



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:23 AM UTC

PDB ID : 7O3N / pdb_00007o3n
Title : Crystal Structure of AcrB Single Mutant - 2
Authors : Ababou, A.
Deposited on : 2021-04-02
Resolution : 3.56 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:

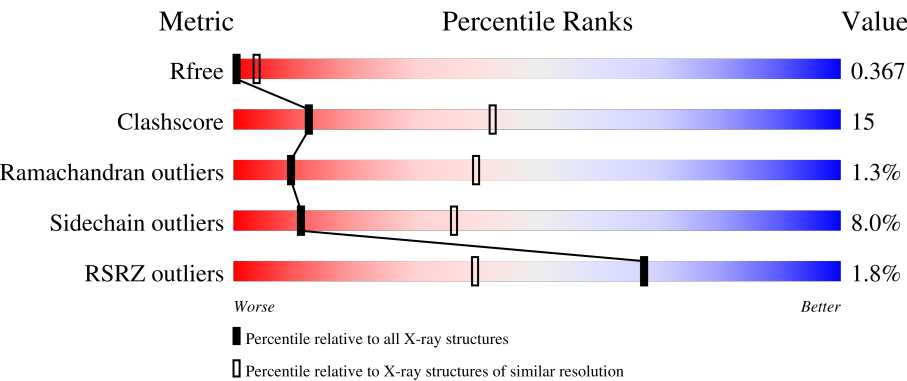
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 3.56 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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	1069	% 58%36% . .
1	B	1069	2% 60%34% . .
1	C	1069	4% 59%34% . .
1	D	1069	% 62%32% . .
1	E	1069	% 62%32% . .

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Mol	Chain	Length	Quality of chain
1	F	1069	 % 62% 31% 5%

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	2000	X	-	-	-
2	LMT	B	2000	X	-	-	-
2	LMT	C	2000	X	-	-	-
2	LMT	D	2000	X	-	-	-
2	LMT	E	2000	X	-	-	-
2	LMT	F	2000	X	-	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 47816 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	1044	Total	C	N	O	S	0	0	0
			7940	5105	1313	1479	43			
1	B	1042	Total	C	N	O	S	0	0	0
			7923	5095	1309	1476	43			
1	C	1044	Total	C	N	O	S	0	0	0
			7940	5105	1313	1479	43			
1	D	1044	Total	C	N	O	S	0	0	0
			7940	5105	1313	1479	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7923	5095	1309	1476	43			
1	F	1044	Total	C	N	O	S	0	0	0
			7940	5105	1313	1479	43			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E2QH56
A	-18	GLY	-	expression tag	UNP E2QH56
A	-17	SER	-	expression tag	UNP E2QH56
A	-16	SER	-	expression tag	UNP E2QH56
A	-15	HIS	-	expression tag	UNP E2QH56
A	-14	HIS	-	expression tag	UNP E2QH56
A	-13	HIS	-	expression tag	UNP E2QH56
A	-12	HIS	-	expression tag	UNP E2QH56
A	-11	HIS	-	expression tag	UNP E2QH56
A	-10	HIS	-	expression tag	UNP E2QH56
A	-9	SER	-	expression tag	UNP E2QH56
A	-8	SER	-	expression tag	UNP E2QH56
A	-7	GLY	-	expression tag	UNP E2QH56
A	-6	LEU	-	expression tag	UNP E2QH56
A	-5	VAL	-	expression tag	UNP E2QH56
A	-4	PRO	-	expression tag	UNP E2QH56
A	-3	ARG	-	expression tag	UNP E2QH56

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP E2QH56
A	-1	SER	-	expression tag	UNP E2QH56
A	0	HIS	-	expression tag	UNP E2QH56
A	620	LYS	ARG	engineered mutation	UNP E2QH56
B	-19	MET	-	initiating methionine	UNP E2QH56
B	-18	GLY	-	expression tag	UNP E2QH56
B	-17	SER	-	expression tag	UNP E2QH56
B	-16	SER	-	expression tag	UNP E2QH56
B	-15	HIS	-	expression tag	UNP E2QH56
B	-14	HIS	-	expression tag	UNP E2QH56
B	-13	HIS	-	expression tag	UNP E2QH56
B	-12	HIS	-	expression tag	UNP E2QH56
B	-11	HIS	-	expression tag	UNP E2QH56
B	-10	HIS	-	expression tag	UNP E2QH56
B	-9	SER	-	expression tag	UNP E2QH56
B	-8	SER	-	expression tag	UNP E2QH56
B	-7	GLY	-	expression tag	UNP E2QH56
B	-6	LEU	-	expression tag	UNP E2QH56
B	-5	VAL	-	expression tag	UNP E2QH56
B	-4	PRO	-	expression tag	UNP E2QH56
B	-3	ARG	-	expression tag	UNP E2QH56
B	-2	GLY	-	expression tag	UNP E2QH56
B	-1	SER	-	expression tag	UNP E2QH56
B	0	HIS	-	expression tag	UNP E2QH56
B	620	LYS	ARG	engineered mutation	UNP E2QH56
C	-19	MET	-	initiating methionine	UNP E2QH56
C	-18	GLY	-	expression tag	UNP E2QH56
C	-17	SER	-	expression tag	UNP E2QH56
C	-16	SER	-	expression tag	UNP E2QH56
C	-15	HIS	-	expression tag	UNP E2QH56
C	-14	HIS	-	expression tag	UNP E2QH56
C	-13	HIS	-	expression tag	UNP E2QH56
C	-12	HIS	-	expression tag	UNP E2QH56
C	-11	HIS	-	expression tag	UNP E2QH56
C	-10	HIS	-	expression tag	UNP E2QH56
C	-9	SER	-	expression tag	UNP E2QH56
C	-8	SER	-	expression tag	UNP E2QH56
C	-7	GLY	-	expression tag	UNP E2QH56
C	-6	LEU	-	expression tag	UNP E2QH56
C	-5	VAL	-	expression tag	UNP E2QH56
C	-4	PRO	-	expression tag	UNP E2QH56
C	-3	ARG	-	expression tag	UNP E2QH56

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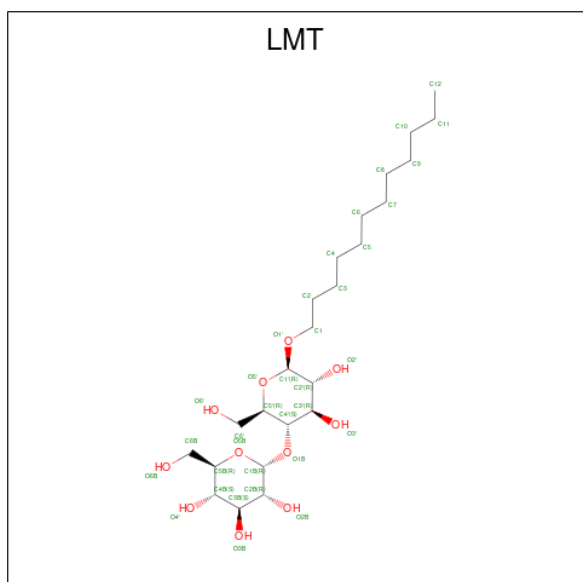
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP E2QH56
C	-1	SER	-	expression tag	UNP E2QH56
C	0	HIS	-	expression tag	UNP E2QH56
C	620	LYS	ARG	engineered mutation	UNP E2QH56
D	-19	MET	-	initiating methionine	UNP E2QH56
D	-18	GLY	-	expression tag	UNP E2QH56
D	-17	SER	-	expression tag	UNP E2QH56
D	-16	SER	-	expression tag	UNP E2QH56
D	-15	HIS	-	expression tag	UNP E2QH56
D	-14	HIS	-	expression tag	UNP E2QH56
D	-13	HIS	-	expression tag	UNP E2QH56
D	-12	HIS	-	expression tag	UNP E2QH56
D	-11	HIS	-	expression tag	UNP E2QH56
D	-10	HIS	-	expression tag	UNP E2QH56
D	-9	SER	-	expression tag	UNP E2QH56
D	-8	SER	-	expression tag	UNP E2QH56
D	-7	GLY	-	expression tag	UNP E2QH56
D	-6	LEU	-	expression tag	UNP E2QH56
D	-5	VAL	-	expression tag	UNP E2QH56
D	-4	PRO	-	expression tag	UNP E2QH56
D	-3	ARG	-	expression tag	UNP E2QH56
D	-2	GLY	-	expression tag	UNP E2QH56
D	-1	SER	-	expression tag	UNP E2QH56
D	0	HIS	-	expression tag	UNP E2QH56
D	620	LYS	ARG	engineered mutation	UNP E2QH56
E	-19	MET	-	initiating methionine	UNP E2QH56
E	-18	GLY	-	expression tag	UNP E2QH56
E	-17	SER	-	expression tag	UNP E2QH56
E	-16	SER	-	expression tag	UNP E2QH56
E	-15	HIS	-	expression tag	UNP E2QH56
E	-14	HIS	-	expression tag	UNP E2QH56
E	-13	HIS	-	expression tag	UNP E2QH56
E	-12	HIS	-	expression tag	UNP E2QH56
E	-11	HIS	-	expression tag	UNP E2QH56
E	-10	HIS	-	expression tag	UNP E2QH56
E	-9	SER	-	expression tag	UNP E2QH56
E	-8	SER	-	expression tag	UNP E2QH56
E	-7	GLY	-	expression tag	UNP E2QH56
E	-6	LEU	-	expression tag	UNP E2QH56
E	-5	VAL	-	expression tag	UNP E2QH56
E	-4	PRO	-	expression tag	UNP E2QH56
E	-3	ARG	-	expression tag	UNP E2QH56

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP E2QH56
E	-1	SER	-	expression tag	UNP E2QH56
E	0	HIS	-	expression tag	UNP E2QH56
E	620	LYS	ARG	engineered mutation	UNP E2QH56
F	-19	MET	-	initiating methionine	UNP E2QH56
F	-18	GLY	-	expression tag	UNP E2QH56
F	-17	SER	-	expression tag	UNP E2QH56
F	-16	SER	-	expression tag	UNP E2QH56
F	-15	HIS	-	expression tag	UNP E2QH56
F	-14	HIS	-	expression tag	UNP E2QH56
F	-13	HIS	-	expression tag	UNP E2QH56
F	-12	HIS	-	expression tag	UNP E2QH56
F	-11	HIS	-	expression tag	UNP E2QH56
F	-10	HIS	-	expression tag	UNP E2QH56
F	-9	SER	-	expression tag	UNP E2QH56
F	-8	SER	-	expression tag	UNP E2QH56
F	-7	GLY	-	expression tag	UNP E2QH56
F	-6	LEU	-	expression tag	UNP E2QH56
F	-5	VAL	-	expression tag	UNP E2QH56
F	-4	PRO	-	expression tag	UNP E2QH56
F	-3	ARG	-	expression tag	UNP E2QH56
F	-2	GLY	-	expression tag	UNP E2QH56
F	-1	SER	-	expression tag	UNP E2QH56
F	0	HIS	-	expression tag	UNP E2QH56
F	620	LYS	ARG	engineered mutation	UNP E2QH56

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

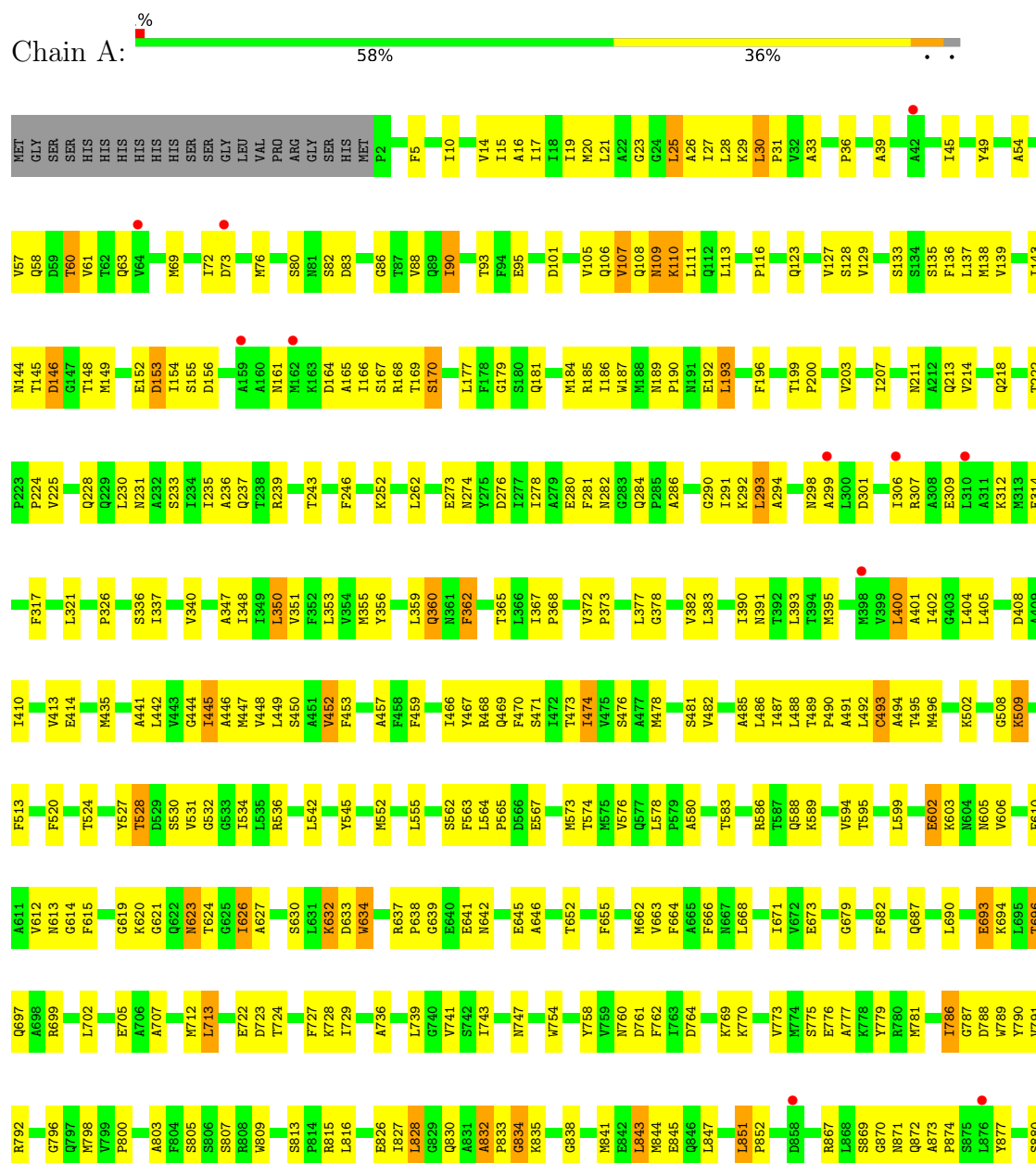


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	C	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		

3 Residue-property plots

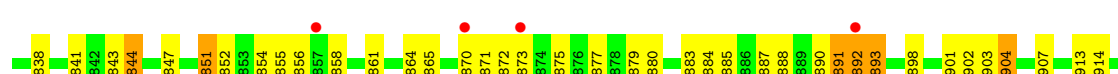
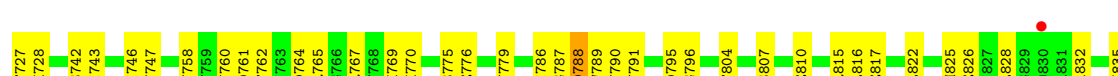
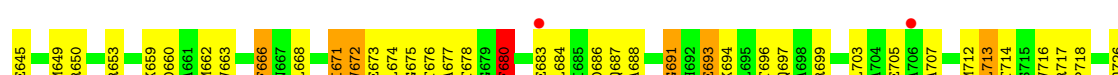
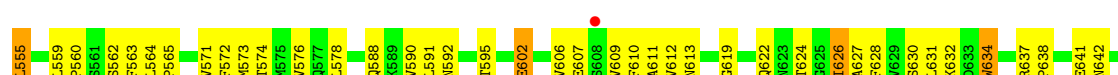
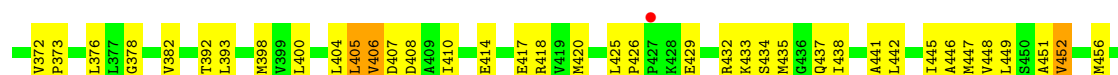
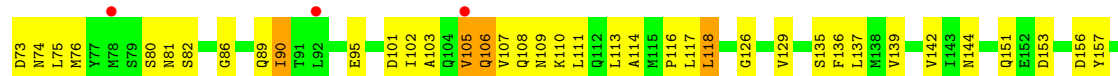
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

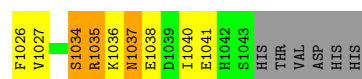
- Molecule 1: Efflux pump membrane transporter



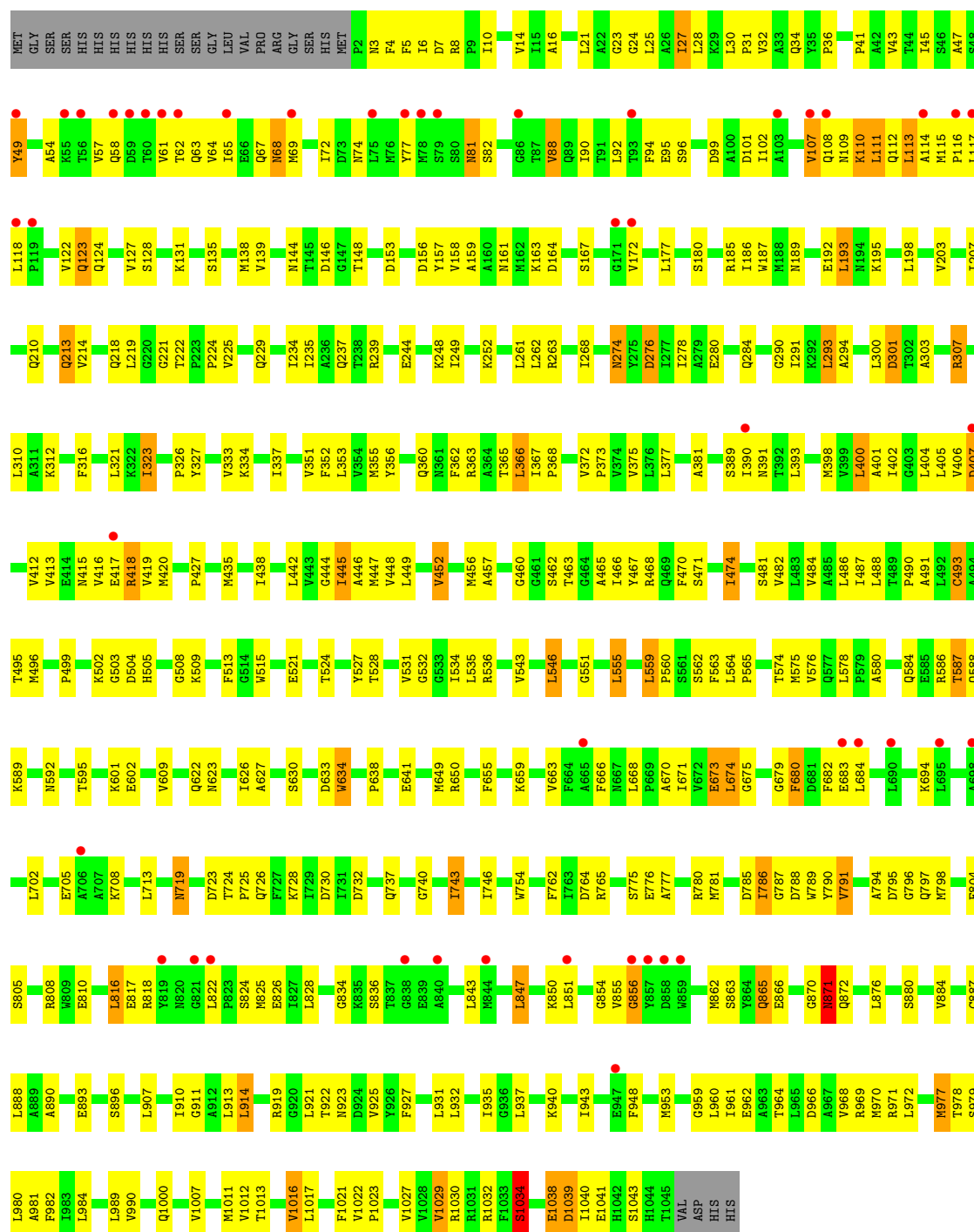


● Molecule 1: Efflux pump membrane transporter

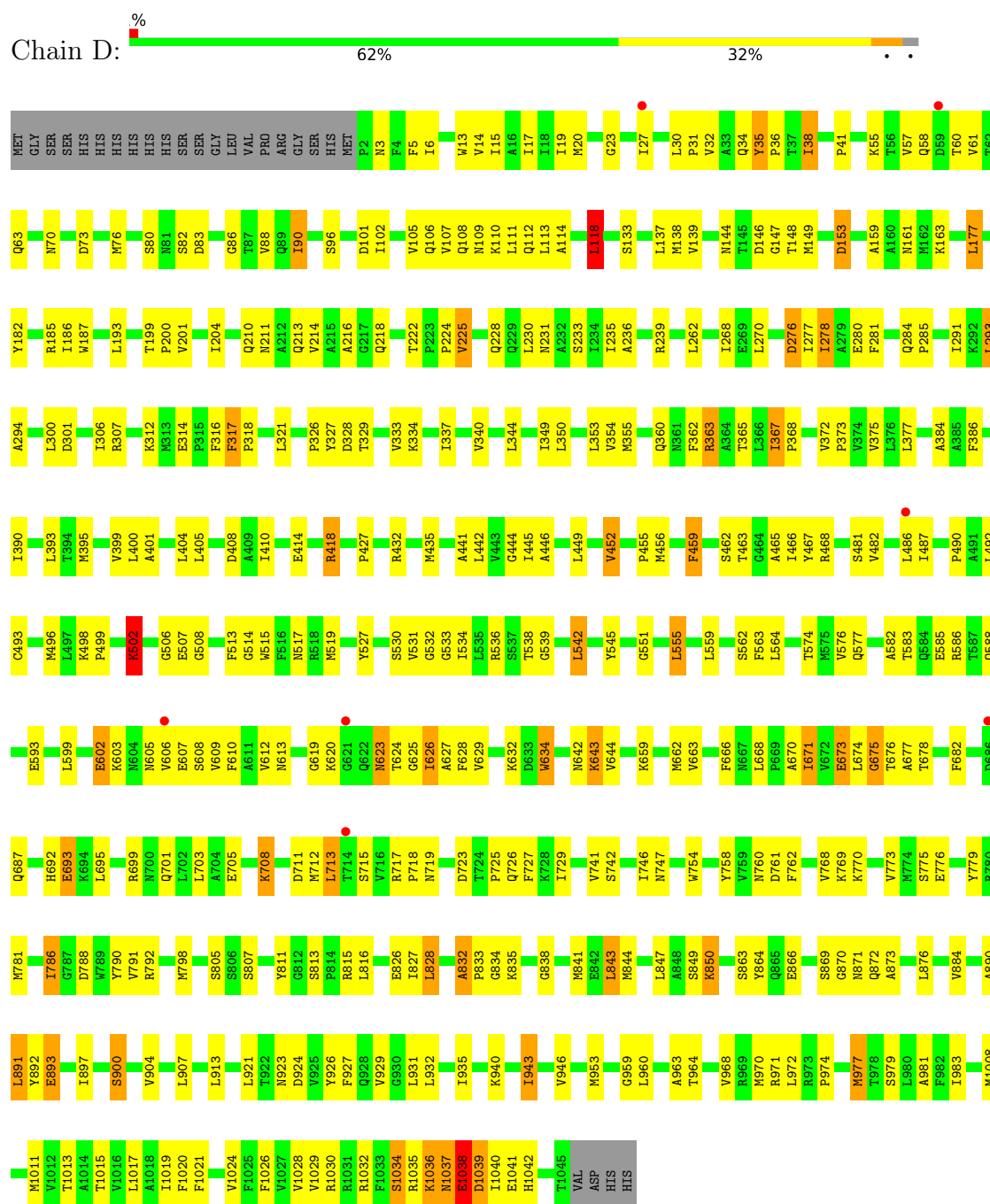




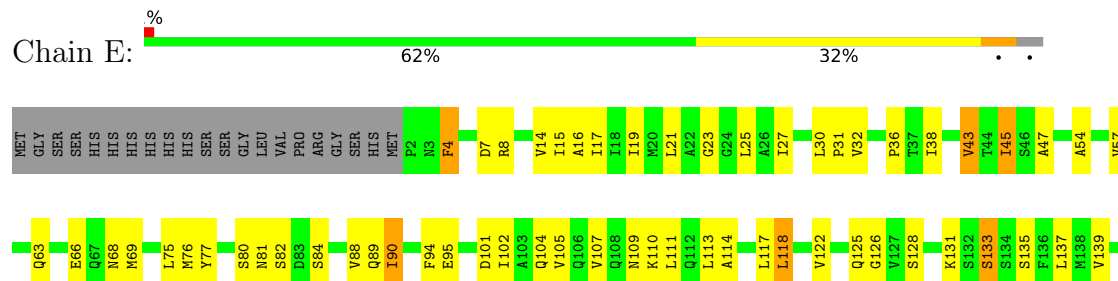
• Molecule 1: Efflux pump membrane transporter

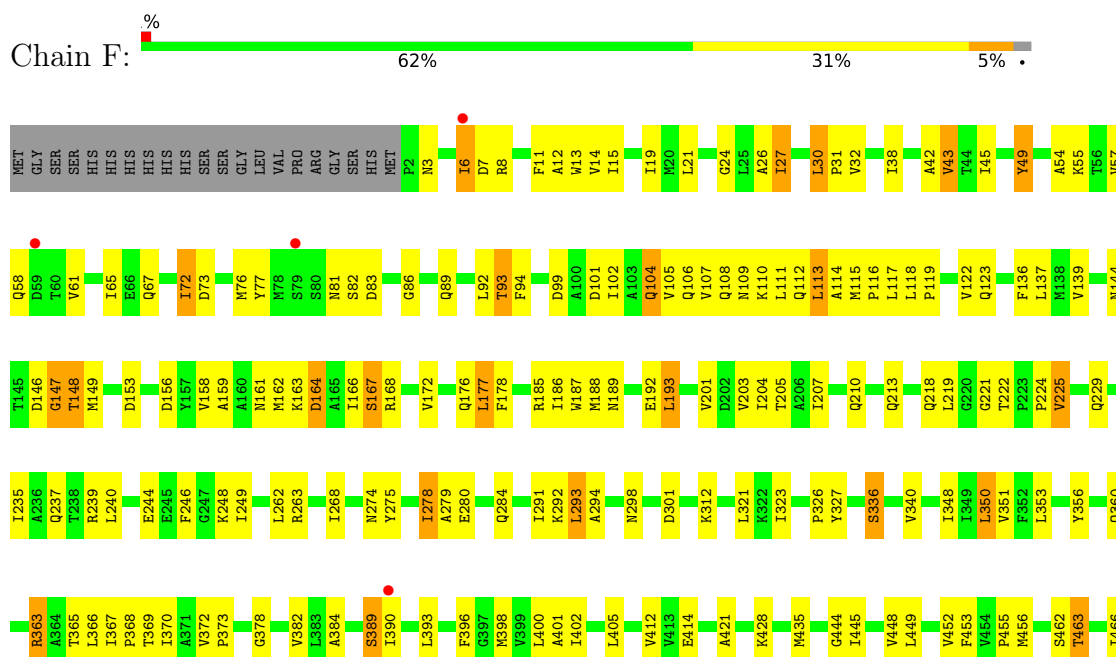
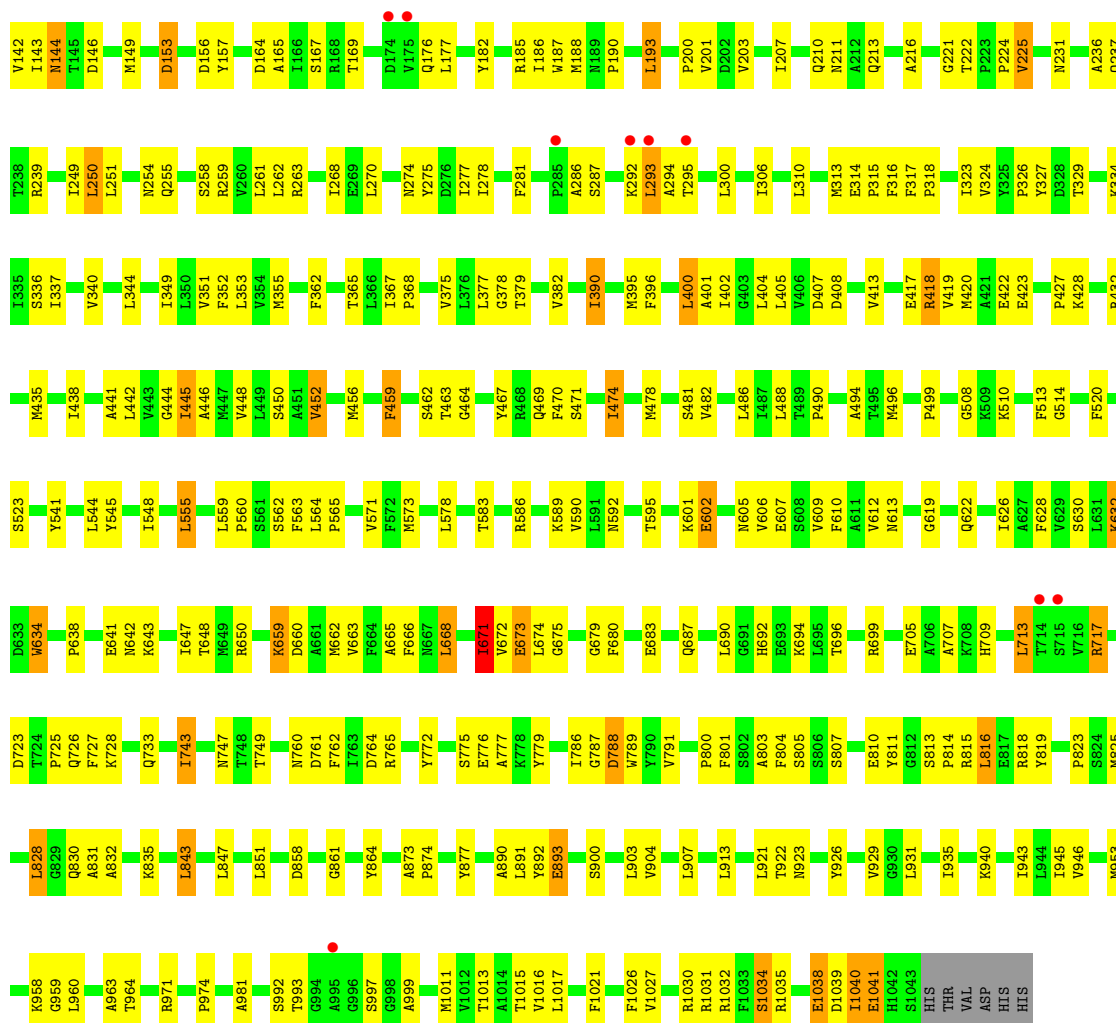


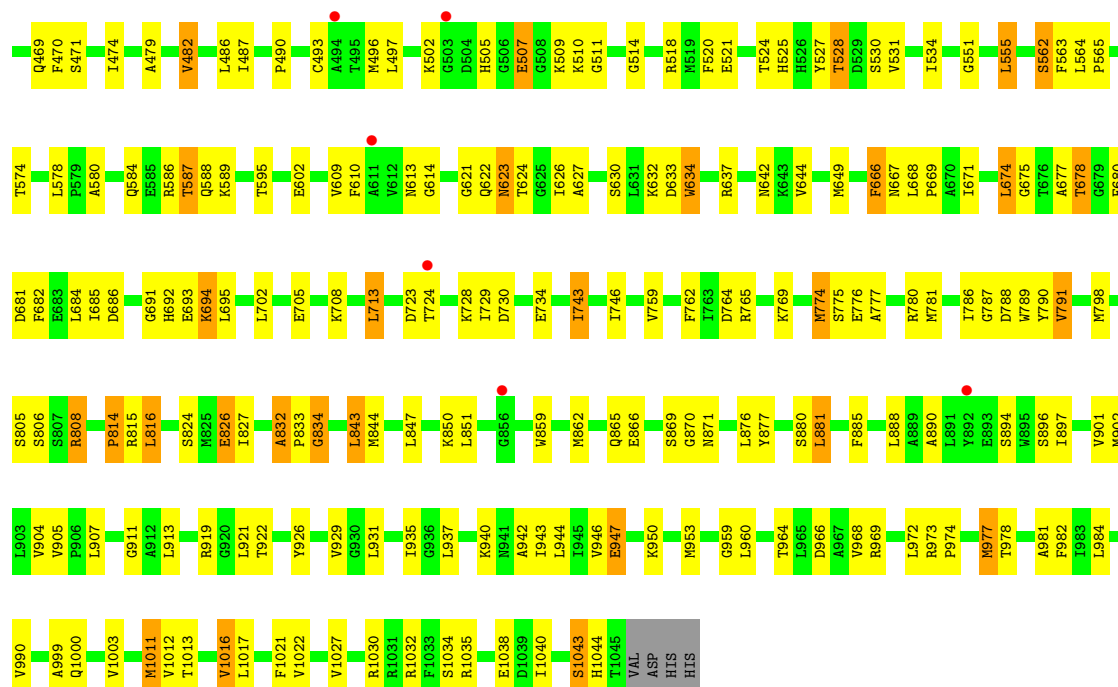
• Molecule 1: Efflux pump membrane transporter



● Molecule 1: Efflux pump membrane transporter







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	152.34Å 157.10Å 218.86Å 90.00° 92.73° 90.00°	Depositor
Resolution (Å)	20.00 – 3.56 20.00 – 3.56	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.56) 98.3 (20.00-3.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 3.52Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.306 , 0.366 0.308 , 0.367	Depositor DCC
R_{free} test set	6118 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	102.9	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 15.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.079 for -k,-h,-l 0.099 for k,h,-l 0.097 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	47816	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0059e-05.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.34	0/8092	0.91	19/10987 (0.2%)
1	B	0.35	0/8074	0.91	21/10962 (0.2%)
1	C	0.36	0/8092	0.95	21/10987 (0.2%)
1	D	0.34	0/8092	0.88	20/10987 (0.2%)
1	E	0.34	0/8074	0.89	13/10962 (0.1%)
1	F	0.34	0/8092	0.91	18/10987 (0.2%)
All	All	0.35	0/48516	0.91	112/65872 (0.2%)

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	C	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	854	GLY	N-CA-C	-11.20	99.73	114.85
1	C	8	ARG	CA-C-N	10.57	130.40	119.19
1	C	8	ARG	C-N-CA	10.57	130.40	119.19
1	B	851	LEU	CA-C-N	9.13	129.49	119.90
1	B	851	LEU	C-N-CA	9.13	129.49	119.90
1	F	30	LEU	CA-C-N	8.87	128.95	119.90
1	F	30	LEU	C-N-CA	8.87	128.95	119.90
1	C	113	LEU	N-CA-C	-8.63	102.67	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	832	ALA	CA-C-N	8.00	129.84	119.84
1	A	832	ALA	C-N-CA	8.00	129.84	119.84
1	D	1034	SER	N-CA-C	7.83	117.50	108.49
1	F	7	ASP	N-CA-C	-7.81	103.33	113.17
1	A	1040	ILE	N-CA-C	7.58	121.48	108.90
1	E	680	PHE	N-CA-C	7.57	118.60	108.38
1	D	1038	GLU	CA-C-N	7.40	135.01	121.70
1	D	1038	GLU	C-N-CA	7.40	135.01	121.70
1	C	1038	GLU	CA-C-N	7.37	134.96	121.70
1	C	1038	GLU	C-N-CA	7.37	134.96	121.70
1	F	666	PHE	N-CA-C	6.95	117.41	108.24
1	B	680	PHE	N-CA-C	6.82	117.58	108.38
1	B	675	GLY	N-CA-C	-6.65	103.58	111.36
1	E	851	LEU	CA-C-N	6.62	126.86	119.90
1	E	851	LEU	C-N-CA	6.62	126.86	119.90
1	A	39	ALA	CA-C-N	6.53	127.11	120.38
1	A	39	ALA	C-N-CA	6.53	127.11	120.38
1	C	164	ASP	N-CA-C	-6.52	104.73	114.64
1	E	118	LEU	CA-C-N	6.52	126.55	119.90
1	E	118	LEU	C-N-CA	6.52	126.55	119.90
1	F	832	ALA	CA-C-N	6.36	127.79	119.84
1	F	832	ALA	C-N-CA	6.36	127.79	119.84
1	D	314	GLU	CA-C-N	-6.30	114.40	120.83
1	D	314	GLU	C-N-CA	-6.30	114.40	120.83
1	D	38	ILE	N-CA-C	6.27	116.90	110.82
1	D	692	HIS	N-CA-C	-6.21	105.86	113.50
1	A	317	PHE	CA-C-N	6.16	127.54	119.84
1	A	317	PHE	C-N-CA	6.16	127.54	119.84
1	B	40	PRO	CA-C-N	6.15	127.52	119.84
1	B	40	PRO	C-N-CA	6.15	127.52	119.84
1	C	683	GLU	N-CA-C	6.12	118.66	108.20
1	B	693	GLU	N-CA-C	-6.09	106.01	113.50
1	D	35	TYR	CA-C-N	-6.08	112.23	119.84
1	D	35	TYR	C-N-CA	-6.08	112.23	119.84
1	E	287	SER	CA-C-N	-6.06	117.08	122.47
1	E	287	SER	C-N-CA	-6.06	117.08	122.47
1	F	8	ARG	CA-C-N	6.04	125.59	119.19
1	F	8	ARG	C-N-CA	6.04	125.59	119.19
1	D	708	LYS	N-CA-C	-5.98	105.57	112.92
1	F	113	LEU	N-CA-C	-5.89	106.63	113.88
1	C	666	PHE	N-CA-C	5.81	116.22	108.38
1	A	314	GLU	CA-C-N	-5.80	114.92	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	GLU	C-N-CA	-5.80	114.92	120.83
1	E	707	ALA	N-CA-C	-5.75	106.24	113.72
1	F	693	GLU	N-CA-C	-5.74	106.26	113.72
1	D	367	ILE	CA-C-N	-5.67	113.92	119.64
1	D	367	ILE	C-N-CA	-5.67	113.92	119.64
1	B	674	LEU	N-CA-C	5.65	117.83	110.43
1	C	195	LYS	N-CA-C	5.63	120.61	111.37
1	A	30	LEU	CA-C-N	5.62	125.63	119.90
1	A	30	LEU	C-N-CA	5.62	125.63	119.90
1	D	317	PHE	CA-C-N	5.61	126.85	119.84
1	D	317	PHE	C-N-CA	5.61	126.85	119.84
1	A	851	LEU	CA-C-N	5.59	125.77	119.90
1	A	851	LEU	C-N-CA	5.59	125.77	119.90
1	F	49	TYR	CA-C-N	5.59	125.52	119.76
1	F	49	TYR	C-N-CA	5.59	125.52	119.76
1	C	460	GLY	N-CA-C	5.57	121.12	112.60
1	C	167	SER	N-CA-C	-5.56	106.09	112.92
1	F	1022	VAL	CB-CA-C	-5.53	108.45	113.70
1	F	1043	SER	N-CA-C	5.53	115.54	108.24
1	C	834	GLY	N-CA-C	-5.50	100.14	113.18
1	A	49	TYR	CA-C-N	5.49	125.42	119.76
1	A	49	TYR	C-N-CA	5.49	125.42	119.76
1	F	685	ILE	N-CA-C	5.48	115.85	108.17
1	B	30	LEU	CA-C-N	5.46	125.47	119.90
1	B	30	LEU	C-N-CA	5.46	125.47	119.90
1	B	637	ARG	CA-C-N	5.45	126.65	119.84
1	B	637	ARG	C-N-CA	5.45	126.65	119.84
1	B	39	ALA	CA-C-N	5.44	123.63	119.66
1	B	39	ALA	C-N-CA	5.44	123.63	119.66
1	E	133	SER	CA-C-O	5.39	121.06	117.94
1	A	707	ALA	N-CA-C	-5.36	106.76	113.72
1	C	49	TYR	CA-C-N	5.33	125.25	119.76
1	C	49	TYR	C-N-CA	5.33	125.25	119.76
1	B	317	PHE	CA-C-N	5.32	126.48	119.84
1	B	317	PHE	C-N-CA	5.32	126.48	119.84
1	C	719	ASN	N-CA-C	5.29	117.83	107.57
1	F	164	ASP	N-CA-C	-5.28	106.62	114.64
1	C	1022	VAL	CB-CA-C	-5.25	108.72	113.70
1	D	832	ALA	CA-C-N	5.22	126.37	119.84
1	D	832	ALA	C-N-CA	5.22	126.37	119.84
1	B	666	PHE	N-CA-C	5.21	115.12	108.24
1	E	1038	GLU	N-CA-C	-5.21	106.25	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	856	GLY	N-CA-C	5.20	118.81	111.42
1	D	666	PHE	N-CA-C	5.19	114.68	107.73
1	E	692	HIS	N-CA-C	-5.17	107.14	113.50
1	B	426	PRO	CA-C-N	5.14	126.27	119.84
1	B	426	PRO	C-N-CA	5.14	126.27	119.84
1	F	729	ILE	N-CA-C	5.12	114.15	106.42
1	C	855	VAL	N-CA-C	-5.09	100.23	107.77
1	D	693	GLU	N-CA-C	-5.09	107.24	113.50
1	B	367	ILE	CA-C-N	-5.08	114.55	120.04
1	B	367	ILE	C-N-CA	-5.08	114.55	120.04
1	C	193	LEU	N-CA-C	-5.06	107.27	113.50
1	A	489	THR	CA-C-N	-5.06	113.52	119.84
1	A	489	THR	C-N-CA	-5.06	113.52	119.84
1	E	438	ILE	N-CA-C	5.06	117.08	112.43
1	A	905	VAL	CB-CA-C	-5.04	108.91	113.70
1	E	110	LYS	N-CA-C	-5.04	107.17	113.72
1	D	118	LEU	CA-C-N	5.03	125.03	119.90
1	D	118	LEU	C-N-CA	5.03	125.03	119.90
1	F	168	ARG	N-CA-C	-5.02	105.88	112.41
1	C	5	PHE	N-CA-C	-5.02	105.89	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	148	THR	Peptide
1	F	834	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7940	0	8080	282	0
1	B	7923	0	8066	262	0
1	C	7940	0	8080	282	0
1	D	7940	0	8080	248	0
1	E	7923	0	8066	234	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	7940	0	8080	255	0
2	A	35	0	46	2	0
2	B	35	0	46	2	0
2	C	35	0	46	0	0
2	D	35	0	46	1	0
2	E	35	0	46	1	0
2	F	35	0	46	3	0
All	All	47816	0	48728	1484	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1484) 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:C:446:ALA:HB2	1:C:482:VAL:HG21	1.50	0.94
1:A:105:VAL:HG21	1:B:105:VAL:HG13	1.52	0.89
1:C:1038:GLU:HA	1:C:1039:ASP:HB2	1.54	0.89
1:D:105:VAL:HG22	1:E:105:VAL:HG11	1.56	0.88
1:E:726:GLN:HG3	1:E:810:GLU:HG3	1.55	0.88
1:C:907:LEU:HD23	1:C:1017:LEU:HB3	1.57	0.87
1:D:355:MET:HE2	1:D:368:PRO:HG2	1.56	0.87
1:A:907:LEU:HD23	1:A:1017:LEU:HB3	1.58	0.84
1:B:726:GLN:HG3	1:B:810:GLU:HG3	1.58	0.83
1:A:400:LEU:HD11	1:A:1003:VAL:HG11	1.60	0.83
1:D:1038:GLU:HB3	1:D:1039:ASP:HB3	1.62	0.82
1:E:444:GLY:HA3	1:E:891:LEU:HD22	1.58	0.82
1:D:367:ILE:HD12	1:D:492:LEU:HB3	1.62	0.82
1:C:393:LEU:HD13	1:C:466:ILE:HA	1.61	0.81
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.61	0.81
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.60	0.81
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.63	0.80
1:A:687:GLN:O	1:C:161:ASN:ND2	2.14	0.80
1:C:144:ASN:O	1:C:284:GLN:NE2	2.15	0.80
1:B:712:MET:HG3	1:B:713:LEU:HD12	1.62	0.79
1:B:919:ARG:NH1	1:B:990:VAL:O	2.14	0.79
1:A:312:LYS:NZ	1:B:858:ASP:OD2	2.14	0.79
1:E:907:LEU:HD23	1:E:1017:LEU:HB3	1.66	0.78
1:C:300:LEU:HD21	1:C:334:LYS:HG3	1.66	0.78
1:D:605:ASN:ND2	1:D:642:ASN:OD1	2.17	0.78
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ALA:HA	1:C:163:LYS:HB3	1.65	0.77
1:C:65:ILE:HD12	1:C:90:ILE:HG13	1.66	0.77
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.67	0.77
1:F:159:ALA:HA	1:F:163:LYS:HB3	1.66	0.76
1:E:236:ALA:O	1:F:728:LYS:NZ	2.19	0.76
1:F:463:THR:HG21	1:F:869:SER:HB2	1.67	0.76
1:D:682:PHE:HB3	1:D:827:ILE:HB	1.66	0.76
1:A:123:GLN:HB3	1:B:116:PRO:HG2	1.68	0.75
1:C:457:ALA:HB2	1:C:471:SER:HB3	1.69	0.75
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.67	0.75
1:B:1037:ASN:OD1	1:B:1037:ASN:N	2.18	0.75
1:D:218:GLN:HG2	1:D:233:SER:HA	1.68	0.75
1:C:69:MET:HB3	1:C:72:ILE:HD11	1.69	0.75
1:C:81:ASN:OD1	1:C:81:ASN:N	2.20	0.75
1:C:959:GLY:HA3	1:C:1040:ILE:HG23	1.67	0.75
1:D:278:ILE:HG13	1:D:613:ASN:HB3	1.68	0.75
1:F:894:SER:HG	1:F:896:SER:HG	1.35	0.74
1:A:138:MET:SD	1:A:307:ARG:NH2	2.60	0.74
1:D:312:LYS:NZ	1:E:858:ASP:OD2	2.20	0.74
1:C:400:LEU:HD11	1:C:1007:VAL:HG21	1.70	0.73
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.68	0.73
1:B:166:ILE:HG12	1:B:310:LEU:HD13	1.70	0.72
1:C:363:ARG:HA	1:C:366:LEU:HD22	1.70	0.72
1:E:671:ILE:HD13	1:E:674:LEU:H	1.55	0.72
1:C:280:GLU:OE2	1:C:588:GLN:NE2	2.23	0.71
1:F:81:ASN:HB2	1:F:89:GLN:HB2	1.71	0.71
1:F:278:ILE:HG13	1:F:613:ASN:HB3	1.72	0.71
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.72	0.71
1:E:54:ALA:HB1	1:E:816:LEU:HG	1.72	0.71
1:A:1041:GLU:H	1:A:1042:HIS:HB2	1.55	0.71
1:D:634:TRP:H	1:D:634:TRP:CD1	2.07	0.71
1:C:112:GLN:HA	1:C:115:MET:HG3	1.72	0.71
1:E:144:ASN:ND2	1:E:146:ASP:OD1	2.23	0.71
1:F:832:ALA:O	1:F:834:GLY:N	2.23	0.71
1:E:157:TYR:OH	1:E:316:PHE:O	2.09	0.71
1:A:214:VAL:HG11	1:B:747:ASN:HB3	1.73	0.70
1:C:393:LEU:HD22	1:C:466:ILE:HG23	1.72	0.70
1:C:368:PRO:HG3	1:C:413:VAL:HG21	1.73	0.70
1:C:445:ILE:HG23	1:C:449:LEU:HD12	1.72	0.70
1:F:713:LEU:HD11	1:F:843:LEU:HD12	1.74	0.70
1:A:193:LEU:HD11	1:A:200:PRO:HD3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:LEU:HD23	1:B:1017:LEU:HB3	1.74	0.70
1:C:1038:GLU:HA	1:C:1039:ASP:CB	2.20	0.70
1:B:108:GLN:NE2	1:C:112:GLN:OE1	2.24	0.70
1:A:218:GLN:HG2	1:A:233:SER:HA	1.72	0.70
1:C:180:SER:OG	1:C:274:ASN:OD1	2.09	0.70
1:A:161:ASN:ND2	1:B:687:GLN:O	2.25	0.69
1:A:211:ASN:O	1:A:760:ASN:ND2	2.25	0.69
1:A:619:GLY:HA3	1:A:815:ARG:HH12	1.55	0.69
1:E:14:VAL:HG11	1:F:890:ALA:HB2	1.73	0.69
1:F:509:LYS:HB3	1:F:514:GLY:H	1.57	0.69
1:C:139:VAL:HG22	1:C:290:GLY:HA2	1.72	0.69
1:B:210:GLN:O	1:B:237:GLN:NE2	2.25	0.69
1:A:679:GLY:HA2	1:A:830:GLN:HA	1.74	0.69
1:C:655:PHE:HB3	1:C:663:VAL:HG23	1.73	0.69
1:E:193:LEU:HD11	1:E:200:PRO:HD3	1.75	0.69
1:E:407:ASP:OD2	1:E:940:LYS:NZ	2.24	0.69
1:F:6:ILE:HG13	1:F:487:ILE:HA	1.75	0.69
1:A:14:VAL:HG11	1:B:890:ALA:HB2	1.75	0.69
1:B:410:ILE:HG23	1:B:977:MET:HE3	1.73	0.69
1:D:435:MET:HG3	1:D:490:PRO:HB3	1.75	0.69
1:F:114:ALA:HA	1:F:117:LEU:HD23	1.74	0.69
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.75	0.69
1:C:863:SER:HA	1:C:866:GLU:HB3	1.75	0.69
1:B:531:VAL:HG21	1:B:968:VAL:HG11	1.75	0.68
1:B:691:GLY:HA3	1:B:694:LYS:HD3	1.75	0.68
1:F:363:ARG:HB2	1:F:496:MET:HG2	1.74	0.68
1:B:14:VAL:HG11	1:C:890:ALA:HB2	1.74	0.68
1:E:541:TYR:OH	2:E:2000:LMT:O2'	2.10	0.68
1:F:393:LEU:HD13	1:F:466:ILE:HA	1.76	0.68
1:B:13:TRP:HE1	1:B:492:LEU:HD21	1.57	0.68
1:F:764:ASP:HB3	1:F:769:LYS:HZ3	1.58	0.68
1:B:126:GLY:HA2	1:C:116:PRO:HG2	1.75	0.68
1:C:57:VAL:HG23	1:C:82:SER:HB2	1.75	0.68
1:C:989:LEU:HD22	1:C:1000:GLN:HB3	1.75	0.68
1:A:280:GLU:OE2	1:A:588:GLN:NE2	2.26	0.67
1:A:781:MET:HE2	1:C:225:VAL:HG22	1.74	0.67
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.74	0.67
1:F:54:ALA:HB1	1:F:816:LEU:HG	1.75	0.67
1:E:239:ARG:NH1	1:E:761:ASP:O	2.27	0.67
1:A:702:LEU:HD11	1:A:851:LEU:HD11	1.75	0.67
1:C:463:THR:HG22	1:C:865:GLN:HE21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:MET:HG3	1:D:713:LEU:HD13	1.77	0.67
1:C:185:ARG:HD2	1:C:187:TRP:HE1	1.58	0.67
1:D:729:ILE:HD13	1:D:786:ILE:HD11	1.77	0.67
1:E:634:TRP:H	1:E:634:TRP:CD1	2.13	0.67
1:A:1019:ILE:HG13	1:A:1020:PHE:HD1	1.59	0.67
1:B:475:VAL:HA	1:B:478:MET:HE3	1.77	0.67
1:B:484:VAL:HG13	1:B:488:LEU:HB3	1.76	0.67
1:A:892:TYR:CE1	1:A:897:ILE:HB	2.30	0.67
1:A:869:SER:OG	1:A:870:GLY:N	2.22	0.66
1:C:47:ALA:HB1	1:C:122:VAL:HG11	1.76	0.66
1:F:686:ASP:HB2	1:F:695:LEU:HD11	1.75	0.66
1:D:213:GLN:HG2	1:D:239:ARG:HG3	1.77	0.66
1:C:790:TYR:HB3	1:C:798:MET:HB3	1.78	0.66
1:D:531:VAL:HG21	1:D:968:VAL:HG11	1.75	0.66
1:D:1036:LYS:O	1:D:1038:GLU:N	2.27	0.66
1:F:137:LEU:HB2	1:F:293:LEU:HB2	1.78	0.66
1:A:30:LEU:HD12	1:A:31:PRO:HD2	1.76	0.66
1:B:634:TRP:H	1:B:634:TRP:CD1	2.13	0.66
1:A:890:ALA:HB2	1:C:14:VAL:HG11	1.78	0.65
1:E:211:ASN:O	1:E:760:ASN:ND2	2.29	0.65
1:D:832:ALA:O	1:D:834:GLY:N	2.29	0.65
1:B:193:LEU:HD21	1:B:200:PRO:HD3	1.79	0.65
1:C:452:VAL:HG12	1:C:884:VAL:HG21	1.79	0.65
1:D:832:ALA:HB3	1:D:835:LYS:HD3	1.76	0.65
1:F:57:VAL:HG11	1:F:86:GLY:HA2	1.78	0.65
1:E:355:MET:HE2	1:E:368:PRO:HG2	1.78	0.65
1:A:82:SER:HB2	1:A:816:LEU:HB2	1.79	0.65
1:B:573:MET:HG2	1:B:628:PHE:HA	1.79	0.65
1:C:576:VAL:HA	1:C:663:VAL:HG12	1.79	0.65
1:D:562:SER:OG	1:D:563:PHE:N	2.29	0.65
1:A:450:SER:HB2	1:A:478:MET:HE1	1.79	0.65
1:B:555:LEU:HD22	1:B:913:LEU:HB3	1.79	0.65
1:B:236:ALA:O	1:C:728:LYS:NZ	2.30	0.65
1:C:427:PRO:HD3	1:C:499:PRO:HB3	1.79	0.65
1:E:671:ILE:HG12	1:E:674:LEU:HB2	1.79	0.65
1:D:108:GLN:NE2	1:E:109:ASN:O	2.29	0.64
1:B:80:SER:HB2	1:B:90:ILE:HG23	1.79	0.64
1:B:57:VAL:HG11	1:B:86:GLY:HA2	1.80	0.64
1:C:555:LEU:HD11	1:C:914:LEU:HD13	1.79	0.64
1:D:280:GLU:OE2	1:D:588:GLN:NE2	2.30	0.64
1:D:211:ASN:O	1:D:760:ASN:ND2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:514:GLY:HA2	1:D:517:ASN:HD22	1.61	0.64
1:D:623:ASN:N	1:D:623:ASN:OD1	2.30	0.64
1:A:54:ALA:HB1	1:A:816:LEU:HG	1.80	0.64
1:C:61:VAL:HG11	1:C:88:VAL:HG21	1.79	0.64
1:C:543:VAL:HA	1:C:546:LEU:HD22	1.79	0.64
1:E:261:LEU:HD12	1:E:263:ARG:HH21	1.61	0.64
1:A:23:GLY:HA3	1:A:377:LEU:HB3	1.80	0.64
1:B:705:GLU:HB3	1:B:847:LEU:HD13	1.80	0.64
1:C:16:ALA:HB2	1:C:488:LEU:HD13	1.80	0.64
1:D:892:TYR:O	1:D:893:GLU:HB2	1.98	0.64
1:F:926:TYR:HE1	1:F:999:ALA:HB1	1.63	0.64
1:A:137:LEU:HB2	1:A:293:LEU:HB2	1.79	0.64
1:D:83:ASP:OD1	1:D:815:ARG:NH1	2.31	0.64
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.81	0.63
1:B:250:LEU:HD23	1:C:737:GLN:HE22	1.63	0.63
1:B:851:LEU:HD13	1:B:855:VAL:HG12	1.79	0.63
1:D:871:ASN:O	1:D:873:ALA:N	2.29	0.63
1:E:187:TRP:HB3	1:E:776:GLU:HG2	1.80	0.63
1:E:679:GLY:HA3	1:E:830:GLN:HA	1.80	0.63
1:E:775:SER:OG	1:E:776:GLU:N	2.30	0.63
1:D:38:ILE:HG23	1:D:462:SER:HB2	1.80	0.63
1:F:30:LEU:HD12	1:F:31:PRO:HD2	1.79	0.63
1:A:1035:ARG:O	1:A:1037:ASN:N	2.32	0.63
1:D:405:LEU:HD22	1:D:481:SER:HB3	1.79	0.63
1:F:144:ASN:O	1:F:284:GLN:NE2	2.31	0.63
1:D:1038:GLU:HB3	1:D:1039:ASP:CB	2.29	0.63
1:E:344:LEU:HD23	1:E:402:ILE:HD11	1.80	0.63
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.80	0.63
1:D:262:LEU:HG	1:D:268:ILE:HD11	1.79	0.63
1:A:144:ASN:O	1:A:284:GLN:NE2	2.32	0.62
1:D:408:ASP:OD2	1:D:940:LYS:NZ	2.32	0.62
1:D:456:MET:HG3	1:D:932:LEU:HD11	1.81	0.62
1:B:82:SER:HB2	1:B:816:LEU:HB2	1.80	0.62
1:B:941:ASN:HB3	1:B:975:ILE:HD12	1.81	0.62
1:C:301:ASP:OD2	1:C:301:ASP:N	2.32	0.62
1:C:531:VAL:HG21	1:C:968:VAL:HG11	1.80	0.62
1:F:669:PRO:HA	1:F:678:THR:HG23	1.81	0.62
1:A:623:ASN:OD1	1:A:623:ASN:N	2.31	0.62
1:B:696:THR:HG23	1:B:699:ARG:HH12	1.64	0.62
1:B:571:VAL:HG13	1:B:628:PHE:HE1	1.64	0.62
1:D:307:ARG:NH2	1:D:328:ASP:OD2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:THR:HA	1:A:284:GLN:HE22	1.64	0.62
1:C:705:GLU:HB3	1:C:847:LEU:HD12	1.82	0.62
1:E:30:LEU:HD12	1:E:31:PRO:HD2	1.81	0.62
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.64	0.62
1:A:888:LEU:HD11	1:A:943:ILE:HD11	1.81	0.62
1:B:231:ASN:OD1	1:C:622:GLN:NE2	2.33	0.62
1:B:239:ARG:NH1	1:B:761:ASP:O	2.31	0.62
1:F:144:ASN:ND2	1:F:149:MET:SD	2.70	0.62
1:B:447:MET:HB3	1:B:887:CYS:SG	2.40	0.62
1:B:971:ARG:HH12	1:B:975:ILE:HD11	1.65	0.62
1:D:1019:ILE:HG13	1:D:1020:PHE:HD1	1.63	0.62
1:F:136:PHE:HA	1:F:292:LYS:HA	1.82	0.62
1:E:210:GLN:O	1:E:237:GLN:NE2	2.33	0.62
1:E:668:LEU:H	1:E:668:LEU:HD23	1.64	0.62
1:C:218:GLN:HG3	1:C:221:GLY:HA2	1.81	0.62
1:A:408:ASP:OD2	1:A:940:LYS:NZ	2.32	0.61
1:C:310:LEU:HD11	1:C:323:ILE:HG21	1.82	0.61
1:C:445:ILE:HG13	1:C:943:ILE:HG21	1.81	0.61
1:B:510:LYS:HB2	1:B:514:GLY:HA3	1.81	0.61
1:C:775:SER:OG	1:C:776:GLU:N	2.33	0.61
1:A:237:GLN:OE1	1:B:747:ASN:ND2	2.32	0.61
1:A:599:LEU:O	1:A:603:LYS:NZ	2.25	0.61
1:C:418:ARG:HH12	1:C:419:VAL:HG23	1.65	0.61
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.81	0.61
1:D:863:SER:HA	1:D:866:GLU:HG2	1.83	0.61
1:F:562:SER:OG	1:F:563:PHE:N	2.32	0.61
1:D:146:ASP:OD2	1:D:147:GLY:N	2.32	0.61
1:A:444:GLY:HA3	1:A:891:LEU:HD22	1.82	0.61
1:B:832:ALA:HB3	1:B:835:LYS:HD3	1.82	0.61
1:C:730:ASP:OD1	1:C:808:ARG:NH2	2.33	0.61
1:F:634:TRP:H	1:F:634:TRP:CD1	2.17	0.61
1:C:521:GLU:O	1:C:524:THR:OG1	2.18	0.61
1:F:72:ILE:HG13	1:F:106:GLN:HB3	1.83	0.61
1:A:410:ILE:HG23	1:A:977:MET:HE3	1.83	0.61
1:B:404:LEU:HD11	1:B:449:LEU:HD13	1.83	0.61
1:B:607:GLU:HB2	1:B:632:LYS:HG3	1.82	0.61
1:E:351:VAL:HG22	1:E:981:ALA:HB1	1.83	0.61
1:C:562:SER:OG	1:C:563:PHE:N	2.33	0.61
1:E:562:SER:OG	1:E:563:PHE:N	2.30	0.61
1:F:189:ASN:HB3	1:F:192:GLU:HB2	1.82	0.61
1:B:513:PHE:N	1:B:513:PHE:CD2	2.68	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:PRO:HD3	1:C:96:SER:HA	1.83	0.60
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.65	0.60
1:F:960:LEU:HD11	1:F:1027:VAL:HA	1.84	0.60
1:B:261:LEU:HD12	1:B:263:ARG:HH21	1.65	0.60
1:B:562:SER:OG	1:B:563:PHE:N	2.32	0.60
1:C:6:ILE:HG21	1:C:487:ILE:HG23	1.83	0.60
1:C:156:ASP:OD1	1:C:765:ARG:NH2	2.34	0.60
1:D:23:GLY:HA3	1:D:377:LEU:HB3	1.83	0.60
1:D:300:LEU:HD11	1:D:333:VAL:HG11	1.83	0.60
1:F:156:ASP:OD1	1:F:765:ARG:NH2	2.34	0.60
1:F:746:ILE:HG22	1:F:791:VAL:HG11	1.83	0.60
1:A:699:ARG:NH2	1:A:722:GLU:OE1	2.35	0.60
1:F:185:ARG:HD2	1:F:187:TRP:HE1	1.67	0.60
1:F:623:ASN:OD1	1:F:623:ASN:N	2.31	0.60
1:A:747:ASN:ND2	1:C:237:GLN:OE1	2.28	0.60
1:C:276:ASP:OD2	1:C:276:ASP:N	2.32	0.60
1:A:146:ASP:OD1	1:A:146:ASP:N	2.29	0.60
1:A:775:SER:OG	1:A:776:GLU:N	2.33	0.60
1:B:137:LEU:HD13	1:B:293:LEU:HG	1.84	0.60
1:C:351:VAL:HG22	1:C:981:ALA:HB1	1.82	0.60
1:D:363:ARG:HD2	1:D:498:LYS:HD3	1.83	0.60
1:E:713:LEU:HA	1:E:831:ALA:HA	1.83	0.60
1:F:728:LYS:HB3	1:F:808:ARG:HD3	1.83	0.60
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.33	0.60
1:C:54:ALA:HB1	1:C:816:LEU:HG	1.82	0.60
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.84	0.60
1:F:137:LEU:HD22	1:F:293:LEU:HD23	1.84	0.60
1:F:966:ASP:OD1	1:F:969:ARG:NH2	2.35	0.60
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.84	0.60
1:A:913:LEU:HD23	1:A:927:PHE:HZ	1.67	0.60
1:E:971:ARG:HG2	1:E:974:PRO:HG3	1.82	0.60
1:D:34:GLN:NE2	1:D:670:ALA:O	2.35	0.59
1:E:699:ARG:HD3	1:E:825:MET:HE2	1.84	0.59
1:A:1019:ILE:HG13	1:A:1020:PHE:CD1	2.36	0.59
1:D:619:GLY:HA3	1:D:815:ARG:HH12	1.68	0.59
1:E:80:SER:HB3	1:E:90:ILE:HG23	1.84	0.59
1:E:114:ALA:HA	1:E:117:LEU:HD13	1.84	0.59
1:E:368:PRO:HG3	1:E:413:VAL:HG21	1.83	0.59
1:E:428:LYS:HG2	1:E:494:ALA:HB1	1.83	0.59
1:E:251:LEU:HD11	1:E:262:LEU:HA	1.84	0.59
1:A:73:ASP:OD2	1:C:131:LYS:NZ	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1034:SER:HB3	1:C:1038:GLU:HG3	1.83	0.59
1:D:953:MET:HG2	1:D:1040:ILE:HD12	1.82	0.59
1:F:524:THR:HG22	1:F:972:LEU:HD12	1.84	0.59
1:A:562:SER:OG	1:A:563:PHE:N	2.34	0.59
1:E:446:ALA:HB2	1:E:482:VAL:HG21	1.84	0.59
1:E:958:LYS:HB3	1:E:963:ALA:HB2	1.84	0.59
1:F:65:ILE:HG23	1:F:111:LEU:HD23	1.85	0.59
1:A:136:PHE:CD2	1:A:292:LYS:HG3	2.37	0.59
1:B:775:SER:OG	1:B:776:GLU:N	2.31	0.59
1:C:634:TRP:CD1	1:C:634:TRP:H	2.21	0.59
1:B:366:LEU:HA	1:B:369:THR:HB	1.85	0.59
1:D:890:ALA:HB2	1:F:14:VAL:HG11	1.85	0.59
1:C:122:VAL:O	1:C:124:GLN:N	2.31	0.58
1:D:13:TRP:HE1	1:D:492:LEU:HD21	1.69	0.58
1:C:139:VAL:HB	1:C:327:TYR:HB3	1.85	0.58
1:D:747:ASN:ND2	1:F:237:GLN:OE1	2.31	0.58
1:D:907:LEU:HD23	1:D:1017:LEU:HB3	1.84	0.58
1:D:1037:ASN:HA	1:D:1040:ILE:HG12	1.83	0.58
1:C:278:ILE:HD11	1:C:584:GLN:HE21	1.67	0.58
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.85	0.58
1:D:1019:ILE:HG13	1:D:1020:PHE:CD1	2.38	0.58
1:F:6:ILE:HG21	1:F:487:ILE:HG23	1.85	0.58
1:A:236:ALA:O	1:B:728:LYS:NZ	2.35	0.58
1:C:244:GLU:HG2	1:C:248:LYS:HE3	1.84	0.58
1:D:214:VAL:HG11	1:E:747:ASN:HB3	1.86	0.58
1:E:250:LEU:HD21	1:F:734:GLU:HG3	1.84	0.58
1:F:186:ILE:HG12	1:F:268:ILE:HG12	1.86	0.58
1:A:33:ALA:HA	1:A:299:ALA:HB3	1.85	0.58
1:A:960:LEU:HD23	1:A:1031:ARG:HE	1.69	0.58
1:C:32:VAL:HG22	1:C:390:ILE:HD11	1.85	0.58
1:E:222:THR:HA	1:E:224:PRO:HD3	1.86	0.58
1:A:404:LEU:HD21	1:A:449:LEU:HD13	1.84	0.58
1:C:65:ILE:HG23	1:C:111:LEU:HD23	1.85	0.58
1:F:105:VAL:O	1:F:109:ASN:ND2	2.36	0.58
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.86	0.57
1:A:168:ARG:NH2	1:B:66:GLU:O	2.36	0.57
1:A:355:MET:HE2	1:A:368:PRO:HG2	1.85	0.57
1:A:901:VAL:HG21	1:A:943:ILE:HG13	1.86	0.57
1:B:459:PHE:HE1	1:B:873:ALA:HB2	1.68	0.57
1:C:966:ASP:OD1	1:C:969:ARG:NH2	2.37	0.57
1:D:80:SER:HB3	1:D:90:ILE:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:775:SER:OG	1:F:776:GLU:N	2.30	0.57
1:A:637:ARG:NH1	1:A:642:ASN:O	2.33	0.57
1:C:63:GLN:OE1	1:C:818:ARG:NH2	2.37	0.57
1:D:186:ILE:HD13	1:D:262:LEU:HD21	1.86	0.57
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.86	0.57
1:A:149:MET:HE2	1:A:154:ILE:HG12	1.85	0.57
1:A:832:ALA:HB3	1:A:835:LYS:HD3	1.86	0.57
1:A:892:TYR:O	1:A:893:GLU:HB2	2.05	0.57
1:B:638:PRO:O	1:B:642:ASN:HB2	2.04	0.57
1:E:139:VAL:HB	1:E:327:TYR:HB3	1.85	0.57
1:F:280:GLU:OE2	1:F:588:GLN:NE2	2.38	0.57
1:F:959:GLY:HA3	1:F:1040:ILE:HG23	1.84	0.57
1:B:448:VAL:HG21	1:B:888:LEU:HG	1.85	0.57
1:E:156:ASP:OD1	1:E:765:ARG:NH2	2.36	0.57
1:E:445:ILE:HG13	1:E:446:ALA:N	2.19	0.57
1:A:445:ILE:HG13	1:A:446:ALA:N	2.18	0.57
1:E:66:GLU:OE2	1:E:80:SER:OG	2.14	0.57
1:E:573:MET:HE2	1:E:668:LEU:HD22	1.87	0.57
1:B:671:ILE:HG22	1:B:672:VAL:HG22	1.87	0.57
1:F:293:LEU:HD22	1:F:294:ALA:H	1.69	0.57
1:F:1043:SER:OG	1:F:1044:HIS:N	2.36	0.57
1:A:441:ALA:HA	1:A:891:LEU:HD21	1.85	0.57
1:D:393:LEU:HD11	1:D:466:ILE:HD12	1.85	0.57
1:A:105:VAL:HG11	1:B:105:VAL:HG22	1.87	0.57
1:A:959:GLY:N	1:A:1040:ILE:HG12	2.20	0.56
1:B:137:LEU:HB2	1:B:293:LEU:HB2	1.87	0.56
1:D:776:GLU:HB3	1:D:779:TYR:HD1	1.70	0.56
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.87	0.56
1:D:367:ILE:HD11	1:D:496:MET:HG3	1.88	0.56
1:E:450:SER:HB3	1:E:478:MET:HE1	1.87	0.56
1:A:453:PHE:O	1:A:471:SER:OG	2.10	0.56
1:B:167:SER:C	1:B:169:THR:H	2.12	0.56
1:B:926:TYR:HE1	1:B:999:ALA:HB1	1.69	0.56
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.87	0.56
1:D:276:ASP:OD2	1:D:276:ASP:N	2.38	0.56
1:D:593:GLU:OE2	1:D:659:LYS:NZ	2.32	0.56
1:E:559:LEU:HD12	1:E:923:ASN:HB2	1.85	0.56
1:B:486:LEU:HB2	1:B:487:ILE:HD12	1.85	0.56
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.30	0.56
1:B:81:ASN:HB2	1:B:89:GLN:HB2	1.88	0.56
1:B:559:LEU:HD22	1:B:560:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ASP:CG	1:D:106:GLN:HE22	2.12	0.56
1:A:136:PHE:HA	1:A:292:LYS:HA	1.88	0.56
1:B:687:GLN:HA	1:B:822:LEU:HD13	1.87	0.56
1:C:448:VAL:HG11	1:C:943:ILE:HD11	1.86	0.56
1:D:57:VAL:HA	1:D:60:THR:HG22	1.88	0.56
1:D:186:ILE:HB	1:D:773:VAL:HG22	1.87	0.56
1:E:904:VAL:HA	1:E:907:LEU:HD13	1.88	0.56
1:F:806:SER:O	1:F:808:ARG:NH1	2.38	0.56
1:A:900:SER:HA	1:A:903:LEU:HD12	1.86	0.56
1:B:376:LEU:HD22	1:B:398:MET:HE3	1.88	0.56
1:C:293:LEU:HD22	1:C:294:ALA:H	1.70	0.56
1:D:609:VAL:HG13	1:D:629:VAL:HG22	1.87	0.56
1:D:699:ARG:HG3	1:D:827:ILE:HD11	1.88	0.56
1:E:776:GLU:HB2	1:E:779:TYR:HD1	1.71	0.56
1:B:707:ALA:HA	1:B:714:THR:HA	1.88	0.56
1:A:447:MET:HB3	1:A:887:CYS:SG	2.46	0.55
1:A:602:GLU:HG3	1:A:605:ASN:HB2	1.88	0.55
1:B:139:VAL:O	1:B:326:PRO:HD2	2.06	0.55
1:D:401:ALA:O	1:D:405:LEU:HG	2.06	0.55
1:E:832:ALA:HB3	1:E:835:LYS:HD3	1.87	0.55
1:F:723:ASP:HA	1:F:814:PRO:HD3	1.88	0.55
1:A:509:LYS:HG2	1:A:513:PHE:HB2	1.88	0.55
1:A:1040:ILE:HB	1:A:1042:HIS:HB2	1.88	0.55
1:C:23:GLY:HA2	1:C:381:ALA:HB2	1.87	0.55
1:C:372:VAL:HG22	1:C:406:VAL:HG12	1.89	0.55
1:D:775:SER:OG	1:D:776:GLU:N	2.32	0.55
1:E:571:VAL:HG22	1:E:630:SER:HA	1.89	0.55
1:F:42:ALA:HB2	1:F:93:THR:HG23	1.87	0.55
1:F:137:LEU:HD13	1:F:293:LEU:HG	1.86	0.55
1:D:14:VAL:HG11	1:E:890:ALA:HB2	1.89	0.55
1:D:1040:ILE:HG22	1:D:1042:HIS:H	1.72	0.55
1:F:901:VAL:HG11	1:F:943:ILE:HG13	1.89	0.55
1:A:870:GLY:O	1:A:872:GLN:N	2.40	0.55
1:B:235:ILE:HD11	1:C:726:GLN:HB3	1.87	0.55
1:B:393:LEU:HD13	1:B:466:ILE:HA	1.88	0.55
1:E:648:THR:OG1	1:E:665:ALA:O	2.22	0.55
1:F:31:PRO:HB2	1:F:389:SER:HB3	1.87	0.55
1:F:595:THR:HG23	1:F:609:VAL:HB	1.89	0.55
1:A:390:ILE:HG23	1:A:395:MET:HG2	1.87	0.55
1:A:805:SER:O	1:A:805:SER:OG	2.23	0.55
1:B:102:ILE:O	1:B:105:VAL:HG12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1013:THR:O	1:D:1017:LEU:HB2	2.07	0.55
1:E:143:ILE:HG22	1:E:286:ALA:HB2	1.89	0.55
1:E:545:TYR:HB2	1:E:1021:PHE:HE2	1.72	0.55
1:F:531:VAL:O	1:F:534:ILE:HG12	2.06	0.55
1:B:114:ALA:O	1:B:118:LEU:HG	2.07	0.55
1:B:688:ALA:H	1:B:854:GLY:HA2	1.70	0.55
1:C:21:LEU:O	1:C:25:LEU:HB2	2.07	0.55
1:C:896:SER:HB2	1:C:1029:VAL:HG13	1.87	0.55
1:D:1035:ARG:O	1:D:1037:ASN:N	2.39	0.55
1:A:1041:GLU:H	1:A:1042:HIS:CB	2.18	0.55
1:C:94:PHE:CE2	1:C:107:VAL:HG21	2.42	0.55
1:F:435:MET:HE3	1:F:490:PRO:HG3	1.89	0.55
1:A:845:GLU:OE2	1:A:867:ARG:NH2	2.40	0.55
1:C:210:GLN:HG3	1:C:249:ILE:HG23	1.88	0.55
1:C:435:MET:HE3	1:C:490:PRO:HB3	1.87	0.55
1:E:36:PRO:HG3	1:E:469:GLN:HG3	1.89	0.55
1:A:235:ILE:HB	1:B:728:LYS:HA	1.88	0.55
1:A:892:TYR:CZ	1:A:946:VAL:HG11	2.42	0.55
1:C:456:MET:HG2	1:C:471:SER:HB2	1.89	0.55
1:D:60:THR:HG23	1:D:61:VAL:HG23	1.89	0.55
1:A:634:TRP:CD1	1:A:634:TRP:H	2.25	0.54
1:C:198:LEU:HD21	1:C:252:LYS:HE3	1.88	0.54
1:C:675:GLY:HA3	1:C:862:MET:HG2	1.90	0.54
1:D:599:LEU:O	1:D:603:LYS:NZ	2.40	0.54
1:E:75:LEU:HA	1:E:94:PHE:HD2	1.72	0.54
1:E:326:PRO:O	1:E:630:SER:OG	2.23	0.54
1:F:667:ASN:O	1:F:678:THR:OG1	2.25	0.54
1:B:103:ALA:HA	1:B:106:GLN:NE2	2.22	0.54
1:B:442:LEU:O	1:B:445:ILE:HG13	2.07	0.54
1:F:705:GLU:HB3	1:F:847:LEU:HD12	1.89	0.54
1:B:157:TYR:OH	1:B:316:PHE:O	2.19	0.54
1:C:172:VAL:HG22	1:C:291:ILE:HG21	1.88	0.54
1:F:55:LYS:HG2	1:F:816:LEU:HD11	1.89	0.54
1:E:45:ILE:HG13	1:E:90:ILE:HB	1.89	0.54
1:A:108:GLN:NE2	1:B:109:ASN:O	2.41	0.54
1:B:531:VAL:O	1:B:534:ILE:HG12	2.08	0.54
1:C:24:GLY:HA2	1:C:377:LEU:HD22	1.88	0.54
1:C:560:PRO:HB2	1:C:836:SER:HB2	1.89	0.54
1:C:870:GLY:C	1:C:872:GLN:H	2.15	0.54
1:F:449:LEU:HD21	1:F:937:LEU:HD23	1.89	0.54
1:D:913:LEU:HD23	1:D:927:PHE:HZ	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:521:GLU:O	1:F:524:THR:OG1	2.19	0.54
1:C:65:ILE:HG12	1:C:111:LEU:HD21	1.90	0.54
1:E:992:SER:O	1:E:997:SER:OG	2.22	0.54
1:F:578:LEU:HD12	1:F:587:THR:HG23	1.89	0.54
1:B:414:GLU:HG2	1:B:973:ARG:HH21	1.72	0.54
1:E:203:VAL:O	1:E:207:ILE:HG13	2.07	0.54
1:E:456:MET:O	1:E:467:TYR:HB3	2.08	0.54
1:F:366:LEU:O	1:F:370:ILE:HG13	2.08	0.54
1:A:583:THR:HG21	1:C:229:GLN:HA	1.91	0.54
1:D:231:ASN:OD1	1:E:622:GLN:NE2	2.41	0.54
1:E:555:LEU:HD22	1:E:913:LEU:HB3	1.90	0.54
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.90	0.53
1:A:470:PHE:O	1:A:474:ILE:HG12	2.08	0.53
1:A:832:ALA:O	1:A:834:GLY:N	2.32	0.53
1:E:125:GLN:OE1	1:E:772:TYR:OH	2.25	0.53
1:B:186:ILE:HD13	1:B:262:LEU:HD21	1.90	0.53
1:D:82:SER:HB2	1:D:816:LEU:HB2	1.90	0.53
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.90	0.53
1:A:491:ALA:O	1:A:495:THR:OG1	2.25	0.53
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.90	0.53
1:E:456:MET:HG2	1:E:471:SER:HB2	1.90	0.53
1:A:139:VAL:HG22	1:A:290:GLY:HA2	1.90	0.53
1:B:448:VAL:HG13	1:B:884:VAL:HG22	1.90	0.53
1:D:582:ALA:HA	1:D:586:ARG:HH21	1.74	0.53
1:E:595:THR:HG23	1:E:609:VAL:HB	1.91	0.53
1:A:776:GLU:HB3	1:A:779:TYR:CD1	2.44	0.53
1:C:30:LEU:HD12	1:C:31:PRO:HD2	1.89	0.53
1:D:602:GLU:HB3	1:D:606:VAL:HG23	1.90	0.53
1:A:16:ALA:HB2	1:A:488:LEU:HD13	1.89	0.53
1:A:712:MET:HG3	1:A:713:LEU:HD13	1.90	0.53
1:A:838:GLY:O	1:A:841:MET:HB2	2.09	0.53
1:F:787:GLY:O	1:F:789:TRP:N	2.42	0.53
1:B:108:GLN:HE22	1:C:112:GLN:HB2	1.74	0.53
1:D:6:ILE:HD12	1:D:432:ARG:HG2	1.91	0.53
1:D:17:ILE:HG12	1:D:20:MET:HE2	1.91	0.53
1:E:165:ALA:HB1	1:E:313:MET:HE3	1.90	0.53
1:B:898:PRO:HA	1:B:901:VAL:HG12	1.91	0.53
1:D:144:ASN:ND2	1:D:146:ASP:OD2	2.41	0.53
1:E:126:GLY:HA2	1:F:116:PRO:HG2	1.89	0.53
1:A:467:TYR:HE2	1:A:925:VAL:HG13	1.73	0.53
1:A:153:ASP:OD1	1:A:153:ASP:N	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:982:PHE:CD2	1:C:1011:MET:HG3	2.44	0.53
1:A:442:LEU:HA	1:A:445:ILE:HG12	1.90	0.52
1:B:228:GLN:NE2	1:B:230:LEU:O	2.36	0.52
1:F:146:ASP:OD1	1:F:147:GLY:N	2.35	0.52
1:B:435:MET:HE1	1:B:486:LEU:HA	1.91	0.52
1:C:595:THR:HG23	1:C:609:VAL:HB	1.92	0.52
1:D:193:LEU:HD11	1:D:200:PRO:HD3	1.92	0.52
1:D:776:GLU:HB3	1:D:779:TYR:CD1	2.44	0.52
1:A:109:ASN:O	1:A:110:LYS:NZ	2.41	0.52
1:A:350:LEU:HD12	1:A:984:LEU:HB3	1.90	0.52
1:A:531:VAL:O	1:A:534:ILE:HG12	2.09	0.52
1:A:926:TYR:CE1	1:A:999:ALA:HB1	2.44	0.52
1:D:946:VAL:HG22	1:D:1026:PHE:HD1	1.74	0.52
1:C:94:PHE:HE2	1:C:107:VAL:HG21	1.74	0.52
1:C:293:LEU:HD22	1:C:294:ALA:N	2.25	0.52
1:C:702:LEU:HG	1:C:851:LEU:HD11	1.92	0.52
1:E:57:VAL:HG13	1:E:82:SER:HB3	1.91	0.52
1:E:470:PHE:O	1:E:474:ILE:HG12	2.10	0.52
1:A:273:GLU:O	1:A:274:ASN:ND2	2.43	0.52
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.09	0.52
1:B:520:PHE:O	1:B:523:SER:OG	2.26	0.52
1:C:907:LEU:HD21	1:C:1021:PHE:CD2	2.44	0.52
1:E:1040:ILE:HG12	1:E:1041:GLU:H	1.74	0.52
1:F:348:ILE:HG12	1:F:372:VAL:HG11	1.91	0.52
1:F:356:TYR:HA	1:F:365:THR:HG21	1.90	0.52
1:B:114:ALA:HA	1:B:117:LEU:HD13	1.92	0.52
1:B:156:ASP:OD1	1:B:765:ARG:NH2	2.37	0.52
1:B:595:THR:HG23	1:B:609:VAL:HB	1.92	0.52
1:E:69:MET:HE1	1:E:111:LEU:HB2	1.91	0.52
1:C:531:VAL:O	1:C:534:ILE:HG12	2.10	0.52
1:D:452:VAL:HG12	1:D:884:VAL:HG21	1.90	0.52
1:D:576:VAL:HA	1:D:663:VAL:HG22	1.92	0.52
1:E:1013:THR:O	1:E:1017:LEU:HB2	2.10	0.52
1:A:239:ARG:HH12	1:A:761:ASP:H	1.58	0.52
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.91	0.52
1:A:612:VAL:N	1:A:626:ILE:O	2.41	0.52
1:A:901:VAL:HG23	1:A:942:ALA:HB3	1.92	0.52
1:E:375:VAL:O	1:E:379:THR:OG1	2.23	0.52
1:F:482:VAL:O	1:F:486:LEU:HG	2.09	0.52
1:A:904:VAL:HA	1:A:907:LEU:HD13	1.92	0.52
1:A:1041:GLU:N	1:A:1042:HIS:HB2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:VAL:HA	1:B:663:VAL:HG22	1.92	0.52
1:B:610:PHE:HB3	1:B:628:PHE:HB3	1.92	0.52
1:B:680:PHE:CZ	1:B:844:MET:HG2	2.45	0.52
1:C:68:ASN:HB2	1:C:114:ALA:HB2	1.92	0.52
1:D:360:GLN:HG2	1:D:513:PHE:HB3	1.92	0.52
1:A:17:ILE:HG12	1:A:20:MET:HE2	1.91	0.52
1:B:7:ASP:OD1	1:B:432:ARG:NH2	2.40	0.52
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.92	0.52
1:D:607:GLU:HB2	1:D:632:LYS:HG3	1.92	0.52
1:D:687:GLN:O	1:F:161:ASN:ND2	2.42	0.52
1:C:111:LEU:C	1:C:113:LEU:H	2.17	0.51
1:D:344:LEU:HD21	1:D:399:VAL:HA	1.92	0.51
1:E:336:SER:O	1:E:340:VAL:HG23	2.10	0.51
1:A:990:VAL:HG21	1:A:1008:MET:HE3	1.92	0.51
1:B:425:LEU:HD13	1:B:429:GLU:HG2	1.90	0.51
1:F:112:GLN:HA	1:F:115:MET:HG3	1.93	0.51
1:A:76:MET:HE3	1:A:95:GLU:HA	1.93	0.51
1:B:189:ASN:HB3	1:B:192:GLU:HB2	1.91	0.51
1:B:441:ALA:O	1:B:445:ILE:HG23	2.09	0.51
1:D:15:ILE:O	1:D:19:ILE:HG13	2.10	0.51
1:D:159:ALA:HA	1:D:163:LYS:HB3	1.92	0.51
1:D:442:LEU:O	1:D:445:ILE:HG13	2.10	0.51
1:C:535:LEU:HD21	1:C:1023:PRO:HB2	1.91	0.51
1:E:926:TYR:HE1	1:E:999:ALA:HB1	1.76	0.51
1:F:445:ILE:HD11	1:F:944:LEU:HD11	1.93	0.51
1:F:730:ASP:H	1:F:808:ARG:HH12	1.57	0.51
1:F:1034:SER:HB3	1:F:1038:GLU:HG2	1.92	0.51
1:D:781:MET:HE2	1:F:225:VAL:HG23	1.93	0.51
1:E:418:ARG:HH21	1:E:419:VAL:HG23	1.76	0.51
1:A:441:ALA:O	1:A:445:ILE:HG23	2.11	0.51
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.91	0.51
1:C:584:GLN:N	1:C:622:GLN:HB3	2.25	0.51
1:C:743:ILE:HA	1:C:746:ILE:HG12	1.93	0.51
1:D:445:ILE:HG22	1:D:943:ILE:HG21	1.92	0.51
1:F:139:VAL:HB	1:F:327:TYR:HB3	1.93	0.51
1:F:412:VAL:HG13	1:F:435:MET:HE1	1.92	0.51
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.93	0.51
1:C:586:ARG:O	1:C:589:LYS:HB2	2.11	0.51
1:C:732:ASP:H	1:C:804:PHE:HB2	1.74	0.51
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.38	0.51
1:B:406:VAL:O	1:B:410:ILE:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:641:GLU:O	1:E:650:ARG:NH1	2.44	0.51
1:F:82:SER:HB2	1:F:816:LEU:HB2	1.93	0.51
1:A:347:ALA:HB1	1:A:402:ILE:HG21	1.92	0.50
1:B:484:VAL:HG12	1:B:489:THR:HG23	1.93	0.50
1:C:457:ALA:HA	1:C:468:ARG:HA	1.93	0.50
1:D:216:ALA:HB2	1:D:236:ALA:HB2	1.91	0.50
1:A:368:PRO:HG3	1:A:413:VAL:HG21	1.93	0.50
1:A:877:TYR:HE2	1:A:932:LEU:HD21	1.75	0.50
1:A:1041:GLU:HB2	1:A:1042:HIS:HA	1.93	0.50
2:B:2000:LMT:O6B	2:B:2000:LMT:O4'	2.27	0.50
1:C:449:LEU:O	1:C:452:VAL:HG22	2.11	0.50
1:C:641:GLU:HB2	1:C:650:ARG:HH22	1.76	0.50
1:D:515:TRP:CD1	1:D:519:MET:HE2	2.46	0.50
1:E:7:ASP:OD1	1:E:432:ARG:NH2	2.44	0.50
1:E:892:TYR:O	1:E:893:GLU:HB2	2.11	0.50
1:A:169:THR:O	1:A:169:THR:OG1	2.27	0.50
1:C:367:ILE:HD11	1:C:496:MET:HB3	1.93	0.50
1:E:776:GLU:HB2	1:E:779:TYR:CD1	2.46	0.50
1:A:790:TYR:HB3	1:A:798:MET:HB3	1.93	0.50
1:B:776:GLU:HB3	1:B:779:TYR:CD1	2.47	0.50
1:C:982:PHE:HD2	1:C:1011:MET:HG3	1.75	0.50
1:D:108:GLN:O	1:D:112:GLN:HG2	2.11	0.50
1:D:671:ILE:HD12	1:D:674:LEU:O	2.11	0.50
1:A:383:LEU:HD21	1:A:473:THR:HA	1.93	0.50
1:A:401:ALA:O	1:A:405:LEU:HG	2.11	0.50
1:A:576:VAL:HA	1:A:663:VAL:HG22	1.93	0.50
1:A:728:LYS:HA	1:C:235:ILE:HB	1.94	0.50
1:A:975:ILE:O	1:A:979:SER:OG	2.22	0.50
1:C:64:VAL:HG12	1:C:117:LEU:HB3	1.93	0.50
1:C:559:LEU:HD13	1:C:923:ASN:HB2	1.93	0.50
1:E:186:ILE:HD13	1:E:262:LEU:HD21	1.94	0.50
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.94	0.50
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.93	0.50
1:C:352:PHE:HE1	1:C:366:LEU:HD12	1.76	0.50
1:C:447:MET:HB3	1:C:887:CYS:SG	2.52	0.50
1:D:790:TYR:HB3	1:D:798:MET:HB3	1.94	0.50
1:C:871:ASN:O	1:C:871:ASN:ND2	2.43	0.50
1:F:509:LYS:CB	1:F:514:GLY:H	2.24	0.50
1:A:580:ALA:HB1	1:A:724:THR:HG22	1.93	0.50
1:B:222:THR:HA	1:B:224:PRO:HD3	1.92	0.50
1:D:871:ASN:C	1:D:873:ALA:H	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.94	0.50
1:B:888:LEU:HD11	1:B:943:ILE:HD11	1.94	0.50
1:D:1038:GLU:N	1:D:1039:ASP:O	2.45	0.50
1:E:104:GLN:NE2	1:F:109:ASN:HB3	2.27	0.50
1:E:185:ARG:HB3	1:E:187:TRP:NE1	2.27	0.50
1:E:259:ARG:HG3	1:E:261:LEU:HG	1.93	0.50
1:A:682:PHE:HB3	1:A:827:ILE:HB	1.94	0.49
1:B:946:VAL:HG13	1:B:1026:PHE:CE1	2.47	0.49
1:B:946:VAL:HG22	1:B:1026:PHE:HD1	1.75	0.49
1:C:805:SER:O	1:C:805:SER:OG	2.24	0.49
1:F:222:THR:HA	1:F:224:PRO:HD3	1.93	0.49
1:A:231:ASN:OD1	1:B:622:GLN:NE2	2.46	0.49
1:B:872:GLN:O	1:B:875:SER:OG	2.21	0.49
1:C:222:THR:HA	1:C:224:PRO:HD3	1.94	0.49
1:D:161:ASN:ND2	1:E:687:GLN:O	2.45	0.49
1:D:239:ARG:HD3	1:D:761:ASP:O	2.13	0.49
1:D:904:VAL:HA	1:D:907:LEU:HD13	1.94	0.49
1:E:76:MET:HB3	1:E:77:TYR:HD2	1.77	0.49
1:E:946:VAL:HG22	1:E:1026:PHE:HD1	1.77	0.49
1:A:26:ALA:O	1:A:30:LEU:HD22	2.12	0.49
1:C:65:ILE:HG21	1:C:90:ILE:HG21	1.94	0.49
1:E:583:THR:HG22	1:E:586:ARG:HE	1.77	0.49
1:E:861:GLY:O	1:E:864:TYR:HB3	2.12	0.49
1:F:453:PHE:HE2	1:F:474:ILE:HD12	1.77	0.49
1:B:979:SER:HB3	1:B:1015:THR:HG21	1.93	0.49
1:E:262:LEU:HG	1:E:268:ILE:HD11	1.93	0.49
1:E:510:LYS:HB2	1:E:514:GLY:HA3	1.95	0.49
1:A:127:VAL:O	1:B:113:LEU:HD22	2.11	0.49
1:A:473:THR:O	1:A:476:SER:OG	2.31	0.49
1:A:632:LYS:HD2	1:A:633:ASP:H	1.77	0.49
1:B:602:GLU:HB3	1:B:606:VAL:HG23	1.95	0.49
1:B:716:VAL:HG22	1:B:717:ARG:H	1.77	0.49
1:B:1013:THR:O	1:B:1017:LEU:HB2	2.11	0.49
1:F:83:ASP:OD1	1:F:815:ARG:NH1	2.42	0.49
1:F:730:ASP:OD1	1:F:808:ARG:NH2	2.45	0.49
1:B:789:TRP:C	1:B:790:TYR:HD2	2.21	0.49
1:B:960:LEU:O	1:B:964:THR:HG23	2.12	0.49
1:C:457:ALA:HB2	1:C:471:SER:CB	2.41	0.49
1:E:43:VAL:HG21	1:E:104:GLN:HB2	1.94	0.49
1:F:178:PHE:HB3	1:F:279:ALA:HB2	1.94	0.49
1:B:787:GLY:O	1:B:789:TRP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:SER:HB2	1:E:816:LEU:HB2	1.95	0.49
1:E:137:LEU:HD22	1:E:293:LEU:HB2	1.95	0.49
1:E:459:PHE:HB3	1:E:464:GLY:HA2	1.95	0.49
1:F:866:GLU:HG2	1:F:866:GLU:O	2.13	0.49
1:B:393:LEU:HD12	1:B:469:GLN:HG3	1.94	0.49
1:B:904:VAL:HA	1:B:907:LEU:HD13	1.95	0.49
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.95	0.49
1:C:671:ILE:HG22	1:C:673:GLU:H	1.76	0.49
1:D:805:SER:O	1:D:805:SER:OG	2.24	0.49
1:A:448:VAL:HG13	1:A:884:VAL:HG22	1.95	0.49
1:C:109:ASN:O	1:C:110:LYS:NZ	2.46	0.49
1:E:873:ALA:N	1:E:874:PRO:HD2	2.28	0.49
1:D:393:LEU:HD13	1:D:466:ILE:HG23	1.95	0.49
1:E:81:ASN:HB2	1:E:89:GLN:HB2	1.95	0.49
1:A:28:LEU:HD22	1:A:29:LYS:HG3	1.94	0.48
1:C:979:SER:HA	1:C:1011:MET:HE1	1.95	0.48
1:D:35:TYR:CZ	1:D:564:LEU:HD21	2.48	0.48
1:D:404:LEU:HD21	1:D:449:LEU:HD13	1.95	0.48
1:F:396:PHE:CZ	1:F:1000:GLN:HG2	2.48	0.48
1:B:56:THR:O	1:B:60:THR:OG1	2.25	0.48
1:C:203:VAL:O	1:C:207:ILE:HG13	2.13	0.48
1:C:465:ALA:O	1:C:468:ARG:HB3	2.13	0.48
1:C:565:PRO:O	1:C:670:ALA:HB2	2.13	0.48
1:D:531:VAL:O	1:D:534:ILE:HG12	2.13	0.48
1:E:201:VAL:HG23	1:E:749:THR:HG23	1.95	0.48
1:F:555:LEU:HD22	1:F:913:LEU:HB3	1.94	0.48
1:F:671:ILE:HG21	1:F:674:LEU:HB2	1.94	0.48
1:F:843:LEU:HD13	1:F:847:LEU:HD23	1.95	0.48
1:A:892:TYR:OH	1:A:946:VAL:HG11	2.14	0.48
1:C:412:VAL:HG13	1:C:435:MET:HE1	1.94	0.48
1:D:719:ASN:HB2	1:D:828:LEU:HG	1.94	0.48
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.48	0.48
1:A:239:ARG:NH1	1:A:761:ASP:O	2.36	0.48
1:A:693:GLU:O	1:A:697:GLN:HB2	2.13	0.48
1:B:5:PHE:CG	1:B:487:ILE:HG13	2.49	0.48
1:B:211:ASN:O	1:B:760:ASN:ND2	2.46	0.48
1:C:312:LYS:HD2	1:C:312:LYS:HA	1.61	0.48
1:E:300:LEU:HD21	1:E:334:LYS:HG2	1.95	0.48
1:A:702:LEU:HD21	1:A:851:LEU:HD21	1.94	0.48
1:A:926:TYR:HD1	1:A:1003:VAL:HG23	1.78	0.48
1:B:280:GLU:OE2	1:B:588:GLN:NE2	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:MET:HE2	1:B:471:SER:HB2	1.95	0.48
1:B:523:SER:HB2	2:B:2000:LMT:H102	1.96	0.48
1:B:892:TYR:O	1:B:893:GLU:HB2	2.14	0.48
1:E:4:PHE:CE1	1:E:8:ARG:HD2	2.47	0.48
1:A:668:LEU:HD23	1:A:668:LEU:H	1.79	0.48
1:D:58:GLN:OE1	1:D:816:LEU:HB3	2.13	0.48
1:D:138:MET:HE1	1:D:307:ARG:HE	1.78	0.48
1:D:414:GLU:CD	1:D:974:PRO:HG3	2.38	0.48
1:D:602:GLU:HG3	1:D:605:ASN:HB2	1.96	0.48
1:E:659:LYS:HD3	1:E:660:ASP:H	1.78	0.48
1:F:911:GLY:HA3	1:F:1013:THR:OG1	2.14	0.48
1:A:777:ALA:HB1	1:C:225:VAL:HG12	1.95	0.48
1:B:224:PRO:HA	1:C:781:MET:HE1	1.94	0.48
1:E:225:VAL:HG13	1:F:777:ALA:HB1	1.96	0.48
1:F:65:ILE:HD11	1:F:118:LEU:HD11	1.96	0.48
1:B:54:ALA:HB1	1:B:816:LEU:HG	1.95	0.48
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.96	0.48
1:D:675:GLY:C	1:D:677:ALA:H	2.22	0.48
1:E:249:ILE:HD11	1:E:262:LEU:HD22	1.96	0.48
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.96	0.48
1:B:885:PHE:HB2	1:B:902:MET:SD	2.54	0.48
1:D:539:GLY:HA2	1:D:542:LEU:HD22	1.96	0.48
1:F:201:VAL:HA	1:F:204:ILE:HD12	1.96	0.48
1:F:901:VAL:HG13	1:F:942:ALA:HB3	1.96	0.48
1:B:516:PHE:HA	1:B:519:MET:HE3	1.96	0.48
1:C:684:LEU:O	1:C:824:SER:HB3	2.14	0.48
1:E:441:ALA:O	1:E:445:ILE:HG23	2.14	0.48
1:E:559:LEU:HD22	1:E:560:PRO:HD2	1.95	0.48
1:A:111:LEU:C	1:A:113:LEU:H	2.22	0.47
1:A:713:LEU:HG	1:A:844:MET:HE3	1.96	0.47
1:A:898:PRO:O	1:A:901:VAL:HG12	2.13	0.47
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.96	0.47
1:E:442:LEU:HA	1:E:445:ILE:HG12	1.96	0.47
1:A:336:SER:O	1:A:340:VAL:HG23	2.14	0.47
1:B:69:MET:HE1	1:B:111:LEU:HB2	1.96	0.47
1:B:216:ALA:HB2	1:B:236:ALA:HB2	1.96	0.47
1:B:683:GLU:HB3	1:B:858:ASP:HB3	1.96	0.47
1:B:946:VAL:HG13	1:B:1026:PHE:HE1	1.80	0.47
1:C:45:ILE:HD12	1:C:65:ILE:HD13	1.95	0.47
1:F:203:VAL:O	1:F:207:ILE:HG13	2.14	0.47
1:F:479:ALA:O	1:F:482:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:TYR:CE1	1:A:770:LYS:HD3	2.49	0.47
1:B:259:ARG:HG3	1:B:261:LEU:HG	1.97	0.47
1:B:619:GLY:HA2	1:B:815:ARG:NH1	2.29	0.47
1:D:13:TRP:NE1	1:D:492:LEU:HD21	2.28	0.47
1:D:101:ASP:O	1:D:105:VAL:HG23	2.15	0.47
1:E:15:ILE:O	1:E:19:ILE:HG13	2.14	0.47
1:E:45:ILE:HA	1:E:128:SER:O	2.14	0.47
1:E:114:ALA:O	1:E:118:LEU:HG	2.14	0.47
1:E:169:THR:HG21	1:E:306:ILE:HG13	1.96	0.47
1:F:455:PRO:HG2	1:F:880:SER:HA	1.96	0.47
1:F:507:GLU:HG2	1:F:518:ARG:HG2	1.96	0.47
1:A:80:SER:HB3	1:A:90:ILE:HG23	1.96	0.47
1:A:282:ASN:HA	1:A:595:THR:HG21	1.95	0.47
1:A:362:PHE:O	1:A:365:THR:OG1	2.24	0.47
1:C:919:ARG:NH1	1:C:990:VAL:O	2.39	0.47
1:A:228:GLN:NE2	1:A:230:LEU:O	2.43	0.47
1:A:727:PHE:CZ	1:A:807:SER:HB2	2.49	0.47
1:B:45:ILE:HD12	1:B:129:VAL:HG22	1.96	0.47
1:B:144:ASN:ND2	1:B:319:SER:O	2.44	0.47
1:B:417:GLU:HA	1:B:420:MET:HE2	1.96	0.47
1:B:885:PHE:CD1	1:B:898:PRO:HB2	2.50	0.47
1:B:1008:MET:HE3	1:B:1008:MET:HB2	1.83	0.47
1:D:532:GLY:O	1:D:536:ARG:HG2	2.14	0.47
1:D:533:GLY:HA2	2:D:2000:LMT:H3B	1.97	0.47
1:E:647:ILE:HD13	1:E:650:ARG:HH11	1.79	0.47
1:B:203:VAL:O	1:B:207:ILE:HG13	2.14	0.47
1:C:1030:ARG:C	1:C:1032:ARG:H	2.23	0.47
1:D:682:PHE:CE1	1:D:844:MET:HB3	2.50	0.47
1:E:105:VAL:HG22	1:F:109:ASN:HD21	1.79	0.47
1:E:723:ASP:HA	1:E:813:SER:HA	1.96	0.47
1:F:172:VAL:HG22	1:F:291:ILE:HG23	1.95	0.47
1:A:69:MET:HE1	1:A:111:LEU:HB2	1.97	0.47
1:A:108:GLN:HE22	1:B:113:LEU:HD21	1.79	0.47
1:A:278:ILE:HB	1:A:613:ASN:HB3	1.97	0.47
1:B:76:MET:HE3	1:B:95:GLU:HA	1.96	0.47
1:B:372:VAL:HG13	1:B:405:LEU:HD21	1.95	0.47
1:B:414:GLU:HG2	1:B:973:ARG:HE	1.79	0.47
1:B:470:PHE:CD1	1:B:929:VAL:HG21	2.49	0.47
1:B:686:ASP:HA	1:B:854:GLY:O	2.15	0.47
1:C:187:TRP:HE3	1:C:776:GLU:HG3	1.80	0.47
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:GLY:O	1:C:536:ARG:HG2	2.14	0.47
1:C:586:ARG:HA	1:C:589:LYS:HD2	1.96	0.47
1:C:980:LEU:O	1:C:984:LEU:HB2	2.14	0.47
1:D:277:ILE:HD11	1:D:620:LYS:HD3	1.96	0.47
1:D:355:MET:HB2	1:D:365:THR:HG23	1.96	0.47
1:D:699:ARG:HD2	1:D:718:PRO:HB3	1.95	0.47
1:D:946:VAL:HG13	1:D:1026:PHE:HE1	1.79	0.47
1:E:16:ALA:HB2	1:E:488:LEU:HD13	1.97	0.47
1:E:32:VAL:HG22	1:E:390:ILE:HG13	1.95	0.47
1:E:638:PRO:O	1:E:642:ASN:HB2	2.15	0.47
1:E:690:LEU:HB3	1:E:694:LYS:HD2	1.96	0.47
1:E:713:LEU:HD11	1:E:843:LEU:HD12	1.97	0.47
1:E:953:MET:HE3	1:E:953:MET:HB2	1.79	0.47
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.96	0.47
1:F:76:MET:H	1:F:94:PHE:HA	1.79	0.47
1:F:112:GLN:HG2	1:F:115:MET:HE3	1.97	0.47
1:F:563:PHE:HB2	1:F:866:GLU:HG3	1.96	0.47
1:F:637:ARG:NH1	1:F:642:ASN:O	2.47	0.47
1:A:58:GLN:OE1	1:A:816:LEU:HB3	2.15	0.47
1:A:181:GLN:HE21	1:A:769:LYS:HG2	1.80	0.47
1:B:151:GLN:HE22	1:B:278:ILE:HG22	1.80	0.47
1:B:434:SER:O	1:B:438:ILE:HG12	2.15	0.47
1:C:719:ASN:HB2	1:C:828:LEU:HD23	1.97	0.47
1:C:960:LEU:HD21	1:C:1027:VAL:HG13	1.95	0.47
1:D:317:PHE:HA	1:D:318:PRO:HD3	1.75	0.47
1:E:137:LEU:O	1:E:329:THR:HG22	2.15	0.47
1:E:400:LEU:HD23	1:E:929:VAL:HG11	1.97	0.47
1:E:641:GLU:HB2	1:E:650:ARG:HH22	1.80	0.47
1:F:574:THR:HG23	1:F:627:ALA:HB3	1.96	0.47
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.96	0.47
1:B:861:GLY:O	1:B:864:TYR:HB3	2.15	0.47
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.97	0.47
1:D:199:THR:HG23	1:D:792:ARG:H	1.79	0.47
1:E:142:VAL:HG13	1:E:323:ILE:HD13	1.97	0.47
1:E:216:ALA:HB2	1:E:236:ALA:HB2	1.96	0.47
1:E:1027:VAL:O	1:E:1031:ARG:HG2	2.15	0.47
1:F:146:ASP:O	1:F:148:THR:N	2.47	0.47
1:F:530:SER:O	2:F:2000:LMT:O3'	2.33	0.47
1:A:185:ARG:HD2	1:A:187:TRP:HE1	1.80	0.47
1:A:1008:MET:HE3	1:A:1008:MET:HB2	1.72	0.47
1:B:72:ILE:HG23	1:B:106:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:MET:HE3	1:B:500:ILE:HB	1.97	0.47
1:C:112:GLN:HB3	1:C:115:MET:HE2	1.96	0.47
1:C:888:LEU:HD23	1:C:888:LEU:HA	1.73	0.47
1:E:68:ASN:OD1	1:E:114:ALA:HB2	2.15	0.47
1:E:709:HIS:CE1	1:E:847:LEU:HD11	2.50	0.47
1:F:99:ASP:HB3	1:F:102:ILE:HB	1.95	0.47
1:F:808:ARG:HD2	1:F:808:ARG:N	2.30	0.47
1:A:72:ILE:HG12	1:A:107:VAL:HG22	1.97	0.46
1:B:142:VAL:HG13	1:B:323:ILE:HD13	1.97	0.46
1:B:758:TYR:CE1	1:B:770:LYS:HD3	2.49	0.46
1:C:261:LEU:HD13	1:C:263:ARG:HH21	1.80	0.46
1:C:574:THR:HG23	1:C:627:ALA:HB3	1.96	0.46
1:C:682:PHE:O	1:C:826:GLU:HB2	2.15	0.46
1:D:185:ARG:HD3	1:D:185:ARG:HA	1.68	0.46
1:E:800:PRO:HG2	1:E:803:ALA:HB2	1.96	0.46
1:F:453:PHE:HB3	1:F:471:SER:HA	1.97	0.46
1:F:787:GLY:C	1:F:789:TRP:H	2.22	0.46
1:A:45:ILE:HA	1:A:128:SER:O	2.15	0.46
1:A:155:SER:OG	1:A:179:GLY:HA3	2.15	0.46
1:B:102:ILE:O	1:B:106:GLN:HG3	2.14	0.46
1:B:641:GLU:HB2	1:B:650:ARG:NH2	2.30	0.46
1:C:575:MET:HA	1:C:626:ILE:HD12	1.96	0.46
1:E:564:LEU:HG	1:E:565:PRO:HD2	1.97	0.46
1:F:691:GLY:HA3	1:F:694:LYS:HD2	1.96	0.46
1:F:790:TYR:HB3	1:F:798:MET:HB3	1.97	0.46
1:A:164:ASP:O	1:A:168:ARG:NH1	2.48	0.46
1:A:520:PHE:O	1:A:524:THR:OG1	2.27	0.46
1:A:892:TYR:CE2	1:A:898:PRO:HA	2.51	0.46
1:A:894:SER:HB3	1:A:897:ILE:HG13	1.97	0.46
1:B:418:ARG:NH1	1:B:418:ARG:HB3	2.30	0.46
1:C:122:VAL:C	1:C:124:GLN:H	2.23	0.46
1:C:555:LEU:HD22	1:C:913:LEU:HB3	1.97	0.46
1:D:3:ASN:O	1:D:6:ILE:HG12	2.15	0.46
1:D:418:ARG:HH12	1:D:970:MET:HE3	1.79	0.46
1:E:367:ILE:HB	1:E:368:PRO:HD3	1.96	0.46
1:E:610:PHE:HB3	1:E:628:PHE:HB2	1.97	0.46
1:F:580:ALA:HB1	1:F:724:THR:HG22	1.97	0.46
1:A:705:GLU:HG3	1:A:847:LEU:HD13	1.96	0.46
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.51	0.46
1:C:36:PRO:HD3	1:C:391:ASN:HB2	1.96	0.46
1:C:405:LEU:HB2	1:C:481:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:VAL:HG21	1:D:86:GLY:O	2.16	0.46
1:F:462:SER:OG	1:F:865:GLN:NE2	2.49	0.46
1:F:509:LYS:O	1:F:511:GLY:N	2.45	0.46
1:A:723:ASP:HA	1:A:813:SER:HA	1.97	0.46
1:B:767:ARG:NH1	1:C:67:GLN:HE22	2.14	0.46
1:C:74:ASN:O	1:C:95:GLU:N	2.37	0.46
1:E:787:GLY:O	1:E:789:TRP:N	2.48	0.46
1:F:158:VAL:HG12	1:F:163:LYS:HB2	1.97	0.46
1:F:682:PHE:CE2	1:F:844:MET:HB3	2.50	0.46
1:B:693:GLU:O	1:B:697:GLN:HB2	2.15	0.46
1:B:742:SER:O	1:B:746:ILE:HG13	2.16	0.46
1:C:4:PHE:O	1:C:7:ASP:HB2	2.16	0.46
1:C:563:PHE:HB2	1:C:866:GLU:HB2	1.97	0.46
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.16	0.46
1:E:619:GLY:HA2	1:E:815:ARG:NH1	2.30	0.46
1:E:971:ARG:HG2	1:E:974:PRO:CG	2.46	0.46
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.97	0.46
1:C:157:TYR:OH	1:C:316:PHE:O	2.20	0.46
1:C:452:VAL:HA	1:C:880:SER:OG	2.15	0.46
1:C:762:PHE:CE1	1:C:764:ASP:HB2	2.50	0.46
1:C:818:ARG:NH2	1:C:822:LEU:HA	2.30	0.46
1:E:417:GLU:HA	1:E:420:MET:HE2	1.98	0.46
1:F:111:LEU:C	1:F:113:LEU:H	2.22	0.46
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.50	0.46
1:B:327:TYR:HD1	1:B:628:PHE:CD1	2.34	0.46
1:C:684:LEU:HD12	1:C:856:GLY:O	2.15	0.46
1:D:30:LEU:HD12	1:D:31:PRO:HD2	1.98	0.46
1:D:111:LEU:C	1:D:113:LEU:H	2.24	0.46
1:D:225:VAL:HG22	1:E:777:ALA:HB1	1.98	0.46
1:F:159:ALA:HB2	1:F:177:LEU:HD12	1.98	0.46
1:F:743:ILE:HA	1:F:746:ILE:HG12	1.98	0.46
1:F:762:PHE:CE1	1:F:764:ASP:HB2	2.50	0.46
1:F:919:ARG:NH1	1:F:990:VAL:O	2.36	0.46
1:A:30:LEU:HD21	1:A:390:ILE:HG13	1.98	0.46
1:A:435:MET:SD	1:A:490:PRO:HB3	2.56	0.46
1:B:185:ARG:HA	1:B:185:ARG:HD3	1.68	0.46
1:C:402:ILE:O	1:C:406:VAL:HG13	2.15	0.46
1:E:231:ASN:OD1	1:F:622:GLN:NE2	2.49	0.46
1:F:218:GLN:HG3	1:F:221:GLY:HA2	1.98	0.46
1:A:116:PRO:HG2	1:C:123:GLN:O	2.15	0.46
1:A:213:GLN:HG2	1:A:239:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:MET:HG2	1:A:843:LEU:HG	1.97	0.46
1:B:513:PHE:N	1:B:513:PHE:HD2	2.13	0.46
1:B:612:VAL:N	1:B:626:ILE:O	2.45	0.46
1:B:838:GLY:O	1:B:841:MET:HB2	2.16	0.46
1:C:467:TYR:HE2	1:C:925:VAL:HG13	1.81	0.46
1:D:727:PHE:CZ	1:D:807:SER:HB2	2.51	0.46
1:D:946:VAL:HG13	1:D:1026:PHE:CE1	2.51	0.46
1:E:21:LEU:O	1:E:25:LEU:HB2	2.16	0.46
1:E:362:PHE:O	1:E:365:THR:OG1	2.23	0.46
1:A:586:ARG:O	1:A:589:LYS:HB3	2.16	0.45
1:B:888:LEU:HA	1:B:888:LEU:HD23	1.66	0.45
1:E:805:SER:O	1:E:805:SER:OG	2.21	0.45
1:F:372:VAL:HG22	1:F:405:LEU:HD11	1.98	0.45
1:F:396:PHE:HZ	1:F:1000:GLN:HG2	1.79	0.45
1:A:693:GLU:HA	1:A:696:THR:HG22	1.98	0.45
1:A:980:LEU:O	1:A:984:LEU:HB2	2.16	0.45
1:E:641:GLU:HB2	1:E:650:ARG:NH2	2.32	0.45
1:F:24:GLY:O	1:F:27:ILE:HG22	2.16	0.45
1:F:293:LEU:HD13	1:F:294:ALA:O	2.17	0.45
1:F:905:VAL:HG22	1:F:935:ILE:HG23	1.98	0.45
2:A:2000:LMT:H2'	2:A:2000:LMT:H12	1.84	0.45
1:B:326:PRO:HB2	1:B:327:TYR:H	1.66	0.45
1:B:451:ALA:HB1	1:B:883:VAL:HG12	1.99	0.45
1:B:564:LEU:HG	1:B:565:PRO:HD2	1.98	0.45
1:C:186:ILE:C	1:C:187:TRP:HD1	2.24	0.45
1:C:563:PHE:CE2	1:C:671:ILE:HD11	2.52	0.45
1:C:679:GLY:O	1:C:863:SER:OG	2.31	0.45
1:C:931:LEU:O	1:C:935:ILE:HG13	2.15	0.45
1:D:897:ILE:HD11	1:D:1030:ARG:NH2	2.31	0.45
1:E:378:GLY:O	1:E:382:VAL:HG23	2.15	0.45
1:E:405:LEU:HD22	1:E:481:SER:HB2	1.98	0.45
1:E:607:GLU:HB2	1:E:632:LYS:HG3	1.99	0.45
1:E:725:PRO:HG3	1:E:811:TYR:HE1	1.82	0.45
1:A:76:MET:HB2	1:A:93:THR:O	2.16	0.45
1:A:485:ALA:O	1:A:490:PRO:HD3	2.17	0.45
1:B:157:TYR:CE1	1:B:161:ASN:HB2	2.52	0.45
1:C:47:ALA:HB2	1:C:127:VAL:HG13	1.98	0.45
1:C:404:LEU:HD12	1:C:937:LEU:HD23	1.98	0.45
1:C:407:ASP:OD2	1:C:937:LEU:HD22	2.16	0.45
1:C:910:ILE:O	1:C:914:LEU:HB2	2.17	0.45
1:D:36:PRO:O	1:D:38:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:LEU:HD23	1:D:334:LYS:HE3	1.98	0.45
1:D:441:ALA:O	1:D:445:ILE:HG23	2.17	0.45
1:E:295:THR:OG1	1:F:73:ASP:OD2	2.34	0.45
1:F:702:LEU:HD12	1:F:851:LEU:HD11	1.97	0.45
1:A:888:LEU:O	1:A:892:TYR:HB2	2.17	0.45
1:B:156:ASP:OD2	1:B:769:LYS:NZ	2.47	0.45
1:B:250:LEU:HD23	1:C:737:GLN:NE2	2.30	0.45
1:B:901:VAL:HG21	1:B:943:ILE:HG13	1.98	0.45
1:C:24:GLY:O	1:C:28:LEU:HG	2.17	0.45
1:D:527:TYR:OH	1:D:1019:ILE:O	2.18	0.45
1:D:668:LEU:HD23	1:D:668:LEU:H	1.82	0.45
1:D:762:PHE:CE2	1:D:769:LYS:HB2	2.51	0.45
1:E:408:ASP:OD1	1:E:940:LYS:NZ	2.49	0.45
1:E:605:ASN:HD22	1:E:647:ILE:HD11	1.80	0.45
1:A:21:LEU:O	1:A:25:LEU:HB3	2.16	0.45
1:C:111:LEU:O	1:C:111:LEU:HD22	2.17	0.45
1:E:47:ALA:HB1	1:E:122:VAL:HG13	1.99	0.45
1:F:6:ILE:CG2	1:F:12:ALA:HB2	2.47	0.45
1:F:445:ILE:HG12	1:F:940:LYS:HG3	1.99	0.45
1:A:776:GLU:HB3	1:A:779:TYR:HD1	1.79	0.45
1:B:136:PHE:HA	1:B:292:LYS:HA	1.98	0.45
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.82	0.45
1:D:32:VAL:HG22	1:D:390:ILE:HB	1.99	0.45
1:D:316:PHE:HD1	1:E:687:GLN:HG2	1.82	0.45
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.99	0.45
1:E:762:PHE:CE1	1:E:764:ASP:HB2	2.51	0.45
1:F:298:ASN:HB3	1:F:301:ASP:HB2	1.99	0.45
1:A:190:PRO:HG3	1:A:779:TYR:HB3	1.97	0.45
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.99	0.45
1:B:507:GLU:C	1:B:509:LYS:H	2.24	0.45
1:C:186:ILE:HD13	1:C:262:LEU:HD21	1.99	0.45
1:D:137:LEU:O	1:D:329:THR:HG22	2.16	0.45
1:E:586:ARG:O	1:E:589:LYS:HB3	2.16	0.45
1:A:729:ILE:HD11	1:C:234:ILE:HD12	1.99	0.45
1:A:988:PRO:O	1:A:992:SER:HB2	2.17	0.45
1:B:314:GLU:N	1:B:315:PRO:HD2	2.32	0.45
1:C:948:PHE:CE2	1:C:971:ARG:HG3	2.51	0.45
1:F:58:GLN:OE1	1:F:816:LEU:HB3	2.17	0.45
1:F:586:ARG:O	1:F:589:LYS:HB2	2.16	0.45
1:A:199:THR:CG2	1:A:792:ARG:H	2.29	0.45
1:C:356:TYR:HA	1:C:365:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:PRO:O	1:D:876:LEU:HD13	2.17	0.45
1:D:530:SER:O	1:D:534:ILE:HG23	2.17	0.45
1:E:254:ASN:HB2	1:E:258:SER:O	2.17	0.45
1:F:188:MET:HB3	1:F:193:LEU:HD13	1.99	0.45
1:F:470:PHE:CE1	1:F:929:VAL:HG11	2.51	0.45
1:F:774:MET:HE3	1:F:774:MET:HB3	1.80	0.45
1:A:110:LYS:HA	1:A:110:LYS:HD3	1.80	0.44
1:A:986:VAL:O	1:A:990:VAL:HG23	2.17	0.44
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.98	0.44
1:B:913:LEU:HD23	1:B:927:PHE:HZ	1.82	0.44
1:B:1036:LYS:HA	1:B:1037:ASN:HA	1.61	0.44
1:C:362:PHE:O	1:C:365:THR:OG1	2.25	0.44
1:C:780:ARG:O	1:C:781:MET:HE2	2.17	0.44
1:C:866:GLU:O	1:C:866:GLU:HG2	2.17	0.44
1:E:188:MET:O	1:E:776:GLU:HG3	2.17	0.44
1:E:683:GLU:HG2	1:E:819:TYR:CG	2.52	0.44
1:F:730:ASP:H	1:F:808:ARG:NH1	2.15	0.44
1:A:203:VAL:O	1:A:207:ILE:HG13	2.16	0.44
1:B:274:ASN:OD1	1:B:275:TYR:N	2.50	0.44
1:C:108:GLN:O	1:C:112:GLN:HG3	2.17	0.44
1:C:977:MET:HE2	1:C:977:MET:HB3	1.91	0.44
1:D:114:ALA:O	1:D:118:LEU:HG	2.17	0.44
1:D:742:SER:O	1:D:746:ILE:HG13	2.18	0.44
1:E:900:SER:HA	1:E:903:LEU:HD12	1.98	0.44
1:F:723:ASP:OD1	1:F:723:ASP:N	2.50	0.44
1:A:594:VAL:HG22	1:A:655:PHE:CE2	2.52	0.44
1:B:187:TRP:HE1	1:B:269:GLU:HG2	1.82	0.44
1:B:891:LEU:HD13	1:B:891:LEU:HA	1.81	0.44
1:C:509:LYS:HG2	1:C:513:PHE:HB2	1.99	0.44
1:C:535:LEU:HD22	1:C:1027:VAL:HG21	2.00	0.44
1:D:897:ILE:O	1:D:900:SER:OG	2.32	0.44
1:E:76:MET:HE3	1:E:95:GLU:HA	1.99	0.44
1:E:463:THR:O	1:E:467:TYR:HD1	2.00	0.44
1:E:578:LEU:HD21	1:E:590:VAL:HG21	2.00	0.44
1:F:61:VAL:HA	1:F:118:LEU:HD22	1.99	0.44
1:F:249:ILE:HB	1:F:262:LEU:HB2	1.99	0.44
1:A:652:THR:HG23	1:A:664:PHE:CD1	2.52	0.44
1:C:723:ASP:OD1	1:C:723:ASP:N	2.51	0.44
1:D:1030:ARG:HD3	1:D:1030:ARG:HA	1.82	0.44
1:E:278:ILE:HB	1:E:613:ASN:HB3	1.99	0.44
1:E:1030:ARG:C	1:E:1032:ARG:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:GLN:O	1:F:112:GLN:HG3	2.18	0.44
1:F:780:ARG:O	1:F:781:MET:HE2	2.18	0.44
1:F:907:LEU:HD21	1:F:1021:PHE:CD2	2.53	0.44
1:A:10:ILE:HB	1:B:893:GLU:HG3	2.00	0.44
1:A:14:VAL:HG21	1:B:890:ALA:HB2	2.00	0.44
1:B:378:GLY:O	1:B:382:VAL:HG23	2.17	0.44
1:B:1040:ILE:HG22	1:B:1041:GLU:N	2.32	0.44
1:C:746:ILE:HG22	1:C:791:VAL:HG11	1.99	0.44
1:D:559:LEU:HD23	1:D:923:ASN:HB2	1.98	0.44
1:D:931:LEU:HD23	1:D:931:LEU:HA	1.80	0.44
1:F:350:LEU:HD13	1:F:984:LEU:HD12	1.98	0.44
1:F:378:GLY:O	1:F:382:VAL:HG23	2.16	0.44
1:A:281:PHE:HD1	1:A:610:PHE:HD1	1.66	0.44
1:A:931:LEU:O	1:A:935:ILE:HG12	2.18	0.44
1:B:470:PHE:HD1	1:B:929:VAL:HG21	1.83	0.44
1:B:668:LEU:HD23	1:B:668:LEU:H	1.82	0.44
1:B:877:TYR:O	1:B:880:SER:HB3	2.18	0.44
1:D:768:VAL:HG12	1:E:63:GLN:OE1	2.17	0.44
1:F:826:GLU:HG2	1:F:827:ILE:N	2.33	0.44
1:A:602:GLU:HB3	1:A:606:VAL:HG23	2.00	0.44
1:A:958:LYS:HD2	1:A:958:LYS:HA	1.52	0.44
1:B:449:LEU:O	1:B:452:VAL:HG22	2.18	0.44
1:D:5:PHE:CD2	1:D:487:ILE:HG23	2.52	0.44
1:D:355:MET:CB	1:D:365:THR:HG23	2.48	0.44
1:D:931:LEU:O	1:D:935:ILE:HG13	2.18	0.44
1:E:496:MET:H	1:E:496:MET:HG2	1.63	0.44
1:E:671:ILE:HB	1:E:672:VAL:H	1.49	0.44
1:A:960:LEU:O	1:A:964:THR:HG23	2.18	0.44
1:C:58:GLN:OE1	1:C:816:LEU:HB3	2.17	0.44
1:C:81:ASN:HA	1:C:817:GLU:HA	1.99	0.44
1:C:578:LEU:HD23	1:C:578:LEU:HA	1.87	0.44
1:D:754:TRP:HZ3	1:F:219:LEU:HD23	1.81	0.44
1:A:15:ILE:O	1:A:19:ILE:HG13	2.17	0.44
1:C:563:PHE:HE2	1:C:671:ILE:HD11	1.81	0.44
1:C:754:TRP:HZ2	1:C:785:ASP:HB2	1.82	0.44
1:F:104:GLN:HG3	1:F:105:VAL:N	2.33	0.44
1:A:359:LEU:O	1:A:360:GLN:HG2	2.17	0.43
1:A:365:THR:O	1:A:368:PRO:HD2	2.18	0.43
1:A:776:GLU:HG2	1:A:777:ALA:H	1.83	0.43
1:C:415:ASN:OD1	1:C:418:ARG:NH2	2.51	0.43
1:C:623:ASN:OD1	1:C:623:ASN:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:668:LEU:H	1:C:668:LEU:HD23	1.83	0.43
1:D:349:ILE:HD13	1:D:349:ILE:HA	1.90	0.43
1:D:612:VAL:N	1:D:626:ILE:O	2.45	0.43
1:E:300:LEU:CD2	1:E:334:LYS:HG2	2.48	0.43
1:F:398:MET:HA	1:F:401:ALA:HB3	2.00	0.43
1:B:137:LEU:HD22	1:B:293:LEU:HD23	1.99	0.43
1:B:699:ARG:HD3	1:B:825:MET:HE2	2.01	0.43
1:D:354:VAL:HG11	1:D:981:ALA:HB2	2.00	0.43
1:D:514:GLY:HA2	1:D:517:ASN:ND2	2.31	0.43
1:D:897:ILE:HD11	1:D:1030:ARG:HH21	1.82	0.43
1:E:340:VAL:HG22	1:E:396:PHE:CE2	2.54	0.43
1:F:372:VAL:HB	1:F:373:PRO:HD3	1.98	0.43
1:F:671:ILE:HG13	1:F:862:MET:HE1	2.00	0.43
1:A:36:PRO:HG3	1:A:469:GLN:HG3	2.01	0.43
1:B:324:VAL:O	1:B:326:PRO:HD3	2.18	0.43
1:B:703:LEU:HD11	1:B:718:PRO:HD3	2.00	0.43
1:C:404:LEU:HA	1:C:937:LEU:HD21	1.99	0.43
1:C:527:TYR:O	1:C:531:VAL:HG23	2.18	0.43
1:D:110:LYS:HA	1:D:110:LYS:HD3	1.69	0.43
1:D:144:ASN:ND2	1:D:149:MET:HG2	2.33	0.43
1:D:701:GLN:O	1:D:705:GLU:HB2	2.18	0.43
1:E:482:VAL:O	1:E:486:LEU:HG	2.18	0.43
1:E:727:PHE:CZ	1:E:807:SER:HB2	2.53	0.43
1:F:805:SER:O	1:F:805:SER:OG	2.24	0.43
1:B:336:SER:O	1:B:340:VAL:HG23	2.18	0.43
1:B:659:LYS:NZ	1:B:660:ASP:OD2	2.43	0.43
1:C:659:LYS:HD3	1:C:659:LYS:HA	1.88	0.43
1:D:185:ARG:HD2	1:D:187:TRP:HE1	1.83	0.43
1:D:235:ILE:HB	1:E:728:LYS:HA	2.01	0.43
1:D:444:GLY:HA3	1:D:891:LEU:HD22	1.99	0.43
1:D:465:ALA:HA	1:D:468:ARG:HD3	2.00	0.43
1:E:190:PRO:HG3	1:E:779:TYR:HB3	2.00	0.43
1:E:390:ILE:H	1:E:390:ILE:HG12	1.60	0.43
1:E:671:ILE:HG21	1:E:674:LEU:HD12	2.00	0.43
1:F:402:ILE:O	1:F:405:LEU:HG	2.18	0.43
1:F:551:GLY:O	1:F:555:LEU:HB2	2.18	0.43
1:A:170:SER:HB3	1:B:74:ASN:H	1.84	0.43
1:A:293:LEU:HD13	1:A:294:ALA:O	2.18	0.43
1:A:578:LEU:HD23	1:A:578:LEU:HA	1.89	0.43
1:A:727:PHE:HD1	1:A:809:TRP:CD1	2.37	0.43
1:A:873:ALA:N	1:A:874:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:LEU:HB3	1:B:611:ALA:HB1	2.00	0.43
1:C:452:VAL:HG12	1:C:884:VAL:CG2	2.49	0.43
1:D:726:GLN:OE1	1:F:235:ILE:HD11	2.18	0.43
1:E:435:MET:SD	1:E:490:PRO:HB3	2.57	0.43
1:F:444:GLY:O	1:F:448:VAL:HG12	2.18	0.43
1:F:453:PHE:CE2	1:F:474:ILE:HD12	2.52	0.43
1:F:904:VAL:HA	1:F:907:LEU:HD13	2.00	0.43
1:B:80:SER:O	1:B:817:GLU:HA	2.18	0.43
1:B:235:ILE:HB	1:C:728:LYS:HA	2.00	0.43
1:B:404:LEU:O	1:B:407:ASP:HB3	2.18	0.43
1:B:851:LEU:HA	1:B:852:PRO:HD3	1.68	0.43
1:D:551:GLY:O	1:D:555:LEU:HB2	2.18	0.43
1:D:725:PRO:HG3	1:D:811:TYR:HE2	1.83	0.43
1:D:983:ILE:HG23	1:D:1008:MET:HE2	2.01	0.43
1:D:1034:SER:HB3	1:D:1035:ARG:H	1.53	0.43
1:E:545:TYR:HA	1:E:548:ILE:HD12	2.01	0.43
1:F:953:MET:HE3	1:F:953:MET:HB2	1.83	0.43
1:A:83:ASP:OD1	1:A:815:ARG:NH1	2.52	0.43
1:A:129:VAL:O	1:B:110:LYS:NZ	2.35	0.43
1:B:101:ASP:N	1:B:101:ASP:OD1	2.52	0.43
1:B:166:ILE:HG21	1:B:310:LEU:HD22	2.00	0.43
1:B:167:SER:C	1:B:169:THR:N	2.76	0.43
1:C:420:MET:HE3	1:C:420:MET:HB2	1.88	0.43
1:C:524:THR:HG22	1:C:972:LEU:HD12	2.00	0.43
1:C:633:ASP:OD1	1:C:633:ASP:N	2.52	0.43
1:D:41:PRO:HD3	1:D:96:SER:HA	1.99	0.43
1:D:153:ASP:OD2	1:D:182:TYR:OH	2.34	0.43
1:D:959:GLY:HA2	1:D:1040:ILE:H	1.82	0.43
1:D:1030:ARG:C	1:D:1032:ARG:H	2.26	0.43
1:F:937:LEU:O	1:F:940:LYS:HB3	2.19	0.43
1:A:58:GLN:O	1:A:63:GLN:HG3	2.18	0.43
1:A:199:THR:HG23	1:A:792:ARG:H	1.84	0.43
1:A:895:TRP:CE2	1:C:10:ILE:HG13	2.54	0.43
1:A:1011:MET:O	1:A:1015:THR:HG23	2.19	0.43
1:B:6:ILE:H	1:B:6:ILE:HG13	1.69	0.43
1:B:162:MET:C	1:B:164:ASP:H	2.27	0.43
1:B:948:PHE:O	1:B:952:LEU:HG	2.19	0.43
1:C:138:MET:HE3	1:C:138:MET:HB2	1.82	0.43
1:C:303:ALA:O	1:C:307:ARG:HB2	2.19	0.43
1:C:680:PHE:N	1:C:680:PHE:CD1	2.85	0.43
1:C:787:GLY:O	1:C:789:TRP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:VAL:HG11	1:D:395:MET:HB3	2.01	0.43
1:D:953:MET:HE2	1:D:963:ALA:HB3	2.01	0.43
1:F:524:THR:O	1:F:527:TYR:HB3	2.18	0.43
1:F:931:LEU:O	1:F:935:ILE:HG13	2.19	0.43
1:A:186:ILE:HD13	1:A:262:LEU:HD21	2.01	0.43
1:A:564:LEU:HG	1:A:565:PRO:HD2	2.01	0.43
1:A:800:PRO:HG2	1:A:803:ALA:HB2	2.00	0.43
1:A:1035:ARG:HH22	1:A:1036:LYS:HB2	1.84	0.43
1:B:278:ILE:CG1	1:B:613:ASN:HB3	2.42	0.43
1:B:650:ARG:HA	1:B:653:ARG:HB2	2.00	0.43
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.53	0.43
1:C:960:LEU:HD11	1:C:1027:VAL:HA	2.00	0.43
1:D:890:ALA:HB1	1:F:11:PHE:CD1	2.54	0.43
1:D:1008:MET:HE3	1:D:1008:MET:HB2	1.82	0.43
1:E:274:ASN:OD1	1:E:275:TYR:N	2.52	0.43
1:E:401:ALA:O	1:E:405:LEU:HG	2.19	0.43
1:E:960:LEU:O	1:E:964:THR:HG23	2.18	0.43
1:F:351:VAL:HG22	1:F:981:ALA:HB1	1.99	0.43
1:F:363:ARG:HG3	1:F:496:MET:O	2.18	0.43
1:F:982:PHE:HD2	1:F:1011:MET:HE3	1.83	0.43
1:A:786:ILE:HD13	1:A:786:ILE:HA	1.83	0.43
1:B:485:ALA:O	1:B:490:PRO:HD3	2.19	0.43
1:C:504:ASP:O	1:C:505:HIS:HB2	2.19	0.43
1:D:31:PRO:O	1:D:390:ILE:N	2.43	0.43
1:D:153:ASP:OD2	1:D:153:ASP:N	2.52	0.43
1:E:317:PHE:HA	1:E:318:PRO:HD2	1.87	0.43
1:E:1040:ILE:HG12	1:E:1041:GLU:N	2.33	0.43
1:F:38:ILE:CG2	1:F:462:SER:HB3	2.49	0.43
1:F:72:ILE:HD12	1:F:72:ILE:HA	1.60	0.43
1:F:162:MET:C	1:F:164:ASP:H	2.27	0.43
1:F:350:LEU:HD12	1:F:984:LEU:O	2.19	0.43
1:F:366:LEU:HA	1:F:369:THR:HB	2.01	0.43
1:F:453:PHE:O	1:F:456:MET:HG2	2.17	0.43
1:F:960:LEU:O	1:F:964:THR:HG23	2.19	0.43
1:A:170:SER:OG	1:B:75:LEU:N	2.41	0.42
1:B:877:TYR:CE2	1:B:932:LEU:HD11	2.54	0.42
1:C:61:VAL:HG13	1:C:118:LEU:HD13	2.02	0.42
1:C:393:LEU:H	1:C:393:LEU:HG	1.62	0.42
1:C:482:VAL:O	1:C:486:LEU:HG	2.19	0.42
1:D:577:GLN:OE1	1:D:624:THR:HG22	2.19	0.42
1:D:758:TYR:CE1	1:D:770:LYS:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:728:LYS:HE3	1:F:730:ASP:OD1	2.19	0.42
1:F:1030:ARG:C	1:F:1032:ARG:H	2.27	0.42
1:A:777:ALA:HB1	1:C:225:VAL:CG1	2.50	0.42
1:B:530:SER:O	1:B:534:ILE:HG23	2.19	0.42
1:B:659:LYS:HA	1:B:659:LYS:HD2	1.83	0.42
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.99	0.42
1:E:281:PHE:CZ	1:E:324:VAL:HG21	2.54	0.42
1:F:43:VAL:HG21	1:F:104:GLN:HB2	2.01	0.42
1:F:185:ARG:HD3	1:F:185:ARG:HA	1.71	0.42
1:F:530:SER:HB3	2:F:2000:LMT:H22	2.01	0.42
1:F:1012:VAL:O	1:F:1016:VAL:HG23	2.20	0.42
1:A:222:THR:HA	1:A:224:PRO:HD3	2.01	0.42
1:A:527:TYR:O	1:A:531:VAL:HG23	2.19	0.42
1:A:641:GLU:HA	1:A:646:ALA:HB3	2.01	0.42
1:B:317:PHE:HA	1:B:318:PRO:HD2	1.82	0.42
1:B:578:LEU:HD21	1:B:590:VAL:HG21	2.01	0.42
1:C:448:VAL:HG21	1:C:888:LEU:HG	2.01	0.42
1:C:913:LEU:HD23	1:C:927:PHE:HZ	1.84	0.42
1:E:104:GLN:OE1	1:E:131:LYS:HG3	2.18	0.42
1:E:105:VAL:CG2	1:F:109:ASN:HD21	2.32	0.42
1:E:717:ARG:O	1:E:828:LEU:N	2.52	0.42
1:E:926:TYR:CE1	1:E:999:ALA:HB1	2.55	0.42
1:F:563:PHE:HB2	1:F:866:GLU:HB2	2.00	0.42
1:F:675:GLY:C	1:F:677:ALA:H	2.26	0.42
1:A:393:LEU:HB3	1:A:470:PHE:CE1	2.54	0.42
1:A:690:LEU:O	1:A:694:LYS:HG3	2.20	0.42
1:A:1015:THR:O	1:A:1019:ILE:HG12	2.19	0.42
1:B:684:LEU:HD12	1:B:856:GLY:O	2.19	0.42
1:C:24:GLY:HA2	1:C:27:ILE:HG23	2.01	0.42
1:C:185:ARG:HD3	1:C:185:ARG:HA	1.75	0.42
1:C:474:ILE:H	1:C:474:ILE:HG12	1.72	0.42
1:D:410:ILE:HD13	1:D:977:MET:HB3	2.02	0.42
1:D:531:VAL:HG11	1:D:968:VAL:HG21	2.01	0.42
1:D:1011:MET:HE3	1:D:1011:MET:HB3	1.91	0.42
1:D:1024:VAL:O	1:D:1028:VAL:HG23	2.20	0.42
1:E:84:SER:HB3	1:E:814:PRO:HB2	2.01	0.42
1:F:110:LYS:HD3	1:F:110:LYS:HA	1.79	0.42
1:F:278:ILE:CG1	1:F:613:ASN:HB3	2.44	0.42
2:F:2000:LMT:H5'	2:F:2000:LMT:H1B	1.64	0.42
1:A:614:GLY:HA2	1:A:621:GLY:O	2.20	0.42
1:B:360:GLN:HB3	1:B:513:PHE:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:VAL:O	1:B:452:VAL:HG13	2.19	0.42
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	2.00	0.42
1:B:641:GLU:HB2	1:B:650:ARG:HH22	1.84	0.42
1:C:578:LEU:HD12	1:C:587:THR:HG23	2.01	0.42
1:C:786:ILE:HD13	1:C:786:ILE:HA	1.83	0.42
1:D:199:THR:CG2	1:D:792:ARG:H	2.33	0.42
1:E:705:GLU:HB3	1:E:847:LEU:HD13	2.01	0.42
1:F:15:ILE:O	1:F:19:ILE:HG13	2.19	0.42
1:A:787:GLY:O	1:A:789:TRP:N	2.52	0.42
1:A:1015:THR:OG1	1:A:1016:VAL:N	2.53	0.42
1:B:110:LYS:HA	1:B:110:LYS:HD3	1.74	0.42
1:B:414:GLU:HG2	1:B:973:ARG:NH2	2.34	0.42
1:C:355:MET:HA	1:C:977:MET:HE1	2.02	0.42
1:D:527:TYR:CD2	1:D:972:LEU:HG	2.54	0.42
1:B:185:ARG:HB3	1:B:187:TRP:NE1	2.34	0.42
1:B:795:ASP:CG	1:B:796:GLY:H	2.26	0.42
1:C:649:MET:HE2	1:C:649:MET:HB2	1.90	0.42
1:C:740:GLY:O	1:C:794:ALA:N	2.45	0.42
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.19	0.42
1:D:281:PHE:CE1	1:D:608:SER:HB2	2.54	0.42
1:D:293:LEU:HD22	1:D:294:ALA:H	1.84	0.42
1:D:924:ASP:OD1	1:D:926:TYR:N	2.51	0.42
1:E:293:LEU:HD22	1:E:294:ALA:H	1.84	0.42
1:E:602:GLU:HB3	1:E:606:VAL:HG23	2.01	0.42
1:E:787:GLY:C	1:E:789:TRP:H	2.27	0.42
1:F:274:ASN:OD1	1:F:275:TYR:N	2.52	0.42
1:F:564:LEU:HG	1:F:565:PRO:HD2	2.00	0.42
1:A:17:ILE:HA	1:A:20:MET:HB2	2.01	0.42
1:A:185:ARG:HA	1:A:185:ARG:HD3	1.69	0.42
1:A:457:ALA:HA	1:A:468:ARG:HA	2.00	0.42
1:A:552:MET:HB2	1:A:910:ILE:HB	2.02	0.42
1:A:888:LEU:HD12	1:A:888:LEU:HA	1.93	0.42
1:B:324:VAL:C	1:B:326:PRO:HD3	2.45	0.42
1:B:452:VAL:HA	1:B:880:SER:OG	2.19	0.42
1:B:545:TYR:OH	1:B:903:LEU:O	2.35	0.42
1:C:462:SER:HB2	1:C:865:GLN:HG2	2.02	0.42
1:D:58:GLN:O	1:D:63:GLN:HG3	2.19	0.42
1:F:11:PHE:HE2	1:F:15:ILE:HD11	1.85	0.42
1:F:960:LEU:HD21	1:F:1027:VAL:HG13	2.02	0.42
1:A:33:ALA:O	1:A:391:ASN:HA	2.20	0.42
1:A:493:CYS:C	1:A:495:THR:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ASP:HB3	1:C:940:LYS:HD2	2.02	0.42
1:C:1012:VAL:O	1:C:1016:VAL:HG23	2.20	0.42
1:D:375:VAL:HG11	1:D:481:SER:HB3	2.02	0.42
1:D:555:LEU:HD22	1:D:913:LEU:HB3	2.01	0.42
1:D:717:ARG:O	1:D:828:LEU:N	2.52	0.42
1:D:741:VAL:HG13	1:D:746:ILE:HD11	2.02	0.42
1:D:786:ILE:HD13	1:D:786:ILE:HA	1.81	0.42
1:F:244:GLU:O	1:F:248:LYS:HG3	2.20	0.42
1:F:312:LYS:HA	1:F:312:LYS:HD2	1.68	0.42
1:F:520:PHE:HE2	1:F:973:ARG:HG3	1.83	0.42
1:F:684:LEU:O	1:F:824:SER:HB2	2.20	0.42
1:F:888:LEU:HD23	1:F:888:LEU:HA	1.67	0.42
1:A:108:GLN:CD	1:B:109:ASN:HB3	2.44	0.42
1:C:564:LEU:HG	1:C:565:PRO:HD2	2.00	0.42
1:D:671:ILE:H	1:D:671:ILE:HG12	1.63	0.42
1:F:877:TYR:O	1:F:881:LEU:HB2	2.20	0.42
1:A:276:ASP:OD2	1:A:276:ASP:N	2.53	0.41
1:A:727:PHE:HD1	1:A:809:TRP:HD1	1.68	0.41
1:D:625:GLY:O	1:D:626:ILE:HD12	2.20	0.41
1:E:133:SER:HG	1:E:292:LYS:HZ1	1.66	0.41
1:E:314:GLU:N	1:E:315:PRO:HD2	2.35	0.41
1:E:590:VAL:HG11	1:E:663:VAL:HG21	2.01	0.41
1:E:709:HIS:ND1	1:E:847:LEU:HD11	2.35	0.41
1:F:102:ILE:O	1:F:105:VAL:HB	2.20	0.41
1:F:178:PHE:CD1	1:F:610:PHE:HE2	2.38	0.41
1:A:5:PHE:CE1	1:A:487:ILE:HG12	2.55	0.41
1:A:729:ILE:HD13	1:A:786:ILE:HD11	2.01	0.41
1:B:471:SER:O	1:B:475:VAL:HB	2.21	0.41
1:C:470:PHE:O	1:C:474:ILE:HG12	2.19	0.41
1:C:491:ALA:O	1:C:495:THR:OG1	2.28	0.41
1:C:684:LEU:HB3	1:C:825:MET:O	2.20	0.41
1:D:76:MET:HE3	1:D:864:TYR:CE2	2.54	0.41
1:D:159:ALA:HB2	1:D:177:LEU:CD1	2.51	0.41
1:D:838:GLY:O	1:D:841:MET:HB2	2.21	0.41
1:D:849:SER:C	1:D:850:LYS:HD2	2.46	0.41
1:E:314:GLU:HG3	1:E:317:PHE:CD2	2.55	0.41
1:F:26:ALA:HB1	1:F:384:ALA:HB3	2.02	0.41
1:F:633:ASP:OD1	1:F:633:ASP:N	2.52	0.41
1:F:743:ILE:O	1:F:746:ILE:HG12	2.20	0.41
1:F:774:MET:HG2	1:F:775:SER:H	1.86	0.41
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:ALA:O	1:A:741:VAL:HG12	2.20	0.41
1:B:126:GLY:HA2	1:C:116:PRO:CG	2.47	0.41
1:C:41:PRO:HD2	1:C:94:PHE:O	2.19	0.41
1:C:158:VAL:HG12	1:C:163:LYS:HB2	2.02	0.41
1:C:189:ASN:HB2	1:C:192:GLU:HB2	2.02	0.41
1:D:210:GLN:OE1	1:E:733:GLN:NE2	2.45	0.41
1:D:482:VAL:O	1:D:486:LEU:HG	2.20	0.41
1:D:506:GLY:O	1:D:508:GLY:N	2.53	0.41
1:D:838:GLY:HA2	1:D:841:MET:SD	2.60	0.41
1:F:943:ILE:O	1:F:947:GLU:HB3	2.19	0.41
1:A:252:LYS:HB3	1:A:252:LYS:HE2	1.89	0.41
1:A:530:SER:O	1:A:534:ILE:HG23	2.21	0.41
1:B:72:ILE:HG12	1:B:107:VAL:HG22	2.03	0.41
1:B:1011:MET:O	1:B:1015:THR:HG23	2.20	0.41
1:C:64:VAL:CG1	1:C:117:LEU:HB3	2.51	0.41
1:C:249:ILE:HB	1:C:262:LEU:HB2	2.02	0.41
1:D:222:THR:HA	1:D:224:PRO:HD3	2.02	0.41
1:D:545:TYR:HB2	1:D:1021:PHE:HE2	1.84	0.41
1:D:705:GLU:HG2	1:D:847:LEU:HD22	2.02	0.41
1:E:76:MET:HB3	1:E:77:TYR:CD2	2.53	0.41
1:E:445:ILE:HG22	1:E:943:ILE:HG21	2.02	0.41
1:E:1011:MET:O	1:E:1015:THR:HG23	2.20	0.41
1:F:977:MET:HE2	1:F:977:MET:HB3	1.86	0.41
1:F:1032:ARG:HD2	1:F:1032:ARG:HA	1.93	0.41
1:A:542:LEU:O	1:A:545:TYR:HB3	2.21	0.41
1:B:649:MET:HE3	1:B:653:ARG:NH2	2.35	0.41
1:C:45:ILE:HA	1:C:128:SER:O	2.20	0.41
1:C:213:GLN:HG2	1:C:239:ARG:HG3	2.01	0.41
1:C:551:GLY:O	1:C:555:LEU:HB2	2.19	0.41
1:C:960:LEU:O	1:C:964:THR:HG23	2.20	0.41
1:D:583:THR:HG21	1:F:229:GLN:HA	2.02	0.41
1:E:520:PHE:O	1:E:523:SER:OG	2.28	0.41
1:F:850:LYS:HE2	1:F:850:LYS:HA	2.03	0.41
1:A:989:LEU:HD23	1:A:989:LEU:HA	1.88	0.41
1:B:45:ILE:HD11	1:B:107:VAL:CG1	2.51	0.41
1:B:293:LEU:HD13	1:B:294:ALA:O	2.20	0.41
1:B:546:LEU:HD23	1:B:546:LEU:HA	1.81	0.41
1:C:58:GLN:HB2	1:C:82:SER:OG	2.21	0.41
1:D:30:LEU:HD13	1:D:384:ALA:HB2	2.02	0.41
1:D:496:MET:H	1:D:496:MET:HG2	1.65	0.41
1:E:221:GLY:O	1:F:780:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:605:ASN:ND2	1:E:647:ILE:HD11	2.36	0.41
1:E:931:LEU:O	1:E:935:ILE:HG13	2.20	0.41
1:F:527:TYR:O	1:F:530:SER:OG	2.26	0.41
1:F:974:PRO:O	1:F:978:THR:HG23	2.20	0.41
1:A:184:MET:HG2	1:A:246:PHE:CZ	2.56	0.41
1:A:452:VAL:HA	1:A:880:SER:OG	2.20	0.41
1:A:508:GLY:O	1:A:509:LYS:C	2.64	0.41
1:C:725:PRO:HA	1:C:810:GLU:O	2.20	0.41
1:D:427:PRO:HD3	1:D:499:PRO:HB3	2.03	0.41
1:E:111:LEU:C	1:E:113:LEU:H	2.29	0.41
1:E:149:MET:HB2	1:E:153:ASP:HB3	2.01	0.41
1:F:158:VAL:O	1:F:163:LYS:N	2.32	0.41
1:F:166:ILE:O	1:F:172:VAL:HG21	2.20	0.41
1:F:921:LEU:HB3	1:F:922:THR:H	1.64	0.41
1:F:931:LEU:HA	1:F:931:LEU:HD23	1.76	0.41
1:A:60:THR:HG23	1:A:61:VAL:HG23	2.02	0.41
1:A:165:ALA:HB1	1:A:309:GLU:OE1	2.20	0.41
1:A:378:GLY:O	1:A:382:VAL:HG23	2.20	0.41
1:B:372:VAL:HB	1:B:373:PRO:HD3	2.03	0.41
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.55	0.41
1:B:931:LEU:HD23	1:B:931:LEU:HA	1.84	0.41
1:D:201:VAL:HA	1:D:204:ILE:HD12	2.03	0.41
1:D:610:PHE:N	1:D:628:PHE:O	2.49	0.41
1:E:84:SER:HB3	1:E:814:PRO:CB	2.51	0.41
1:E:101:ASP:OD1	1:E:101:ASP:N	2.53	0.41
1:E:310:LEU:HD21	1:E:323:ILE:HG21	2.03	0.41
1:F:21:LEU:HD23	1:F:21:LEU:HA	1.88	0.41
1:F:38:ILE:HG23	1:F:462:SER:HB3	2.02	0.41
1:F:350:LEU:HD22	1:F:350:LEU:HA	1.96	0.41
1:A:143:ILE:HG22	1:A:286:ALA:HB2	2.03	0.41
1:A:467:TYR:CE2	1:A:925:VAL:HG13	2.55	0.41
1:B:6:ILE:HG23	1:B:490:PRO:HB2	2.02	0.41
1:B:513:PHE:HD2	1:B:513:PHE:H	1.61	0.41
1:C:416:VAL:HG21	1:C:493:CYS:SG	2.61	0.41
1:C:680:PHE:HB3	1:C:863:SER:OG	2.21	0.41
1:C:787:GLY:C	1:C:789:TRP:H	2.28	0.41
1:C:795:ASP:OD2	1:C:797:GLN:HG2	2.20	0.41
1:C:921:LEU:HB3	1:C:922:THR:H	1.68	0.41
1:D:270:LEU:HD12	1:D:270:LEU:HA	1.94	0.41
1:D:284:GLN:HA	1:D:285:PRO:HD3	1.87	0.41
1:D:527:TYR:O	1:D:531:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:921:LEU:HD13	1:D:921:LEU:HA	1.94	0.41
1:E:349:ILE:O	1:E:352:PHE:HB3	2.21	0.41
1:E:564:LEU:HD12	1:E:564:LEU:HA	1.99	0.41
1:E:612:VAL:HB	1:E:626:ILE:HG13	2.02	0.41
1:E:801:PHE:O	1:E:805:SER:HB3	2.20	0.41
1:E:921:LEU:HB3	1:E:922:THR:H	1.65	0.41
1:E:945:ILE:CG1	1:E:971:ARG:HH12	2.34	0.41
1:F:32:VAL:O	1:F:298:ASN:ND2	2.51	0.41
1:F:101:ASP:OD1	1:F:101:ASP:N	2.53	0.41
1:F:336:SER:O	1:F:340:VAL:HG23	2.21	0.41
1:F:421:ALA:HB1	1:F:505:HIS:H	1.86	0.41
1:F:584:GLN:N	1:F:622:GLN:HB3	2.36	0.41
1:C:444:GLY:O	1:C:448:VAL:HG12	2.20	0.41
1:C:588:GLN:NE2	1:C:592:ASN:OD1	2.54	0.41
1:D:70:ASN:HB2	1:F:167:SER:OG	2.20	0.41
1:D:228:GLN:NE2	1:D:230:LEU:O	2.52	0.41
1:D:502:LYS:H	1:D:502:LYS:HG3	1.62	0.41
1:D:869:SER:OG	1:D:870:GLY:N	2.53	0.41
1:E:456:MET:CG	1:E:471:SER:HB2	2.51	0.41
1:E:818:ARG:HH12	1:E:823:PRO:HG3	1.86	0.41
1:E:931:LEU:HD23	1:E:931:LEU:HA	1.88	0.41
1:E:959:GLY:HA2	1:E:1039:ASP:HA	2.03	0.41
1:F:525:HIS:O	1:F:528:THR:HG22	2.21	0.41
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.21	0.41
1:A:356:TYR:HD1	1:A:365:THR:HG21	1.86	0.40
1:A:445:ILE:HD13	1:A:940:LYS:NZ	2.36	0.40
1:A:828:LEU:HD23	1:A:828:LEU:HA	1.86	0.40
1:B:219:LEU:HD12	1:B:232:ALA:HB3	2.03	0.40
1:B:559:LEU:HD12	1:B:923:ASN:HB2	2.02	0.40
1:B:727:PHE:CZ	1:B:807:SER:HB2	2.56	0.40
1:C:375:VAL:HG22	1:C:484:VAL:HG21	2.02	0.40
1:D:35:TYR:CE2	1:D:564:LEU:HD11	2.56	0.40
1:D:101:ASP:OD1	1:D:101:ASP:N	2.53	0.40
1:D:139:VAL:HB	1:D:327:TYR:HB3	2.02	0.40
1:D:463:THR:O	1:D:467:TYR:HD1	2.04	0.40
1:E:418:ARG:HD2	1:E:422:GLU:HG3	2.03	0.40
1:E:743:ILE:H	1:E:743:ILE:HG12	1.50	0.40
1:F:527:TYR:CE2	1:F:968:VAL:HG13	2.56	0.40
1:F:614:GLY:HA2	1:F:621:GLY:O	2.22	0.40
1:A:101:ASP:OD1	1:A:101:ASP:N	2.51	0.40
1:A:105:VAL:HG11	1:B:105:VAL:CG2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ILE:HG22	1:A:166:ILE:O	2.21	0.40
1:A:482:VAL:O	1:A:486:LEU:HG	2.21	0.40
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.56	0.40
1:B:433:LYS:O	1:B:437:GLN:HG3	2.21	0.40
1:B:572:PHE:CD2	1:B:631:LEU:HD11	2.56	0.40
1:C:418:ARG:HE	1:C:970:MET:HB2	1.86	0.40
1:C:438:ILE:O	1:C:442:LEU:HG	2.20	0.40
1:C:754:TRP:CZ2	1:C:780:ARG:HA	2.56	0.40
1:D:372:VAL:HB	1:D:373:PRO:HD3	2.03	0.40
1:D:715:SER:O	1:D:717:ARG:HG2	2.21	0.40
1:D:850:LYS:HD2	1:D:850:LYS:N	2.36	0.40
1:D:929:VAL:O	1:D:932:LEU:HB2	2.22	0.40
1:F:45:ILE:HD13	1:F:111:LEU:HG	2.01	0.40
1:F:210:GLN:HG3	1:F:249:ILE:HG23	2.03	0.40
1:F:414:GLU:HG2	1:F:973:ARG:HD3	2.03	0.40
1:F:493:CYS:O	1:F:497:LEU:HB3	2.22	0.40
1:A:524:THR:O	1:A:528:THR:OG1	2.38	0.40
1:A:532:GLY:O	1:A:536:ARG:HG2	2.21	0.40
1:A:1011:MET:HE3	1:A:1011:MET:HB3	1.87	0.40
1:B:355:MET:HE3	1:B:355:MET:HA	2.02	0.40
1:B:1035:ARG:O	1:B:1038:GLU:HG3	2.21	0.40
1:C:776:GLU:HG2	1:C:777:ALA:H	1.87	0.40
1:C:961:ILE:HG13	1:C:962:GLU:H	1.86	0.40
1:D:459:PHE:HZ	1:D:873:ALA:HB2	1.86	0.40
1:D:574:THR:HG23	1:D:627:ALA:HB3	2.04	0.40
1:D:723:ASP:HA	1:D:813:SER:HA	2.04	0.40
1:D:960:LEU:O	1:D:964:THR:HG23	2.22	0.40
1:D:979:SER:HB2	1:D:1015:THR:HG21	2.03	0.40
1:E:126:GLY:HA2	1:F:116:PRO:CG	2.52	0.40
1:E:448:VAL:O	1:E:452:VAL:HG13	2.21	0.40
1:F:13:TRP:HH2	1:F:370:ILE:HD13	1.86	0.40
1:F:119:PRO:HB2	1:F:122:VAL:HG23	2.02	0.40
1:A:196:PHE:O	1:A:252:LYS:NZ	2.39	0.40
1:A:348:ILE:HG12	1:A:372:VAL:HG11	2.04	0.40
1:A:851:LEU:HA	1:A:852:PRO:HD3	1.84	0.40
1:A:919:ARG:NH1	1:A:990:VAL:O	2.54	0.40
1:A:1016:VAL:HG13	2:A:2000:LMT:H102	2.03	0.40
1:B:184:MET:HE3	1:B:184:MET:HA	2.03	0.40
1:B:680:PHE:HZ	1:B:844:MET:HG2	1.86	0.40
1:C:58:GLN:O	1:C:62:THR:HB	2.21	0.40
1:C:101:ASP:N	1:C:101:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:SER:O	1:C:391:ASN:ND2	2.55	0.40
1:C:398:MET:HB3	1:C:398:MET:HE3	1.85	0.40
1:C:398:MET:HA	1:C:401:ALA:HB3	2.04	0.40
1:C:527:TYR:CD2	1:C:972:LEU:HG	2.57	0.40
1:D:643:LYS:HG3	1:D:644:VAL:N	2.35	0.40
1:E:643:LYS:NZ	1:E:993:THR:HG21	2.36	0.40
1:F:176:GLN:NE2	1:F:177:LEU:O	2.53	0.40
1:F:680:PHE:HB2	1:F:859:TRP:CZ3	2.57	0.40
1:F:885:PHE:HB2	1:F:902:MET:SD	2.62	0.40
1:F:888:LEU:HD21	1:F:943:ILE:CD1	2.52	0.40
1:A:186:ILE:HB	1:A:773:VAL:HG22	2.02	0.40
1:A:492:LEU:O	1:A:496:MET:HG2	2.20	0.40
1:B:24:GLY:O	1:B:27:ILE:HG22	2.21	0.40
1:B:776:GLU:HB3	1:B:779:TYR:HD1	1.86	0.40
1:C:870:GLY:C	1:C:872:GLN:N	2.79	0.40
1:C:932:LEU:HD23	1:C:932:LEU:HA	1.81	0.40
1:D:363:ARG:H	1:D:363:ARG:HG2	1.63	0.40
1:D:695:LEU:HD23	1:D:695:LEU:HA	1.83	0.40
1:E:38:ILE:HG22	1:E:462:SER:HB3	2.03	0.40
1:E:270:LEU:HD12	1:E:270:LEU:HA	1.95	0.40
1:E:1011:MET:HE3	1:E:1011:MET:HB3	1.87	0.40
1:F:159:ALA:HB2	1:F:177:LEU:CD1	2.52	0.40
1:F:365:THR:O	1:F:368:PRO:HD2	2.22	0.40

There are no symmetry-related clashes.

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	1042/1069 (98%)	908 (87%)	115 (11%)	19 (2%)	6	34
1	B	1040/1069 (97%)	909 (87%)	116 (11%)	15 (1%)	9	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1042/1069 (98%)	898 (86%)	128 (12%)	16 (2%)	8	37
1	D	1042/1069 (98%)	904 (87%)	123 (12%)	15 (1%)	9	38
1	E	1040/1069 (97%)	913 (88%)	120 (12%)	7 (1%)	18	51
1	F	1042/1069 (98%)	905 (87%)	126 (12%)	11 (1%)	11	43
All	All	6248/6414 (97%)	5437 (87%)	728 (12%)	83 (1%)	9	40

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	SER
1	A	167	SER
1	A	833	PRO
1	A	871	ASN
1	A	893	GLU
1	A	1036	LYS
1	B	326	PRO
1	B	671	ILE
1	B	871	ASN
1	B	893	GLU
1	B	1034	SER
1	C	123	GLN
1	C	1039	ASP
1	D	133	SER
1	D	833	PRO
1	D	872	GLN
1	D	893	GLU
1	D	1036	LYS
1	D	1037	ASN
1	D	1039	ASP
1	E	671	ILE
1	E	675	GLY
1	E	893	GLU
1	E	1034	SER
1	F	510	LYS
1	F	788	ASP
1	F	833	PRO
1	A	148	THR
1	A	170	SER
1	A	502	LYS
1	A	638	PRO
1	A	639	GLY

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Mol	Chain	Res	Type
1	A	788	ASP
1	B	508	GLY
1	B	788	ASP
1	C	3	ASN
1	C	638	PRO
1	C	788	ASP
1	C	871	ASN
1	D	502	LYS
1	D	507	GLU
1	E	508	GLY
1	E	788	ASP
1	F	147	GLY
1	F	502	LYS
1	A	1043	SER
1	B	164	ASP
1	C	508	GLY
1	C	674	LEU
1	C	1034	SER
1	C	1043	SER
1	D	148	THR
1	D	673	GLU
1	D	788	ASP
1	F	870	GLY
1	A	494	ALA
1	A	509	LYS
1	B	327	TYR
1	C	503	GLY
1	F	507	GLU
1	F	814	PRO
1	A	834	GLY
1	A	1042	HIS
1	B	672	VAL
1	B	677	ALA
1	B	678	THR
1	C	146	ASP
1	C	502	LYS
1	C	1041	GLU
1	E	673	GLU
1	F	123	GLN
1	F	326	PRO
1	C	326	PRO
1	D	676	THR

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Mol	Chain	Res	Type
1	F	148	THR
1	B	870	GLY
1	B	71	GLY
1	B	691	GLY
1	A	326	PRO
1	D	326	PRO
1	A	796	GLY
1	C	796	GLY
1	D	675	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	850/872 (98%)	784 (92%)	66 (8%)	11	37
1	B	848/872 (97%)	776 (92%)	72 (8%)	10	35
1	C	850/872 (98%)	782 (92%)	68 (8%)	11	36
1	D	850/872 (98%)	790 (93%)	60 (7%)	13	40
1	E	848/872 (97%)	782 (92%)	66 (8%)	11	37
1	F	850/872 (98%)	776 (91%)	74 (9%)	9	34
All	All	5096/5232 (97%)	4690 (92%)	406 (8%)	11	36

All (406) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	27	ILE
1	A	60	THR
1	A	88	VAL
1	A	90	ILE
1	A	106	GLN
1	A	107	VAL
1	A	109	ASN
1	A	110	LYS

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Mol	Chain	Res	Type
1	A	135	SER
1	A	146	ASP
1	A	152	GLU
1	A	153	ASP
1	A	177	LEU
1	A	193	LEU
1	A	225	VAL
1	A	243	THR
1	A	293	LEU
1	A	321	LEU
1	A	337	ILE
1	A	350	LEU
1	A	353	LEU
1	A	360	GLN
1	A	362	PHE
1	A	400	LEU
1	A	445	ILE
1	A	452	VAL
1	A	459	PHE
1	A	474	ILE
1	A	493	CYS
1	A	528	THR
1	A	555	LEU
1	A	567	GLU
1	A	573	MET
1	A	602	GLU
1	A	615	PHE
1	A	620	LYS
1	A	623	ASN
1	A	624	THR
1	A	626	ILE
1	A	630	SER
1	A	632	LYS
1	A	634	TRP
1	A	645	GLU
1	A	662	MET
1	A	666	PHE
1	A	671	ILE
1	A	673	GLU
1	A	693	GLU
1	A	696	THR
1	A	713	LEU

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Mol	Chain	Res	Type
1	A	739	LEU
1	A	743	ILE
1	A	786	ILE
1	A	791	VAL
1	A	826	GLU
1	A	828	LEU
1	A	843	LEU
1	A	888	LEU
1	A	897	ILE
1	A	943	ILE
1	A	958	LYS
1	A	1016	VAL
1	A	1034	SER
1	A	1035	ARG
1	A	1038	GLU
1	B	3	ASN
1	B	10	ILE
1	B	25	LEU
1	B	27	ILE
1	B	73	ASP
1	B	90	ILE
1	B	105	VAL
1	B	106	GLN
1	B	118	LEU
1	B	135	SER
1	B	153	ASP
1	B	164	ASP
1	B	172	VAL
1	B	177	LEU
1	B	193	LEU
1	B	205	THR
1	B	213	GLN
1	B	243	THR
1	B	255	GLN
1	B	278	ILE
1	B	293	LEU
1	B	310	LEU
1	B	337	ILE
1	B	350	LEU
1	B	353	LEU
1	B	392	THR
1	B	400	LEU

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Mol	Chain	Res	Type
1	B	405	LEU
1	B	406	VAL
1	B	452	VAL
1	B	459	PHE
1	B	470	PHE
1	B	484	VAL
1	B	513	PHE
1	B	522	LYS
1	B	528	THR
1	B	540	ARG
1	B	546	LEU
1	B	555	LEU
1	B	592	ASN
1	B	602	GLU
1	B	624	THR
1	B	626	ILE
1	B	630	SER
1	B	634	TRP
1	B	645	GLU
1	B	662	MET
1	B	666	PHE
1	B	673	GLU
1	B	676	THR
1	B	680	PHE
1	B	713	LEU
1	B	743	ILE
1	B	786	ILE
1	B	788	ASP
1	B	791	VAL
1	B	804	PHE
1	B	826	GLU
1	B	828	LEU
1	B	843	LEU
1	B	844	MET
1	B	865	GLN
1	B	879	ILE
1	B	891	LEU
1	B	892	TYR
1	B	904	VAL
1	B	914	LEU
1	B	943	ILE
1	B	1016	VAL

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Mol	Chain	Res	Type
1	B	1034	SER
1	B	1035	ARG
1	B	1037	ASN
1	C	27	ILE
1	C	43	VAL
1	C	68	ASN
1	C	77	TYR
1	C	81	ASN
1	C	88	VAL
1	C	92	LEU
1	C	107	VAL
1	C	110	LYS
1	C	111	LEU
1	C	135	SER
1	C	153	ASP
1	C	177	LEU
1	C	193	LEU
1	C	213	GLN
1	C	274	ASN
1	C	276	ASP
1	C	293	LEU
1	C	301	ASP
1	C	307	ARG
1	C	321	LEU
1	C	323	ILE
1	C	337	ILE
1	C	353	LEU
1	C	360	GLN
1	C	366	LEU
1	C	400	LEU
1	C	407	ASP
1	C	417	GLU
1	C	418	ARG
1	C	445	ILE
1	C	452	VAL
1	C	474	ILE
1	C	493	CYS
1	C	515	TRP
1	C	528	THR
1	C	546	LEU
1	C	555	LEU
1	C	559	LEU

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Mol	Chain	Res	Type
1	C	587	THR
1	C	601	LYS
1	C	602	GLU
1	C	630	SER
1	C	634	TRP
1	C	673	GLU
1	C	674	LEU
1	C	680	PHE
1	C	694	LYS
1	C	708	LYS
1	C	713	LEU
1	C	743	ILE
1	C	786	ILE
1	C	791	VAL
1	C	816	LEU
1	C	843	LEU
1	C	847	LEU
1	C	850	LYS
1	C	865	GLN
1	C	871	ASN
1	C	876	LEU
1	C	893	GLU
1	C	914	LEU
1	C	953	MET
1	C	977	MET
1	C	978	THR
1	C	1016	VAL
1	C	1029	VAL
1	C	1034	SER
1	D	27	ILE
1	D	55	LYS
1	D	88	VAL
1	D	90	ILE
1	D	102	ILE
1	D	107	VAL
1	D	109	ASN
1	D	118	LEU
1	D	153	ASP
1	D	177	LEU
1	D	225	VAL
1	D	276	ASP
1	D	278	ILE

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Mol	Chain	Res	Type
1	D	293	LEU
1	D	301	ASP
1	D	321	LEU
1	D	337	ILE
1	D	350	LEU
1	D	353	LEU
1	D	362	PHE
1	D	363	ARG
1	D	386	PHE
1	D	400	LEU
1	D	418	ARG
1	D	452	VAL
1	D	459	PHE
1	D	493	CYS
1	D	502	LYS
1	D	538	THR
1	D	542	LEU
1	D	555	LEU
1	D	585	GLU
1	D	602	GLU
1	D	623	ASN
1	D	626	ILE
1	D	634	TRP
1	D	643	LYS
1	D	662	MET
1	D	671	ILE
1	D	673	GLU
1	D	678	THR
1	D	693	GLU
1	D	703	LEU
1	D	708	LYS
1	D	711	ASP
1	D	713	LEU
1	D	786	ILE
1	D	791	VAL
1	D	826	GLU
1	D	828	LEU
1	D	843	LEU
1	D	850	LYS
1	D	891	LEU
1	D	900	SER
1	D	943	ILE

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Mol	Chain	Res	Type
1	D	971	ARG
1	D	977	MET
1	D	1029	VAL
1	D	1038	GLU
1	D	1041	GLU
1	E	4	PHE
1	E	17	ILE
1	E	27	ILE
1	E	43	VAL
1	E	45	ILE
1	E	88	VAL
1	E	90	ILE
1	E	102	ILE
1	E	107	VAL
1	E	135	SER
1	E	144	ASN
1	E	153	ASP
1	E	164	ASP
1	E	167	SER
1	E	176	GLN
1	E	177	LEU
1	E	182	TYR
1	E	193	LEU
1	E	213	GLN
1	E	225	VAL
1	E	250	LEU
1	E	255	GLN
1	E	277	ILE
1	E	293	LEU
1	E	337	ILE
1	E	353	LEU
1	E	390	ILE
1	E	400	LEU
1	E	404	LEU
1	E	418	ARG
1	E	423	GLU
1	E	445	ILE
1	E	452	VAL
1	E	459	PHE
1	E	474	ILE
1	E	513	PHE
1	E	544	LEU

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Mol	Chain	Res	Type
1	E	555	LEU
1	E	592	ASN
1	E	601	LYS
1	E	602	GLU
1	E	632	LYS
1	E	634	TRP
1	E	659	LYS
1	E	662	MET
1	E	666	PHE
1	E	668	LEU
1	E	671	ILE
1	E	673	GLU
1	E	713	LEU
1	E	717	ARG
1	E	743	ILE
1	E	786	ILE
1	E	788	ASP
1	E	791	VAL
1	E	804	PHE
1	E	816	LEU
1	E	828	LEU
1	E	843	LEU
1	E	877	TYR
1	E	1016	VAL
1	E	1034	SER
1	E	1035	ARG
1	E	1038	GLU
1	E	1040	ILE
1	E	1041	GLU
1	F	3	ASN
1	F	6	ILE
1	F	27	ILE
1	F	43	VAL
1	F	67	GLN
1	F	72	ILE
1	F	77	TYR
1	F	92	LEU
1	F	93	THR
1	F	104	GLN
1	F	107	VAL
1	F	153	ASP
1	F	167	SER

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Mol	Chain	Res	Type
1	F	177	LEU
1	F	193	LEU
1	F	205	THR
1	F	225	VAL
1	F	263	ARG
1	F	278	ILE
1	F	293	LEU
1	F	321	LEU
1	F	323	ILE
1	F	336	SER
1	F	350	LEU
1	F	353	LEU
1	F	360	GLN
1	F	363	ARG
1	F	389	SER
1	F	400	LEU
1	F	428	LYS
1	F	452	VAL
1	F	463	THR
1	F	482	VAL
1	F	528	THR
1	F	555	LEU
1	F	562	SER
1	F	587	THR
1	F	602	GLU
1	F	623	ASN
1	F	624	THR
1	F	626	ILE
1	F	630	SER
1	F	632	LYS
1	F	634	TRP
1	F	644	VAL
1	F	649	MET
1	F	666	PHE
1	F	668	LEU
1	F	674	LEU
1	F	678	THR
1	F	681	ASP
1	F	692	HIS
1	F	694	LYS
1	F	708	LYS
1	F	713	LEU

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Mol	Chain	Res	Type
1	F	743	ILE
1	F	759	VAL
1	F	774	MET
1	F	786	ILE
1	F	791	VAL
1	F	808	ARG
1	F	816	LEU
1	F	826	GLU
1	F	843	LEU
1	F	871	ASN
1	F	876	LEU
1	F	881	LEU
1	F	947	GLU
1	F	950	LYS
1	F	977	MET
1	F	1003	VAL
1	F	1011	MET
1	F	1016	VAL
1	F	1035	ARG

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	58	GLN
1	A	74	ASN
1	A	106	GLN
1	A	108	GLN
1	A	211	ASN
1	A	274	ASN
1	A	284	GLN
1	A	505	HIS
1	A	588	GLN
1	A	592	ASN
1	A	667	ASN
1	A	928	GLN
1	B	74	ASN
1	B	109	ASN
1	B	161	ASN
1	B	415	ASN
1	B	437	GLN
1	B	596	HIS
1	B	667	ASN

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Mol	Chain	Res	Type
1	B	865	GLN
1	C	67	GLN
1	C	120	GLN
1	C	123	GLN
1	C	213	GLN
1	C	525	HIS
1	C	584	GLN
1	C	737	GLN
1	C	760	ASN
1	C	865	GLN
1	D	67	GLN
1	D	125	GLN
1	D	144	ASN
1	D	161	ASN
1	D	284	GLN
1	D	760	ASN
1	D	872	GLN
1	D	1037	ASN
1	E	74	ASN
1	E	106	GLN
1	E	108	GLN
1	E	161	ASN
1	E	189	ASN
1	E	284	GLN
1	E	596	HIS
1	E	865	GLN
1	F	58	GLN
1	F	68	ASN
1	F	104	GLN
1	F	109	ASN
1	F	161	ASN
1	F	211	ASN
1	F	525	HIS
1	F	737	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	2000	-	36,36,36	1.71	10 (27%)	47,47,47	1.30	4 (8%)
2	LMT	C	2000	-	36,36,36	1.75	10 (27%)	47,47,47	1.27	4 (8%)
2	LMT	B	2000	-	36,36,36	1.74	9 (25%)	47,47,47	0.97	3 (6%)
2	LMT	D	2000	-	36,36,36	1.76	9 (25%)	47,47,47	0.94	1 (2%)
2	LMT	E	2000	-	36,36,36	1.73	9 (25%)	47,47,47	1.22	6 (12%)
2	LMT	A	2000	-	36,36,36	1.74	9 (25%)	47,47,47	1.25	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	2000	-	3/3/10/10	13/21/61/61	0/2/2/2
2	LMT	C	2000	-	3/3/10/10	7/21/61/61	0/2/2/2
2	LMT	B	2000	-	2/2/10/10	11/21/61/61	0/2/2/2
2	LMT	D	2000	-	2/2/10/10	13/21/61/61	0/2/2/2
2	LMT	E	2000	-	5/5/10/10	10/21/61/61	0/2/2/2
2	LMT	A	2000	-	2/2/10/10	9/21/61/61	0/2/2/2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2000	LMT	O5'-C5'	4.00	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	LMT	O5'-C5'	3.92	1.53	1.44
2	E	2000	LMT	O5'-C5'	3.88	1.53	1.44
2	C	2000	LMT	O5'-C5'	3.81	1.53	1.44
2	A	2000	LMT	O5'-C5'	3.78	1.53	1.44
2	F	2000	LMT	O5'-C5'	3.70	1.53	1.44
2	A	2000	LMT	O1'-C1'	3.69	1.46	1.40
2	F	2000	LMT	O1'-C1'	3.52	1.46	1.40
2	C	2000	LMT	O1'-C1'	3.49	1.46	1.40
2	C	2000	LMT	O5B-C1B	3.49	1.50	1.41
2	E	2000	LMT	O1'-C1'	3.49	1.46	1.40
2	B	2000	LMT	O5B-C1B	3.45	1.50	1.41
2	A	2000	LMT	O5B-C1B	3.45	1.50	1.41
2	D	2000	LMT	O1'-C1'	3.37	1.45	1.40
2	B	2000	LMT	O1'-C1'	3.37	1.45	1.40
2	D	2000	LMT	O5B-C1B	3.35	1.50	1.41
2	F	2000	LMT	O5B-C1B	3.34	1.50	1.41
2	E	2000	LMT	O5B-C1B	3.26	1.50	1.41
2	D	2000	LMT	C6'-C5'	-3.25	1.40	1.51
2	A	2000	LMT	C6'-C5'	-3.24	1.40	1.51
2	C	2000	LMT	C6'-C5'	-3.22	1.41	1.51
2	B	2000	LMT	O5'-C1'	3.20	1.50	1.41
2	E	2000	LMT	C6'-C5'	-3.20	1.41	1.51
2	D	2000	LMT	O5'-C1'	3.10	1.49	1.41
2	C	2000	LMT	O5'-C1'	3.08	1.49	1.41
2	B	2000	LMT	C6'-C5'	-3.08	1.41	1.51
2	F	2000	LMT	C6'-C5'	-3.06	1.41	1.51
2	F	2000	LMT	O5'-C1'	2.98	1.49	1.41
2	E	2000	LMT	O3B-C3B	2.81	1.49	1.43
2	E	2000	LMT	O5'-C1'	2.79	1.49	1.41
2	C	2000	LMT	O3B-C3B	2.79	1.49	1.43
2	B	2000	LMT	O3B-C3B	2.77	1.49	1.43
2	F	2000	LMT	O3B-C3B	2.77	1.49	1.43
2	D	2000	LMT	O3B-C3B	2.76	1.49	1.43
2	A	2000	LMT	O3B-C3B	2.76	1.49	1.43
2	A	2000	LMT	O5'-C1'	2.75	1.48	1.41
2	D	2000	LMT	C3'-C2'	-2.69	1.45	1.52
2	E	2000	LMT	C3'-C2'	-2.48	1.45	1.52
2	C	2000	LMT	C3'-C2'	-2.39	1.46	1.52
2	B	2000	LMT	C3'-C2'	-2.28	1.46	1.52
2	F	2000	LMT	O2'-C2'	2.25	1.48	1.43
2	A	2000	LMT	O2'-C2'	2.23	1.48	1.43
2	B	2000	LMT	O2'-C2'	2.21	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2000	LMT	O2'-C2'	2.20	1.48	1.43
2	A	2000	LMT	C3'-C2'	-2.19	1.46	1.52
2	D	2000	LMT	O2'-C2'	2.12	1.48	1.43
2	C	2000	LMT	C3B-C2B	-2.08	1.46	1.52
2	E	2000	LMT	C5-C4	2.06	1.62	1.51
2	A	2000	LMT	C5-C4	2.04	1.61	1.51
2	E	2000	LMT	O2'-C2'	2.03	1.48	1.43
2	C	2000	LMT	C5-C4	2.03	1.61	1.51
2	F	2000	LMT	C5-C4	2.02	1.61	1.51
2	F	2000	LMT	C3B-C2B	-2.02	1.47	1.52
2	F	2000	LMT	C3'-C2'	-2.01	1.47	1.52
2	D	2000	LMT	C5-C4	2.01	1.61	1.51
2	B	2000	LMT	C5-C4	2.00	1.61	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2000	LMT	C2'-C3'-C4'	4.81	120.59	109.68
2	C	2000	LMT	O5B-C5B-C4B	4.07	117.03	109.70
2	A	2000	LMT	C3'-C4'-C5'	3.90	119.58	110.93
2	C	2000	LMT	C3B-C4B-C5B	3.90	117.30	110.23
2	A	2000	LMT	C2'-C3'-C4'	3.77	118.23	109.68
2	F	2000	LMT	C3'-C4'-C5'	3.67	119.06	110.93
2	C	2000	LMT	C1B-O1B-C4'	-3.51	109.66	117.98
2	E	2000	LMT	C3'-C4'-C5'	3.42	118.52	110.93
2	D	2000	LMT	C1B-O1B-C4'	-3.39	109.94	117.98
2	F	2000	LMT	C1'-C2'-C3'	3.15	116.63	110.01
2	A	2000	LMT	C1B-O1B-C4'	-2.93	111.03	117.98
2	E	2000	LMT	C1B-O1B-C4'	-2.93	111.04	117.98
2	B	2000	LMT	C1B-O1B-C4'	-2.81	111.31	117.98
2	E	2000	LMT	C4B-C3B-C2B	2.62	115.43	110.83
2	E	2000	LMT	C2'-C3'-C4'	2.59	115.56	109.68
2	A	2000	LMT	O1'-C1'-C2'	2.49	112.05	108.27
2	B	2000	LMT	O5'-C5'-C6'	2.31	112.17	106.44
2	B	2000	LMT	C2'-C3'-C4'	2.27	114.82	109.68
2	C	2000	LMT	C4B-C3B-C2B	2.26	114.79	110.83
2	F	2000	LMT	C1B-O1B-C4'	-2.22	112.71	117.98
2	E	2000	LMT	C1B-C2B-C3B	2.13	114.48	110.01
2	E	2000	LMT	O1'-C1'-C2'	2.05	111.38	108.27

All (17) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2000	LMT	C4B
2	A	2000	LMT	C3'
2	B	2000	LMT	C4B
2	B	2000	LMT	C3'
2	C	2000	LMT	C4B
2	C	2000	LMT	C2'
2	C	2000	LMT	C3'
2	D	2000	LMT	C4B
2	D	2000	LMT	C3'
2	E	2000	LMT	C4B
2	E	2000	LMT	C5B
2	E	2000	LMT	C2B
2	E	2000	LMT	C1B
2	E	2000	LMT	C3'
2	F	2000	LMT	C4B
2	F	2000	LMT	C2B
2	F	2000	LMT	C1B

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2000	LMT	C2-C1-O1'-C1'
2	C	2000	LMT	O5B-C5B-C6B-O6B
2	E	2000	LMT	O5B-C5B-C6B-O6B
2	C	2000	LMT	C4B-C5B-C6B-O6B
2	F	2000	LMT	O5B-C5B-C6B-O6B
2	A	2000	LMT	O5'-C5'-C6'-O6'
2	F	2000	LMT	O5'-C5'-C6'-O6'
2	D	2000	LMT	O5'-C1'-O1'-C1
2	B	2000	LMT	O5'-C5'-C6'-O6'
2	D	2000	LMT	O5'-C5'-C6'-O6'
2	F	2000	LMT	C5'-C4'-O1B-C1B
2	F	2000	LMT	C4'-C5'-C6'-O6'
2	A	2000	LMT	C4'-C5'-C6'-O6'
2	A	2000	LMT	C2'-C1'-O1'-C1
2	D	2000	LMT	C2'-C1'-O1'-C1
2	B	2000	LMT	C4'-C5'-C6'-O6'
2	E	2000	LMT	C4B-C5B-C6B-O6B
2	D	2000	LMT	C4'-C5'-C6'-O6'
2	B	2000	LMT	C7-C8-C9-C10
2	C	2000	LMT	C7-C8-C9-C10
2	F	2000	LMT	C3'-C4'-O1B-C1B
2	E	2000	LMT	C4'-C5'-C6'-O6'

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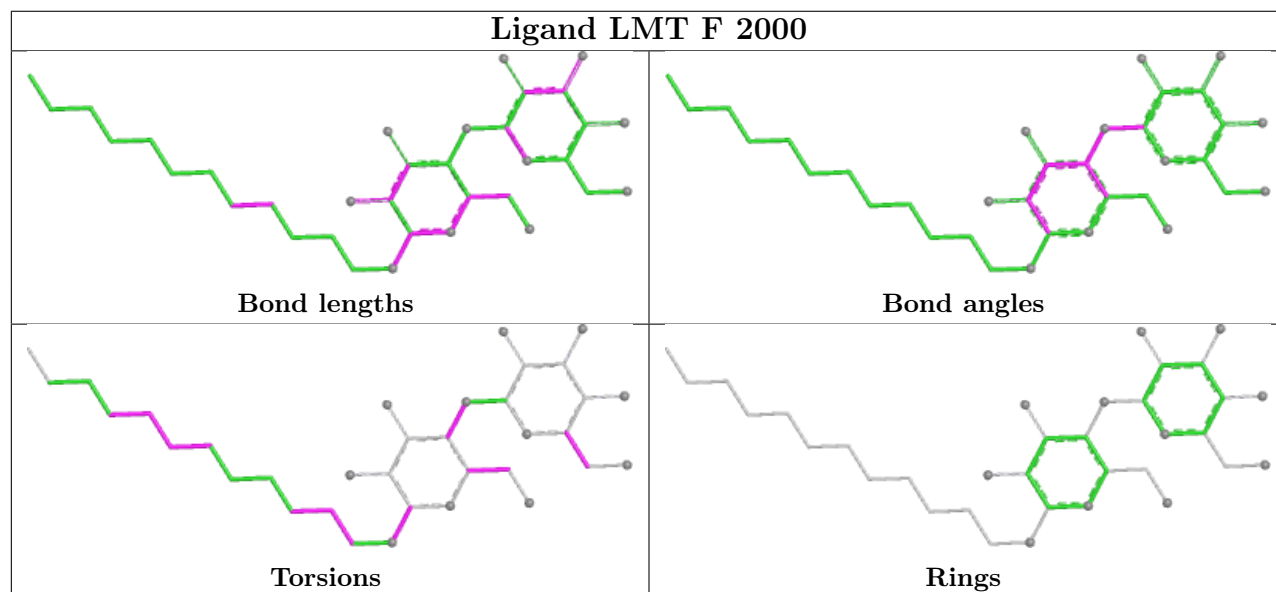
Mol	Chain	Res	Type	Atoms
2	F	2000	LMT	C7-C8-C9-C10
2	A	2000	LMT	O1'-C1-C2-C3
2	D	2000	LMT	C4B-C5B-C6B-O6B
2	C	2000	LMT	O1'-C1-C2-C3
2	B	2000	LMT	O1'-C1-C2-C3
2	E	2000	LMT	O5'-C5'-C6'-O6'
2	F	2000	LMT	C2'-C1'-O1'-C1
2	F	2000	LMT	C4B-C5B-C6B-O6B
2	B	2000	LMT	O5'-C1'-O1'-C1
2	D	2000	LMT	O1'-C1-C2-C3
2	D	2000	LMT	C2-C1-O1'-C1'
2	E	2000	LMT	C2-C1-O1'-C1'
2	D	2000	LMT	C1-C2-C3-C4
2	D	2000	LMT	O5B-C5B-C6B-O6B
2	C	2000	LMT	C2-C3-C4-C5
2	E	2000	LMT	C1-C2-C3-C4
2	F	2000	LMT	C5-C6-C7-C8
2	E	2000	LMT	C3-C4-C5-C6
2	C	2000	LMT	C1-C2-C3-C4
2	E	2000	LMT	C2'-C1'-O1'-C1
2	B	2000	LMT	O5B-C5B-C6B-O6B
2	A	2000	LMT	C6-C7-C8-C9
2	D	2000	LMT	C6-C7-C8-C9
2	A	2000	LMT	C4-C5-C6-C7
2	A	2000	LMT	C11-C10-C9-C8
2	A	2000	LMT	C2-C1-O1'-C1'
2	B	2000	LMT	C1-C2-C3-C4
2	F	2000	LMT	O5'-C1'-O1'-C1
2	E	2000	LMT	C7-C8-C9-C10
2	F	2000	LMT	O1'-C1-C2-C3
2	B	2000	LMT	C2-C3-C4-C5
2	F	2000	LMT	C6-C7-C8-C9
2	B	2000	LMT	C5'-C4'-O1B-C1B
2	D	2000	LMT	C3'-C4'-O1B-C1B
2	D	2000	LMT	C5-C6-C7-C8
2	F	2000	LMT	C1-C2-C3-C4
2	E	2000	LMT	C2-C3-C4-C5
2	B	2000	LMT	C3'-C4'-O1B-C1B
2	A	2000	LMT	C4B-C5B-C6B-O6B
2	C	2000	LMT	C4-C5-C6-C7
2	D	2000	LMT	C5'-C4'-O1B-C1B

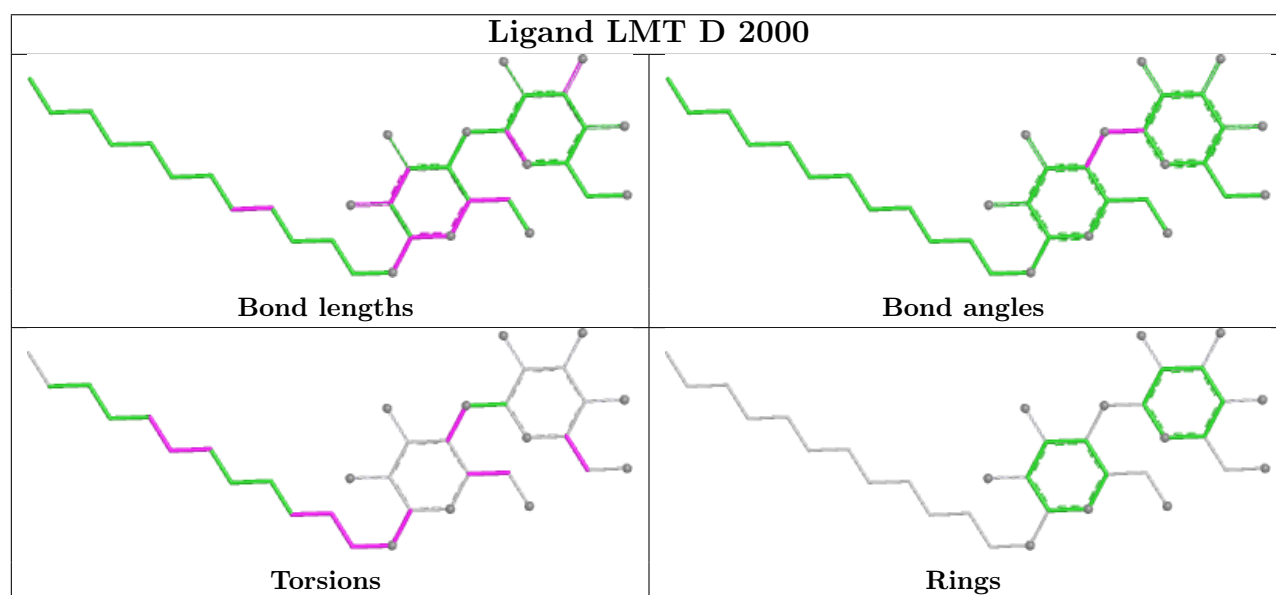
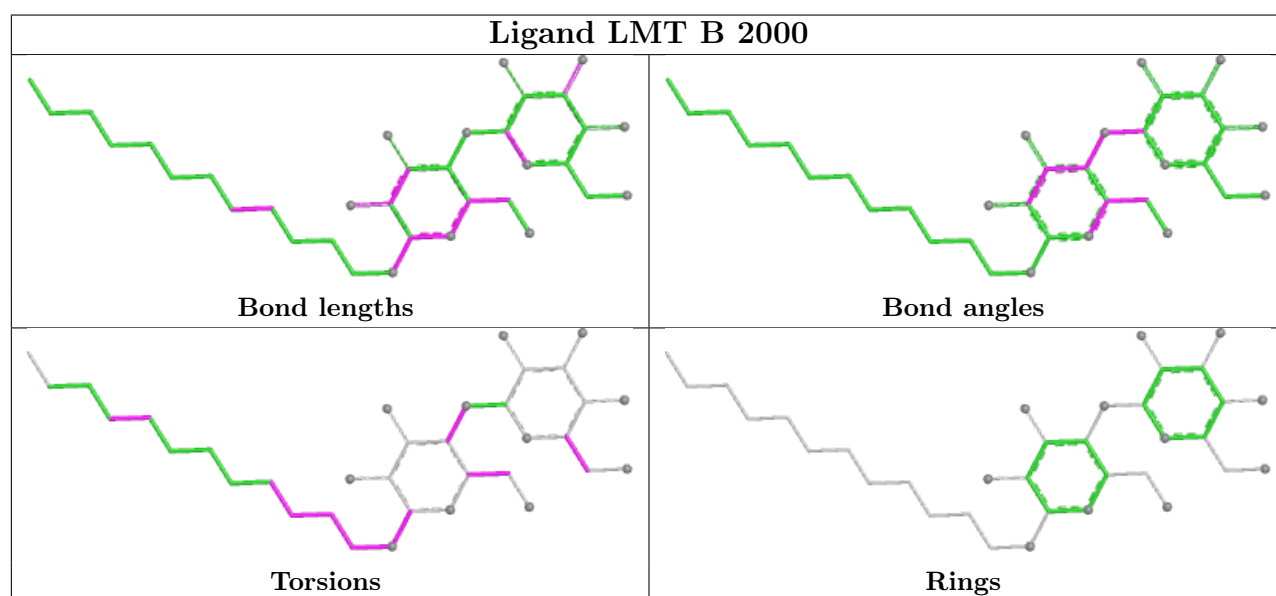
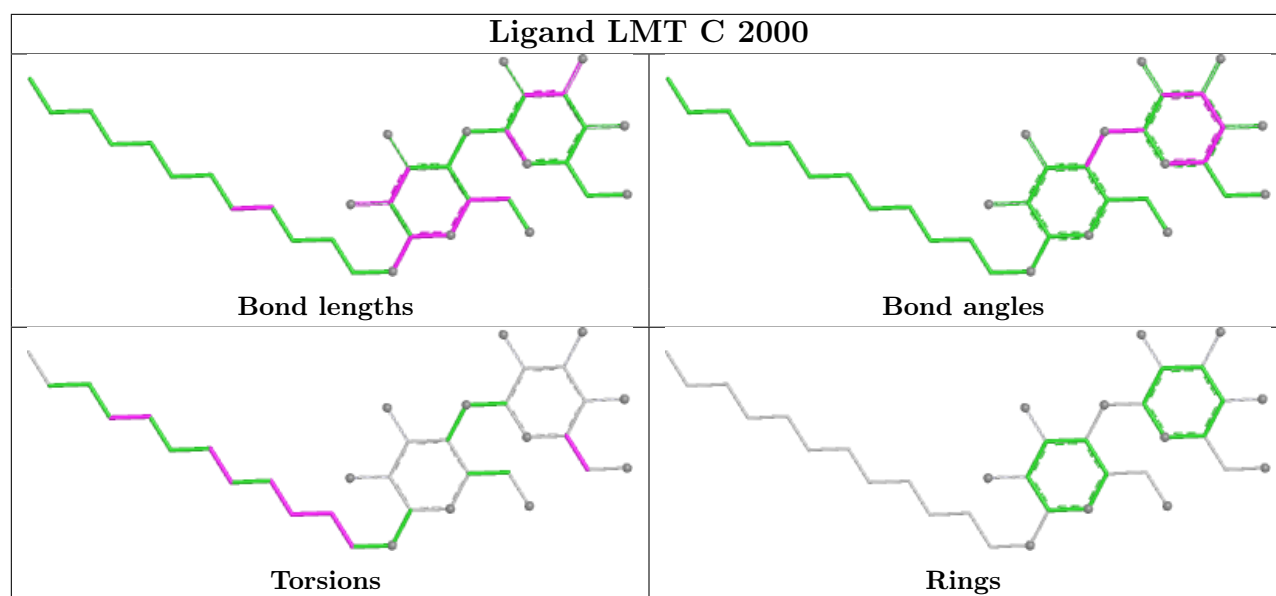
There are no ring outliers.

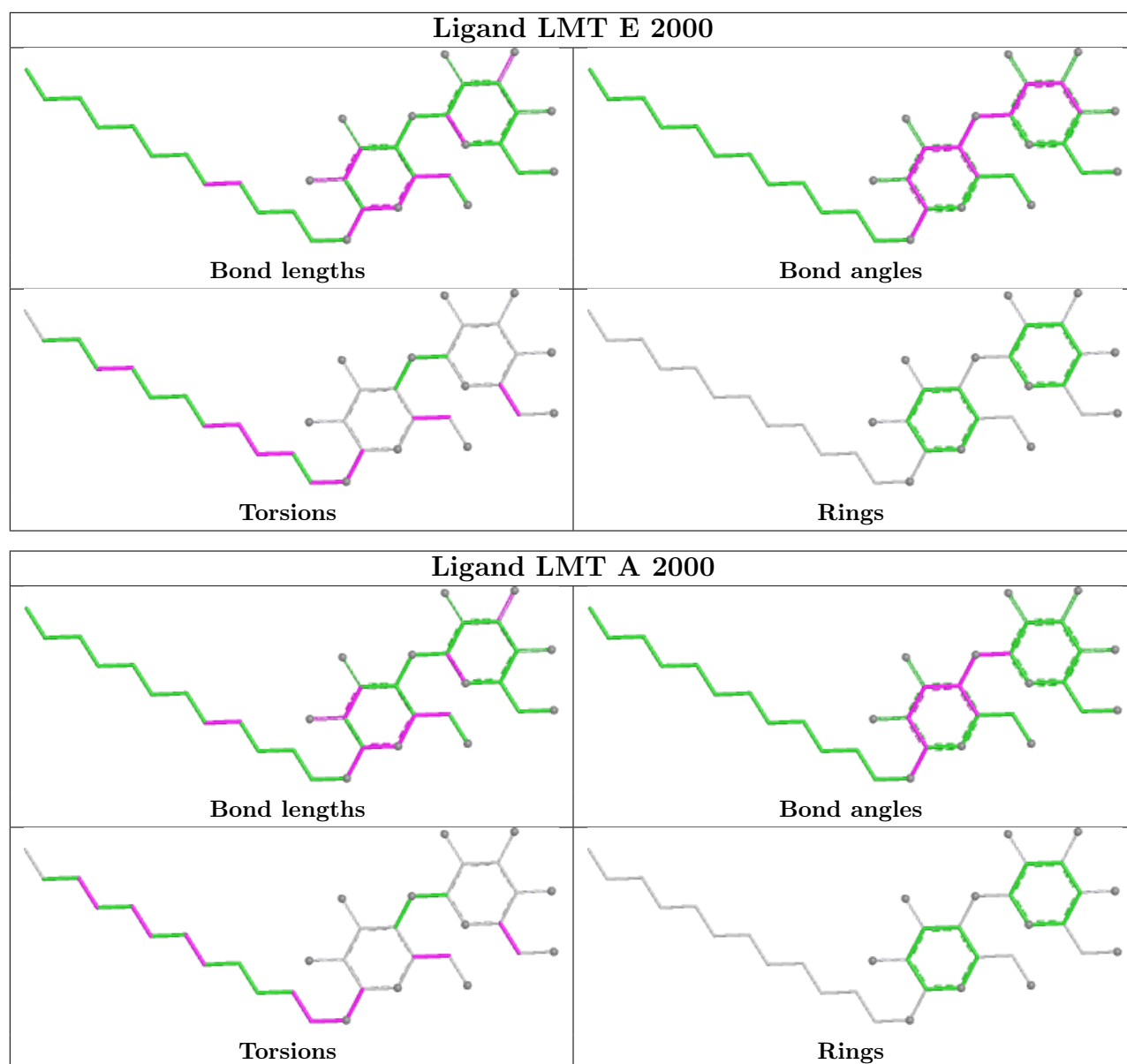
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2000	LMT	3	0
2	B	2000	LMT	2	0
2	D	2000	LMT	1	0
2	E	2000	LMT	1	0
2	A	2000	LMT	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1044/1069 (97%)	0.07	11 (1%)	78 52	15, 54, 96, 123	0
1	B	1042/1069 (97%)	0.11	25 (2%)	59 33	8, 53, 102, 133	0
1	C	1044/1069 (97%)	0.19	48 (4%)	37 20	10, 57, 103, 141	0
1	D	1044/1069 (97%)	0.00	7 (0%)	84 61	13, 45, 89, 128	0
1	E	1042/1069 (97%)	-0.16	9 (0%)	81 56	10, 36, 75, 99	0
1	F	1044/1069 (97%)	-0.06	10 (0%)	79 54	6, 37, 71, 95	0
All	All	6260/6414 (97%)	0.03	110 (1%)	67 40	6, 46, 93, 141	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	856	GLY	6.2
1	C	171	GLY	6.2
1	B	78	MET	5.6
1	F	856	GLY	5.2
1	A	306	ILE	5.1
1	C	116	PRO	4.3
1	C	947	GLU	4.2
1	E	175	VAL	4.2
1	C	118	LEU	4.1
1	C	107	VAL	3.9
1	B	167	SER	3.9
1	C	117	LEU	3.8
1	A	299	ALA	3.6
1	C	390	ILE	3.3
1	C	49	TYR	3.2
1	C	840	ALA	3.2
1	F	79	SER	3.2
1	B	92	LEU	3.2
1	F	390	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	857	TYR	3.1
1	C	417	GLU	3.0
1	B	995	ALA	3.0
1	C	69	MET	2.9
1	D	606	VAL	2.9
1	C	859	TRP	2.9
1	D	686	ASP	2.8
1	C	851	LEU	2.8
1	F	494	ALA	2.8
1	E	174	ASP	2.8
1	B	463	THR	2.8
1	C	60	THR	2.8
1	C	108	GLN	2.7
1	B	171	GLY	2.7
1	D	486	LEU	2.7
1	C	93	THR	2.7
1	A	159	ALA	2.7
1	B	706	ALA	2.7
1	C	857	TYR	2.7
1	B	427	PRO	2.6
1	C	114	ALA	2.6
1	E	995	ALA	2.6
1	C	79	SER	2.6
1	B	494	ALA	2.6
1	C	684	LEU	2.6
1	D	59	ASP	2.6
1	E	715	SER	2.6
1	D	714	THR	2.5
1	A	858	ASP	2.5
1	B	873	ALA	2.5
1	E	293	LEU	2.5
1	C	75	LEU	2.5
1	C	61	VAL	2.5
1	C	62	THR	2.5
1	B	65	ILE	2.4
1	C	65	ILE	2.4
1	E	292	LYS	2.4
1	C	665	ALA	2.4
1	B	59	ASP	2.4
1	B	170	SER	2.4
1	B	166	ILE	2.4
1	C	56	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	892	TYR	2.3
1	C	858	ASP	2.3
1	C	86	GLY	2.3
1	C	119	PRO	2.3
1	B	1010	GLY	2.3
1	C	821	GLY	2.3
1	C	838	GLY	2.3
1	C	683	GLU	2.3
1	C	103	ALA	2.3
1	B	105	VAL	2.3
1	A	876	LEU	2.2
1	B	246	PHE	2.2
1	A	42	ALA	2.2
1	A	398	MET	2.2
1	C	690	LEU	2.2
1	C	844	MET	2.2
1	B	683	GLU	2.2
1	E	714	THR	2.2
1	A	162	MET	2.2
1	A	310	LEU	2.2
1	B	608	SER	2.2
1	A	64	VAL	2.2
1	C	77	TYR	2.2
1	D	27	ILE	2.2
1	F	724	THR	2.2
1	C	695	LEU	2.1
1	A	73	ASP	2.1
1	F	6	ILE	2.1
1	B	493	CYS	2.1
1	E	295	THR	2.1
1	C	58	GLN	2.1
1	C	407	ASP	2.1
1	B	870	GLY	2.1
1	D	621	GLY	2.1
1	C	822	LEU	2.1
1	C	819	TYR	2.1
1	F	611	ALA	2.1
1	C	55	LYS	2.0
1	C	706	ALA	2.0
1	B	830	GLN	2.0
1	E	285	PRO	2.0
1	C	698	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	172	VAL	2.0
1	C	78	MET	2.0
1	B	936	GLY	2.0
1	F	503	GLY	2.0
1	B	892	TYR	2.0
1	C	59	ASP	2.0
1	F	59	ASP	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](#)

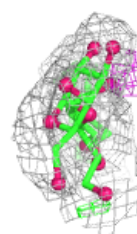
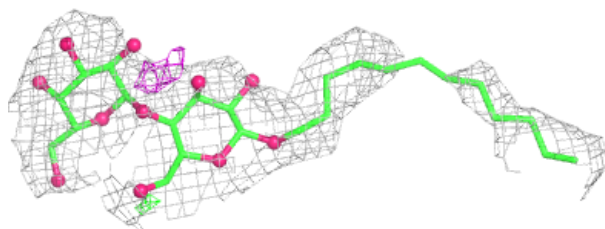
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	2000	35/35	0.72	0.11	21,41,61,68	0
2	LMT	E	2000	35/35	0.81	0.11	3,42,59,66	0
2	LMT	B	2000	35/35	0.82	0.09	2,48,54,66	0
2	LMT	A	2000	35/35	0.83	0.09	11,44,65,67	0
2	LMT	F	2000	35/35	0.86	0.10	6,45,57,63	0
2	LMT	C	2000	35/35	0.89	0.08	10,44,55,59	0

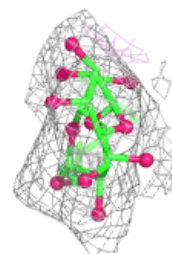
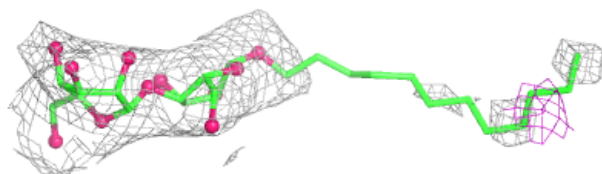
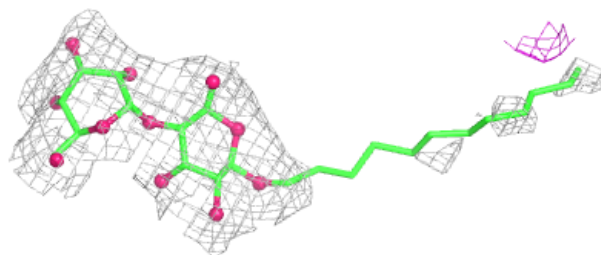
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT D 2000:

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

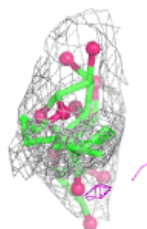
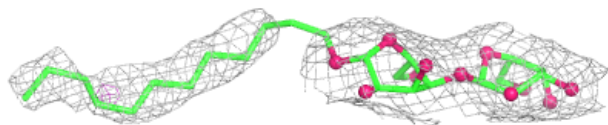
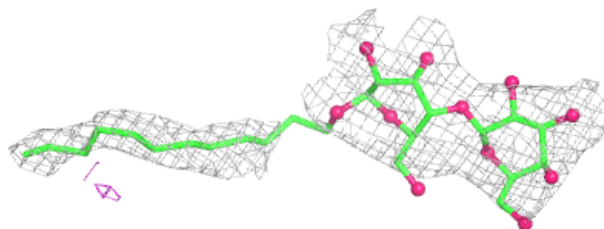
**Electron density around LMT E 2000:**

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

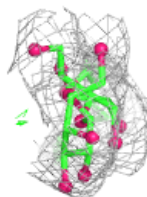
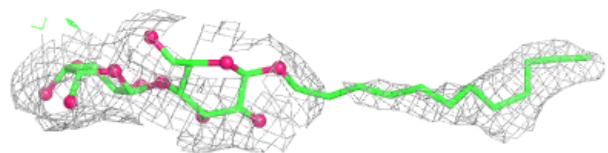
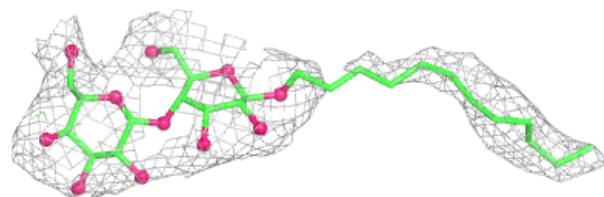


Electron density around LMT B 2000:

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

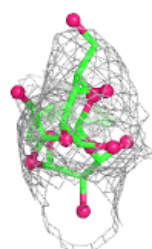
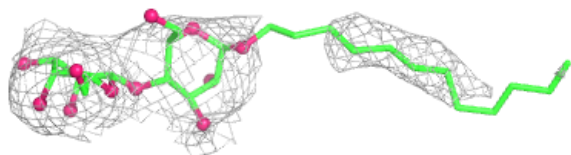
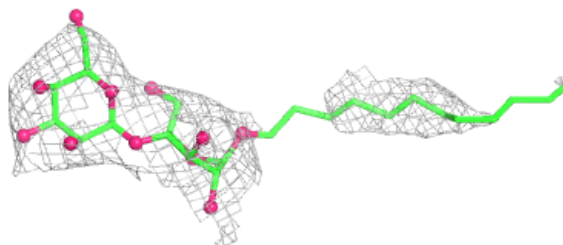
**Electron density around LMT A 2000:**

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

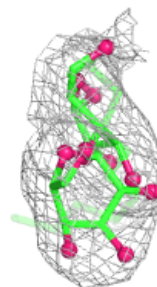
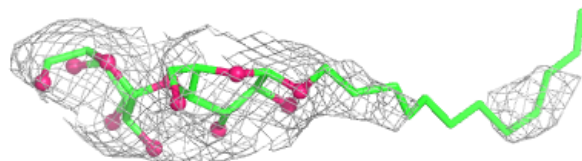
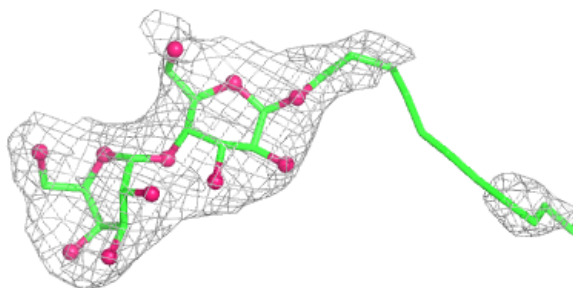


Electron density around LMT F 2000:

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

**Electron density around LMT C 2000:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.