Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2026 – 12:36 pm GMT

PDB ID	:	33WJ / pdb_000033wj
Title	:	Structural and functional evaluation of the classical RND efflux pumps inhibitor PAbN, a systematic study.
Authors	:	Wehbi, H.; Megret, M.; Phan, G.; Broutin, I.
Deposited on	:	2026-08-27
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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

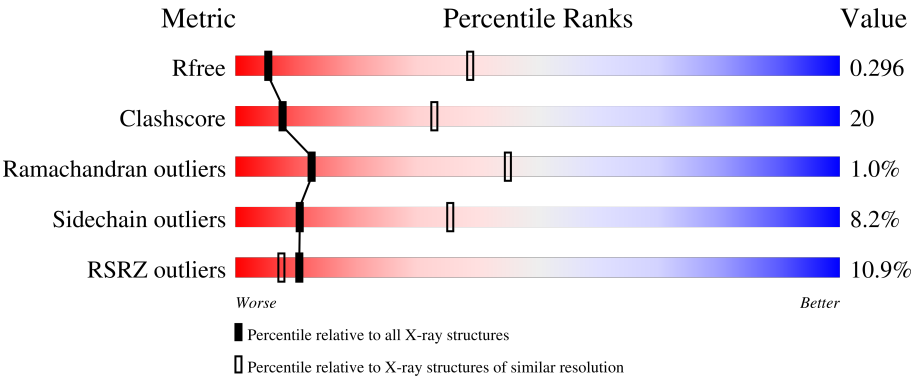
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



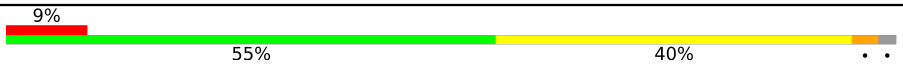
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1056	12% 54% 37%
1	B	1056	11% 56% 38%
1	C	1056	9% 57% 37%
1	D	1056	11% 55% 36%
1	E	1056	11% 57% 37%

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Mol	Chain	Length	Quality of chain
1	F	1056	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 47031 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Multidrug resistance protein MexB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1013	Total	C	N	O	S	6	0	0
			7690	4955	1276	1420	39			
1	B	1030	Total	C	N	O	S	0	0	0
			7812	5027	1299	1446	40			
1	C	1030	Total	C	N	O	S	12	0	0
			7812	5027	1299	1446	40			
1	D	1012	Total	C	N	O	S	6	0	0
			7682	4949	1275	1419	39			
1	E	1030	Total	C	N	O	S	0	0	0
			7812	5027	1299	1446	40			
1	F	1032	Total	C	N	O	S	12	0	0
			7832	5042	1302	1448	40			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	407	ASN	ASP	engineered mutation	UNP P52002
A	1047	LEU	-	expression tag	UNP P52002
A	1048	GLU	-	expression tag	UNP P52002
A	1049	HIS	-	expression tag	UNP P52002
A	1050	HIS	-	expression tag	UNP P52002
A	1051	HIS	-	expression tag	UNP P52002
A	1052	HIS	-	expression tag	UNP P52002
A	1053	HIS	-	expression tag	UNP P52002
A	1054	HIS	-	expression tag	UNP P52002
A	1055	HIS	-	expression tag	UNP P52002
A	1056	HIS	-	expression tag	UNP P52002
B	407	ASN	ASP	engineered mutation	UNP P52002
B	1047	LEU	-	expression tag	UNP P52002
B	1048	GLU	-	expression tag	UNP P52002
B	1049	HIS	-	expression tag	UNP P52002
B	1050	HIS	-	expression tag	UNP P52002
B	1051	HIS	-	expression tag	UNP P52002

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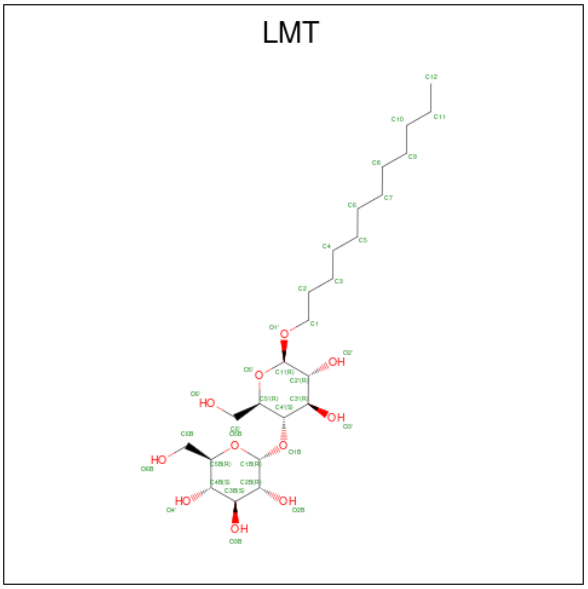
Chain	Residue	Modelled	Actual	Comment	Reference
B	1052	HIS	-	expression tag	UNP P52002
B	1053	HIS	-	expression tag	UNP P52002
B	1054	HIS	-	expression tag	UNP P52002
B	1055	HIS	-	expression tag	UNP P52002
B	1056	HIS	-	expression tag	UNP P52002
C	407	ASN	ASP	engineered mutation	UNP P52002
C	1047	LEU	-	expression tag	UNP P52002
C	1048	GLU	-	expression tag	UNP P52002
C	1049	HIS	-	expression tag	UNP P52002
C	1050	HIS	-	expression tag	UNP P52002
C	1051	HIS	-	expression tag	UNP P52002
C	1052	HIS	-	expression tag	UNP P52002
C	1053	HIS	-	expression tag	UNP P52002
C	1054	HIS	-	expression tag	UNP P52002
C	1055	HIS	-	expression tag	UNP P52002
C	1056	HIS	-	expression tag	UNP P52002
D	407	ASN	ASP	engineered mutation	UNP P52002
D	1047	LEU	-	expression tag	UNP P52002
D	1048	GLU	-	expression tag	UNP P52002
D	1049	HIS	-	expression tag	UNP P52002
D	1050	HIS	-	expression tag	UNP P52002
D	1051	HIS	-	expression tag	UNP P52002
D	1052	HIS	-	expression tag	UNP P52002
D	1053	HIS	-	expression tag	UNP P52002
D	1054	HIS	-	expression tag	UNP P52002
D	1055	HIS	-	expression tag	UNP P52002
D	1056	HIS	-	expression tag	UNP P52002
E	407	ASN	ASP	engineered mutation	UNP P52002
E	1047	LEU	-	expression tag	UNP P52002
E	1048	GLU	-	expression tag	UNP P52002
E	1049	HIS	-	expression tag	UNP P52002
E	1050	HIS	-	expression tag	UNP P52002
E	1051	HIS	-	expression tag	UNP P52002
E	1052	HIS	-	expression tag	UNP P52002
E	1053	HIS	-	expression tag	UNP P52002
E	1054	HIS	-	expression tag	UNP P52002
E	1055	HIS	-	expression tag	UNP P52002
E	1056	HIS	-	expression tag	UNP P52002
F	407	ASN	ASP	engineered mutation	UNP P52002
F	1047	LEU	-	expression tag	UNP P52002
F	1048	GLU	-	expression tag	UNP P52002
F	1049	HIS	-	expression tag	UNP P52002

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1050	HIS	-	expression tag	UNP P52002
F	1051	HIS	-	expression tag	UNP P52002
F	1052	HIS	-	expression tag	UNP P52002
F	1053	HIS	-	expression tag	UNP P52002
F	1054	HIS	-	expression tag	UNP P52002
F	1055	HIS	-	expression tag	UNP P52002
F	1056	HIS	-	expression tag	UNP P52002

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



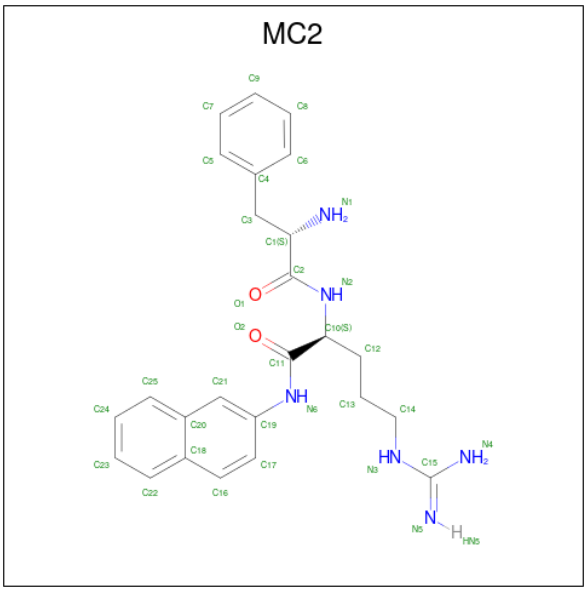
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	A	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		

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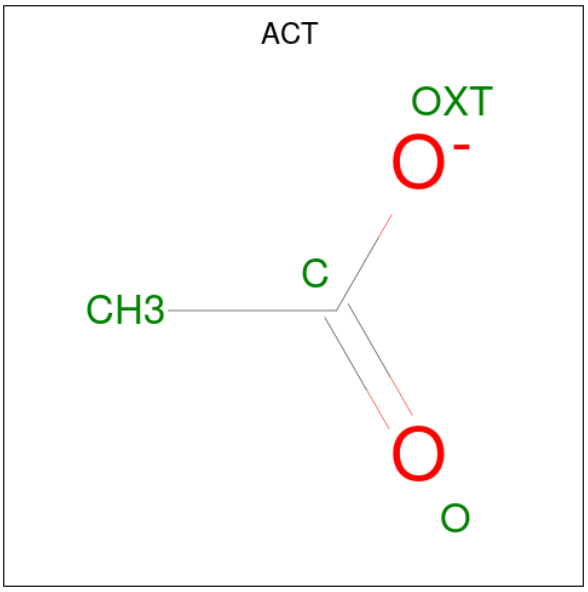
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0
2	E	1	Total C O 35 24 11	0	0

- Molecule 3 is N2-(L-PHENYLALANYL)-N1-(NAPHTHALENYL)-L-ARIGNINAMIDE (CCD ID: MC2) (formula: $C_{25}H_{30}N_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 33 25 6 2	0	0

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0

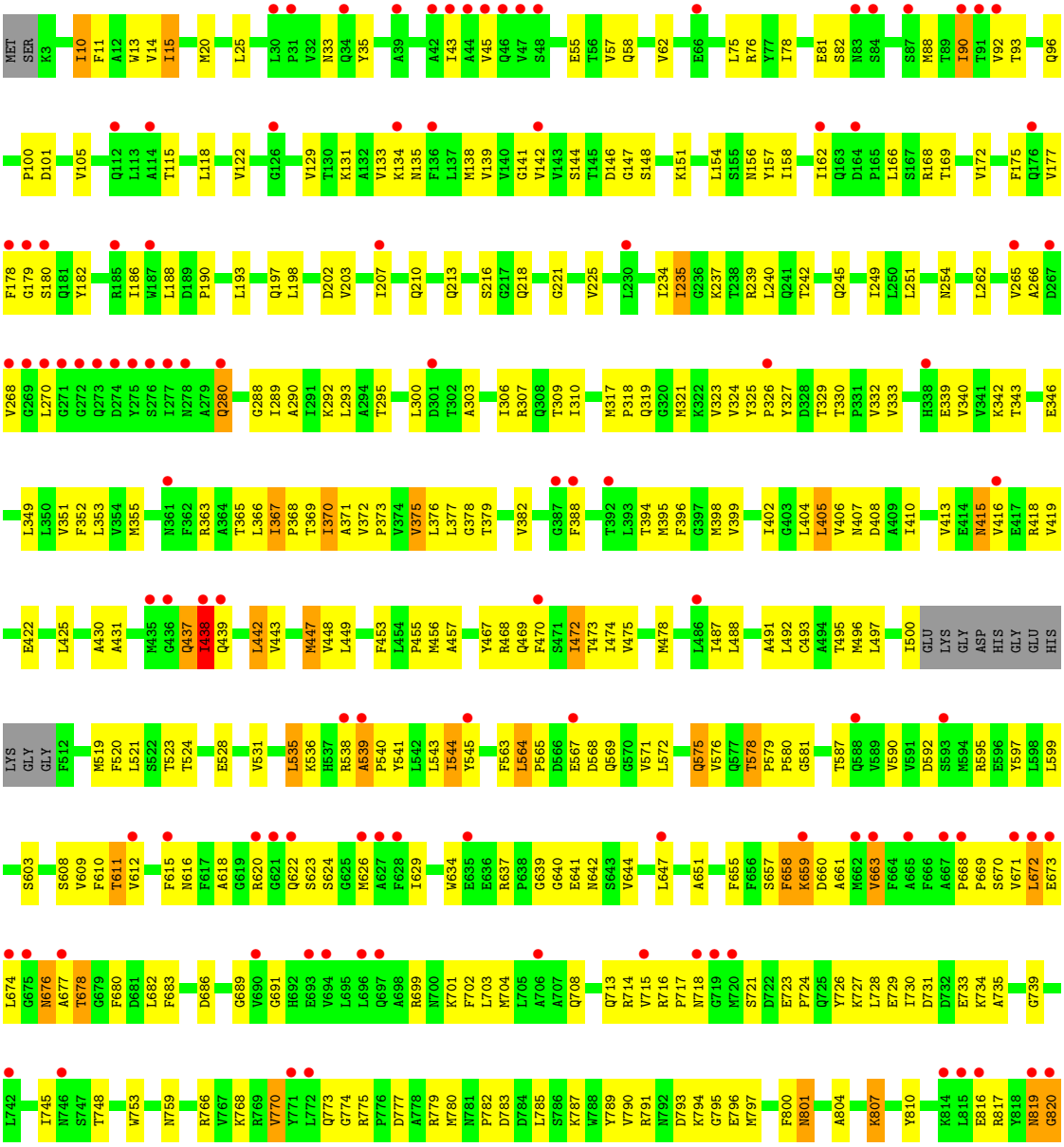
3 Residue-property plots (i)

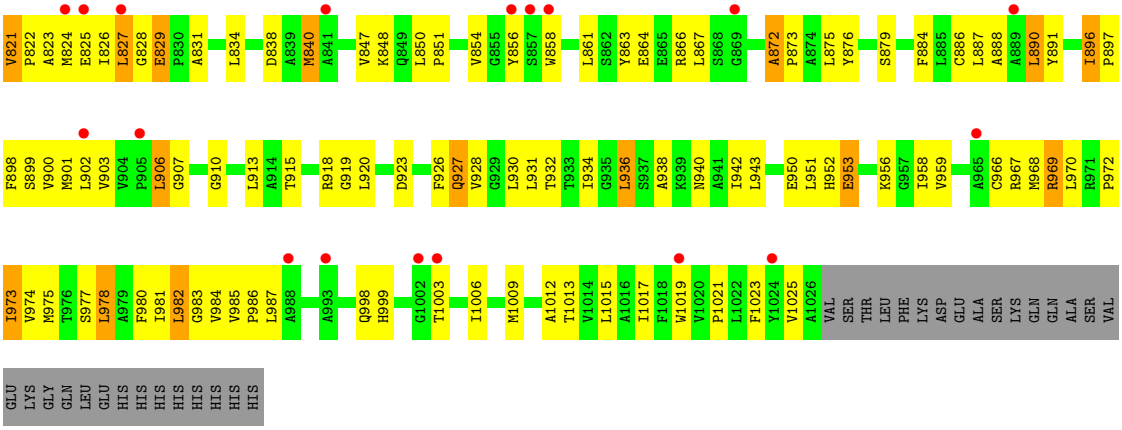
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:



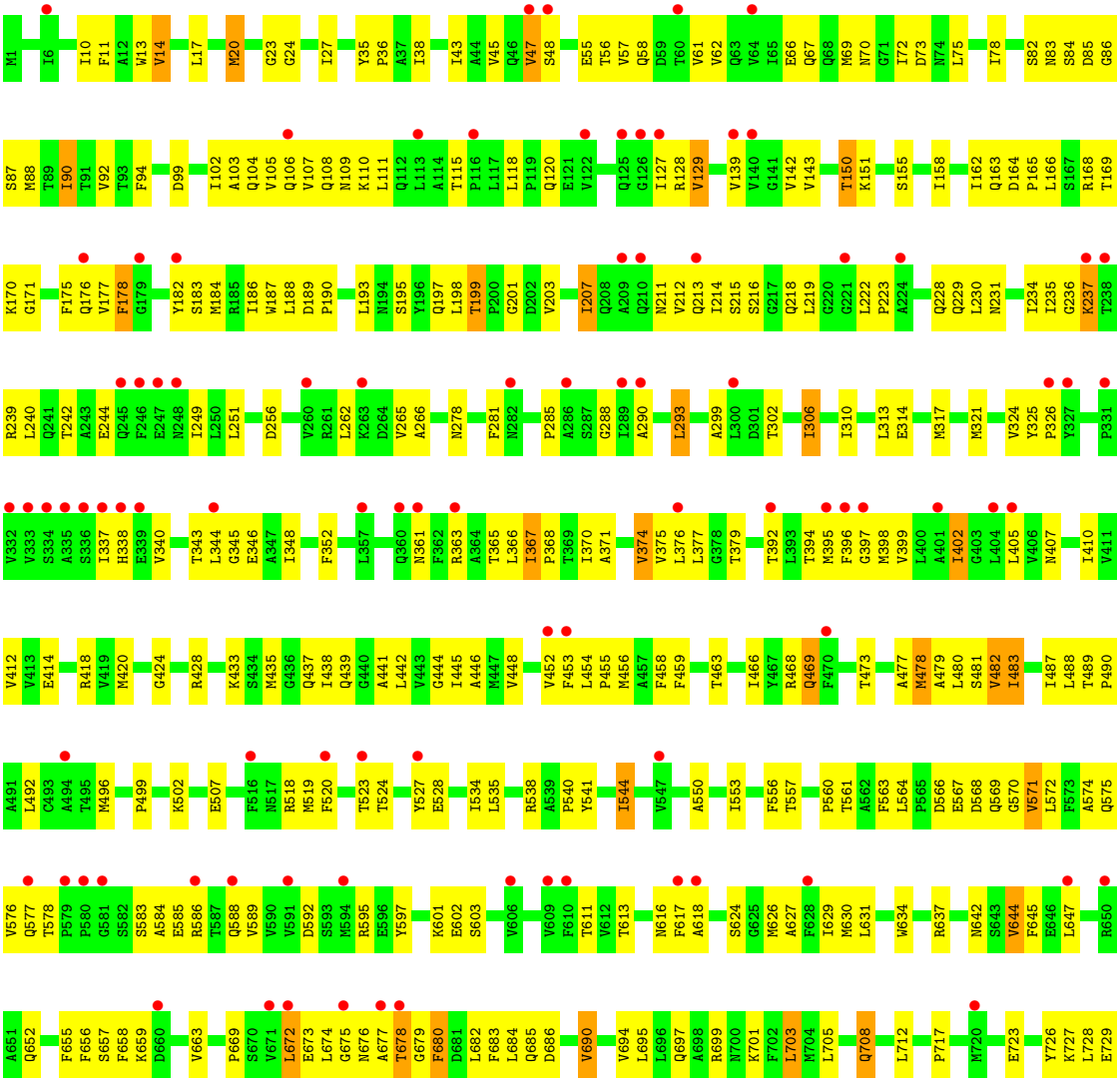


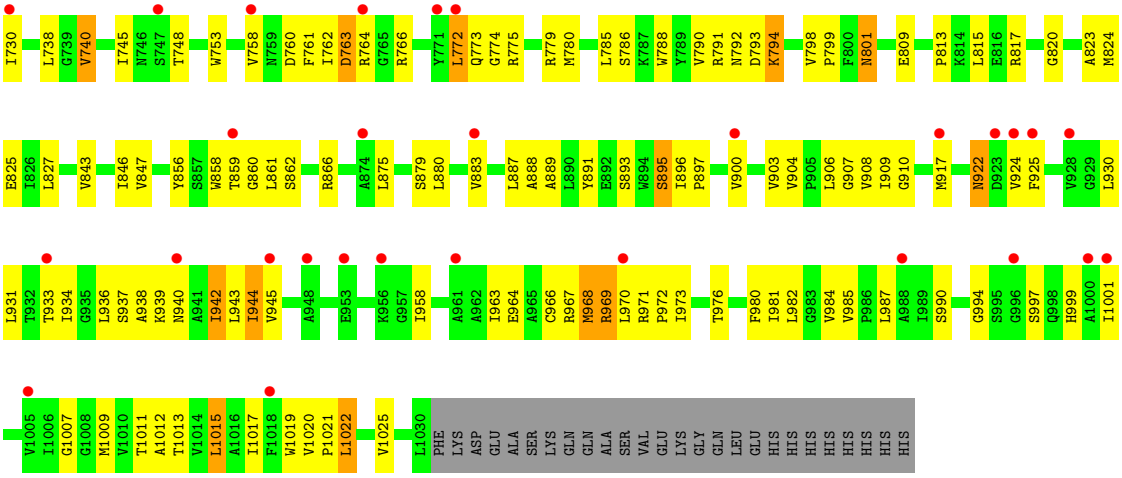


• Molecule 1: Multidrug resistance protein MexB

Chain B:



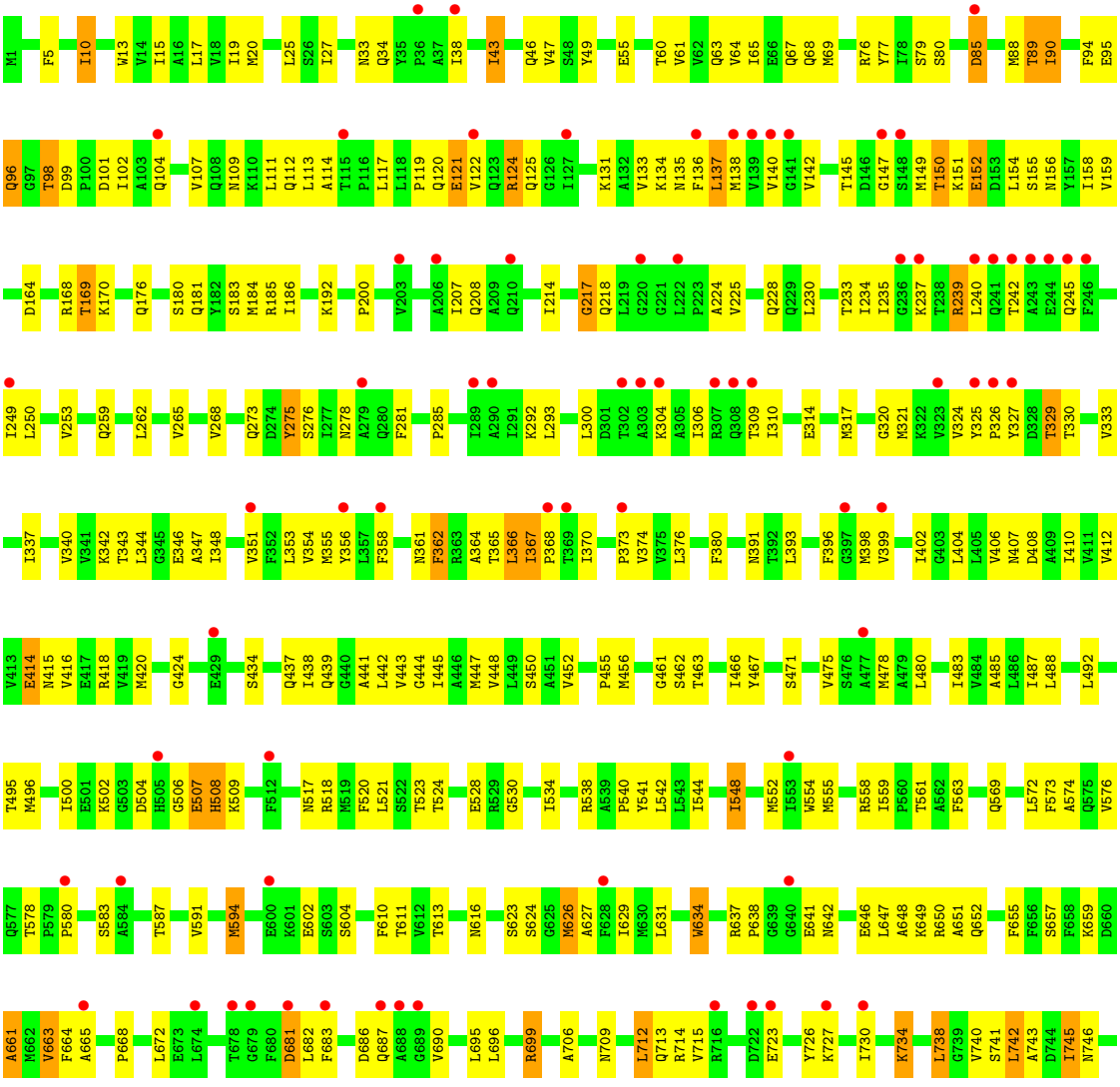


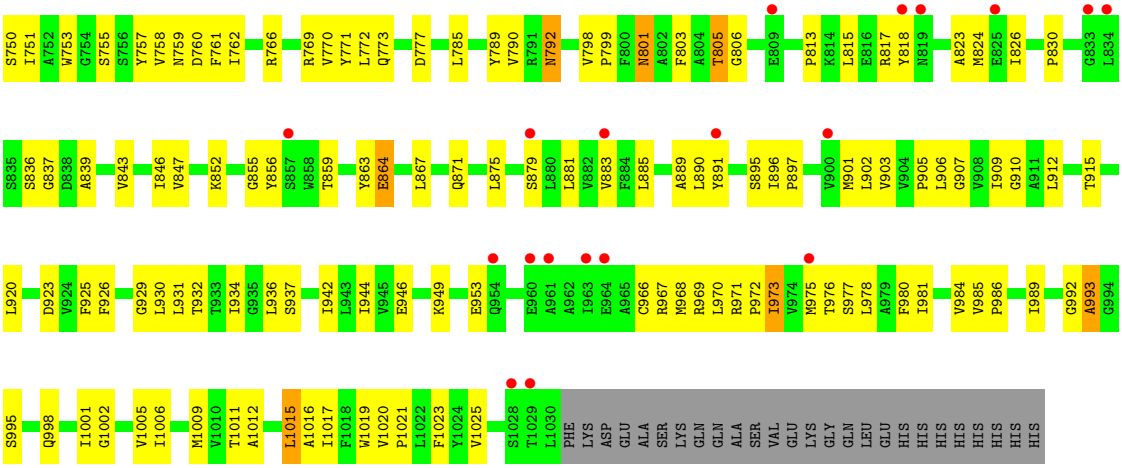


• Molecule 1: Multidrug resistance protein MexB

Chain C:



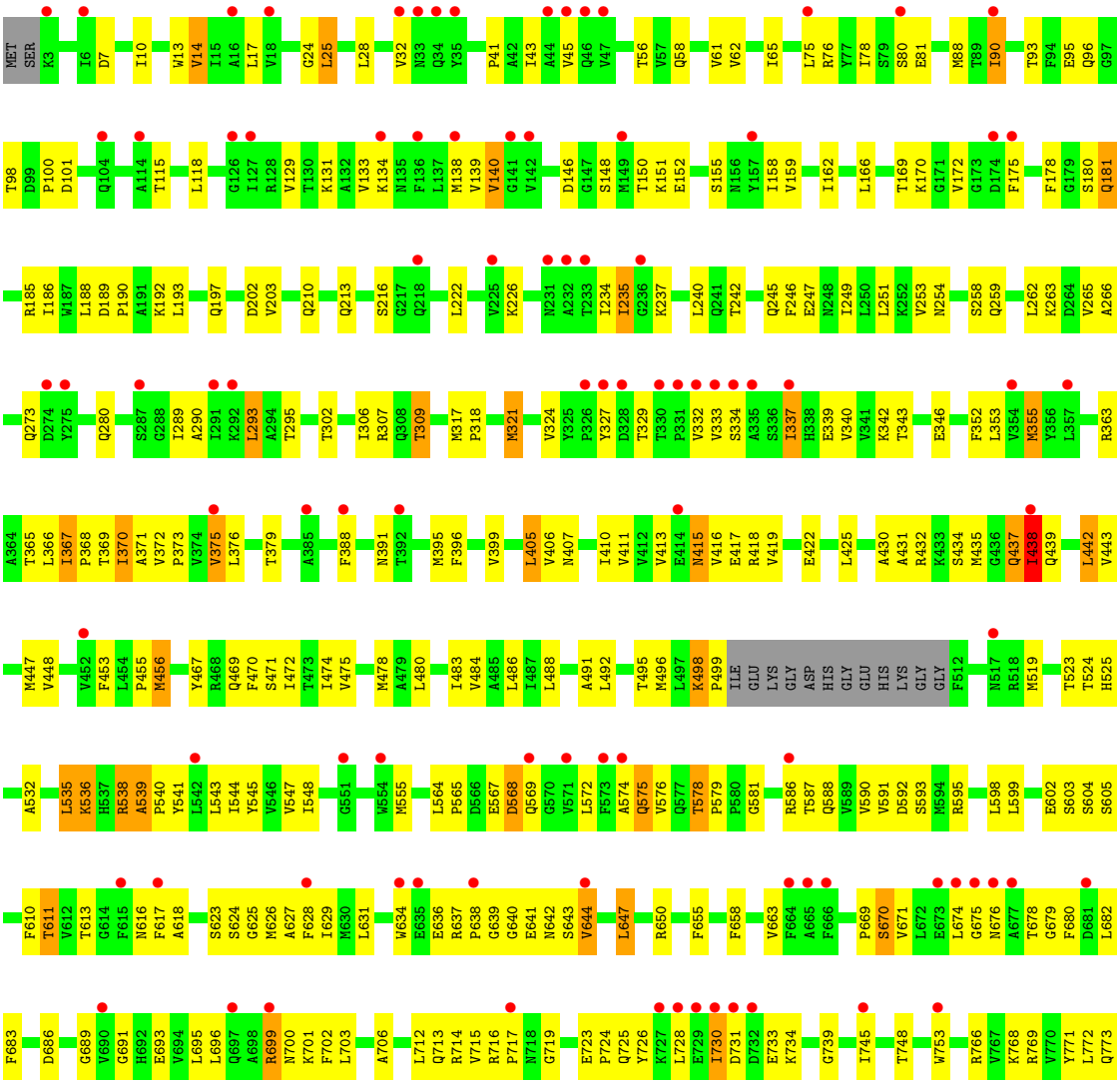


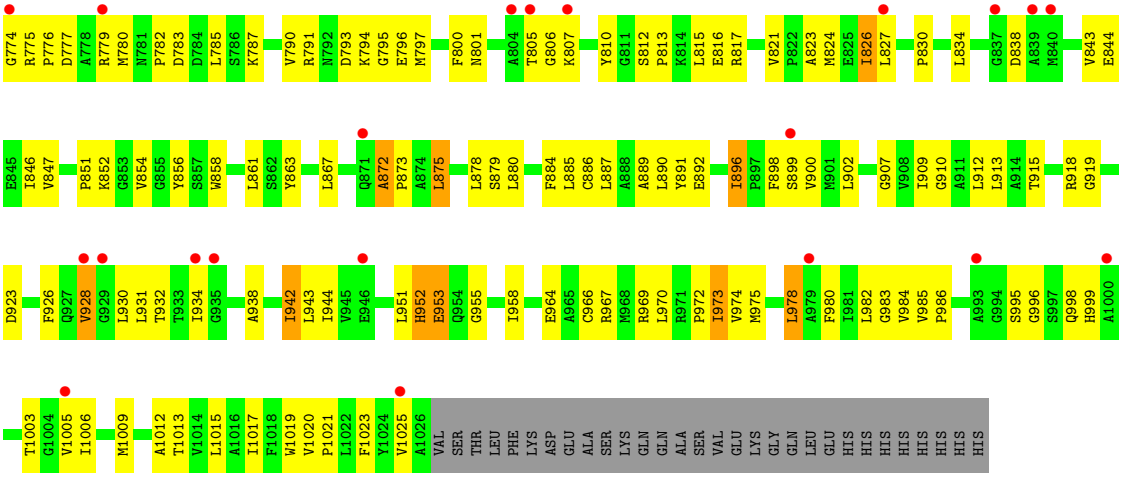


- Molecule 1: Multidrug resistance protein MexB

Chain D:



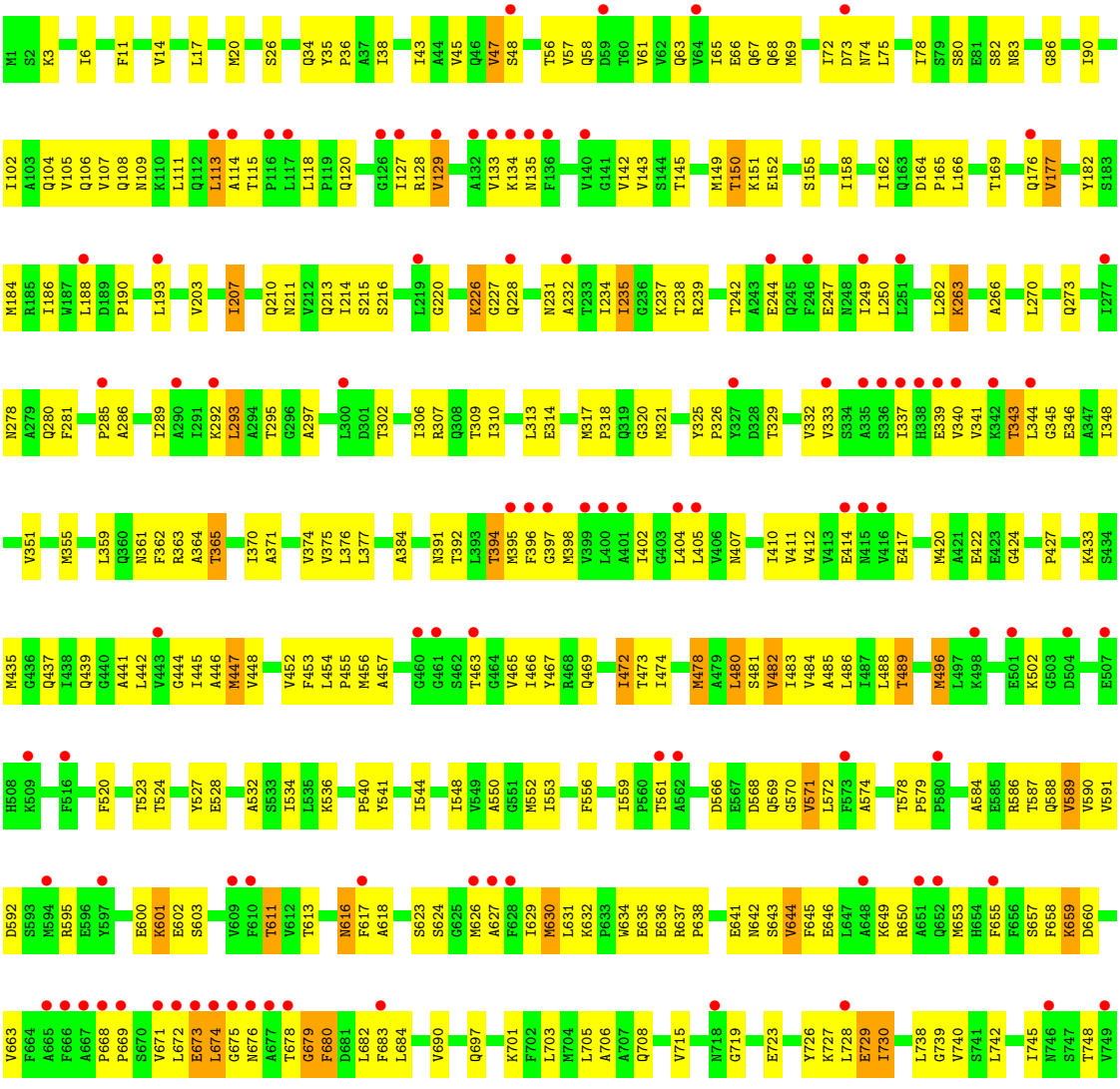


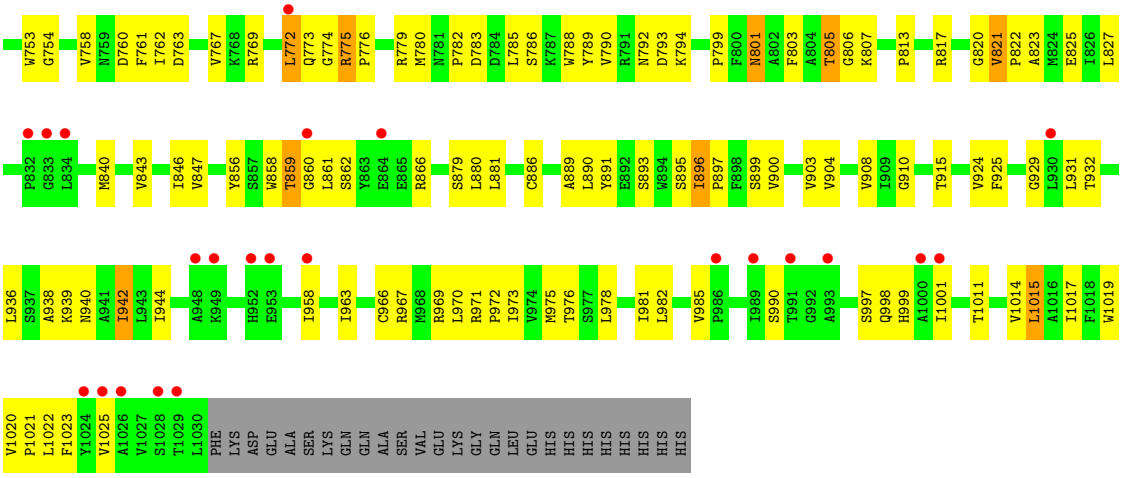


• Molecule 1: Multidrug resistance protein MexB

Chain E:



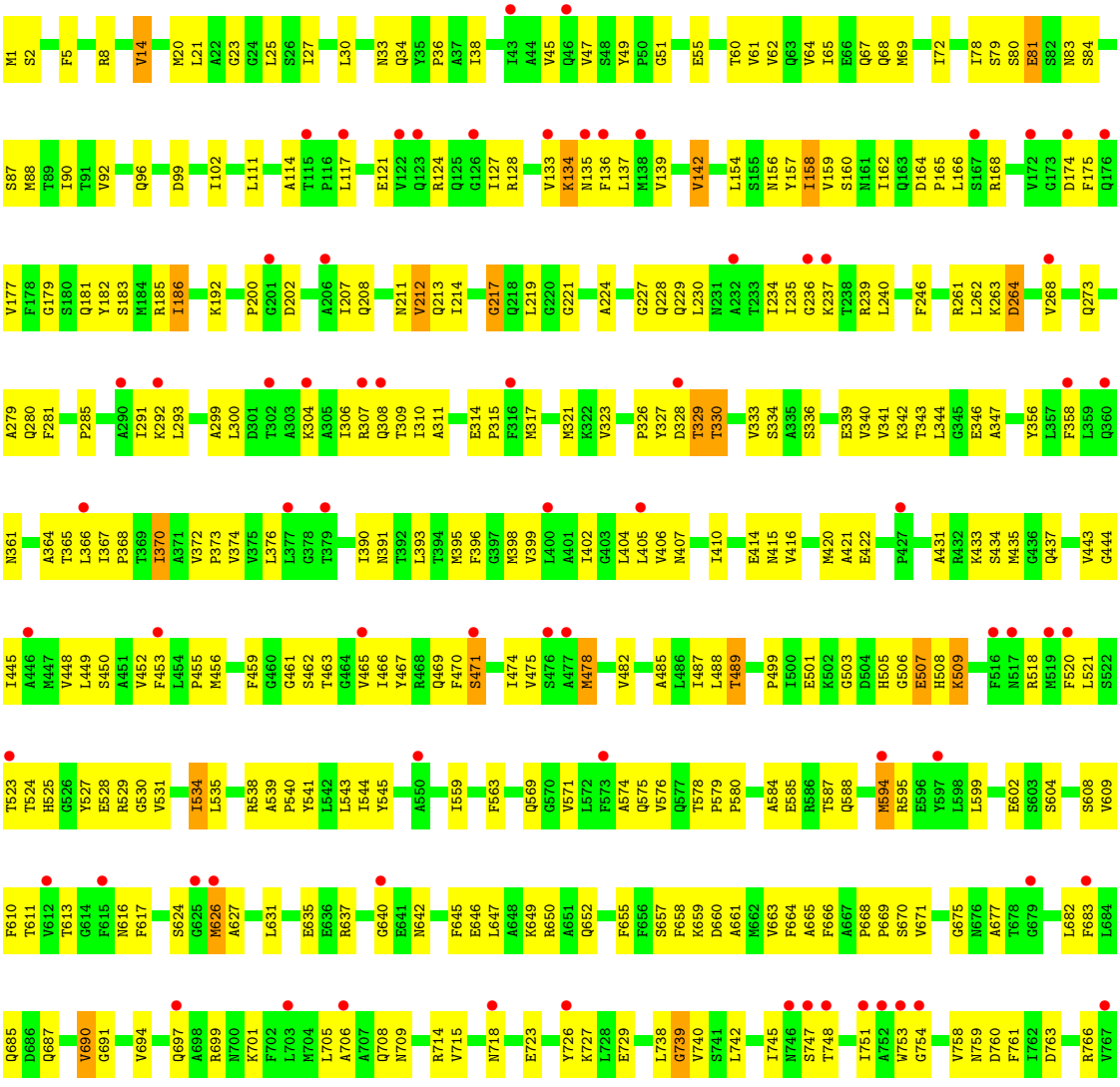


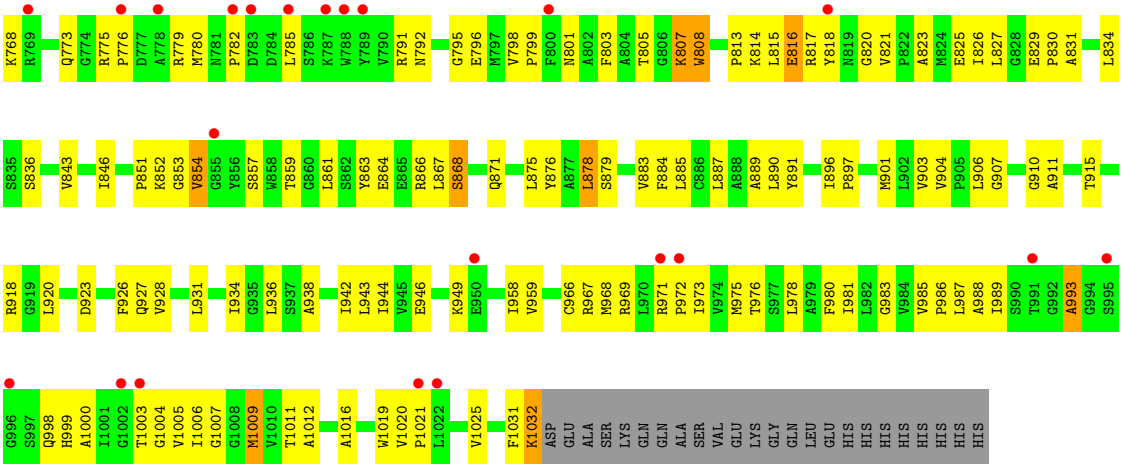


• Molecule 1: Multidrug resistance protein MexB

Chain F:






K768 R769 Q773 G774 R775 P776 D777 A778 R779 M780 N781 P782 D783 D784 L785 S786 K787 W788 Y789 V790 R791 N792 G795 E796 M797 V798 P799 F800 N801 A802 F803 A804 T805 G806 K807 W808 P813 K814 L815 E816 R817 Y818 N819 G820 V821 P822 A823 M824 E825 I826 L827 G828 E829 P830 A831 L834
S835 S836 V843 I846 P851 K852 G853 V854 G855 Y856 S857 W858 T859 G860 L861 S862 Y863 E864 E865 R866 L867 S868 Q871 L875 Y876 A877 L878 S879 V883 F884 L885 C886 L887 A888 A889 L890 Y891 I896 P897 M901 L902 V903 V904 P905 L906 G907 G910 A911 T915
R918 G919 L920 D923 F926 Q927 V928 L931 I934 G935 L936 S937 A938 I942 L943 I944 V945 E946 K949 E950 I958 V959 C966 R967 M968 R969 L970 R971 P972 I973 V974 M975 T976 S977 L978 A979 F980 I981 L982 G983 V984 V985 P986 L987 A988 I989 S990 T991 G992 A993 G994 S995
G996 S997 Q998 H999 A1000 I1001 G1002 T1003 G1004 V1005 I1006 G1007 G1008 M1009 V1010 T1011 A1012 A1016 W1019 V1020 P1021 L1022 V1025 F1031 K1032 ASP GLU ALA SER LYS GLN GLN ALA SER VAL GLU LYS GLY GLN LEU GLU HIS HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	125.93Å 135.71Å 153.21Å 86.19° 69.11° 87.56°	Depositor
Resolution (Å)	45.81 – 3.56 45.81 – 3.56	Depositor EDS
% Data completeness (in resolution range)	92.5 (45.81-3.56) 92.7 (45.81-3.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.285 , 0.297 0.279 , 0.296	Depositor DCC
R_{free} test set	1711 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	109.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 65.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	47031	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, ACT, MC2

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	0.26	0/7846	0.61	1/10666 (0.0%)
1	B	0.26	0/7971	0.59	0/10833
1	C	0.25	0/7971	0.59	0/10833
1	D	0.24	0/7838	0.60	0/10655
1	E	0.25	0/7971	0.60	1/10833 (0.0%)
1	F	0.26	0/7992	0.58	0/10860
All	All	0.26	0/47589	0.59	2/64680 (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	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	820	GLY	N-CA-C	-5.65	108.25	115.42
1	E	602	GLU	N-CA-C	-5.02	106.90	112.57

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	678	THR	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	7690	0	7828	336	0
1	B	7812	0	7946	329	0
1	C	7812	0	7946	311	0
1	D	7682	0	7817	320	0
1	E	7812	0	7946	310	0
1	F	7832	0	7968	360	0
2	A	70	0	92	5	0
2	B	140	0	184	7	0
2	D	70	0	92	8	0
2	E	70	0	92	6	0
3	B	33	0	29	3	0
4	C	4	0	3	0	0
4	F	4	0	3	0	0
All	All	47031	0	47946	1885	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 20.

All (1885) 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:F:414:GLU:HG2	1:F:972:PRO:HG3	1.41	1.01
1:B:617:PHE:HB3	3:B:1101:MC2:H17	1.46	0.97
1:E:446:ALA:HB2	1:E:482:VAL:HG21	1.53	0.90
1:F:738:LEU:HB2	1:F:803:PHE:HZ	1.36	0.88
1:A:135:ASN:HA	1:A:674:LEU:HG	1.55	0.88
1:E:38:ILE:HD11	1:E:671:VAL:HG21	1.53	0.87
1:F:317:MET:HE2	1:F:321:MET:HG2	1.56	0.87
1:A:724:PRO:HA	1:A:810:TYR:HB2	1.54	0.87
1:B:78:ILE:HD11	1:B:90:ILE:HD11	1.55	0.87
1:B:14:VAL:HG11	1:C:889:ALA:HB2	1.55	0.87
1:E:774:GLY:O	1:E:779:ARG:NH1	2.08	0.87
1:D:794:LYS:O	1:D:796:GLU:N	2.07	0.86
1:F:604:SER:O	1:F:642:ASN:ND2	2.08	0.86
1:D:730:ILE:HD11	1:F:237:LYS:HD3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:774:GLY:O	1:B:779:ARG:NH1	2.09	0.85
1:A:682:LEU:HD21	1:A:856:TYR:HB2	1.58	0.85
1:B:249:ILE:HD11	1:B:262:LEU:HD12	1.59	0.85
1:D:900:VAL:HG21	1:D:942:ILE:HD13	1.57	0.84
1:D:419:VAL:HG23	1:D:430:ALA:HB1	1.60	0.84
1:A:780:MET:HE1	1:C:224:ALA:HA	1.59	0.84
1:E:641:GLU:O	1:E:650:ARG:NH2	2.10	0.84
1:E:278:ASN:HB2	1:E:613:THR:HG22	1.59	0.84
1:A:639:GLY:O	1:A:641:GLU:N	2.10	0.83
1:D:139:VAL:HG12	1:D:327:TYR:HB3	1.58	0.83
1:F:185:ARG:HH21	1:F:773:GLN:HB2	1.40	0.83
1:A:708:GLN:HB2	1:D:807:LYS:HD3	1.59	0.82
1:C:641:GLU:O	1:C:650:ARG:NH2	2.13	0.81
1:B:412:VAL:HG13	1:B:435:MET:HE1	1.62	0.81
1:E:376:LEU:HD21	1:E:402:ILE:HD11	1.60	0.81
1:C:253:VAL:HG13	1:C:259:GLN:HG2	1.63	0.81
1:D:175:PHE:HB2	1:D:289:ILE:HD11	1.63	0.81
1:A:794:LYS:O	1:A:796:GLU:N	2.12	0.80
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.62	0.80
1:A:372:VAL:HG22	1:A:405:LEU:HD21	1.63	0.80
1:D:317:MET:HE2	1:D:321:MET:HG3	1.63	0.80
1:A:581:GLY:N	1:A:723:GLU:OE1	2.13	0.79
1:F:96:GLN:NE2	1:F:462:SER:OG	2.15	0.79
1:C:903:VAL:HG21	1:C:1020:VAL:HG22	1.65	0.79
1:C:414:GLU:HG2	1:C:972:PRO:HG3	1.63	0.79
1:B:216:SER:HB3	1:B:236:GLY:HA2	1.65	0.79
1:D:140:VAL:HG23	1:D:289:ILE:HG23	1.64	0.79
1:A:419:VAL:HG23	1:A:430:ALA:HB1	1.64	0.79
1:E:1014:VAL:HG13	1:E:1015:LEU:HD13	1.65	0.78
1:F:875:LEU:HD11	1:F:931:LEU:HD11	1.64	0.78
1:E:344:LEU:HD22	1:E:376:LEU:HD11	1.64	0.78
1:B:682:LEU:HD11	1:B:856:TYR:HD2	1.48	0.78
1:B:344:LEU:HD22	1:B:376:LEU:HD11	1.66	0.77
1:A:918:ARG:HH21	1:A:1003:THR:HB	1.49	0.77
1:E:45:VAL:HG22	1:E:129:VAL:HG12	1.67	0.77
1:B:407:ASN:HD22	1:B:936:LEU:HD22	1.49	0.77
1:F:280:GLN:HG2	1:F:285:PRO:HA	1.66	0.76
1:D:682:LEU:HD21	1:D:856:TYR:HB2	1.67	0.76
1:D:943:LEU:HB3	1:D:969:ARG:NH1	1.99	0.76
1:D:456:MET:HG3	1:D:467:TYR:HB3	1.67	0.76
1:E:682:LEU:HD11	1:E:856:TYR:HD2	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:925:PHE:HB3	1:E:1001:ILE:HG23	1.67	0.76
1:C:742:LEU:HD13	1:C:746:ASN:HD21	1.51	0.76
1:D:151:LYS:NZ	1:D:178:PHE:O	2.19	0.75
1:D:370:ILE:HD11	1:D:492:LEU:HD11	1.67	0.75
1:A:372:VAL:HA	1:A:405:LEU:HD11	1.68	0.75
1:D:367:ILE:HG23	1:D:368:PRO:HD3	1.68	0.75
1:E:569:GLN:O	1:E:571:VAL:N	2.15	0.75
1:A:810:TYR:HE1	1:D:701:LYS:HE3	1.50	0.75
1:A:567:GLU:HB2	1:A:670:SER:HB3	1.68	0.75
1:F:459:PHE:HB3	1:F:871:GLN:HE21	1.51	0.75
1:B:966:CYS:SG	1:B:1021:PRO:HG3	2.26	0.75
1:F:727:LYS:HB3	1:F:807:LYS:HB3	1.68	0.75
1:D:943:LEU:HB3	1:D:969:ARG:HH12	1.51	0.74
1:E:410:ILE:HD11	1:E:976:THR:HG22	1.69	0.74
1:B:379:THR:HG21	1:B:477:ALA:HA	1.69	0.74
1:C:151:LYS:HG2	1:C:285:PRO:HB3	1.67	0.74
1:B:900:VAL:HG11	1:B:942:ILE:HG23	1.70	0.74
1:C:580:PRO:HB3	1:C:723:GLU:HG2	1.68	0.74
1:E:63:GLN:HG2	1:E:817:ARG:HH12	1.53	0.74
1:A:151:LYS:NZ	1:A:178:PHE:O	2.19	0.74
1:F:158:ILE:HD11	1:F:177:VAL:HG13	1.70	0.74
1:A:355:MET:HE1	1:A:406:VAL:HG11	1.69	0.74
1:E:186:ILE:HD11	1:E:772:LEU:HG	1.69	0.74
1:A:969:ARG:O	1:A:973:ILE:HG12	1.88	0.74
1:D:581:GLY:N	1:D:723:GLU:OE1	2.21	0.73
1:D:723:GLU:HG3	1:D:813:PRO:HG3	1.70	0.73
1:A:317:MET:HE2	1:A:321:MET:HG3	1.69	0.73
1:C:19:ILE:HD11	1:C:374:VAL:HG12	1.70	0.73
1:F:918:ARG:NH2	1:F:988:ALA:O	2.21	0.73
1:B:45:VAL:HB	1:B:90:ILE:HG23	1.70	0.73
1:B:569:GLN:O	1:B:571:VAL:N	2.16	0.73
1:E:592:ASP:OD1	1:E:595:ARG:NH2	2.21	0.73
1:A:456:MET:HE3	1:A:931:LEU:HD12	1.67	0.73
1:A:918:ARG:O	1:A:920:LEU:N	2.21	0.73
1:A:139:VAL:HG12	1:A:327:TYR:HB3	1.70	0.73
1:D:32:VAL:HG11	1:D:337:ILE:HD13	1.69	0.73
1:D:713:GLN:HE21	1:D:714:ARG:HD2	1.54	0.73
1:E:650:ARG:HA	1:E:653:MET:HE2	1.70	0.73
1:A:669:PRO:HB3	1:A:678:THR:HG22	1.70	0.72
1:A:332:VAL:HG21	1:A:569:GLN:HA	1.71	0.72
1:C:574:ALA:HB3	1:C:627:ALA:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PHE:HB2	1:A:289:ILE:HD11	1.70	0.72
1:C:561:THR:HG23	1:C:837:GLY:HA3	1.71	0.72
1:D:456:MET:HG2	1:D:471:SER:HB2	1.72	0.72
1:F:81:GLU:HB2	1:F:814:LYS:HE3	1.71	0.72
1:C:604:SER:O	1:C:642:ASN:ND2	2.22	0.72
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.70	0.72
1:F:422:GLU:HG2	1:F:505:HIS:NE2	2.05	0.72
1:A:616:ASN:HB2	1:A:624:SER:HB2	1.72	0.72
1:B:925:PHE:HB3	1:B:1001:ILE:HG23	1.72	0.71
1:E:414:GLU:CD	1:E:972:PRO:HG3	2.14	0.71
1:A:367:ILE:HG23	1:A:368:PRO:HD3	1.72	0.71
1:A:578:THR:HG22	1:A:579:PRO:HD2	1.71	0.71
1:B:527:TYR:HE2	1:B:966:CYS:HB3	1.54	0.71
1:D:7:ASP:OD2	1:D:432:ARG:NH2	2.19	0.71
1:B:891:TYR:HB3	1:B:896:ILE:HD11	1.71	0.71
1:C:152:GLU:O	1:C:156:ASN:ND2	2.23	0.71
1:B:182:TYR:HD2	1:B:764:ARG:HH22	1.36	0.71
1:A:186:ILE:HG13	1:A:268:VAL:HG22	1.72	0.71
1:D:62:VAL:HG22	1:D:88:MET:HE2	1.73	0.71
1:D:604:SER:O	1:D:642:ASN:ND2	2.24	0.71
1:E:524:THR:HG22	1:E:970:LEU:HD13	1.73	0.71
1:E:938:ALA:O	1:E:942:ILE:HG12	1.90	0.70
1:D:544:ILE:HG23	1:D:1019:TRP:HH2	1.56	0.70
1:E:753:TRP:HZ2	1:E:785:LEU:HA	1.56	0.70
1:A:370:ILE:HD11	1:A:492:LEU:HD11	1.73	0.70
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.72	0.70
1:B:766:ARG:HH22	1:C:67:GLN:HE22	1.39	0.70
1:E:317:MET:HE3	1:E:321:MET:HB3	1.72	0.70
1:C:552:MET:HB2	1:C:909:ILE:HG22	1.74	0.70
1:C:985:VAL:HG23	1:C:986:PRO:HD3	1.73	0.69
1:A:727:LYS:HB3	1:A:807:LYS:HG3	1.73	0.69
1:C:524:THR:HG22	1:C:970:LEU:HD12	1.74	0.69
1:E:337:ILE:HG22	1:E:395:MET:HG3	1.75	0.69
1:F:576:VAL:HA	1:F:663:VAL:HG12	1.74	0.69
1:A:216:SER:OG	1:A:234:ILE:O	2.09	0.69
1:A:969:ARG:HH21	1:A:972:PRO:HB2	1.57	0.69
1:A:669:PRO:HG2	1:A:671:VAL:HG12	1.73	0.69
1:D:578:THR:HG22	1:D:579:PRO:HD2	1.75	0.69
1:C:43:ILE:HD13	1:C:104:GLN:HA	1.74	0.69
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.75	0.68
1:C:682:LEU:HD11	1:C:843:VAL:HG11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:ARG:HD2	1:E:762:ILE:HG23	1.75	0.68
1:B:936:LEU:HB2	1:B:1009:MET:HE1	1.76	0.68
1:D:332:VAL:HG21	1:D:569:GLN:HA	1.75	0.68
1:F:174:ASP:HB3	1:F:292:LYS:HD2	1.75	0.68
1:B:62:VAL:HG22	1:B:88:MET:HE2	1.75	0.68
1:A:493:CYS:HA	1:A:497:LEU:HD23	1.75	0.68
1:F:753:TRP:HZ3	1:F:779:ARG:HA	1.58	0.68
1:A:731:ASP:HB3	1:A:734:LYS:HB2	1.73	0.68
1:B:981:ILE:O	1:B:985:VAL:HG23	1.94	0.68
1:D:197:GLN:HB3	1:D:797:MET:HE3	1.76	0.68
1:B:47:VAL:HG13	1:B:127:ILE:HA	1.75	0.68
1:E:441:ALA:O	1:E:445:ILE:HG23	1.93	0.68
1:E:544:ILE:HG23	1:E:1019:TRP:HH2	1.59	0.68
1:E:232:ALA:HB3	1:F:726:TYR:HE1	1.58	0.68
1:F:980:PHE:CD2	1:F:1009:MET:HG3	2.29	0.67
1:B:45:VAL:HG22	1:B:129:VAL:HG12	1.77	0.67
1:E:972:PRO:O	1:E:976:THR:HG23	1.94	0.67
1:D:969:ARG:O	1:D:973:ILE:HG12	1.94	0.67
1:E:188:LEU:HD13	1:E:193:LEU:HD11	1.77	0.67
1:C:239:ARG:HD3	1:C:761:PHE:HA	1.77	0.67
1:C:655:PHE:HB3	1:C:663:VAL:HG23	1.77	0.67
1:B:48:SER:HA	1:B:87:SER:HA	1.76	0.67
1:D:76:ARG:HD2	1:D:863:TYR:CE2	2.30	0.67
1:D:535:LEU:O	1:D:538:ARG:NH1	2.28	0.67
1:E:149:MET:HE1	1:E:318:PRO:HB2	1.77	0.67
1:A:544:ILE:HG23	1:A:1019:TRP:HH2	1.60	0.67
1:F:541:TYR:O	1:F:1019:TRP:HH2	1.78	0.67
1:A:138:MET:HE3	1:A:306:ILE:HD11	1.77	0.66
1:A:699:ARG:NH1	1:A:824:MET:SD	2.67	0.66
1:D:13:TRP:NE1	2:D:1101:LMT:O2'	2.28	0.66
1:F:666:PHE:HA	1:F:714:ARG:NH2	2.09	0.66
1:A:188:LEU:HB3	1:A:193:LEU:HD21	1.78	0.66
1:C:905:PRO:O	1:C:909:ILE:HG23	1.95	0.66
1:D:669:PRO:HA	1:D:678:THR:HG22	1.76	0.66
1:F:372:VAL:HG22	1:F:405:LEU:HD11	1.77	0.66
1:A:352:PHE:HD2	1:A:369:THR:HG21	1.61	0.66
1:B:592:ASP:OD1	1:B:595:ARG:NH2	2.29	0.66
1:C:973:ILE:HD12	1:C:1017:ILE:HG22	1.77	0.66
1:E:424:GLY:HA3	1:E:502:LYS:HG2	1.76	0.66
1:B:528:GLU:HB3	1:B:963:ILE:HD11	1.76	0.66
1:E:182:TYR:HB3	1:E:270:LEU:HD22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:900:VAL:HG11	1:E:942:ILE:HG23	1.77	0.66
1:A:973:ILE:HD12	1:A:1017:ILE:HG22	1.78	0.66
1:B:544:ILE:HG23	1:B:1019:TRP:HH2	1.61	0.66
1:F:456:MET:HB2	1:F:467:TYR:HB3	1.77	0.66
1:B:302:THR:O	1:B:306:ILE:HG12	1.95	0.65
1:B:1015:LEU:O	1:B:1019:TRP:HD1	1.80	0.65
1:C:376:LEU:HD22	1:C:398:MET:HE2	1.77	0.65
1:C:883:VAL:HG12	1:C:901:MET:HE1	1.78	0.65
1:D:14:VAL:HG11	1:E:889:ALA:HB2	1.77	0.65
1:D:780:MET:HE1	1:F:224:ALA:HA	1.78	0.65
1:E:762:ILE:HG22	1:E:767:VAL:HG22	1.79	0.65
1:F:281:PHE:CE1	1:F:608:SER:HB2	2.32	0.65
1:D:437:GLN:O	1:D:439:GLN:N	2.30	0.65
1:A:958:ILE:HD12	1:A:1025:VAL:HG13	1.77	0.65
1:F:137:LEU:HD23	1:F:291:ILE:HD11	1.79	0.65
1:F:682:LEU:HD11	1:F:843:VAL:HG11	1.78	0.65
1:E:302:THR:O	1:E:306:ILE:HG12	1.97	0.65
1:F:646:GLU:HA	1:F:649:LYS:HD2	1.78	0.65
1:B:352:PHE:CD2	1:B:365:THR:HG21	2.32	0.65
1:F:459:PHE:HB3	1:F:871:GLN:NE2	2.11	0.65
1:C:980:PHE:CD2	1:C:1009:MET:HG3	2.31	0.65
1:F:137:LEU:HD11	1:F:330:THR:HG23	1.78	0.65
1:C:358:PHE:CG	1:C:975:MET:HG2	2.32	0.64
1:B:213:GLN:HG3	1:B:239:ARG:HG3	1.79	0.64
1:D:371:ALA:O	1:D:375:VAL:HG22	1.97	0.64
1:B:424:GLY:HA3	1:B:502:LYS:HG2	1.78	0.64
1:F:535:LEU:HD13	1:F:959:VAL:HG13	1.77	0.64
1:E:234:ILE:HG22	1:F:726:TYR:HB2	1.77	0.64
1:E:213:GLN:HG3	1:E:239:ARG:HG3	1.79	0.64
1:E:637:ARG:HB2	1:E:642:ASN:HB3	1.80	0.64
1:B:527:TYR:CE2	1:B:966:CYS:HB3	2.33	0.64
1:C:90:ILE:O	1:C:90:ILE:HG13	1.98	0.64
1:D:101:ASP:OD1	1:D:131:LYS:NZ	2.31	0.64
1:A:748:THR:HG21	1:A:790:VAL:HG22	1.79	0.64
1:F:538:ARG:HH12	1:F:1025:VAL:CG1	2.11	0.64
1:A:131:LYS:NZ	1:B:73:ASP:OD2	2.30	0.64
1:B:197:GLN:O	1:B:791:ARG:NH2	2.28	0.64
1:C:60:THR:HG23	1:C:61:VAL:HG23	1.79	0.64
1:B:186:ILE:HD11	1:B:772:LEU:HG	1.79	0.64
1:C:616:ASN:HB2	1:C:624:SER:HB2	1.79	0.64
1:F:36:PRO:HG3	1:F:469:GLN:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:NH2	1:B:66:GLU:O	2.29	0.63
1:B:203:VAL:O	1:B:207:ILE:HG12	1.97	0.63
1:D:17:LEU:HD21	2:D:1101:LMT:H51	1.79	0.63
1:A:225:VAL:HG12	1:B:780:MET:HE2	1.80	0.63
1:B:222:LEU:HD12	1:C:276:SER:HA	1.79	0.63
1:C:758:VAL:O	1:C:759:ASN:ND2	2.31	0.63
1:A:974:VAL:O	1:A:978:LEU:HB2	1.97	0.63
1:C:903:VAL:HG12	1:C:937:SER:HB2	1.80	0.63
1:D:878:LEU:HD11	1:F:25:LEU:HD11	1.80	0.63
1:E:801:ASN:OD1	1:E:801:ASN:N	2.32	0.63
1:F:186:ILE:HG22	1:F:268:VAL:HG22	1.80	0.63
1:A:197:GLN:O	1:A:791:ARG:NH2	2.25	0.63
1:B:568:ASP:OD2	1:B:644:VAL:N	2.23	0.63
1:C:572:LEU:HD21	1:C:665:ALA:HB1	1.81	0.63
1:D:973:ILE:HD12	1:D:1017:ILE:HG22	1.81	0.63
1:E:569:GLN:NE2	1:E:669:PRO:O	2.30	0.63
1:B:36:PRO:HD2	1:B:38:ILE:HD11	1.80	0.63
1:B:222:LEU:HB3	1:C:275:TYR:HB2	1.79	0.63
1:D:699:ARG:NH2	1:D:824:MET:HB2	2.13	0.63
1:D:915:THR:HG21	1:D:926:PHE:HD2	1.63	0.63
1:E:527:TYR:CD2	1:E:970:LEU:HD12	2.34	0.63
1:D:13:TRP:NE1	2:D:1101:LMT:H2O2	1.96	0.62
1:E:72:ILE:HD11	1:E:75:LEU:HD22	1.81	0.62
1:D:568:ASP:HB3	1:D:634:TRP:CH2	2.34	0.62
1:A:492:LEU:HB3	1:A:496:MET:HE2	1.80	0.62
1:A:900:VAL:HG21	1:A:942:ILE:HD13	1.81	0.62
1:B:72:ILE:HG22	1:B:106:GLN:HB3	1.82	0.62
1:D:1015:LEU:O	1:D:1019:TRP:HD1	1.82	0.62
1:E:528:GLU:HB3	1:E:963:ILE:HD11	1.81	0.62
1:A:524:THR:HG22	1:A:970:LEU:HD12	1.81	0.62
1:D:188:LEU:HD23	1:D:266:ALA:HB2	1.81	0.62
1:F:753:TRP:CZ3	1:F:779:ARG:HA	2.35	0.62
1:B:188:LEU:HD23	1:B:266:ALA:HB2	1.81	0.62
1:B:459:PHE:O	1:B:468:ARG:NH2	2.33	0.62
1:D:372:VAL:HG22	1:D:405:LEU:HD21	1.82	0.62
1:E:158:ILE:HD11	1:E:177:VAL:HG13	1.80	0.62
1:A:618:ALA:HB2	1:A:716:ARG:HH22	1.65	0.61
1:A:938:ALA:O	1:A:942:ILE:HG12	2.01	0.61
1:B:441:ALA:O	1:B:445:ILE:HG23	1.99	0.61
1:D:61:VAL:HG12	1:D:88:MET:HE3	1.82	0.61
1:E:343:THR:HA	1:E:346:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:ILE:HG12	1:F:237:LYS:HB2	1.81	0.61
1:F:617:PHE:CD1	1:F:626:MET:HE1	2.35	0.61
1:A:182:TYR:HB3	1:A:270:LEU:HD22	1.82	0.61
1:A:352:PHE:HD1	1:A:353:LEU:HD22	1.65	0.61
1:C:47:VAL:HG12	1:C:88:MET:HE3	1.82	0.61
1:D:45:VAL:HB	1:D:90:ILE:HG23	1.82	0.61
1:E:484:VAL:HG13	1:E:488:LEU:HD13	1.82	0.61
1:E:571:VAL:HG23	1:E:668:PRO:HG2	1.82	0.61
1:F:462:SER:O	1:F:466:ILE:HG12	2.00	0.61
1:F:575:GLN:HG3	1:F:666:PHE:CE1	2.35	0.61
1:F:666:PHE:HA	1:F:714:ARG:HH22	1.65	0.61
1:B:352:PHE:HA	1:B:365:THR:HG23	1.82	0.61
1:C:96:GLN:NE2	1:C:462:SER:HB3	2.14	0.61
1:E:47:VAL:HG13	1:E:127:ILE:HA	1.83	0.61
1:F:578:THR:HG21	1:F:587:THR:HA	1.81	0.61
1:A:237:LYS:HD2	1:B:730:ILE:HD11	1.83	0.61
1:A:773:GLN:HG2	1:A:774:GLY:H	1.65	0.61
1:E:280:GLN:HB2	1:E:611:THR:HG23	1.82	0.61
1:A:847:VAL:HG11	1:A:856:TYR:CD1	2.35	0.61
1:B:910:GLY:H	1:B:1011:THR:HG21	1.64	0.61
1:D:775:ARG:NH2	1:D:777:ASP:OD2	2.34	0.61
1:B:801:ASN:OD1	1:B:801:ASN:N	2.30	0.61
1:C:830:PRO:HB3	1:C:839:ALA:HB2	1.82	0.61
1:D:352:PHE:HD2	1:D:369:THR:HG21	1.66	0.61
1:D:780:MET:SD	1:F:228:GLN:HG3	2.41	0.61
1:D:958:ILE:HD12	1:D:1025:VAL:HG13	1.82	0.61
1:E:57:VAL:HG13	1:E:82:SER:HB2	1.81	0.61
1:E:847:VAL:HG11	1:E:856:TYR:CD1	2.35	0.61
1:F:60:THR:HG23	1:F:61:VAL:HG23	1.82	0.61
1:F:485:ALA:HA	1:F:489:THR:OG1	2.01	0.61
1:A:203:VAL:O	1:A:207:ILE:HG12	2.00	0.61
1:D:899:SER:HA	1:D:1023:PHE:HB3	1.81	0.61
1:E:213:GLN:HG2	1:E:238:THR:HA	1.82	0.61
1:E:568:ASP:OD2	1:E:644:VAL:N	2.24	0.61
1:F:539:ALA:O	1:F:543:LEU:HG	2.00	0.61
1:B:637:ARG:HB2	1:B:642:ASN:HB3	1.83	0.60
1:C:907:GLY:HA2	1:C:1011:THR:HG23	1.82	0.60
1:E:862:SER:O	1:E:866:ARG:HG3	2.01	0.60
1:A:455:PRO:HG2	1:A:879:SER:HA	1.81	0.60
1:A:817:ARG:NH2	1:A:820:GLY:O	2.34	0.60
1:B:188:LEU:HD13	1:B:193:LEU:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:HG3	1:A:365:THR:HG23	1.82	0.60
1:B:231:ASN:OD1	1:C:583:SER:HA	2.00	0.60
1:C:184:MET:HB2	1:C:770:VAL:HG12	1.84	0.60
1:E:188:LEU:HD23	1:E:266:ALA:HB2	1.83	0.60
1:B:903:VAL:HG23	1:B:906:LEU:HD12	1.83	0.60
1:C:713:GLN:HG3	1:C:714:ARG:HD3	1.83	0.60
1:D:138:MET:HE3	1:D:306:ILE:HD11	1.82	0.60
1:E:14:VAL:HG11	1:F:889:ALA:HB2	1.84	0.60
1:B:455:PRO:HB2	1:B:456:MET:HE2	1.84	0.60
1:A:733:GLU:HG2	1:C:250:LEU:HD11	1.84	0.60
1:C:755:SER:HB3	1:C:773:GLN:HE21	1.66	0.60
1:D:131:LYS:O	1:D:295:THR:HG22	2.01	0.60
1:E:210:GLN:HG2	1:F:742:LEU:HD12	1.84	0.60
1:F:907:GLY:HA2	1:F:1011:THR:HG23	1.82	0.60
1:C:281:PHE:CE2	1:C:324:VAL:HG11	2.37	0.60
1:A:713:GLN:HE21	1:A:714:ARG:HD2	1.64	0.60
1:B:278:ASN:HB2	1:B:613:THR:HG22	1.84	0.60
1:D:189:ASP:HB2	1:D:775:ARG:HD3	1.82	0.60
1:E:485:ALA:HA	1:E:489:THR:OG1	2.02	0.60
1:F:904:VAL:HG13	1:F:934:ILE:HG12	1.83	0.60
1:F:906:LEU:O	1:F:1011:THR:OG1	2.20	0.60
1:A:980:PHE:O	1:A:984:VAL:HG23	2.02	0.60
1:B:414:GLU:HG2	1:B:971:ARG:HH11	1.67	0.60
1:C:64:VAL:HG11	1:C:117:LEU:HB2	1.82	0.60
1:E:782:PRO:O	1:E:785:LEU:HB2	2.02	0.60
1:F:200:PRO:HB2	1:F:751:ILE:HD11	1.84	0.60
1:A:730:ILE:HD11	1:C:237:LYS:HD3	1.84	0.59
1:C:249:ILE:HD11	1:C:262:LEU:HD22	1.84	0.59
1:D:773:GLN:HG2	1:D:774:GLY:H	1.66	0.59
1:E:273:GLN:OE1	1:E:769:ARG:NH1	2.35	0.59
1:F:228:GLN:NE2	1:F:230:LEU:O	2.27	0.59
1:C:637:ARG:HG2	1:C:642:ASN:HD22	1.66	0.59
1:C:648:ALA:HB1	1:C:714:ARG:HH12	1.66	0.59
1:C:949:LYS:NZ	1:C:953:GLU:OE2	2.34	0.59
1:C:977:SER:O	1:C:981:ILE:HG12	2.01	0.59
1:D:76:ARG:HD2	1:D:863:TYR:HE2	1.67	0.59
1:F:300:LEU:O	1:F:304:LYS:HG3	2.02	0.59
1:B:930:LEU:O	1:B:934:ILE:HG12	2.02	0.59
1:C:137:LEU:HD22	1:C:138:MET:HG2	1.85	0.59
1:F:463:THR:HG22	1:F:563:PHE:HE1	1.67	0.59
1:F:817:ARG:NH2	1:F:820:GLY:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:GLU:O	1:A:343:THR:HG23	2.02	0.59
1:B:340:VAL:HG21	1:B:395:MET:HB3	1.84	0.59
1:C:361:ASN:HB3	1:C:364:ALA:HB3	1.84	0.59
1:C:969:ARG:O	1:C:973:ILE:HG12	2.02	0.59
1:D:188:LEU:HB3	1:D:193:LEU:HD21	1.83	0.59
1:D:966:CYS:SG	1:D:1021:PRO:HG3	2.42	0.59
1:E:655:PHE:HB3	1:E:663:VAL:HB	1.83	0.59
1:D:415:ASN:O	1:D:419:VAL:HG22	2.02	0.59
1:C:530:GLY:O	1:C:534:ILE:HG23	2.02	0.59
1:F:185:ARG:NH2	1:F:773:GLN:HB2	2.16	0.59
1:A:188:LEU:HD23	1:A:266:ALA:HB2	1.83	0.59
1:C:399:VAL:O	1:C:402:ILE:HG13	2.03	0.59
1:C:572:LEU:HD22	1:C:629:ILE:HD12	1.84	0.59
1:D:339:GLU:O	1:D:343:THR:HG23	2.02	0.59
1:B:964:GLU:O	1:B:968:MET:HG3	2.02	0.59
1:D:65:ILE:HD11	1:D:90:ILE:HG21	1.85	0.59
1:E:958:ILE:HD12	1:E:1025:VAL:HG13	1.85	0.59
1:F:361:ASN:HB3	1:F:364:ALA:HB3	1.85	0.59
1:F:897:PRO:O	1:F:901:MET:HG2	2.03	0.59
1:A:210:GLN:OE1	1:A:249:ILE:HG13	2.02	0.59
1:B:455:PRO:HG2	1:B:879:SER:HB3	1.85	0.59
1:C:652:GLN:NE2	1:C:714:ARG:HG2	2.16	0.59
1:D:280:GLN:HG3	1:D:595:ARG:HH21	1.67	0.59
1:E:617:PHE:CE2	1:E:626:MET:HE1	2.38	0.59
1:E:676:ASN:HB2	1:E:679:GLY:HA3	1.85	0.59
1:A:415:ASN:O	1:A:419:VAL:HG22	2.03	0.58
1:C:342:LYS:O	1:C:346:GLU:HG3	2.02	0.58
1:D:438:ILE:O	1:D:442:LEU:HD13	2.02	0.58
1:A:58:GLN:HG3	1:A:817:ARG:HD2	1.85	0.58
1:E:595:ARG:HH21	1:E:611:THR:HG21	1.67	0.58
1:F:406:VAL:HG22	1:F:410:ILE:HG13	1.85	0.58
1:A:540:PRO:O	1:A:544:ILE:HG22	2.03	0.58
1:B:723:GLU:HG3	1:B:813:PRO:HG3	1.84	0.58
1:D:45:VAL:HG22	1:D:129:VAL:HG13	1.85	0.58
1:E:391:ASN:H	1:E:394:THR:HG22	1.67	0.58
1:A:368:PRO:HB2	1:A:406:VAL:HG13	1.85	0.58
1:B:616:ASN:HB2	1:B:624:SER:HB2	1.86	0.58
1:C:217:GLY:O	1:C:234:ILE:HG12	2.02	0.58
1:C:576:VAL:HG22	1:C:663:VAL:HG12	1.85	0.58
1:D:545:TYR:HB2	1:D:1019:TRP:CZ3	2.39	0.58
1:E:603:SER:O	1:E:632:LYS:NZ	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:818:TYR:CD2	1:F:823:ALA:HB3	2.39	0.58
1:D:847:VAL:HG11	1:D:856:TYR:CD1	2.38	0.58
1:E:773:GLN:HG2	1:E:774:GLY:H	1.68	0.58
1:F:463:THR:OG1	1:F:871:GLN:OE1	2.18	0.58
1:A:166:LEU:O	1:A:172:VAL:HG21	2.04	0.58
1:A:780:MET:SD	1:C:228:GLN:HG3	2.43	0.58
1:B:108:GLN:NE2	1:B:109:ASN:OD1	2.36	0.58
1:E:455:PRO:HG2	1:E:879:SER:HB3	1.85	0.58
1:E:1015:LEU:O	1:E:1019:TRP:HD1	1.87	0.58
1:F:775:ARG:O	1:F:779:ARG:HG2	2.03	0.58
1:A:899:SER:HA	1:A:1023:PHE:HB3	1.86	0.58
1:C:300:LEU:HD23	1:C:330:THR:HG23	1.84	0.58
1:C:337:ILE:HA	1:C:340:VAL:HG12	1.84	0.58
1:A:78:ILE:HD11	1:A:90:ILE:HD12	1.85	0.58
1:B:773:GLN:HG2	1:B:774:GLY:H	1.68	0.58
1:C:120:GLN:O	1:C:124:ARG:HG3	2.04	0.58
1:C:723:GLU:HG3	1:C:813:PRO:HG3	1.85	0.58
1:D:974:VAL:O	1:D:978:LEU:HB2	2.04	0.58
1:E:211:ASN:ND2	1:E:760:ASP:O	2.36	0.58
1:E:969:ARG:C	1:E:972:PRO:HD2	2.29	0.58
1:F:527:TYR:CE2	1:F:966:CYS:HB3	2.39	0.58
1:A:775:ARG:NH2	1:A:777:ASP:OD2	2.29	0.57
1:C:847:VAL:HG11	1:C:856:TYR:CD1	2.39	0.57
1:C:1002:GLY:O	1:C:1006:ILE:HG12	2.04	0.57
1:D:969:ARG:HH21	1:D:972:PRO:HB2	1.68	0.57
1:D:980:PHE:O	1:D:984:VAL:HG23	2.03	0.57
1:F:530:GLY:O	1:F:534:ILE:HG23	2.04	0.57
1:A:310:ILE:HD11	1:A:325:TYR:OH	2.03	0.57
1:A:840:MET:N	1:A:840:MET:SD	2.77	0.57
1:D:907:GLY:HA2	1:D:1012:ALA:HB2	1.84	0.57
1:E:232:ALA:HB3	1:F:726:TYR:CE1	2.37	0.57
1:F:936:LEU:HB3	1:F:1009:MET:HE3	1.86	0.57
1:B:410:ILE:HD11	1:B:976:THR:HG22	1.86	0.57
1:B:677:ALA:O	1:B:679:GLY:N	2.38	0.57
1:B:990:SER:O	1:B:999:HIS:NE2	2.36	0.57
1:F:207:ILE:HB	1:F:758:VAL:HG11	1.86	0.57
1:C:745:ILE:HG23	1:C:790:VAL:HG11	1.85	0.57
1:E:748:THR:HG21	1:E:790:VAL:HG22	1.86	0.57
1:F:714:ARG:HE	1:F:829:GLU:CD	2.13	0.57
1:A:753:TRP:CH2	1:A:785:LEU:HA	2.39	0.57
1:B:235:ILE:HG12	1:C:727:LYS:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:TRP:CD1	1:A:634:TRP:H	2.21	0.57
1:C:142:VAL:HG12	1:C:154:LEU:HD22	1.86	0.57
1:C:1015:LEU:O	1:C:1019:TRP:HD1	1.87	0.57
1:F:655:PHE:HB3	1:F:663:VAL:HG23	1.86	0.57
1:F:569:GLN:NE2	1:F:669:PRO:O	2.38	0.57
1:A:76:ARG:HD2	1:A:863:TYR:CE2	2.39	0.57
1:C:183:SER:OG	1:C:273:GLN:HG3	2.05	0.57
1:B:634:TRP:H	1:B:634:TRP:CD1	2.21	0.57
1:D:532:ALA:O	1:D:536:LYS:HG2	2.05	0.57
1:E:805:THR:OG1	1:E:806:GLY:N	2.38	0.57
1:F:574:ALA:HB3	1:F:627:ALA:HB3	1.87	0.57
1:B:379:THR:CG2	1:B:477:ALA:HA	2.33	0.56
1:D:56:THR:HG22	1:F:213:GLN:HB3	1.86	0.56
1:A:310:ILE:HD12	1:A:323:VAL:HG11	1.86	0.56
1:B:466:ILE:HD11	1:B:924:VAL:HG21	1.87	0.56
1:B:527:TYR:CD2	1:B:970:LEU:HD12	2.40	0.56
1:D:396:PHE:HA	1:D:399:VAL:HG12	1.87	0.56
1:B:375:VAL:O	1:B:379:THR:HG23	2.05	0.56
1:D:456:MET:HE3	1:D:931:LEU:HD12	1.86	0.56
1:E:203:VAL:O	1:E:207:ILE:HG12	2.05	0.56
1:E:618:ALA:O	1:E:719:GLY:HA2	2.05	0.56
1:D:13:TRP:CD1	2:D:1101:LMT:H2O2	2.23	0.56
1:D:723:GLU:O	1:D:810:TYR:HB2	2.05	0.56
1:E:249:ILE:HD11	1:E:262:LEU:HD12	1.87	0.56
1:E:359:LEU:HD21	1:E:971:ARG:HH12	1.71	0.56
1:E:371:ALA:O	1:E:374:VAL:HG12	2.05	0.56
1:A:438:ILE:O	1:A:442:LEU:HD13	2.06	0.56
1:F:160:SER:HA	1:F:766:ARG:CZ	2.36	0.56
1:A:15:ILE:HD13	1:A:487:ILE:HG21	1.87	0.56
1:C:578:THR:HG21	1:C:587:THR:HA	1.87	0.56
1:E:35:TYR:CE2	1:E:671:VAL:HG23	2.41	0.56
1:E:454:LEU:HD11	2:E:1102:LMT:H101	1.88	0.56
1:D:237:LYS:HG3	1:E:730:ILE:HD11	1.88	0.56
1:D:753:TRP:CH2	1:D:785:LEU:HA	2.40	0.56
1:E:940:ASN:O	1:E:944:ILE:HG23	2.05	0.56
1:F:157:TYR:HB3	1:F:321:MET:HE1	1.87	0.56
1:C:17:LEU:HA	1:C:20:MET:HE2	1.87	0.56
1:C:137:LEU:HD12	1:C:293:LEU:HG	1.88	0.56
1:C:867:LEU:O	1:C:871:GLN:HG3	2.06	0.56
1:C:930:LEU:O	1:C:934:ILE:HG23	2.06	0.56
1:F:396:PHE:CE1	1:F:998:GLN:HG2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HD2	1:A:863:TYR:HE2	1.71	0.56
1:B:940:ASN:O	1:B:944:ILE:HG23	2.05	0.56
1:C:208:GLN:HG2	1:C:759:ASN:HD21	1.71	0.56
1:E:448:VAL:O	1:E:452:VAL:HG23	2.06	0.56
1:E:745:ILE:HD11	1:E:803:PHE:CD1	2.40	0.56
1:F:200:PRO:CB	1:F:751:ILE:HD11	2.36	0.56
1:B:69:MET:HE1	1:B:107:VAL:O	2.06	0.56
1:B:150:THR:OG1	1:B:151:LYS:N	2.38	0.56
1:C:406:VAL:O	1:C:410:ILE:HG12	2.06	0.56
1:C:757:TYR:OH	1:C:760:ASP:OD1	2.20	0.56
1:E:572:LEU:HD22	1:E:629:ILE:HD12	1.87	0.56
1:F:398:MET:O	1:F:402:ILE:HG23	2.06	0.56
1:F:602:GLU:HG2	1:F:647:LEU:CD1	2.36	0.56
1:B:847:VAL:HG11	1:B:856:TYR:CD1	2.41	0.55
1:C:978:LEU:HD23	1:C:981:ILE:HD11	1.88	0.55
1:E:158:ILE:HA	1:E:162:ILE:HG12	1.87	0.55
1:E:729:GLU:HB3	1:E:805:THR:HG23	1.87	0.55
1:F:142:VAL:HG11	1:F:321:MET:HE2	1.88	0.55
1:F:758:VAL:HG12	1:F:759:ASN:ND2	2.20	0.55
1:A:521:LEU:O	1:A:524:THR:OG1	2.23	0.55
1:A:969:ARG:NH2	1:A:972:PRO:HB2	2.20	0.55
1:B:166:LEU:HD22	1:B:306:ILE:HG22	1.87	0.55
1:C:462:SER:O	1:C:466:ILE:HG22	2.06	0.55
1:D:793:ASP:O	1:D:794:LYS:HD3	2.05	0.55
1:E:339:GLU:O	1:E:343:THR:HG23	2.06	0.55
1:F:421:ALA:HB1	1:F:505:HIS:HD2	1.72	0.55
1:F:422:GLU:HG2	1:F:505:HIS:CE1	2.41	0.55
1:A:14:VAL:HG11	1:B:889:ALA:HB2	1.87	0.55
1:F:534:ILE:HG22	1:F:541:TYR:CZ	2.42	0.55
1:B:47:VAL:HG11	1:B:127:ILE:HG12	1.89	0.55
1:B:697:GLN:O	1:B:701:LYS:HG3	2.06	0.55
1:C:455:PRO:HG2	1:C:879:SER:HA	1.89	0.55
1:C:544:ILE:O	1:C:548:ILE:HG23	2.06	0.55
1:A:524:THR:O	1:A:528:GLU:HG3	2.07	0.55
1:C:910:GLY:HA3	1:C:1011:THR:HG21	1.88	0.55
1:D:588:GLN:HG2	1:D:613:THR:HG21	1.87	0.55
1:E:362:PHE:O	1:E:365:THR:HG22	2.06	0.55
1:F:159:VAL:HG11	1:F:181:GLN:HB2	1.86	0.55
1:F:709:ASN:HB2	1:F:846:ILE:HD11	1.87	0.55
1:A:907:GLY:HA2	1:A:1012:ALA:HB2	1.87	0.55
1:D:366:LEU:O	1:D:370:ILE:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:669:PRO:HB2	1:D:671:VAL:HG22	1.87	0.55
1:D:733:GLU:CD	1:F:261:ARG:HH22	2.12	0.55
1:E:981:ILE:O	1:E:985:VAL:HG23	2.06	0.55
1:B:550:ALA:O	1:B:553:ILE:HG12	2.07	0.55
1:C:695:LEU:HD13	1:C:699:ARG:HH22	1.71	0.55
1:D:139:VAL:HA	1:D:290:ALA:HA	1.89	0.55
1:D:181:GLN:NE2	1:D:273:GLN:OE1	2.36	0.55
1:D:416:VAL:HG22	1:D:431:ALA:HA	1.88	0.55
1:D:674:LEU:HD11	1:D:861:LEU:HB3	1.89	0.55
1:A:207:ILE:HD13	1:A:249:ILE:HD13	1.88	0.55
1:A:415:ASN:HA	1:A:418:ARG:HG2	1.89	0.55
1:A:569:GLN:H	1:A:634:TRP:HH2	1.53	0.55
1:B:84:SER:N	1:B:813:PRO:O	2.40	0.55
1:B:399:VAL:O	1:B:402:ILE:HG13	2.07	0.55
1:D:830:PRO:HA	1:D:838:ASP:OD2	2.06	0.55
1:E:20:MET:HE2	1:E:374:VAL:HG23	1.89	0.55
1:A:365:THR:O	1:A:368:PRO:HD2	2.07	0.55
1:A:766:ARG:NE	1:B:67:GLN:OE1	2.39	0.55
1:B:340:VAL:HG22	1:B:399:VAL:CG2	2.37	0.55
1:D:572:LEU:HB3	1:D:629:ILE:HB	1.89	0.55
1:F:1016:ALA:HB1	1:F:1020:VAL:HG23	1.88	0.55
1:B:405:LEU:HD22	1:B:481:SER:HB3	1.89	0.55
1:C:818:TYR:CD2	1:C:823:ALA:HB3	2.42	0.55
1:D:388:PHE:CE2	1:D:472:ILE:HG12	2.42	0.55
1:E:407:ASN:HD22	1:E:936:LEU:CD2	2.20	0.55
1:A:190:PRO:HG2	1:A:787:LYS:HG2	1.89	0.54
1:A:343:THR:HG21	1:A:998:GLN:OE1	2.07	0.54
1:C:367:ILE:HG12	1:C:496:MET:HE2	1.89	0.54
1:D:805:THR:HG22	1:D:806:GLY:H	1.72	0.54
1:D:930:LEU:O	1:D:934:ILE:HG12	2.07	0.54
1:E:899:SER:HA	1:E:1023:PHE:HB3	1.89	0.54
1:A:1015:LEU:O	1:A:1019:TRP:HD1	1.91	0.54
1:B:190:PRO:HG3	1:B:788:TRP:CE2	2.43	0.54
1:B:766:ARG:HH22	1:C:67:GLN:NE2	2.06	0.54
1:C:340:VAL:O	1:C:343:THR:HG22	2.08	0.54
1:D:234:ILE:HG22	1:E:726:TYR:HB3	1.89	0.54
1:A:793:ASP:O	1:A:794:LYS:HD2	2.07	0.54
1:B:164:ASP:HB2	1:C:67:GLN:NE2	2.22	0.54
1:D:575:GLN:HG3	1:D:616:ASN:ND2	2.23	0.54
1:A:146:ASP:C	1:A:148:SER:H	2.15	0.54
1:A:470:PHE:CE2	1:A:474:ILE:HD13	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ALA:HA	1:B:478:MET:SD	2.47	0.54
1:C:396:PHE:CE1	1:C:998:GLN:HG2	2.42	0.54
1:C:637:ARG:HD2	1:C:642:ASN:HB3	1.89	0.54
1:C:745:ILE:HG22	1:C:790:VAL:HG21	1.90	0.54
1:E:164:ASP:HB2	1:F:67:GLN:NE2	2.22	0.54
1:A:782:PRO:HA	1:A:785:LEU:HD13	1.90	0.54
1:B:617:PHE:CD2	3:B:1101:MC2:H7	2.42	0.54
1:C:407:ASN:OD1	1:C:976:THR:HG23	2.07	0.54
1:D:539:ALA:HB3	1:D:540:PRO:HD3	1.90	0.54
1:E:910:GLY:H	1:E:1011:THR:HG21	1.72	0.54
1:B:753:TRP:HZ2	1:B:785:LEU:HA	1.72	0.54
1:C:55:GLU:HG3	1:C:815:LEU:HD11	1.89	0.54
1:C:452:VAL:HG11	1:C:931:LEU:O	2.07	0.54
1:C:456:MET:HB2	1:C:467:TYR:HB3	1.88	0.54
1:E:446:ALA:HA	1:E:478:MET:SD	2.47	0.54
1:F:96:GLN:HG3	1:F:461:GLY:HA2	1.90	0.54
1:F:217:GLY:O	1:F:234:ILE:HG12	2.07	0.54
1:F:506:GLY:HA3	1:F:521:LEU:HD11	1.90	0.54
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.89	0.54
1:A:366:LEU:O	1:A:370:ILE:HG23	2.08	0.54
1:F:366:LEU:O	1:F:370:ILE:HD12	2.08	0.54
1:F:415:ASN:HB3	1:F:434:SER:HB2	1.89	0.54
1:A:133:VAL:HG22	1:A:134:LYS:H	1.72	0.54
1:D:210:GLN:CD	1:D:249:ILE:HG13	2.33	0.54
1:E:457:ALA:HB1	2:E:1102:LMT:H42	1.90	0.54
1:F:20:MET:HE3	1:F:373:PRO:HB2	1.88	0.54
1:A:876:TYR:OH	1:A:927:GLN:HG3	2.07	0.54
1:D:80:SER:OG	1:D:817:ARG:HB2	2.08	0.54
1:D:634:TRP:CD1	1:D:634:TRP:H	2.26	0.54
1:E:740:VAL:HG23	1:E:792:ASN:OD1	2.07	0.54
1:F:545:TYR:HB2	1:F:1019:TRP:CH2	2.43	0.54
1:A:590:VAL:HG11	1:A:661:ALA:HB3	1.88	0.54
1:C:587:THR:O	1:C:591:VAL:HG23	2.08	0.54
1:D:591:VAL:HG11	1:D:611:THR:HG23	1.89	0.54
1:E:214:ILE:HG23	1:E:237:LYS:HB2	1.90	0.54
1:E:840:MET:HG2	1:E:858:TRP:CH2	2.42	0.54
1:F:202:ASP:OD2	1:F:791:ARG:NH2	2.38	0.54
1:F:1007:GLY:O	1:F:1011:THR:HG22	2.08	0.54
1:E:108:GLN:HG3	1:E:129:VAL:HG21	1.89	0.53
1:E:162:ILE:HG22	1:E:313:LEU:HD13	1.89	0.53
1:F:445:ILE:HD11	1:F:943:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:HG13	1:A:135:ASN:H	1.73	0.53
1:B:748:THR:HG21	1:B:790:VAL:HG22	1.90	0.53
1:C:434:SER:O	1:C:438:ILE:HG12	2.08	0.53
1:D:686:ASP:OD2	1:D:691:GLY:HA2	2.08	0.53
1:E:843:VAL:HA	1:E:846:ILE:HG12	1.90	0.53
1:F:448:VAL:HG21	1:F:942:ILE:CD1	2.38	0.53
1:F:958:ILE:HD12	1:F:1025:VAL:HG13	1.90	0.53
1:B:657:SER:O	1:B:659:LYS:N	2.40	0.53
1:C:306:ILE:O	1:C:309:THR:HG22	2.09	0.53
1:E:150:THR:OG1	1:E:151:LYS:N	2.39	0.53
1:E:444:GLY:O	1:E:448:VAL:HG23	2.09	0.53
1:F:68:GLN:HG3	1:F:114:ALA:HB2	1.89	0.53
1:C:805:THR:OG1	1:C:806:GLY:N	2.34	0.53
1:F:111:LEU:HD11	1:F:127:ILE:HD12	1.89	0.53
1:F:142:VAL:HG13	1:F:321:MET:HG3	1.89	0.53
1:F:538:ARG:HH12	1:F:1025:VAL:HG11	1.73	0.53
1:A:671:VAL:HG22	1:A:672:LEU:H	1.73	0.53
1:B:11:PHE:O	1:B:14:VAL:HG12	2.08	0.53
1:B:931:LEU:HD23	1:B:934:ILE:HD11	1.90	0.53
1:C:207:ILE:HB	1:C:758:VAL:HG11	1.89	0.53
1:E:396:PHE:HE2	1:E:998:GLN:HG2	1.74	0.53
1:F:524:THR:O	1:F:528:GLU:HG3	2.08	0.53
1:F:851:PRO:C	1:F:853:GLY:H	2.17	0.53
1:A:162:ILE:O	1:A:166:LEU:HD23	2.09	0.53
1:A:448:VAL:HG22	1:A:886:CYS:HB3	1.90	0.53
1:C:439:GLN:O	1:C:443:VAL:HG23	2.09	0.53
1:C:699:ARG:HE	1:C:824:MET:HG2	1.73	0.53
1:D:367:ILE:HD13	1:D:413:VAL:HG22	1.90	0.53
1:E:215:SER:HA	1:F:51:GLY:HA3	1.90	0.53
1:A:977:SER:HB3	1:A:1013:THR:HG21	1.89	0.53
1:B:24:GLY:O	1:B:27:ILE:HG12	2.08	0.53
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.91	0.53
1:B:575:GLN:OE1	1:B:617:PHE:HB2	2.09	0.53
1:B:680:PHE:HD1	1:B:858:TRP:HZ3	1.57	0.53
1:C:661:ALA:O	1:C:663:VAL:HG22	2.08	0.53
1:C:966:CYS:SG	1:C:1021:PRO:HG3	2.49	0.53
1:F:239:ARG:HH21	1:F:760:ASP:H	1.56	0.53
1:A:726:TYR:CZ	1:A:782:PRO:HB3	2.44	0.53
1:B:57:VAL:HG13	1:B:82:SER:HB3	1.91	0.53
1:D:368:PRO:HB2	1:D:406:VAL:HG13	1.91	0.53
1:D:418:ARG:O	1:D:422:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:715:VAL:HG22	1:D:826:ILE:HD11	1.90	0.53
1:F:342:LYS:O	1:F:346:GLU:HG3	2.09	0.53
1:F:525:HIS:O	1:F:529:ARG:HG3	2.07	0.53
1:F:863:TYR:O	1:F:867:LEU:HD23	2.09	0.53
1:A:396:PHE:HA	1:A:399:VAL:HG12	1.90	0.53
1:A:915:THR:HG21	1:A:926:PHE:HD1	1.73	0.53
1:B:371:ALA:O	1:B:374:VAL:HG12	2.09	0.53
1:C:404:LEU:HD21	1:C:936:LEU:HD21	1.90	0.53
1:C:408:ASP:HB3	1:C:485:ALA:CB	2.39	0.53
1:C:508:HIS:CD2	1:C:521:LEU:HD12	2.43	0.53
1:E:442:LEU:O	1:E:445:ILE:HG12	2.08	0.53
1:E:971:ARG:O	1:E:975:MET:HG2	2.09	0.53
1:F:154:LEU:O	1:F:158:ILE:HG23	2.09	0.53
1:A:472:ILE:HA	1:A:475:VAL:HG12	1.90	0.53
1:A:714:ARG:HB2	1:A:829:GLU:HG3	1.91	0.53
1:B:158:ILE:HD11	1:B:177:VAL:HG13	1.90	0.53
1:C:159:VAL:HG11	1:C:181:GLN:HB2	1.90	0.53
1:C:164:ASP:OD2	1:C:766:ARG:NH2	2.41	0.53
1:D:439:GLN:HG3	1:D:486:LEU:HD22	1.91	0.53
1:E:72:ILE:HG22	1:E:106:GLN:HB3	1.90	0.53
1:E:753:TRP:CZ2	1:E:785:LEU:HA	2.39	0.53
1:F:99:ASP:HB3	1:F:102:ILE:HG12	1.91	0.53
1:A:847:VAL:HA	1:A:850:LEU:HG	1.91	0.52
1:B:943:LEU:HB3	1:B:969:ARG:HD2	1.91	0.52
1:C:753:TRP:CZ2	1:C:785:LEU:HD23	2.44	0.52
1:E:43:ILE:HG21	1:E:107:VAL:HG11	1.91	0.52
1:F:509:LYS:H	1:F:509:LYS:HE2	1.74	0.52
1:B:214:ILE:H	1:B:237:LYS:HB2	1.74	0.52
1:B:344:LEU:HD23	1:B:402:ILE:HD13	1.90	0.52
1:B:843:VAL:HA	1:B:846:ILE:HG12	1.91	0.52
1:B:896:ILE:N	1:B:897:PRO:HD2	2.24	0.52
1:C:239:ARG:HE	1:C:760:ASP:C	2.17	0.52
1:C:683:PHE:O	1:C:856:TYR:HA	2.08	0.52
1:D:437:GLN:C	1:D:439:GLN:H	2.17	0.52
1:D:565:PRO:HG3	1:D:923:ASP:OD2	2.09	0.52
1:D:610:PHE:HB3	1:D:628:PHE:HB2	1.91	0.52
1:E:340:VAL:HG21	1:E:395:MET:HB3	1.90	0.52
1:F:317:MET:HE2	1:F:321:MET:CG	2.36	0.52
1:F:631:LEU:HD23	1:F:637:ARG:NH1	2.25	0.52
1:A:528:GLU:OE2	1:A:967:ARG:NH2	2.42	0.52
1:A:819:ASN:C	1:A:821:VAL:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:VAL:O	1:B:452:VAL:HG23	2.08	0.52
1:C:984:VAL:HG11	1:C:1005:VAL:CG1	2.39	0.52
1:D:538:ARG:NE	1:D:538:ARG:O	2.42	0.52
1:E:143:VAL:HG12	1:E:286:ALA:HB2	1.90	0.52
1:B:340:VAL:HG22	1:B:399:VAL:HG23	1.92	0.52
1:C:418:ARG:NH2	1:C:968:MET:O	2.42	0.52
1:C:758:VAL:HB	1:C:770:VAL:HG23	1.91	0.52
1:E:11:PHE:O	1:E:14:VAL:HG12	2.08	0.52
1:F:181:GLN:OE1	1:F:768:LYS:HG2	2.09	0.52
1:A:657:SER:O	1:A:659:LYS:N	2.42	0.52
1:A:910:GLY:HA2	1:A:913:LEU:HB2	1.90	0.52
1:B:72:ILE:HD11	1:B:75:LEU:HD22	1.91	0.52
1:D:703:LEU:HD11	1:D:717:PRO:HD3	1.91	0.52
1:E:680:PHE:HD1	1:E:858:TRP:HZ3	1.58	0.52
1:A:612:VAL:HG12	1:A:615:PHE:HB3	1.91	0.52
1:B:190:PRO:HG3	1:B:788:TRP:CZ2	2.45	0.52
1:B:958:ILE:HD12	1:B:1025:VAL:HG13	1.92	0.52
1:D:575:GLN:HE22	1:D:617:PHE:H	1.57	0.52
1:E:929:GLY:HA2	1:E:932:THR:HG22	1.92	0.52
1:A:810:TYR:CE1	1:D:701:LYS:HE3	2.39	0.52
1:A:985:VAL:HA	1:A:1006:ILE:HD11	1.92	0.52
1:C:520:PHE:HA	1:C:523:THR:HG22	1.92	0.52
1:D:470:PHE:CE2	1:D:474:ILE:HD13	2.45	0.52
1:F:23:GLY:O	1:F:27:ILE:HG13	2.10	0.52
1:F:211:ASN:OD1	1:F:239:ARG:HG3	2.10	0.52
1:A:142:VAL:HG12	1:A:154:LEU:HD22	1.92	0.52
1:A:329:THR:O	1:A:332:VAL:HG12	2.10	0.52
1:A:951:LEU:C	1:A:953:GLU:H	2.17	0.52
1:B:862:SER:O	1:B:866:ARG:HG3	2.09	0.52
1:C:95:GLU:O	1:C:98:THR:HG23	2.10	0.52
1:D:872:ALA:HA	1:D:875:LEU:HD23	1.91	0.52
1:F:38:ILE:HD11	1:F:671:VAL:HG21	1.92	0.52
1:F:157:TYR:CB	1:F:321:MET:HE1	2.39	0.52
1:F:281:PHE:HE1	1:F:608:SER:HB2	1.73	0.52
1:F:344:LEU:HD11	1:F:395:MET:CE	2.40	0.52
1:F:665:ALA:O	1:F:714:ARG:NH1	2.35	0.52
1:A:569:GLN:OE1	1:A:670:SER:HA	2.09	0.52
1:A:686:ASP:OD2	1:A:691:GLY:HA2	2.10	0.52
1:B:479:ALA:O	1:B:483:ILE:HG23	2.10	0.52
1:D:133:VAL:HG22	1:D:134:LYS:H	1.75	0.52
1:E:345:GLY:O	1:E:348:ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:ASN:ND2	1:A:977:SER:OG	2.42	0.52
1:E:890:LEU:HA	2:E:1101:LMT:H42	1.91	0.52
1:C:843:VAL:HA	1:C:846:ILE:HG12	1.92	0.51
1:E:36:PRO:HG3	1:E:469:GLN:HG3	1.92	0.51
1:E:728:LEU:HD11	1:E:785:LEU:HD21	1.91	0.51
1:F:575:GLN:O	1:F:663:VAL:HA	2.10	0.51
1:F:903:VAL:HG13	1:F:906:LEU:HD12	1.92	0.51
1:B:345:GLY:O	1:B:348:ILE:HG12	2.10	0.51
1:F:393:LEU:HD22	1:F:470:PHE:HE1	1.76	0.51
1:F:580:PRO:HB3	1:F:723:GLU:HG2	1.92	0.51
1:F:705:LEU:O	1:F:708:GLN:HG2	2.11	0.51
1:F:981:ILE:O	1:F:985:VAL:HG23	2.11	0.51
1:F:1009:MET:HA	1:F:1009:MET:HE2	1.93	0.51
1:A:448:VAL:HG11	1:A:887:LEU:HD21	1.92	0.51
1:B:85:ASP:O	1:B:87:SER:N	2.43	0.51
1:B:937:SER:HB2	1:B:1012:ALA:HB1	1.91	0.51
1:C:681:ASP:OD1	1:C:681:ASP:N	2.44	0.51
1:C:706:ALA:HB1	1:C:715:VAL:HG21	1.92	0.51
1:D:75:LEU:CD2	1:F:168:ARG:HG2	2.41	0.51
1:D:242:THR:HG22	1:D:245:GLN:HG3	1.92	0.51
1:D:715:VAL:CG2	1:D:826:ILE:HD11	2.40	0.51
1:E:207:ILE:HG13	1:E:758:VAL:HG11	1.93	0.51
1:E:396:PHE:CE2	1:E:998:GLN:HG2	2.45	0.51
1:F:452:VAL:HG11	1:F:931:LEU:O	2.11	0.51
1:F:640:GLY:O	1:F:646:GLU:HG3	2.10	0.51
1:B:14:VAL:HG23	1:C:885:LEU:HD22	1.91	0.51
1:D:616:ASN:HB2	1:D:624:SER:HB2	1.93	0.51
1:E:634:TRP:H	1:E:634:TRP:CD1	2.26	0.51
1:E:944:ILE:HD11	1:E:1020:VAL:HB	1.90	0.51
1:F:465:VAL:O	1:F:469:GLN:HG2	2.11	0.51
1:A:680:PHE:CD2	1:A:858:TRP:HZ3	2.29	0.51
1:A:715:VAL:HA	1:A:827:LEU:O	2.11	0.51
3:B:1101:MC2:C2	3:B:1101:MC2:H5	2.40	0.51
1:C:184:MET:HE1	1:C:268:VAL:HG13	1.92	0.51
1:C:214:ILE:HG12	1:C:237:LYS:HB2	1.92	0.51
1:D:680:PHE:CZ	1:D:843:VAL:HG21	2.45	0.51
1:E:65:ILE:HD11	1:E:118:LEU:HD21	1.92	0.51
1:E:586:ARG:O	1:E:589:VAL:HG12	2.10	0.51
1:F:575:GLN:HG3	1:F:666:PHE:HE1	1.75	0.51
1:F:814:LYS:HE2	1:F:816:GLU:HG2	1.93	0.51
1:B:216:SER:HB3	1:B:236:GLY:CA	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:GLN:HB2	1:C:461:GLY:HA2	1.93	0.51
1:C:408:ASP:HB3	1:C:485:ALA:HB2	1.93	0.51
1:C:699:ARG:NE	1:C:824:MET:HG2	2.26	0.51
1:C:910:GLY:HA3	1:C:1011:THR:CG2	2.40	0.51
1:C:936:LEU:HB3	1:C:1009:MET:SD	2.51	0.51
1:D:166:LEU:O	1:D:172:VAL:HG21	2.10	0.51
1:E:786:SER:HB2	1:E:801:ASN:ND2	2.25	0.51
1:F:88:MET:SD	1:F:90:ILE:HG23	2.51	0.51
1:F:341:VAL:HA	1:F:344:LEU:HD12	1.92	0.51
1:A:703:LEU:HD11	1:A:717:PRO:HD3	1.93	0.51
1:B:799:PRO:HB2	1:B:801:ASN:OD1	2.10	0.51
1:B:944:ILE:HD11	1:B:1020:VAL:HB	1.93	0.51
1:C:5:PHE:CG	1:C:487:ILE:HG23	2.45	0.51
1:C:792:ASN:OD1	1:C:798:VAL:HG23	2.11	0.51
1:D:706:ALA:HA	1:D:846:ILE:HD13	1.93	0.51
1:F:443:VAL:HG23	1:F:890:LEU:HD11	1.92	0.51
1:F:807:LYS:NZ	1:F:808:TRP:O	2.44	0.51
1:A:216:SER:O	1:B:753:TRP:HB2	2.10	0.51
1:A:437:GLN:O	1:A:439:GLN:N	2.44	0.51
1:B:176:GLN:HG3	2:B:1103:LMT:H51	1.93	0.51
1:C:43:ILE:HD11	1:C:107:VAL:HB	1.92	0.51
1:D:602:GLU:CD	1:D:650:ARG:HE	2.18	0.51
1:E:134:LYS:HE2	1:E:674:LEU:HD23	1.92	0.51
1:F:347:ALA:CB	1:F:402:ILE:HD11	2.40	0.51
1:B:166:LEU:O	1:B:169:THR:OG1	2.28	0.51
1:B:528:GLU:CD	1:B:967:ARG:HG3	2.36	0.51
1:C:310:ILE:HD11	1:C:325:TYR:OH	2.11	0.51
1:C:891:TYR:CE1	1:C:946:GLU:HG3	2.46	0.51
1:D:273:GLN:CD	1:D:769:ARG:HD2	2.36	0.51
1:D:472:ILE:HA	1:D:475:VAL:HG12	1.93	0.51
1:D:540:PRO:O	1:D:543:LEU:HG	2.10	0.51
1:E:532:ALA:HB2	1:E:963:ILE:HD12	1.93	0.51
1:A:213:GLN:HG3	1:B:56:THR:HG23	1.93	0.51
1:B:151:LYS:HE3	1:B:285:PRO:HB3	1.91	0.51
1:B:189:ASP:HB2	1:B:775:ARG:HD3	1.93	0.51
1:C:150:THR:OG1	1:C:151:LYS:N	2.43	0.51
1:C:347:ALA:HB1	1:C:402:ILE:HD11	1.92	0.51
1:D:131:LYS:NZ	1:E:73:ASP:OD2	2.42	0.51
1:D:592:ASP:HA	1:D:595:ARG:HB2	1.92	0.51
1:E:17:LEU:HA	1:E:20:MET:HE3	1.93	0.51
1:F:782:PRO:O	1:F:785:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:OE1	1:B:820:GLY:HA2	2.11	0.50
1:B:367:ILE:HD13	1:B:492:LEU:HB3	1.93	0.50
1:B:686:ASP:HB2	1:B:690:VAL:HG12	1.93	0.50
1:B:925:PHE:CE2	1:B:997:SER:HB3	2.46	0.50
1:B:972:PRO:O	1:B:976:THR:HG23	2.11	0.50
1:C:164:ASP:HB3	1:C:168:ARG:NH2	2.26	0.50
1:B:703:LEU:HD11	1:B:717:PRO:HD3	1.93	0.50
1:B:1015:LEU:HD12	1:B:1019:TRP:NE1	2.26	0.50
1:C:897:PRO:O	1:C:901:MET:HG2	2.11	0.50
1:D:437:GLN:O	1:D:438:ILE:HG13	2.11	0.50
1:F:414:GLU:OE2	1:F:971:ARG:NH2	2.45	0.50
1:A:169:THR:O	1:A:172:VAL:HG22	2.11	0.50
1:A:676:ASN:N	1:A:676:ASN:HD22	2.09	0.50
1:B:184:MET:HG2	1:B:761:PHE:CZ	2.46	0.50
1:D:938:ALA:O	1:D:942:ILE:HG12	2.10	0.50
1:E:318:PRO:HD2	1:E:321:MET:HG3	1.94	0.50
1:E:534:ILE:HG22	1:E:1022:LEU:HD23	1.92	0.50
1:E:683:PHE:CD2	1:E:859:THR:HG21	2.46	0.50
1:A:404:LEU:HD13	1:A:449:LEU:HD11	1.94	0.50
1:B:20:MET:HG2	1:B:377:LEU:HD12	1.93	0.50
1:B:73:ASP:N	1:B:106:GLN:OE1	2.43	0.50
1:D:985:VAL:HA	1:D:1006:ILE:HD11	1.94	0.50
1:E:326:PRO:O	1:E:630:MET:HG3	2.11	0.50
1:E:361:ASN:HB3	1:E:364:ALA:H	1.76	0.50
1:E:407:ASN:HD22	1:E:936:LEU:HD21	1.75	0.50
1:E:540:PRO:O	1:E:544:ILE:HG22	2.12	0.50
1:F:609:VAL:HG12	1:F:611:THR:HG23	1.93	0.50
1:A:587:THR:HG21	1:A:622:GLN:O	2.11	0.50
1:A:587:THR:HG21	1:A:623:SER:HA	1.93	0.50
1:A:966:CYS:SG	1:A:1021:PRO:HG3	2.51	0.50
1:B:61:VAL:HG12	1:B:88:MET:HE3	1.94	0.50
1:B:397:GLY:HA3	1:B:473:THR:HG21	1.94	0.50
1:C:99:ASP:HB3	1:C:102:ILE:CG1	2.40	0.50
1:C:709:ASN:HB3	1:C:712:LEU:HD21	1.94	0.50
1:C:741:SER:O	1:C:743:ALA:N	2.39	0.50
1:A:682:LEU:HD23	1:A:683:PHE:C	2.37	0.50
1:A:731:ASP:O	1:A:735:ALA:N	2.37	0.50
1:A:915:THR:HG21	1:A:926:PHE:CD1	2.46	0.50
1:B:162:ILE:HG22	1:B:313:LEU:HD13	1.93	0.50
1:B:164:ASP:OD2	1:B:168:ARG:NH2	2.45	0.50
1:C:682:LEU:HB2	1:C:826:ILE:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:MET:HG2	1:E:761:PHE:CZ	2.47	0.50
1:F:535:LEU:O	1:F:538:ARG:NE	2.43	0.50
1:F:588:GLN:HG2	1:F:613:THR:HG21	1.94	0.50
1:A:135:ASN:HB3	1:A:672:LEU:O	2.12	0.50
1:A:539:ALA:HB3	1:A:540:PRO:HD3	1.93	0.50
1:A:851:PRO:O	1:A:854:VAL:HG12	2.12	0.50
1:D:162:ILE:O	1:D:166:LEU:HD23	2.11	0.50
1:D:388:PHE:HE2	1:D:469:GLN:HA	1.77	0.50
1:D:753:TRP:HH2	1:D:785:LEU:HA	1.75	0.50
1:A:115:THR:HA	1:A:118:LEU:HD13	1.93	0.50
1:A:437:GLN:O	1:A:438:ILE:HG12	2.12	0.50
1:B:407:ASN:HD22	1:B:936:LEU:CD2	2.22	0.50
1:B:520:PHE:HA	1:B:523:THR:HG22	1.92	0.50
1:E:66:GLU:OE1	1:E:820:GLY:HA2	2.11	0.50
1:E:310:ILE:HD11	1:E:325:TYR:CE2	2.47	0.50
1:F:448:VAL:O	1:F:452:VAL:HG23	2.12	0.50
1:A:351:VAL:O	1:A:355:MET:HG2	2.11	0.50
1:A:578:THR:OG1	1:A:587:THR:HG22	2.12	0.50
1:B:973:ILE:HD12	1:B:1017:ILE:HG22	1.94	0.50
1:D:202:ASP:OD2	1:D:791:ARG:NH2	2.35	0.50
1:D:498:LYS:H	1:D:499:PRO:HD3	1.77	0.50
1:E:143:VAL:HG11	1:E:281:PHE:HD2	1.77	0.50
1:E:344:LEU:O	1:E:348:ILE:HG23	2.11	0.50
1:F:208:GLN:HA	1:F:759:ASN:HD21	1.77	0.50
1:F:575:GLN:HG2	1:F:616:ASN:OD1	2.12	0.50
1:F:683:PHE:CZ	1:F:859:THR:HG21	2.47	0.50
1:B:193:LEU:HG	1:B:265:VAL:HG13	1.94	0.49
1:B:234:ILE:HG23	1:C:726:TYR:HB2	1.94	0.49
1:B:763:ASP:OD1	1:B:764:ARG:HG3	2.11	0.49
1:C:616:ASN:HA	1:C:626:MET:HG3	1.94	0.49
1:A:379:THR:HG23	1:A:398:MET:HE1	1.94	0.49
1:C:1012:ALA:O	1:C:1016:ALA:HB3	2.12	0.49
1:D:448:VAL:HG11	1:D:887:LEU:HD21	1.93	0.49
1:F:831:ALA:HB3	1:F:834:LEU:HD12	1.95	0.49
1:A:131:LYS:O	1:A:295:THR:HG22	2.13	0.49
1:C:909:ILE:HG13	1:C:910:GLY:N	2.26	0.49
1:C:1016:ALA:O	1:C:1020:VAL:HG23	2.12	0.49
1:D:189:ASP:HB3	1:D:192:LYS:HG3	1.94	0.49
1:E:584:ALA:O	1:E:588:GLN:HB2	2.13	0.49
1:E:646:GLU:HA	1:E:649:LYS:HD2	1.94	0.49
1:E:783:ASP:O	1:E:786:SER:OG	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:GLN:NE2	1:F:273:GLN:HE22	2.11	0.49
1:D:234:ILE:HA	1:E:726:TYR:O	2.12	0.49
1:D:578:THR:OG1	1:D:587:THR:HG22	2.13	0.49
1:D:944:ILE:HD11	1:D:1020:VAL:HB	1.94	0.49
1:D:370:ILE:O	1:D:373:PRO:HD2	2.12	0.49
1:F:306:ILE:O	1:F:310:ILE:HG12	2.13	0.49
1:F:399:VAL:HG11	1:F:987:LEU:HD21	1.94	0.49
1:C:912:LEU:HD23	1:C:926:PHE:HZ	1.76	0.49
1:F:192:LYS:HD3	1:F:264:ASP:O	2.13	0.49
1:F:261:ARG:HD2	1:F:263:LYS:HE3	1.95	0.49
1:F:966:CYS:SG	1:F:1021:PRO:HG3	2.52	0.49
1:A:572:LEU:HD13	1:A:644:VAL:HG13	1.95	0.49
1:A:753:TRP:HB2	1:C:217:GLY:H	1.76	0.49
1:B:102:ILE:HA	1:B:105:VAL:HG12	1.94	0.49
1:D:343:THR:HG21	1:D:998:GLN:OE1	2.12	0.49
1:D:375:VAL:HG12	1:D:480:LEU:HB3	1.93	0.49
1:D:453:PHE:CG	1:D:474:ILE:HD11	2.47	0.49
1:D:567:GLU:HB2	1:D:670:SER:HB2	1.93	0.49
1:E:445:ILE:HG22	1:E:942:ILE:HG13	1.94	0.49
1:F:135:ASN:O	1:F:292:LYS:HG2	2.13	0.49
1:F:910:GLY:HA3	1:F:1011:THR:HG21	1.94	0.49
1:C:218:GLN:HB3	1:C:233:THR:HA	1.95	0.49
1:D:728:LEU:HD21	1:D:785:LEU:HD22	1.93	0.49
1:D:816:GLU:HB2	1:D:823:ALA:O	2.12	0.49
1:E:47:VAL:CG1	1:E:127:ILE:HA	2.42	0.49
1:F:314:GLU:HA	1:F:317:MET:HB2	1.94	0.49
1:F:455:PRO:HB3	1:F:878:LEU:HD21	1.94	0.49
1:F:685:GLN:HG2	1:F:823:ALA:HB2	1.94	0.49
1:A:90:ILE:O	1:A:90:ILE:HG13	2.12	0.49
1:A:326:PRO:CB	1:A:610:PHE:HB2	2.43	0.49
1:B:211:ASN:ND2	1:B:760:ASP:O	2.44	0.49
1:B:394:THR:HG23	1:B:469:GLN:HG3	1.94	0.49
1:C:344:LEU:O	1:C:348:ILE:HG23	2.13	0.49
1:F:416:VAL:HG22	1:F:431:ALA:HA	1.95	0.49
1:A:453:PHE:CZ	1:A:932:THR:HA	2.48	0.49
1:A:831:ALA:HB3	1:A:834:LEU:HD23	1.94	0.49
1:B:433:LYS:O	1:B:437:GLN:HG3	2.13	0.49
1:C:906:LEU:HD22	1:C:1015:LEU:HB3	1.94	0.49
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.48	0.49
1:E:47:VAL:HG11	1:E:127:ILE:HG12	1.93	0.49
1:E:216:SER:HB2	1:E:234:ILE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:467:TYR:HE1	1:E:924:VAL:HG13	1.78	0.49
1:E:550:ALA:O	1:E:553:ILE:HG12	2.13	0.49
1:F:339:GLU:HG3	1:F:993:ALA:HB3	1.95	0.49
1:D:555:MET:HB3	1:D:912:LEU:HD13	1.95	0.48
1:D:812:SER:OG	1:D:815:LEU:HD13	2.13	0.48
1:E:392:THR:O	1:E:396:PHE:HD1	1.95	0.48
1:A:906:LEU:HD23	1:A:906:LEU:H	1.77	0.48
1:D:766:ARG:NE	1:E:67:GLN:OE1	2.43	0.48
1:F:531:VAL:O	1:F:534:ILE:HG13	2.14	0.48
1:F:683:PHE:HB2	1:F:857:SER:OG	2.12	0.48
1:F:818:TYR:HD2	1:F:823:ALA:HB3	1.76	0.48
1:A:10:ILE:HD11	1:B:888:ALA:O	2.12	0.48
1:A:405:LEU:HG	1:A:406:VAL:N	2.28	0.48
1:B:569:GLN:NE2	1:B:669:PRO:O	2.45	0.48
1:C:638:PRO:HD2	1:C:642:ASN:CG	2.38	0.48
1:D:411:VAL:HG12	1:D:438:ILE:HD13	1.95	0.48
1:E:226:LYS:HA	1:F:585:GLU:OE2	2.14	0.48
1:F:55:GLU:HG3	1:F:815:LEU:HD11	1.94	0.48
1:F:183:SER:OG	1:F:273:GLN:HG3	2.13	0.48
1:F:339:GLU:O	1:F:343:THR:HG23	2.13	0.48
1:F:910:GLY:HA3	1:F:1011:THR:CG2	2.43	0.48
1:F:969:ARG:C	1:F:972:PRO:HD2	2.38	0.48
1:A:193:LEU:HD22	1:A:265:VAL:HG13	1.94	0.48
1:B:55:GLU:HG2	1:B:815:LEU:HD11	1.96	0.48
1:B:980:PHE:O	1:B:984:VAL:HG22	2.12	0.48
1:C:507:GLU:HB3	1:C:509:LYS:HE3	1.95	0.48
1:D:100:PRO:HB3	1:D:295:THR:HG21	1.95	0.48
1:D:329:THR:O	1:D:332:VAL:HG12	2.13	0.48
1:D:631:LEU:HD21	1:D:647:LEU:HD12	1.95	0.48
1:D:745:ILE:HA	1:D:748:THR:HG22	1.95	0.48
1:F:356:TYR:HE1	1:F:361:ASN:C	2.22	0.48
1:A:394:THR:O	1:A:398:MET:HG2	2.13	0.48
1:A:753:TRP:HZ3	1:A:779:ARG:HA	1.78	0.48
1:B:544:ILE:HG23	1:B:1019:TRP:CH2	2.47	0.48
1:B:566:ASP:HB3	1:B:645:PHE:CZ	2.48	0.48
1:C:792:ASN:OD1	1:C:792:ASN:N	2.46	0.48
1:D:910:GLY:HA2	1:D:913:LEU:HB2	1.94	0.48
1:F:212:VAL:HA	1:F:239:ARG:HH11	1.78	0.48
1:A:319:GLN:CD	1:A:319:GLN:H	2.20	0.48
1:A:439:GLN:O	1:A:443:VAL:HG23	2.13	0.48
1:C:101:ASP:OD1	1:C:131:LYS:NZ	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:ARG:NH1	1:C:1025:VAL:HG12	2.29	0.48
1:F:450:SER:OG	1:F:475:VAL:HG13	2.13	0.48
1:A:186:ILE:HG12	1:A:262:LEU:HD21	1.95	0.48
1:A:370:ILE:O	1:A:373:PRO:HD2	2.13	0.48
1:A:567:GLU:HB2	1:A:670:SER:CB	2.43	0.48
1:A:569:GLN:CD	1:A:670:SER:HA	2.39	0.48
1:A:682:LEU:HD11	1:A:856:TYR:CD2	2.49	0.48
1:B:99:ASP:HB3	1:B:102:ILE:CG1	2.44	0.48
1:B:507:GLU:HB3	1:B:518:ARG:HG3	1.96	0.48
1:B:728:LEU:HD21	1:B:785:LEU:HD13	1.95	0.48
1:C:404:LEU:CD2	1:C:936:LEU:HD21	2.44	0.48
1:D:455:PRO:HG2	1:D:879:SER:HA	1.96	0.48
1:D:699:ARG:NH1	1:D:824:MET:SD	2.87	0.48
1:E:520:PHE:HA	1:E:523:THR:HG22	1.95	0.48
1:F:343:THR:HG21	1:F:998:GLN:OE1	2.13	0.48
1:F:753:TRP:CZ2	1:F:785:LEU:HD23	2.48	0.48
1:F:923:ASP:OD1	1:F:926:PHE:N	2.40	0.48
1:A:468:ARG:O	1:A:472:ILE:HG23	2.14	0.48
1:A:592:ASP:O	1:A:595:ARG:HB2	2.14	0.48
1:A:682:LEU:HD11	1:A:856:TYR:HD2	1.79	0.48
1:B:240:LEU:O	1:B:761:PHE:HB2	2.14	0.48
1:B:445:ILE:HG22	1:B:942:ILE:CD1	2.43	0.48
1:C:5:PHE:CD2	1:C:487:ILE:HG23	2.49	0.48
1:C:420:MET:HE3	1:C:500:ILE:HG12	1.96	0.48
1:E:566:ASP:HB3	1:E:645:PHE:CZ	2.48	0.48
1:E:729:GLU:OE1	1:E:807:LYS:HE3	2.13	0.48
1:F:697:GLN:O	1:F:701:LYS:HG2	2.14	0.48
1:F:761:PHE:CE2	1:F:763:ASP:HB2	2.49	0.48
1:B:444:GLY:O	1:B:448:VAL:HG23	2.14	0.48
1:C:278:ASN:HB2	1:C:613:THR:HG22	1.95	0.48
1:E:544:ILE:HG23	1:E:1019:TRP:CH2	2.45	0.48
1:F:980:PHE:HD2	1:F:1009:MET:HG3	1.76	0.48
1:B:17:LEU:HD23	1:C:885:LEU:HD21	1.95	0.48
1:C:43:ILE:HD11	1:C:107:VAL:CB	2.44	0.48
1:C:524:THR:O	1:C:528:GLU:HG3	2.13	0.48
1:D:318:PRO:HG2	1:D:321:MET:SD	2.54	0.48
1:E:314:GLU:HA	1:E:317:MET:SD	2.54	0.48
1:A:470:PHE:O	1:A:473:THR:HG22	2.14	0.47
1:A:701:LYS:HB3	1:A:701:LYS:HE2	1.63	0.47
1:A:702:PHE:HE2	1:A:847:VAL:HG23	1.79	0.47
1:B:786:SER:HB2	1:B:801:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:GLY:HA2	1:B:1011:THR:HG23	1.96	0.47
1:D:146:ASP:C	1:D:148:SER:H	2.21	0.47
1:D:618:ALA:HB1	1:D:719:GLY:H	1.78	0.47
1:D:674:LEU:O	1:D:676:ASN:N	2.47	0.47
1:D:753:TRP:CH2	1:D:785:LEU:HG	2.49	0.47
1:F:799:PRO:HB2	1:F:801:ASN:OD1	2.13	0.47
1:A:704:MET:HG2	1:D:693:GLU:OE2	2.14	0.47
1:B:455:PRO:O	1:B:875:LEU:HD13	2.13	0.47
1:B:938:ALA:O	1:B:942:ILE:HG12	2.13	0.47
1:E:616:ASN:HB2	1:E:624:SER:HB2	1.95	0.47
1:F:69:MET:O	1:F:72:ILE:HG13	2.14	0.47
1:F:470:PHE:CD2	1:F:928:VAL:HG11	2.48	0.47
1:F:579:PRO:HG3	1:F:660:ASP:CG	2.39	0.47
1:F:726:TYR:HE2	1:F:782:PRO:HG3	1.79	0.47
1:A:943:LEU:HB2	1:A:969:ARG:NH1	2.29	0.47
1:D:851:PRO:O	1:D:854:VAL:HG22	2.14	0.47
1:F:99:ASP:HB3	1:F:102:ILE:CG1	2.44	0.47
1:B:524:THR:HG22	1:B:970:LEU:HD13	1.96	0.47
1:B:708:GLN:H	1:B:708:GLN:HG2	1.51	0.47
1:D:748:THR:HG21	1:D:790:VAL:HG22	1.96	0.47
1:E:68:GLN:HG3	1:E:114:ALA:HB2	1.96	0.47
1:E:404:LEU:HD13	1:E:478:MET:HG3	1.96	0.47
1:F:541:TYR:O	1:F:544:ILE:HG12	2.14	0.47
1:A:437:GLN:C	1:A:439:GLN:H	2.21	0.47
1:A:759:ASN:H	1:A:770:VAL:HG22	1.79	0.47
1:B:223:PRO:HB3	1:C:275:TYR:CD2	2.49	0.47
1:C:138:MET:HB2	1:C:327:TYR:O	2.14	0.47
1:D:170:LYS:NZ	1:E:74:ASN:H	2.13	0.47
1:D:226:LYS:H	1:D:226:LYS:HD2	1.79	0.47
1:D:240:LEU:HD22	1:D:245:GLN:HB3	1.96	0.47
1:D:453:PHE:CZ	1:D:932:THR:HA	2.49	0.47
1:D:918:ARG:HH21	1:D:1003:THR:HB	1.79	0.47
1:E:151:LYS:HE3	1:E:285:PRO:HB3	1.96	0.47
1:E:220:GLY:O	1:E:231:ASN:ND2	2.47	0.47
1:F:336:SER:HA	1:F:993:ALA:HB1	1.96	0.47
1:F:571:VAL:HG23	1:F:668:PRO:HG2	1.97	0.47
1:F:1012:ALA:O	1:F:1016:ALA:HB3	2.14	0.47
1:A:863:TYR:O	1:A:867:LEU:N	2.47	0.47
1:B:314:GLU:HA	1:B:317:MET:HE2	1.97	0.47
1:B:527:TYR:OH	1:B:1017:ILE:O	2.22	0.47
1:C:77:TYR:CZ	1:C:859:THR:HG23	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:456:MET:HE3	1:E:931:LEU:HD11	1.95	0.47
1:E:723:GLU:HG3	1:E:813:PRO:HG3	1.97	0.47
1:A:280:GLN:HG2	1:A:611:THR:HB	1.97	0.47
1:A:371:ALA:O	1:A:375:VAL:HG13	2.14	0.47
1:A:724:PRO:HA	1:A:810:TYR:CB	2.35	0.47
1:A:724:PRO:CA	1:A:810:TYR:HB2	2.36	0.47
1:A:816:GLU:HB2	1:A:823:ALA:O	2.15	0.47
1:B:207:ILE:HG13	1:B:758:VAL:HG11	1.97	0.47
1:B:219:LEU:HD13	1:B:230:LEU:HD21	1.96	0.47
1:B:445:ILE:HG22	1:B:942:ILE:HD12	1.97	0.47
1:B:740:VAL:HG23	1:B:792:ASN:OD1	2.15	0.47
1:B:762:ILE:O	1:B:762:ILE:HG13	2.14	0.47
1:C:281:PHE:CZ	1:C:324:VAL:HG11	2.49	0.47
1:D:302:THR:O	1:D:306:ILE:HG23	2.15	0.47
1:D:453:PHE:CD1	1:D:474:ILE:HD11	2.50	0.47
1:D:519:MET:O	1:D:523:THR:HG23	2.14	0.47
1:D:1015:LEU:O	1:D:1019:TRP:CD1	2.67	0.47
1:E:69:MET:SD	1:E:107:VAL:HG23	2.55	0.47
1:E:235:ILE:O	1:E:235:ILE:HG13	2.14	0.47
1:E:643:SER:OG	1:E:646:GLU:OE1	2.33	0.47
1:F:463:THR:HG21	1:F:868:SER:HB2	1.96	0.47
1:F:637:ARG:HB3	1:F:642:ASN:HB3	1.96	0.47
1:A:816:GLU:OE1	1:A:824:MET:HA	2.15	0.47
1:B:553:ILE:O	1:B:557:THR:HG23	2.14	0.47
1:C:540:PRO:O	1:C:544:ILE:HG23	2.14	0.47
1:C:555:MET:O	1:C:559:ILE:HG23	2.15	0.47
1:C:985:VAL:O	1:C:989:ILE:HG12	2.15	0.47
1:D:169:THR:O	1:D:172:VAL:HG22	2.15	0.47
1:D:193:LEU:HD22	1:D:265:VAL:HG13	1.97	0.47
1:E:20:MET:HG2	1:E:377:LEU:HD12	1.96	0.47
1:E:38:ILE:HG22	1:E:465:VAL:CG1	2.45	0.47
1:E:162:ILE:C	1:E:165:PRO:HD2	2.40	0.47
1:E:344:LEU:HD23	1:E:402:ILE:HG12	1.97	0.47
1:E:925:PHE:CE2	1:E:997:SER:HB3	2.49	0.47
1:F:690:VAL:HG12	1:F:691:GLY:H	1.78	0.47
1:F:763:ASP:OD2	1:F:768:LYS:NZ	2.45	0.47
1:F:983:GLY:O	1:F:986:PRO:HD2	2.15	0.47
1:A:457:ALA:O	1:A:468:ARG:HD3	2.15	0.47
1:A:727:LYS:HD3	1:C:235:ILE:HD11	1.97	0.47
1:C:548:ILE:HD11	1:C:906:LEU:HD23	1.96	0.47
1:D:213:GLN:HG3	1:E:56:THR:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:726:TYR:CZ	1:D:782:PRO:HB3	2.49	0.47
1:E:990:SER:O	1:E:999:HIS:NE2	2.44	0.47
1:F:20:MET:SD	1:F:374:VAL:HG22	2.55	0.47
1:F:181:GLN:CD	1:F:766:ARG:HH11	2.22	0.47
1:F:520:PHE:HA	1:F:523:THR:HG22	1.97	0.47
1:F:920:LEU:HD13	1:F:1000:ALA:HA	1.96	0.47
1:A:376:LEU:O	1:A:379:THR:HG22	2.15	0.47
1:A:655:PHE:HA	1:A:658:PHE:HD2	1.80	0.47
1:A:729:GLU:O	1:A:804:ALA:HA	2.14	0.47
1:B:306:ILE:O	1:B:310:ILE:HG12	2.15	0.47
1:B:563:PHE:CD2	1:B:564:LEU:HD22	2.49	0.47
1:B:684:LEU:O	1:B:823:ALA:HA	2.15	0.47
1:E:280:GLN:OE1	1:E:588:GLN:NE2	2.48	0.47
1:E:657:SER:O	1:E:659:LYS:N	2.48	0.47
1:F:99:ASP:O	1:F:102:ILE:HG13	2.14	0.47
1:F:740:VAL:HG23	1:F:798:VAL:HG21	1.95	0.47
1:A:326:PRO:HB3	1:A:610:PHE:HB2	1.97	0.46
1:A:540:PRO:O	1:A:543:LEU:HG	2.14	0.46
1:C:445:ILE:HA	1:C:942:ILE:HD11	1.97	0.46
1:C:891:TYR:CB	1:C:896:ILE:HD11	2.44	0.46
1:D:365:THR:O	1:D:368:PRO:HD2	2.15	0.46
1:F:635:GLU:OE1	1:F:635:GLU:N	2.43	0.46
1:F:910:GLY:H	1:F:1011:THR:HG21	1.80	0.46
1:F:918:ARG:NH1	1:F:1003:THR:OG1	2.44	0.46
1:B:23:GLY:HA3	1:B:377:LEU:O	2.15	0.46
1:B:178:PHE:HB2	1:B:288:GLY:H	1.79	0.46
1:C:85:ASP:OD1	1:C:85:ASP:N	2.48	0.46
1:C:393:LEU:HD13	1:C:466:ILE:HG13	1.97	0.46
1:C:412:VAL:O	1:C:416:VAL:HG23	2.16	0.46
1:C:969:ARG:O	1:C:972:PRO:HD2	2.15	0.46
1:D:616:ASN:OD1	1:D:626:MET:HB3	2.15	0.46
1:D:863:TYR:O	1:D:867:LEU:HB2	2.15	0.46
2:D:1101:LMT:H81	2:D:1101:LMT:H52	1.67	0.46
1:E:145:THR:N	1:E:320:GLY:O	2.37	0.46
1:F:137:LEU:HD12	1:F:329:THR:HG22	1.97	0.46
1:F:328:ASP:OD1	1:F:330:THR:OG1	2.32	0.46
1:F:726:TYR:CE2	1:F:782:PRO:HG3	2.50	0.46
1:A:453:PHE:HZ	1:A:932:THR:HA	1.81	0.46
1:A:616:ASN:CB	1:A:624:SER:HB2	2.44	0.46
1:B:683:PHE:CE1	1:B:825:GLU:HB2	2.50	0.46
1:C:111:LEU:HA	1:C:111:LEU:HD23	1.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.96	0.46
1:C:646:GLU:HA	1:C:649:LYS:HD2	1.97	0.46
1:C:682:LEU:HD11	1:C:843:VAL:CG1	2.44	0.46
1:C:931:LEU:O	1:C:934:ILE:HG12	2.15	0.46
1:D:716:ARG:O	1:D:826:ILE:HD12	2.15	0.46
1:E:143:VAL:HG11	1:E:281:PHE:CD2	2.51	0.46
1:E:363:ARG:HD3	1:E:496:MET:O	2.15	0.46
1:F:212:VAL:HA	1:F:239:ARG:NH1	2.30	0.46
1:F:825:GLU:OE2	1:F:827:LEU:HD21	2.15	0.46
1:B:712:LEU:HD21	1:B:843:VAL:HG23	1.98	0.46
1:C:65:ILE:O	1:C:69:MET:HG2	2.16	0.46
1:C:99:ASP:HB3	1:C:102:ILE:HG13	1.97	0.46
1:C:145:THR:N	1:C:320:GLY:O	2.49	0.46
1:D:10:ILE:HD11	1:E:893:SER:N	2.30	0.46
1:D:631:LEU:HD22	1:D:644:VAL:HG23	1.96	0.46
1:F:740:VAL:CG2	1:F:798:VAL:HG21	2.45	0.46
1:A:139:VAL:HA	1:A:290:ALA:HA	1.97	0.46
1:A:141:GLY:HA2	1:A:288:GLY:HA2	1.97	0.46
1:A:580:PRO:HG3	1:A:721:SER:HB2	1.97	0.46
1:B:540:PRO:O	1:B:544:ILE:HG22	2.15	0.46
1:D:41:PRO:HG2	1:D:98:THR:HB	1.98	0.46
1:F:293:LEU:HD11	1:F:299:ALA:HA	1.97	0.46
1:A:655:PHE:HA	1:A:658:PHE:CD2	2.50	0.46
1:B:178:PHE:HA	2:B:1103:LMT:H52	1.96	0.46
1:C:324:VAL:HG12	1:C:325:TYR:N	2.31	0.46
1:C:508:HIS:NE2	1:C:521:LEU:HD12	2.31	0.46
1:D:453:PHE:HZ	1:D:932:THR:HA	1.81	0.46
1:D:575:GLN:NE2	1:D:617:PHE:H	2.13	0.46
1:D:592:ASP:O	1:D:595:ARG:HB2	2.16	0.46
1:E:762:ILE:O	1:E:762:ILE:HG13	2.15	0.46
1:A:210:GLN:CD	1:A:249:ILE:HG13	2.41	0.46
1:B:142:VAL:HG21	1:B:158:ILE:HG21	1.98	0.46
1:B:1013:THR:O	1:B:1017:ILE:HG23	2.16	0.46
1:C:444:GLY:O	1:C:448:VAL:HG23	2.15	0.46
1:C:448:VAL:O	1:C:452:VAL:HG23	2.16	0.46
1:D:983:GLY:O	1:D:986:PRO:HD2	2.16	0.46
1:F:134:LYS:HG3	1:F:675:GLY:HA2	1.97	0.46
1:F:958:ILE:HG13	1:F:959:VAL:N	2.31	0.46
1:A:156:ASN:OD1	1:A:768:LYS:NZ	2.47	0.46
1:A:739:GLY:O	1:A:793:ASP:HB2	2.16	0.46
1:B:178:PHE:HA	2:B:1103:LMT:H32	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:VAL:HG12	1:D:259:GLN:HA	1.98	0.46
1:D:363:ARG:NH2	2:D:1101:LMT:O3B	2.45	0.46
1:E:3:LYS:HA	1:E:6:ILE:HD12	1.98	0.46
1:E:775:ARG:CZ	1:E:776:PRO:HD2	2.46	0.46
1:F:20:MET:HG2	1:F:374:VAL:HA	1.97	0.46
1:F:617:PHE:CE1	1:F:626:MET:HE1	2.51	0.46
1:F:866:ARG:HA	1:F:866:ARG:HE	1.80	0.46
1:A:157:TYR:CG	1:A:321:MET:HE1	2.51	0.46
1:A:355:MET:HB3	1:A:355:MET:HE2	1.49	0.46
1:A:367:ILE:HD13	1:A:413:VAL:HG22	1.98	0.46
1:C:184:MET:HE1	1:C:268:VAL:CG1	2.45	0.46
1:D:951:LEU:C	1:D:953:GLU:H	2.23	0.46
1:E:166:LEU:HD22	1:E:306:ILE:HG22	1.96	0.46
1:F:65:ILE:O	1:F:69:MET:HG2	2.16	0.46
1:F:444:GLY:O	1:F:448:VAL:HG23	2.15	0.46
1:F:448:VAL:HG11	1:F:938:ALA:CB	2.46	0.46
1:A:352:PHE:CD2	1:A:369:THR:HG21	2.46	0.46
1:A:745:ILE:HG22	1:A:790:VAL:HG11	1.97	0.46
1:B:893:SER:OG	1:B:896:ILE:HG12	2.16	0.46
1:C:634:TRP:CD1	1:C:634:TRP:H	2.33	0.46
1:E:340:VAL:HG11	1:E:395:MET:HE3	1.98	0.46
1:B:20:MET:HE2	1:B:374:VAL:HG23	1.98	0.45
1:B:43:ILE:HG21	1:B:107:VAL:HG11	1.98	0.45
1:B:104:GLN:HA	1:B:107:VAL:HG12	1.98	0.45
1:B:171:GLY:HA3	1:B:302:THR:HB	1.98	0.45
1:B:616:ASN:CB	1:B:624:SER:HB2	2.46	0.45
1:B:626:MET:HG3	1:B:627:ALA:N	2.31	0.45
1:C:192:LYS:HB3	1:C:265:VAL:HA	1.96	0.45
1:C:367:ILE:O	1:C:370:ILE:HG22	2.16	0.45
1:D:969:ARG:HH21	1:D:972:PRO:CB	2.28	0.45
1:E:164:ASP:HB3	1:E:165:PRO:HD3	1.97	0.45
1:E:190:PRO:HB3	1:E:788:TRP:CD2	2.51	0.45
1:E:559:ILE:HD11	1:E:915:THR:HG22	1.98	0.45
1:E:579:PRO:HD3	1:E:660:ASP:O	2.17	0.45
1:A:235:ILE:HD12	1:B:727:LYS:HG3	1.98	0.45
1:B:70:ASN:O	1:B:110:LYS:HE2	2.16	0.45
1:B:199:THR:HG22	1:B:201:GLY:H	1.81	0.45
1:B:576:VAL:HG22	1:B:663:VAL:HG22	1.98	0.45
1:C:186:ILE:HG22	1:C:268:VAL:HG22	1.97	0.45
1:C:362:PHE:HA	1:C:365:THR:HG22	1.97	0.45
1:D:669:PRO:O	1:D:671:VAL:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:701:LYS:HE2	1:D:701:LYS:HB3	1.78	0.45
1:E:630:MET:N	1:E:630:MET:SD	2.88	0.45
1:F:936:LEU:HB3	1:F:1009:MET:CE	2.46	0.45
1:A:637:ARG:HB2	1:A:642:ASN:HB3	1.98	0.45
1:B:281:PHE:CE2	1:B:324:VAL:HG11	2.51	0.45
1:B:483:ILE:O	1:B:487:ILE:HG12	2.16	0.45
1:C:79:SER:HB2	1:C:818:TYR:CE1	2.52	0.45
1:C:88:MET:SD	1:C:90:ILE:HG23	2.56	0.45
1:D:388:PHE:CE2	1:D:469:GLN:HA	2.52	0.45
1:D:491:ALA:O	1:D:495:THR:HG23	2.17	0.45
1:D:779:ARG:NH1	1:F:221:GLY:O	2.39	0.45
1:E:683:PHE:HD2	1:E:859:THR:HG21	1.82	0.45
1:F:45:VAL:HB	1:F:90:ILE:HG13	1.97	0.45
1:F:121:GLU:HG3	1:F:124:ARG:NH2	2.31	0.45
1:F:685:GLN:O	1:F:854:VAL:HA	2.17	0.45
1:A:300:LEU:HD21	1:A:333:VAL:HG11	1.99	0.45
1:A:377:LEU:HD11	2:A:1101:LMT:H101	1.98	0.45
1:A:699:ARG:HE	1:A:699:ARG:HB2	1.42	0.45
1:A:896:ILE:HG12	1:A:897:PRO:HD3	1.98	0.45
1:C:356:TYR:HD2	1:C:365:THR:HG21	1.80	0.45
1:C:925:PHE:HB3	1:C:1001:ILE:HG23	1.99	0.45
1:D:185:ARG:NH1	1:D:771:TYR:HB3	2.32	0.45
1:E:78:ILE:HD11	1:E:90:ILE:HD11	1.98	0.45
1:A:239:ARG:HE	1:A:239:ARG:HB3	1.62	0.45
1:A:332:VAL:HG23	1:A:634:TRP:HZ2	1.81	0.45
1:B:572:LEU:HD22	1:B:629:ILE:HD12	1.99	0.45
1:D:703:LEU:HD21	1:D:826:ILE:HD13	1.97	0.45
1:F:718:ASN:HB3	1:F:825:GLU:HB3	1.98	0.45
1:F:739:GLY:O	1:F:792:ASN:HA	2.16	0.45
1:A:888:ALA:O	1:C:10:ILE:HD11	2.16	0.45
1:B:677:ALA:H	1:B:861:LEU:HD12	1.81	0.45
1:D:24:GLY:O	1:D:28:LEU:HG	2.16	0.45
1:D:134:LYS:HE2	1:D:674:LEU:HD23	1.99	0.45
1:E:433:LYS:O	1:E:437:GLN:HG3	2.17	0.45
1:F:455:PRO:HG2	1:F:879:SER:HA	1.98	0.45
1:F:456:MET:HE2	1:F:467:TYR:HA	1.99	0.45
1:A:202:ASP:OD2	1:A:791:ARG:NH2	2.43	0.45
1:A:728:LEU:HD11	1:A:785:LEU:HD23	1.99	0.45
1:B:128:ARG:NH1	1:C:113:LEU:HD22	2.31	0.45
1:B:158:ILE:HA	1:B:162:ILE:HG12	1.98	0.45
1:B:215:SER:HB2	1:C:750:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ARG:CZ	1:B:968:MET:HE3	2.46	0.45
1:B:566:ASP:HB3	1:B:645:PHE:HZ	1.81	0.45
1:C:242:THR:HG22	1:C:245:GLN:HG3	1.99	0.45
1:D:10:ILE:HA	1:D:13:TRP:HB2	1.98	0.45
1:D:115:THR:HA	1:D:118:LEU:HD13	1.99	0.45
1:D:334:SER:O	1:D:337:ILE:HG13	2.17	0.45
1:D:576:VAL:HB	1:D:625:GLY:O	2.17	0.45
1:A:595:ARG:HH12	1:A:609:VAL:HB	1.81	0.45
1:C:46:GLN:HG2	1:C:89:THR:HB	1.99	0.45
1:C:121:GLU:H	1:C:121:GLU:HG2	1.44	0.45
1:C:915:THR:HG23	1:C:920:LEU:HB2	1.99	0.45
1:D:492:LEU:HD22	1:D:496:MET:HE2	1.99	0.45
1:D:637:ARG:HB2	1:D:642:ASN:HB3	1.98	0.45
1:E:397:GLY:HA3	1:E:473:THR:HG21	1.99	0.45
1:E:411:VAL:HG13	1:E:969:ARG:HH12	1.81	0.45
1:E:467:TYR:CE1	1:E:924:VAL:HG13	2.52	0.45
1:E:534:ILE:HG12	1:E:541:TYR:CZ	2.52	0.45
1:E:742:LEU:O	1:E:745:ILE:HG22	2.17	0.45
2:E:1101:LMT:H62	2:E:1101:LMT:H32	1.54	0.45
1:F:433:LYS:NZ	1:F:437:GLN:OE1	2.49	0.45
1:F:652:GLN:HE22	1:F:664:PHE:HD1	1.64	0.45
1:A:416:VAL:HG22	1:A:431:ALA:HA	1.98	0.45
1:A:565:PRO:HG3	1:A:923:ASP:OD2	2.17	0.45
1:A:576:VAL:HG22	1:A:663:VAL:HG13	1.98	0.45
1:A:864:GLU:O	1:A:866:ARG:N	2.49	0.45
1:B:685:GLN:HB3	1:B:823:ALA:HB2	1.98	0.45
1:C:136:PHE:CE1	1:C:292:LYS:HE3	2.51	0.45
1:C:240:LEU:O	1:C:761:PHE:HB2	2.17	0.45
1:C:424:GLY:HA3	1:C:502:LYS:HG2	1.98	0.45
1:D:181:GLN:OE1	1:D:768:LYS:HG2	2.17	0.45
1:D:492:LEU:HB3	1:D:496:MET:HE2	1.98	0.45
1:E:65:ILE:HG12	1:E:111:LEU:HD23	1.98	0.45
1:E:188:LEU:HD11	1:E:772:LEU:HD21	1.98	0.45
1:F:64:VAL:HG11	1:F:117:LEU:HB2	1.98	0.45
1:A:840:MET:CE	1:A:866:ARG:HE	2.29	0.45
1:A:983:GLY:O	1:A:986:PRO:HD2	2.16	0.45
1:B:218:GLN:HG2	1:B:219:LEU:O	2.17	0.45
1:B:290:ALA:HB2	2:B:1103:LMT:H91	1.99	0.45
1:D:680:PHE:CD2	1:D:858:TRP:HZ3	2.35	0.45
1:E:237:LYS:NZ	1:F:742:LEU:O	2.49	0.45
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:VAL:HG13	1:E:435:MET:CE	2.46	0.45
1:E:574:ALA:HB3	1:E:627:ALA:HB3	1.98	0.45
1:F:158:ILE:HB	1:F:162:ILE:HD11	1.98	0.45
1:F:540:PRO:O	1:F:544:ILE:HG23	2.16	0.45
1:F:602:GLU:OE2	1:F:650:ARG:HD2	2.16	0.45
1:F:967:ARG:HG3	1:F:968:MET:N	2.32	0.45
1:B:535:LEU:O	1:B:538:ARG:NH1	2.50	0.44
1:C:27:ILE:HD11	1:C:380:PHE:CD2	2.52	0.44
1:D:76:ARG:HE	1:D:95:GLU:CD	2.25	0.44
1:D:796:GLU:O	1:D:797:MET:HE2	2.17	0.44
1:D:872:ALA:HB3	1:D:873:PRO:HD3	1.99	0.44
1:E:48:SER:HA	1:E:86:GLY:O	2.17	0.44
1:E:447:MET:HE1	2:E:1101:LMT:H121	1.99	0.44
1:E:817:ARG:NH2	1:E:820:GLY:O	2.50	0.44
1:F:182:TYR:HD2	1:F:768:LYS:HZ3	1.64	0.44
1:F:540:PRO:HA	1:F:543:LEU:HD12	1.99	0.44
1:F:738:LEU:HB2	1:F:803:PHE:CZ	2.29	0.44
1:F:981:ILE:HG23	1:F:1006:ILE:HG23	1.98	0.44
1:A:810:TYR:OH	1:D:701:LYS:HG2	2.17	0.44
1:B:524:THR:O	1:B:528:GLU:HG3	2.18	0.44
1:B:904:VAL:O	1:B:908:VAL:HG23	2.18	0.44
1:D:235:ILE:HD12	1:E:727:LYS:HG3	1.98	0.44
1:D:574:ALA:HB3	1:D:627:ALA:HB3	1.99	0.44
1:D:898:PHE:O	1:D:902:LEU:HD13	2.17	0.44
1:E:359:LEU:HD22	1:E:417:GLU:OE1	2.18	0.44
1:E:398:MET:O	1:E:402:ILE:HD13	2.16	0.44
1:E:636:GLU:C	1:E:638:PRO:HD3	2.42	0.44
1:F:918:ARG:HD3	1:F:1003:THR:OG1	2.16	0.44
1:A:538:ARG:HA	1:A:541:TYR:HD2	1.81	0.44
1:B:577:GLN:HE21	1:B:616:ASN:HD22	1.66	0.44
1:B:910:GLY:N	1:B:1011:THR:HG21	2.31	0.44
1:C:109:ASN:HA	1:C:112:GLN:CD	2.42	0.44
1:C:789:TYR:CE2	1:C:799:PRO:HB3	2.52	0.44
1:D:376:LEU:HA	1:D:379:THR:HG22	1.98	0.44
1:E:104:GLN:HA	1:E:107:VAL:HG12	1.99	0.44
1:E:247:GLU:HB3	1:E:263:LYS:HG2	1.99	0.44
1:F:635:GLU:H	1:F:635:GLU:CD	2.24	0.44
1:F:896:ILE:HD11	1:F:949:LYS:HD3	1.98	0.44
1:A:378:GLY:O	1:A:382:VAL:HG23	2.17	0.44
1:A:680:PHE:HD2	1:A:858:TRP:HZ3	1.66	0.44
1:A:817:ARG:NH1	1:A:822:PRO:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:ALA:HB3	1:A:873:PRO:HD3	2.00	0.44
1:A:903:VAL:O	1:A:906:LEU:HG	2.17	0.44
1:B:164:ASP:HB3	1:B:165:PRO:HD3	1.99	0.44
1:B:344:LEU:O	1:B:348:ILE:HG23	2.18	0.44
1:B:407:ASN:ND2	1:B:936:LEU:HD22	2.25	0.44
1:B:407:ASN:OD1	1:B:976:THR:HB	2.18	0.44
1:B:442:LEU:O	1:B:445:ILE:HG12	2.17	0.44
1:C:480:LEU:HA	1:C:483:ILE:HG22	1.99	0.44
1:D:155:SER:OG	1:D:180:SER:N	2.51	0.44
1:D:541:TYR:HA	1:D:544:ILE:HG22	1.99	0.44
1:D:669:PRO:C	1:D:671:VAL:H	2.25	0.44
1:E:58:GLN:OE1	1:E:817:ARG:HD3	2.17	0.44
1:E:115:THR:HA	1:E:118:LEU:HD13	1.98	0.44
1:F:729:GLU:HB2	1:F:805:THR:OG1	2.17	0.44
1:F:944:ILE:HG13	1:F:973:ILE:CD1	2.47	0.44
1:A:197:GLN:HB3	1:A:797:MET:HE3	2.00	0.44
1:A:801:ASN:OD1	1:A:801:ASN:N	2.49	0.44
1:B:62:VAL:HG21	1:B:82:SER:OG	2.18	0.44
1:B:85:ASP:C	1:B:87:SER:H	2.26	0.44
1:B:887:LEU:HB3	1:B:897:PRO:HB3	2.00	0.44
1:B:895:SER:C	1:B:897:PRO:HD2	2.43	0.44
1:C:300:LEU:O	1:C:304:LYS:HG3	2.18	0.44
1:C:447:MET:HE2	1:C:447:MET:HB3	1.70	0.44
1:C:655:PHE:HB3	1:C:663:VAL:CG2	2.46	0.44
1:C:936:LEU:HD13	1:C:1009:MET:CG	2.47	0.44
1:D:150:THR:HG23	1:D:152:GLU:H	1.82	0.44
1:F:807:LYS:HZ2	1:F:808:TRP:H	1.64	0.44
1:B:435:MET:O	1:B:439:GLN:HB2	2.18	0.44
1:B:930:LEU:O	1:B:933:THR:HG22	2.18	0.44
1:C:80:SER:HB2	1:C:90:ILE:HG22	1.99	0.44
1:C:362:PHE:O	1:C:366:LEU:HB2	2.18	0.44
1:C:626:MET:HE3	1:C:626:MET:HB3	1.80	0.44
1:D:188:LEU:HD21	1:D:203:VAL:HG11	2.00	0.44
1:D:242:THR:HG23	1:D:245:GLN:H	1.81	0.44
1:E:155:SER:O	1:E:158:ILE:HG12	2.18	0.44
1:E:249:ILE:HD11	1:E:262:LEU:CD1	2.47	0.44
1:E:532:ALA:O	1:E:536:LYS:HG3	2.17	0.44
1:E:817:ARG:HD2	1:E:822:PRO:HA	2.00	0.44
1:F:718:ASN:CB	1:F:825:GLU:HB3	2.48	0.44
1:F:754:GLY:O	1:F:773:GLN:HG3	2.17	0.44
1:A:168:ARG:NE	1:B:69:MET:O	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:ALA:O	1:A:678:THR:C	2.61	0.44
1:B:519:MET:HE3	1:B:519:MET:HB3	1.84	0.44
1:B:686:ASP:HB3	1:B:695:LEU:HG	1.99	0.44
1:C:20:MET:CG	1:C:374:VAL:HA	2.47	0.44
1:C:49:TYR:CE2	1:C:119:PRO:HG2	2.53	0.44
1:C:936:LEU:HD23	1:C:936:LEU:HA	1.82	0.44
1:D:333:VAL:O	1:D:337:ILE:HG12	2.18	0.44
1:D:696:LEU:O	1:D:700:ASN:ND2	2.42	0.44
1:D:995:SER:HB3	1:D:999:HIS:HE2	1.83	0.44
1:E:102:ILE:O	1:E:105:VAL:HG12	2.18	0.44
1:E:578:THR:HG21	1:E:587:THR:HB	2.00	0.44
1:F:264:ASP:OD1	1:F:264:ASP:N	2.51	0.44
1:F:545:TYR:HB2	1:F:1019:TRP:CZ3	2.53	0.44
1:A:75:LEU:CD2	1:C:168:ARG:HG2	2.48	0.44
1:A:456:MET:HB3	1:A:467:TYR:HB3	1.98	0.44
1:A:789:TYR:HB3	1:A:797:MET:HB3	2.00	0.44
1:B:115:THR:HA	1:B:118:LEU:HD13	2.00	0.44
1:B:567:GLU:OE1	1:B:994:GLY:HA2	2.17	0.44
1:C:80:SER:OG	1:C:817:ARG:HB2	2.18	0.44
1:C:273:GLN:OE1	1:C:769:ARG:HD2	2.18	0.44
1:C:738:LEU:HB2	1:C:803:PHE:HE1	1.83	0.44
1:D:76:ARG:HB3	1:D:93:THR:O	2.18	0.44
1:D:375:VAL:HG21	1:D:405:LEU:HG	1.99	0.44
1:E:861:LEU:HD23	1:E:861:LEU:HA	1.74	0.44
1:A:568:ASP:HB3	1:A:634:TRP:CZ3	2.52	0.44
1:A:609:VAL:HG13	1:A:629:ILE:HD13	1.98	0.44
1:A:680:PHE:HD1	1:A:828:GLY:O	2.00	0.44
1:B:78:ILE:HD12	1:B:92:VAL:HG22	2.00	0.44
1:B:213:GLN:HA	1:B:237:LYS:HB3	1.99	0.44
1:B:343:THR:HA	1:B:346:GLU:HG2	1.99	0.44
1:B:534:ILE:HG12	1:B:541:TYR:CZ	2.52	0.44
1:C:186:ILE:HD11	1:C:772:LEU:HG	2.00	0.44
1:D:478:MET:HE2	1:D:478:MET:HB2	1.79	0.44
1:D:548:ILE:HG23	1:D:909:ILE:HD13	2.00	0.44
1:D:555:MET:HG3	1:D:912:LEU:HB3	2.00	0.44
1:D:753:TRP:C	1:F:217:GLY:HA3	2.43	0.44
1:E:109:ASN:O	1:E:113:LEU:HD13	2.18	0.44
1:F:666:PHE:CD2	1:F:677:ALA:HB2	2.52	0.44
1:F:727:LYS:HB3	1:F:807:LYS:CB	2.43	0.44
1:A:57:VAL:CG1	1:A:88:MET:HB3	2.48	0.43
1:A:234:ILE:HA	1:B:726:TYR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:MET:HE2	1:B:499:PRO:HA	2.00	0.43
1:B:616:ASN:CG	1:B:624:SER:HB2	2.43	0.43
1:B:631:LEU:HD12	1:B:644:VAL:HG23	2.00	0.43
1:C:569:GLN:HA	1:C:634:TRP:HH2	1.82	0.43
1:D:342:LYS:O	1:D:346:GLU:HG3	2.17	0.43
1:D:590:VAL:O	1:D:593:SER:HB2	2.18	0.43
1:E:14:VAL:HG23	1:F:885:LEU:HD22	2.00	0.43
1:E:891:TYR:HB3	1:E:896:ILE:HD11	1.99	0.43
1:F:279:ALA:HB1	1:F:610:PHE:CE1	2.53	0.43
1:F:876:TYR:OH	1:F:927:GLN:HG2	2.17	0.43
1:A:218:GLN:HG3	1:A:221:GLY:HA2	2.00	0.43
1:A:363:ARG:NH2	2:A:1102:LMT:O4'	2.51	0.43
1:A:418:ARG:O	1:A:422:GLU:HG3	2.18	0.43
1:A:478:MET:HE2	1:A:478:MET:HB2	1.85	0.43
1:A:519:MET:O	1:A:523:THR:HG23	2.19	0.43
1:B:753:TRP:CZ2	1:B:785:LEU:HA	2.53	0.43
1:C:137:LEU:O	1:C:329:THR:HB	2.18	0.43
1:C:929:GLY:HA2	1:C:932:THR:HG22	2.00	0.43
1:D:739:GLY:O	1:D:793:ASP:HB2	2.17	0.43
1:E:422:GLU:OE2	1:E:967:ARG:NH1	2.51	0.43
1:E:527:TYR:OH	1:E:1017:ILE:O	2.27	0.43
1:E:738:LEU:O	1:E:792:ASN:ND2	2.49	0.43
1:F:453:PHE:O	1:F:471:SER:OG	2.28	0.43
1:F:896:ILE:CD1	1:F:949:LYS:HD3	2.48	0.43
1:A:58:GLN:HA	1:A:62:VAL:HB	2.00	0.43
1:A:101:ASP:OD1	1:A:131:LYS:NZ	2.51	0.43
1:B:187:TRP:HB3	1:B:775:ARG:HA	2.00	0.43
1:B:293:LEU:HD11	1:B:299:ALA:HB2	1.99	0.43
1:C:228:GLN:NE2	1:C:230:LEU:H	2.16	0.43
1:C:370:ILE:HG21	1:C:492:LEU:CD1	2.48	0.43
1:C:462:SER:OG	1:C:864:GLU:HG3	2.19	0.43
1:C:587:THR:OG1	1:C:623:SER:HA	2.19	0.43
1:C:602:GLU:HG2	1:C:647:LEU:CD2	2.48	0.43
1:D:753:TRP:HZ3	1:D:779:ARG:HA	1.84	0.43
1:E:61:VAL:O	1:E:65:ILE:HD12	2.17	0.43
1:E:176:GLN:O	1:E:289:ILE:HA	2.18	0.43
1:E:453:PHE:HZ	1:E:932:THR:HA	1.83	0.43
1:E:466:ILE:HD11	1:E:924:VAL:HG21	2.01	0.43
1:E:587:THR:O	1:E:591:VAL:HG23	2.18	0.43
1:F:20:MET:CE	1:F:373:PRO:HB2	2.48	0.43
1:F:390:ILE:HG23	1:F:395:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:699:ARG:HG3	1:F:826:ILE:HD11	2.00	0.43
1:A:699:ARG:O	1:A:703:LEU:HD23	2.18	0.43
1:B:120:GLN:CD	1:B:120:GLN:H	2.27	0.43
1:B:1007:GLY:O	1:B:1011:THR:HG22	2.19	0.43
1:C:370:ILE:O	1:C:373:PRO:HD2	2.17	0.43
1:C:554:TRP:CZ2	1:C:558:ARG:HD2	2.53	0.43
1:C:890:LEU:HD22	1:C:891:TYR:CE1	2.54	0.43
1:D:249:ILE:HG23	1:D:262:LEU:HB2	1.99	0.43
1:D:352:PHE:HD1	1:D:353:LEU:HD22	1.83	0.43
1:D:375:VAL:HG13	1:D:484:VAL:HG21	1.99	0.43
1:D:456:MET:CG	1:D:471:SER:HB2	2.45	0.43
1:D:669:PRO:HG2	1:D:674:LEU:HB2	1.99	0.43
1:E:480:LEU:HA	1:E:483:ILE:HG22	2.00	0.43
1:E:684:LEU:O	1:E:823:ALA:HA	2.19	0.43
1:A:780:MET:HE3	1:C:225:VAL:HG23	2.00	0.43
1:A:975:MET:HE2	1:A:975:MET:HB3	1.86	0.43
1:B:94:PHE:CE2	1:B:103:ALA:HB1	2.53	0.43
1:B:361:ASN:ND2	1:B:363:ARG:HB2	2.33	0.43
1:C:38:ILE:O	1:C:96:GLN:NE2	2.51	0.43
1:C:651:ALA:HB1	1:C:655:PHE:CE2	2.54	0.43
1:C:672:LEU:HA	1:C:672:LEU:HD23	1.68	0.43
1:D:139:VAL:HG23	1:D:289:ILE:C	2.44	0.43
1:D:915:THR:HG21	1:D:926:PHE:CD2	2.48	0.43
1:F:317:MET:HE1	1:F:323:VAL:HG23	2.00	0.43
1:F:376:LEU:HD11	1:F:402:ILE:HG22	2.01	0.43
1:A:177:VAL:HG13	1:A:179:GLY:O	2.18	0.43
1:A:388:PHE:CE2	1:A:469:GLN:HA	2.53	0.43
1:A:568:ASP:HB3	1:A:634:TRP:CH2	2.53	0.43
1:B:13:TRP:CH2	1:B:370:ILE:HD13	2.54	0.43
1:B:234:ILE:HG22	1:B:235:ILE:N	2.34	0.43
1:B:478:MET:HE3	1:B:478:MET:HB3	1.53	0.43
1:C:138:MET:HE2	1:C:306:ILE:HD11	2.00	0.43
1:C:180:SER:HB2	1:C:273:GLN:HB2	2.00	0.43
1:C:418:ARG:HD3	1:C:968:MET:SD	2.59	0.43
1:C:687:GLN:NE2	1:C:855:GLY:HA3	2.34	0.43
1:C:734:LYS:HE2	1:C:734:LYS:HB3	1.40	0.43
1:D:76:ARG:NH2	1:D:96:GLN:HG2	2.33	0.43
1:D:186:ILE:HD12	1:D:186:ILE:N	2.33	0.43
1:D:884:PHE:HD2	1:D:885:LEU:HD12	1.82	0.43
1:A:349:LEU:O	1:A:353:LEU:HD23	2.19	0.43
1:B:178:PHE:CE1	2:B:1103:LMT:H61	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ILE:HD11	1:B:325:TYR:CE2	2.54	0.43
1:B:428:ARG:H	1:B:428:ARG:HG3	1.42	0.43
1:C:169:THR:HG21	1:C:306:ILE:HG22	2.01	0.43
1:C:631:LEU:HD11	1:C:647:LEU:HD12	2.01	0.43
1:D:190:PRO:HG2	1:D:787:LYS:HG2	2.01	0.43
1:D:415:ASN:HB3	1:D:434:SER:HB2	2.01	0.43
1:D:878:LEU:HD13	1:D:878:LEU:HA	1.85	0.43
1:E:45:VAL:HB	1:E:90:ILE:CG2	2.49	0.43
1:E:420:MET:HE3	1:E:427:PRO:HA	2.00	0.43
1:E:578:THR:OG1	1:E:579:PRO:HD2	2.19	0.43
1:F:347:ALA:HB3	1:F:402:ILE:HD11	2.01	0.43
1:F:690:VAL:HG11	1:F:694:VAL:HG11	2.01	0.43
1:F:792:ASN:CB	1:F:796:GLU:HG3	2.49	0.43
1:F:887:LEU:HD21	1:F:942:ILE:HD11	2.00	0.43
1:A:545:TYR:HB2	1:A:1019:TRP:CZ3	2.53	0.43
1:A:887:LEU:HA	1:A:887:LEU:HD23	1.62	0.43
1:B:1015:LEU:O	1:B:1019:TRP:CD1	2.66	0.43
1:C:450:SER:OG	1:C:475:VAL:HG13	2.19	0.43
1:C:863:TYR:O	1:C:867:LEU:HD23	2.19	0.43
1:D:435:MET:O	1:D:439:GLN:HB2	2.18	0.43
1:D:448:VAL:HG22	1:D:886:CYS:HB3	2.00	0.43
1:E:45:VAL:HA	1:E:128:ARG:O	2.17	0.43
1:E:226:LYS:HD2	1:E:227:GLY:N	2.33	0.43
1:A:13:TRP:CD2	2:A:1102:LMT:H32	2.53	0.43
1:A:318:PRO:HD2	1:A:321:MET:SD	2.59	0.43
1:A:447:MET:HE2	1:A:447:MET:HB2	1.76	0.43
1:A:733:GLU:CG	1:C:250:LEU:HD11	2.48	0.43
1:B:99:ASP:HB3	1:B:102:ILE:HG12	2.00	0.43
1:B:212:VAL:O	1:B:237:LYS:HD3	2.19	0.43
1:B:987:LEU:O	1:B:999:HIS:HD2	2.02	0.43
1:C:354:VAL:HG11	1:C:978:LEU:HB3	2.01	0.43
1:C:376:LEU:HD11	1:C:402:ILE:HG22	2.01	0.43
1:D:733:GLU:OE2	1:F:261:ARG:NH2	2.36	0.43
1:E:26:SER:HB2	1:E:384:ALA:HB2	2.00	0.43
1:E:80:SER:HB3	1:E:90:ILE:HG13	2.01	0.43
1:E:343:THR:HA	1:E:346:GLU:CG	2.48	0.43
1:F:645:PHE:O	1:F:649:LYS:HG3	2.19	0.43
1:A:144:SER:HA	1:A:321:MET:HA	2.00	0.43
1:A:730:ILE:O	1:A:730:ILE:HG13	2.18	0.43
1:C:155:SER:O	1:C:158:ILE:HG12	2.19	0.43
1:D:543:LEU:O	1:D:547:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:VAL:HG11	1:E:158:ILE:HG21	2.00	0.43
2:E:1101:LMT:H82	2:E:1101:LMT:H112	1.52	0.43
1:F:358:PHE:CG	1:F:975:MET:HG2	2.53	0.43
1:F:367:ILE:HB	1:F:368:PRO:HD3	2.00	0.43
1:A:135:ASN:CA	1:A:674:LEU:HG	2.39	0.42
1:B:338:HIS:C	1:B:340:VAL:H	2.26	0.42
1:B:602:GLU:HG2	1:B:647:LEU:HD12	2.01	0.42
1:C:434:SER:HA	1:C:437:GLN:HG3	2.01	0.42
1:D:470:PHE:CE2	1:D:928:VAL:HG13	2.54	0.42
1:D:578:THR:HG21	1:D:586:ARG:HD2	2.01	0.42
1:D:807:LYS:HB2	1:D:807:LYS:HE2	1.79	0.42
1:F:281:PHE:CD1	1:F:326:PRO:HB3	2.54	0.42
1:F:503:GLY:C	1:F:505:HIS:H	2.27	0.42
1:F:616:ASN:HB2	1:F:624:SER:HB3	2.02	0.42
1:A:20:MET:HE3	1:A:373:PRO:HB2	2.00	0.42
1:A:45:VAL:HG22	1:A:129:VAL:HG13	2.01	0.42
1:A:388:PHE:HE2	1:A:469:GLN:HA	1.83	0.42
1:A:563:PHE:O	1:A:564:LEU:HB2	2.19	0.42
1:B:198:LEU:HA	1:B:791:ARG:HH22	1.84	0.42
1:B:234:ILE:HG12	1:C:726:TYR:HB2	2.01	0.42
1:C:353:LEU:HD23	1:C:353:LEU:HA	1.92	0.42
1:C:365:THR:O	1:C:368:PRO:HD2	2.19	0.42
1:C:508:HIS:ND1	1:C:518:ARG:HG2	2.33	0.42
1:C:652:GLN:HE22	1:C:664:PHE:HD1	1.67	0.42
1:D:439:GLN:O	1:D:443:VAL:HG23	2.18	0.42
1:D:682:LEU:HD23	1:D:683:PHE:C	2.45	0.42
1:E:568:ASP:OD1	1:E:637:ARG:NH1	2.47	0.42
1:F:49:TYR:CE2	1:F:60:THR:HG21	2.53	0.42
1:F:234:ILE:HG13	1:F:234:ILE:O	2.18	0.42
1:F:520:PHE:HE2	1:F:971:ARG:HB2	1.85	0.42
1:F:915:THR:HG23	1:F:920:LEU:HB2	2.00	0.42
1:A:76:ARG:HB3	1:A:93:THR:O	2.19	0.42
1:A:796:GLU:O	1:A:797:MET:HE2	2.18	0.42
1:B:162:ILE:C	1:B:165:PRO:HD2	2.44	0.42
1:C:138:MET:HE3	1:C:140:VAL:HG22	2.01	0.42
1:C:145:THR:HG22	1:C:320:GLY:C	2.44	0.42
1:C:759:ASN:O	1:C:770:VAL:HG22	2.19	0.42
1:D:785:LEU:HD11	1:F:219:LEU:HD21	2.01	0.42
1:E:262:LEU:HD23	1:E:262:LEU:O	2.18	0.42
1:E:344:LEU:HD21	1:E:402:ILE:HD11	2.01	0.42
1:E:566:ASP:HB3	1:E:645:PHE:HZ	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:508:HIS:HB3	1:F:518:ARG:HG2	2.01	0.42
1:F:706:ALA:HB1	1:F:715:VAL:HG21	2.01	0.42
1:A:669:PRO:HG3	1:A:673:GLU:OE2	2.19	0.42
1:B:214:ILE:HG12	1:B:237:LYS:HB2	2.01	0.42
1:B:445:ILE:HD12	1:B:939:LYS:NZ	2.35	0.42
1:B:669:PRO:HD2	1:B:672:LEU:HD13	2.02	0.42
1:B:936:LEU:HA	1:B:936:LEU:HD23	1.62	0.42
1:C:463:THR:HA	1:C:466:ILE:CG2	2.49	0.42
1:D:439:GLN:HG3	1:D:486:LEU:CD2	2.50	0.42
1:E:143:VAL:O	1:E:321:MET:HA	2.19	0.42
1:E:235:ILE:HD11	1:F:727:LYS:HD3	2.01	0.42
1:E:760:ASP:HB3	1:E:767:VAL:HG13	2.01	0.42
1:F:2:SER:OG	1:F:435:MET:HE2	2.20	0.42
1:F:174:ASP:OD1	1:F:175:PHE:N	2.51	0.42
1:F:637:ARG:HA	1:F:642:ASN:HD22	1.84	0.42
1:F:745:ILE:HA	1:F:748:THR:HG22	2.01	0.42
1:F:1032:LYS:HE3	1:F:1032:LYS:HB2	1.75	0.42
1:A:138:MET:HE1	1:A:307:ARG:NH1	2.35	0.42
1:A:981:ILE:HG22	1:A:1009:MET:HB3	2.02	0.42
1:A:984:VAL:HG13	1:A:987:LEU:HD12	2.01	0.42
1:B:57:VAL:HG21	1:B:88:MET:HB3	2.02	0.42
1:B:234:ILE:HG22	1:B:235:ILE:H	1.84	0.42
1:B:459:PHE:CE1	1:B:875:LEU:HD12	2.54	0.42
1:C:696:LEU:HA	1:C:699:ARG:NH1	2.35	0.42
1:D:776:PRO:O	1:D:780:MET:HG2	2.19	0.42
1:E:478:MET:HE3	1:E:478:MET:HB3	1.49	0.42
1:F:5:PHE:CD2	1:F:487:ILE:HG23	2.54	0.42
1:F:181:GLN:OE1	1:F:766:ARG:HD3	2.20	0.42
1:F:452:VAL:HG22	1:F:883:VAL:HG21	2.00	0.42
1:F:980:PHE:CE2	1:F:1009:MET:HG3	2.54	0.42
1:F:1016:ALA:HB1	1:F:1020:VAL:CG2	2.50	0.42
1:A:33:ASN:ND2	1:A:35:TYR:O	2.37	0.42
1:A:342:LYS:O	1:A:346:GLU:HG3	2.20	0.42
1:A:680:PHE:CD1	1:A:828:GLY:O	2.73	0.42
1:D:541:TYR:HA	1:D:544:ILE:CG2	2.49	0.42
1:E:307:ARG:HG3	1:E:325:TYR:CZ	2.54	0.42
1:E:329:THR:O	1:E:333:VAL:HG23	2.19	0.42
1:E:359:LEU:HA	1:E:359:LEU:HD23	1.85	0.42
1:E:568:ASP:OD1	1:E:637:ARG:NH2	2.47	0.42
1:F:78:ILE:HG22	1:F:92:VAL:HG13	2.01	0.42
1:F:449:LEU:HD12	1:F:478:MET:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:453:PHE:CD2	1:F:474:ILE:HG21	2.55	0.42
1:A:234:ILE:HG22	1:B:726:TYR:HB3	2.01	0.42
1:D:13:TRP:CZ2	2:D:1101:LMT:H31	2.55	0.42
1:E:414:GLU:OE1	1:E:972:PRO:HG3	2.19	0.42
1:F:83:ASN:HD22	1:F:87:SER:HB2	1.85	0.42
1:F:84:SER:HB3	1:F:813:PRO:HA	2.01	0.42
1:F:407:ASN:HA	1:F:976:THR:HG22	2.02	0.42
1:F:584:ALA:O	1:F:588:GLN:HB2	2.20	0.42
1:B:584:ALA:O	1:B:588:GLN:HB2	2.20	0.42
1:C:992:GLY:O	1:C:995:SER:HB3	2.18	0.42
1:D:669:PRO:CA	1:D:678:THR:HG22	2.46	0.42
1:E:465:VAL:O	1:E:469:GLN:HG2	2.19	0.42
1:E:683:PHE:CE1	1:E:825:GLU:HB2	2.55	0.42
1:F:595:ARG:HG2	1:F:599:LEU:HD12	2.01	0.42
1:A:303:ALA:HA	1:A:306:ILE:HG12	2.02	0.42
1:A:541:TYR:HA	1:A:544:ILE:CG2	2.49	0.42
1:A:775:ARG:O	1:A:779:ARG:HG2	2.19	0.42
1:B:448:VAL:HG13	1:B:883:VAL:HG22	2.01	0.42
1:B:560:PRO:O	1:B:922:ASN:HB2	2.20	0.42
1:B:597:TYR:CD1	1:B:601:LYS:HD2	2.54	0.42
1:B:672:LEU:HD13	1:B:672:LEU:HA	1.79	0.42
1:D:655:PHE:HA	1:D:658:PHE:CD2	2.55	0.42
1:E:234:ILE:HG22	1:F:726:TYR:CB	2.48	0.42
1:E:472:ILE:HD13	1:E:472:ILE:HA	1.94	0.42
1:A:406:VAL:HG12	1:A:410:ILE:HG12	2.02	0.42
1:A:898:PHE:O	1:A:902:LEU:HD13	2.19	0.42
1:B:541:TYR:O	1:B:1019:TRP:CZ3	2.73	0.42
1:D:25:LEU:HD12	1:D:25:LEU:HA	1.86	0.42
1:D:246:PHE:O	1:D:262:LEU:HD23	2.19	0.42
1:E:56:THR:O	1:E:56:THR:HG22	2.20	0.42
1:E:120:GLN:CD	1:E:120:GLN:H	2.27	0.42
1:E:893:SER:OG	1:E:896:ILE:HG23	2.19	0.42
1:F:541:TYR:C	1:F:1019:TRP:HH2	2.27	0.42
1:B:394:THR:O	1:B:398:MET:HG3	2.19	0.41
1:C:695:LEU:O	1:C:699:ARG:NH1	2.53	0.41
1:D:639:GLY:O	1:D:641:GLU:N	2.44	0.41
1:F:45:VAL:HA	1:F:128:ARG:O	2.19	0.41
1:F:164:ASP:HB2	1:F:165:PRO:HD3	2.02	0.41
1:F:652:GLN:HG3	1:F:714:ARG:HH11	1.85	0.41
1:A:863:TYR:OH	1:C:170:LYS:NZ	2.53	0.41
1:B:143:VAL:O	1:B:321:MET:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:MET:HG2	2:B:1102:LMT:O6B	2.20	0.41
1:C:573:PHE:CE2	1:C:668:PRO:HG3	2.54	0.41
1:C:594:MET:HE2	1:C:594:MET:HB3	1.59	0.41
1:C:902:LEU:HD13	1:C:1023:PHE:CD1	2.55	0.41
1:D:188:LEU:HD11	1:D:772:LEU:HD21	2.02	0.41
1:D:293:LEU:HD12	1:D:302:THR:HG21	2.02	0.41
1:D:702:PHE:CE1	1:D:826:ILE:HG12	2.54	0.41
1:D:724:PRO:HA	1:D:810:TYR:HB2	2.02	0.41
1:D:725:GLN:OE1	1:F:235:ILE:HD11	2.20	0.41
1:E:412:VAL:HG13	1:E:435:MET:HE1	2.02	0.41
1:F:79:SER:HB2	1:F:818:TYR:CE1	2.55	0.41
1:F:637:ARG:HD2	1:F:642:ASN:O	2.20	0.41
1:F:884:PHE:CE2	1:F:897:PRO:HB2	2.54	0.41
1:F:911:ALA:HA	1:F:1004:GLY:O	2.20	0.41
1:F:985:VAL:O	1:F:989:ILE:HG12	2.19	0.41
1:A:198:LEU:HA	1:A:791:ARG:NH2	2.35	0.41
1:A:571:VAL:HG23	1:A:668:PRO:HG2	2.02	0.41
1:A:931:LEU:HD23	1:A:931:LEU:HA	1.80	0.41
1:B:399:VAL:HG11	1:B:987:LEU:HD11	2.01	0.41
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.20	0.41
1:B:904:VAL:HG13	1:B:934:ILE:CG2	2.50	0.41
1:D:598:LEU:O	1:D:602:GLU:HB2	2.21	0.41
1:D:696:LEU:HD13	1:D:699:ARG:HH11	1.86	0.41
1:D:793:ASP:C	1:D:794:LYS:HD3	2.45	0.41
1:E:541:TYR:HA	1:E:544:ILE:CG2	2.49	0.41
1:E:697:GLN:O	1:E:701:LYS:HG3	2.20	0.41
1:E:904:VAL:O	1:E:908:VAL:HG23	2.19	0.41
1:F:33:ASN:O	1:F:391:ASN:HA	2.20	0.41
1:F:987:LEU:O	1:F:999:HIS:HD2	2.03	0.41
1:A:491:ALA:O	1:A:495:THR:HG23	2.20	0.41
1:A:950:GLU:O	1:A:953:GLU:HG3	2.21	0.41
1:B:23:GLY:O	1:B:27:ILE:HG23	2.19	0.41
1:B:454:LEU:O	1:B:458:PHE:HD1	2.04	0.41
1:B:586:ARG:O	1:B:589:VAL:HG12	2.20	0.41
1:B:738:LEU:HD13	1:B:798:VAL:HG11	2.01	0.41
1:C:185:ARG:HH11	1:C:771:TYR:CB	2.32	0.41
1:C:563:PHE:O	1:C:923:ASP:HB2	2.20	0.41
1:D:158:ILE:HG12	1:D:162:ILE:HD11	2.01	0.41
1:D:166:LEU:HD22	1:D:309:THR:HG21	2.02	0.41
1:D:405:LEU:HD23	1:D:406:VAL:N	2.35	0.41
1:E:453:PHE:CD1	1:E:474:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:PHE:O	1:F:327:TYR:HE2	2.02	0.41
1:F:139:VAL:HG11	1:F:610:PHE:CE2	2.55	0.41
1:F:448:VAL:HG13	1:F:883:VAL:HG13	2.01	0.41
1:F:747:SER:O	1:F:751:ILE:HG12	2.20	0.41
1:F:890:LEU:HD22	1:F:891:TYR:CE1	2.55	0.41
1:A:62:VAL:HG21	1:A:82:SER:OG	2.21	0.41
1:A:135:ASN:HA	1:A:674:LEU:CG	2.38	0.41
1:A:318:PRO:HD2	1:A:321:MET:CE	2.50	0.41
1:A:535:LEU:HD23	1:A:959:VAL:HG13	2.02	0.41
1:A:753:TRP:CZ2	1:A:785:LEU:HA	2.55	0.41
1:B:155:SER:O	1:B:158:ILE:HG12	2.20	0.41
1:B:207:ILE:HG12	1:B:207:ILE:H	1.71	0.41
1:B:574:ALA:HB3	1:B:627:ALA:HB3	2.02	0.41
1:C:68:GLN:HG3	1:C:114:ALA:HB2	2.01	0.41
1:C:149:MET:HE3	1:C:321:MET:HB3	2.03	0.41
1:C:903:VAL:CG2	1:C:1020:VAL:HG22	2.42	0.41
1:D:524:THR:HG22	1:D:970:LEU:HD12	2.02	0.41
1:D:892:GLU:HG3	1:F:8:ARG:HD3	2.02	0.41
1:E:527:TYR:CE2	1:E:966:CYS:HB3	2.56	0.41
1:F:393:LEU:HD13	1:F:466:ILE:HG23	2.03	0.41
1:A:456:MET:HE1	1:A:928:VAL:HA	2.02	0.41
1:A:884:PHE:HB2	1:A:901:MET:HE2	2.02	0.41
1:A:930:LEU:O	1:A:934:ILE:HG23	2.20	0.41
1:B:106:GLN:O	1:B:110:LYS:HG2	2.20	0.41
1:B:655:PHE:HB3	1:B:663:VAL:HB	2.02	0.41
1:C:10:ILE:HA	1:C:13:TRP:HB2	2.03	0.41
1:C:792:ASN:CG	1:C:798:VAL:HG23	2.46	0.41
1:D:170:LYS:HZ3	1:E:74:ASN:H	1.68	0.41
1:D:480:LEU:O	1:D:483:ILE:HG22	2.20	0.41
1:D:702:PHE:HE2	1:D:847:VAL:HG23	1.84	0.41
1:E:102:ILE:HA	1:E:105:VAL:HG12	2.02	0.41
1:E:973:ILE:HD11	1:E:1017:ILE:HG22	2.01	0.41
1:F:80:SER:OG	1:F:817:ARG:HB2	2.20	0.41
1:F:687:GLN:CD	1:F:821:VAL:HG11	2.44	0.41
1:A:796:GLU:C	1:A:797:MET:HE2	2.46	0.41
1:A:840:MET:HE2	1:A:866:ARG:HH21	1.85	0.41
1:A:864:GLU:C	1:A:866:ARG:H	2.28	0.41
1:B:163:GLN:HG3	1:B:175:PHE:HE1	1.85	0.41
1:B:262:LEU:O	1:B:262:LEU:HD23	2.20	0.41
1:B:817:ARG:NH1	1:B:820:GLY:O	2.54	0.41
1:C:76:ARG:HG2	1:C:77:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:GLN:HG3	1:D:817:ARG:HD2	2.02	0.41
1:F:365:THR:O	1:F:368:PRO:HD2	2.21	0.41
1:A:20:MET:HE1	2:A:1102:LMT:H111	2.03	0.41
1:A:146:ASP:C	1:A:148:SER:N	2.78	0.41
1:B:35:TYR:HB3	1:B:38:ILE:HD12	2.02	0.41
1:B:84:SER:HB3	1:B:813:PRO:HA	2.02	0.41
1:C:138:MET:HE2	1:C:306:ILE:CD1	2.50	0.41
1:C:351:VAL:O	1:C:355:MET:HG3	2.21	0.41
1:C:572:LEU:HD23	1:C:573:PHE:O	2.21	0.41
1:C:985:VAL:CG2	1:C:986:PRO:HD3	2.44	0.41
1:E:439:GLN:HG2	1:E:486:LEU:HD22	2.03	0.41
1:E:445:ILE:HD12	1:E:939:LYS:NZ	2.36	0.41
1:E:601:LYS:H	1:E:601:LYS:HG2	1.71	0.41
1:E:671:VAL:O	1:E:673:GLU:HG2	2.21	0.41
1:E:789:TYR:CZ	1:E:799:PRO:HB3	2.56	0.41
1:F:891:TYR:CE1	1:F:946:GLU:OE1	2.74	0.41
1:F:958:ILE:HG13	1:F:959:VAL:H	1.84	0.41
1:A:375:VAL:CG2	1:A:405:LEU:HD13	2.51	0.41
1:A:520:PHE:O	1:A:524:THR:HG23	2.21	0.41
1:A:647:LEU:HD12	1:A:647:LEU:HA	1.89	0.41
1:A:673:GLU:OE1	1:A:861:LEU:HD13	2.21	0.41
1:A:848:LYS:HE3	1:A:848:LYS:HB3	1.87	0.41
1:A:951:LEU:HD22	1:A:956:LYS:HE3	2.03	0.41
1:A:982:LEU:HA	1:A:985:VAL:HG23	2.03	0.41
1:B:139:VAL:O	1:B:326:PRO:HD2	2.21	0.41
1:B:228:GLN:O	1:B:229:GLN:NE2	2.50	0.41
1:B:453:PHE:CE1	1:B:931:LEU:HB3	2.55	0.41
1:C:200:PRO:HB2	1:C:751:ILE:HD11	2.02	0.41
1:C:208:GLN:HA	1:C:759:ASN:OD1	2.21	0.41
1:D:75:LEU:HD21	1:F:168:ARG:HG2	2.02	0.41
1:D:138:MET:HE1	1:D:307:ARG:NH1	2.35	0.41
1:D:247:GLU:HB3	1:D:263:LYS:HB2	2.03	0.41
1:D:355:MET:HE1	1:D:410:ILE:HG13	2.03	0.41
1:D:525:HIS:CD2	1:D:967:ARG:HH22	2.39	0.41
1:D:540:PRO:O	1:D:544:ILE:HG22	2.21	0.41
1:D:586:ARG:O	1:D:590:VAL:HG23	2.21	0.41
1:D:603:SER:C	1:D:605:SER:H	2.29	0.41
1:D:636:GLU:C	1:D:638:PRO:HD3	2.46	0.41
1:D:712:LEU:HD23	1:D:838:ASP:OD2	2.21	0.41
1:D:731:ASP:OD2	1:D:734:LYS:HD3	2.21	0.41
1:E:69:MET:HE1	1:E:107:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:VAL:O	1:E:355:MET:HB2	2.21	0.41
1:E:524:THR:O	1:E:528:GLU:HG3	2.20	0.41
1:E:527:TYR:HE2	1:E:966:CYS:HB3	1.86	0.41
1:E:635:GLU:H	1:E:635:GLU:CD	2.29	0.41
1:E:659:LYS:HE3	1:E:659:LYS:HB3	1.78	0.41
1:E:739:GLY:O	1:E:793:ASP:N	2.54	0.41
1:E:821:VAL:HG12	1:E:822:PRO:HD2	2.03	0.41
1:E:973:ILE:CD1	1:E:1017:ILE:HG22	2.51	0.41
1:F:27:ILE:HA	1:F:30:LEU:HD12	2.03	0.41
1:F:47:VAL:HG12	1:F:88:MET:CE	2.50	0.41
1:F:156:ASN:OD1	1:F:156:ASN:N	2.54	0.41
1:F:177:VAL:HG12	1:F:179:GLY:N	2.36	0.41
1:F:186:ILE:HG21	1:F:262:LEU:HD21	2.03	0.41
1:F:240:LEU:HB2	1:F:246:PHE:CZ	2.56	0.41
1:F:341:VAL:O	1:F:344:LEU:HB2	2.21	0.41
1:F:594:MET:HE3	1:F:594:MET:HB3	1.59	0.41
1:F:595:ARG:HD2	1:F:595:ARG:C	2.46	0.41
1:F:690:VAL:HG21	1:F:853:GLY:HA3	2.03	0.41
1:F:830:PRO:HG3	1:F:836:SER:HA	2.03	0.41
1:A:402:ILE:HA	1:A:405:LEU:CD2	2.51	0.41
1:A:708:GLN:HB2	1:D:807:LYS:CD	2.41	0.41
1:A:936:LEU:HD12	1:A:1009:MET:CE	2.51	0.41
1:B:251:LEU:HD11	1:B:262:LEU:HA	2.02	0.41
1:B:455:PRO:HG3	2:B:1105:LMT:H51	2.02	0.41
1:B:616:ASN:HB3	1:B:618:ALA:H	1.85	0.41
1:C:441:ALA:O	1:C:445:ILE:HG12	2.20	0.41
1:D:889:ALA:HB2	1:F:14:VAL:HG11	2.03	0.41
1:E:375:VAL:HG11	1:E:405:LEU:HD22	2.03	0.41
1:E:671:VAL:O	1:E:671:VAL:HG13	2.21	0.41
1:E:1020:VAL:N	1:E:1021:PRO:HD2	2.36	0.41
1:F:55:GLU:OE1	1:F:55:GLU:N	2.51	0.41
1:F:697:GLN:HB3	1:F:701:LYS:HE3	2.03	0.41
1:A:135:ASN:O	1:A:292:LYS:HG3	2.20	0.40
1:A:240:LEU:HD13	1:A:245:GLN:HB3	2.03	0.40
1:B:58:GLN:NE2	1:B:815:LEU:HD13	2.36	0.40
1:B:281:PHE:CZ	1:B:324:VAL:HG11	2.57	0.40
1:B:410:ILE:HD11	1:B:976:THR:HA	2.03	0.40
1:D:498:LYS:H	1:D:499:PRO:CD	2.34	0.40
1:D:1009:MET:O	1:D:1013:THR:HG23	2.21	0.40
1:E:966:CYS:SG	1:E:1021:PRO:HG3	2.60	0.40
1:F:62:VAL:HG11	1:F:817:ARG:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:VAL:O	1:F:766:ARG:NH2	2.54	0.40
1:F:509:LYS:H	1:F:509:LYS:CE	2.34	0.40
1:A:718:ASN:HB3	1:A:825:GLU:HB3	2.03	0.40
2:A:1102:LMT:H72	2:A:1102:LMT:H101	1.65	0.40
1:B:163:GLN:HG3	1:B:175:PHE:CE1	2.56	0.40
1:B:652:GLN:O	1:B:656:PHE:HB2	2.21	0.40
1:B:909:ILE:HG13	1:B:910:GLY:N	2.36	0.40
1:C:326:PRO:HB3	1:C:610:PHE:HB2	2.02	0.40
1:C:534:ILE:HG22	1:C:541:TYR:CZ	2.55	0.40
1:C:969:ARG:C	1:C:972:PRO:HD2	2.46	0.40
1:D:240:LEU:HD13	1:D:245:GLN:C	2.46	0.40
1:D:355:MET:SD	1:D:410:ILE:HD11	2.61	0.40
1:D:891:TYR:CG	1:D:896:ILE:HD11	2.56	0.40
1:E:586:ARG:O	1:E:590:VAL:HG23	2.21	0.40
1:E:706:ALA:HB1	1:E:715:VAL:HG21	2.02	0.40
1:F:340:VAL:HG11	1:F:395:MET:HB3	2.02	0.40
1:A:11:PHE:O	1:A:15:ILE:HG22	2.21	0.40
1:A:977:SER:O	1:A:981:ILE:HG23	2.21	0.40
1:A:999:HIS:O	1:A:1003:THR:HG22	2.20	0.40
1:B:45:VAL:HB	1:B:90:ILE:CG2	2.46	0.40
1:B:392:THR:O	1:B:396:PHE:HD1	2.05	0.40
1:B:534:ILE:HG22	1:B:1022:LEU:HG	2.03	0.40
1:B:563:PHE:O	1:B:924:VAL:HG23	2.21	0.40
1:C:133:VAL:HG12	1:C:135:ASN:H	1.86	0.40
1:C:508:HIS:HD2	1:C:517:ASN:HB3	1.86	0.40
1:C:992:GLY:O	1:C:993:ALA:C	2.65	0.40
1:D:159:VAL:HB	1:D:181:GLN:HB3	2.04	0.40
1:D:696:LEU:CD1	1:D:699:ARG:HH11	2.35	0.40
1:E:293:LEU:HD22	1:E:297:ALA:HB3	2.03	0.40
1:E:341:VAL:HA	1:E:344:LEU:HD12	2.02	0.40
1:F:214:ILE:HD11	1:F:236:GLY:HA3	2.02	0.40
1:F:227:GLY:O	1:F:229:GLN:HG2	2.21	0.40
1:F:1009:MET:HE2	1:F:1012:ALA:HB3	2.02	0.40
1:A:100:PRO:HB3	1:A:295:THR:HG21	2.03	0.40
1:A:453:PHE:CD1	1:A:474:ILE:HD11	2.56	0.40
1:A:890:LEU:HD12	1:A:891:TYR:CE1	2.57	0.40
1:A:907:GLY:CA	1:A:1012:ALA:HB2	2.51	0.40
1:B:235:ILE:CG1	1:C:727:LYS:HA	2.51	0.40
1:B:900:VAL:O	1:B:903:VAL:HG12	2.22	0.40
1:C:145:THR:HG22	1:C:320:GLY:O	2.22	0.40
1:C:438:ILE:O	1:C:442:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ARG:HD3	1:D:771:TYR:HB2	2.02	0.40
1:D:410:ILE:HD13	1:D:410:ILE:HA	1.94	0.40
2:D:1102:LMT:H102	2:D:1102:LMT:H72	1.85	0.40
1:E:135:ASN:O	1:E:292:LYS:HG2	2.21	0.40
1:E:893:SER:OG	1:E:897:PRO:HD3	2.22	0.40
1:F:753:TRP:CH2	1:F:785:LEU:HD23	2.56	0.40
1:F:776:PRO:O	1:F:780:MET:HG2	2.22	0.40
1:A:158:ILE:HG12	1:A:162:ILE:HD11	2.02	0.40
1:A:575:GLN:O	1:A:663:VAL:HA	2.21	0.40
1:A:597:TYR:CE2	1:A:651:ALA:HA	2.57	0.40
1:B:229:GLN:HA	1:C:583:SER:HB3	2.04	0.40
1:B:453:PHE:HE1	1:B:931:LEU:HB3	1.87	0.40
1:B:699:ARG:HH21	1:B:824:MET:HE2	1.86	0.40
1:B:727:LYS:HD2	1:B:809:GLU:OE1	2.22	0.40
1:C:15:ILE:O	1:C:19:ILE:HG23	2.22	0.40
1:C:33:ASN:O	1:C:391:ASN:HA	2.21	0.40
1:C:314:GLU:HA	1:C:317:MET:HG3	2.03	0.40
1:C:358:PHE:CD2	1:C:975:MET:HG2	2.56	0.40
1:C:971:ARG:HB3	1:C:972:PRO:HD3	2.04	0.40
1:D:216:SER:O	1:E:754:GLY:N	2.55	0.40
1:D:753:TRP:HB3	1:F:217:GLY:HA3	2.03	0.40
1:E:166:LEU:O	1:E:169:THR:OG1	2.38	0.40
1:E:447:MET:HE3	1:E:886:CYS:SG	2.62	0.40
1:F:166:LEU:HD23	1:F:166:LEU:HA	1.87	0.40
1:F:311:ALA:O	1:F:315:PRO:HD3	2.21	0.40
1:F:420:MET:CE	1:F:499:PRO:HA	2.52	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	1009/1056 (96%)	951 (94%)	46 (5%)	12 (1%)	10	42
1	B	1028/1056 (97%)	987 (96%)	34 (3%)	7 (1%)	18	51
1	C	1028/1056 (97%)	980 (95%)	39 (4%)	9 (1%)	14	47
1	D	1008/1056 (96%)	954 (95%)	37 (4%)	17 (2%)	7	35
1	E	1028/1056 (97%)	987 (96%)	35 (3%)	6 (1%)	21	54
1	F	1030/1056 (98%)	981 (95%)	38 (4%)	11 (1%)	11	43
All	All	6131/6336 (97%)	5840 (95%)	229 (4%)	62 (1%)	12	45

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	ILE
1	A	640	GLY
1	A	658	PHE
1	A	795	GLY
1	A	872	ALA
1	A	919	GLY
1	B	570	GLY
1	B	658	PHE
1	B	678	THR
1	D	438	ILE
1	D	539	ALA
1	D	675	GLY
1	D	795	GLY
1	D	872	ALA
1	E	570	GLY
1	E	658	PHE
1	E	672	LEU
1	E	679	GLY
1	F	658	PHE
1	F	690	VAL
1	F	739	GLY
1	F	993	ALA
1	A	689	GLY
1	A	953	GLU
1	B	86	GLY
1	C	96	GLN
1	C	217	GLY
1	C	690	VAL
1	C	993	ALA
1	D	568	ASP

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Mol	Chain	Res	Type
1	D	919	GLY
1	D	953	GLU
1	F	217	GLY
1	F	661	ALA
1	F	852	LYS
1	A	147	GLY
1	A	539	ALA
1	C	661	ALA
1	D	670	SER
1	E	860	GLY
1	F	657	SER
1	F	808	TRP
1	A	564	LEU
1	C	801	ASN
1	D	498	LYS
1	A	819	ASN
1	B	794	LYS
1	C	657	SER
1	D	564	LEU
1	D	679	GLY
1	D	689	GLY
1	D	952	HIS
1	F	507	GLU
1	B	860	GLY
1	F	795	GLY
1	E	675	GLY
1	B	675	GLY
1	C	506	GLY
1	D	996	GLY
1	C	147	GLY
1	D	640	GLY
1	D	955	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	828/864 (96%)	752 (91%)	76 (9%)	8 32
1	B	841/864 (97%)	763 (91%)	78 (9%)	8 32
1	C	841/864 (97%)	774 (92%)	67 (8%)	11 36
1	D	827/864 (96%)	756 (91%)	71 (9%)	10 34
1	E	841/864 (97%)	764 (91%)	77 (9%)	8 32
1	F	843/864 (98%)	798 (95%)	45 (5%)	20 47
All	All	5021/5184 (97%)	4607 (92%)	414 (8%)	10 35

All (414) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	15	ILE
1	A	25	LEU
1	A	43	ILE
1	A	55	GLU
1	A	81	GLU
1	A	90	ILE
1	A	92	VAL
1	A	96	GLN
1	A	105	VAL
1	A	122	VAL
1	A	180	SER
1	A	235	ILE
1	A	242	THR
1	A	251	LEU
1	A	254	ASN
1	A	280	GLN
1	A	293	LEU
1	A	309	THR
1	A	324	VAL
1	A	330	THR
1	A	367	ILE
1	A	370	ILE
1	A	375	VAL
1	A	405	LEU
1	A	407	ASN
1	A	408	ASP
1	A	415	ASN
1	A	425	LEU
1	A	437	GLN

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Mol	Chain	Res	Type
1	A	438	ILE
1	A	442	LEU
1	A	447	MET
1	A	472	ILE
1	A	488	LEU
1	A	500	ILE
1	A	531	VAL
1	A	535	LEU
1	A	536	LYS
1	A	544	ILE
1	A	575	GLN
1	A	578	THR
1	A	599	LEU
1	A	603	SER
1	A	608	SER
1	A	611	THR
1	A	620	ARG
1	A	626	MET
1	A	659	LYS
1	A	660	ASP
1	A	663	VAL
1	A	672	LEU
1	A	676	ASN
1	A	770	VAL
1	A	783	ASP
1	A	800	PHE
1	A	801	ASN
1	A	807	LYS
1	A	821	VAL
1	A	826	ILE
1	A	827	LEU
1	A	829	GLU
1	A	838	ASP
1	A	840	MET
1	A	875	LEU
1	A	890	LEU
1	A	896	ILE
1	A	906	LEU
1	A	927	GLN
1	A	936	LEU
1	A	952	HIS
1	A	968	MET

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Mol	Chain	Res	Type
1	A	969	ARG
1	A	973	ILE
1	A	978	LEU
1	A	982	LEU
1	B	10	ILE
1	B	14	VAL
1	B	20	MET
1	B	47	VAL
1	B	83	ASN
1	B	90	ILE
1	B	111	LEU
1	B	129	VAL
1	B	150	THR
1	B	170	LYS
1	B	178	PHE
1	B	183	SER
1	B	195	SER
1	B	199	THR
1	B	207	ILE
1	B	237	LYS
1	B	242	THR
1	B	244	GLU
1	B	256	ASP
1	B	293	LEU
1	B	306	ILE
1	B	337	ILE
1	B	366	LEU
1	B	367	ILE
1	B	374	VAL
1	B	402	ILE
1	B	438	ILE
1	B	463	THR
1	B	469	GLN
1	B	478	MET
1	B	480	LEU
1	B	482	VAL
1	B	483	ILE
1	B	488	LEU
1	B	544	ILE
1	B	556	PHE
1	B	561	THR
1	B	571	VAL

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Mol	Chain	Res	Type
1	B	578	THR
1	B	583	SER
1	B	585	GLU
1	B	603	SER
1	B	611	THR
1	B	630	MET
1	B	644	VAL
1	B	672	LEU
1	B	673	GLU
1	B	674	LEU
1	B	676	ASN
1	B	678	THR
1	B	680	PHE
1	B	690	VAL
1	B	694	VAL
1	B	703	LEU
1	B	705	LEU
1	B	708	GLN
1	B	729	GLU
1	B	740	VAL
1	B	745	ILE
1	B	763	ASP
1	B	772	LEU
1	B	793	ASP
1	B	794	LYS
1	B	801	ASN
1	B	827	LEU
1	B	859	THR
1	B	880	LEU
1	B	895	SER
1	B	917	MET
1	B	922	ASN
1	B	942	ILE
1	B	944	ILE
1	B	945	VAL
1	B	968	MET
1	B	969	ARG
1	B	982	LEU
1	B	1015	LEU
1	B	1022	LEU
1	C	10	ILE
1	C	25	LEU

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Mol	Chain	Res	Type
1	C	43	ILE
1	C	63	GLN
1	C	85	ASP
1	C	89	THR
1	C	90	ILE
1	C	94	PHE
1	C	98	THR
1	C	121	GLU
1	C	122	VAL
1	C	124	ARG
1	C	125	GLN
1	C	134	LYS
1	C	137	LEU
1	C	150	THR
1	C	152	GLU
1	C	169	THR
1	C	176	GLN
1	C	239	ARG
1	C	275	TYR
1	C	329	THR
1	C	362	PHE
1	C	366	LEU
1	C	367	ILE
1	C	414	GLU
1	C	415	ASN
1	C	471	SER
1	C	478	MET
1	C	488	LEU
1	C	495	THR
1	C	504	ASP
1	C	507	GLU
1	C	508	HIS
1	C	542	LEU
1	C	548	ILE
1	C	594	MET
1	C	611	THR
1	C	626	MET
1	C	634	TRP
1	C	659	LYS
1	C	663	VAL
1	C	681	ASP
1	C	686	ASP

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Mol	Chain	Res	Type
1	C	699	ARG
1	C	712	LEU
1	C	730	ILE
1	C	734	LYS
1	C	738	LEU
1	C	740	VAL
1	C	742	LEU
1	C	745	ILE
1	C	762	ILE
1	C	777	ASP
1	C	792	ASN
1	C	801	ASN
1	C	805	THR
1	C	836	SER
1	C	852	LYS
1	C	864	GLU
1	C	875	LEU
1	C	881	LEU
1	C	895	SER
1	C	944	ILE
1	C	967	ARG
1	C	973	ILE
1	C	1015	LEU
1	D	14	VAL
1	D	25	LEU
1	D	43	ILE
1	D	78	ILE
1	D	81	GLU
1	D	90	ILE
1	D	140	VAL
1	D	181	GLN
1	D	222	LEU
1	D	235	ILE
1	D	251	LEU
1	D	254	ASN
1	D	258	SER
1	D	293	LEU
1	D	309	THR
1	D	321	MET
1	D	324	VAL
1	D	337	ILE
1	D	355	MET

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Mol	Chain	Res	Type
1	D	367	ILE
1	D	370	ILE
1	D	375	VAL
1	D	391	ASN
1	D	405	LEU
1	D	407	ASN
1	D	415	ASN
1	D	417	GLU
1	D	425	LEU
1	D	437	GLN
1	D	438	ILE
1	D	442	LEU
1	D	447	MET
1	D	456	MET
1	D	488	LEU
1	D	535	LEU
1	D	536	LYS
1	D	538	ARG
1	D	575	GLN
1	D	578	THR
1	D	599	LEU
1	D	611	THR
1	D	623	SER
1	D	643	SER
1	D	644	VAL
1	D	647	LEU
1	D	663	VAL
1	D	695	LEU
1	D	699	ARG
1	D	730	ILE
1	D	783	ASP
1	D	800	PHE
1	D	801	ASN
1	D	821	VAL
1	D	826	ILE
1	D	827	LEU
1	D	834	LEU
1	D	844	GLU
1	D	852	LYS
1	D	875	LEU
1	D	880	LEU
1	D	890	LEU

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Mol	Chain	Res	Type
1	D	896	ILE
1	D	928	VAL
1	D	942	ILE
1	D	952	HIS
1	D	964	GLU
1	D	973	ILE
1	D	975	MET
1	D	978	LEU
1	D	982	LEU
1	D	1005	VAL
1	E	34	GLN
1	E	47	VAL
1	E	83	ASN
1	E	113	LEU
1	E	129	VAL
1	E	133	VAL
1	E	150	THR
1	E	152	GLU
1	E	177	VAL
1	E	207	ILE
1	E	226	LYS
1	E	228	GLN
1	E	235	ILE
1	E	242	THR
1	E	244	GLU
1	E	250	LEU
1	E	263	LYS
1	E	293	LEU
1	E	295	THR
1	E	309	THR
1	E	332	VAL
1	E	343	THR
1	E	365	THR
1	E	370	ILE
1	E	394	THR
1	E	447	MET
1	E	463	THR
1	E	472	ILE
1	E	478	MET
1	E	480	LEU
1	E	482	VAL
1	E	489	THR

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Mol	Chain	Res	Type
1	E	496	MET
1	E	548	ILE
1	E	552	MET
1	E	556	PHE
1	E	561	THR
1	E	571	VAL
1	E	589	VAL
1	E	600	GLU
1	E	601	LYS
1	E	611	THR
1	E	616	ASN
1	E	623	SER
1	E	630	MET
1	E	631	LEU
1	E	644	VAL
1	E	659	LYS
1	E	673	GLU
1	E	674	LEU
1	E	678	THR
1	E	680	PHE
1	E	690	VAL
1	E	703	LEU
1	E	705	LEU
1	E	708	GLN
1	E	729	GLU
1	E	730	ILE
1	E	763	ASP
1	E	772	LEU
1	E	775	ARG
1	E	780	MET
1	E	794	LYS
1	E	801	ASN
1	E	805	THR
1	E	821	VAL
1	E	827	LEU
1	E	859	THR
1	E	880	LEU
1	E	881	LEU
1	E	895	SER
1	E	896	ILE
1	E	903	VAL
1	E	942	ILE

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Mol	Chain	Res	Type
1	E	978	LEU
1	E	982	LEU
1	E	1015	LEU
1	F	1	MET
1	F	14	VAL
1	F	21	LEU
1	F	81	GLU
1	F	133	VAL
1	F	134	LYS
1	F	142	VAL
1	F	158	ILE
1	F	186	ILE
1	F	212	VAL
1	F	264	ASP
1	F	307	ARG
1	F	308	GLN
1	F	309	THR
1	F	329	THR
1	F	330	THR
1	F	334	SER
1	F	370	ILE
1	F	404	LEU
1	F	471	SER
1	F	478	MET
1	F	482	VAL
1	F	488	LEU
1	F	489	THR
1	F	501	GLU
1	F	507	GLU
1	F	509	LYS
1	F	534	ILE
1	F	559	ILE
1	F	594	MET
1	F	626	MET
1	F	659	LYS
1	F	670	SER
1	F	807	LYS
1	F	816	GLU
1	F	854	VAL
1	F	861	LEU
1	F	864	GLU
1	F	868	SER

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Mol	Chain	Res	Type
1	F	878	LEU
1	F	978	LEU
1	F	1005	VAL
1	F	1009	MET
1	F	1031	PHE
1	F	1032	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	176	GLN
1	A	181	GLN
1	A	273	GLN
1	A	437	GLN
1	A	654	HIS
1	A	713	GLN
1	A	725	GLN
1	A	940	ASN
1	B	58	GLN
1	B	163	GLN
1	B	181	GLN
1	B	194	ASN
1	B	213	GLN
1	B	273	GLN
1	B	280	GLN
1	B	407	ASN
1	B	415	ASN
1	B	469	GLN
1	B	616	ASN
1	C	67	GLN
1	C	231	ASN
1	C	254	ASN
1	C	259	GLN
1	C	517	ASN
1	C	642	ASN
1	C	746	ASN
1	D	96	GLN
1	D	161	ASN
1	D	229	GLN
1	D	241	GLN
1	D	278	ASN

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Mol	Chain	Res	Type
1	D	407	ASN
1	D	525	HIS
1	D	575	GLN
1	D	577	GLN
1	D	676	ASN
1	D	708	GLN
1	D	713	GLN
1	D	927	GLN
1	E	68	GLN
1	E	70	ASN
1	E	161	ASN
1	E	163	GLN
1	E	194	ASN
1	E	231	ASN
1	E	407	ASN
1	E	588	GLN
1	E	922	ASN
1	F	68	GLN
1	F	83	ASN
1	F	96	GLN
1	F	108	GLN
1	F	176	GLN
1	F	229	GLN
1	F	391	ASN
1	F	505	HIS
1	F	676	ASN
1	F	713	GLN
1	F	759	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	D	1101	-	36,36,36	1.14	2 (5%)	47,47,47	0.96	1 (2%)
3	MC2	B	1101	-	35,35,35	1.81	6 (17%)	45,46,46	1.91	9 (20%)
2	LMT	E	1101	-	36,36,36	1.19	2 (5%)	47,47,47	0.89	1 (2%)
4	ACT	F	1101	-	3,3,3	0.93	0	3,3,3	0.80	0
2	LMT	B	1102	-	36,36,36	1.17	2 (5%)	47,47,47	0.90	0
2	LMT	B	1104	-	36,36,36	1.22	3 (8%)	47,47,47	1.22	4 (8%)
2	LMT	B	1105	-	36,36,36	1.13	2 (5%)	47,47,47	0.89	1 (2%)
2	LMT	A	1102	-	36,36,36	1.14	2 (5%)	47,47,47	0.83	1 (2%)
4	ACT	C	1101	-	3,3,3	0.92	0	3,3,3	0.87	0
2	LMT	E	1102	-	36,36,36	1.14	2 (5%)	47,47,47	0.89	1 (2%)
2	LMT	B	1103	-	36,36,36	1.12	2 (5%)	47,47,47	1.03	1 (2%)
2	LMT	D	1102	-	36,36,36	1.13	2 (5%)	47,47,47	1.06	2 (4%)
2	LMT	A	1101	-	36,36,36	1.23	3 (8%)	47,47,47	1.27	7 (14%)

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	D	1101	-	-	9/21/61/61	0/2/2/2
3	MC2	B	1101	-	-	10/27/27/27	0/3/3/3
2	LMT	E	1101	-	-	14/21/61/61	0/2/2/2
2	LMT	B	1102	-	-	13/21/61/61	0/2/2/2
2	LMT	B	1104	-	-	7/21/61/61	0/2/2/2
2	LMT	B	1105	-	-	8/21/61/61	0/2/2/2
2	LMT	A	1102	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	E	1102	-	-	13/21/61/61	0/2/2/2
2	LMT	B	1103	-	-	14/21/61/61	0/2/2/2
2	LMT	D	1102	-	-	13/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	15/21/61/61	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1101	MC2	C15-N3	5.95	1.45	1.33
3	B	1101	MC2	C2-N2	5.11	1.45	1.34
3	B	1101	MC2	C11-N6	4.27	1.45	1.35
2	A	1101	LMT	O5'-C1'	3.87	1.51	1.41
2	B	1104	LMT	O5B-C1B	3.71	1.51	1.41
2	E	1101	LMT	O5'-C1'	3.63	1.51	1.41
2	B	1102	LMT	O5'-C1'	3.62	1.51	1.41
2	B	1104	LMT	O5'-C1'	3.47	1.50	1.41
2	D	1102	LMT	O5'-C1'	3.39	1.50	1.41
2	A	1102	LMT	O5'-C1'	3.38	1.50	1.41
2	E	1101	LMT	O5B-C1B	3.36	1.50	1.41
2	D	1101	LMT	O5B-C1B	3.35	1.50	1.41
2	B	1102	LMT	O5B-C1B	3.34	1.50	1.41
2	E	1102	LMT	O5'-C1'	3.33	1.50	1.41
2	A	1101	LMT	O5B-C1B	3.32	1.50	1.41
2	D	1101	LMT	O5'-C1'	3.31	1.50	1.41
2	E	1102	LMT	O5B-C1B	3.31	1.50	1.41
2	B	1105	LMT	O5'-C1'	3.30	1.50	1.41
2	B	1105	LMT	O5B-C1B	3.29	1.50	1.41
2	A	1102	LMT	O5B-C1B	3.24	1.50	1.41
2	B	1103	LMT	O5'-C1'	3.23	1.50	1.41
2	B	1103	LMT	O5B-C1B	3.17	1.49	1.41
2	D	1102	LMT	O5B-C1B	3.12	1.49	1.41
3	B	1101	MC2	C15-N4	2.64	1.45	1.34
3	B	1101	MC2	O2-C11	-2.30	1.18	1.23
3	B	1101	MC2	O1-C2	-2.30	1.18	1.23
2	B	1104	LMT	O5B-C5B	2.16	1.49	1.44
2	A	1101	LMT	O5'-C5'	2.09	1.49	1.44

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1101	MC2	C17-C19-N6	-5.61	101.54	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1101	MC2	C19-N6-C11	5.33	140.17	127.40
2	B	1104	LMT	O5B-C5B-C4B	4.29	117.48	109.69
3	B	1101	MC2	C13-C12-C10	-3.81	102.17	113.92
3	B	1101	MC2	C12-C10-C11	3.80	119.06	110.20
3	B	1101	MC2	C21-C19-N6	3.33	134.23	123.13
2	B	1104	LMT	C1B-O5B-C5B	3.32	120.21	113.69
2	A	1101	LMT	O1B-C4'-C3'	3.28	116.01	107.28
3	B	1101	MC2	C11-C10-N2	-3.27	102.27	111.16
2	D	1102	LMT	C1B-O5B-C5B	-3.23	107.36	113.69
2	D	1101	LMT	C1B-O1B-C4'	-3.16	110.15	117.96
2	B	1105	LMT	C1B-O1B-C4'	-2.93	110.70	117.96
2	A	1101	LMT	C1'-O5'-C5'	2.91	119.41	113.69
3	B	1101	MC2	C17-C19-C21	2.90	123.70	119.33
3	B	1101	MC2	O2-C11-C10	2.87	126.48	120.45
2	A	1102	LMT	C1B-O1B-C4'	-2.86	110.89	117.96
2	A	1101	LMT	O5B-C5B-C4B	2.79	114.77	109.69
2	B	1104	LMT	C1B-O1B-C4'	-2.74	111.18	117.96
2	E	1102	LMT	C1B-O1B-C4'	-2.73	111.21	117.96
3	B	1101	MC2	C10-C11-N6	-2.59	107.34	115.10
2	E	1101	LMT	C1B-O1B-C4'	-2.59	111.55	117.96
2	B	1103	LMT	C1B-O1B-C4'	-2.58	111.59	117.96
2	A	1101	LMT	C3B-C4B-C5B	2.57	114.83	110.24
2	D	1102	LMT	C1B-O1B-C4'	-2.49	111.81	117.96
2	B	1104	LMT	C6B-C5B-C4B	-2.44	107.29	113.00
2	A	1101	LMT	O5'-C5'-C4'	2.35	114.70	109.75
2	A	1101	LMT	O5'-C1'-C2'	2.11	114.82	110.35
2	A	1101	LMT	C6B-C5B-C4B	-2.07	108.16	113.00

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	LMT	C2'-C1'-O1'-C1
2	A	1101	LMT	O5'-C1'-O1'-C1
2	B	1102	LMT	C2-C1-O1'-C1'
2	B	1105	LMT	O5'-C1'-O1'-C1
2	D	1101	LMT	C2-C1-O1'-C1'
2	E	1101	LMT	C2'-C1'-O1'-C1
2	E	1101	LMT	O5'-C1'-O1'-C1
2	E	1101	LMT	C2-C1-O1'-C1'
2	E	1102	LMT	O5'-C1'-O1'-C1
3	B	1101	MC2	C3-C1-C2-N2

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Mol	Chain	Res	Type	Atoms
3	B	1101	MC2	C3-C1-C2-O1
2	D	1102	LMT	C4B-C5B-C6B-O6B
2	A	1101	LMT	C3'-C4'-O1B-C1B
2	B	1104	LMT	O5B-C5B-C6B-O6B
2	E	1102	LMT	O5'-C5'-C6'-O6'
2	B	1102	LMT	O5'-C5'-C6'-O6'
3	B	1101	MC2	N2-C10-C12-C13
2	B	1103	LMT	O5'-C5'-C6'-O6'
2	D	1102	LMT	O5B-C5B-C6B-O6B
2	A	1102	LMT	C7-C8-C9-C10
2	A	1102	LMT	C1-C2-C3-C4
2	E	1101	LMT	C5-C6-C7-C8
2	D	1102	LMT	O5'-C5'-C6'-O6'
2	A	1101	LMT	C4B-C5B-C6B-O6B
2	E	1102	LMT	C4'-C5'-C6'-O6'
2	A	1102	LMT	O5'-C1'-O1'-C1
2	D	1102	LMT	O5'-C1'-O1'-C1
2	E	1101	LMT	C11-C10-C9-C8
3	B	1101	MC2	C11-C10-C12-C13
2	B	1104	LMT	C4B-C5B-C6B-O6B
2	B	1102	LMT	C3'-C4'-O1B-C1B
2	E	1101	LMT	C3-C4-C5-C6
2	E	1102	LMT	O5B-C5B-C6B-O6B
2	E	1101	LMT	C3'-C4'-O1B-C1B
2	E	1101	LMT	C5'-C4'-O1B-C1B
2	D	1102	LMT	C4'-C5'-C6'-O6'
2	A	1101	LMT	O5B-C5B-C6B-O6B
2	B	1103	LMT	O1'-C1-C2-C3
2	B	1102	LMT	O1'-C1-C2-C3
2	D	1101	LMT	O1'-C1-C2-C3
2	B	1102	LMT	C4'-C5'-C6'-O6'
2	B	1103	LMT	C4'-C5'-C6'-O6'
2	B	1103	LMT	C2-C3-C4-C5
3	B	1101	MC2	C17-C19-N6-C11
2	B	1102	LMT	C3-C4-C5-C6
2	B	1103	LMT	C11-C10-C9-C8
2	D	1102	LMT	C11-C10-C9-C8
2	D	1102	LMT	O1'-C1-C2-C3
2	A	1101	LMT	C3-C4-C5-C6
2	D	1101	LMT	C6-C7-C8-C9
2	E	1101	LMT	C2-C3-C4-C5
2	A	1102	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	B	1104	LMT	C7-C8-C9-C10
2	B	1105	LMT	C4-C5-C6-C7
2	D	1101	LMT	C3-C4-C5-C6
2	D	1102	LMT	C4-C5-C6-C7
2	B	1102	LMT	C7-C8-C9-C10
2	A	1102	LMT	C6-C7-C8-C9
2	B	1103	LMT	C2-C1-O1'-C1'
2	B	1104	LMT	C2-C1-O1'-C1'
2	B	1105	LMT	C2-C1-O1'-C1'
2	D	1102	LMT	C2-C1-O1'-C1'
2	A	1102	LMT	C5-C6-C7-C8
2	D	1102	LMT	C5-C6-C7-C8
2	A	1101	LMT	C1-C2-C3-C4
2	E	1101	LMT	C6-C7-C8-C9
3	B	1101	MC2	C12-C13-C14-N3
2	B	1103	LMT	C1-C2-C3-C4
2	D	1102	LMT	C1-C2-C3-C4
2	A	1102	LMT	O1'-C1-C2-C3
2	A	1101	LMT	C2-C3-C4-C5
3	B	1101	MC2	C21-C19-N6-C11
2	D	1101	LMT	C5-C6-C7-C8
2	B	1102	LMT	C5'-C4'-O1B-C1B
2	B	1103	LMT	C9-C10-C11-C12
2	A	1101	LMT	C11-C10-C9-C8
2	B	1102	LMT	C2-C3-C4-C5
2	B	1103	LMT	C3-C4-C5-C6
2	D	1102	LMT	C2-C3-C4-C5
2	A	1101	LMT	C9-C10-C11-C12
2	E	1101	LMT	C7-C8-C9-C10
2	E	1102	LMT	C4B-C5B-C6B-O6B
3	B	1101	MC2	C1-C3-C4-C6
2	E	1102	LMT	C2-C1-O1'-C1'
3	B	1101	MC2	C1-C3-C4-C5
2	A	1101	LMT	C7-C8-C9-C10
2	B	1105	LMT	C11-C10-C9-C8
2	A	1102	LMT	C9-C10-C11-C12
2	E	1101	LMT	O5'-C5'-C6'-O6'
2	B	1102	LMT	O5B-C5B-C6B-O6B
2	E	1102	LMT	C2-C3-C4-C5
2	B	1105	LMT	C3-C4-C5-C6
2	A	1101	LMT	C4'-C5'-C6'-O6'
2	B	1103	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	E	1101	LMT	C9-C10-C11-C12
2	E	1102	LMT	C4-C5-C6-C7
2	B	1104	LMT	C11-C10-C9-C8
2	E	1102	LMT	C9-C10-C11-C12
2	B	1102	LMT	C9-C10-C11-C12
2	E	1101	LMT	C4-C5-C6-C7
2	B	1102	LMT	C11-C10-C9-C8
2	E	1102	LMT	C5-C6-C7-C8
2	B	1104	LMT	C3-C4-C5-C6
2	B	1103	LMT	O5'-C1'-O1'-C1
2	B	1103	LMT	C2'-C1'-O1'-C1
2	D	1101	LMT	C11-C10-C9-C8
2	B	1105	LMT	C9-C10-C11-C12
2	A	1101	LMT	O1'-C1-C2-C3
2	D	1101	LMT	O5B-C5B-C6B-O6B
2	D	1101	LMT	C2-C3-C4-C5
2	B	1103	LMT	C4-C5-C6-C7
2	A	1102	LMT	C11-C10-C9-C8
2	D	1101	LMT	C1-C2-C3-C4
2	B	1105	LMT	C1-C2-C3-C4
2	B	1103	LMT	O5B-C5B-C6B-O6B
2	A	1101	LMT	O5'-C5'-C6'-O6'
3	B	1101	MC2	C12-C10-C11-O2
2	D	1102	LMT	C3-C4-C5-C6
2	E	1102	LMT	C7-C8-C9-C10
2	E	1102	LMT	C11-C10-C9-C8
2	E	1102	LMT	C6-C7-C8-C9
2	B	1105	LMT	C2-C3-C4-C5
2	B	1102	LMT	C5-C6-C7-C8
2	A	1101	LMT	C5'-C4'-O1B-C1B
2	B	1104	LMT	C4-C5-C6-C7

There are no ring outliers.

10 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1101	LMT	7	0
3	B	1101	MC2	3	0
2	E	1101	LMT	4	0
2	B	1102	LMT	1	0
2	B	1105	LMT	1	0
2	A	1102	LMT	4	0

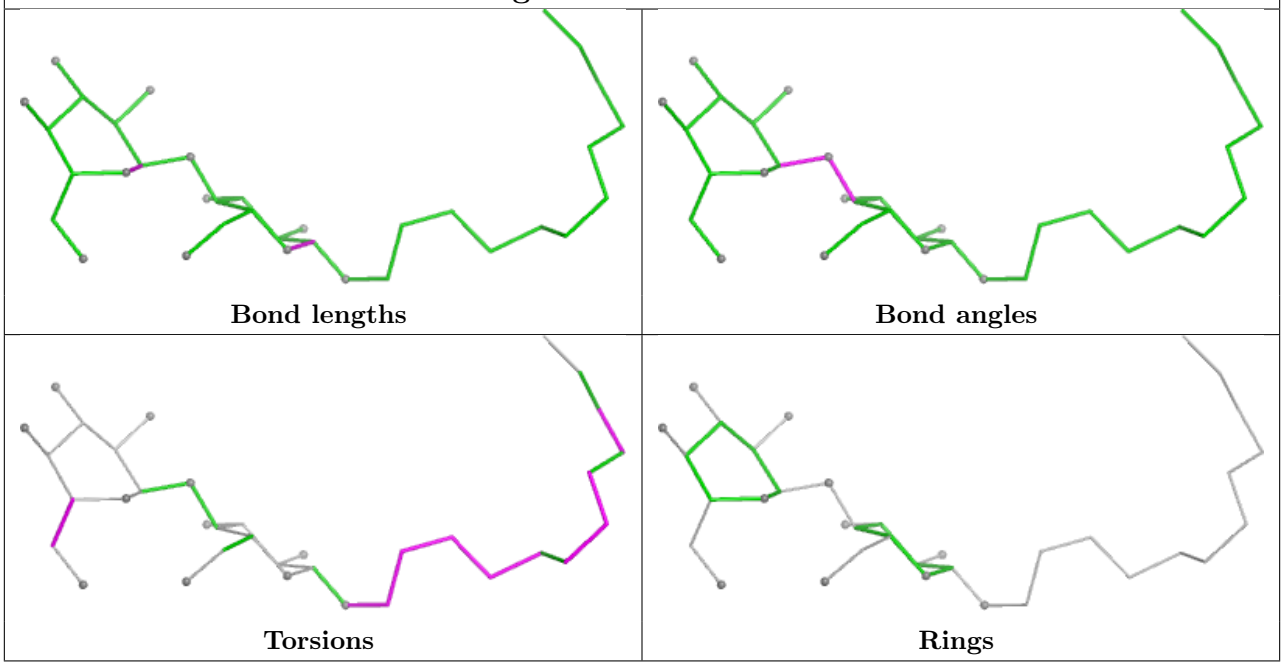
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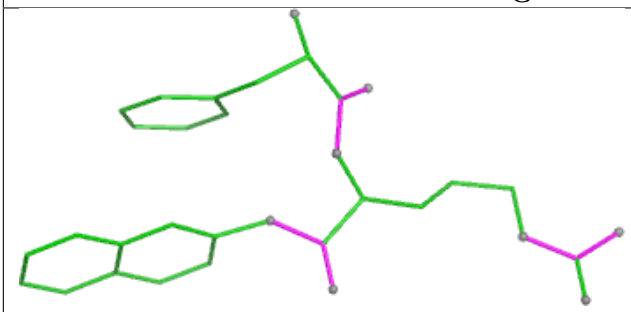
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1102	LMT	2	0
2	B	1103	LMT	5	0
2	D	1102	LMT	1	0
2	A	1101	LMT	1	0

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.

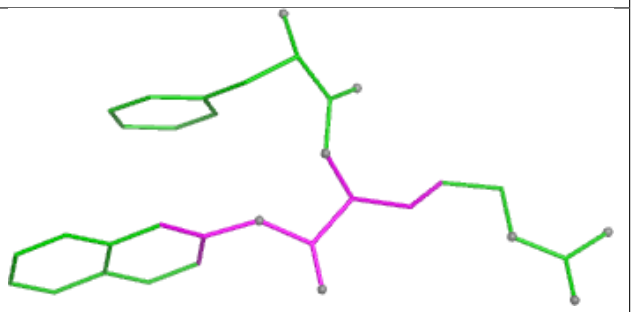
Ligand LMT D 1101



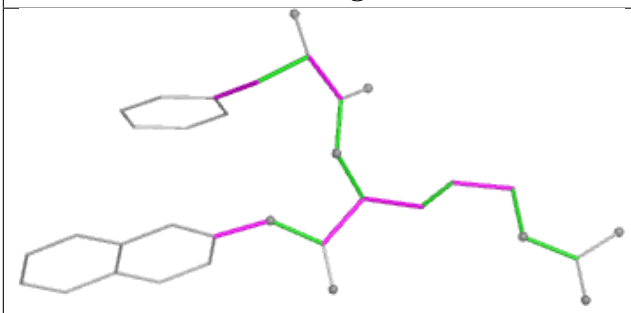
Ligand MC2 B 1101



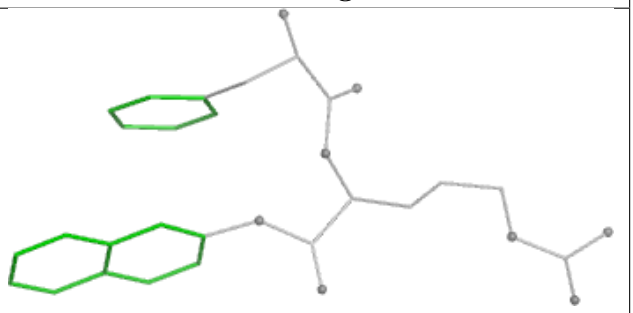
Bond lengths



Bond angles

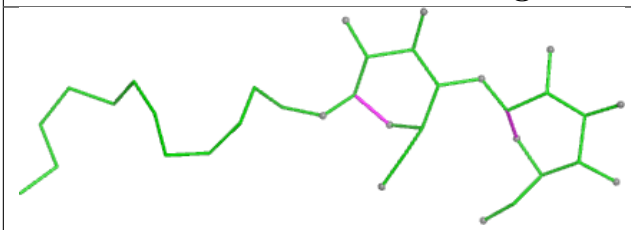


Torsions

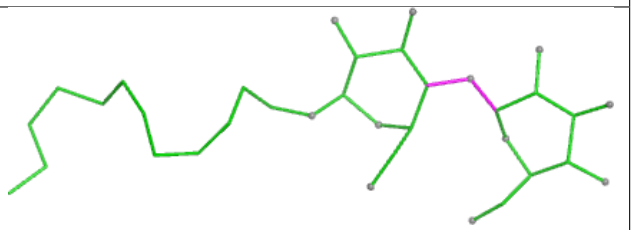


Rings

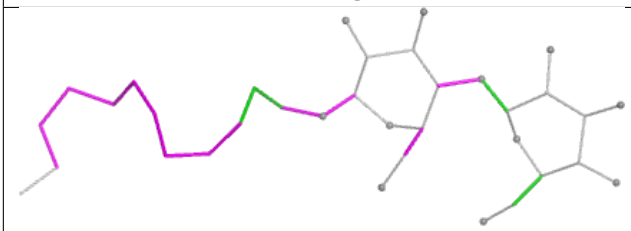
Ligand LMT E 1101



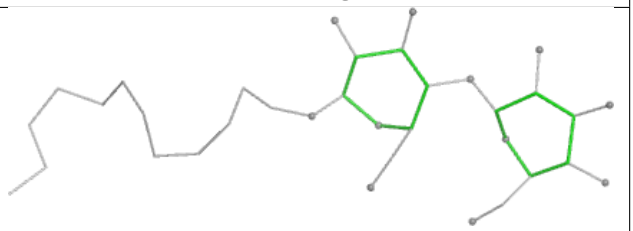
Bond lengths



Bond angles

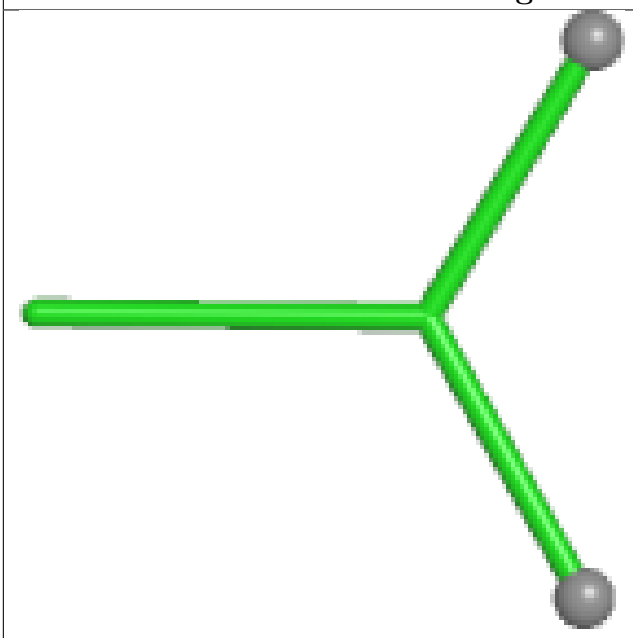


Torsions

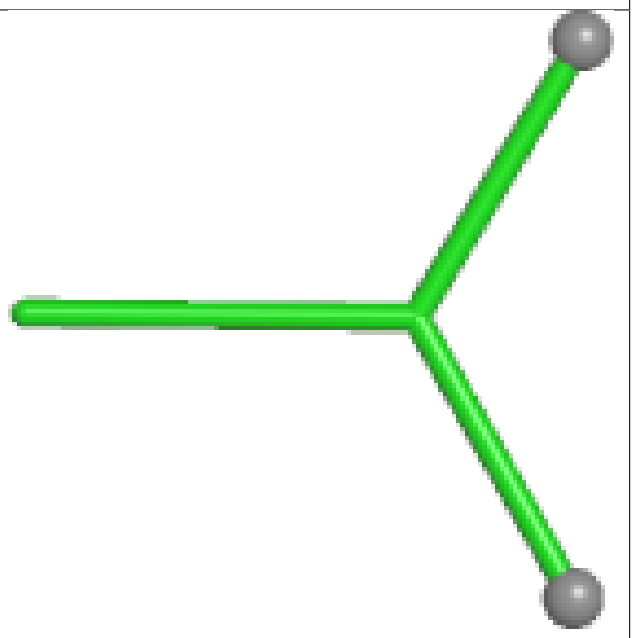


Rings

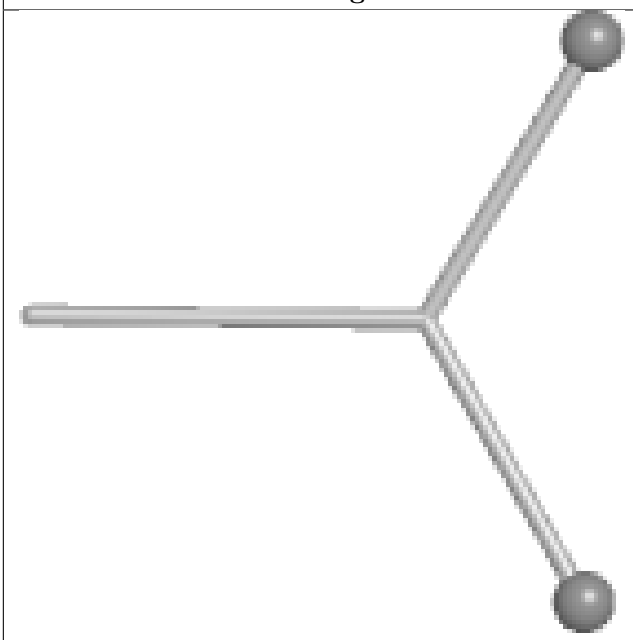
Ligand ACT F 1101



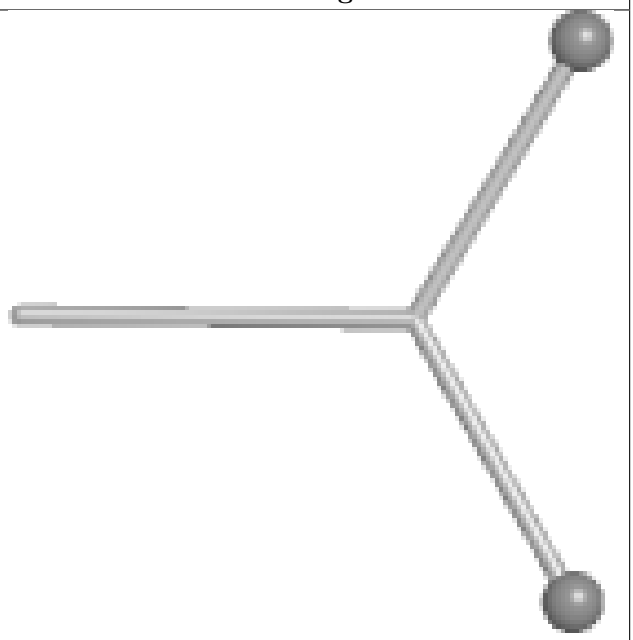
Bond lengths



Bond angles

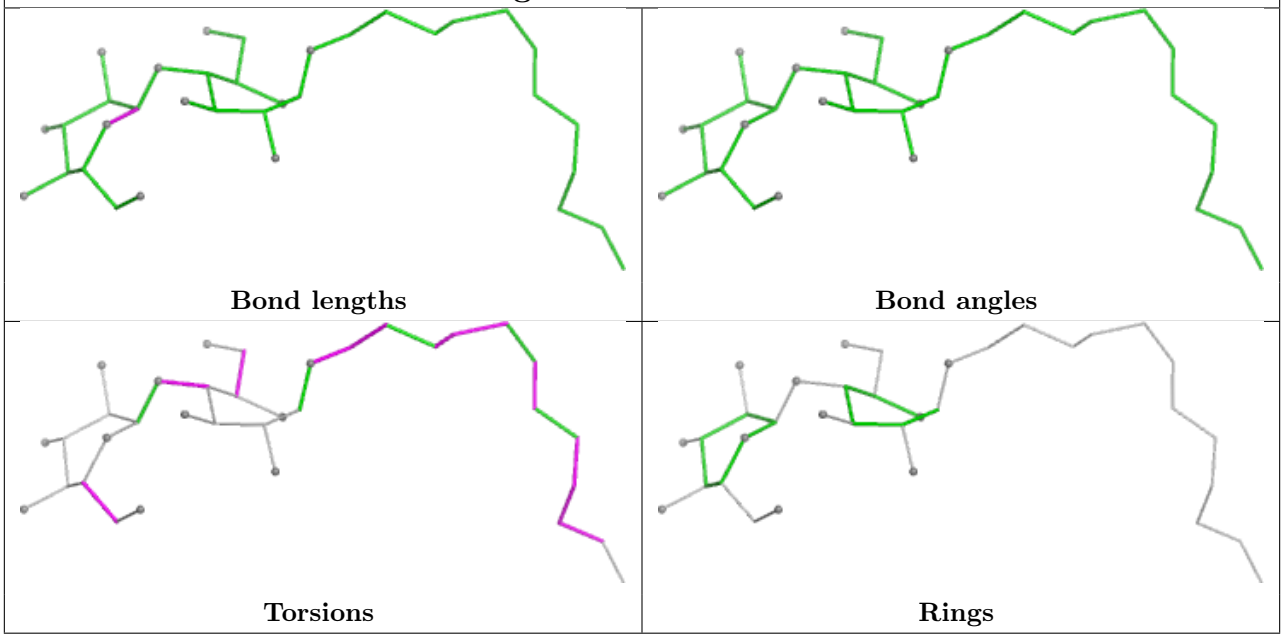


Torsions

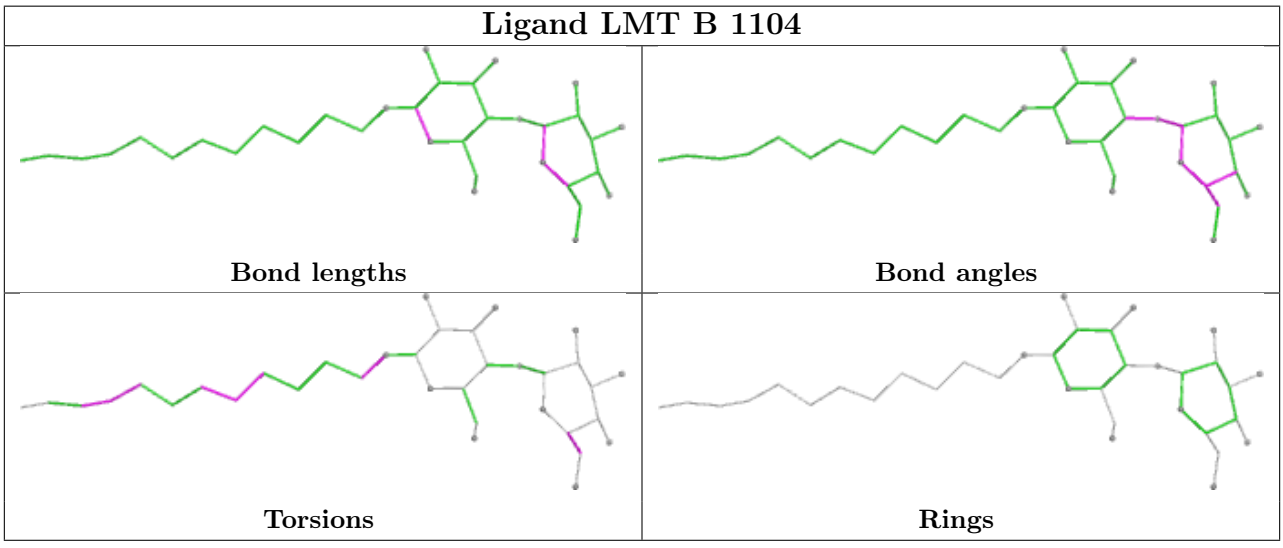


Rings

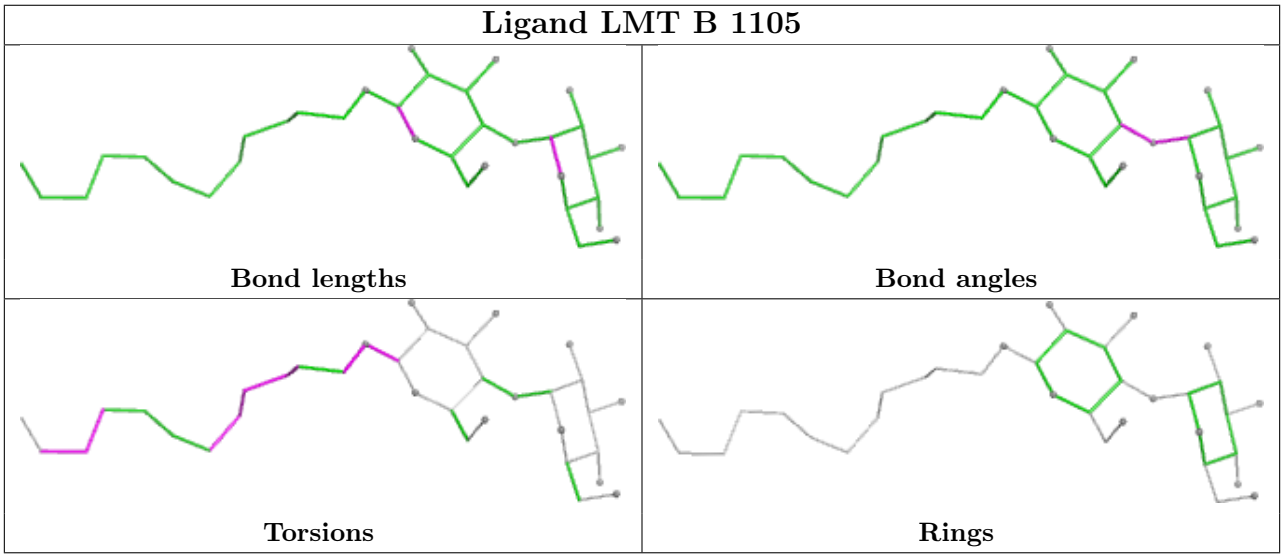
Ligand LMT B 1102



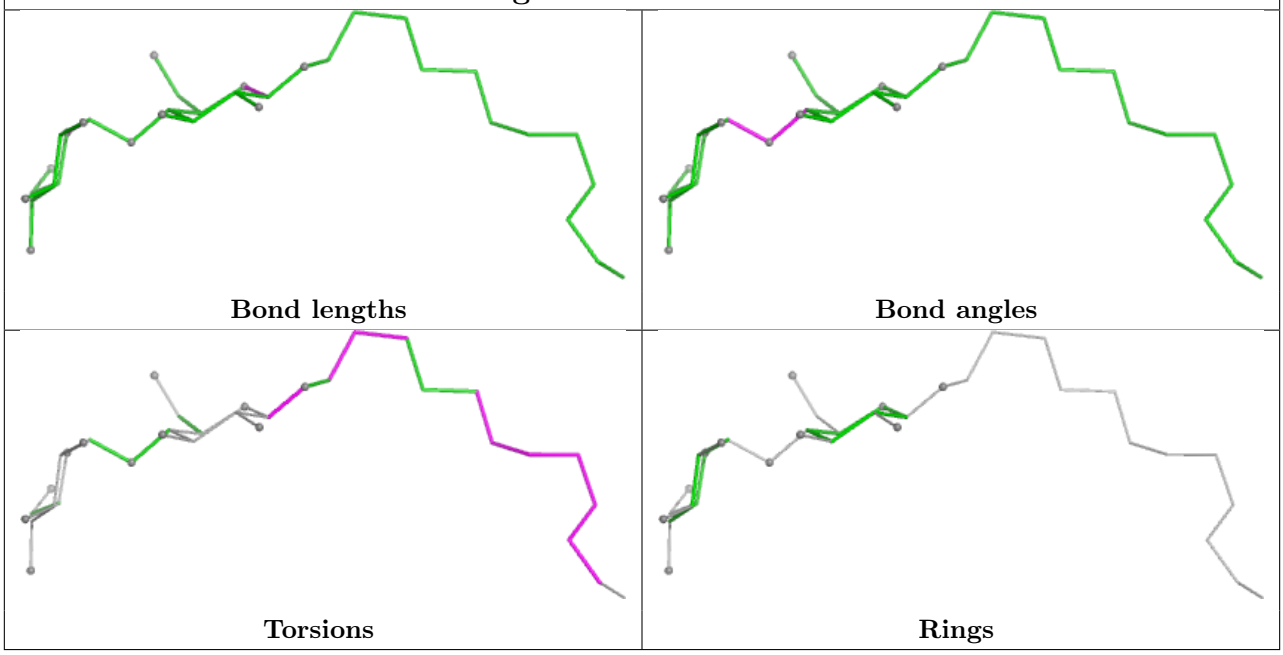
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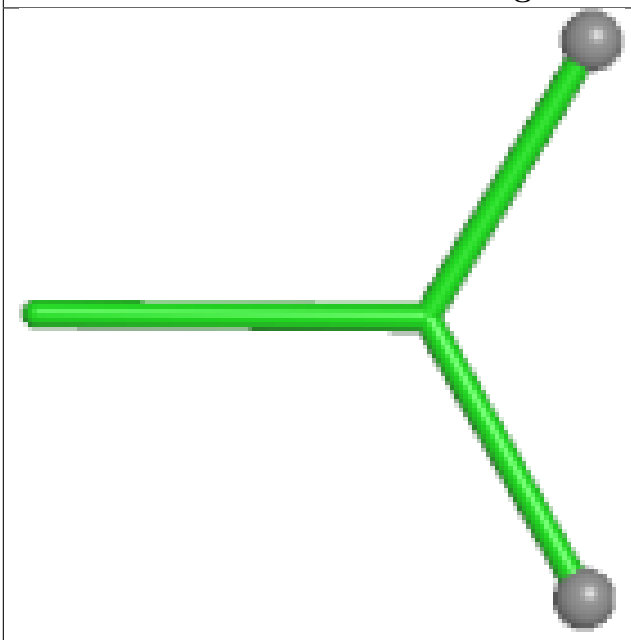
Ligand LMT B 1105



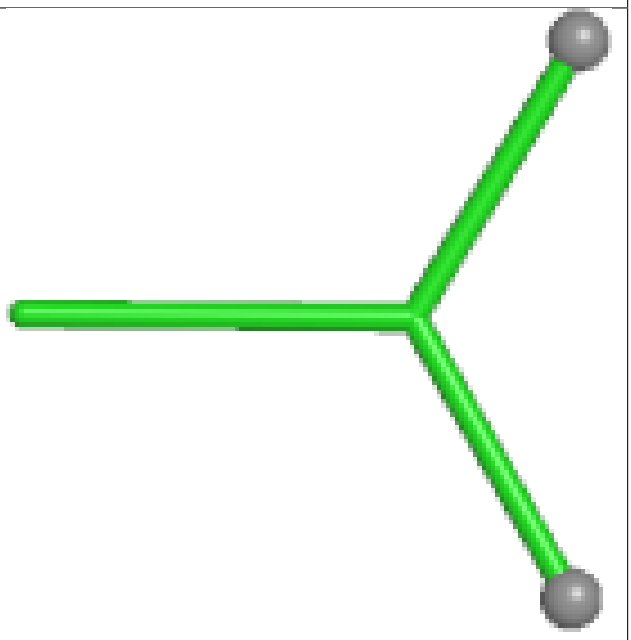
Ligand LMT A 1102



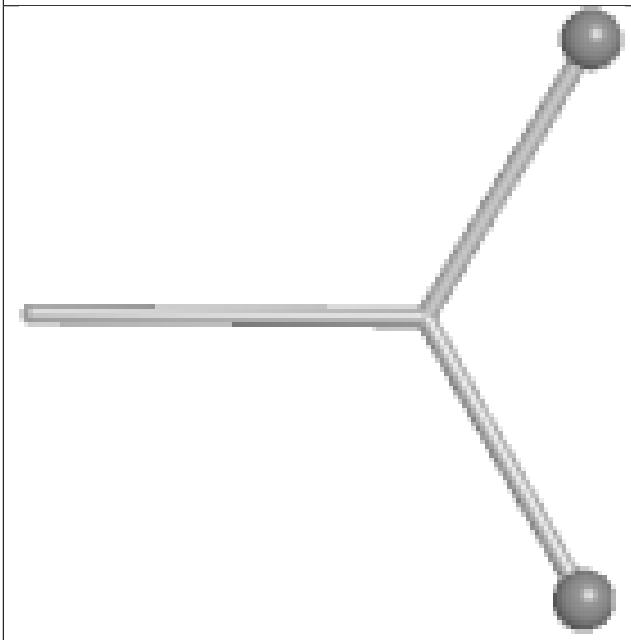
Ligand ACT C 1101



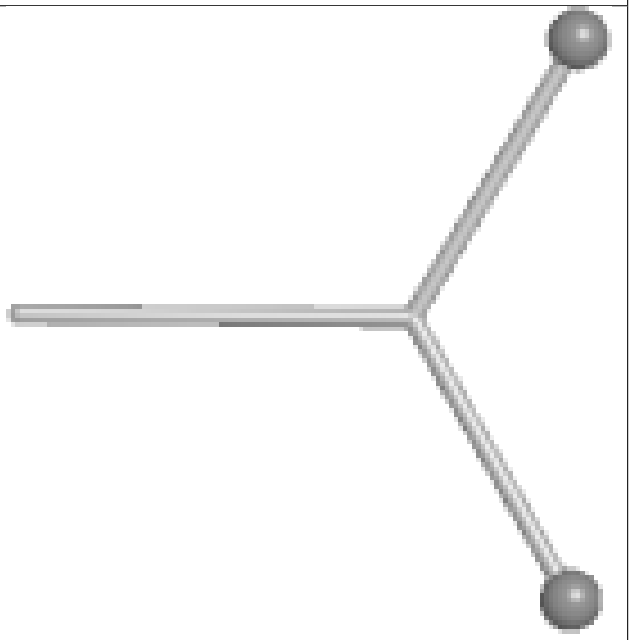
Bond lengths



Bond angles

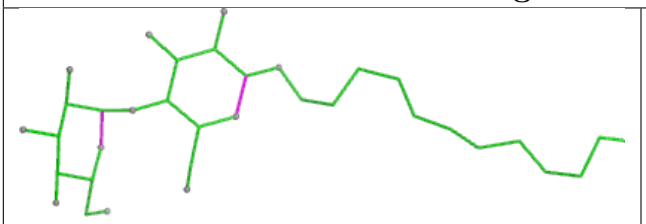


Torsions

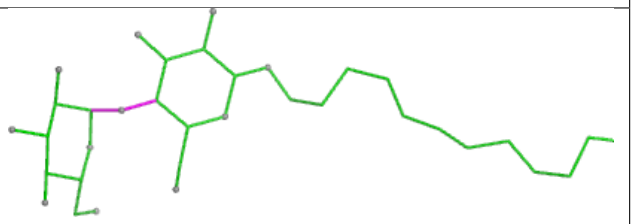


Rings

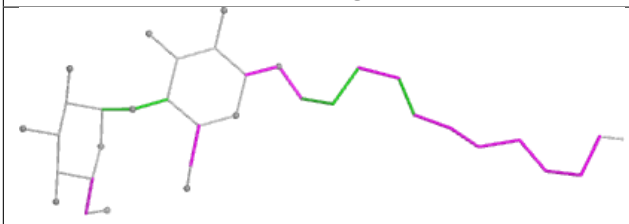
Ligand LMT E 1102



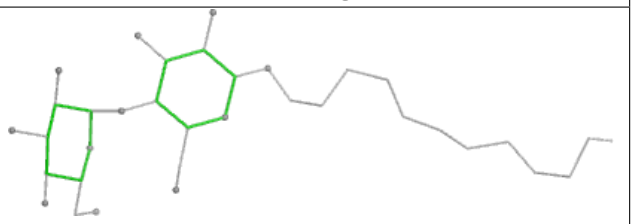
Bond lengths



Bond angles

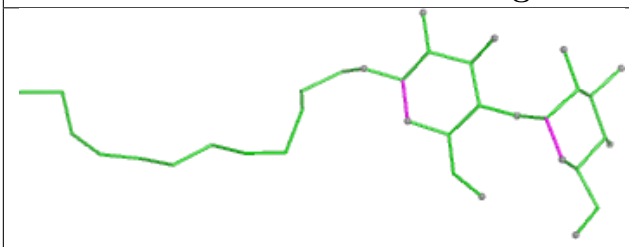


Torsions

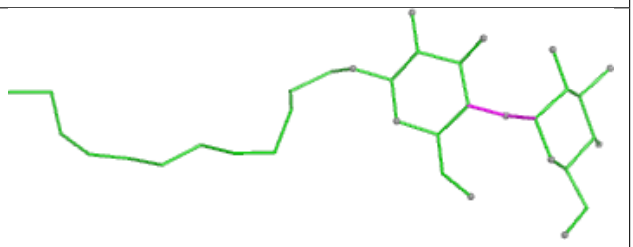


Rings

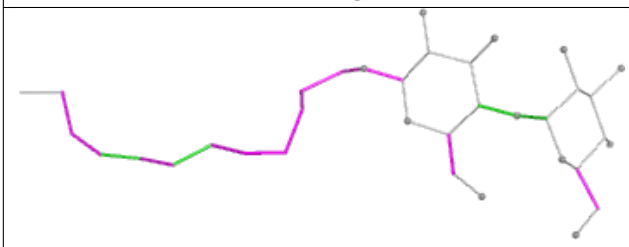
Ligand LMT B 1103



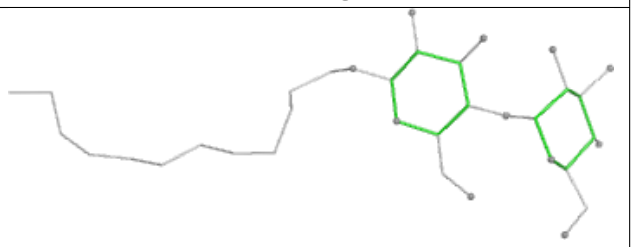
Bond lengths



Bond angles

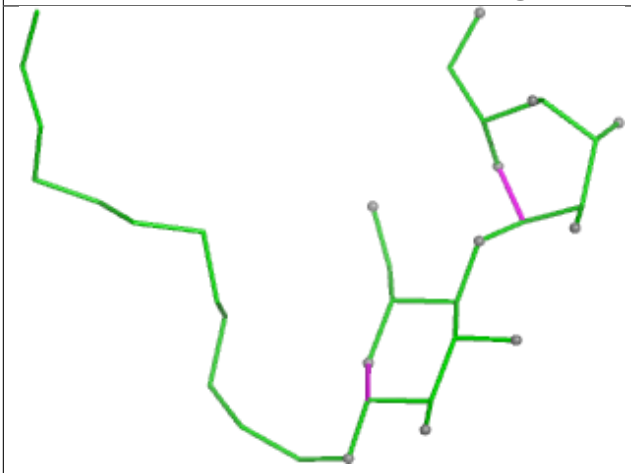


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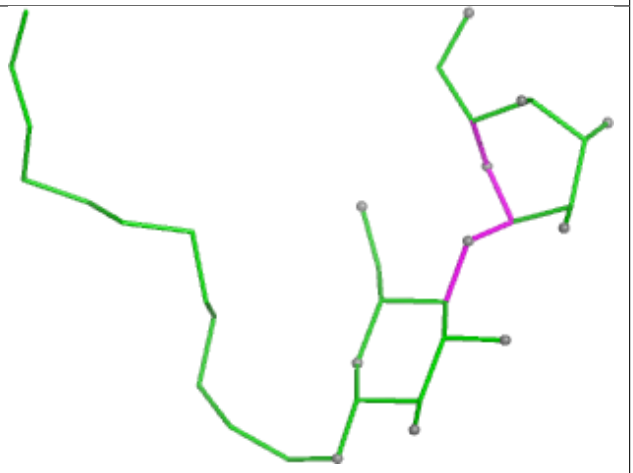


Rings

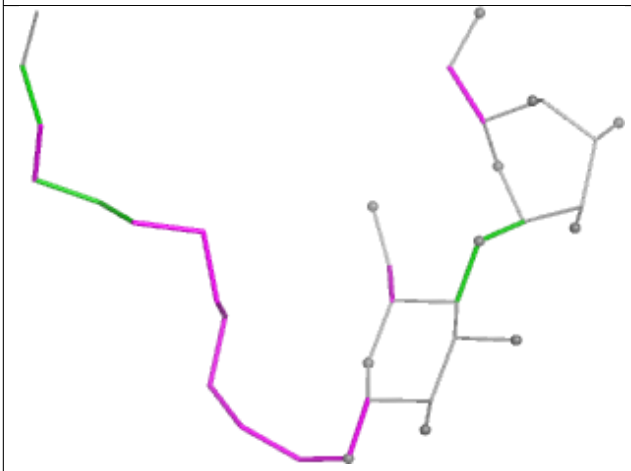
Ligand LMT D 1102



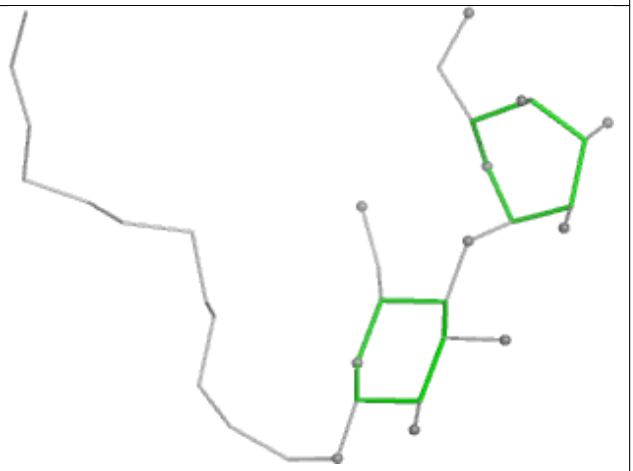
Bond lengths



Bond angles

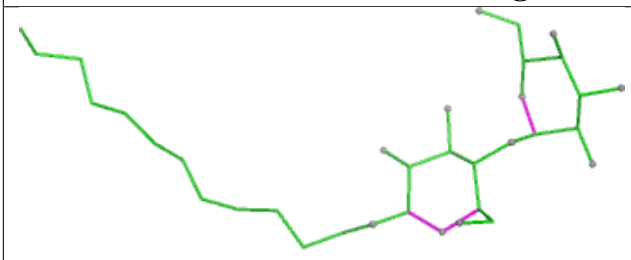


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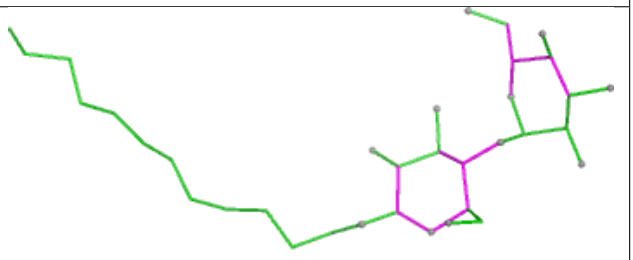


Rings

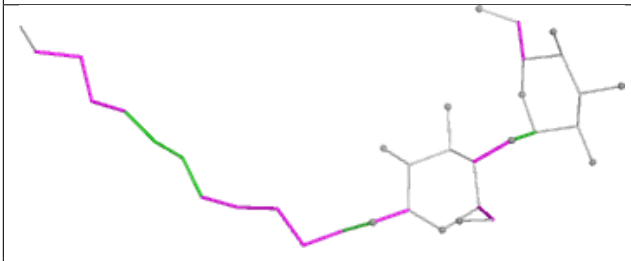
Ligand LMT A 1101



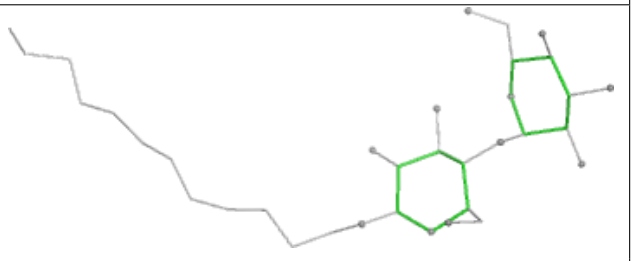
Bond lengths



Bond angles



Torsions



Rings

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	1012/1056 (95%)	0.83	127 (12%) 8 6	84, 117, 146, 168	0
1	B	1030/1056 (97%)	0.83	120 (11%) 9 7	78, 115, 160, 194	0
1	C	1028/1056 (97%)	0.67	93 (9%) 15 10	88, 132, 186, 229	0
1	D	1011/1056 (95%)	0.87	116 (11%) 9 7	87, 123, 159, 192	0
1	E	1030/1056 (97%)	0.80	120 (11%) 9 7	85, 123, 170, 189	0
1	F	1030/1056 (97%)	0.72	94 (9%) 15 9	87, 128, 181, 224	0
All	All	6141/6336 (96%)	0.79	670 (10%) 10 7	78, 123, 170, 229	0

All (670) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	675	GLY	10.7
1	D	676	ASN	10.5
1	B	126	GLY	10.3
1	A	44	ALA	10.2
1	D	728	LEU	10.1
1	D	732	ASP	9.9
1	D	730	ILE	9.8
1	E	573	PHE	9.7
1	E	666	PHE	9.4
1	D	332	VAL	9.1
1	D	665	ALA	8.8
1	D	675	GLY	8.7
1	F	236	GLY	8.5
1	D	753	TRP	8.5
1	F	778	ALA	8.4
1	E	628	PHE	8.3
1	B	335	ALA	8.2
1	A	268	VAL	7.9
1	D	729	GLU	7.9

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Mol	Chain	Res	Type	RSRZ
1	E	117	LEU	7.4
1	A	439	GLN	7.2
1	E	399	VAL	7.1
1	E	672	LEU	6.7
1	D	35	TYR	6.7
1	C	240	LEU	6.7
1	D	635	GLU	6.7
1	C	210	GLN	6.4
1	E	952	HIS	6.4
1	A	269	GLY	6.3
1	E	132	ALA	6.1
1	E	669	PRO	6.1
1	D	34	GLN	6.1
1	D	126	GLY	6.0
1	A	672	LEU	6.0
1	B	392	THR	6.0
1	F	788	TRP	5.9
1	A	275	TYR	5.9
1	D	674	LEU	5.8
1	F	748	THR	5.8
1	D	33	ASN	5.8
1	A	91	THR	5.8
1	B	339	GLU	5.7
1	B	660	ASP	5.7
1	E	336	SER	5.7
1	D	44	ALA	5.6
1	D	727	LYS	5.5
1	C	138	MET	5.5
1	F	167	SER	5.5
1	E	675	GLY	5.5
1	F	752	ALA	5.5
1	D	335	ALA	5.4
1	B	516	PHE	5.4
1	C	244	GLU	5.3
1	F	516	PHE	5.3
1	E	667	ALA	5.3
1	E	617	PHE	5.3
1	F	800	PHE	5.3
1	F	753	TRP	5.3
1	E	397	GLY	5.2
1	C	141	GLY	5.2
1	A	46	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	340	VAL	5.1
1	B	327	TYR	5.1
1	D	666	PHE	5.1
1	D	292	LYS	5.1
1	E	676	ASN	5.0
1	E	290	ALA	5.0
1	A	276	SER	5.0
1	E	626	MET	5.0
1	E	136	PHE	4.9
1	A	436	GLY	4.9
1	D	330	THR	4.9
1	E	665	ALA	4.8
1	E	989	ILE	4.8
1	D	326	PRO	4.8
1	E	833	GLY	4.7
1	D	225	VAL	4.7
1	B	127	ILE	4.5
1	E	655	PHE	4.5
1	A	361	ASN	4.5
1	B	397	GLY	4.5
1	C	960	GLU	4.5
1	C	307	ARG	4.5
1	F	782	PRO	4.5
1	B	924	VAL	4.5
1	A	31	PRO	4.5
1	B	282	ASN	4.5
1	D	644	VAL	4.5
1	C	242	THR	4.5
1	E	246	PHE	4.5
1	A	674	LEU	4.4
1	A	693	GLU	4.4
1	B	331	PRO	4.4
1	A	673	GLU	4.4
1	A	438	ILE	4.4
1	C	327	TYR	4.4
1	C	600	GLU	4.4
1	D	327	TYR	4.4
1	A	627	ALA	4.4
1	B	401	ALA	4.3
1	A	274	ASP	4.3
1	B	591	VAL	4.3
1	A	126	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	36	PRO	4.3
1	A	272	GLY	4.2
1	B	336	SER	4.2
1	B	263	LYS	4.2
1	B	396	PHE	4.2
1	B	618	ALA	4.2
1	E	651	ALA	4.2
1	E	958	ILE	4.2
1	D	681	ASP	4.2
1	A	671	VAL	4.2
1	A	267	ASP	4.1
1	F	446	ALA	4.1
1	A	277	ILE	4.1
1	A	690	VAL	4.1
1	F	292	LYS	4.1
1	A	667	ALA	4.1
1	A	677	ALA	4.1
1	F	855	GLY	4.1
1	E	746	ASN	4.1
1	F	785	LEU	4.0
1	A	45	VAL	4.0
1	B	247	GLU	4.0
1	D	334	SER	4.0
1	A	176	GLN	3.9
1	E	652	GLN	3.9
1	D	628	PHE	3.9
1	F	626	MET	3.9
1	E	113	LEU	3.9
1	B	610	PHE	3.9
1	E	674	LEU	3.9
1	D	142	VAL	3.9
1	F	477	ALA	3.9
1	C	245	GLN	3.9
1	E	396	PHE	3.8
1	A	134	LYS	3.8
1	F	519	MET	3.8
1	E	949	LYS	3.8
1	D	745	ILE	3.8
1	B	520	PHE	3.8
1	B	139	VAL	3.8
1	C	140	VAL	3.8
1	D	3	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	677	ALA	3.8
1	A	857	SER	3.7
1	C	687	GLN	3.7
1	F	123	GLN	3.7
1	A	179	GLY	3.7
1	B	363	ARG	3.7
1	A	178	PHE	3.7
1	C	246	PHE	3.7
1	C	883	VAL	3.7
1	D	697	GLN	3.7
1	D	328	ASP	3.7
1	A	185	ARG	3.7
1	C	819	ASN	3.6
1	E	580	PRO	3.6
1	B	1000	ALA	3.6
1	B	60	THR	3.6
1	D	840	MET	3.6
1	B	237	LYS	3.6
1	F	747	SER	3.6
1	E	251	LEU	3.6
1	F	136	PHE	3.6
1	F	615	PHE	3.6
1	F	358	PHE	3.6
1	A	43	ILE	3.6
1	B	125	GLN	3.6
1	E	673	GLU	3.6
1	F	726	TYR	3.6
1	A	697	GLN	3.5
1	F	308	GLN	3.5
1	B	925	PHE	3.5
1	E	339	GLU	3.5
1	B	47	VAL	3.5
1	D	231	ASN	3.5
1	E	498	LYS	3.5
1	B	140	VAL	3.5
1	B	606	VAL	3.5
1	C	302	THR	3.5
1	B	948	ALA	3.5
1	E	864	GLU	3.4
1	B	113	LEU	3.4
1	B	289	ILE	3.4
1	A	715	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	357	LEU	3.4
1	E	1025	VAL	3.4
1	C	368	PRO	3.4
1	E	344	LEU	3.4
1	D	45	VAL	3.4
1	E	133	VAL	3.4
1	A	486	LEU	3.4
1	C	683	PHE	3.4
1	D	136	PHE	3.4
1	D	174	ASP	3.4
1	B	579	PRO	3.4
1	F	133	VAL	3.4
1	F	520	PHE	3.4
1	E	678	THR	3.3
1	C	290	ALA	3.3
1	D	331	PRO	3.3
1	E	832	PRO	3.3
1	A	47	VAL	3.3
1	C	723	GLU	3.3
1	A	720	MET	3.3
1	E	627	ALA	3.3
1	B	617	PHE	3.3
1	D	452	VAL	3.3
1	C	857	SER	3.3
1	A	270	LEU	3.3
1	F	751	ILE	3.3
1	C	220	GLY	3.3
1	D	946	GLU	3.3
1	C	85	ASP	3.3
1	B	671	VAL	3.3
1	F	746	ASN	3.3
1	A	1019	TRP	3.3
1	B	580	PRO	3.3
1	D	114	ALA	3.3
1	D	127	ILE	3.3
1	D	392	THR	3.3
1	C	512	PHE	3.2
1	C	203	VAL	3.2
1	F	172	VAL	3.2
1	C	833	GLY	3.2
1	E	501	GLU	3.2
1	B	404	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	573	PHE	3.2
1	E	1001	ILE	3.2
1	C	809	GLU	3.2
1	E	461	GLY	3.2
1	F	679	GLY	3.2
1	C	681	ASP	3.2
1	B	182	TYR	3.2
1	D	673	GLU	3.2
1	D	333	VAL	3.2
1	E	338	HIS	3.2
1	C	954	GLN	3.2
1	F	176	GLN	3.2
1	F	597	TYR	3.2
1	E	460	GLY	3.1
1	A	187	TRP	3.1
1	B	332	VAL	3.1
1	C	429	GLU	3.1
1	E	285	PRO	3.1
1	D	993	ALA	3.1
1	E	335	ALA	3.1
1	C	308	GLN	3.0
1	A	180	SER	3.0
1	C	963	ILE	3.0
1	A	539	ALA	3.0
1	D	807	LYS	3.0
1	A	902	LEU	3.0
1	B	675	GLY	3.0
1	B	338	HIS	3.0
1	E	953	GLU	3.0
1	E	59	ASP	3.0
1	D	586	ARG	3.0
1	D	634	TRP	3.0
1	F	754	GLY	3.0
1	A	92	VAL	3.0
1	C	206	ALA	3.0
1	E	401	ALA	3.0
1	E	594	MET	3.0
1	E	1000	ALA	3.0
1	B	116	PRO	3.0
1	A	827	LEU	3.0
1	E	1028	SER	3.0
1	B	209	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	722	ASP	3.0
1	D	1000	ALA	3.0
1	A	819	ASN	3.0
1	B	248	ASN	3.0
1	E	507	GLU	3.0
1	D	218	GLN	3.0
1	F	115	THR	3.0
1	D	517	ASN	2.9
1	B	594	MET	2.9
1	D	287	SER	2.9
1	C	249	ILE	2.9
1	D	134	LYS	2.9
1	A	470	PHE	2.9
1	D	664	PHE	2.9
1	C	678	THR	2.9
1	D	32	VAL	2.9
1	D	46	GLN	2.9
1	F	995	SER	2.9
1	F	174	ASP	2.9
1	A	719	GLY	2.9
1	D	375	VAL	2.9
1	F	268	VAL	2.9
1	D	690	VAL	2.9
1	C	309	THR	2.9
1	B	246	PHE	2.9
1	C	325	TYR	2.9
1	B	213	GLN	2.9
1	F	787	LYS	2.9
1	B	678	THR	2.9
1	A	90	ILE	2.9
1	A	665	ALA	2.9
1	D	385	ALA	2.9
1	E	728	LEU	2.9
1	A	538	ARG	2.9
1	A	856	TYR	2.9
1	C	716	ARG	2.9
1	C	237	LYS	2.9
1	D	731	ASP	2.8
1	E	292	LYS	2.9
1	D	571	VAL	2.8
1	E	277	ILE	2.8
1	E	609	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	718	ASN	2.8
1	C	834	LEU	2.8
1	D	569	GLN	2.8
1	A	615	PHE	2.8
1	E	129	VAL	2.8
1	C	477	ALA	2.8
1	B	917	MET	2.8
1	F	316	PHE	2.8
1	B	764	ARG	2.8
1	E	671	VAL	2.8
1	A	621	GLY	2.8
1	B	210	GLN	2.8
1	A	42	ALA	2.8
1	A	965	ALA	2.8
1	F	453	PHE	2.8
1	D	554	TRP	2.8
1	C	139	VAL	2.8
1	C	148	SER	2.8
1	A	718	ASN	2.8
1	B	290	ALA	2.8
1	D	805	THR	2.8
1	F	304	LYS	2.8
1	B	376	LEU	2.8
1	B	772	LEU	2.8
1	A	545	TYR	2.8
1	E	597	TYR	2.8
1	A	628	PHE	2.8
1	C	241	GLN	2.8
1	D	774	GLY	2.8
1	B	6	ILE	2.7
1	C	399	VAL	2.7
1	A	271	GLY	2.7
1	D	236	GLY	2.7
1	D	677	ALA	2.7
1	A	435	MET	2.7
1	A	659	LYS	2.7
1	C	580	PRO	2.7
1	B	527	TYR	2.7
1	E	176	GLN	2.7
1	F	1002	GLY	2.7
1	E	404	LEU	2.7
1	F	971	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	337	ILE	2.7
1	A	87	SER	2.7
1	A	694	VAL	2.7
1	B	64	VAL	2.7
1	B	900	VAL	2.7
1	D	615	PHE	2.7
1	E	193	LEU	2.7
1	F	302	THR	2.7
1	A	83	ASN	2.7
1	A	988	ALA	2.7
1	C	289	ILE	2.7
1	D	542	LEU	2.7
1	D	827	LEU	2.7
1	E	228	GLN	2.7
1	E	414	GLU	2.7
1	A	626	MET	2.7
1	B	672	LEU	2.7
1	B	758	VAL	2.6
1	C	147	GLY	2.6
1	C	304	LYS	2.6
1	B	609	VAL	2.6
1	B	928	VAL	2.6
1	E	562	ALA	2.6
1	C	628	PHE	2.6
1	A	84	SER	2.6
1	A	416	VAL	2.6
1	E	333	VAL	2.6
1	E	668	PRO	2.6
1	C	243	ALA	2.6
1	C	674	LEU	2.6
1	A	612	VAL	2.6
1	C	373	PRO	2.6
1	B	628	PHE	2.6
1	D	617	PHE	2.6
1	B	48	SER	2.6
1	E	337	ILE	2.6
1	D	232	ALA	2.6
1	D	935	GLY	2.6
1	F	683	PHE	2.6
1	C	369	THR	2.6
1	A	816	GLU	2.6
1	B	300	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	400	LEU	2.6
1	A	905	PRO	2.6
1	A	207	ILE	2.5
1	C	356	TYR	2.5
1	A	620	ARG	2.5
1	C	351	VAL	2.5
1	D	839	ALA	2.5
1	F	201	GLY	2.5
1	C	1029	THR	2.5
1	E	991	THR	2.5
1	F	379	THR	2.5
1	B	586	ARG	2.5
1	B	883	VAL	2.5
1	E	443	VAL	2.5
1	B	577	GLN	2.5
1	F	573	PHE	2.5
1	E	986	PRO	2.5
1	F	706	ALA	2.5
1	C	640	GLY	2.5
1	B	1001	ILE	2.5
1	D	47	VAL	2.5
1	C	975	MET	2.5
1	B	106	GLN	2.5
1	C	127	ILE	2.5
1	C	397	GLY	2.5
1	D	141	GLY	2.5
1	F	996	GLY	2.5
1	C	222	LEU	2.5
1	E	64	VAL	2.5
1	F	135	ASN	2.5
1	A	706	ALA	2.5
1	B	956	LYS	2.5
1	B	326	PRO	2.5
1	C	730	ILE	2.5
1	E	232	ALA	2.5
1	F	550	ALA	2.5
1	B	933	THR	2.5
1	D	149	MET	2.5
1	A	825	GLU	2.5
1	A	622	GLN	2.5
1	A	841	ALA	2.5
1	A	993	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	581	GLY	2.5
1	B	996	GLY	2.5
1	B	859	THR	2.5
1	B	720	MET	2.5
1	C	900	VAL	2.5
1	A	858	TRP	2.4
1	F	43	ILE	2.4
1	F	232	ALA	2.4
1	B	970	LEU	2.4
1	F	377	LEU	2.4
1	F	400	LEU	2.4
1	A	164	ASP	2.4
1	A	746	ASN	2.4
1	B	245	GLN	2.4
1	B	588	GLN	2.4
1	F	972	PRO	2.4
1	E	134	LYS	2.4
1	F	237	LYS	2.4
1	C	679	GLY	2.4
1	E	463	THR	2.4
1	E	1029	THR	2.4
1	C	825	GLU	2.4
1	E	1026	ALA	2.4
1	F	307	ARG	2.4
1	A	392	THR	2.4
1	B	333	VAL	2.4
1	D	1025	VAL	2.4
1	A	1024	TYR	2.4
1	C	964	GLU	2.4
1	C	236	GLY	2.4
1	C	122	VAL	2.4
1	E	127	ILE	2.4
1	E	219	LEU	2.4
1	F	328	ASP	2.4
1	E	395	MET	2.4
1	F	625	GLY	2.3
1	A	663	VAL	2.3
1	E	504	ASP	2.3
1	A	114	ALA	2.3
1	C	688	ALA	2.3
1	F	360	GLN	2.3
1	A	30	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	358	PHE	2.3
1	C	505	HIS	2.3
1	D	357	LEU	2.3
1	A	273	GLN	2.3
1	F	46	GLN	2.3
1	F	950	GLU	2.3
1	E	300	LEU	2.3
1	E	405	LEU	2.3
1	F	405	LEU	2.3
1	D	929	GLY	2.3
1	D	275	TYR	2.3
1	F	640	GLY	2.3
1	A	136	PHE	2.3
1	F	789	TYR	2.3
1	D	871	GLN	2.3
1	D	717	PRO	2.3
1	E	73	ASP	2.3
1	F	612	VAL	2.3
1	B	940	ASN	2.3
1	F	1003	THR	2.3
1	B	730	ILE	2.3
1	D	6	ILE	2.3
1	E	610	PHE	2.3
1	A	34	GLN	2.3
1	D	157	TYR	2.3
1	A	567	GLU	2.3
1	D	80	SER	2.3
1	D	899	SER	2.3
1	E	244	GLU	2.3
1	E	135	ASN	2.2
1	F	523	THR	2.2
1	E	1024	TYR	2.2
1	B	547	VAL	2.2
1	B	945	VAL	2.2
1	D	699	ARG	2.2
1	E	188	LEU	2.2
1	E	249	ILE	2.2
1	A	39	ALA	2.2
1	D	979	ALA	2.2
1	A	588	GLN	2.2
1	B	360	GLN	2.2
1	D	104	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	334	SER	2.2
1	E	48	SER	2.2
1	A	265	VAL	2.2
1	A	230	LEU	2.2
1	B	238	THR	2.2
1	D	233	THR	2.2
1	A	301	ASP	2.2
1	D	337	ILE	2.2
1	F	206	ALA	2.2
1	A	635	GLU	2.2
1	F	1021	PRO	2.2
1	B	470	PHE	2.2
1	A	338	HIS	2.2
1	B	961	ALA	2.2
1	D	804	ALA	2.2
1	E	948	ALA	2.2
1	C	104	GLN	2.2
1	C	1028	SER	2.2
1	F	703	LEU	2.2
1	E	516	PHE	2.2
1	A	814	LYS	2.2
1	E	342	LYS	2.2
1	B	988	ALA	2.2
1	C	303	ALA	2.2
1	D	274	ASP	2.2
1	F	783	ASP	2.2
1	A	696	LEU	2.2
1	B	344	LEU	2.2
1	E	834	LEU	2.2
1	F	117	LEU	2.2
1	D	354	VAL	2.2
1	F	122	VAL	2.2
1	F	465	VAL	2.2
1	A	66	GLU	2.2
1	C	326	PRO	2.2
1	D	837	GLY	2.2
1	B	523	THR	2.2
1	F	991	THR	2.2
1	A	278	ASN	2.2
1	A	112	GLN	2.1
1	A	162	ILE	2.1
1	B	452	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	388	PHE	2.1
1	E	116	PRO	2.1
1	F	126	GLY	2.1
1	E	561	THR	2.1
1	B	874	ALA	2.1
1	C	665	ALA	2.1
1	F	290	ALA	2.1
1	F	471	SER	2.1
1	C	818	TYR	2.1
1	E	327	TYR	2.1
1	A	387	GLY	2.1
1	A	668	PRO	2.1
1	A	820	GLY	2.1
1	A	1002	GLY	2.1
1	C	689	GLY	2.1
1	D	551	GLY	2.1
1	B	953	GLU	2.1
1	E	772	LEU	2.1
1	F	1022	LEU	2.1
1	D	574	ALA	2.1
1	E	718	ASN	2.1
1	A	48	SER	2.1
1	A	280	GLN	2.1
1	C	38	ILE	2.1
1	A	142	VAL	2.1
1	B	122	VAL	2.1
1	C	323	VAL	2.1
1	C	727	LYS	2.1
1	D	18	VAL	2.1
1	E	509	LYS	2.1
1	F	818	TYR	2.1
1	A	869	GLY	2.1
1	B	179	GLY	2.1
1	E	126	GLY	2.1
1	A	772	LEU	2.1
1	B	395	MET	2.1
1	B	224	ALA	2.1
1	C	279	ALA	2.1
1	E	114	ALA	2.1
1	C	879	SER	2.1
1	B	176	GLN	2.1
1	A	388	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1018	PHE	2.1
1	E	860	GLY	2.1
1	A	824	MET	2.1
1	A	1003	THR	2.1
1	B	677	ALA	2.1
1	D	90	ILE	2.1
1	F	517	ASN	2.1
1	F	697	GLN	2.1
1	B	405	LEU	2.1
1	A	771	TYR	2.1
1	D	138	MET	2.1
1	F	138	MET	2.1
1	D	638	PRO	2.1
1	D	779	ARG	2.1
1	B	494	ALA	2.1
1	D	16	ALA	2.1
1	E	683	PHE	2.1
1	B	647	LEU	2.1
1	B	1005	VAL	2.1
1	D	75	LEU	2.1
1	D	928	VAL	2.1
1	D	1005	VAL	2.1
1	A	662	MET	2.1
1	F	594	MET	2.1
1	B	221	GLY	2.0
1	B	771	TYR	2.0
1	C	553	ILE	2.0
1	D	438	ILE	2.0
1	B	747	SER	2.0
1	E	930	LEU	2.0
1	B	260	VAL	2.0
1	E	140	VAL	2.0
1	E	749	VAL	2.0
1	F	767	VAL	2.0
1	B	361	ASN	2.0
1	C	891	TYR	2.0
1	F	427	PRO	2.0
1	D	291	ILE	2.0
1	F	769	ARG	2.0
1	C	115	THR	2.0
1	B	923	ASP	2.0
1	D	414	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	136	PHE	2.0
1	A	742	LEU	2.0
1	A	815	LEU	2.0
1	C	961	ALA	2.0
1	E	993	ALA	2.0
1	E	415	ASN	2.0
1	A	326	PRO	2.0
1	B	650	ARG	2.0
1	D	934	ILE	2.0
1	F	776	PRO	2.0
1	A	647	LEU	2.0
1	B	453	PHE	2.0
1	D	175	PHE	2.0
1	F	366	LEU	2.0
1	A	593	SER	2.0
1	A	889	ALA	2.0
1	B	286	ALA	2.0
1	C	584	ALA	2.0
1	E	648	ALA	2.0
1	F	476	SER	2.0
1	E	416	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	ACT	F	1101	4/4	0.36	0.30	130,130,131,131	0
4	ACT	C	1101	4/4	0.50	0.21	112,112,112,112	0

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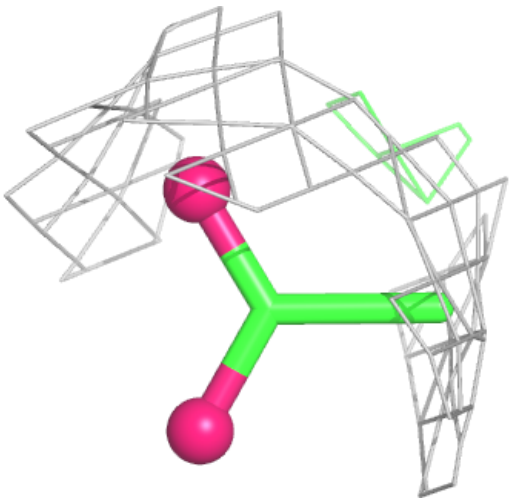
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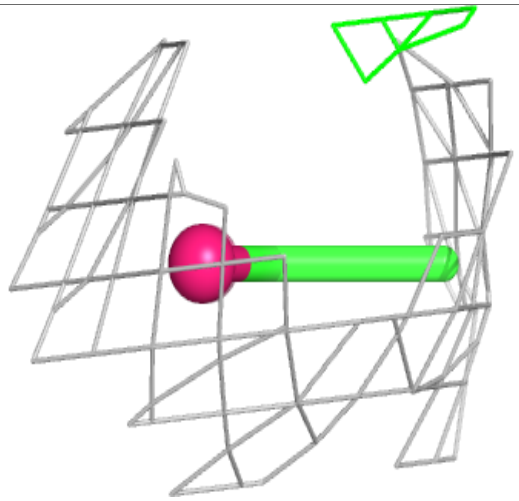
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LMT	B	1102	35/35	0.56	0.19	120,123,128,129	0
3	MC2	B	1101	33/33	0.56	0.27	137,138,139,139	0
2	LMT	B	1103	35/35	0.71	0.30	122,135,152,160	0
2	LMT	D	1102	35/35	0.75	0.17	98,104,120,123	0
2	LMT	B	1104	35/35	0.76	0.14	106,115,128,132	0
2	LMT	E	1101	35/35	0.79	0.18	107,126,138,143	0
2	LMT	A	1101	35/35	0.79	0.17	102,116,141,146	0
2	LMT	E	1102	35/35	0.81	0.14	103,120,131,140	0
2	LMT	D	1101	35/35	0.84	0.12	112,127,148,154	0
2	LMT	A	1102	35/35	0.85	0.15	102,119,134,138	0
2	LMT	B	1105	35/35	0.88	0.11	98,104,109,113	0

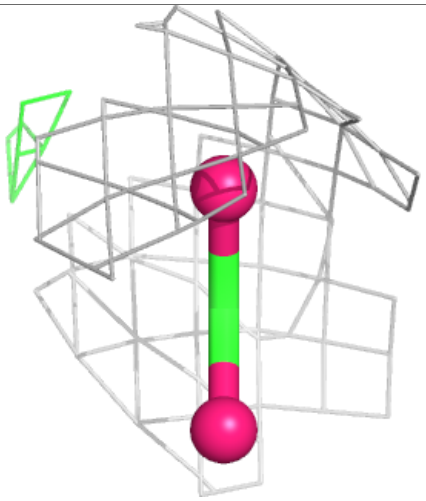
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACT F 1101:

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

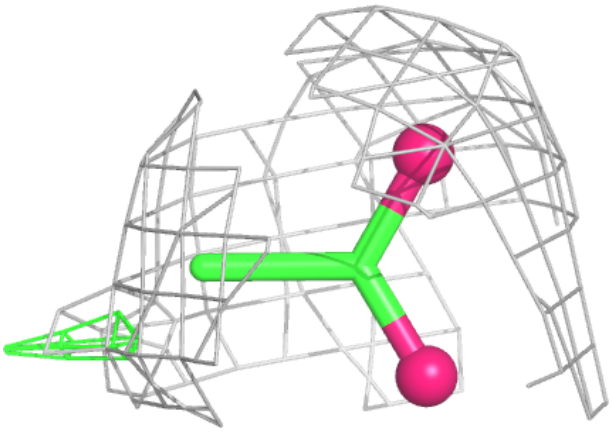


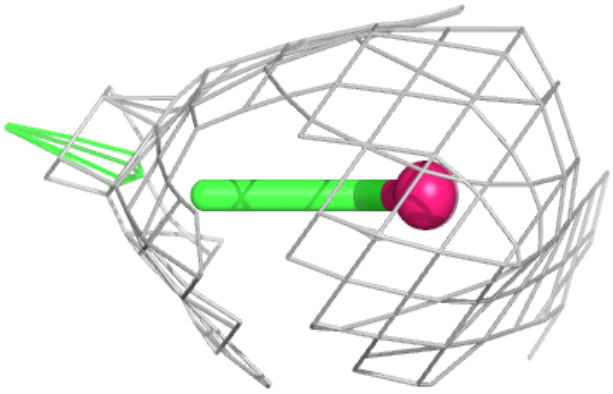


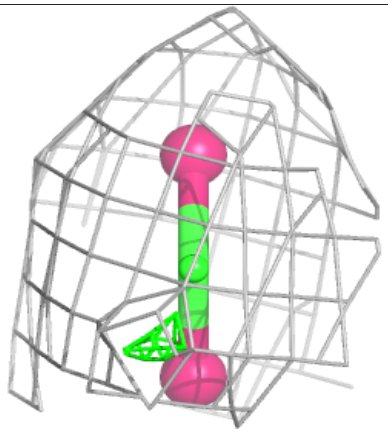


Electron density around ACT C 1101:

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

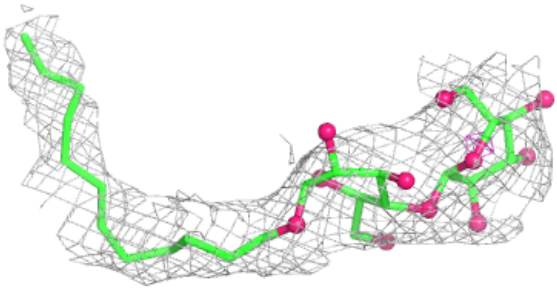


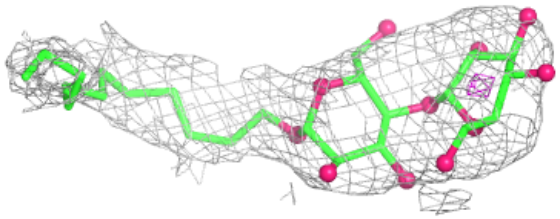


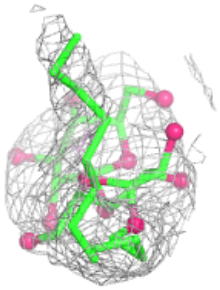


Electron density around LMT B 1102:

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

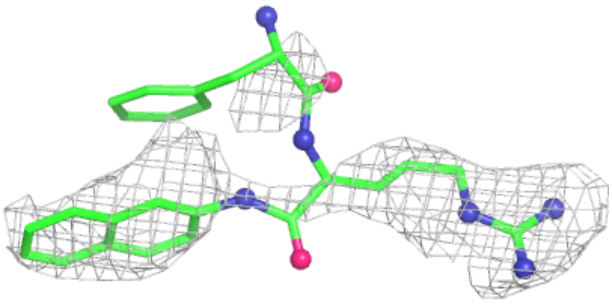


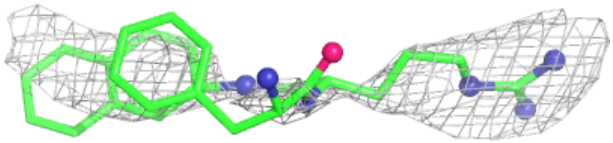


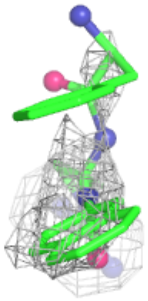


Electron density around MC2 B 1101:

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

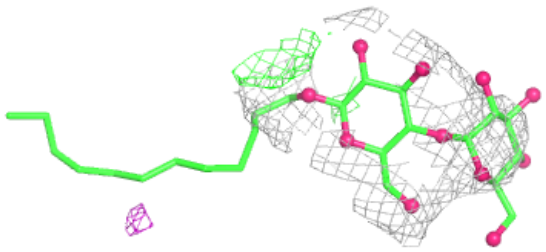


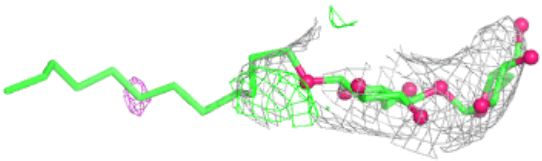




Electron density around LMT B 1103:

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

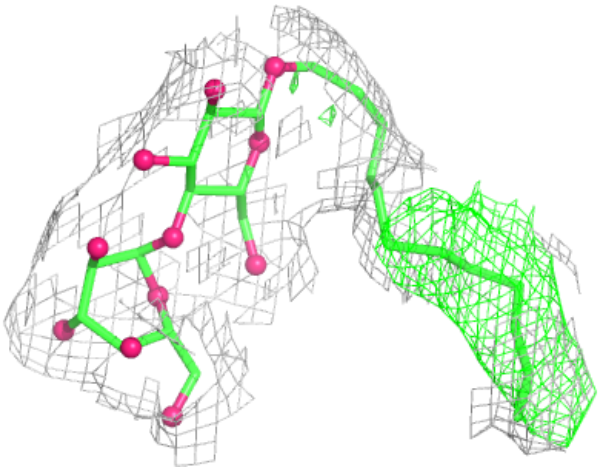


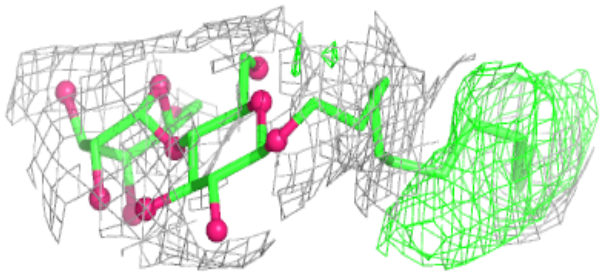


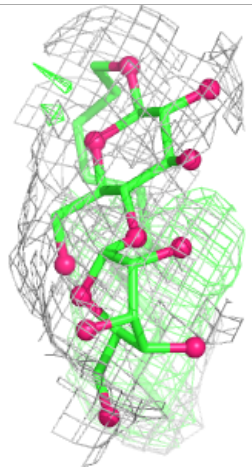


Electron density around LMT D 1102:

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

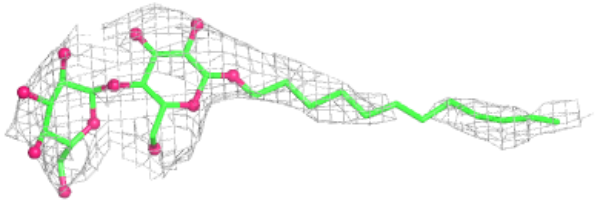


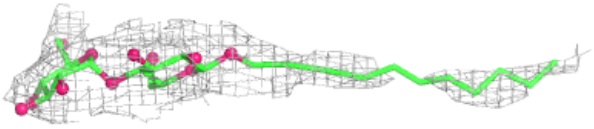


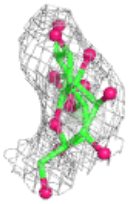


Electron density around LMT B 1104:

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

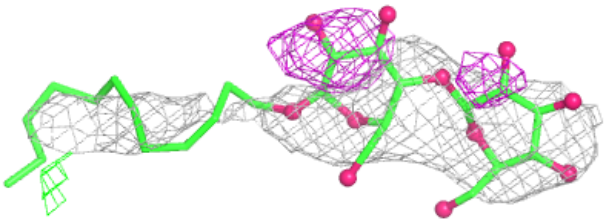


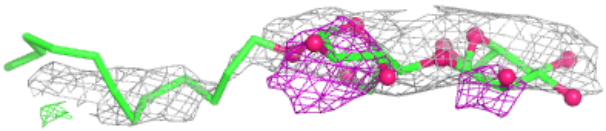


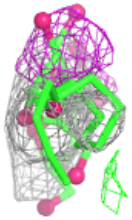


Electron density around LMT E 1101:

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

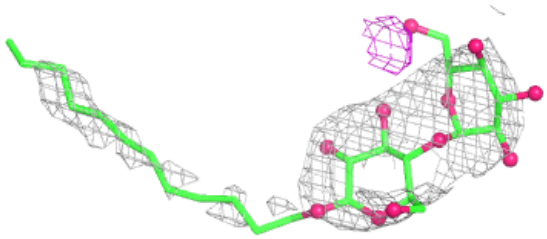


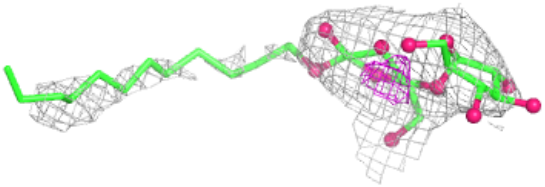




Electron density around LMT A 1101:

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

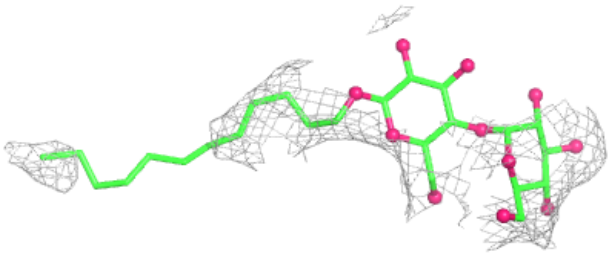


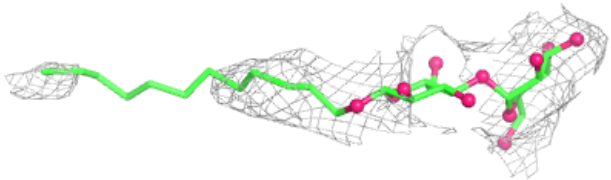


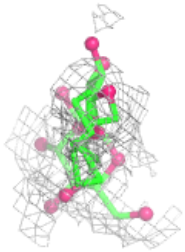


Electron density around LMT E 1102:

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

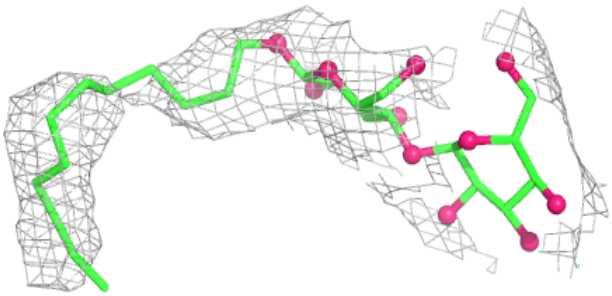


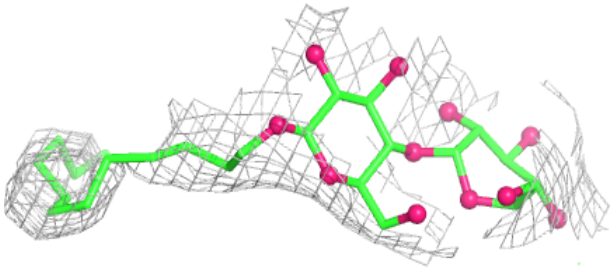




Electron density around LMT D 1101:

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

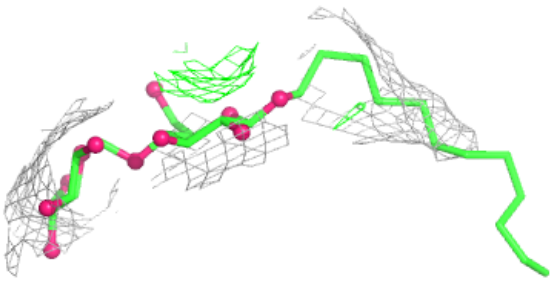


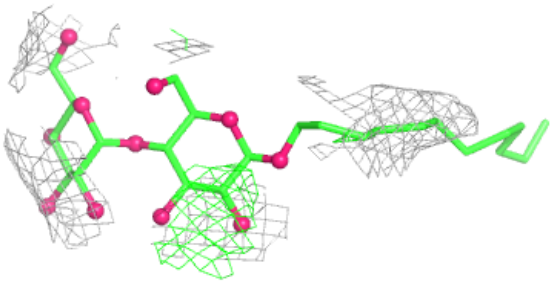


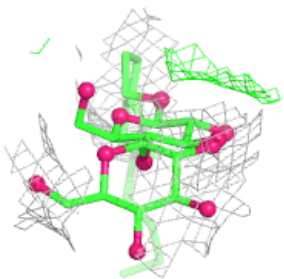


Electron density around LMT A 1102:

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

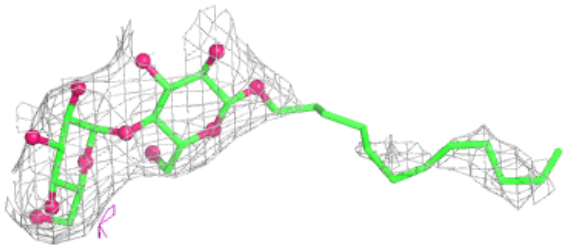


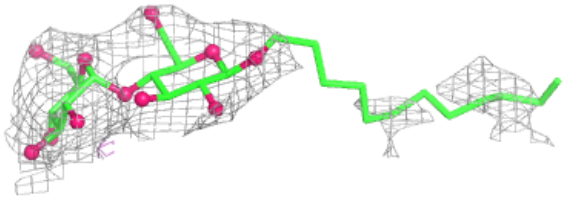


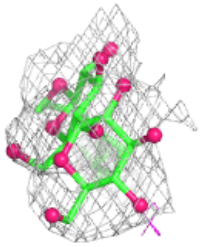


Electron density around LMT B 1105:

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







6.5 Other polymers

There are no such residues in this entry.