Full wwPDB X-ray Structure Validation Report (i)

Apr 5, 2022 – 01:18 pm BST

PDB ID	:	7O3N
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

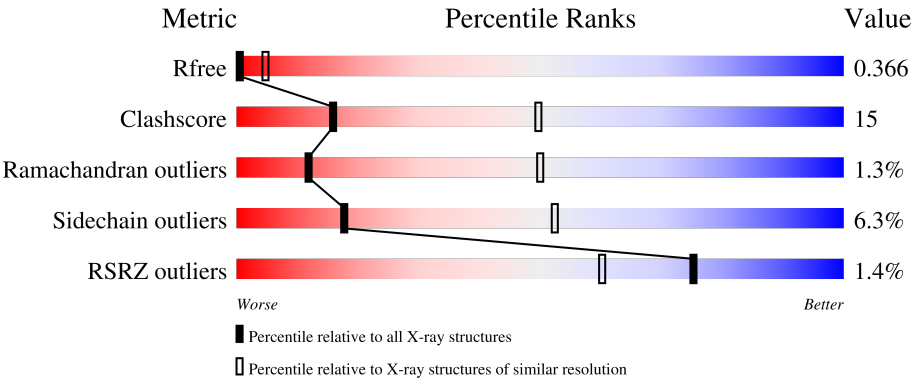
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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}	130704	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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

Mol	Chain	Length	Quality of chain
1	A	1069	60% 35%
1	B	1069	62% 32%
1	C	1069	3% 61% 33%
1	D	1069	63% 32%
1	E	1069	65% 31%

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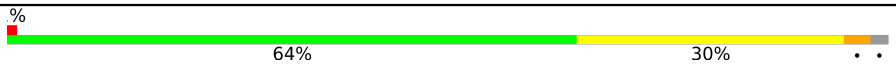
Mol	Chain	Length	Quality of chain
1	F	1069	

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 (i)

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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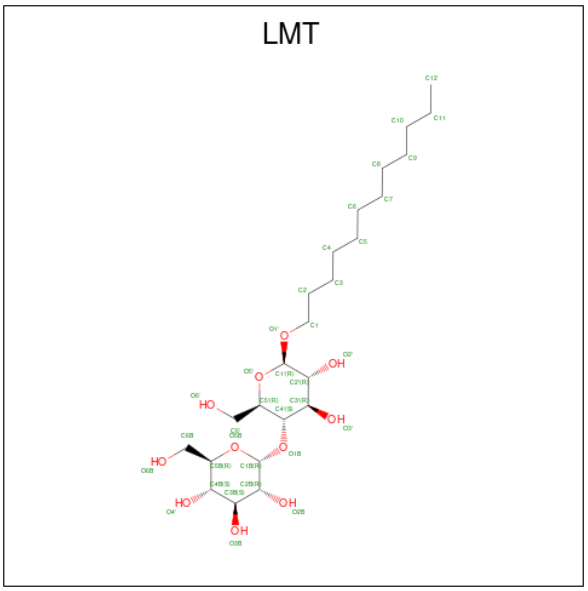
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP E2QH56
E	-1	SER	-	expression tag	UNP E2QH56
E	0	HIS	-	expression tag	UNP E2QH56
E	620	LYS	ARG	engineered mutation	UNP E2QH56
F	-19	MET	-	initiating methionine	UNP E2QH56
F	-18	GLY	-	expression tag	UNP E2QH56
F	-17	SER	-	expression 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 (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



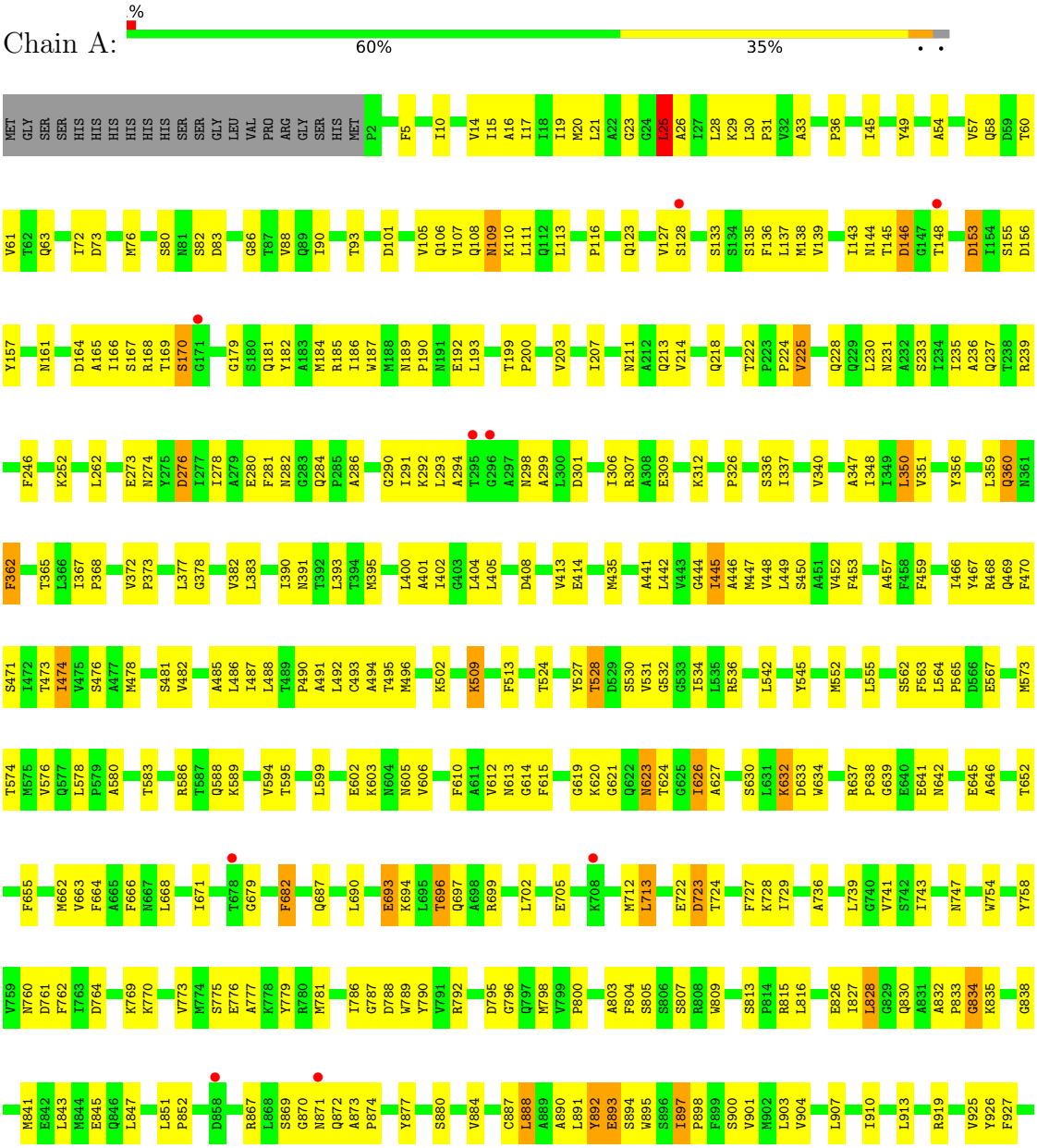
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	C	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		

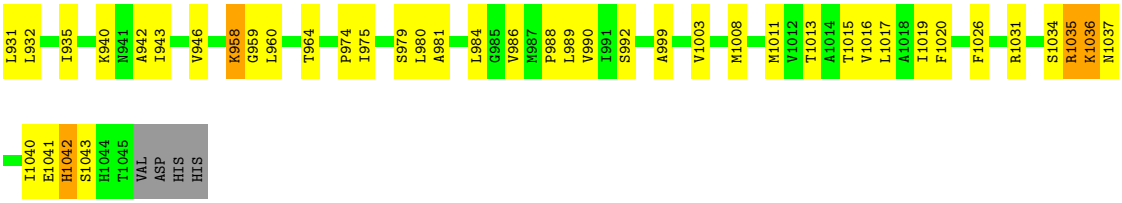
3 Residue-property plots (i)

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

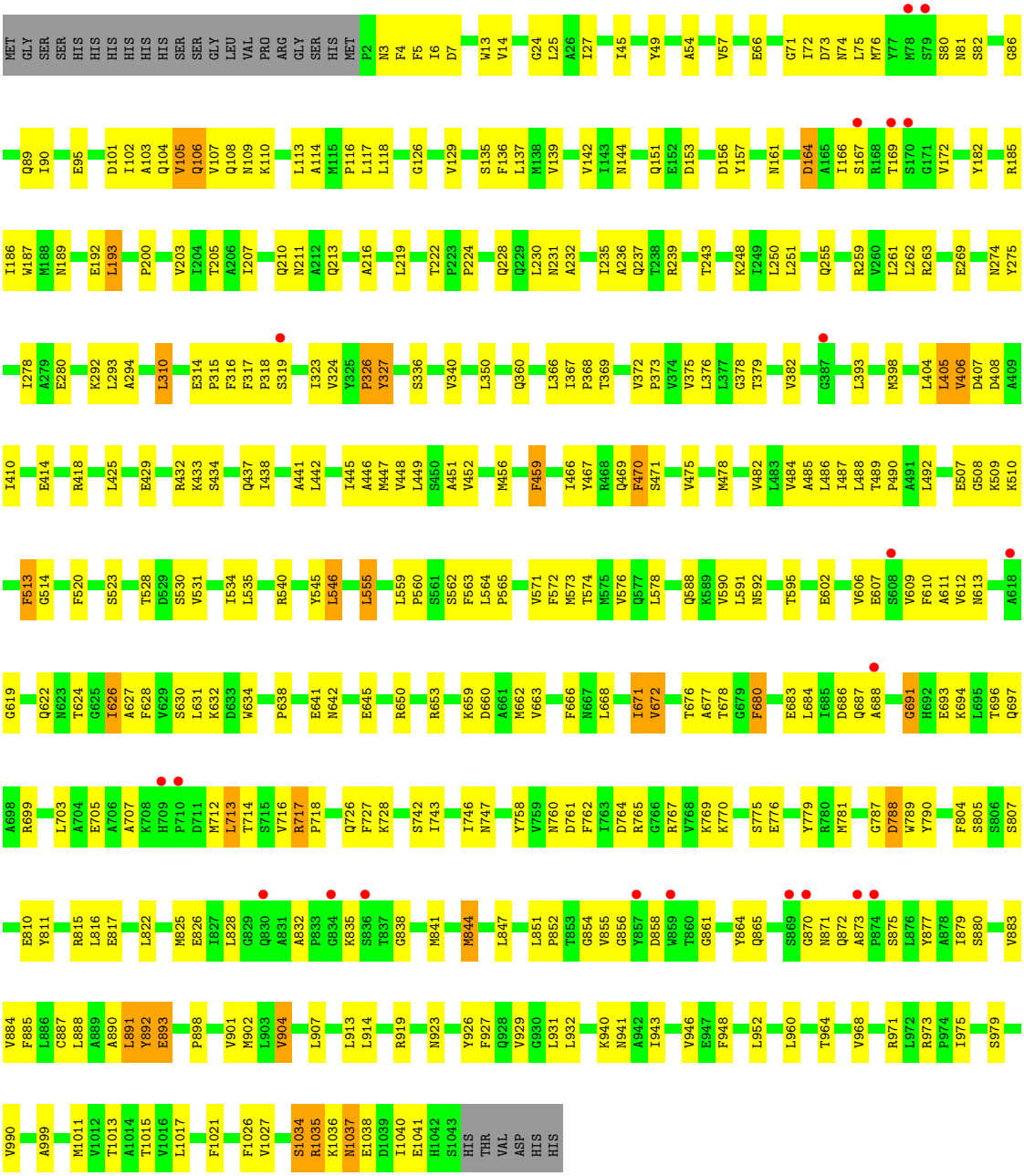
Chain A:





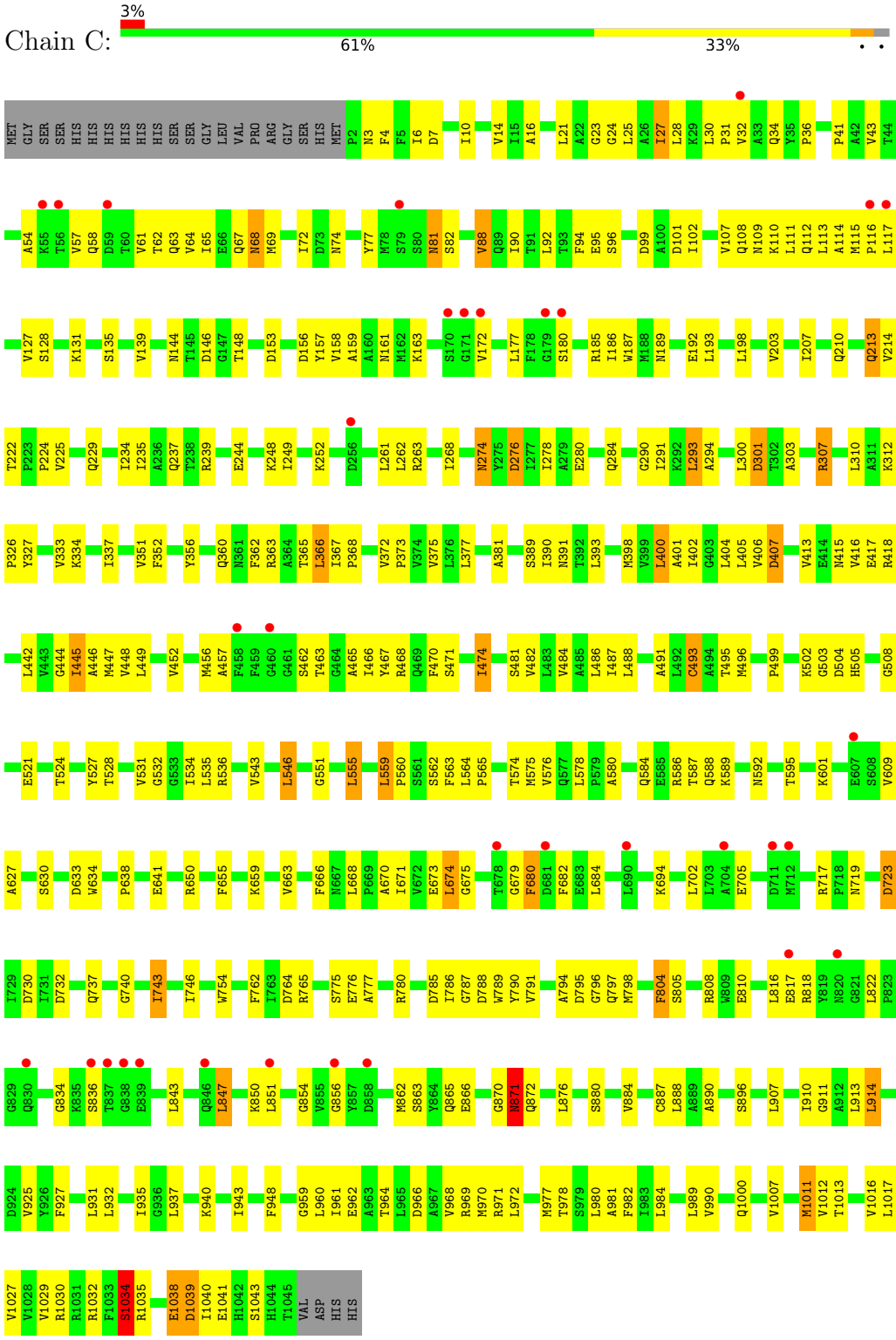
• Molecule 1: Efflux pump membrane transporter

Chain B:



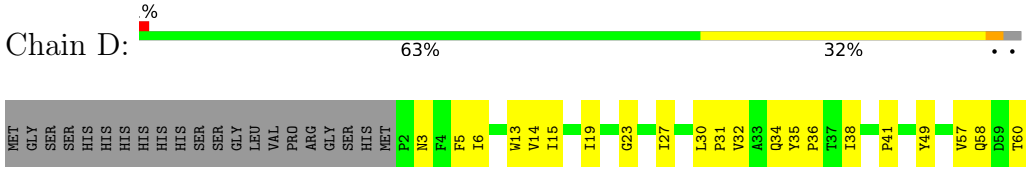
• Molecule 1: Efflux pump membrane transporter

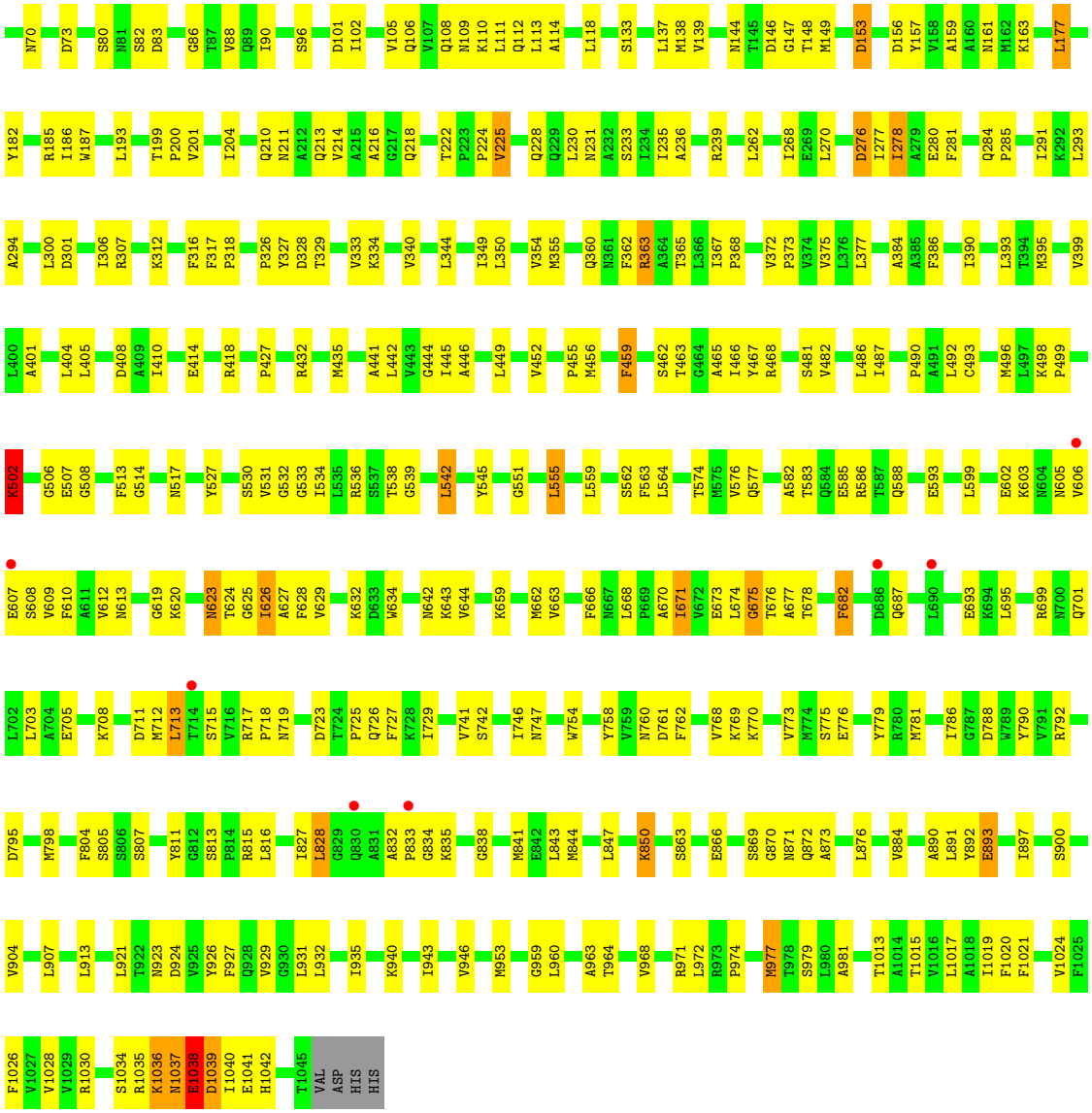
Chain C:



• Molecule 1: Efflux pump membrane transporter

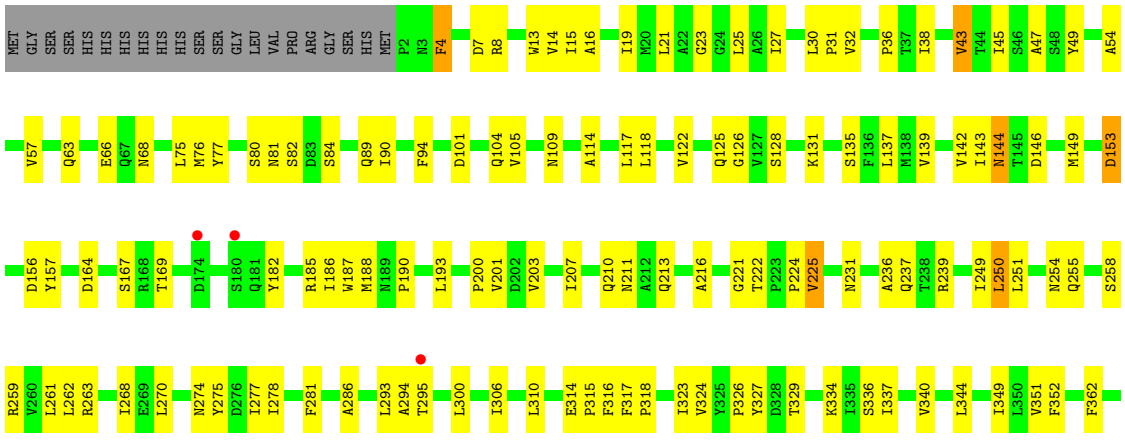
Chain D:

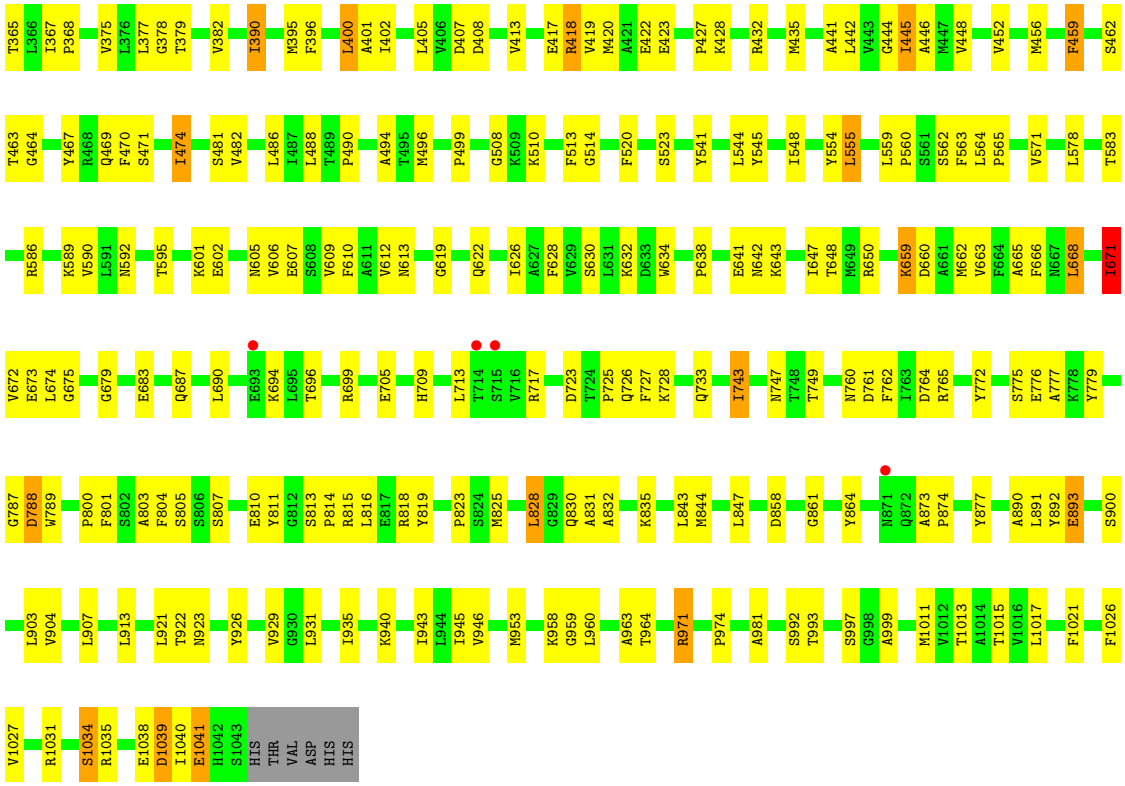




• Molecule 1: Efflux pump membrane transporter

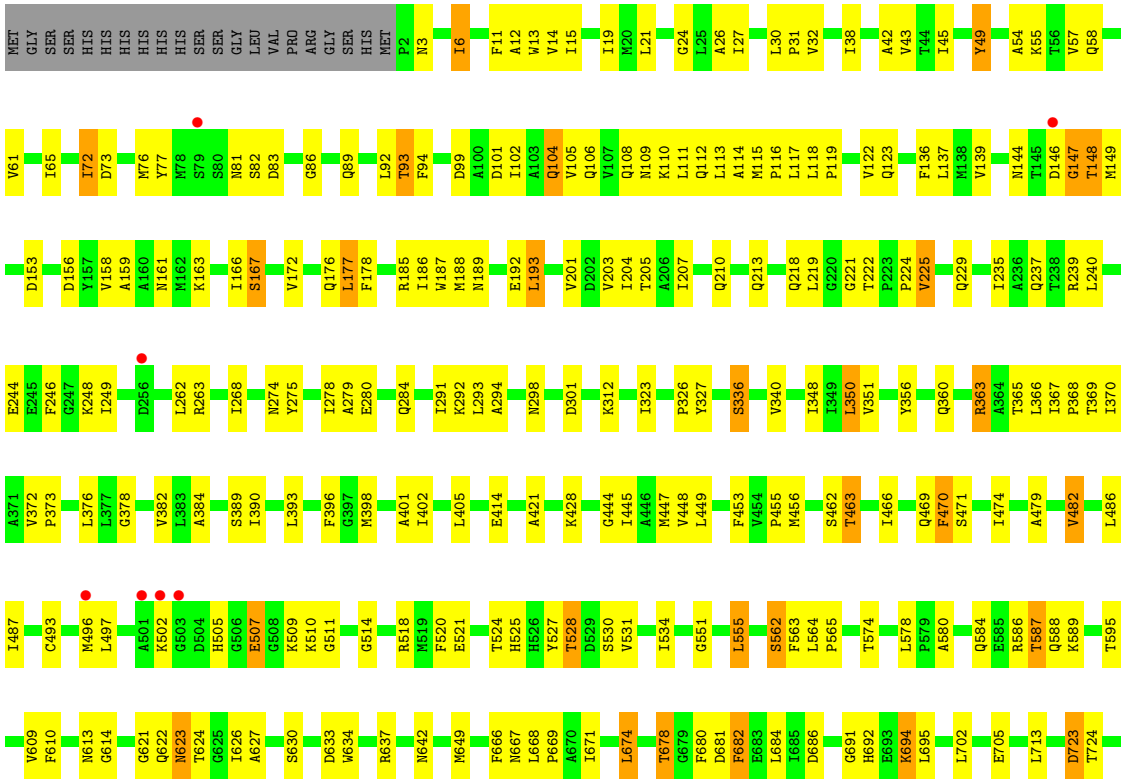
Chain E:

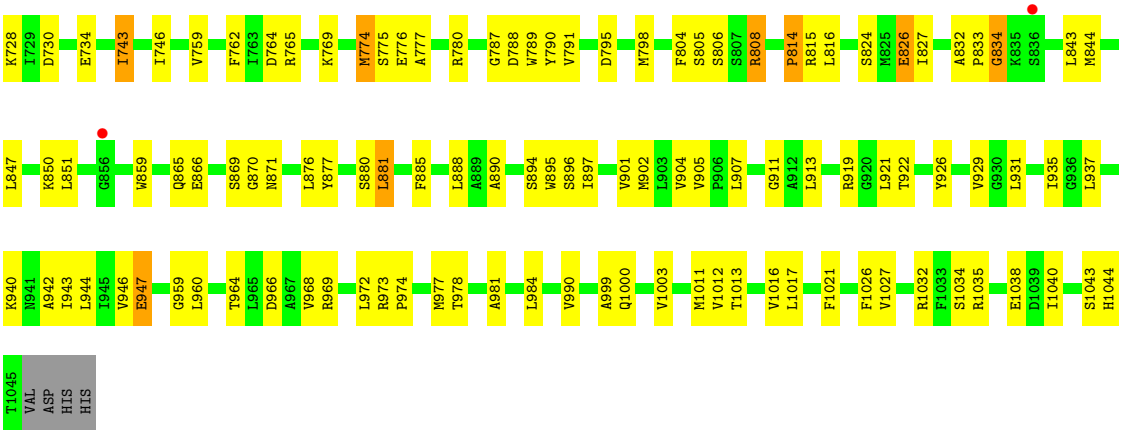




• Molecule 1: Efflux pump membrane transporter

Chain F:




K728 I729 D730 E734 I743 I746 V759 F762 I763 D764 R765 K769 M774 S775 E776 A777 R780 G787 D788 W789 Y790 V791 D795 M798 F804 S805 S806 S807 R808 P814 R815 L816 S824 M825 E826 I827 A832 P833 G834 K835 S836 L843 M844
L847 K850 L851 Q856 W859 Q865 E866 S869 G870 N871 L876 Y877 S880 L881 F885 L888 A889 A890 S894 W895 S896 I897 V901 M902 L903 V904 V905 P906 L907 G911 A912 L913 R919 G920 L921 T922 Y926 V929 G930 L931 I935 G936 L937
K940 N941 A942 I943 L944 I945 V946 E947 G959 L960 T964 L965 D966 A967 V968 R969 L972 R973 P974 M977 T978 A981 L984 V990 A999 Q1000 V1003 M1011 V1012 T1013 V1016 L1017 F1021 F1026 V1027 R1032 F1033 S1034 R1035 E1038 D1039 I1040 S1043 H1044
T1045 VAL ASP HIS HIS

4 Data and refinement statistics (i)

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) 98.9 (20.00-3.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 3.52Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.306 , 0.366 0.306 , 0.366	Depositor DCC
R_{free} test set	6063 reflections (5.00%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	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	0.88	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.25	0/8092	0.52	1/10987 (0.0%)
1	B	0.25	0/8074	0.51	1/10962 (0.0%)
1	C	0.26	0/8092	0.55	3/10987 (0.0%)
1	D	0.25	0/8092	0.50	1/10987 (0.0%)
1	E	0.25	0/8074	0.51	0/10962
1	F	0.25	0/8092	0.51	0/10987
All	All	0.25	0/48516	0.52	6/65872 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	713	LEU	CA-CB-CG	6.31	129.82	115.30
1	A	25	LEU	CA-CB-CG	6.08	129.28	115.30
1	C	854	GLY	N-CA-C	-5.35	99.73	113.10
1	D	1038	GLU	C-N-CA	5.33	135.01	121.70
1	C	1038	GLU	C-N-CA	5.30	134.96	121.70
1	C	834	GLY	N-CA-C	-5.18	100.14	113.10

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	268	0
1	B	7923	0	8066	246	0
1	C	7940	0	8080	266	0
1	D	7940	0	8080	239	0
1	E	7923	0	8066	223	0
1	F	7940	0	8080	243	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	1407	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 (1407) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:781:MET:HE1	1:C:225:VAL:H	1.47	0.79
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:781:MET:HE1	1:F:225:VAL:H	1.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:990:VAL:HG21	1:A:1008:MET:HE3	1.74	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
1:B:475:VAL:HA	1:B:478:MET:HE3	1.77	0.67
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:A:1019:ILE:HG13	1:A:1020:PHE:HD1	1.59	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:H	1:B:781:MET:HE1	1.60	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:B:555:LEU:HD22	1:B:913:LEU:HB3	1.79	0.65
1:F:775:SER:OG	1:F:776:GLU:N	2.30	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
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:B:775:SER:OG	1:B:776:GLU:N	2.31	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:D:775:SER:OG	1:D:776:GLU:N	2.32	0.63
1:F:144:ASN:O	1:F:284:GLN:NE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:562:SER:OG	1:F:563:PHE:N	2.32	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:B:562:SER:OG	1:B:563:PHE:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:366:LEU:HA	1:B:369:THR:HB	1.85	0.59
1:D:138:MET:HE3	1:D:307:ARG:HH21	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:376:LEU:HD22	1:B:398:MET:HE3	1.86	0.57
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: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
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: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:805:SER:O	1:E:805:SER:OG	2.21	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:A:453:PHE:O	1:A:471:SER:OG	2.10	0.56
1:B:926:TYR:HE1	1:B:999:ALA:HB1	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:805:SER:OG	1:B:805:SER:O	2.19	0.55
1:C:94:PHE:CE2	1:C:107:VAL:HG21	2.42	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:E:36:PRO:HG3	1:E:469:GLN:HG3	1.89	0.55
1:F:805:SER:O	1:F:805:SER:OG	2.24	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: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: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:F:449:LEU:HD21	1:F:937:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:913:LEU:HD23	1:D:927:PHE:HZ	1.71	0.54
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:167:SER:C	1:B:169:THR:H	2.12	0.52
1:F:482:VAL:O	1:F:486:LEU:HG	2.09	0.52
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:417:GLU:HA	1:E:420:MET:HE2	1.90	0.52
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:B:425:LEU:HD13	1:B:429:GLU:HG2	1.90	0.51
1:D:73:ASP:CG	1:D:106:GLN:HE22	2.12	0.51
1:F:112:GLN:HA	1:F:115:MET:HG3	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:HG22	1:B:1026:PHE:HD1	1.75	0.49
1:B:946:VAL:HG13	1:B:1026:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:870:GLY:C	1:C:872:GLN:H	2.15	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:375:VAL:O	1:B:379:THR:OG1	2.26	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: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
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:D:953:MET:HE2	1:D:963:ALA:HB3	1.95	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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:885:PHE:CD1	1:B:898:PRO:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:491:ALA:O	1:C:495:THR:OG1	2.28	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: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: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:111:LEU:C	1:C:113:LEU:H	2.17	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:953:MET:HE1	1:E:960:LEU:HD12	1.97	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:B:72:ILE:HG23	1:B:106:GLN:OE1	2.15	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ARG:NH1	1:B:418:ARG:HB3	2.30	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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:979:SER:HA	1:B:1011:MET:HE1	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:871:ASN:C	1:D:873:ALA:H	2.20	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: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:E:699:ARG:HH11	1:E:825:MET:HE1	1.80	0.45
1:A:729:ILE:HD11	1:C:234:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:953:MET:HE1	1:D:960:LEU:HD12	1.98	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
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: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: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:376:LEU:HD22	1:F:398:MET:HE3	1.98	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:B:789:TRP:C	1:B:790:TYR:HD2	2.21	0.44
1:C:108:GLN:O	1:C:112:GLN:HG3	2.17	0.44
1:D:114:ALA:O	1:D:118:LEU:HG	2.17	0.44
1:D:156:ASP:OD2	1:D:769:LYS:NZ	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:108:GLN:O	1:F:112:GLN:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:414:GLU:CD	1:D:974:PRO:HG3	2.38	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:E:844:MET:HE1	1:E:847:LEU:HD12	1.99	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: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: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: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:527:TYR:O	1:F:530:SER:OG	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:675:GLY:C	1:D:677:ALA:H	2.22	0.43
1:D:726:GLN:OE1	1:F:235:ILE:HD11	2.18	0.43
1:E:326:PRO:O	1:E:630:SER:OG	2.23	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: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:A:83:ASP:OD1	1:A:815:ARG:NH1	2.52	0.43
1:A:101:ASP:OD1	1:A:101:ASP:N	2.51	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: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: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:111:LEU:C	1:A:113:LEU:H	2.22	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:76:MET:HE3	1:B:95:GLU:OE2	2.19	0.43
1:B:948:PHE:O	1:B:952:LEU:HG	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:787:GLY:O	1:C:789:TRP:N	2.52	0.43
1:D:340:VAL:HG11	1:D:395:MET: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:491:ALA:O	1:A:495:THR:OG1	2.25	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:B:699:ARG:HH11	1:B:825:MET:HE1	1.84	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: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: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: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:764:ASP:HB3	1:F:769:LYS:NZ	2.34	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: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:C:1030:ARG:C	1:C:1032:ARG:H	2.23	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:A:225:VAL:HG23	1:B:781:MET:HE1	2.01	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: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
1:B:448:VAL:O	1:B:452:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:452:VAL:HA	1:B:880:SER:OG	2.19	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:111:LEU:C	1:F:113:LEU:H	2.22	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: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:101:ASP:OD1	1:D:101:ASP:N	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:786:ILE:HD13	1:D:786:ILE:HA	1.81	0.42
1:D:953:MET:HE3	1:D:953:MET:HB2	1.95	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:787:GLY:C	1:F:789:TRP:H	2.22	0.42
1:F:888:LEU:HD23	1:F:888:LEU:HA	1.67	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:E:375:VAL:O	1:E:379:THR:OG1	2.23	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: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:684:LEU:HB3	1:C:825:MET:O	2.20	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:473:THR:O	1:A:476:SER:OG	2.31	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: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: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
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:186:ILE:C	1:C:187:TRP:HD1	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:450:SER:HB2	1:A:478:MET:HE1	2.03	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: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:105:VAL:HG11	1:B:105:VAL:CG2	2.49	0.40
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:N	1:D:850:LYS:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:111:LEU:C	1:D:113:LEU:H	2.24	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: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:507:GLU:C	1:B:509:LYS:H	2.24	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
1:C:389:SER:O	1:C:391:ASN:ND2	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	8	43
1	B	1040/1069 (97%)	909 (87%)	116 (11%)	15 (1%)	11	48
1	C	1042/1069 (98%)	898 (86%)	128 (12%)	16 (2%)	10	47
1	D	1042/1069 (98%)	904 (87%)	123 (12%)	15 (1%)	11	48
1	E	1040/1069 (97%)	913 (88%)	120 (12%)	7 (1%)	22	62
1	F	1042/1069 (98%)	905 (87%)	126 (12%)	11 (1%)	14	54
All	All	6248/6414 (97%)	5437 (87%)	728 (12%)	83 (1%)	12	50

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	850/872 (98%)	796 (94%)	54 (6%)	17	51
1	B	848/872 (97%)	792 (93%)	56 (7%)	16	50
1	C	850/872 (98%)	795 (94%)	55 (6%)	17	51
1	D	850/872 (98%)	803 (94%)	47 (6%)	21	56
1	E	848/872 (97%)	801 (94%)	47 (6%)	21	56
1	F	850/872 (98%)	789 (93%)	61 (7%)	14	47
All	All	5096/5232 (97%)	4776 (94%)	320 (6%)	18	52

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	49	TYR
1	A	88	VAL
1	A	106	GLN
1	A	109	ASN
1	A	135	SER
1	A	146	ASP
1	A	153	ASP
1	A	157	TYR
1	A	182	TYR
1	A	225	VAL
1	A	276	ASP
1	A	337	ILE
1	A	350	LEU
1	A	360	GLN
1	A	362	PHE
1	A	445	ILE
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	615	PHE
1	A	620	LYS
1	A	623	ASN
1	A	624	THR
1	A	626	ILE
1	A	630	SER

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Mol	Chain	Res	Type
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	682	PHE
1	A	693	GLU
1	A	696	THR
1	A	713	LEU
1	A	723	ASP
1	A	739	LEU
1	A	743	ILE
1	A	795	ASP
1	A	804	PHE
1	A	826	GLU
1	A	828	LEU
1	A	888	LEU
1	A	892	TYR
1	A	897	ILE
1	A	958	LYS
1	A	1026	PHE
1	A	1034	SER
1	A	1035	ARG
1	B	3	ASN
1	B	4	PHE
1	B	25	LEU
1	B	49	TYR
1	B	73	ASP
1	B	104	GLN
1	B	105	VAL
1	B	106	GLN
1	B	135	SER
1	B	153	ASP
1	B	164	ASP
1	B	172	VAL
1	B	182	TYR
1	B	193	LEU
1	B	205	THR
1	B	213	GLN
1	B	243	THR
1	B	255	GLN

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Mol	Chain	Res	Type
1	B	310	LEU
1	B	350	LEU
1	B	405	LEU
1	B	406	VAL
1	B	459	PHE
1	B	470	PHE
1	B	513	PHE
1	B	528	THR
1	B	540	ARG
1	B	546	LEU
1	B	555	LEU
1	B	592	ASN
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	676	THR
1	B	680	PHE
1	B	717	ARG
1	B	743	ILE
1	B	788	ASP
1	B	804	PHE
1	B	811	TYR
1	B	826	GLU
1	B	828	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	1034	SER
1	B	1035	ARG
1	B	1037	ASN
1	C	27	ILE
1	C	43	VAL
1	C	49	TYR
1	C	68	ASN

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Mol	Chain	Res	Type
1	C	77	TYR
1	C	81	ASN
1	C	88	VAL
1	C	92	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	323	ILE
1	C	337	ILE
1	C	360	GLN
1	C	366	LEU
1	C	400	LEU
1	C	407	ASP
1	C	417	GLU
1	C	445	ILE
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
1	C	601	LYS
1	C	630	SER
1	C	634	TRP
1	C	666	PHE
1	C	674	LEU
1	C	680	PHE
1	C	694	LYS
1	C	717	ARG
1	C	723	ASP
1	C	743	ILE
1	C	804	PHE
1	C	843	LEU
1	C	847	LEU

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Mol	Chain	Res	Type
1	C	850	LYS
1	C	871	ASN
1	C	876	LEU
1	C	914	LEU
1	C	977	MET
1	C	978	THR
1	C	1011	MET
1	C	1034	SER
1	C	1035	ARG
1	D	27	ILE
1	D	49	TYR
1	D	67	GLN
1	D	88	VAL
1	D	102	ILE
1	D	109	ASN
1	D	153	ASP
1	D	157	TYR
1	D	177	LEU
1	D	225	VAL
1	D	276	ASP
1	D	278	ILE
1	D	301	ASP
1	D	350	LEU
1	D	362	PHE
1	D	363	ARG
1	D	386	PHE
1	D	418	ARG
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	623	ASN
1	D	626	ILE
1	D	634	TRP
1	D	662	MET
1	D	666	PHE
1	D	671	ILE
1	D	678	THR
1	D	682	PHE

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Mol	Chain	Res	Type
1	D	693	GLU
1	D	703	LEU
1	D	708	LYS
1	D	711	ASP
1	D	713	LEU
1	D	795	ASP
1	D	804	PHE
1	D	828	LEU
1	D	850	LYS
1	D	900	SER
1	D	971	ARG
1	D	977	MET
1	D	1038	GLU
1	D	1041	GLU
1	E	4	PHE
1	E	13	TRP
1	E	27	ILE
1	E	43	VAL
1	E	49	TYR
1	E	135	SER
1	E	144	ASN
1	E	153	ASP
1	E	164	ASP
1	E	167	SER
1	E	182	TYR
1	E	213	GLN
1	E	225	VAL
1	E	250	LEU
1	E	255	GLN
1	E	277	ILE
1	E	337	ILE
1	E	390	ILE
1	E	400	LEU
1	E	418	ARG
1	E	423	GLU
1	E	445	ILE
1	E	459	PHE
1	E	474	ILE
1	E	513	PHE
1	E	544	LEU
1	E	554	TYR
1	E	555	LEU

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Mol	Chain	Res	Type
1	E	592	ASN
1	E	601	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	743	ILE
1	E	788	ASP
1	E	804	PHE
1	E	828	LEU
1	E	877	TYR
1	E	971	ARG
1	E	1034	SER
1	E	1035	ARG
1	E	1038	GLU
1	E	1039	ASP
1	E	1041	GLU
1	F	3	ASN
1	F	6	ILE
1	F	49	TYR
1	F	72	ILE
1	F	77	TYR
1	F	92	LEU
1	F	93	THR
1	F	104	GLN
1	F	153	ASP
1	F	167	SER
1	F	177	LEU
1	F	193	LEU
1	F	205	THR
1	F	225	VAL
1	F	263	ARG
1	F	323	ILE
1	F	336	SER
1	F	350	LEU
1	F	360	GLN
1	F	363	ARG
1	F	428	LYS
1	F	447	MET
1	F	463	THR

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Mol	Chain	Res	Type
1	F	470	PHE
1	F	482	VAL
1	F	528	THR
1	F	555	LEU
1	F	562	SER
1	F	587	THR
1	F	623	ASN
1	F	624	THR
1	F	626	ILE
1	F	630	SER
1	F	634	TRP
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	682	PHE
1	F	692	HIS
1	F	694	LYS
1	F	723	ASP
1	F	743	ILE
1	F	759	VAL
1	F	774	MET
1	F	795	ASP
1	F	804	PHE
1	F	808	ARG
1	F	826	GLU
1	F	871	ASN
1	F	876	LEU
1	F	881	LEU
1	F	895	TRP
1	F	947	GLU
1	F	977	MET
1	F	1003	VAL
1	F	1011	MET
1	F	1026	PHE
1	F	1035	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	274	ASN
1	A	284	GLN
1	A	709	HIS
1	A	923	ASN
1	A	928	GLN
1	B	109	ASN
1	B	865	GLN
1	C	584	GLN
1	C	737	GLN
1	C	865	GLN
1	D	144	ASN
1	D	360	GLN
1	D	517	ASN
1	D	760	ASN
1	E	108	GLN
1	E	865	GLN
1	F	108	GLN
1	F	109	ASN
1	F	642	ASN
1	F	865	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	A	2000	-	36,36,36	1.75	9 (25%)	47,47,47	1.23	4 (8%)
2	LMT	F	2000	-	36,36,36	1.71	9 (25%)	47,47,47	1.29	4 (8%)
2	LMT	B	2000	-	36,36,36	1.74	8 (22%)	47,47,47	0.95	3 (6%)
2	LMT	C	2000	-	36,36,36	1.76	9 (25%)	47,47,47	1.26	4 (8%)
2	LMT	E	2000	-	36,36,36	1.73	8 (22%)	47,47,47	1.20	5 (10%)
2	LMT	D	2000	-	36,36,36	1.77	9 (25%)	47,47,47	0.93	1 (2%)

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	A	2000	-	2/2/10/10	9/21/61/61	0/2/2/2
2	LMT	F	2000	-	3/3/10/10	13/21/61/61	0/2/2/2
2	LMT	B	2000	-	2/2/10/10	11/21/61/61	0/2/2/2
2	LMT	C	2000	-	3/3/10/10	7/21/61/61	0/2/2/2
2	LMT	E	2000	-	5/5/10/10	10/21/61/61	0/2/2/2
2	LMT	D	2000	-	2/2/10/10	12/21/61/61	0/2/2/2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2000	LMT	O5'-C5'	4.04	1.54	1.44
2	B	2000	LMT	O5'-C5'	3.96	1.53	1.44
2	E	2000	LMT	O5'-C5'	3.92	1.53	1.44
2	C	2000	LMT	O5'-C5'	3.85	1.53	1.44
2	A	2000	LMT	O5'-C5'	3.82	1.53	1.44
2	F	2000	LMT	O5'-C5'	3.74	1.53	1.44
2	A	2000	LMT	O1'-C1'	3.60	1.46	1.40
2	C	2000	LMT	O5B-C1B	3.52	1.50	1.41
2	B	2000	LMT	O5B-C1B	3.48	1.50	1.41
2	A	2000	LMT	O5B-C1B	3.48	1.50	1.41
2	F	2000	LMT	O1'-C1'	3.44	1.46	1.40
2	C	2000	LMT	O1'-C1'	3.41	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2000	LMT	O1'-C1'	3.41	1.46	1.40
2	D	2000	LMT	O5B-C1B	3.38	1.50	1.41
2	F	2000	LMT	O5B-C1B	3.37	1.50	1.41
2	E	2000	LMT	O5B-C1B	3.29	1.50	1.41
2	D	2000	LMT	O1'-C1'	3.29	1.45	1.40
2	B	2000	LMT	O1'-C1'	3.29	1.45	1.40
2	D	2000	LMT	C6'-C5'	-3.26	1.40	1.51
2	A	2000	LMT	C6'-C5'	-3.25	1.40	1.51
2	C	2000	LMT	C6'-C5'	-3.23	1.41	1.51
2	B	2000	LMT	O5'-C1'	3.23	1.50	1.41
2	E	2000	LMT	C6'-C5'	-3.21	1.41	1.51
2	D	2000	LMT	O5'-C1'	3.13	1.49	1.41
2	C	2000	LMT	O5'-C1'	3.11	1.49	1.41
2	B	2000	LMT	C6'-C5'	-3.09	1.41	1.51
2	F	2000	LMT	C6'-C5'	-3.08	1.41	1.51
2	F	2000	LMT	O5'-C1'	3.01	1.49	1.41
2	E	2000	LMT	O3B-C3B	2.95	1.49	1.43
2	C	2000	LMT	O3B-C3B	2.92	1.49	1.43
2	B	2000	LMT	O3B-C3B	2.90	1.49	1.43
2	F	2000	LMT	O3B-C3B	2.90	1.49	1.43
2	D	2000	LMT	O3B-C3B	2.90	1.49	1.43
2	A	2000	LMT	O3B-C3B	2.89	1.49	1.43
2	E	2000	LMT	O5'-C1'	2.82	1.49	1.41
2	A	2000	LMT	O5'-C1'	2.78	1.48	1.41
2	D	2000	LMT	C3'-C2'	-2.74	1.45	1.52
2	E	2000	LMT	C3'-C2'	-2.52	1.45	1.52
2	C	2000	LMT	C3'-C2'	-2.43	1.46	1.52
2	F	2000	LMT	O2'-C2'	2.36	1.48	1.43
2	A	2000	LMT	O2'-C2'	2.33	1.48	1.43
2	B	2000	LMT	O2'-C2'	2.32	1.48	1.43
2	B	2000	LMT	C3'-C2'	-2.32	1.46	1.52
2	C	2000	LMT	O2'-C2'	2.31	1.48	1.43
2	A	2000	LMT	C3'-C2'	-2.23	1.46	1.52
2	D	2000	LMT	O2'-C2'	2.22	1.48	1.43
2	E	2000	LMT	O2'-C2'	2.13	1.48	1.43
2	C	2000	LMT	C3B-C2B	-2.11	1.46	1.52
2	F	2000	LMT	C3B-C2B	-2.05	1.47	1.52
2	F	2000	LMT	C3'-C2'	-2.05	1.47	1.52
2	A	2000	LMT	C3B-C2B	-2.03	1.47	1.52
2	D	2000	LMT	C3B-C2B	-2.01	1.47	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2000	LMT	C2'-C3'-C4'	4.78	120.59	109.68
2	C	2000	LMT	O5B-C5B-C4B	4.04	117.03	109.69
2	C	2000	LMT	C3B-C4B-C5B	3.96	117.30	110.24
2	A	2000	LMT	C3'-C4'-C5'	3.77	119.58	110.93
2	A	2000	LMT	C2'-C3'-C4'	3.74	118.23	109.68
2	F	2000	LMT	C3'-C4'-C5'	3.55	119.06	110.93
2	C	2000	LMT	C1B-O1B-C4'	-3.36	109.66	117.96
2	E	2000	LMT	C3'-C4'-C5'	3.31	118.52	110.93
2	D	2000	LMT	C1B-O1B-C4'	-3.24	109.94	117.96
2	F	2000	LMT	C1'-C2'-C3'	3.19	116.63	110.00
2	A	2000	LMT	C1B-O1B-C4'	-2.80	111.03	117.96
2	E	2000	LMT	C1B-O1B-C4'	-2.80	111.04	117.96
2	B	2000	LMT	C1B-O1B-C4'	-2.69	111.31	117.96
2	E	2000	LMT	C4B-C3B-C2B	2.64	115.43	110.82
2	E	2000	LMT	C2'-C3'-C4'	2.57	115.56	109.68
2	A	2000	LMT	O1'-C1'-C2'	2.40	112.05	108.30
2	B	2000	LMT	O5'-C5'-C6'	2.31	112.17	106.44
2	C	2000	LMT	C4B-C3B-C2B	2.27	114.79	110.82
2	B	2000	LMT	C2'-C3'-C4'	2.25	114.82	109.68
2	E	2000	LMT	C1B-C2B-C3B	2.15	114.48	110.00
2	F	2000	LMT	C1B-O1B-C4'	-2.12	112.71	117.96

All (17) chirality outliers are listed below:

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

All (62) torsion outliers are listed below:

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

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

There are no ring outliers.

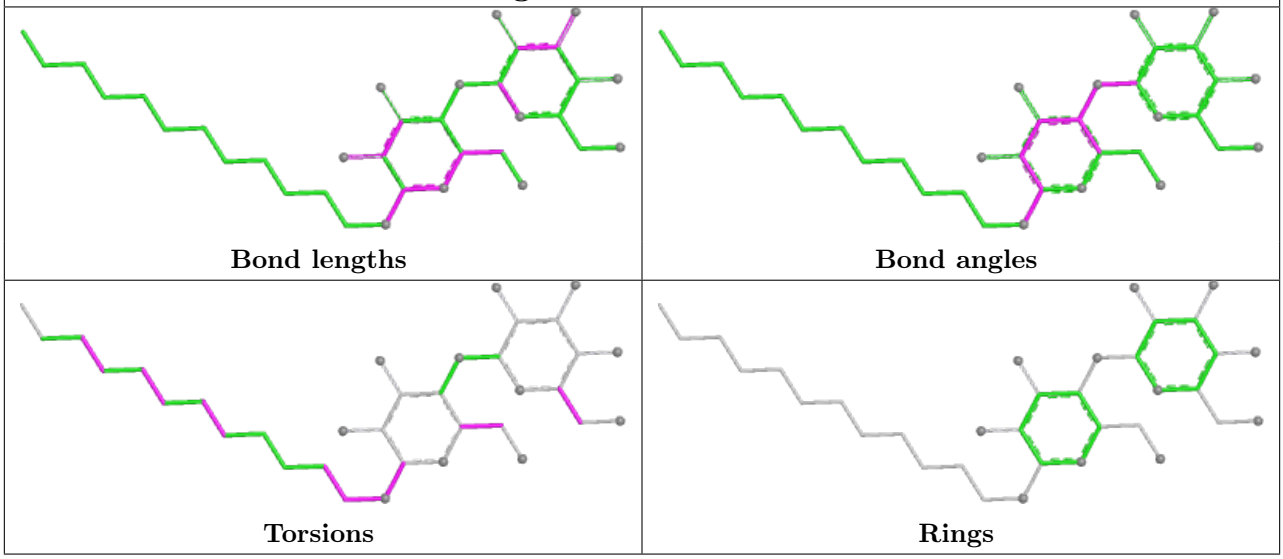
5 monomers are involved in 9 short contacts:

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

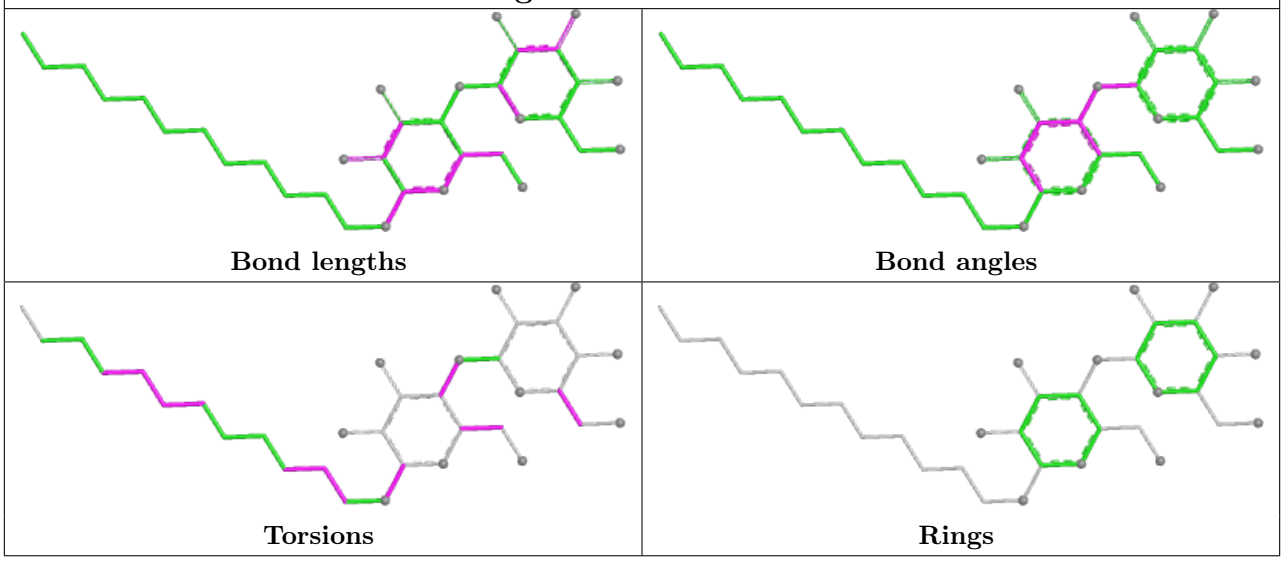
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

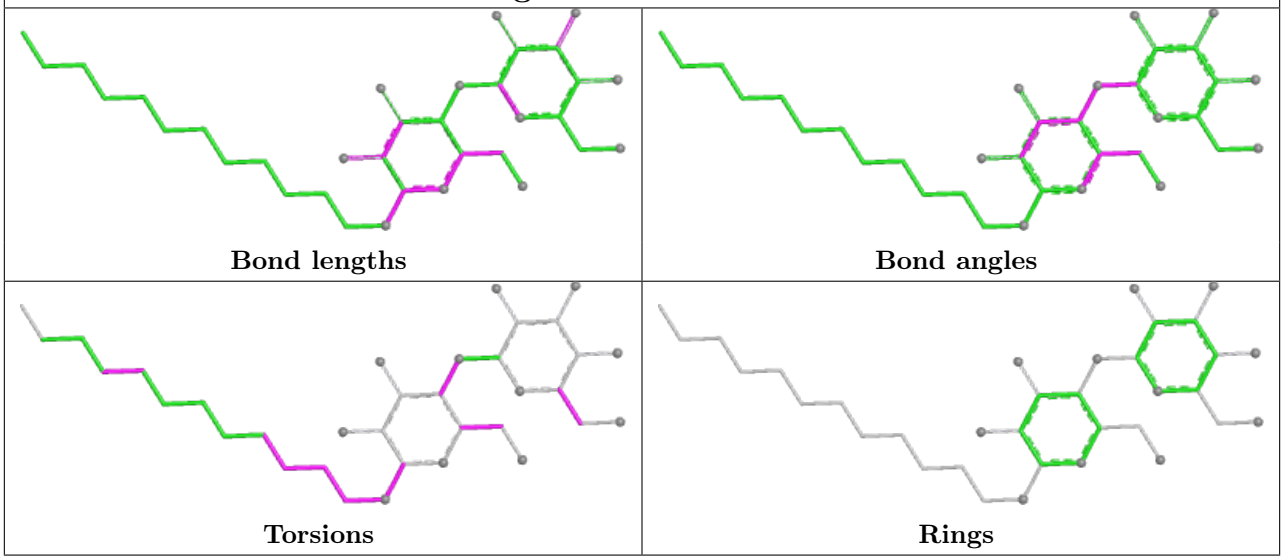
Ligand LMT A 2000



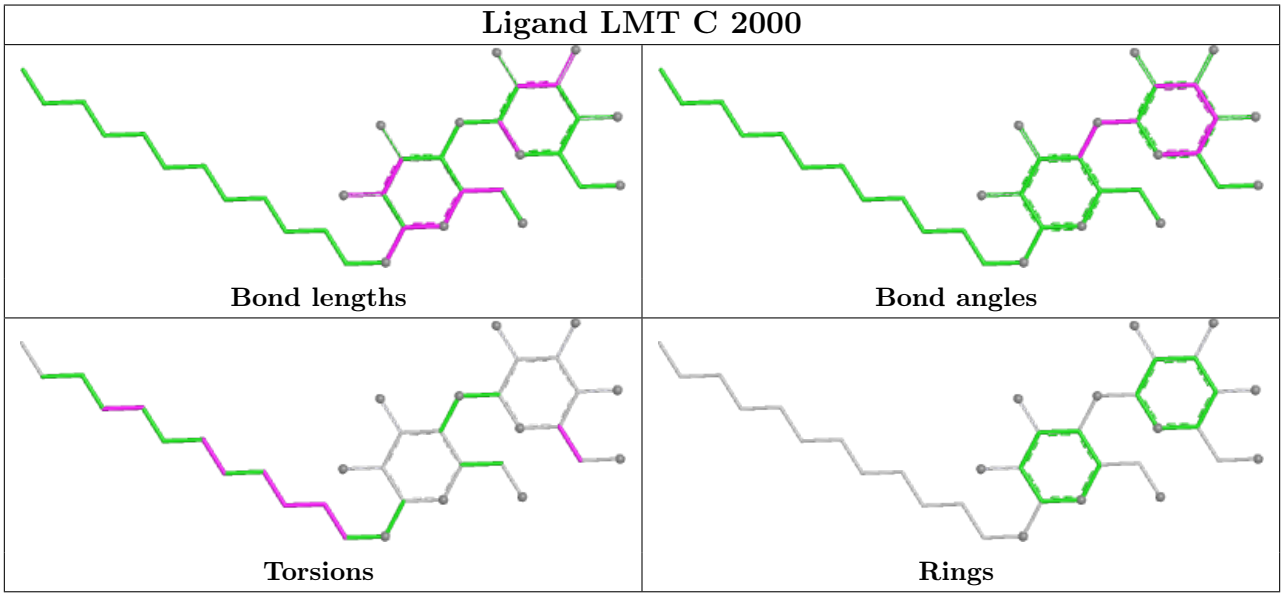
Ligand LMT F 2000



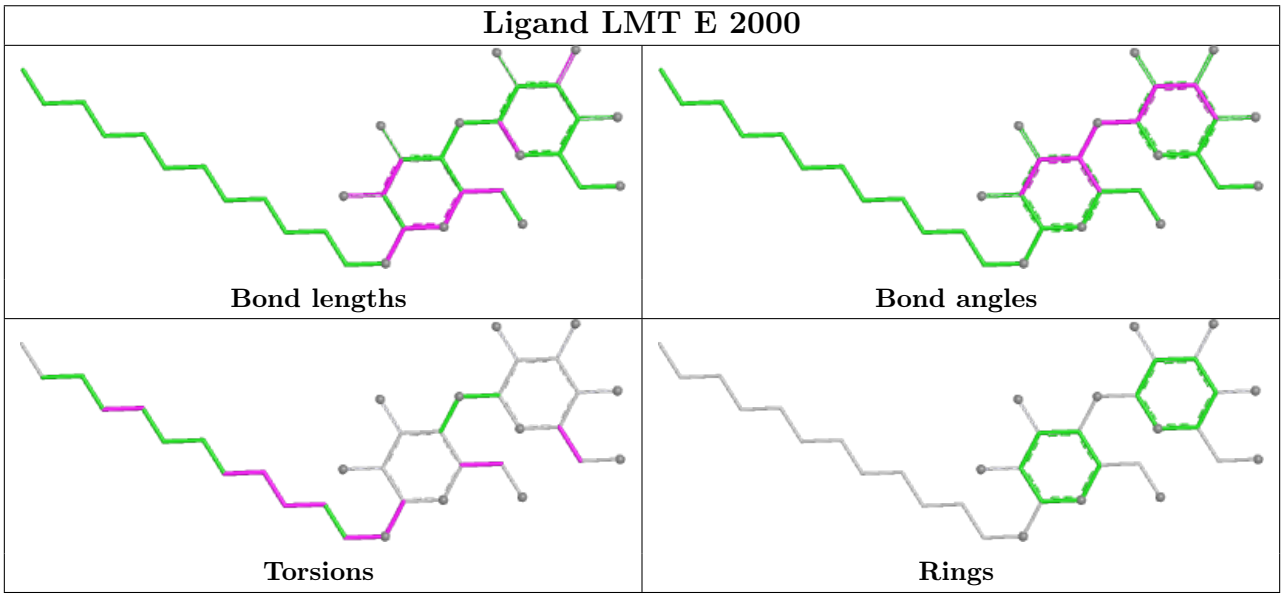
Ligand LMT B 2000



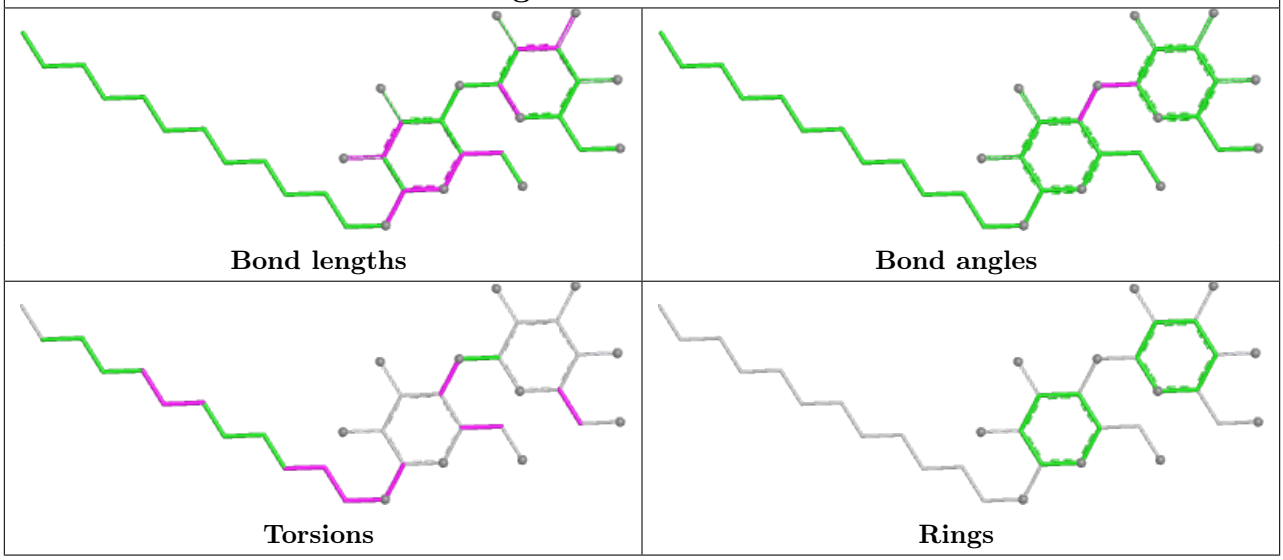
Ligand LMT C 2000



Ligand LMT E 2000



Ligand LMT D 2000



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, 95^{th} 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%)	-0.25	9 (0%)	84	72	15, 54, 96, 123	0
1	B	1042/1069 (97%)	-0.18	21 (2%)	65	49	8, 53, 102, 133	0
1	C	1044/1069 (97%)	-0.10	34 (3%)	46	32	10, 57, 103, 141	0
1	D	1044/1069 (97%)	-0.34	7 (0%)	87	78	13, 45, 89, 128	0
1	E	1042/1069 (97%)	-0.39	7 (0%)	87	78	10, 36, 75, 99	0
1	F	1044/1069 (97%)	-0.36	9 (0%)	84	72	6, 37, 71, 95	0
All	All	6260/6414 (97%)	-0.27	87 (1%)	75	60	6, 46, 93, 141	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	MET	5.5
1	C	171	GLY	5.2
1	C	116	PRO	4.7
1	B	870	GLY	4.5
1	C	856	GLY	4.2
1	E	714	THR	3.8
1	E	715	SER	3.8
1	D	833	PRO	3.7
1	F	856	GLY	3.7
1	B	869	SER	3.6
1	E	295	THR	3.4
1	C	836	SER	3.4
1	C	458	PHE	3.3
1	C	32	VAL	3.2
1	C	858	ASP	3.2
1	E	693	GLU	3.1
1	B	857	TYR	3.1
1	B	79	SER	3.1
1	C	79	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	59	ASP	3.0
1	B	836	SER	3.0
1	E	871	ASN	3.0
1	B	319	SER	3.0
1	C	817	GLU	2.9
1	E	174	ASP	2.8
1	A	708	LYS	2.8
1	B	170	SER	2.8
1	C	690	LEU	2.8
1	C	704	ALA	2.8
1	C	170	SER	2.7
1	C	820	ASN	2.7
1	C	837	THR	2.7
1	D	830	GLN	2.7
1	B	169	THR	2.7
1	C	172	VAL	2.7
1	D	714	THR	2.7
1	C	839	GLU	2.6
1	C	180	SER	2.6
1	C	55	LYS	2.6
1	D	607	GLU	2.6
1	A	148	THR	2.6
1	F	79	SER	2.6
1	B	710	PRO	2.5
1	C	117	LEU	2.5
1	F	496	MET	2.5
1	A	296	GLY	2.5
1	B	387	GLY	2.5
1	B	167	SER	2.4
1	E	180	SER	2.4
1	F	256	ASP	2.4
1	F	503	GLY	2.4
1	A	171	GLY	2.4
1	F	501	ALA	2.4
1	C	49	TYR	2.4
1	C	179	GLY	2.3
1	D	686	ASP	2.3
1	B	830	GLN	2.3
1	C	838	GLY	2.3
1	C	851	LEU	2.3
1	C	712	MET	2.3
1	D	606	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	618	ALA	2.2
1	A	871	ASN	2.2
1	A	295	THR	2.2
1	C	830	GLN	2.2
1	B	873	ALA	2.2
1	A	128	SER	2.2
1	C	607	GLU	2.2
1	C	846	GLN	2.2
1	A	678	THR	2.2
1	B	834	GLY	2.1
1	B	688	ALA	2.1
1	C	711	ASP	2.1
1	F	146	ASP	2.1
1	C	56	THR	2.1
1	C	256	ASP	2.1
1	F	836	SER	2.1
1	A	858	ASP	2.1
1	C	460	GLY	2.1
1	B	608	SER	2.1
1	B	859	TRP	2.1
1	C	678	THR	2.1
1	C	681	ASP	2.1
1	B	874	PRO	2.0
1	B	709	HIS	2.0
1	D	690	LEU	2.0
1	F	502	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

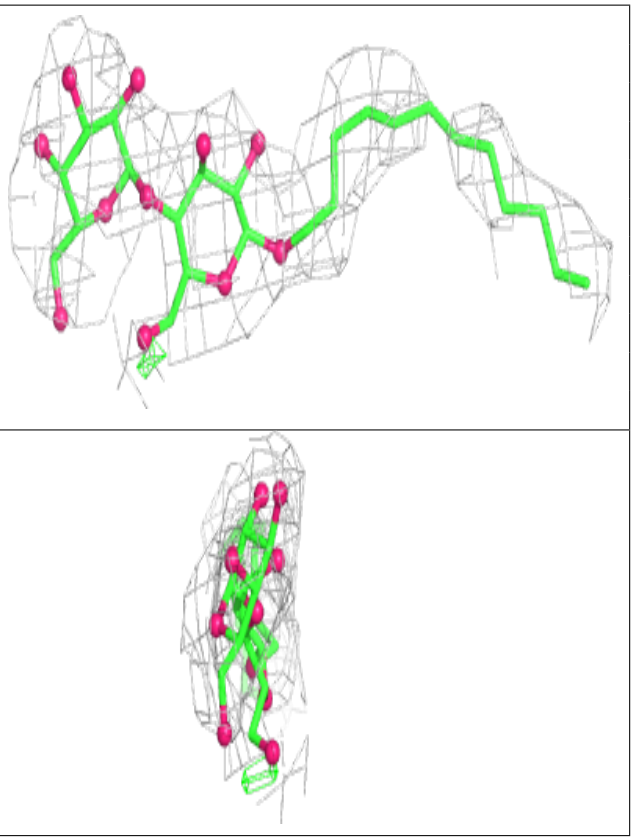
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

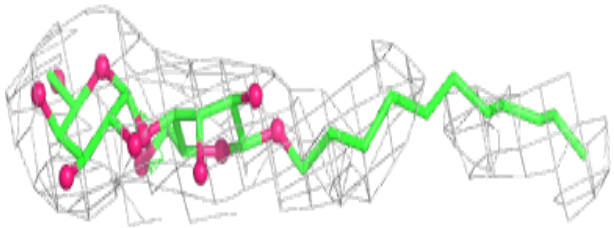
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LMT	D	2000	35/35	0.81	0.33	21,41,61,68	0
2	LMT	A	2000	35/35	0.86	0.31	11,44,65,67	0
2	LMT	E	2000	35/35	0.86	0.34	3,42,59,66	0
2	LMT	C	2000	35/35	0.87	0.43	10,44,55,59	0
2	LMT	F	2000	35/35	0.87	0.39	6,45,57,63	0
2	LMT	B	2000	35/35	0.90	0.42	2,48,54,66	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:

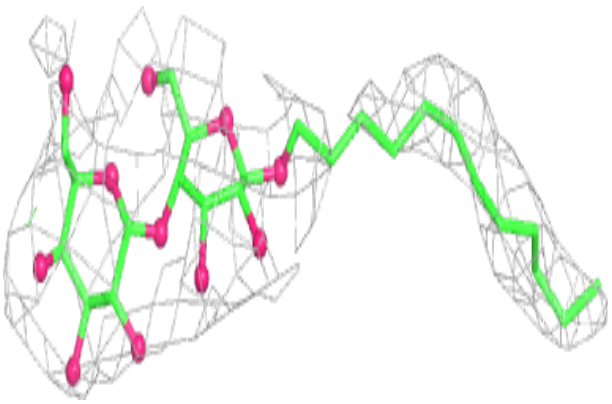
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

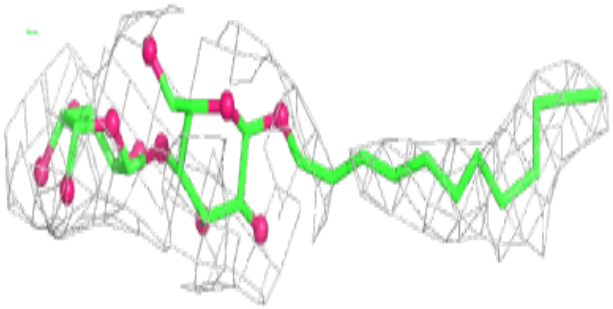




Electron density around LMT A 2000:

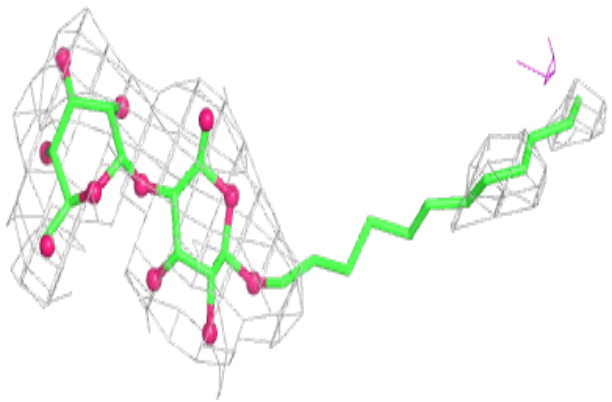
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

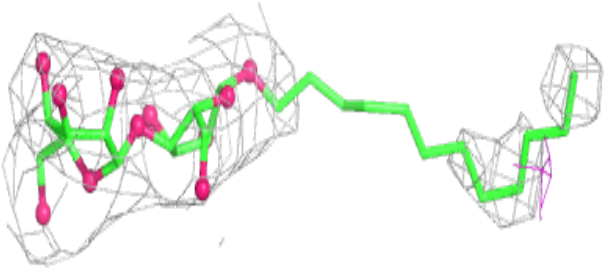


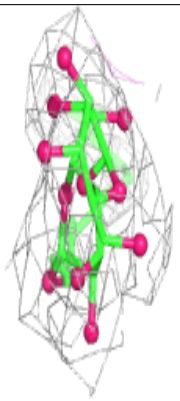


Electron density around LMT E 2000:

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

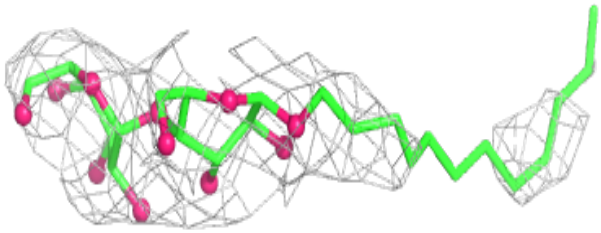


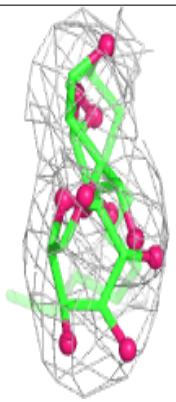




Electron density around LMT C 2000:

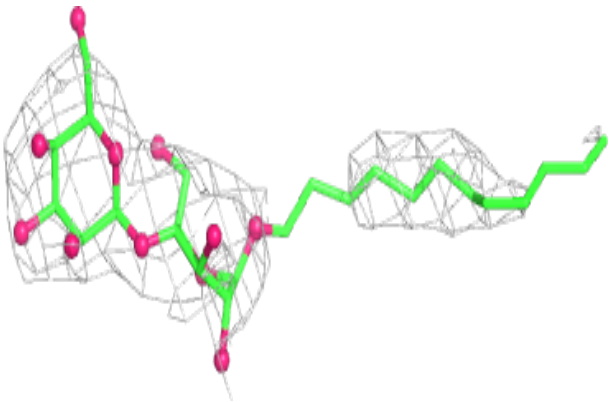
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

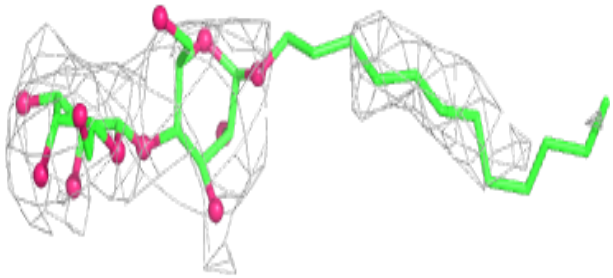


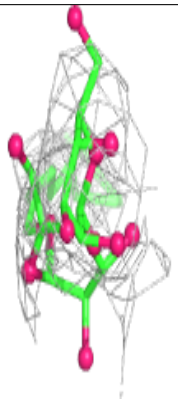


Electron density around LMT F 2000:

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







<table>
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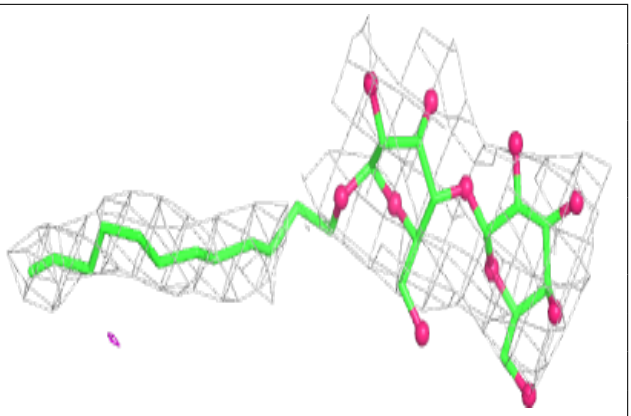
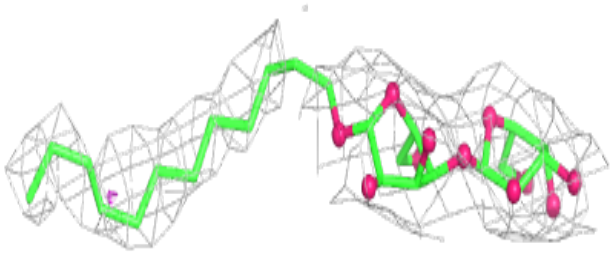
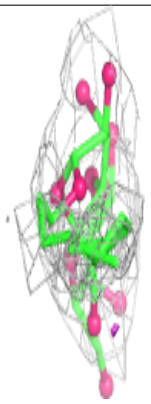
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)</td><td>  </td></tr>
<tr><td>  </td><td>  </td></tr>
</table>

6.5 Other polymers

There are no such residues in this entry.