



Full wwPDB X-ray Structure Validation Report i

Nov 23, 2023 – 02:30 AM JST

PDB ID : 7WLV
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 i 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

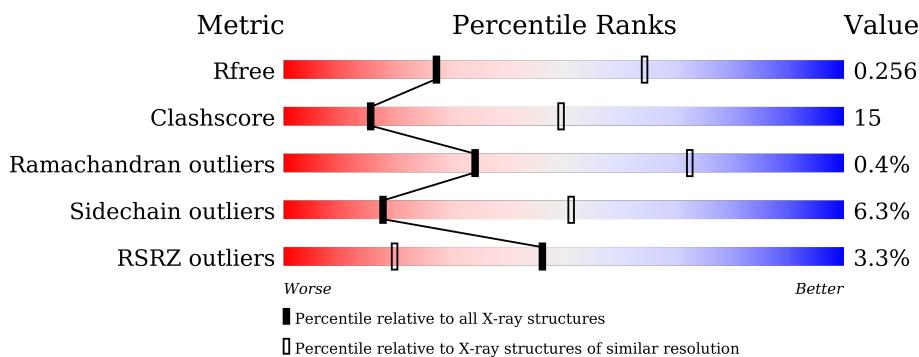
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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.



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Mol	Chain	Length	Quality of chain			
1	F	1067	2%	63%	31%	..

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

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

2 Entry composition (i)

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 7920	N 5106	O 1341	S 1442	31	0	0
1	B	1042	Total	C 7920	N 5106	O 1341	S 1442	31	0	0
1	C	1043	Total	C 7929	N 5112	O 1343	S 1443	31	0	0
1	D	1042	Total	C 7920	N 5106	O 1341	S 1442	31	0	0
1	E	1042	Total	C 7921	N 5107	O 1342	S 1442	30	0	0
1	F	1043	Total	C 7929	N 5112	O 1343	S 1443	31	0	0

There are 36 discrepancies between the modelled and reference sequences:

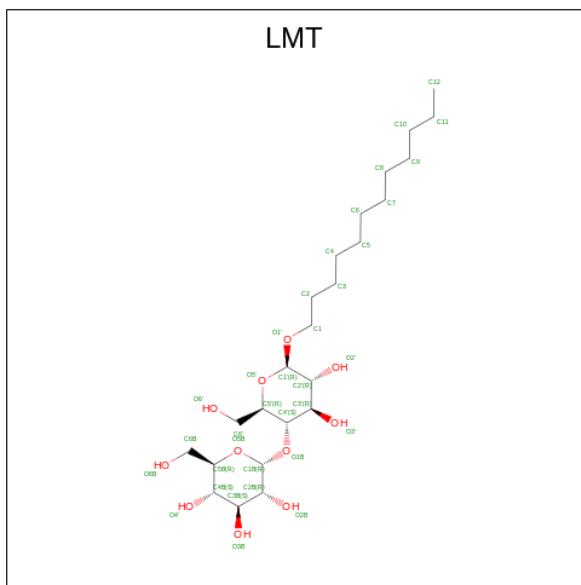
Chain	Residue	Modelled	Actual	Comment	Reference
A	1062	HIS	-	expression tag	UNP Q63NK6
A	1063	HIS	-	expression tag	UNP Q63NK6
A	1064	HIS	-	expression tag	UNP Q63NK6
A	1065	HIS	-	expression tag	UNP Q63NK6
A	1066	HIS	-	expression tag	UNP Q63NK6
A	1067	HIS	-	expression tag	UNP Q63NK6
B	1062	HIS	-	expression 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 (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	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	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

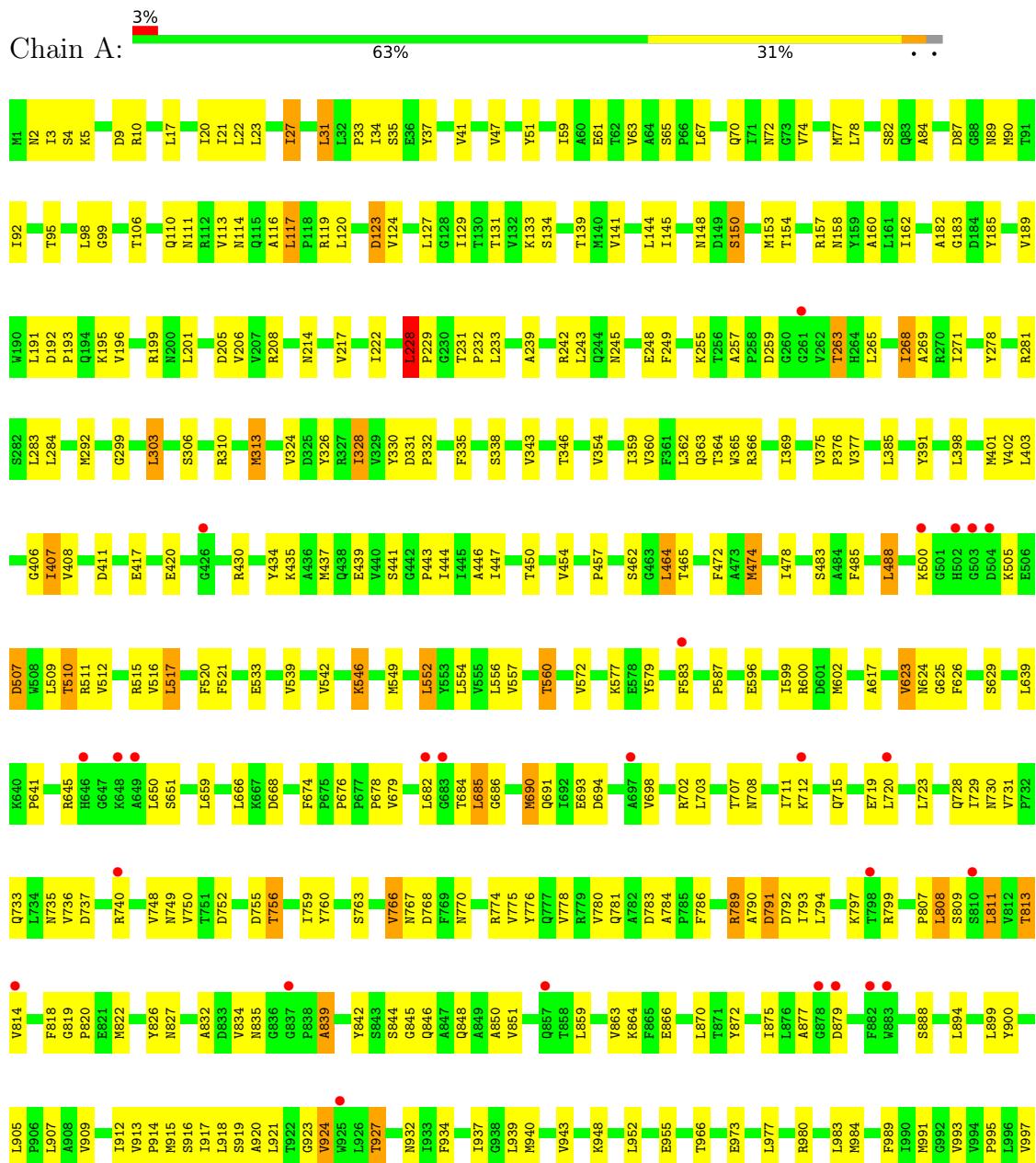
- Molecule 3 is water.

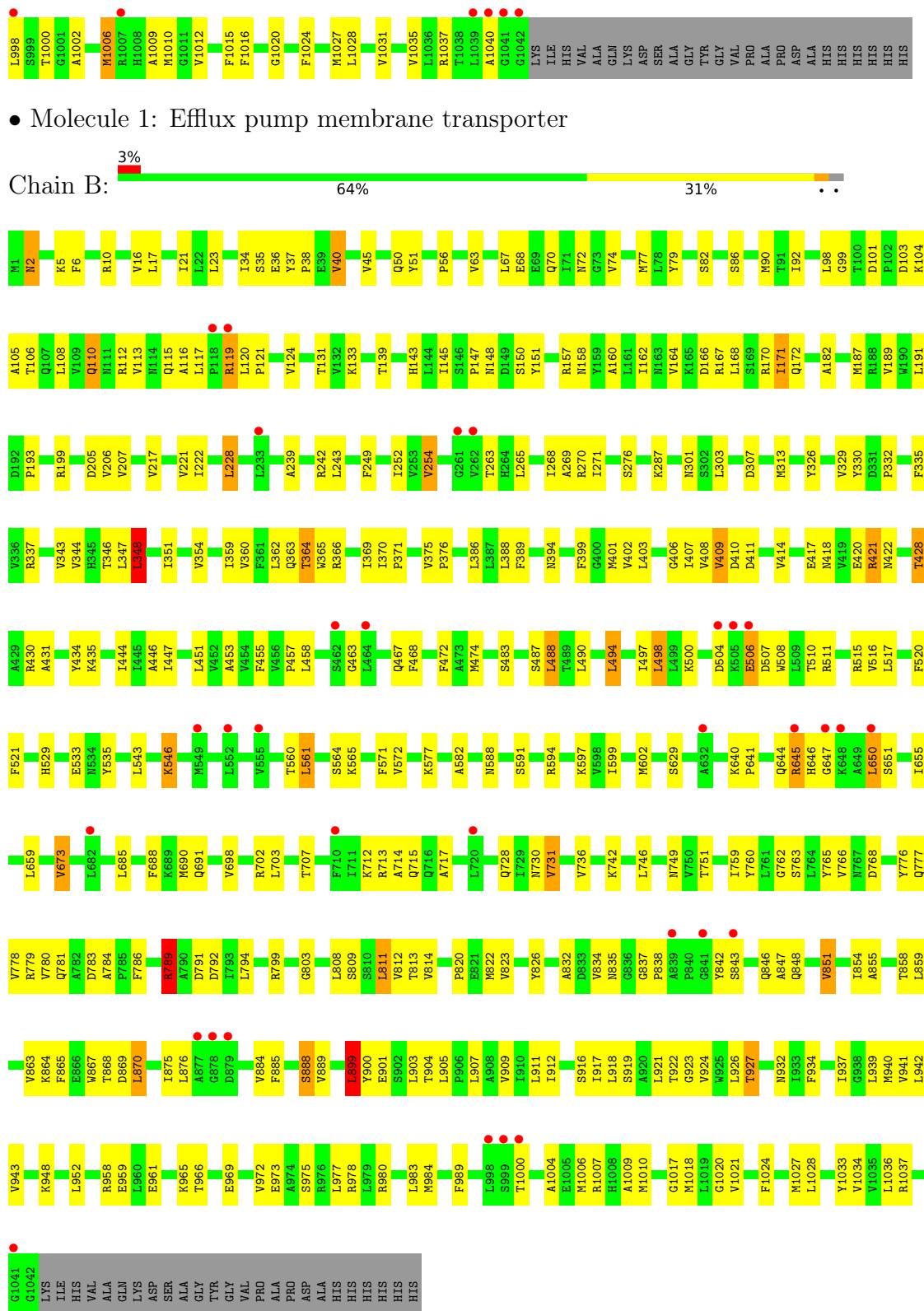
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	10	Total O 10 10	0	0
3	C	8	Total O 8 8	0	0
3	D	7	Total O 7 7	0	0
3	E	5	Total O 5 5	0	0
3	F	6	Total O 6 6	0	0

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.

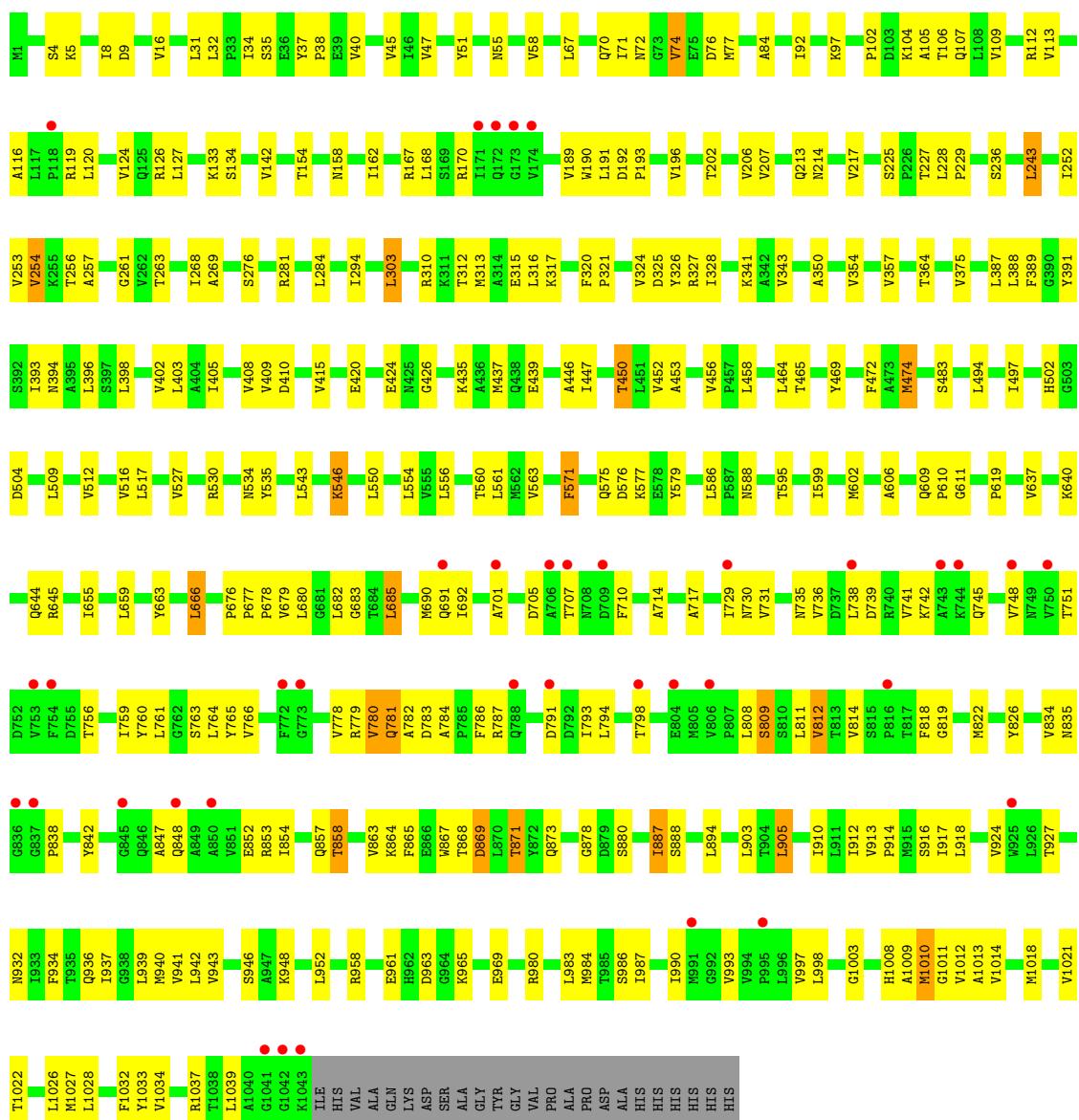
- Molecule 1: Efflux pump membrane transporter



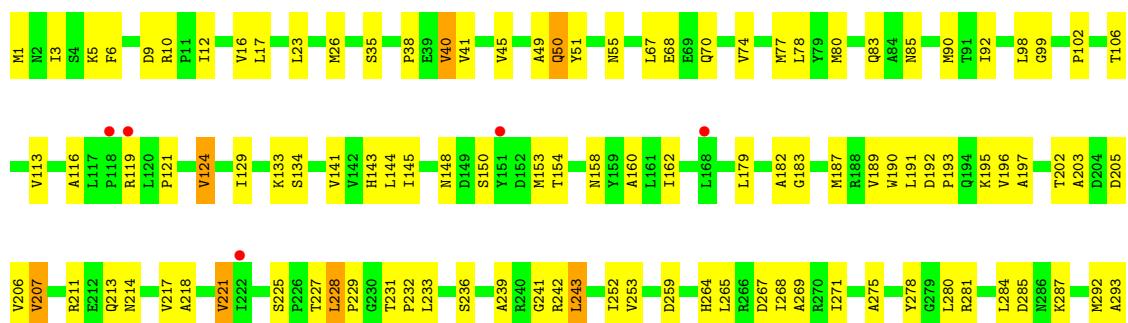


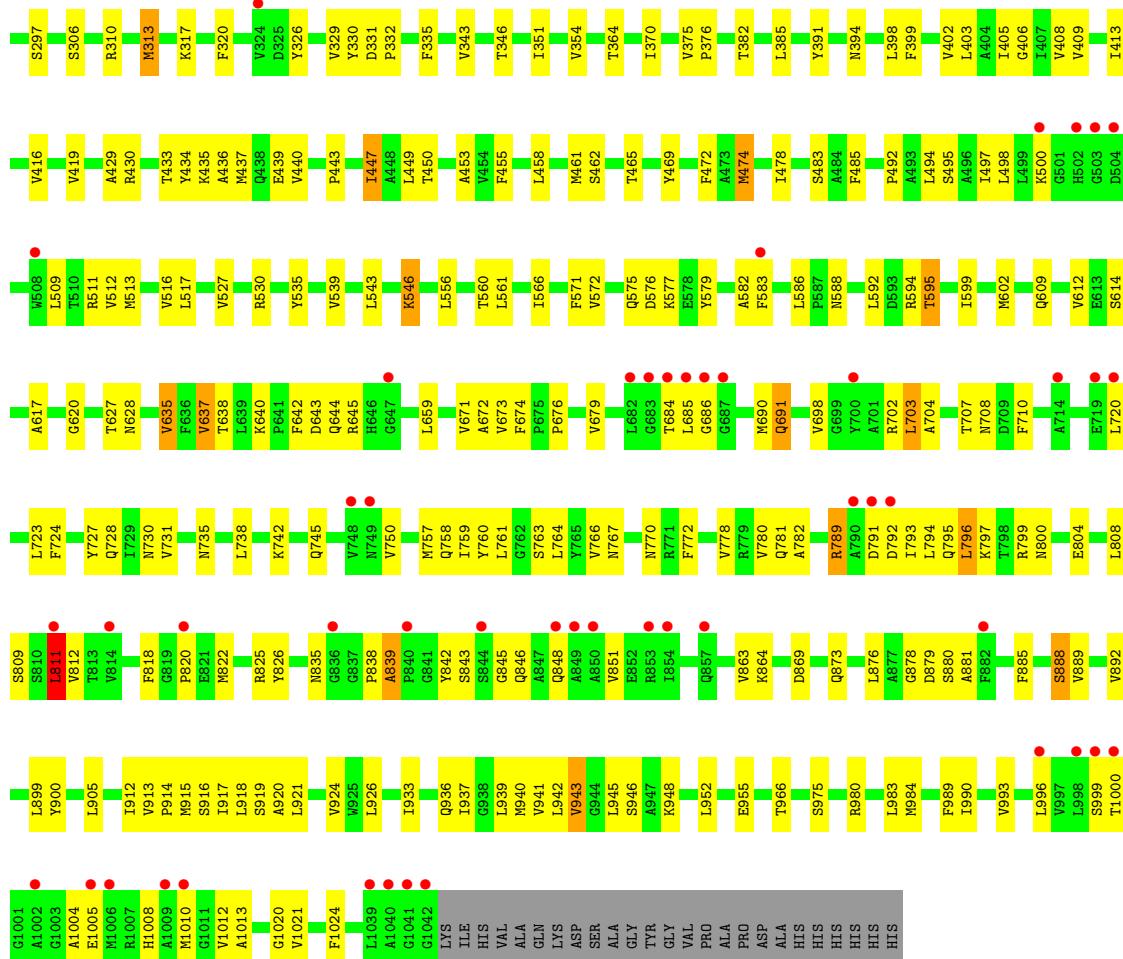
- Molecule 1: Efflux pump membrane transporter



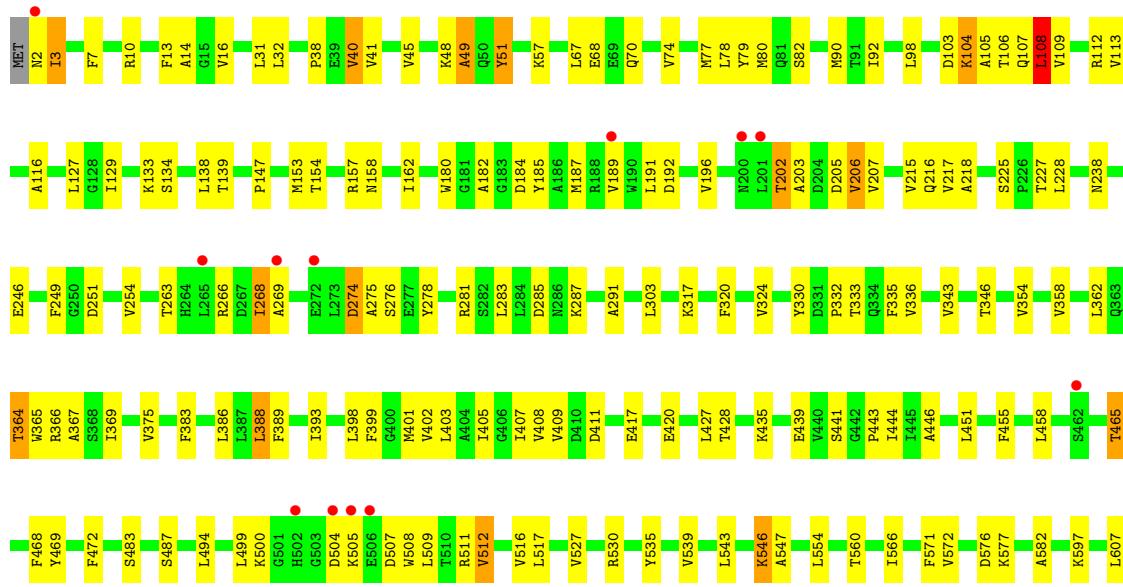


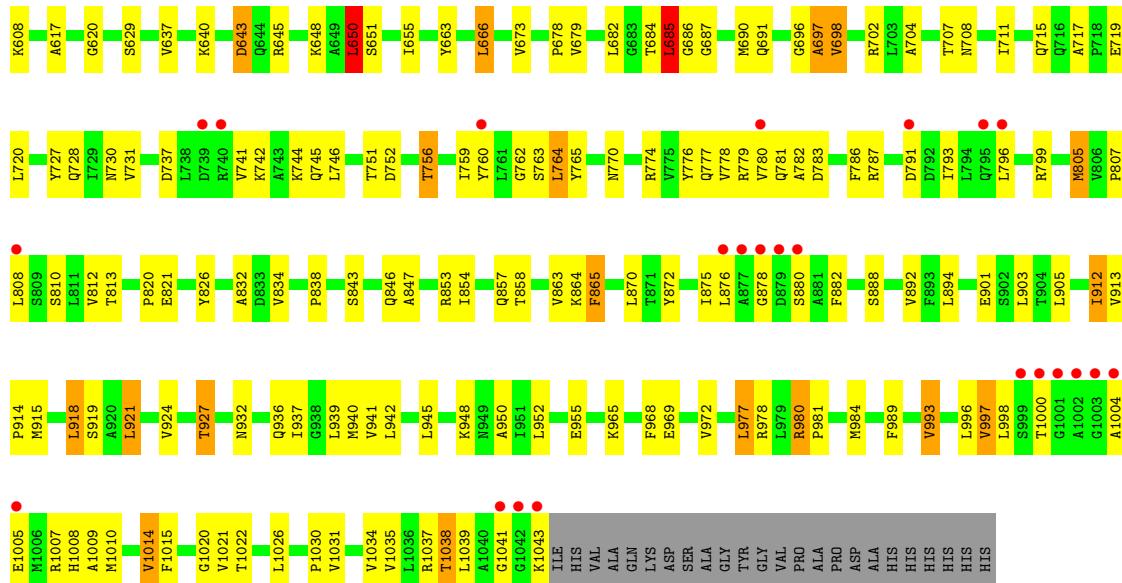
- Molecule 1: Efflux pump membrane transporter



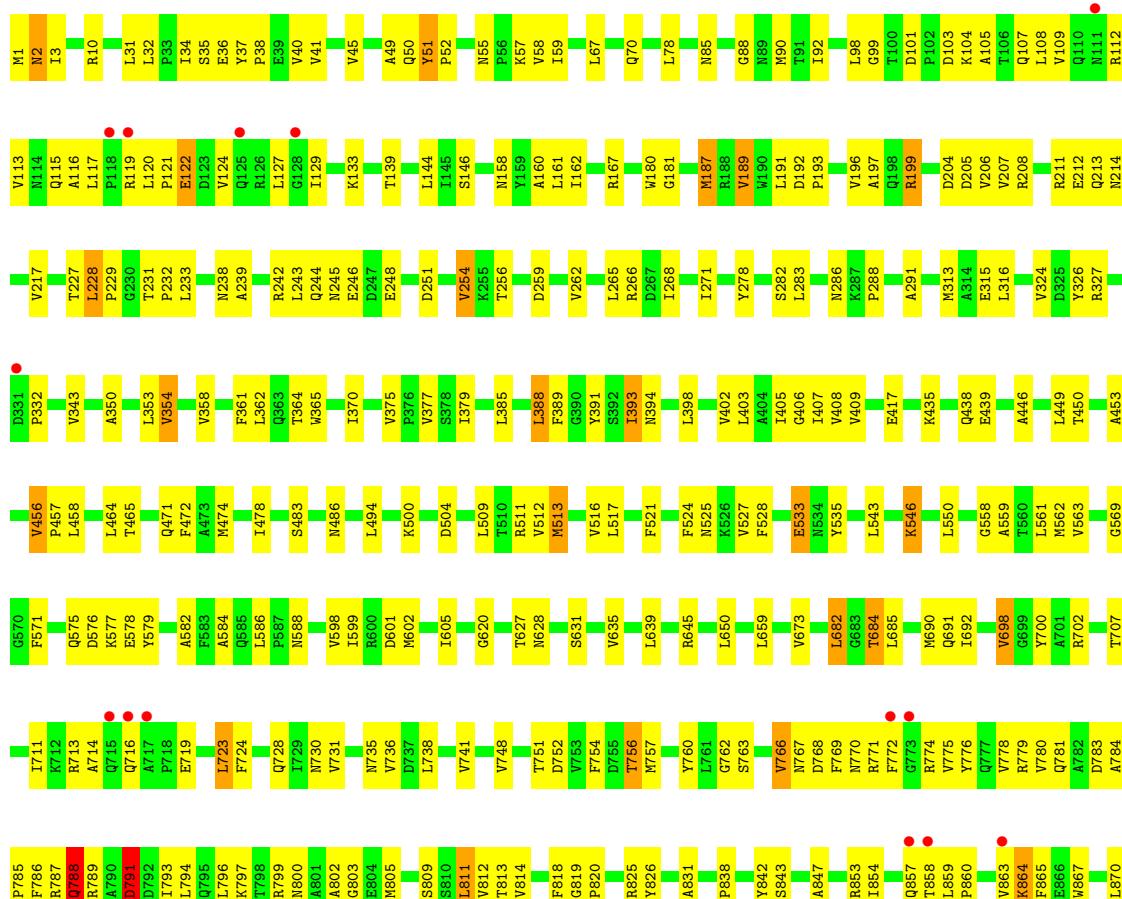


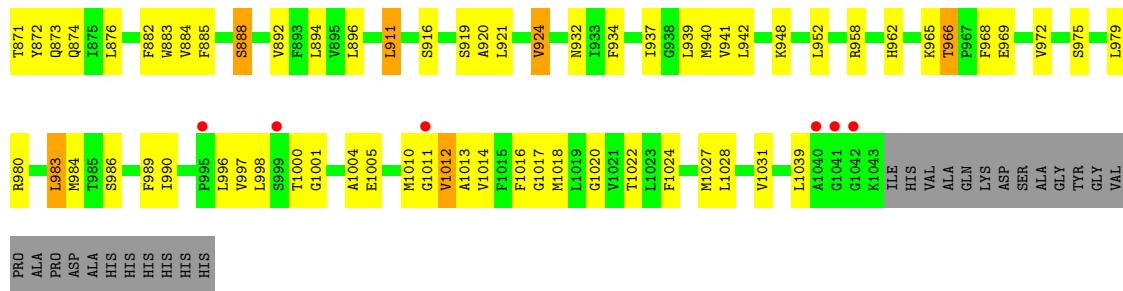
- Molecule 1: Efflux pump membrane transporter





- Molecule 1: Efflux pump membrane transporter





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ ¹	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R , R_{free}	0.211 , 0.259 0.208 , 0.256	Depositor DCC
R_{free} test set	7880 reflections (4.91%)	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)	0.32 , 89.0	EDS
L-test for twinning ²	$< L > = 0.50$, $< L^2 > = 0.33$	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	0/8072	0.74	5/10990 (0.0%)
1	B	0.47	0/8072	0.75	6/10990 (0.1%)
1	C	0.46	0/8081	0.71	1/11001 (0.0%)
1	D	0.47	0/8072	0.71	3/10990 (0.0%)
1	E	0.44	0/8073	0.73	4/10991 (0.0%)
1	F	0.50	0/8081	0.76	7/11001 (0.1%)
All	All	0.47	0/48451	0.73	26/65963 (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 (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	808	LEU	CA-CB-CG	7.51	132.58	115.30
1	A	552	LEU	CA-CB-CG	6.26	129.70	115.30
1	F	388	LEU	CA-CB-CG	-6.22	100.99	115.30
1	F	682	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	31	LEU	C-N-CA	-5.99	106.74	121.70
1	F	811	LEU	CA-CB-CG	5.88	128.83	115.30
1	E	108	LEU	CA-CB-CG	5.65	128.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	650	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	A	228	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	899	LEU	CA-CB-CG	5.54	128.03	115.30
1	B	348	LEU	CA-CB-CG	5.53	128.02	115.30
1	B	650	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	811	LEU	CA-CB-CG	5.44	127.82	115.30
1	F	31	LEU	C-N-CA	-5.40	108.20	121.70
1	C	228	LEU	CA-CB-CG	5.32	127.54	115.30
1	F	791	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	E	31	LEU	C-N-CA	-5.24	108.60	121.70
1	B	685	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	789	ARG	CG-CD-NE	5.17	122.66	111.80
1	F	911	LEU	CA-CB-CG	5.13	127.11	115.30
1	B	386	LEU	CA-CB-CG	5.12	127.07	115.30
1	D	796	LEU	CA-CB-CG	5.12	127.07	115.30
1	E	685	LEU	CA-CB-CG	5.11	127.06	115.30
1	F	996	LEU	CA-CB-CG	5.09	127.01	115.30
1	D	811	LEU	CA-CB-CG	5.05	126.91	115.30
1	D	498	LEU	CA-CB-CG	5.01	126.83	115.30

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 MolProbit. 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	242	0
1	B	7920	0	8168	263	1
1	C	7929	0	8181	219	0
1	D	7920	0	8168	244	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	7921	0	8169	232	0
1	F	7929	0	8181	270	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	5	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	1436	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 15.

All (1436) 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
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:599:ILE:HD13	1:F:602:MET:HE3	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: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:E:698:VAL:HG13	1:E:702:ARG:HB3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
1:C:1010:MET:O	1:C:1014:VAL:N	2.15	0.78
1:F:101:ASP:H	1:F:104:LYS:HZ3	1.30	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:A:599:ILE:HA	1:A:602:MET:HE2	1.65	0.78
1:C:276:SER:O	1:C:779:ARG:NH1	2.17	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: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: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:C:313:MET:HE1	1:C:316:LEU:HD12	1.68	0.74
1:F:799:ARG:HE	1:F:805:MET:HE1	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:417:GLU:HG3	1:F:984:MET:HE3	1.72	0.72
1:D:102:PRO:O	1:D:106:THR:HG23	1.90	0.72
1:F:122:GLU:H	1:F:122:GLU:CD	1.94	0.72
1:D:265:LEU:HG	1:D:271:ILE:HD11	1.72	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:217:VAL:HG11	1:F:754:PHE:CD2	2.28	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
1:A:447:ILE:HD13	1:A:948:LYS:HZ3	1.59	0.67
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: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:F:736:VAL:HG21	1:F:757:MET:HE1	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:599:ILE:HD13	1:A:602:MET:HE1	1.78	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
1:A:736:VAL:HG22	1:A:814:VAL:HG22	1.77	0.65
1:F:1001:GLY:H	1:F:1004:ALA:CB	2.09	0.65
1:E:411:ASP:OD1	1:E:948:LYS:NZ	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:576:ASP:OD2	1:F:645:ARG:NH2	2.31	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
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:F:1010:MET:HE3	1:F:1014:VAL:HG21	1.80	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:F:199:ARG:HG2	1:F:199:ARG:HH11	1.65	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:999:SER:HB2	1:D:1004:ALA:HB2	1.82	0.61
1:A:790:ALA:O	1:A:793:ILE:HB	2.00	0.61
1:C:599:ILE:HA	1:C:602:MET:HE2	1.82	0.61
1:E:32:LEU:HD13	1:E:393:ILE:HD11	1.83	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:411:ASP:OD1	1:A:948:LYS:NZ	2.25	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
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: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:A:444:ILE:HG21	1:A:488:LEU:HD13	1.84	0.60
1:A:72:ASN:HA	1:A:77:MET:HE1	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:B:10:ARG:NH1	2:C:1101:LMT:O6'	2.35	0.59
1:D:738:LEU:HD13	1:D:812:VAL:HG12	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:68:GLU:HB3	1:E:80:MET:HE3	1.86	0.58
1:E:516:VAL:HG13	1:E:517:LEU:HG	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:939:LEU:O	1:B:943:VAL:HG13	2.02	0.57
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: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:A:437:MET:HA	1:A:437:MET:HE3	1.86	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:D:763:SER:HB3	1:D:781:GLN:CD	2.25	0.57
1:C:403:LEU:HB3	1:C:941:VAL:HG21	1.87	0.56
1:D:153:MET:HE1	1:D:281:ARG:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:742:LYS:HA	1:E:745:GLN:NE2	2.20	0.56
1:B:599:ILE:HA	1:B:602:MET:HE2	1.86	0.56
1:B:843:SER:O	1:B:846:GLN:NE2	2.38	0.56
1:E:180:TRP:HB2	1:E:291:ALA:HB3	1.87	0.56
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:B:868:THR:HG23	1:B:868:THR:O	2.04	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: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:D:70:GLN:HG3	1:D:116:ALA:HB2	1.88	0.56
1:E:153:MET:HE3	1:E:182:ALA:HB2	1.86	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:B:375:VAL:HG22	1:B:408:VAL:HG12	1.87	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:E:107:GLN:CD	1:F:107:GLN:HG3	2.26	0.55
1:A:5:LYS:HD3	1:A:434:TYR:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:599:ILE:HD13	1:D:602:MET:HE1	1.87	0.55
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:F:863:VAL:O	1:F:863:VAL:HG13	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:640:LYS:HD3	1:C:644:GLN:HG2	1.89	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:F:598:VAL:HG12	1:F:602:MET:HE1	1.87	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:A:185:TYR:HB2	1:A:776:TYR:CE2	2.42	0.54
1:D:191:LEU:HD11	1:D:206:VAL:HG11	1.89	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:763:SER:HB3	1:F:781:GLN:CD	2.28	0.54
1:F:990:ILE:HD11	1:F:1018:MET:HB3	1.89	0.54
1:A:74:VAL:HG12	1:A:77:MET:HE2	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:599:ILE:HA	1:F:602:MET:HE2	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:72:ASN:HA	1:C:77:MET:HE1	1.90	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:HG1	1.90	0.53
1:F:791:ASP:C	1:F:793:ILE:N	2.62	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:187:MET:HE1	1:F:246:GLU:HG3	1.90	0.53
1:F:398:LEU:O	1:F:402:VAL:HG13	2.08	0.53
1:C:55:ASN:HB3	1:C:58:VAL:HG23	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:B:591:SER:OG	1:B:594:ARG:HG3	2.08	0.53
1:A:98:LEU:HD12	1:A:99:GLY:H	1.74	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:VAL:HG13	1:A:517:LEU:HD13	1.90	0.53
1:B:749:ASN:CG	1:B:751:THR:HG22	2.29	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:147:PRO:O	1:E:287:LYS:NZ	2.30	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: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:A:153:MET:HE1	1:A:281:ARG:HG2	1.92	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: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:B:599:ILE:HD13	1:B:602:MET:HE1	1.92	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:B:763:SER:HB3	1:B:781:GLN:CD	2.31	0.51
1:E:225:SER:HB2	1:F:278:TYR:HB3	1.93	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:763:SER:HB3	1:E:781:GLN:CD	2.30	0.51
1:E:774:ARG:HB2	1:E:776:TYR:HE1	1.76	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: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: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:A:763:SER:HB3	1:A:781:GLN:CD	2.32	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
1:D:143:HIS:O	1:D:326:TYR:HA	2.11	0.50
1:F:736:VAL:HG11	1:F:757:MET:CE	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:205:ASP:CG	1:D:799:ARG:HH22	2.15	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:599:ILE:HA	1:F:602:MET:CE	2.41	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: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
1:E:202:THR:HG22	1:E:805:MET:HE1	1.94	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:F:391:TYR:CZ	1:F:474:MET:HG2	2.47	0.49
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:74:VAL:HG12	1:E:77:MET:HE2	2.03	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: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
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: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:C:325:ASP:OD1	1:C:326:TYR:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:978:ARG:C	1:E:981:PRO:HD2	2.41	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: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:762:GLY:O	1:F:763:SER:OG	2.38	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
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:410:ASP:OD2	1:C:948:LYS:NZ	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:965:LYS:HB3	1:F:969:GLU:HG3	2.03	0.40
1:A:698:VAL:CG1	1:A:702:ARG:HB3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:609:GLN:CD	1:C:610:PRO:HD2	2.41	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: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: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
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%)	25 64
1	B	1040/1067 (98%)	985 (95%)	50 (5%)	5 (0%)	29 68
1	C	1041/1067 (98%)	984 (94%)	55 (5%)	2 (0%)	47 82
1	D	1040/1067 (98%)	989 (95%)	47 (4%)	4 (0%)	34 72
1	E	1040/1067 (98%)	989 (95%)	47 (4%)	4 (0%)	34 72
1	F	1041/1067 (98%)	993 (95%)	46 (4%)	2 (0%)	47 82
All	All	6242/6402 (98%)	5923 (95%)	296 (5%)	23 (0%)	34 72

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
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 [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	849/868 (98%)	794 (94%)	55 (6%)	17 50
1	B	849/868 (98%)	801 (94%)	48 (6%)	20 56
1	C	850/868 (98%)	800 (94%)	50 (6%)	19 54
1	D	849/868 (98%)	796 (94%)	53 (6%)	18 52
1	E	849/868 (98%)	785 (92%)	64 (8%)	13 43
1	F	850/868 (98%)	798 (94%)	52 (6%)	18 53
All	All	5096/5208 (98%)	4774 (94%)	322 (6%)	18 51

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	27	ILE
1	A	31	LEU
1	A	41	VAL
1	A	51	TYR
1	A	117	LEU
1	A	123	ASP
1	A	134	SER
1	A	150	SER
1	A	228	LEU
1	A	243	LEU
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	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

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Mol	Chain	Res	Type
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
1	A	756	THR
1	A	766	VAL
1	A	789	ARG
1	A	791	ASP
1	A	813	THR
1	A	864	LYS
1	A	870	LEU
1	A	907	LEU
1	A	916	SER
1	A	924	VAL
1	A	927	THR
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	40	VAL
1	B	51	TYR
1	B	79	TYR
1	B	110	GLN
1	B	119	ARG
1	B	206	VAL
1	B	221	VAL
1	B	228	LEU
1	B	254	VAL
1	B	337	ARG
1	B	348	LEU
1	B	364	THR
1	B	401	MET

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Mol	Chain	Res	Type
1	B	409	VAL
1	B	421	ARG
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	546	LYS
1	B	561	LEU
1	B	673	VAL
1	B	690	MET
1	B	713	ARG
1	B	731	VAL
1	B	789	ARG
1	B	811	LEU
1	B	813	THR
1	B	834	VAL
1	B	835	ASN
1	B	851	VAL
1	B	864	LYS
1	B	865	PHE
1	B	870	LEU
1	B	875	ILE
1	B	888	SER
1	B	899	LEU
1	B	927	THR
1	B	983	LEU
1	B	1000	THR
1	B	1010	MET
1	B	1018	MET
1	B	1027	MET
1	C	51	TYR
1	C	74	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

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Mol	Chain	Res	Type
1	C	254	VAL
1	C	256	THR
1	C	263	THR
1	C	303	LEU
1	C	357	VAL
1	C	364	THR
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	571	PHE
1	C	637	VAL
1	C	666	LEU
1	C	685	LEU
1	C	705	ASP
1	C	735	ASN
1	C	741	VAL
1	C	751	THR
1	C	756	THR
1	C	780	VAL
1	C	791	ASP
1	C	809	SER
1	C	812	VAL
1	C	835	ASN
1	C	858	THR
1	C	864	LYS
1	C	869	ASP
1	C	871	THR
1	C	887	ILE
1	C	905	LEU
1	C	912	ILE
1	C	916	SER
1	C	963	ASP
1	C	1010	MET
1	C	1012	VAL
1	C	1022	THR
1	C	1027	MET
1	C	1034	VAL

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Mol	Chain	Res	Type
1	D	3	ILE
1	D	23	LEU
1	D	26	MET
1	D	40	VAL
1	D	41	VAL
1	D	50	GLN
1	D	51	TYR
1	D	67	LEU
1	D	113	VAL
1	D	124	VAL
1	D	134	SER
1	D	207	VAL
1	D	221	VAL
1	D	228	LEU
1	D	243	LEU
1	D	297	SER
1	D	313	MET
1	D	346	THR
1	D	364	THR
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	595	THR
1	D	635	VAL
1	D	637	VAL
1	D	642	PHE
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	789	ARG
1	D	796	LEU
1	D	811	LEU
1	D	888	SER
1	D	889	VAL

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Mol	Chain	Res	Type
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	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
1	E	51	TYR
1	E	79	TYR
1	E	98	LEU
1	E	104	LYS
1	E	108	LEU
1	E	127	LEU
1	E	134	SER
1	E	138	LEU
1	E	202	THR
1	E	206	VAL
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	346	THR
1	E	364	THR
1	E	388	LEU
1	E	401	MET
1	E	407	ILE
1	E	427	LEU
1	E	428	THR
1	E	465	THR
1	E	508	TRP
1	E	511	ARG
1	E	512	VAL

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Mol	Chain	Res	Type
1	E	546	LYS
1	E	554	LEU
1	E	637	VAL
1	E	643	ASP
1	E	666	LEU
1	E	685	LEU
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	793	ILE
1	E	796	LEU
1	E	805	MET
1	E	813	THR
1	E	834	VAL
1	E	865	PHE
1	E	870	LEU
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	51	TYR
1	F	117	LEU
1	F	122	GLU
1	F	187	MET
1	F	189	VAL
1	F	199	ARG
1	F	212	GLU
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	324	VAL
1	F	354	VAL
1	F	364	THR
1	F	456	VAL
1	F	465	THR
1	F	511	ARG
1	F	513	MET
1	F	533	GLU
1	F	546	LYS
1	F	550	LEU
1	F	561	LEU
1	F	684	THR
1	F	685	LEU
1	F	690	MET
1	F	698	VAL
1	F	723	LEU
1	F	724	PHE
1	F	735	ASN
1	F	741	VAL
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	813	THR
1	F	825	ARG
1	F	858	THR
1	F	864	LYS
1	F	888	SER
1	F	911	LEU
1	F	916	SER
1	F	924	VAL
1	F	948	LYS
1	F	966	THR
1	F	983	LEU
1	F	1012	VAL

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Mol	Chain	Res	Type
1	F	1027	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	846	GLN
1	B	534	ASN
1	B	644	GLN
1	B	733	GLN
1	C	83	GLN
1	C	85	ASN
1	C	502	HIS
1	C	691	GLN
1	C	745	GLN
1	D	70	GLN
1	D	575	GLN
1	D	745	GLN
1	D	846	GLN
1	E	111	ASN
1	E	394	ASN
1	F	55	ASN
1	F	83	GLN
1	F	107	GLN
1	F	733	GLN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

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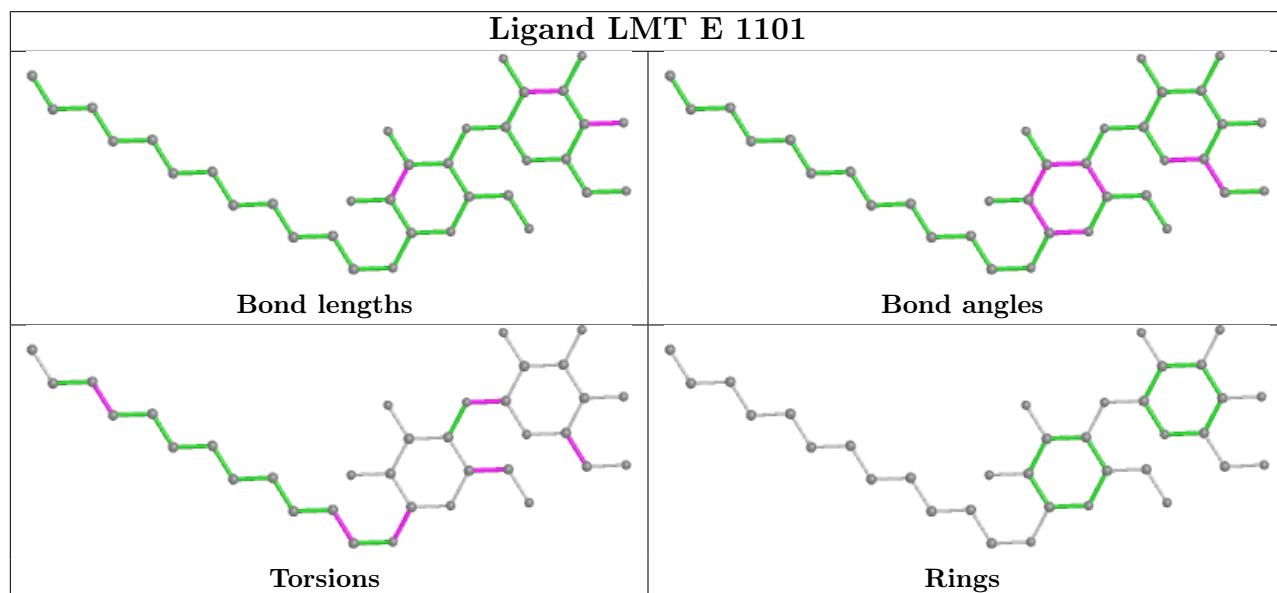
Mol	Chain	Res	Type	Atoms
2	D	1101	LMT	C5-C6-C7-C8
2	D	1101	LMT	C2'-C1'-O1'-C1
2	A	1101	LMT	O5B-C5B-C6B-O6B
2	F	1101	LMT	C4B-C5B-C6B-O6B
2	C	1101	LMT	C4B-C5B-C6B-O6B
2	C	1101	LMT	C3-C4-C5-C6
2	F	1101	LMT	C1-C2-C3-C4
2	C	1101	LMT	C7-C8-C9-C10
2	B	1102	LMT	C1-C2-C3-C4
2	B	1102	LMT	C2-C1-O1'-C1'
2	C	1101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

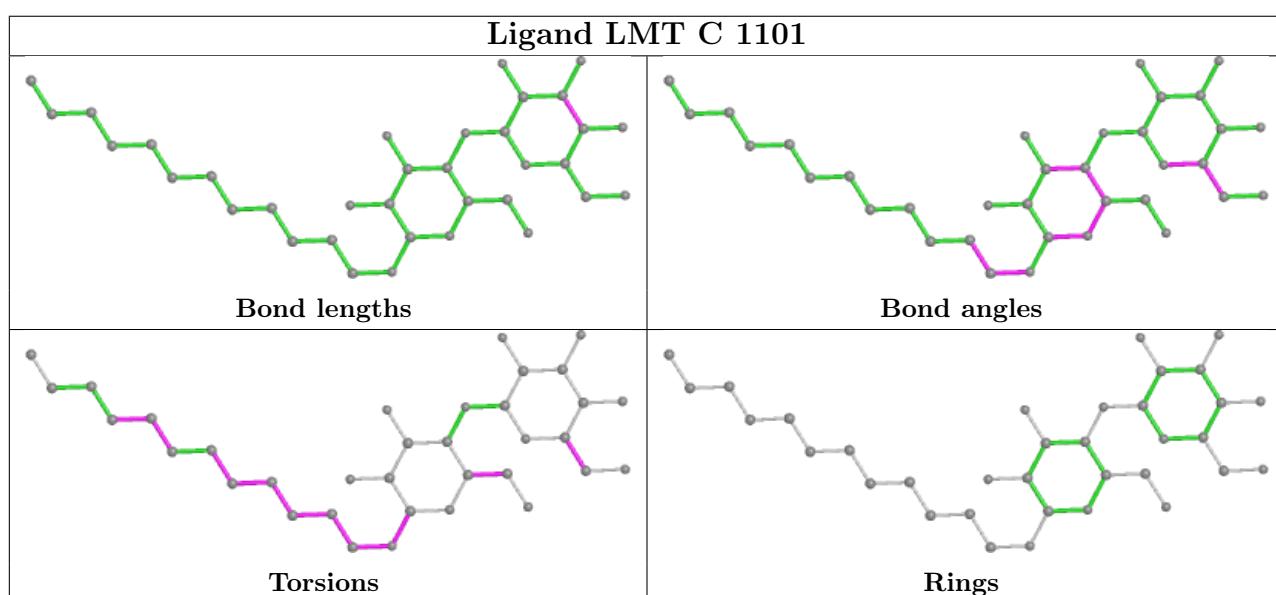
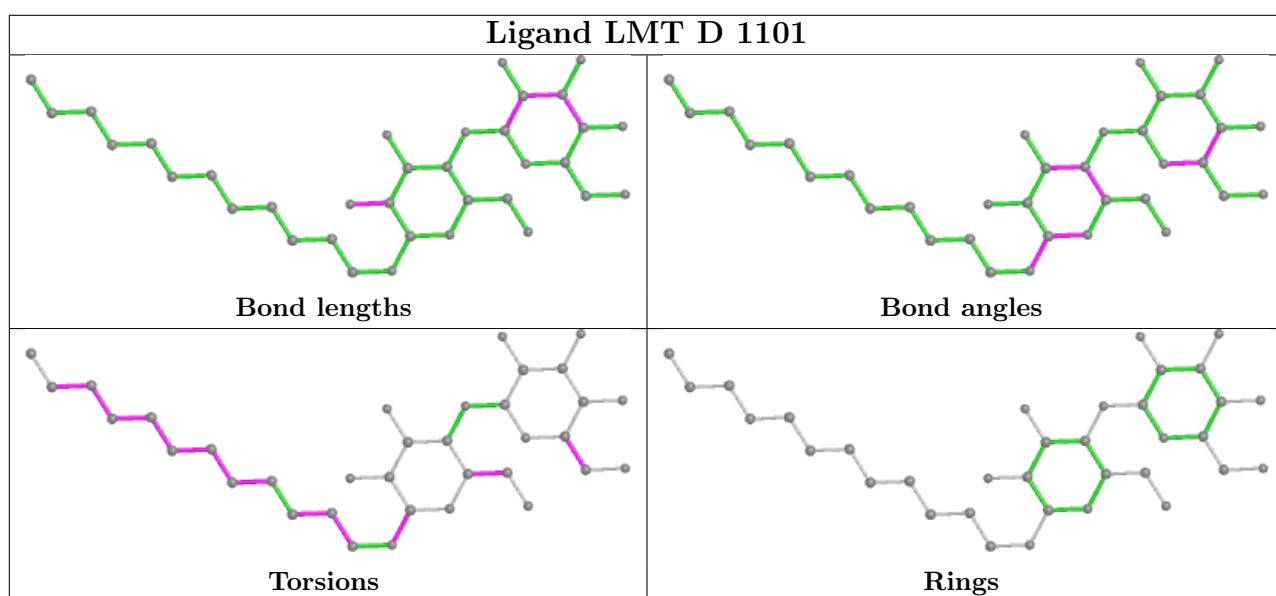
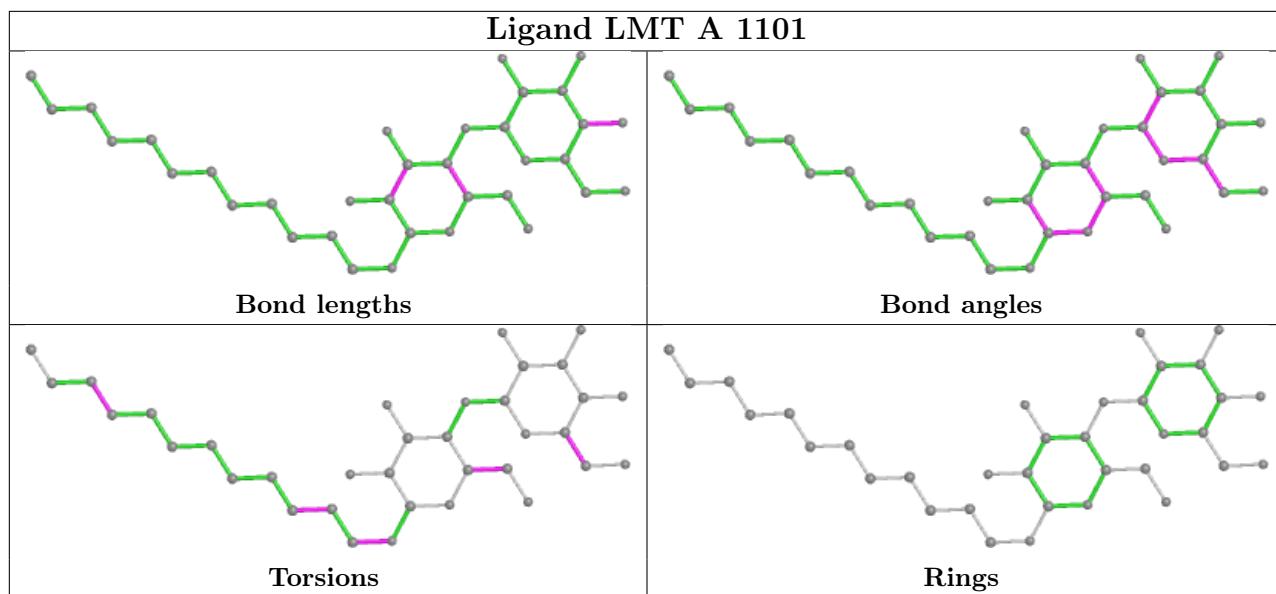
There are no ring outliers.

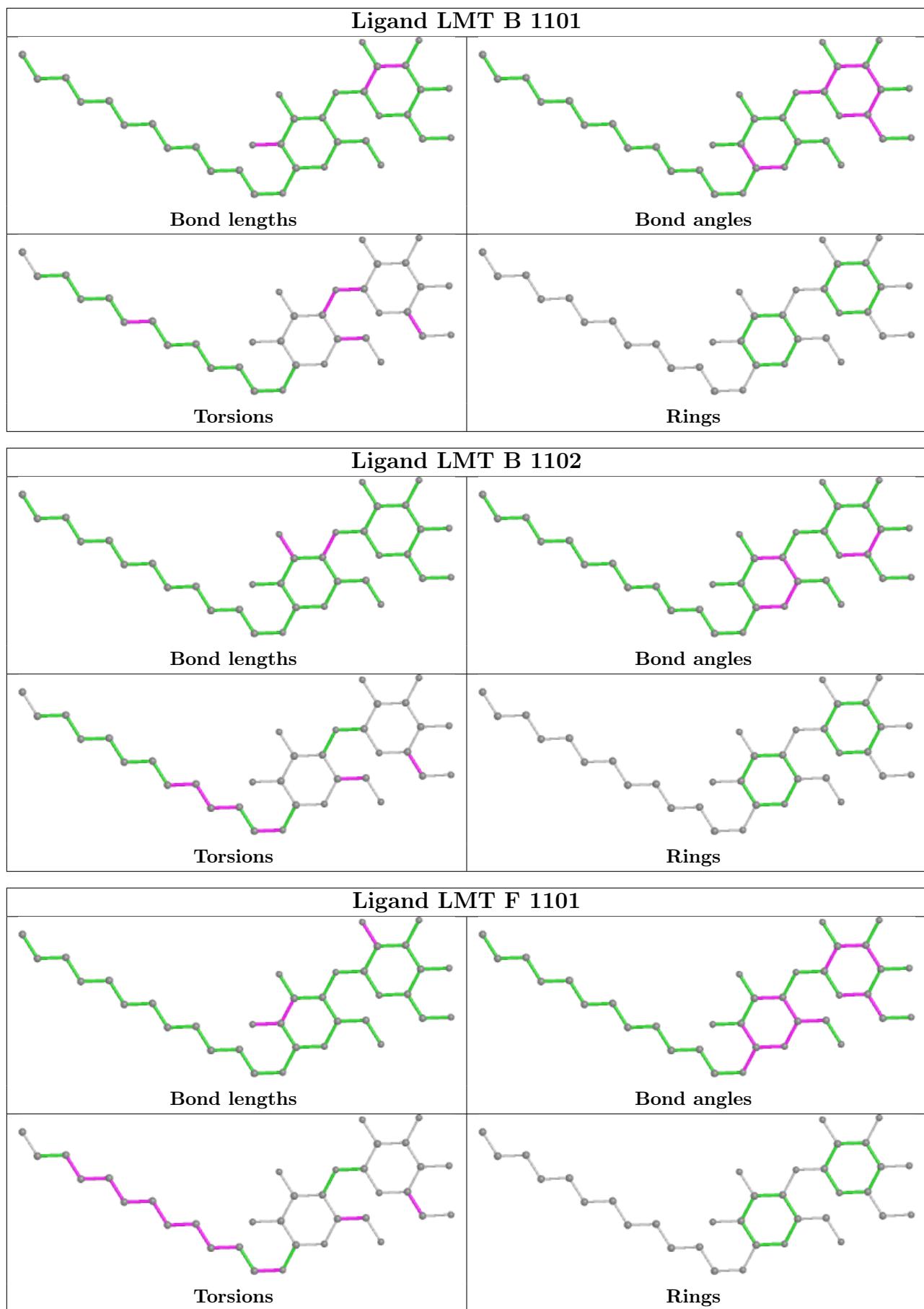
7 monomers are involved in 26 short contacts:

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

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Mol	Chain	Res	Type	RSRZ
1	A	1041	GLY	6.3
1	A	682	LEU	6.1
1	E	880	SER	5.9
1	B	999	SER	5.9
1	E	1003	GLY	5.8
1	A	878	GLY	5.7
1	D	999	SER	5.6
1	A	503	GLY	5.5
1	C	772	PHE	5.4
1	A	683	GLY	5.2
1	E	1043	LYS	5.1
1	F	773	GLY	5.0
1	B	998	LEU	4.9
1	F	1011	GLY	4.9
1	B	506	GLU	4.9
1	C	743	ALA	4.8
1	B	877	ALA	4.8
1	F	1040	ALA	4.6
1	B	879	ASP	4.4
1	B	878	GLY	4.4
1	D	1006	MET	4.4
1	E	999	SER	4.3
1	D	853	ARG	4.3
1	F	995	PRO	4.3
1	D	996	LEU	4.2
1	D	502	HIS	4.2
1	A	837	GLY	4.2
1	D	686	GLY	4.2
1	B	505	LYS	4.1
1	C	806	VAL	4.1
1	A	1039	LEU	4.0
1	E	2	ASN	4.0
1	E	1004	ALA	4.0
1	C	709	ASP	4.0
1	C	172	GLN	4.0
1	A	1040	ALA	4.0
1	C	707	THR	4.0
1	E	1005	GLU	3.9
1	C	750	VAL	3.8
1	B	682	LEU	3.8
1	A	998	LEU	3.8
1	C	788	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	863	VAL	3.7
1	E	878	GLY	3.7
1	E	200	ASN	3.7
1	E	877	ALA	3.7
1	A	1042	GLY	3.7
1	A	1007	ARG	3.7
1	F	715	GLN	3.7
1	C	744	LYS	3.6
1	E	462	SER	3.6
1	C	753	VAL	3.6
1	D	748	VAL	3.6
1	C	754	PHE	3.6
1	C	804	GLU	3.5
1	C	706	ALA	3.5
1	E	502	HIS	3.5
1	D	583	PHE	3.5
1	D	882	PHE	3.5
1	E	791	ASP	3.5
1	F	716	GLN	3.4
1	C	845	GLY	3.4
1	A	857	GLN	3.4
1	F	857	GLN	3.4
1	D	503	GLY	3.3
1	F	128	GLY	3.3
1	E	201	LEU	3.3
1	D	119	ARG	3.3
1	A	261	GLY	3.3
1	D	1009	ALA	3.3
1	D	687	GLY	3.3
1	D	840	PRO	3.3
1	D	811	LEU	3.3
1	D	998	LEU	3.2
1	D	1039	LEU	3.2
1	A	814	VAL	3.2
1	A	720	LEU	3.2
1	A	649	ALA	3.2
1	C	798	THR	3.2
1	C	701	ALA	3.2
1	A	648	LYS	3.2
1	E	760	TYR	3.1
1	E	808	LEU	3.1
1	A	882	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	272	GLU	3.1
1	B	648	LYS	3.1
1	D	685	LEU	3.1
1	C	173	GLY	3.0
1	C	738	LEU	3.0
1	D	790	ALA	3.0
1	C	691	GLN	3.0
1	D	504	ASP	3.0
1	B	645	ARG	2.9
1	C	925	TRP	2.9
1	D	814	VAL	2.9
1	D	1002	ALA	2.9
1	D	222	ILE	2.9
1	E	189	VAL	2.9
1	A	500	LYS	2.9
1	B	552	LEU	2.9
1	D	1000	THR	2.8
1	D	682	LEU	2.8
1	E	506	GLU	2.8
1	F	125	GLN	2.8
1	E	740	ARG	2.8
1	B	841	GLY	2.8
1	A	883	TRP	2.8
1	B	632	ALA	2.8
1	B	839	ALA	2.8
1	D	151	TYR	2.8
1	B	262	VAL	2.8
1	A	798	THR	2.7
1	C	729	ILE	2.7
1	F	331	ASP	2.7
1	D	848	GLN	2.7
1	E	796	LEU	2.7
1	B	549	MET	2.7
1	E	780	VAL	2.7
1	D	850	ALA	2.7
1	F	858	THR	2.6
1	F	772	PHE	2.6
1	D	1005	GLU	2.6
1	B	710	PHE	2.6
1	E	739	ASP	2.6
1	F	717	ALA	2.6
1	B	555	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	118	PRO	2.6
1	B	720	LEU	2.6
1	C	773	GLY	2.5
1	D	792	ASP	2.5
1	D	684	THR	2.5
1	C	991	MET	2.5
1	C	837	GLY	2.5
1	E	795	GLN	2.5
1	C	850	ALA	2.5
1	A	925	TRP	2.5
1	B	462	SER	2.5
1	D	857	GLN	2.5
1	C	748	VAL	2.5
1	D	508	TRP	2.5
1	D	700	TYR	2.4
1	B	233	LEU	2.4
1	B	118	PRO	2.4
1	D	324	VAL	2.4
1	F	119	ARG	2.4
1	D	647	GLY	2.4
1	D	849	ALA	2.4
1	C	791	ASP	2.4
1	B	1000	THR	2.4
1	D	714	ALA	2.3
1	A	426	GLY	2.3
1	D	168	LEU	2.3
1	B	1041	GLY	2.3
1	D	720	LEU	2.3
1	B	261	GLY	2.3
1	C	848	GLN	2.3
1	A	712	LYS	2.3
1	B	843	SER	2.3
1	F	111	ASN	2.3
1	D	820	PRO	2.2
1	F	118	PRO	2.2
1	A	583	PHE	2.2
1	B	464	LEU	2.2
1	A	740	ARG	2.2
1	B	647	GLY	2.2
1	C	171	ILE	2.2
1	E	879	ASP	2.2
1	D	500	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	174	VAL	2.2
1	A	697	ALA	2.2
1	D	844	SER	2.1
1	D	791	ASP	2.1
1	B	119	ARG	2.1
1	D	749	ASN	2.1
1	B	650	LEU	2.1
1	E	1001	GLY	2.1
1	A	810	SER	2.1
1	D	1010	MET	2.1
1	E	269	ALA	2.1
1	C	836	GLY	2.1
1	D	836	GLY	2.1
1	C	816	PRO	2.1
1	E	876	LEU	2.0
1	E	505	LYS	2.0
1	A	646	HIS	2.0
1	D	854	ILE	2.0
1	E	265	LEU	2.0
1	D	719	GLU	2.0
1	A	879	ASP	2.0
1	C	118	PRO	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 monosaccharides 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.

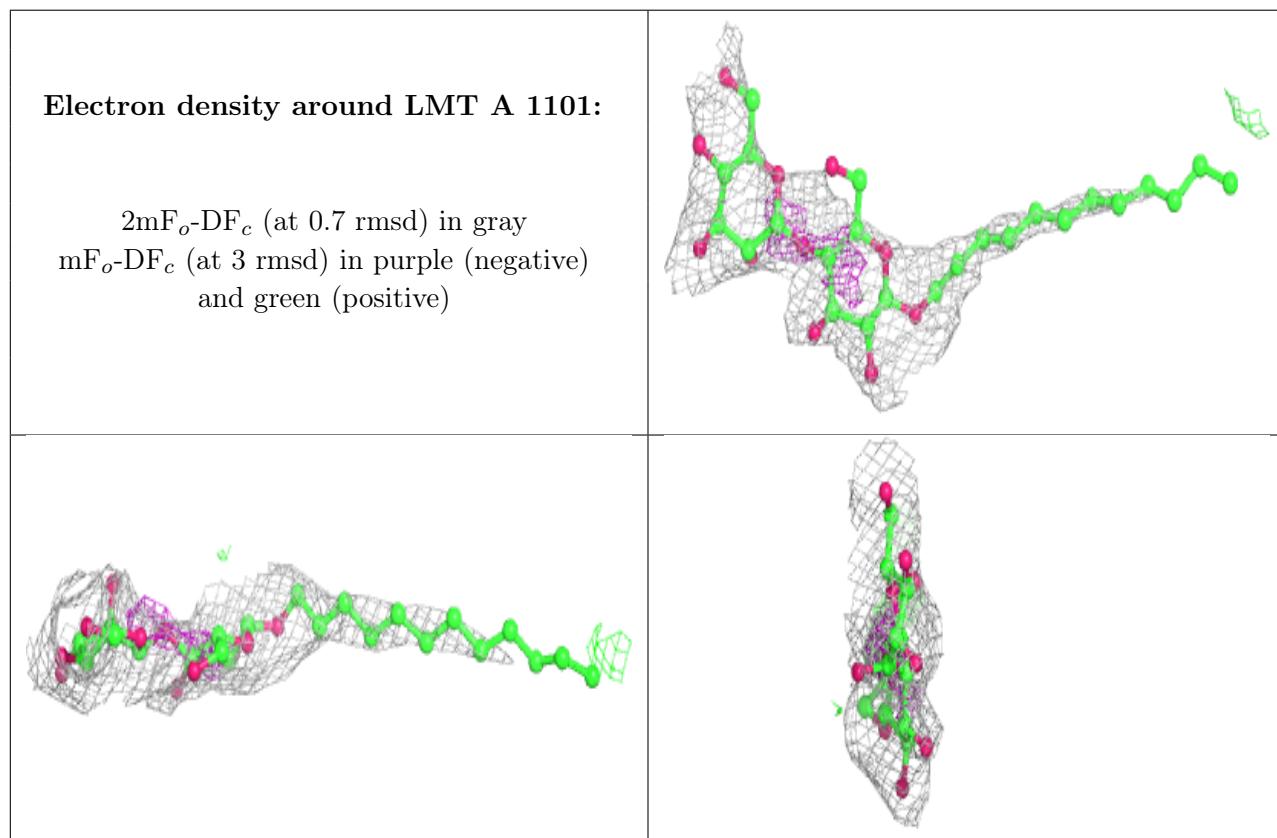
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LMT	A	1101	35/35	0.70	0.42	88,129,148,154	0

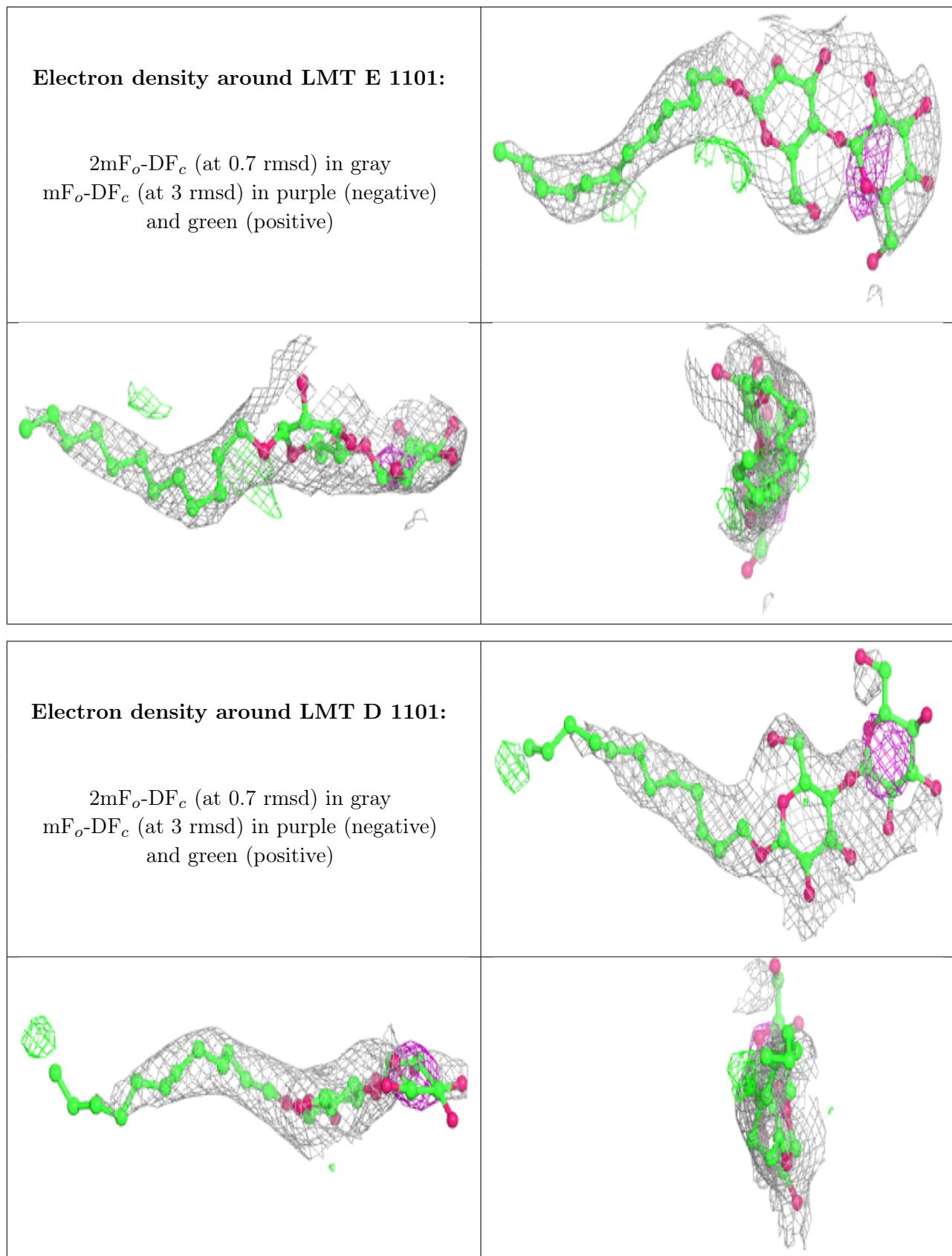
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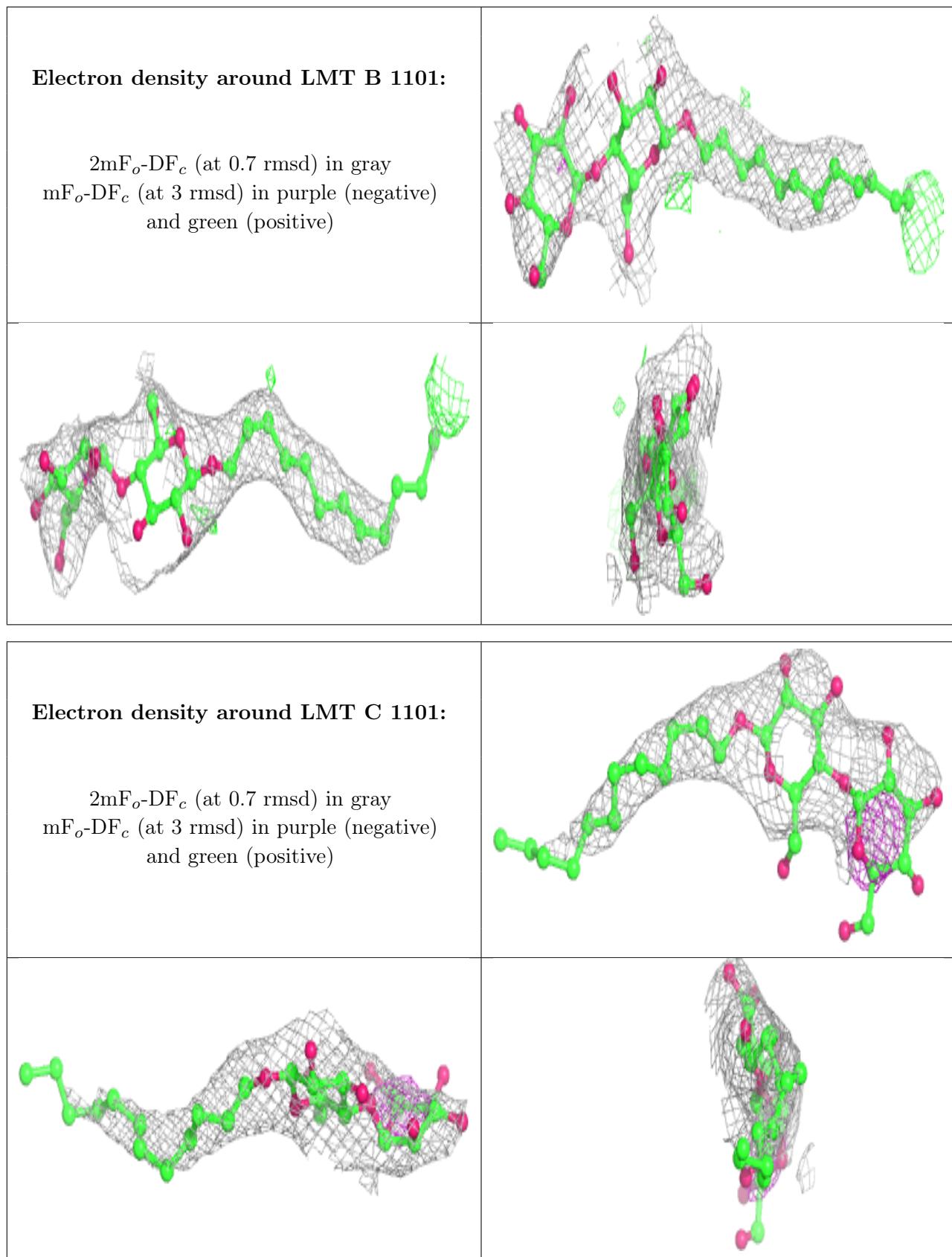
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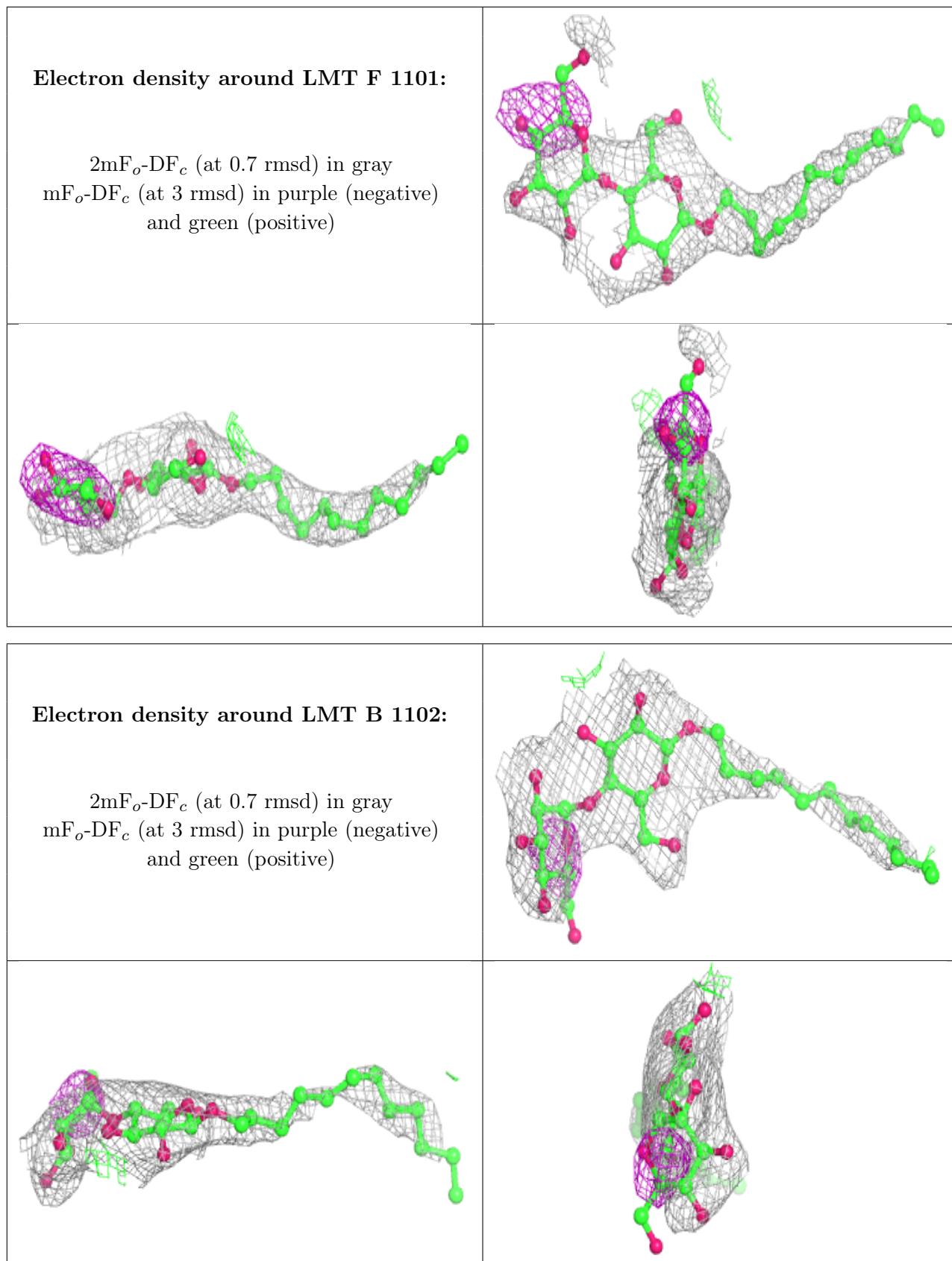
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LMT	E	1101	35/35	0.71	0.22	83,126,137,138	0
2	LMT	D	1101	35/35	0.72	0.30	82,132,147,148	0
2	LMT	B	1101	35/35	0.77	0.24	83,122,135,137	0
2	LMT	C	1101	35/35	0.77	0.41	86,131,141,145	0
2	LMT	F	1101	35/35	0.77	0.30	85,126,134,138	0
2	LMT	B	1102	35/35	0.83	0.36	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.









6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.