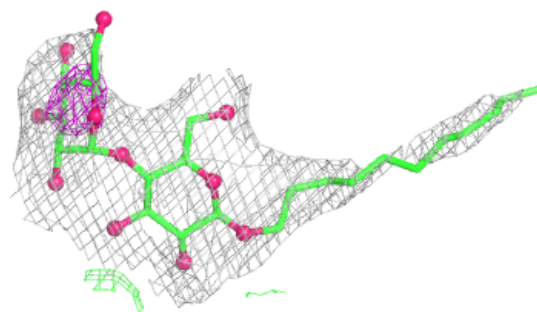
**Electron density around LMT C 1101:**

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



Electron density around LMT B 1102:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.