Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:06 PM EDT

PDB ID	:	3W9J
Title	:	Structural basis for the inhibition of bacterial multidrug exporters
Authors	:	Sakurai, K.; Nakashima, R.; Hayashi, K.; Yamaguchi, A.
Deposited on	:	2013-04-04
Resolution	:	3.15 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:

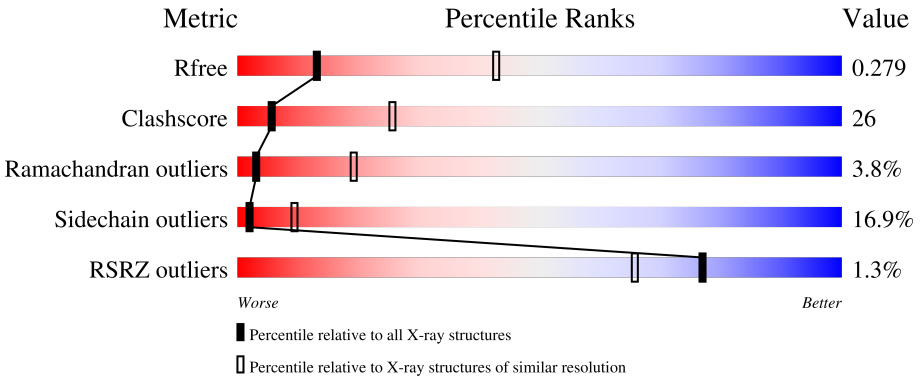
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	1052	52% 37% 8%
1	B	1052	52% 38% 8%
1	C	1052	3% 46% 40% 12%
1	D	1052	48% 40% 8%
1	E	1052	50% 38% 10%

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Mol	Chain	Length	Quality of chain
1	F	1052	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	D	2001	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 47358 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	1018	Total	C	N	O	S	0	0	0
			7724	4975	1280	1429	40			
1	B	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	C	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	D	1019	Total	C	N	O	S	0	0	0
			7735	4984	1281	1430	40			
1	E	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	F	1033	Total	C	N	O	S	0	0	0
			7840	5046	1302	1452	40			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	expression tag	UNP P52002
A	1048	HIS	-	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
B	1047	HIS	-	expression tag	UNP P52002
B	1048	HIS	-	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
B	1052	HIS	-	expression tag	UNP P52002
C	1047	HIS	-	expression tag	UNP P52002
C	1048	HIS	-	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

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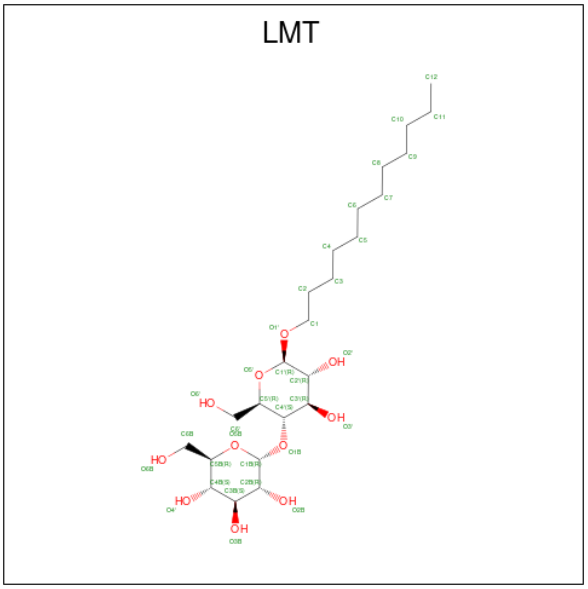
Chain	Residue	Modelled	Actual	Comment	Reference
C	1052	HIS	-	expression tag	UNP P52002
D	1047	HIS	-	expression tag	UNP P52002
D	1048	HIS	-	expression tag	UNP P52002
D	1049	HIS	-	expression tag	UNP P52002
D	1050	HIS	-	expression tag	UNP P52002
D	1051	HIS	-	expression tag	UNP P52002
D	1052	HIS	-	expression tag	UNP P52002
E	1047	HIS	-	expression tag	UNP P52002
E	1048	HIS	-	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
F	1047	HIS	-	expression tag	UNP P52002
F	1048	HIS	-	expression tag	UNP P52002
F	1049	HIS	-	expression tag	UNP P52002
F	1050	HIS	-	expression tag	UNP P52002
F	1051	HIS	-	expression tag	UNP P52002
F	1052	HIS	-	expression tag	UNP P52002

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



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

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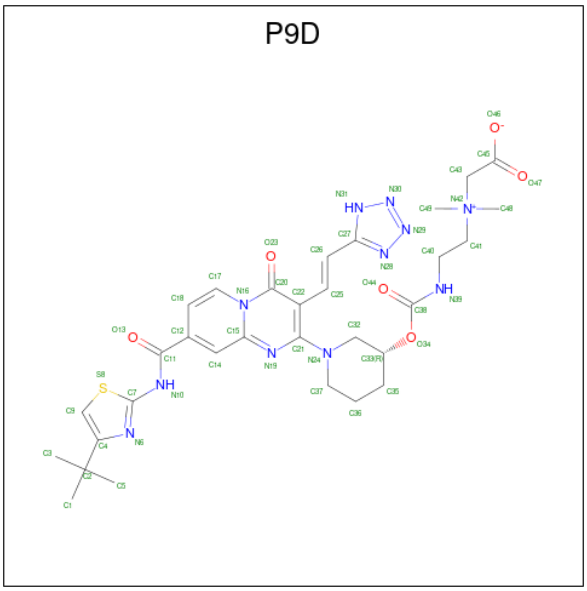
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 35 24 11	0	0
2	A	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	B	1	Total C O 35 24 11	0	0
2	C	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0
2	D	1	Total C O 35 24 11	0	0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

- Molecule 3 is [{2-[({[(3R)-1-{8-[(4-tert-butyl-1,3-thiazol-2-yl)carbamoyl]-4-oxo-3-[(E)-2-(1H-tetrazol-5-yl)ethenyl]-4H-pyrido[1,2-a]pyrimidin-2-yl}piperidin-3-yl]oxy}carbonyl)amino]ethyl}(dimethyl)ammonio]acetate (three-letter code: P9D) (formula: $C_{31}H_{39}N_{11}O_6S$).



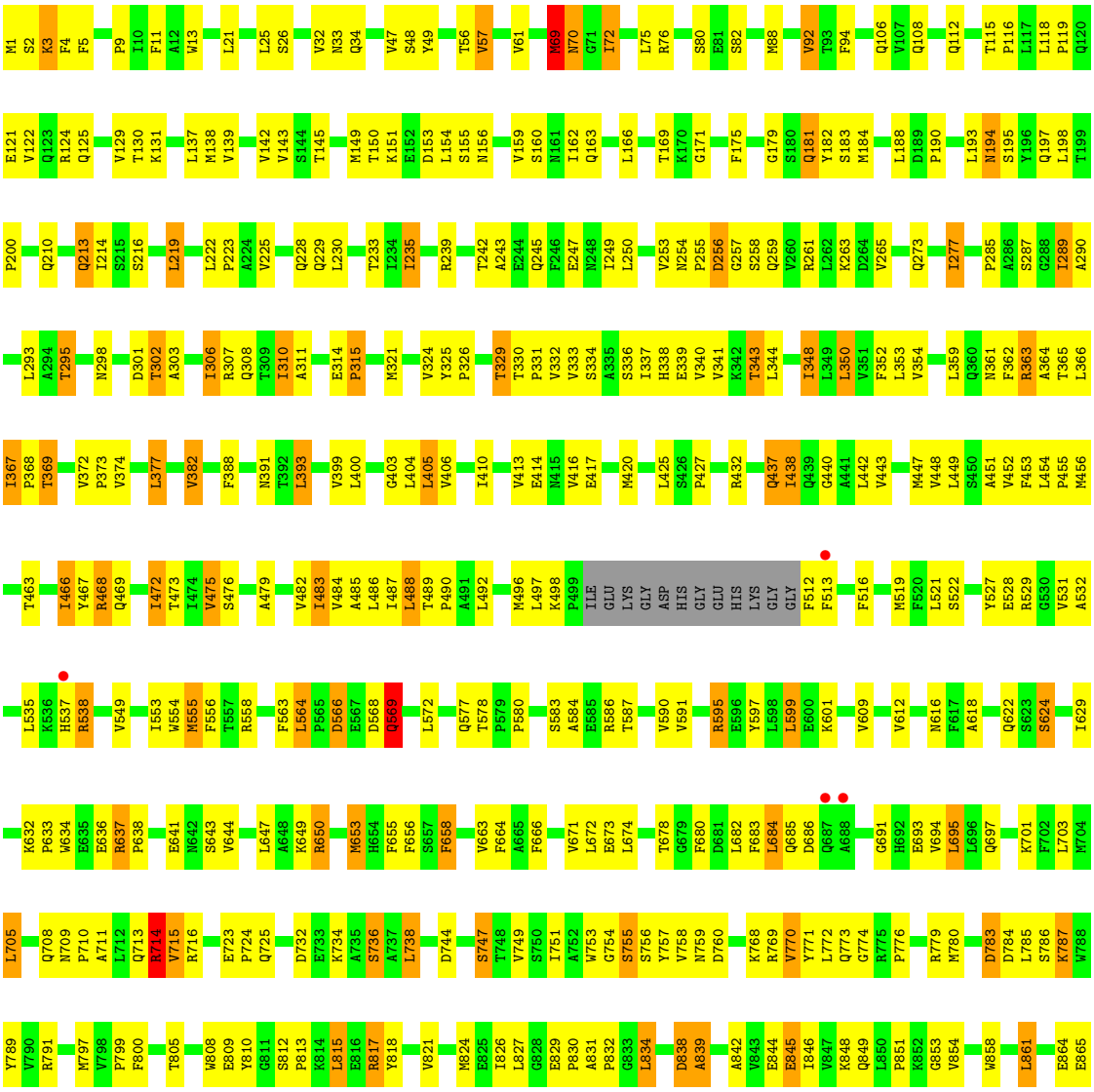
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			49	31	11	6	1		
3	E	1	Total	C	N	O	S	0	0
			49	31	11	6	1		

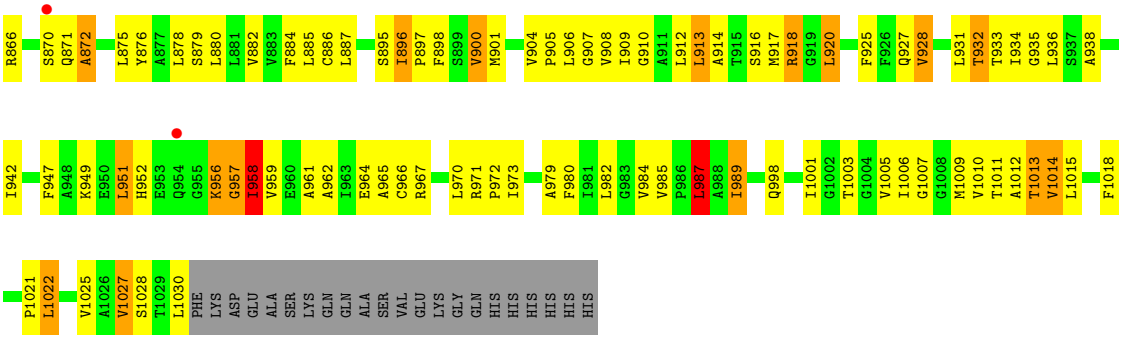
3 Residue-property plots (i)

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

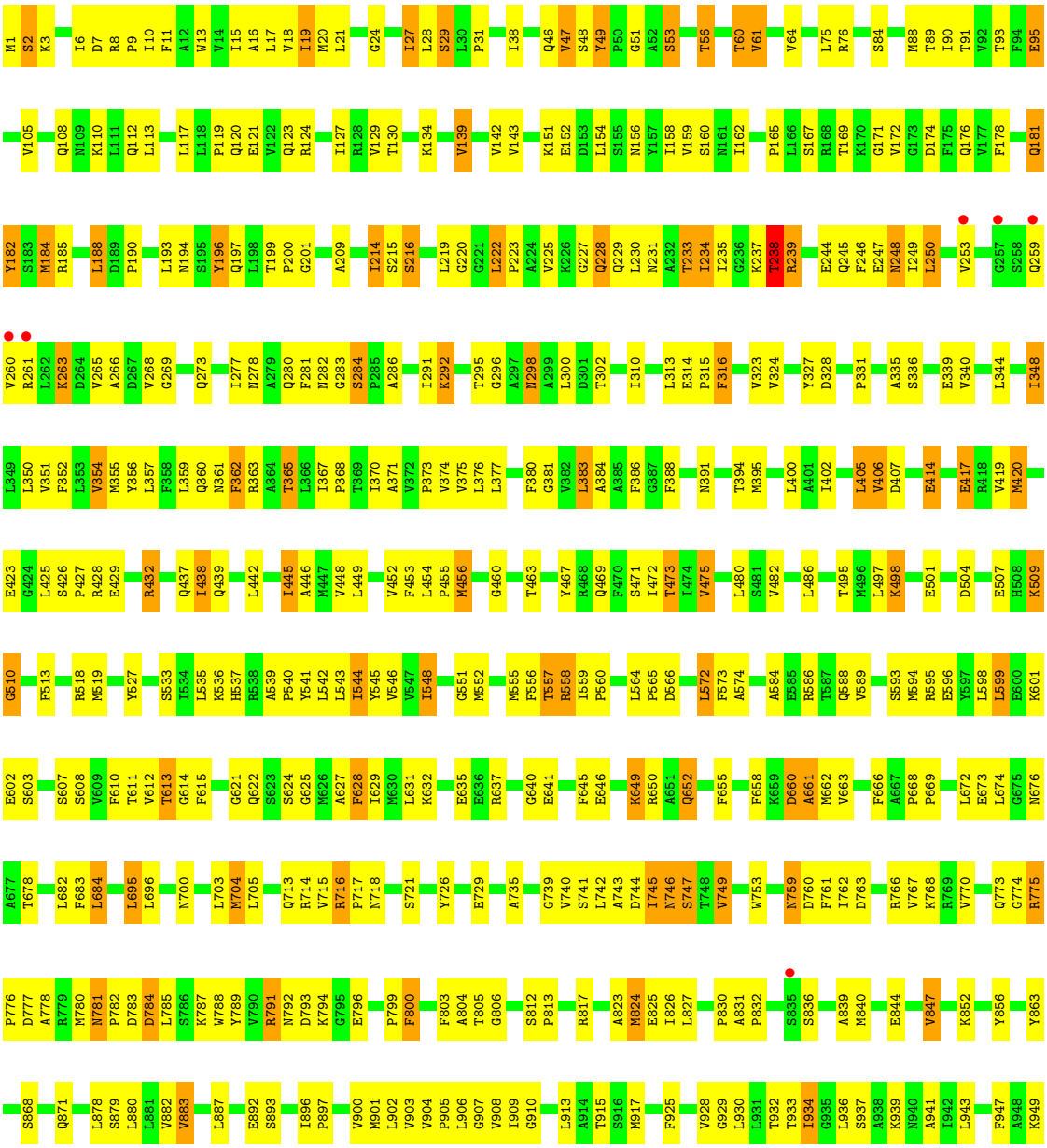
Chain A:

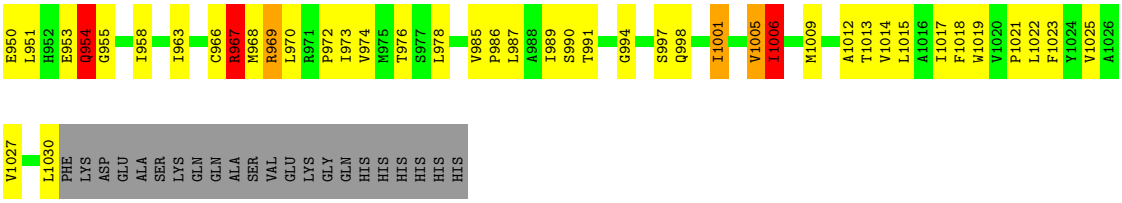




• Molecule 1: Multidrug resistance protein MexB

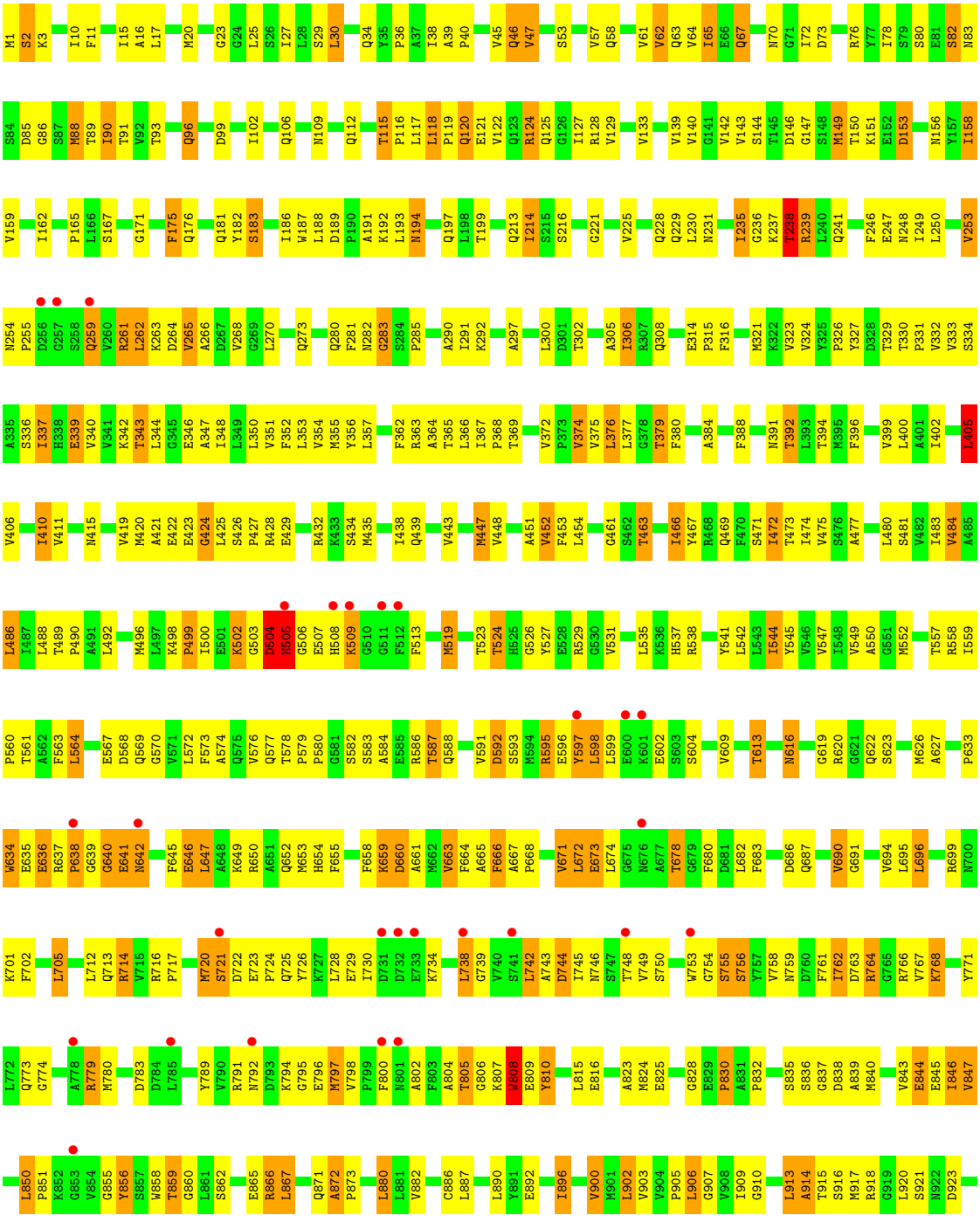
Chain B:

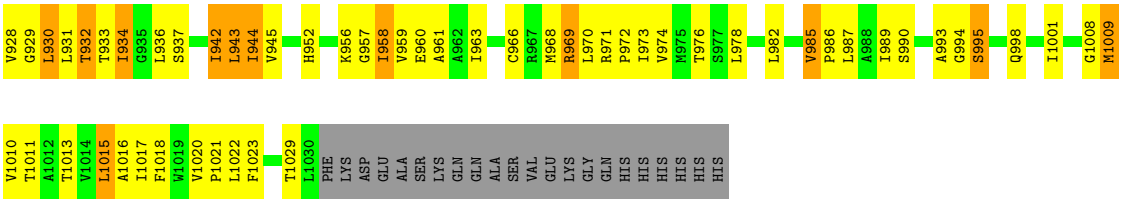




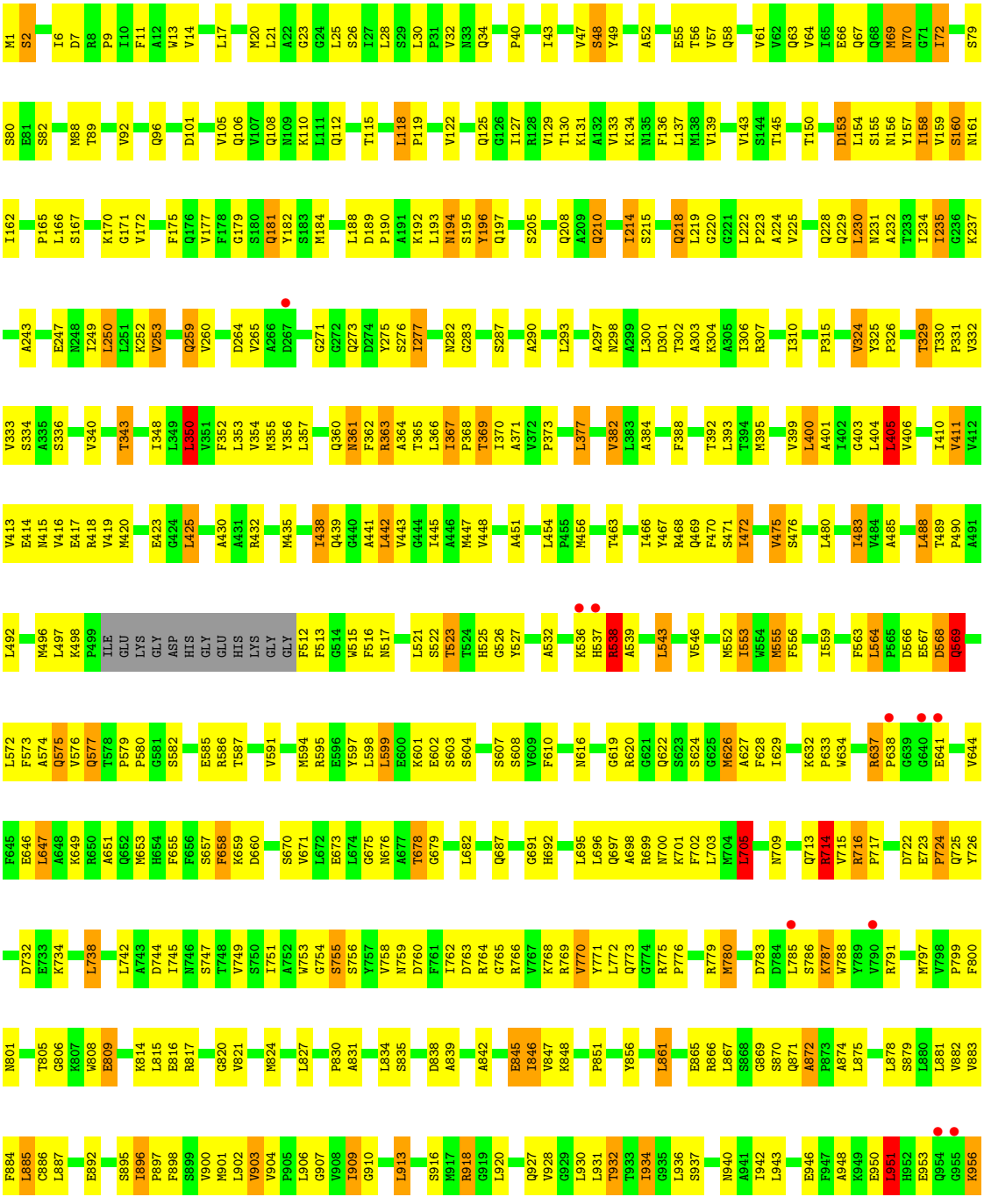
• Molecule 1: Multidrug resistance protein MexB

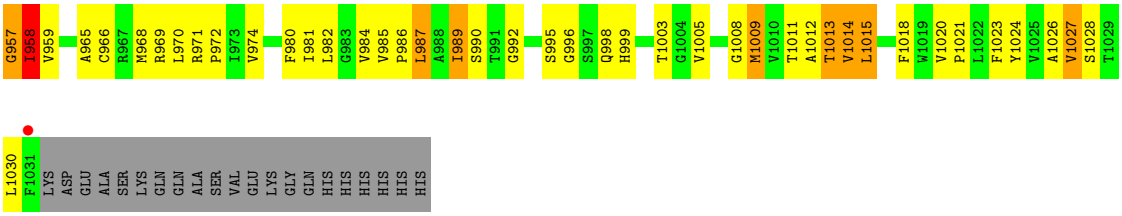
Chain C:





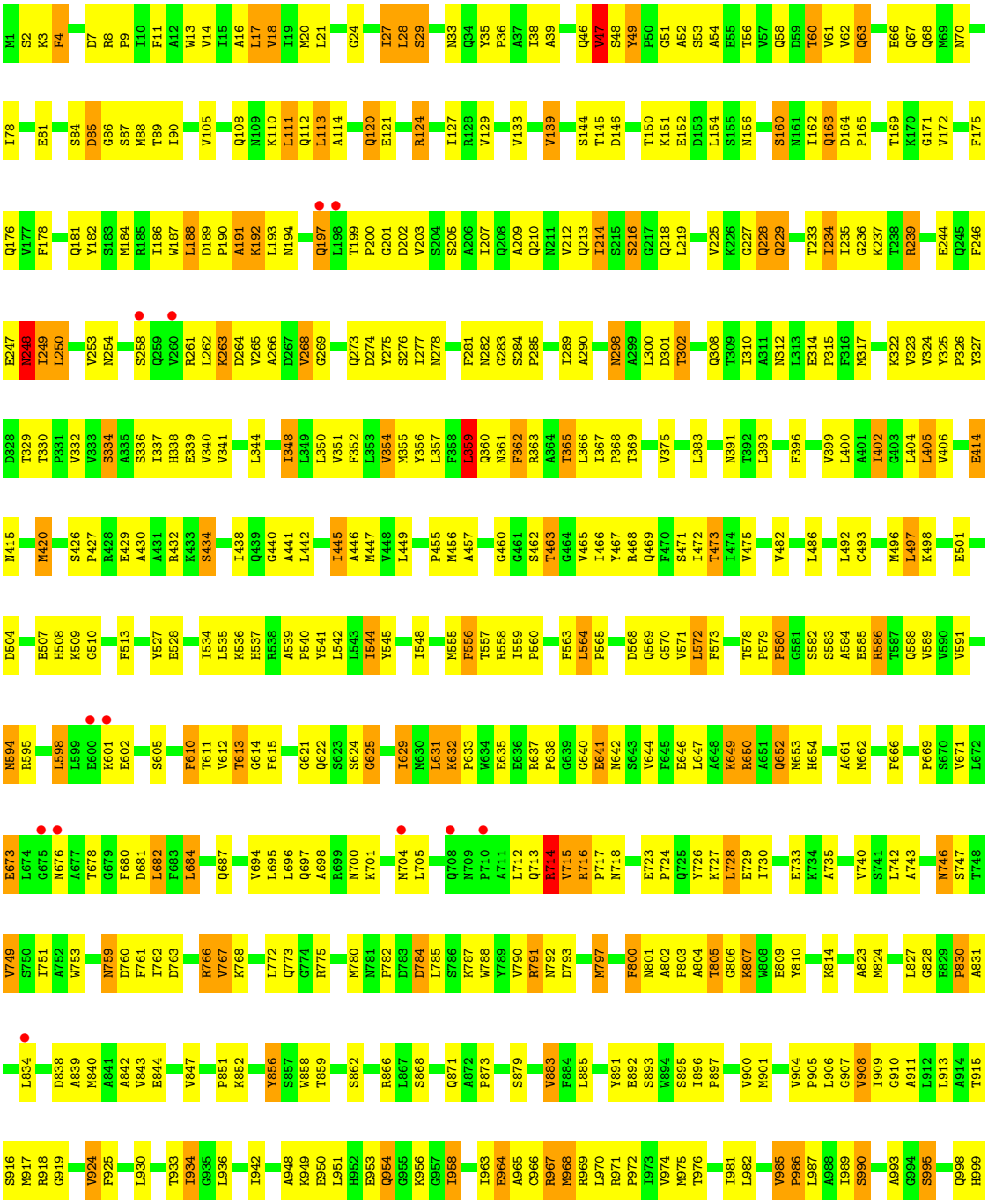
• Molecule 1: Multidrug resistance protein MexB

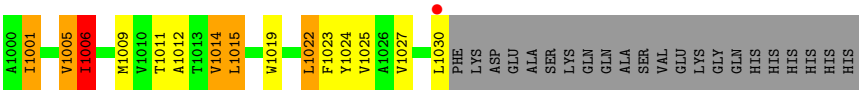




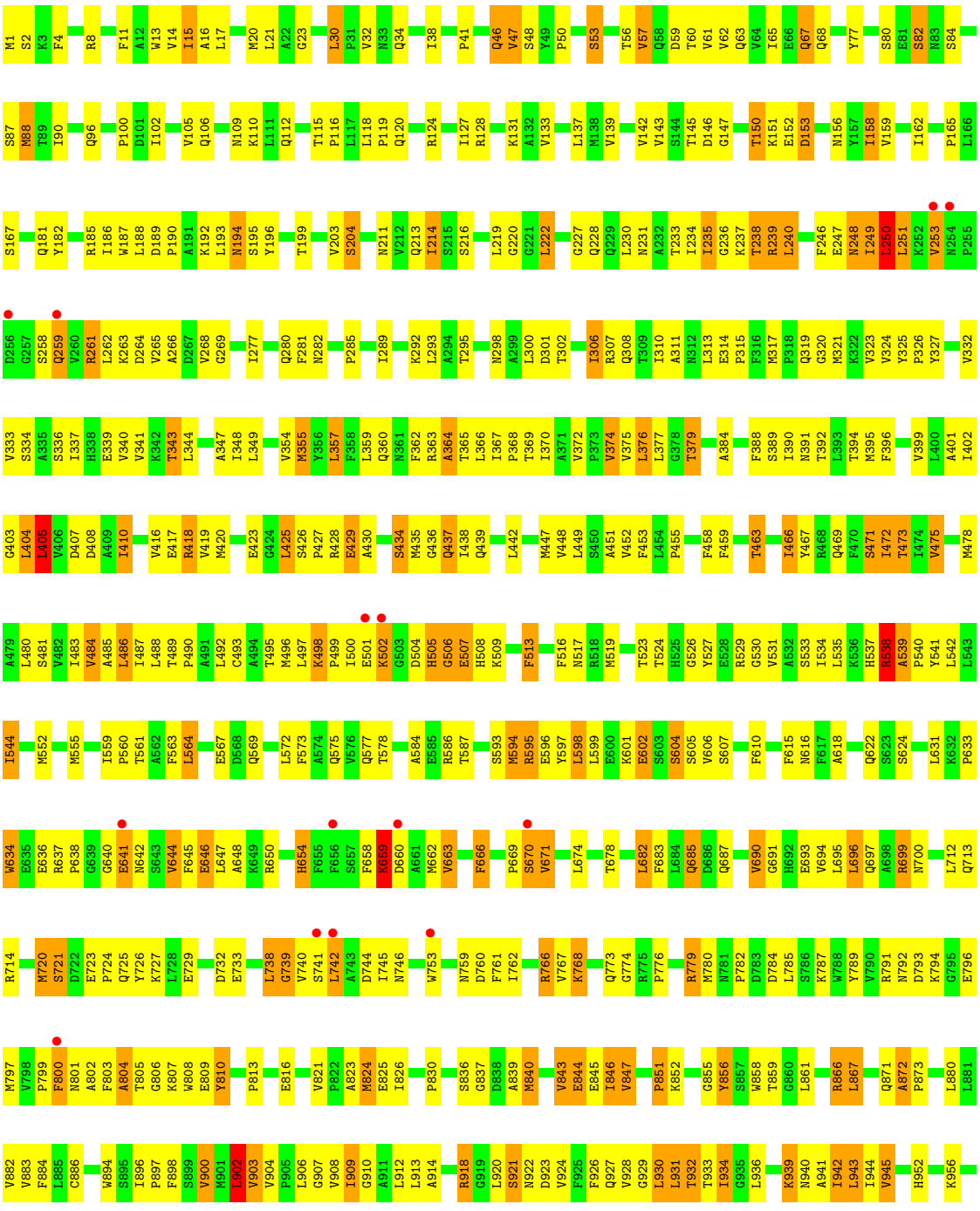
• Molecule 1: Multidrug resistance protein MexB

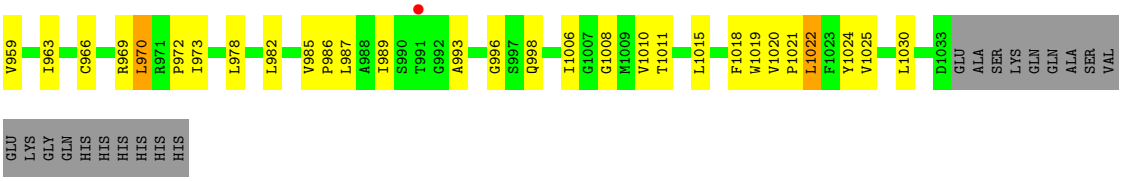
Chain E:





• Molecule 1: Multidrug resistance protein MexB




V959
I963
C966
R969
L970
R971
P972
I973
L978
L982
V985
P986
L987
A988
I989
S990
T991
G992
A993
G996
S997
Q998
I1006
G1007
G1008
M1009
V1010
T1011
L1015
F1018
W1019
V1020
P1021
L1022
F1023
Y1024
V1025
L1030
D1033
GLU
ALA
SER
LYS
GLN
GLN
ALA
SER
VAL
GLU
LYS
GLY
GLN
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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	126.20Å 137.03Å 152.28Å 85.75° 68.93° 87.39°	Depositor
Resolution (Å)	42.19 – 3.15 42.19 – 3.15	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.19-3.15) 97.4 (42.19-3.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.279 0.202 , 0.279	Depositor DCC
R_{free} test set	7980 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	80.1	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	47358	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: P9D, LMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.55	0/7880	0.81	4/10712 (0.0%)
1	B	0.54	0/7971	0.79	0/10833
1	C	0.51	0/7971	0.78	3/10833 (0.0%)
1	D	0.52	0/7892	0.79	6/10728 (0.1%)
1	E	0.53	0/7971	0.79	3/10833 (0.0%)
1	F	0.53	0/8000	0.80	6/10871 (0.1%)
All	All	0.53	0/47685	0.79	22/64810 (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
1	D	0	2
All	All	0	3

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	405	LEU	CA-CB-CG	8.26	134.30	115.30
1	D	705	LEU	CA-CB-CG	7.54	132.64	115.30
1	E	359	LEU	CA-CB-CG	7.48	132.51	115.30
1	D	405	LEU	CA-CB-CG	7.38	132.28	115.30
1	A	393	LEU	CA-CB-CG	-7.24	98.65	115.30
1	D	218	GLN	CB-CA-C	7.17	124.74	110.40
1	E	28	LEU	CA-CB-CG	6.52	130.30	115.30
1	F	405	LEU	CA-CB-CG	6.47	130.17	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	539	ALA	C-N-CD	-6.32	106.69	120.60
1	F	250	LEU	CA-CB-CG	6.30	129.79	115.30
1	C	867	LEU	CA-CB-CG	5.95	128.98	115.30
1	F	867	LEU	CA-CB-CG	5.88	128.83	115.30
1	A	987	LEU	CA-CB-CG	5.79	128.62	115.30
1	F	931	LEU	CB-CG-CD1	-5.42	101.78	111.00
1	D	350	LEU	CA-CB-CG	5.40	127.72	115.30
1	D	867	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	405	LEU	CA-CB-CG	5.39	127.70	115.30
1	C	262	LEU	CA-CB-CG	5.17	127.19	115.30
1	D	987	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	1022	LEU	CA-CB-CG	5.14	127.13	115.30
1	E	47	VAL	CB-CA-C	-5.11	101.69	111.40
1	F	539	ALA	C-N-CA	5.11	143.45	122.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	951	LEU	Peptide
1	D	691	GLY	Peptide
1	D	951	LEU	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	7724	0	7864	375	0
1	B	7812	0	7944	395	0
1	C	7812	0	7944	484	0
1	D	7735	0	7873	417	0
1	E	7812	0	7944	421	0
1	F	7840	0	7970	439	0
2	A	105	0	138	6	0
2	B	105	0	138	5	0
2	C	35	0	46	6	0
2	D	105	0	138	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	105	0	138	10	0
2	F	70	0	92	7	0
3	B	49	0	39	8	0
3	E	49	0	39	8	0
All	All	47358	0	48307	2452	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 26.

All (2452) 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:D:780:MET:CE	1:F:220:GLY:HA2	1.75	1.17
1:E:958:ILE:HD12	1:E:958:ILE:H	1.11	1.10
1:F:239:ARG:HG2	1:F:239:ARG:HH11	1.11	1.10
1:B:469:GLN:O	1:B:473:THR:HG22	1.52	1.10
1:C:239:ARG:HG2	1:C:239:ARG:HH11	0.96	1.09
1:C:261:ARG:HG2	1:C:261:ARG:HH11	1.12	1.08
3:E:2001:P9D:H37	3:E:2001:P9D:C25	1.79	1.07
1:F:524:THR:HG22	1:F:970:LEU:HD12	1.37	1.06
1:D:367:ILE:HG13	1:D:368:PRO:HD3	1.11	1.06
1:A:56:THR:HG23	1:C:213:GLN:HG2	1.09	1.05
1:A:749:VAL:HG22	1:A:753:TRP:CZ3	1.93	1.04
1:E:652:GLN:HA	1:E:652:GLN:HE21	1.17	1.04
1:F:910:GLY:HA3	1:F:1011:THR:HG21	1.37	1.04
1:A:966:CYS:SG	1:A:1021:PRO:HG3	1.99	1.03
1:C:340:VAL:HA	1:C:343:THR:HG23	1.40	1.03
1:E:985:VAL:HG12	1:E:986:PRO:HD3	1.39	1.03
1:C:193:LEU:HD12	1:C:265:VAL:HG12	1.39	1.03
1:C:542:LEU:HD12	1:C:1022:LEU:HD11	1.37	1.03
1:C:723:GLU:O	1:C:810:TYR:HB2	1.59	1.02
1:A:749:VAL:HG22	1:A:753:TRP:HZ3	1.21	1.02
1:A:845:GLU:O	1:A:848:LYS:HG2	1.60	1.01
1:E:469:GLN:O	1:E:473:THR:HG22	1.60	1.01
1:E:228:GLN:HE22	1:F:622:GLN:HE22	1.09	1.00
1:E:1006:ILE:HA	1:E:1009:MET:HB2	1.40	1.00
1:E:375:VAL:HG11	1:E:405:LEU:HD11	1.43	1.00
1:F:211:ASN:HA	1:F:240:LEU:HD13	1.44	1.00
2:F:2001:LMT:H4'	2:F:2001:LMT:O2B	1.63	0.99
1:D:845:GLU:OE1	1:D:845:GLU:HA	1.61	0.99
1:A:34:GLN:HG3	1:A:333:VAL:HG12	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:ILE:HG13	1:D:368:PRO:CD	1.93	0.99
1:C:542:LEU:CD1	1:C:1022:LEU:HD11	1.93	0.98
1:D:574:ALA:HB3	1:D:627:ALA:HB3	1.46	0.98
1:E:156:ASN:ND2	1:E:182:TYR:H	1.61	0.98
1:F:542:LEU:HD12	1:F:1022:LEU:HD11	1.45	0.97
1:C:40:PRO:HD3	1:C:96:GLN:HE22	1.28	0.97
1:C:142:VAL:HG21	1:C:321:MET:HE2	1.43	0.97
1:E:156:ASN:HD22	1:E:182:TYR:N	1.63	0.96
1:B:967:ARG:HG2	1:B:967:ARG:HH11	1.29	0.96
1:D:156:ASN:ND2	1:D:182:TYR:H	1.61	0.96
1:B:193:LEU:HD12	1:B:265:VAL:HG21	1.48	0.96
1:A:225:VAL:H	1:B:780:MET:HE2	1.28	0.96
1:E:156:ASN:HD22	1:E:182:TYR:H	1.13	0.95
2:F:2002:LMT:H3'	2:F:2002:LMT:O5B	1.64	0.95
1:D:369:THR:O	1:D:373:PRO:HD2	1.66	0.95
1:E:640:GLY:O	1:E:646:GLU:HG3	1.67	0.95
1:F:418:ARG:HH22	1:F:437:GLN:HE22	1.14	0.94
1:A:684:LEU:HD22	1:A:826:ILE:HD11	1.48	0.94
1:C:194:ASN:HB2	1:C:797:MET:HG2	1.49	0.94
1:A:56:THR:HG23	1:C:213:GLN:CG	1.98	0.93
1:C:239:ARG:HG2	1:C:239:ARG:NH1	1.71	0.93
1:F:910:GLY:HA3	1:F:1011:THR:CG2	1.98	0.93
1:A:210:GLN:HE22	1:A:250:LEU:H	0.97	0.93
1:C:197:GLN:O	1:C:791:ARG:HD3	1.68	0.92
1:E:791:ARG:NH1	1:E:791:ARG:HB2	1.83	0.92
1:C:918:ARG:HG3	1:C:918:ARG:O	1.69	0.92
1:F:723:GLU:O	1:F:810:TYR:HB2	1.69	0.92
1:E:162:ILE:O	1:E:165:PRO:HD2	1.69	0.92
1:B:1023:PHE:O	1:B:1027:VAL:HG23	1.69	0.92
1:F:908:VAL:HG13	1:F:930:LEU:HD21	1.50	0.92
1:A:684:LEU:CD2	1:A:826:ILE:HD11	1.98	0.92
1:B:1006:ILE:HA	1:B:1009:MET:HB2	1.50	0.92
1:D:283:GLY:HA2	1:D:595:ARG:NH1	1.83	0.92
1:B:129:VAL:H	1:C:112:GLN:HE22	1.15	0.91
1:C:340:VAL:HA	1:C:343:THR:CG2	1.98	0.91
1:D:343:THR:HG21	1:D:998:GLN:HE22	1.32	0.91
1:F:261:ARG:HG2	1:F:261:ARG:HH11	1.31	0.91
1:A:367:ILE:HG13	1:A:368:PRO:HD3	1.52	0.91
1:C:57:VAL:HG12	1:C:82:SER:HB3	1.52	0.91
1:E:193:LEU:CD1	1:E:265:VAL:HG21	2.00	0.90
1:A:210:GLN:HE22	1:A:250:LEU:N	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLN:HG2	1:C:586:ARG:HH21	1.33	0.90
1:A:987:LEU:HB2	1:A:998:GLN:HE21	1.35	0.90
1:D:918:ARG:HE	1:D:1003:THR:HG21	1.37	0.90
1:E:455:PRO:HG2	1:E:879:SER:HB2	1.51	0.90
1:F:469:GLN:O	1:F:473:THR:HG22	1.72	0.90
1:B:594:MET:HA	1:B:655:PHE:HZ	1.38	0.89
1:E:958:ILE:HD12	1:E:958:ILE:N	1.86	0.89
1:E:958:ILE:H	1:E:958:ILE:CD1	1.83	0.89
1:F:47:VAL:HG13	1:F:127:ILE:HA	1.53	0.89
1:D:156:ASN:HD22	1:D:182:TYR:H	1.07	0.89
1:B:156:ASN:HD22	1:B:182:TYR:H	1.19	0.89
1:E:556:PHE:O	1:E:559:ILE:HG22	1.72	0.89
1:F:156:ASN:ND2	1:F:182:TYR:H	1.70	0.89
1:A:684:LEU:HD22	1:A:826:ILE:CD1	2.02	0.88
1:B:228:GLN:HE22	1:C:622:GLN:HE22	1.20	0.88
1:C:830:PRO:HB3	1:C:839:ALA:HB2	1.54	0.88
1:D:537:HIS:O	1:D:538:ARG:HB2	1.69	0.88
1:F:57:VAL:HG12	1:F:82:SER:HB3	1.55	0.88
1:C:253:VAL:HG13	1:C:259:GLN:HB3	1.54	0.88
1:E:129:VAL:H	1:F:112:GLN:HE22	1.20	0.88
1:B:507:GLU:HB3	1:B:518:ARG:HG3	1.54	0.88
1:D:780:MET:HB3	1:F:228:GLN:NE2	1.88	0.87
1:A:156:ASN:ND2	1:A:182:TYR:H	1.72	0.87
1:E:308:GLN:HE21	1:E:312:ASN:HD21	1.20	0.87
1:F:690:VAL:HG22	1:F:694:VAL:HG21	1.55	0.87
1:F:239:ARG:HG2	1:F:239:ARG:NH1	1.88	0.87
1:B:985:VAL:HG12	1:B:986:PRO:HD3	1.53	0.87
1:E:440:GLY:HA3	2:E:2002:LMT:O2'	1.75	0.87
1:F:507:GLU:HG3	1:F:509:LYS:HB2	1.57	0.86
1:C:928:VAL:O	1:C:932:THR:HG22	1.75	0.86
1:E:746:ASN:HA	1:E:749:VAL:HG23	1.57	0.86
1:A:138:MET:SD	1:A:306:ILE:HD11	2.16	0.86
1:D:160:SER:HB3	1:D:766:ARG:HD3	1.58	0.86
1:E:139:VAL:HG13	1:E:327:TYR:HB3	1.55	0.86
1:C:1011:THR:O	1:C:1015:LEU:HB2	1.76	0.86
1:C:142:VAL:HG21	1:C:321:MET:CE	2.06	0.86
1:C:261:ARG:HG2	1:C:261:ARG:NH1	1.90	0.86
1:E:254:ASN:HB2	1:E:258:SER:OG	1.76	0.86
1:A:485:ALA:O	1:A:490:PRO:HD3	1.76	0.85
1:C:402:ILE:HA	1:C:405:LEU:HD13	1.57	0.85
1:F:933:THR:HA	1:F:936:LEU:HD12	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ASP:HB3	1:A:634:TRP:CH2	2.11	0.85
1:D:69:MET:O	1:D:70:ASN:O	1.94	0.85
1:B:640:GLY:O	1:B:646:GLU:HG3	1.77	0.85
1:D:780:MET:HE3	1:F:220:GLY:HA2	1.59	0.85
1:E:441:ALA:O	1:E:445:ILE:HG23	1.77	0.85
1:F:800:PHE:O	1:F:804:ALA:HB2	1.76	0.85
1:A:2:SER:HB3	1:A:486:LEU:O	1.77	0.84
1:B:193:LEU:HD12	1:B:265:VAL:CG2	2.08	0.84
1:C:729:GLU:HB3	1:C:805:THR:HB	1.57	0.84
1:F:80:SER:HB3	1:F:90:ILE:HG13	1.58	0.84
1:B:56:THR:O	1:B:60:THR:HB	1.76	0.84
1:A:310:ILE:HD11	1:A:325:TYR:OH	1.78	0.84
1:B:594:MET:HA	1:B:655:PHE:CZ	2.12	0.84
1:A:156:ASN:HD22	1:A:182:TYR:H	1.26	0.83
1:A:210:GLN:NE2	1:A:250:LEU:H	1.76	0.83
1:F:931:LEU:HA	1:F:934:ILE:HG23	1.60	0.83
1:E:277:ILE:HG21	3:E:2001:P9D:H25	1.60	0.83
1:F:910:GLY:CA	1:F:1011:THR:HG21	2.06	0.83
1:F:402:ILE:HD12	1:F:403:GLY:N	1.94	0.83
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.59	0.83
1:B:791:ARG:HH11	1:B:791:ARG:HG3	1.43	0.83
1:E:193:LEU:HD13	1:E:265:VAL:HG21	1.58	0.83
1:B:718:ASN:HB2	1:B:827:LEU:CD1	2.07	0.83
1:D:845:GLU:O	1:D:848:LYS:HG2	1.77	0.83
1:D:568:ASP:HB3	1:D:634:TRP:CH2	2.14	0.83
1:A:367:ILE:HD11	1:A:413:VAL:CG2	2.10	0.82
1:D:356:TYR:CE1	1:D:513:PHE:HZ	1.96	0.82
1:D:448:VAL:HG22	1:D:886:CYS:HB3	1.62	0.82
1:B:184:MET:HB2	1:B:761:PHE:CE1	2.16	0.81
1:A:705:LEU:HD13	1:A:846:ILE:HG23	1.63	0.81
1:C:541:TYR:HA	1:C:544:ILE:HG23	1.61	0.81
1:F:402:ILE:HA	1:F:405:LEU:HD13	1.61	0.81
1:A:302:THR:O	1:A:306:ILE:HG23	1.80	0.81
1:B:761:PHE:CE2	1:B:763:ASP:HB2	2.16	0.81
1:B:277:ILE:HG21	3:B:2001:P9D:H25	1.63	0.81
1:B:753:TRP:CH2	1:B:785:LEU:HD22	2.16	0.81
3:E:2001:P9D:C25	3:E:2001:P9D:C37	2.58	0.81
1:C:942:ILE:HA	1:C:945:VAL:HG12	1.62	0.81
1:E:199:THR:O	1:E:202:ASP:HB2	1.81	0.80
1:A:705:LEU:CD1	1:A:846:ILE:HG23	2.12	0.80
1:C:638:PRO:HD2	1:C:642:ASN:HD22	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:559:ILE:HG13	1:E:560:PRO:HD2	1.64	0.80
1:B:229:GLN:HG2	1:C:586:ARG:NH2	1.96	0.80
1:D:108:GLN:HE21	1:E:112:GLN:HE21	1.29	0.80
1:D:115:THR:HA	1:D:118:LEU:CD2	2.11	0.80
1:F:539:ALA:HB2	1:F:542:LEU:HB2	1.61	0.80
1:D:72:ILE:HG22	1:D:106:GLN:HB3	1.64	0.80
1:C:910:GLY:HA3	1:C:1011:THR:HG21	1.63	0.80
1:D:423:GLU:HB3	1:D:425:LEU:CD1	2.12	0.80
1:A:708:GLN:HE22	1:D:809:GLU:HG3	1.46	0.79
1:D:713:GLN:HG2	1:D:714:ARG:HG3	1.64	0.79
1:C:690:VAL:HG22	1:C:694:VAL:HG21	1.63	0.79
1:E:605:SER:O	1:E:632:LYS:HG2	1.81	0.79
1:C:40:PRO:HD3	1:C:96:GLN:NE2	1.97	0.79
1:D:156:ASN:HD22	1:D:182:TYR:N	1.80	0.79
1:A:468:ARG:O	1:A:469:GLN:HB2	1.83	0.79
1:E:281:PHE:CE2	1:E:324:VAL:HG11	2.17	0.79
1:B:767:VAL:HG11	1:C:119:PRO:HD3	1.63	0.79
1:B:469:GLN:O	1:B:473:THR:CG2	2.30	0.79
1:B:584:ALA:H	1:B:622:GLN:HG2	1.47	0.79
1:F:469:GLN:O	1:F:473:THR:CG2	2.31	0.79
1:B:966:CYS:O	1:B:967:ARG:CB	2.29	0.79
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.65	0.78
1:C:247:GLU:HG2	1:C:263:LYS:HB3	1.65	0.78
1:C:187:TRP:O	1:C:266:ALA:HB1	1.82	0.78
1:B:407:ASP:OD1	1:B:976:THR:HG21	1.83	0.78
1:B:344:LEU:O	1:B:348:ILE:HG23	1.83	0.78
1:C:661:ALA:O	1:C:663:VAL:HG23	1.83	0.78
1:F:593:SER:HG	1:F:658:PHE:HE1	1.32	0.78
1:F:247:GLU:HG2	1:F:263:LYS:HB3	1.64	0.78
1:C:695:LEU:HD23	1:C:824:MET:SD	2.23	0.78
1:E:652:GLN:HA	1:E:652:GLN:NE2	1.98	0.78
1:C:471:SER:O	1:C:475:VAL:HG13	1.84	0.78
1:B:735:ALA:O	1:B:740:VAL:HG12	1.85	0.77
1:C:61:VAL:HG23	1:C:62:VAL:H	1.50	0.77
1:E:967:ARG:HG2	1:E:967:ARG:HH11	1.48	0.77
1:B:966:CYS:O	1:B:967:ARG:HB3	1.84	0.77
1:C:507:GLU:HG3	1:C:509:LYS:H	1.50	0.77
1:E:989:ILE:O	1:E:989:ILE:HG22	1.85	0.77
1:E:791:ARG:HH11	1:E:791:ARG:CG	1.98	0.77
1:A:987:LEU:HB2	1:A:998:GLN:NE2	1.99	0.77
1:B:541:TYR:HA	1:B:544:ILE:HG23	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:GLY:HA3	1:D:302:THR:HG21	1.67	0.77
1:F:247:GLU:CG	1:F:263:LYS:HB3	2.15	0.77
1:D:575:GLN:HG2	1:D:616:ASN:OD1	1.83	0.76
1:E:695:LEU:HD11	1:E:824:MET:HG3	1.67	0.76
1:A:363:ARG:HD3	1:A:496:MET:O	1.85	0.76
1:A:416:VAL:O	1:A:420:MET:HB2	1.85	0.76
1:A:403:GLY:HA3	1:A:980:PHE:HD1	1.50	0.76
1:E:713:GLN:HG2	1:E:714:ARG:N	2.01	0.76
1:C:910:GLY:HA3	1:C:1011:THR:CG2	2.16	0.76
1:E:624:SER:O	1:E:625:GLY:O	2.03	0.76
1:B:541:TYR:HA	1:B:544:ILE:CG2	2.16	0.76
1:E:746:ASN:HA	1:E:749:VAL:CG2	2.16	0.76
1:B:967:ARG:HG2	1:B:967:ARG:NH1	1.91	0.76
1:D:451:ALA:HB1	1:D:882:VAL:HG12	1.66	0.76
1:D:780:MET:HE1	1:F:220:GLY:HA2	1.65	0.76
1:B:972:PRO:O	1:B:976:THR:HG22	1.84	0.76
1:C:989:ILE:HD12	1:C:989:ILE:O	1.86	0.76
1:C:121:GLU:HA	1:C:124:ARG:HH21	1.51	0.76
1:C:602:GLU:HG2	1:C:650:ARG:NH1	2.01	0.75
1:E:63:GLN:O	1:E:67:GLN:HG3	1.86	0.75
1:E:330:THR:O	1:E:334:SER:HB2	1.85	0.75
1:A:362:PHE:O	1:A:363:ARG:HB2	1.84	0.75
1:E:414:GLU:HG2	1:E:972:PRO:HB3	1.67	0.75
1:A:188:LEU:HD11	1:A:772:LEU:HD11	1.68	0.75
1:B:559:ILE:HD11	1:B:915:THR:HG22	1.67	0.75
1:D:82:SER:O	1:D:814:LYS:HA	1.87	0.75
1:F:156:ASN:HD22	1:F:182:TYR:H	1.35	0.75
1:D:472:ILE:H	1:D:475:VAL:HG13	1.52	0.75
1:E:53:SER:OG	1:E:56:THR:HG23	1.86	0.75
1:F:944:ILE:HG23	1:F:973:ILE:HD11	1.68	0.75
1:B:28:LEU:HD12	1:B:28:LEU:O	1.86	0.75
1:B:414:GLU:HG2	1:B:972:PRO:HB3	1.69	0.75
1:E:1005:VAL:HG23	1:E:1006:ILE:HG23	1.66	0.75
1:F:985:VAL:O	1:F:989:ILE:HG13	1.85	0.75
1:D:918:ARG:HH21	1:D:1003:THR:HG23	1.51	0.75
1:F:253:VAL:HG12	1:F:259:GLN:HB3	1.69	0.75
1:B:174:ASP:O	1:B:292:LYS:HB2	1.87	0.74
1:D:360:GLN:HG2	1:D:513:PHE:CD1	2.22	0.74
1:D:568:ASP:HB3	1:D:634:TRP:CZ3	2.22	0.74
1:D:830:PRO:HB3	1:D:839:ALA:HB2	1.67	0.74
1:B:129:VAL:N	1:C:112:GLN:HE22	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:TRP:HE1	1:C:993:ALA:HB2	1.52	0.74
1:C:726:TYR:CZ	1:C:806:GLY:HA3	2.21	0.74
1:E:652:GLN:HE21	1:E:652:GLN:CA	1.96	0.74
1:C:120:GLN:HA	1:C:120:GLN:HE21	1.53	0.74
1:D:866:ARG:HA	1:D:866:ARG:HE	1.52	0.74
1:A:732:ASP:O	1:A:736:SER:HB2	1.87	0.74
1:E:631:LEU:N	1:E:631:LEU:HD23	2.02	0.74
1:F:928:VAL:O	1:F:932:THR:HG22	1.88	0.74
1:E:375:VAL:CG1	1:E:405:LEU:HD11	2.18	0.74
1:D:416:VAL:O	1:D:420:MET:HB2	1.88	0.74
1:E:214:ILE:HG12	1:E:236:GLY:HA3	1.70	0.74
1:A:664:PHE:HE2	1:A:666:PHE:HB3	1.53	0.74
1:A:115:THR:HA	1:A:118:LEU:HD23	1.68	0.74
1:E:614:GLY:HA2	1:E:621:GLY:O	1.87	0.74
1:E:760:ASP:HB3	1:E:767:VAL:HG23	1.69	0.74
1:F:561:THR:HG22	1:F:922:ASN:HB3	1.68	0.74
1:D:115:THR:HA	1:D:118:LEU:HD23	1.69	0.73
1:E:28:LEU:O	1:E:29:SER:HB3	1.88	0.73
1:F:84:SER:OG	1:F:813:PRO:HA	1.88	0.73
1:E:193:LEU:HD12	1:E:265:VAL:HG21	1.70	0.73
1:A:377:LEU:HD13	2:A:2002:LMT:H101	1.69	0.73
1:B:310:ILE:CG2	1:B:323:VAL:HG21	2.19	0.73
1:D:388:PHE:HE2	1:D:472:ILE:HG12	1.51	0.73
1:F:944:ILE:HD11	1:F:1020:VAL:HB	1.70	0.73
1:A:451:ALA:HB1	1:A:882:VAL:CG1	2.19	0.73
1:F:332:VAL:O	1:F:336:SER:HB2	1.88	0.73
1:F:507:GLU:CG	1:F:509:LYS:HB2	2.18	0.73
1:D:423:GLU:HB3	1:D:425:LEU:HD13	1.70	0.73
1:E:791:ARG:HH11	1:E:791:ARG:HG3	1.53	0.73
1:D:356:TYR:HE1	1:D:513:PHE:HZ	1.37	0.73
1:E:985:VAL:HG12	1:E:986:PRO:CD	2.19	0.73
1:B:535:LEU:HD13	1:B:1025:VAL:HG21	1.69	0.73
1:B:718:ASN:HB2	1:B:827:LEU:HD13	1.70	0.73
1:F:776:PRO:O	1:F:780:MET:HG2	1.89	0.73
1:B:156:ASN:HD21	1:B:768:LYS:NZ	1.87	0.72
1:A:119:PRO:HG2	1:A:122:VAL:HG22	1.71	0.72
1:B:878:LEU:HD13	2:B:2004:LMT:H32	1.68	0.72
1:C:734:LYS:HG2	1:C:802:ALA:O	1.89	0.72
1:D:966:CYS:SG	1:D:1021:PRO:HG3	2.29	0.72
1:C:61:VAL:HG23	1:C:62:VAL:N	2.03	0.72
1:E:568:ASP:OD1	1:E:644:VAL:HG23	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:LEU:HD23	1:C:609:VAL:HG21	1.71	0.72
1:E:298:ASN:O	1:E:302:THR:HG23	1.90	0.72
1:F:690:VAL:HG13	1:F:691:GLY:H	1.53	0.72
1:E:612:VAL:HG11	1:E:615:PHE:HD2	1.53	0.72
1:E:649:LYS:HA	1:E:649:LYS:HE2	1.72	0.72
1:F:942:ILE:HA	1:F:945:VAL:HG12	1.71	0.72
1:C:944:ILE:HG22	1:C:973:ILE:HD11	1.72	0.72
1:F:402:ILE:HA	1:F:405:LEU:CD1	2.20	0.72
1:F:985:VAL:HG23	1:F:986:PRO:HD3	1.70	0.72
1:E:1011:THR:O	1:E:1015:LEU:HB2	1.90	0.72
1:F:779:ARG:HG2	1:F:779:ARG:HH11	1.54	0.72
1:E:228:GLN:NE2	1:F:622:GLN:HE22	1.87	0.71
1:F:343:THR:HG21	1:F:998:GLN:HE22	1.55	0.71
1:F:360:GLN:HE22	1:F:517:ASN:HD21	1.37	0.71
1:F:739:GLY:HA3	1:F:792:ASN:OD1	1.90	0.71
1:F:903:VAL:HG21	1:F:1020:VAL:HG22	1.71	0.71
1:A:909:ILE:HD12	1:A:910:GLY:H	1.55	0.71
1:A:918:ARG:HE	1:A:1003:THR:HG21	1.53	0.71
1:C:140:VAL:HG21	1:C:306:ILE:HD11	1.72	0.71
1:F:359:LEU:HD12	1:F:365:THR:HA	1.72	0.71
1:F:685:GLN:HE21	1:F:687:GLN:HE21	1.38	0.71
1:B:901:MET:O	1:B:904:VAL:HG23	1.89	0.71
1:D:903:VAL:HA	1:D:906:LEU:HD12	1.72	0.71
1:B:1009:MET:HE2	1:B:1009:MET:HA	1.73	0.71
1:E:583:SER:HA	1:E:622:GLN:HE21	1.55	0.71
1:B:228:GLN:NE2	1:C:622:GLN:HE22	1.89	0.71
1:B:209:ALA:HB1	1:C:742:LEU:HB3	1.72	0.71
1:D:759:ASN:O	1:D:770:VAL:HG13	1.91	0.71
1:A:131:LYS:O	1:A:295:THR:HG23	1.90	0.71
1:D:188:LEU:HD11	1:D:772:LEU:HD11	1.72	0.71
1:D:215:SER:HB2	1:E:51:GLY:O	1.91	0.71
1:E:192:LYS:HD2	1:E:264:ASP:O	1.90	0.71
1:B:958:ILE:HD12	1:B:958:ILE:H	1.55	0.70
1:C:302:THR:O	1:C:306:ILE:HG23	1.91	0.70
1:D:139:VAL:O	1:D:326:PRO:HD2	1.90	0.70
1:B:791:ARG:HH11	1:B:791:ARG:CG	2.04	0.70
1:C:690:VAL:HG13	1:C:691:GLY:H	1.55	0.70
1:D:34:GLN:HG3	1:D:333:VAL:HG12	1.73	0.70
1:A:568:ASP:HB3	1:A:634:TRP:HH2	1.55	0.70
1:C:724:PRO:HA	1:C:810:TYR:HB3	1.73	0.70
1:C:903:VAL:HG21	1:C:1020:VAL:HG22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:984:VAL:HG11	1:D:1005:VAL:CG2	2.21	0.70
1:E:535:LEU:HD22	1:E:1025:VAL:HG21	1.73	0.70
1:D:842:ALA:O	1:D:846:ILE:HG12	1.90	0.70
1:E:193:LEU:HD13	1:E:265:VAL:CG2	2.20	0.70
1:E:228:GLN:HE22	1:F:622:GLN:NE2	1.87	0.70
1:E:308:GLN:NE2	1:E:312:ASN:HD21	1.88	0.70
1:B:60:THR:HG22	1:B:61:VAL:HG12	1.74	0.70
1:B:753:TRP:CZ2	1:B:785:LEU:HD13	2.26	0.70
1:C:448:VAL:O	1:C:452:VAL:HG22	1.91	0.70
1:D:101:ASP:O	1:D:105:VAL:HG23	1.91	0.70
1:A:834:LEU:HB3	1:A:838:ASP:OD1	1.90	0.70
1:B:455:PRO:HG2	1:B:879:SER:HB2	1.74	0.70
1:C:635:GLU:HG3	1:C:636:GLU:HG3	1.74	0.70
1:C:45:VAL:O	1:C:88:MET:HE1	1.92	0.70
1:E:791:ARG:HB2	1:E:791:ARG:HH11	1.56	0.70
1:F:302:THR:O	1:F:306:ILE:HG23	1.92	0.70
1:F:453:PHE:HZ	1:F:932:THR:HB	1.56	0.70
1:F:631:LEU:HD11	1:F:644:VAL:HG23	1.74	0.70
1:A:367:ILE:HD11	1:A:413:VAL:HG21	1.72	0.70
1:B:602:GLU:OE2	1:B:650:ARG:HD2	1.92	0.70
1:E:344:LEU:HD23	1:E:402:ILE:HG13	1.74	0.69
1:A:365:THR:O	1:A:369:THR:HG23	1.91	0.69
1:D:568:ASP:O	1:D:569:GLN:HB2	1.89	0.69
1:E:904:VAL:HB	1:E:905:PRO:HD3	1.74	0.69
1:A:242:THR:OG1	1:A:245:GLN:HG3	1.93	0.69
1:A:361:ASN:HB3	1:A:364:ALA:HB3	1.74	0.69
1:C:354:VAL:HG11	1:C:978:LEU:HB3	1.74	0.69
1:D:951:LEU:O	1:D:956:LYS:HB2	1.91	0.69
1:F:843:VAL:HA	1:F:846:ILE:HG23	1.75	0.69
1:A:759:ASN:O	1:A:770:VAL:HG13	1.92	0.69
1:B:8:ARG:HH11	1:B:8:ARG:HG3	1.56	0.69
1:E:767:VAL:HG11	1:F:119:PRO:HD3	1.74	0.69
1:D:303:ALA:HB2	1:D:330:THR:HG21	1.72	0.69
1:F:425:LEU:HD22	1:F:429:GLU:HB3	1.74	0.69
1:A:568:ASP:HB3	1:A:634:TRP:CZ3	2.27	0.69
1:E:209:ALA:HB1	1:F:742:LEU:HB3	1.73	0.69
1:E:534:ILE:HG22	1:E:1022:LEU:HD23	1.74	0.69
1:C:602:GLU:HG2	1:C:650:ARG:HH11	1.56	0.69
1:E:239:ARG:HG2	1:E:239:ARG:HH11	1.56	0.69
1:A:753:TRP:CZ2	1:A:785:LEU:HG	2.27	0.69
1:B:612:VAL:HG11	1:B:615:PHE:HD2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:PHE:CE2	1:C:564:LEU:HD22	2.28	0.69
1:C:680:PHE:CD2	1:C:828:GLY:O	2.45	0.69
1:E:214:ILE:HA	1:F:746:ASN:HD21	1.58	0.69
1:A:845:GLU:OE1	1:A:845:GLU:HA	1.92	0.69
1:C:687:GLN:HE22	1:C:855:GLY:H	1.41	0.69
1:E:791:ARG:NH1	1:E:791:ARG:CB	2.55	0.69
1:D:698:ALA:HB2	1:D:851:PRO:HG2	1.75	0.68
1:A:339:GLU:O	1:A:343:THR:HG23	1.94	0.68
1:A:195:SER:O	1:A:197:GLN:NE2	2.23	0.68
1:B:761:PHE:HE2	1:B:763:ASP:HB2	1.57	0.68
1:E:950:GLU:HG2	2:E:2002:LMT:H4B	1.76	0.68
1:F:314:GLU:HA	1:F:317:MET:HG3	1.74	0.68
1:A:9:PRO:HD2	1:B:892:GLU:OE1	1.93	0.68
1:A:749:VAL:HG13	1:A:753:TRP:HE3	1.59	0.68
1:E:178:PHE:HA	3:E:2001:P9D:H26	1.74	0.68
1:F:641:GLU:HA	1:F:646:GLU:HG2	1.75	0.68
1:E:39:ALA:HB2	1:E:673:GLU:HG2	1.74	0.68
1:E:910:GLY:CA	1:E:1011:THR:HG21	2.23	0.68
1:A:479:ALA:O	1:A:482:VAL:HG22	1.94	0.68
1:B:557:THR:O	1:B:558:ARG:HG2	1.93	0.68
1:C:80:SER:HB3	1:C:90:ILE:HG23	1.76	0.68
1:D:361:ASN:HB3	1:D:364:ALA:HB3	1.75	0.68
1:D:367:ILE:CD1	1:D:489:THR:HG23	2.24	0.68
1:D:369:THR:O	1:D:373:PRO:CD	2.40	0.68
1:D:709:ASN:HD22	1:D:846:ILE:HD11	1.58	0.68
1:A:904:VAL:HB	1:A:905:PRO:HD3	1.76	0.67
1:B:794:LYS:HB3	1:B:796:GLU:OE1	1.93	0.67
1:C:426:SER:HB3	1:C:429:GLU:HB2	1.74	0.67
1:E:631:LEU:HD11	1:E:644:VAL:HG22	1.76	0.67
1:A:664:PHE:CE2	1:A:666:PHE:HB3	2.29	0.67
1:E:910:GLY:HA3	1:E:1011:THR:CG2	2.24	0.67
1:A:1:MET:O	1:A:4:PHE:HB3	1.95	0.67
1:A:156:ASN:HD21	1:A:768:LYS:NZ	1.92	0.67
1:C:726:TYR:OH	1:C:806:GLY:HA3	1.93	0.67
1:E:191:ALA:O	1:E:193:LEU:N	2.27	0.67
1:E:233:THR:HG23	1:F:725:GLN:HG2	1.75	0.67
1:C:156:ASN:ND2	1:C:182:TYR:H	1.93	0.67
1:D:713:GLN:HG2	1:D:714:ARG:N	2.09	0.67
3:E:2001:P9D:H37	3:E:2001:P9D:C26	2.25	0.67
1:C:47:VAL:HG13	1:C:127:ILE:HA	1.76	0.67
1:F:1020:VAL:HB	1:F:1021:PRO:HD3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:CD1	1:A:277:ILE:H	2.07	0.67
1:A:684:LEU:CD2	1:A:826:ILE:CD1	2.66	0.67
1:A:966:CYS:SG	1:A:1021:PRO:CG	2.81	0.67
1:B:310:ILE:HG21	1:B:323:VAL:HG21	1.76	0.67
1:B:559:ILE:HG13	1:B:560:PRO:HD2	1.77	0.67
1:B:682:LEU:CD2	1:B:826:ILE:HB	2.25	0.67
1:C:567:GLU:OE2	1:C:994:GLY:HA2	1.95	0.67
1:D:678:THR:HG22	1:D:679:GLY:H	1.59	0.67
1:F:402:ILE:HD12	1:F:403:GLY:H	1.59	0.67
1:C:236:GLY:O	1:C:238:THR:HG23	1.94	0.67
1:C:332:VAL:HG11	1:C:569:GLN:HE21	1.60	0.67
1:C:560:PRO:O	1:C:921:SER:HB2	1.94	0.67
1:D:119:PRO:HG2	1:D:122:VAL:HG22	1.77	0.67
1:E:718:ASN:HB2	1:E:827:LEU:HD13	1.75	0.67
1:D:861:LEU:HD22	1:D:861:LEU:H	1.60	0.67
1:E:700:ASN:O	1:E:704:MET:HG2	1.95	0.67
1:F:340:VAL:HA	1:F:343:THR:HG23	1.77	0.67
1:C:139:VAL:HG23	1:C:327:TYR:HB3	1.76	0.66
1:E:47:VAL:CG2	1:E:127:ILE:HG13	2.25	0.66
1:F:410:ILE:C	1:F:410:ILE:HD12	2.15	0.66
1:C:906:LEU:O	1:C:1011:THR:HG23	1.94	0.66
1:F:420:MET:SD	1:F:427:PRO:HA	2.35	0.66
1:E:447:MET:CE	2:E:2002:LMT:H72	2.25	0.66
1:E:791:ARG:HH11	1:E:791:ARG:CB	2.09	0.66
1:A:13:TRP:HE1	2:A:2003:LMT:H2O2	1.43	0.66
1:F:133:VAL:O	1:F:292:LYS:HE2	1.94	0.66
1:D:709:ASN:ND2	1:D:846:ILE:HD11	2.10	0.66
1:E:723:GLU:HB2	1:E:724:PRO:HD2	1.78	0.66
1:F:343:THR:HG21	1:F:998:GLN:NE2	2.11	0.66
1:A:159:VAL:HG11	1:A:181:GLN:HG2	1.77	0.66
1:A:854:VAL:O	1:A:854:VAL:HG12	1.94	0.66
1:F:560:PRO:HG2	1:F:921:SER:HB3	1.76	0.66
1:F:616:ASN:ND2	1:F:624:SER:HB2	2.11	0.66
1:A:791:ARG:HB2	1:A:797:MET:CE	2.26	0.66
1:C:420:MET:CE	1:C:500:ILE:HG22	2.26	0.66
1:C:726:TYR:HD1	1:C:808:TRP:HD1	1.43	0.66
1:D:1:MET:O	1:D:2:SER:HB2	1.94	0.66
1:E:966:CYS:O	1:E:967:ARG:CB	2.43	0.66
1:F:792:ASN:HB2	1:F:796:GLU:O	1.95	0.66
1:F:872:ALA:HB3	1:F:873:PRO:HD3	1.77	0.66
1:F:388:PHE:CZ	1:F:472:ILE:HG12	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:690:VAL:CG2	1:F:694:VAL:HG21	2.25	0.66
1:A:909:ILE:HD12	1:A:910:GLY:N	2.11	0.66
1:B:215:SER:HB3	1:C:750:SER:HB3	1.77	0.66
1:E:695:LEU:CD1	1:E:824:MET:HG3	2.25	0.66
1:E:951:LEU:HD11	1:E:968:MET:HE1	1.78	0.66
1:F:784:ASP:HA	1:F:787:LYS:HD3	1.76	0.66
1:D:403:GLY:HA3	1:D:980:PHE:HD1	1.60	0.66
1:C:792:ASN:HB2	1:C:796:GLU:O	1.96	0.65
1:E:186:ILE:CG2	1:E:772:LEU:HD12	2.26	0.65
1:F:527:TYR:CD2	1:F:970:LEU:HG	2.31	0.65
1:F:634:TRP:H	1:F:634:TRP:HE3	1.44	0.65
1:D:404:LEU:HD22	1:D:936:LEU:HD12	1.78	0.65
1:D:616:ASN:HA	1:D:626:MET:HG2	1.78	0.65
1:E:227:GLY:O	1:E:229:GLN:N	2.29	0.65
1:F:1:MET:O	1:F:4:PHE:HB3	1.96	0.65
1:F:194:ASN:C	1:F:196:TYR:H	2.00	0.65
1:A:2:SER:O	1:A:3:LYS:HB2	1.97	0.65
1:C:649:LYS:NZ	1:C:713:GLN:HE21	1.93	0.65
1:D:119:PRO:HG2	1:D:122:VAL:CG2	2.27	0.65
1:A:115:THR:HA	1:A:118:LEU:CD2	2.27	0.65
1:B:930:LEU:O	1:B:934:ILE:HG23	1.97	0.65
1:C:560:PRO:HG2	1:C:921:SER:HB3	1.79	0.65
1:A:2:SER:O	1:A:3:LYS:CB	2.45	0.65
1:B:879:SER:O	1:B:883:VAL:HG12	1.96	0.65
1:C:372:VAL:O	1:C:376:LEU:HB2	1.95	0.65
1:D:616:ASN:HB3	1:D:619:GLY:H	1.61	0.65
1:F:616:ASN:HD22	1:F:624:SER:HB2	1.60	0.65
1:A:749:VAL:HG13	1:A:753:TRP:CE3	2.31	0.65
1:E:541:TYR:HA	1:E:544:ILE:HG23	1.79	0.65
1:F:391:ASN:H	1:F:394:THR:CG2	2.09	0.65
1:F:723:GLU:O	1:F:810:TYR:CB	2.43	0.65
1:F:766:ARG:HG2	1:F:766:ARG:HH11	1.61	0.65
1:C:902:LEU:O	1:C:905:PRO:HD2	1.97	0.65
1:E:800:PHE:HD2	1:E:804:ALA:HB2	1.62	0.65
1:F:68:GLN:O	1:F:110:LYS:HD2	1.97	0.65
1:D:622:GLN:HB2	1:F:231:ASN:ND2	2.11	0.65
1:D:958:ILE:HG21	1:D:1028:SER:HB3	1.79	0.65
1:E:967:ARG:HG2	1:E:967:ARG:NH1	2.07	0.65
1:A:861:LEU:H	1:A:861:LEU:CD2	2.10	0.65
1:E:108:GLN:HB3	1:E:129:VAL:HG21	1.79	0.65
1:F:250:LEU:HB3	1:F:261:ARG:HH12	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:ASN:HA	1:B:749:VAL:HG22	1.79	0.64
1:D:861:LEU:H	1:D:861:LEU:CD2	2.11	0.64
1:F:418:ARG:HH22	1:F:437:GLN:NE2	1.91	0.64
1:D:228:GLN:NE2	1:D:229:GLN:H	1.94	0.64
1:D:456:MET:HE2	1:D:931:LEU:HD13	1.78	0.64
1:E:540:PRO:O	1:E:544:ILE:HG22	1.97	0.64
1:E:714:ARG:O	1:E:716:ARG:HD3	1.96	0.64
1:F:816:GLU:OE1	1:F:824:MET:HA	1.97	0.64
1:E:129:VAL:H	1:F:112:GLN:NE2	1.94	0.64
1:A:210:GLN:NE2	1:A:249:ILE:HA	2.12	0.64
1:A:780:MET:HB3	1:C:228:GLN:NE2	2.13	0.64
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.78	0.64
1:F:782:PRO:O	1:F:785:LEU:HG	1.98	0.64
1:A:655:PHE:HD2	1:A:658:PHE:HE2	1.46	0.64
1:C:552:MET:HB2	1:C:909:ILE:HG23	1.80	0.64
1:D:228:GLN:HE21	1:D:229:GLN:H	1.43	0.64
1:B:753:TRP:CZ2	1:B:785:LEU:HA	2.33	0.64
1:B:951:LEU:HD11	1:B:968:MET:HE1	1.79	0.64
1:C:761:PHE:CE1	1:C:763:ASP:HB2	2.32	0.64
1:C:931:LEU:HA	1:C:934:ILE:HG23	1.79	0.64
1:D:419:VAL:HG23	1:D:430:ALA:HB1	1.80	0.64
1:D:847:VAL:HG11	1:D:856:TYR:CD2	2.33	0.64
1:E:127:ILE:H	1:E:127:ILE:HD12	1.62	0.64
1:E:669:PRO:HG3	1:E:676:ASN:HA	1.79	0.64
1:A:188:LEU:CD1	1:A:772:LEU:HD11	2.27	0.64
1:C:362:PHE:O	1:C:364:ALA:N	2.26	0.64
1:D:189:ASP:HA	1:D:775:ARG:HD3	1.80	0.64
1:E:176:GLN:HB2	3:E:2001:P9D:H48A	1.79	0.64
1:E:966:CYS:O	1:E:967:ARG:HB3	1.98	0.64
1:F:337:ILE:HA	1:F:340:VAL:HG12	1.79	0.64
1:D:70:ASN:HB2	1:F:167:SER:HB2	1.79	0.64
1:E:298:ASN:C	1:E:298:ASN:HD22	2.01	0.64
1:D:13:TRP:HE1	2:D:2003:LMT:H2O2	1.45	0.64
1:D:907:GLY:CA	1:D:1012:ALA:HB2	2.28	0.64
1:B:171:GLY:HA3	1:B:302:THR:HG21	1.80	0.64
1:D:713:GLN:HG2	1:D:714:ARG:H	1.62	0.64
1:E:559:ILE:HD11	1:E:915:THR:HG22	1.78	0.64
1:B:354:VAL:HG11	1:B:978:LEU:HD22	1.80	0.63
1:C:61:VAL:CG2	1:C:62:VAL:H	2.11	0.63
1:A:108:GLN:NE2	1:B:113:LEU:HD13	2.13	0.63
1:C:420:MET:HE3	1:C:500:ILE:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:VAL:O	1:E:207:ILE:HG13	1.98	0.63
1:E:534:ILE:CG2	1:E:1022:LEU:HD23	2.28	0.63
1:F:944:ILE:CG2	1:F:973:ILE:HD11	2.29	0.63
1:B:156:ASN:HD22	1:B:182:TYR:N	1.93	0.63
1:B:555:MET:CE	1:B:913:LEU:HD12	2.28	0.63
1:C:96:GLN:HB2	1:C:461:GLY:HA2	1.80	0.63
1:C:167:SER:HB2	1:C:175:PHE:HE2	1.63	0.63
1:D:210:GLN:HE22	1:D:250:LEU:H	1.46	0.63
1:E:868:SER:HA	1:E:871:GLN:HE21	1.63	0.63
1:B:544:ILE:O	1:B:548:ILE:HG23	1.98	0.63
1:C:343:THR:HG21	1:C:998:GLN:NE2	2.14	0.63
1:C:944:ILE:HG22	1:C:973:ILE:CD1	2.29	0.63
1:F:314:GLU:N	1:F:315:PRO:HD2	2.14	0.63
1:A:472:ILE:H	1:A:475:VAL:HG13	1.63	0.63
1:C:563:PHE:O	1:C:923:ASP:HB2	1.98	0.63
1:D:150:THR:HG22	1:D:153:ASP:OD1	1.99	0.63
1:A:448:VAL:HG22	1:A:886:CYS:HB3	1.81	0.63
1:A:884:PHE:HB2	1:A:901:MET:CE	2.29	0.63
1:D:934:ILE:HD12	1:D:934:ILE:O	1.99	0.63
1:D:1009:MET:O	1:D:1013:THR:HG23	1.99	0.63
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.81	0.63
1:F:729:GLU:HB3	1:F:805:THR:HB	1.81	0.63
1:F:659:LYS:HG3	1:F:660:ASP:H	1.63	0.62
1:F:690:VAL:HG13	1:F:691:GLY:N	2.14	0.62
1:C:451:ALA:HB1	1:C:882:VAL:HG12	1.82	0.62
1:A:910:GLY:HA2	1:A:1011:THR:HG21	1.81	0.62
1:D:1009:MET:O	1:D:1013:THR:CG2	2.47	0.62
1:A:907:GLY:HA2	1:A:1012:ALA:HB2	1.81	0.62
1:B:214:ILE:HG23	1:B:237:LYS:H	1.63	0.62
1:B:298:ASN:C	1:B:298:ASN:HD22	2.03	0.62
1:D:772:LEU:O	1:D:773:GLN:HB2	1.98	0.62
1:F:452:VAL:HG22	1:F:883:VAL:HG21	1.81	0.62
1:A:70:ASN:HB3	1:C:167:SER:OG	1.99	0.62
1:C:913:LEU:O	1:C:915:THR:N	2.32	0.62
1:D:415:ASN:ND2	1:D:418:ARG:HH21	1.97	0.62
1:B:649:LYS:HA	1:B:649:LYS:HE2	1.82	0.62
1:C:463:THR:HB	1:C:871:GLN:HE22	1.64	0.62
1:D:909:ILE:HD12	1:D:910:GLY:H	1.65	0.62
1:A:584:ALA:HB2	1:A:622:GLN:HG2	1.82	0.62
1:E:49:TYR:CE1	1:E:121:GLU:HG3	2.35	0.62
1:F:896:ILE:O	1:F:900:VAL:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:PHE:HA	3:B:2001:P9D:H26	1.81	0.62
1:C:343:THR:HG21	1:C:998:GLN:HE22	1.65	0.62
1:C:375:VAL:O	1:C:379:THR:HG23	1.99	0.62
1:E:612:VAL:HG11	1:E:615:PHE:CD2	2.34	0.62
1:F:156:ASN:HD22	1:F:182:TYR:N	1.97	0.62
1:F:362:PHE:HA	1:F:365:THR:HG22	1.80	0.62
1:D:362:PHE:O	1:D:363:ARG:HB2	1.99	0.62
1:D:576:VAL:HG22	1:D:594:MET:HE1	1.82	0.62
1:F:541:TYR:HA	1:F:544:ILE:HG23	1.82	0.62
1:F:602:GLU:HG2	1:F:647:LEU:HD13	1.82	0.62
1:F:500:ILE:HD11	1:F:504:ASP:HB3	1.82	0.62
1:C:229:GLN:HA	1:C:229:GLN:HE21	1.64	0.61
1:C:241:GLN:HG3	1:C:762:ILE:O	2.01	0.61
1:C:248:ASN:HA	1:C:261:ARG:HD3	1.80	0.61
1:D:214:ILE:HD12	1:D:237:LYS:HB2	1.81	0.61
1:F:559:ILE:HG23	1:F:560:PRO:HD2	1.82	0.61
1:A:150:THR:HG22	1:A:153:ASP:CG	2.20	0.61
1:A:655:PHE:HD2	1:A:658:PHE:CE2	2.18	0.61
1:C:355:MET:CE	1:C:410:ILE:HG22	2.30	0.61
1:D:602:GLU:O	1:D:604:SER:N	2.33	0.61
1:E:1023:PHE:O	1:E:1027:VAL:HG23	2.00	0.61
1:F:416:VAL:O	1:F:416:VAL:HG12	1.99	0.61
1:A:372:VAL:HG22	1:A:405:LEU:HD22	1.82	0.61
1:A:568:ASP:O	1:A:569:GLN:HB2	1.99	0.61
1:B:188:LEU:HD12	1:B:266:ALA:HB2	1.82	0.61
1:B:985:VAL:HG12	1:B:986:PRO:CD	2.28	0.61
1:C:281:PHE:CE2	1:C:324:VAL:HG21	2.35	0.61
1:D:219:LEU:N	1:D:232:ALA:O	2.32	0.61
1:F:16:ALA:HB1	1:F:374:VAL:HG21	1.81	0.61
1:F:332:VAL:HG11	1:F:569:GLN:HG3	1.82	0.61
1:B:746:ASN:HA	1:B:749:VAL:CG2	2.30	0.61
1:B:950:GLU:HG2	2:B:2002:LMT:H3B	1.83	0.61
1:C:649:LYS:HZ2	1:C:713:GLN:HE21	1.48	0.61
1:D:336:SER:O	1:D:340:VAL:HG23	2.00	0.61
1:D:423:GLU:HB3	1:D:425:LEU:HD11	1.81	0.61
1:E:393:LEU:HD13	1:E:466:ILE:HG23	1.81	0.61
1:F:504:ASP:O	1:F:506:GLY:N	2.34	0.61
1:F:766:ARG:HB3	1:F:768:LYS:CE	2.31	0.61
1:B:753:TRP:HZ2	1:B:785:LEU:HA	1.65	0.61
1:C:1013:THR:O	1:C:1017:ILE:HG12	2.00	0.61
1:E:800:PHE:CD2	1:E:804:ALA:HB2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:TYR:CD1	1:B:970:LEU:HD22	2.36	0.61
1:B:740:VAL:CG1	1:B:745:ILE:HD11	2.30	0.61
1:C:187:TRP:HA	1:C:773:GLN:O	2.01	0.61
1:D:989:ILE:HG12	1:D:989:ILE:O	2.01	0.61
1:B:953:GLU:OE1	2:B:2002:LMT:H6'2	2.01	0.61
1:F:966:CYS:SG	1:F:1021:PRO:CG	2.88	0.61
1:A:632:LYS:HB2	1:A:633:PRO:HD2	1.82	0.61
1:B:830:PRO:HB3	1:B:839:ALA:HB2	1.82	0.61
1:D:108:GLN:NE2	1:E:112:GLN:HE21	1.98	0.61
1:D:943:LEU:HD13	1:D:969:ARG:HH21	1.64	0.61
1:E:308:GLN:HE21	1:E:312:ASN:ND2	1.95	0.61
1:F:966:CYS:SG	1:F:1021:PRO:HG3	2.40	0.61
1:C:659:LYS:NZ	1:C:661:ALA:HB2	2.15	0.61
1:A:247:GLU:HB3	1:A:263:LYS:HB3	1.83	0.60
1:C:102:ILE:O	1:C:106:GLN:HG3	2.01	0.60
1:C:352:PHE:HD2	1:C:353:LEU:HD23	1.66	0.60
1:E:214:ILE:HA	1:F:746:ASN:ND2	2.16	0.60
1:F:1:MET:HE3	1:F:486:LEU:HB3	1.82	0.60
1:F:448:VAL:O	1:F:452:VAL:HG23	2.01	0.60
1:A:156:ASN:HD22	1:A:182:TYR:N	1.96	0.60
1:B:527:TYR:CE1	1:B:966:CYS:HB3	2.36	0.60
1:B:729:GLU:HB3	1:B:805:THR:HG23	1.83	0.60
1:F:211:ASN:CA	1:F:240:LEU:HD13	2.26	0.60
1:A:691:GLY:H	1:A:694:VAL:CG2	2.13	0.60
1:C:355:MET:HE1	1:C:410:ILE:HG22	1.83	0.60
1:D:228:GLN:HE21	1:D:229:GLN:N	1.98	0.60
1:D:751:ILE:CG2	1:D:772:LEU:HD23	2.32	0.60
1:D:918:ARG:NE	1:D:1003:THR:HG21	2.12	0.60
1:E:171:GLY:HA3	1:E:302:THR:HG21	1.83	0.60
1:A:213:GLN:HB2	1:A:239:ARG:HG3	1.82	0.60
1:B:228:GLN:HA	1:C:780:MET:HE3	1.84	0.60
1:C:133:VAL:O	1:C:292:LYS:HE2	2.02	0.60
1:C:213:GLN:HA	1:C:238:THR:HA	1.84	0.60
1:E:250:LEU:HA	1:E:261:ARG:HG2	1.84	0.60
1:E:830:PRO:HB3	1:E:839:ALA:HB2	1.84	0.60
1:E:930:LEU:O	1:E:934:ILE:HG23	2.01	0.60
1:B:278:ASN:HB3	1:B:613:THR:HG22	1.82	0.60
1:C:194:ASN:HB2	1:C:797:MET:CG	2.29	0.60
1:D:907:GLY:HA3	1:D:1012:ALA:HB2	1.83	0.60
1:E:193:LEU:HB2	1:E:265:VAL:HG23	1.82	0.60
1:E:598:LEU:O	1:E:602:GLU:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:718:ASN:HB2	1:E:827:LEU:CD1	2.31	0.60
1:E:948:ALA:HB1	1:E:1024:TYR:CE2	2.36	0.60
1:B:663:VAL:O	1:B:663:VAL:HG12	2.01	0.60
1:C:247:GLU:CG	1:C:263:LYS:HB3	2.29	0.60
1:E:471:SER:O	1:E:475:VAL:HG13	2.02	0.60
1:E:784:ASP:HA	1:E:787:LYS:HE3	1.83	0.60
1:F:375:VAL:O	1:F:379:THR:HG23	2.02	0.60
1:A:92:VAL:HG22	1:A:94:PHE:CE2	2.36	0.60
1:C:40:PRO:HG3	1:C:76:ARG:NH1	2.16	0.60
1:C:453:PHE:HZ	1:C:932:THR:HB	1.66	0.60
1:D:568:ASP:O	1:D:569:GLN:CB	2.50	0.60
1:D:937:SER:HB3	1:D:1009:MET:HE1	1.84	0.60
1:E:193:LEU:CD1	1:E:265:VAL:CG2	2.78	0.60
1:E:641:GLU:O	1:E:650:ARG:NH2	2.34	0.60
1:E:972:PRO:HA	1:E:975:MET:HB2	1.84	0.60
1:F:32:VAL:HG22	1:F:390:ILE:HB	1.81	0.60
1:A:303:ALA:HB2	1:A:330:THR:HG21	1.82	0.60
1:C:158:ILE:HG22	1:C:159:VAL:N	2.16	0.60
1:C:910:GLY:CA	1:C:1011:THR:HG21	2.30	0.60
1:D:987:LEU:HB2	1:D:998:GLN:HE21	1.66	0.60
1:E:753:TRP:CZ2	1:E:785:LEU:HA	2.37	0.60
1:F:563:PHE:CE2	1:F:564:LEU:HD22	2.37	0.60
1:B:139:VAL:HG13	1:B:327:TYR:HB3	1.83	0.60
1:B:381:GLY:O	1:B:384:ALA:HB3	2.02	0.60
1:F:654:HIS:ND1	1:F:654:HIS:O	2.35	0.60
1:B:682:LEU:HD21	1:B:826:ILE:HB	1.84	0.59
1:C:507:GLU:HG3	1:C:509:LYS:HB2	1.84	0.59
1:F:23:GLY:HA3	1:F:377:LEU:O	2.02	0.59
1:A:188:LEU:HD23	1:A:200:PRO:HG3	1.84	0.59
1:A:467:TYR:OH	1:A:927:GLN:NE2	2.35	0.59
1:C:65:ILE:HD11	1:C:90:ILE:HG13	1.84	0.59
1:D:871:GLN:O	1:D:872:ALA:HB2	2.01	0.59
1:E:120:GLN:O	1:E:124:ARG:HG2	2.02	0.59
1:E:447:MET:HE3	2:E:2002:LMT:H72	1.83	0.59
1:F:120:GLN:HA	1:F:120:GLN:HE21	1.67	0.59
1:F:158:ILE:HG22	1:F:159:VAL:N	2.17	0.59
1:F:214:ILE:CD1	1:F:237:LYS:H	2.15	0.59
1:D:657:SER:O	1:D:659:LYS:N	2.35	0.59
1:E:189:ASP:HB3	1:E:192:LYS:HB2	1.82	0.59
1:E:713:GLN:CG	1:E:714:ARG:N	2.65	0.59
2:F:2001:LMT:O2B	2:F:2001:LMT:C4'	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:902:LEU:O	1:B:905:PRO:HD2	2.03	0.59
1:C:447:MET:HE1	1:C:886:CYS:HB3	1.83	0.59
1:C:573:PHE:HB2	1:C:666:PHE:CE1	2.37	0.59
1:F:695:LEU:HD23	1:F:824:MET:SD	2.42	0.59
1:A:632:LYS:HB2	1:A:633:PRO:CD	2.33	0.59
1:B:76:ARG:HD3	1:B:863:TYR:CE2	2.37	0.59
1:B:471:SER:O	1:B:475:VAL:HG13	2.02	0.59
1:C:1020:VAL:HB	1:C:1021:PRO:HD3	1.85	0.59
1:D:190:PRO:HG2	1:D:787:LYS:HG2	1.84	0.59
1:D:400:LEU:CD2	1:D:932:THR:HG21	2.32	0.59
1:E:186:ILE:HG22	1:E:772:LEU:HD12	1.83	0.59
1:E:572:LEU:HB3	1:E:629:ILE:HG13	1.84	0.59
1:F:542:LEU:CD1	1:F:1022:LEU:HD11	2.26	0.59
1:F:726:TYR:CZ	1:F:806:GLY:HA3	2.37	0.59
1:A:190:PRO:HG2	1:A:787:LYS:HG2	1.85	0.59
1:C:193:LEU:HD12	1:C:265:VAL:CG1	2.24	0.59
1:E:528:GLU:OE1	1:E:967:ARG:HD3	2.02	0.59
1:B:760:ASP:HB3	1:B:767:VAL:HG23	1.85	0.59
1:B:782:PRO:O	1:B:785:LEU:HB2	2.02	0.59
1:C:281:PHE:HE2	1:C:324:VAL:HG21	1.68	0.59
1:E:949:LYS:NZ	2:E:2002:LMT:O6B	2.26	0.59
1:F:404:LEU:HD22	1:F:449:LEU:HD13	1.84	0.59
1:F:606:VAL:CG1	1:F:607:SER:N	2.66	0.59
1:C:909:ILE:HG13	1:C:910:GLY:H	1.68	0.59
1:D:576:VAL:HG22	1:D:594:MET:CE	2.33	0.59
1:E:28:LEU:O	1:E:29:SER:CB	2.51	0.59
1:E:225:VAL:HG22	1:F:780:MET:HG3	1.84	0.59
1:E:578:THR:HG22	1:E:661:ALA:HB2	1.84	0.59
1:F:261:ARG:HG2	1:F:261:ARG:NH1	2.01	0.59
1:F:969:ARG:C	1:F:972:PRO:HD2	2.23	0.59
1:A:780:MET:HB3	1:C:228:GLN:HE22	1.67	0.59
1:C:952:HIS:HD2	1:C:956:LYS:O	1.85	0.59
1:E:701:LYS:O	1:E:705:LEU:HB3	2.03	0.59
1:C:27:ILE:HD11	1:C:380:PHE:CD2	2.38	0.59
1:C:447:MET:CE	1:C:886:CYS:HB3	2.32	0.59
1:C:567:GLU:O	1:C:569:GLN:N	2.36	0.59
1:C:713:GLN:O	1:C:714:ARG:CB	2.51	0.59
1:D:293:LEU:HG	1:D:297:ALA:HB3	1.83	0.59
1:E:559:ILE:HG13	1:E:560:PRO:CD	2.32	0.59
1:F:362:PHE:O	1:F:364:ALA:N	2.36	0.59
1:B:652:GLN:HE21	1:B:652:GLN:HA	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:TRP:HB3	1:C:637:ARG:NH2	2.18	0.58
1:C:646:GLU:O	1:C:649:LYS:N	2.36	0.58
1:D:577:GLN:HA	1:D:577:GLN:HE21	1.66	0.58
1:B:323:VAL:HG23	1:B:323:VAL:O	2.02	0.58
1:D:569:GLN:H	1:D:634:TRP:HH2	1.46	0.58
1:E:472:ILE:HD11	2:E:2003:LMT:H62	1.85	0.58
1:B:540:PRO:O	1:B:544:ILE:HG22	2.03	0.58
1:C:367:ILE:HG23	1:C:492:LEU:HD12	1.85	0.58
1:D:300:LEU:HD11	1:D:333:VAL:HG23	1.85	0.58
1:B:247:GLU:HB3	1:B:263:LYS:HB3	1.84	0.58
1:C:197:GLN:HA	1:C:797:MET:SD	2.43	0.58
1:D:356:TYR:CE1	1:D:513:PHE:CZ	2.86	0.58
1:A:488:LEU:HD22	1:A:492:LEU:HG	1.86	0.58
1:A:569:GLN:H	1:A:634:TRP:HH2	1.51	0.58
1:C:36:PRO:HG2	1:C:38:ILE:CG2	2.33	0.58
1:E:247:GLU:HG3	1:E:268:VAL:CG1	2.32	0.58
1:F:389:SER:O	1:F:394:THR:HG21	2.03	0.58
1:B:214:ILE:HA	1:C:746:ASN:ND2	2.18	0.58
1:D:456:MET:CE	1:D:931:LEU:HD13	2.34	0.58
1:D:468:ARG:O	1:D:470:PHE:N	2.35	0.58
1:D:884:PHE:HB2	1:D:901:MET:CE	2.33	0.58
1:D:898:PHE:O	1:D:902:LEU:HG	2.03	0.58
1:E:784:ASP:OD2	1:E:784:ASP:N	2.37	0.58
1:A:156:ASN:HD21	1:A:768:LYS:HZ3	1.49	0.58
1:A:367:ILE:HG13	1:A:368:PRO:CD	2.30	0.58
1:C:283:GLY:HA2	1:C:595:ARG:NH1	2.18	0.58
1:D:468:ARG:O	1:D:469:GLN:HB2	2.02	0.58
1:F:945:VAL:HG23	1:F:1024:TYR:HB2	1.85	0.58
1:B:196:TYR:N	1:B:196:TYR:CD1	2.70	0.58
1:B:314:GLU:N	1:B:315:PRO:HD2	2.19	0.58
1:D:48:SER:O	1:D:125:GLN:HG2	2.03	0.58
1:E:367:ILE:HB	1:E:368:PRO:HD3	1.86	0.58
1:F:194:ASN:HB2	1:F:797:MET:HG3	1.85	0.58
1:A:80:SER:OG	1:A:817:ARG:HG3	2.04	0.58
1:B:584:ALA:N	1:B:622:GLN:HG2	2.18	0.58
1:B:684:LEU:O	1:B:823:ALA:HA	2.04	0.58
1:B:1005:VAL:HG23	1:B:1006:ILE:HG23	1.85	0.58
1:A:314:GLU:N	1:A:315:PRO:HD2	2.19	0.57
1:B:904:VAL:HB	1:B:905:PRO:HD3	1.85	0.57
1:D:527:TYR:CD1	1:D:970:LEU:HG	2.39	0.57
1:D:887:LEU:HD22	1:D:942:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:VAL:HG21	1:E:406:VAL:HG22	1.86	0.57
1:E:806:GLY:O	1:E:807:LYS:HB2	2.04	0.57
1:A:875:LEU:O	1:A:876:TYR:HB2	2.03	0.57
1:B:24:GLY:O	1:B:27:ILE:HG22	2.05	0.57
1:C:805:THR:HG22	1:C:807:LYS:HG3	1.85	0.57
1:D:162:ILE:HG22	1:D:166:LEU:HD22	1.86	0.57
1:F:830:PRO:HB3	1:F:839:ALA:HB2	1.84	0.57
1:B:227:GLY:O	1:B:229:GLN:N	2.37	0.57
1:C:149:MET:HB3	1:C:153:ASP:HB3	1.87	0.57
1:D:831:ALA:HB3	1:D:834:LEU:CD1	2.35	0.57
1:F:530:GLY:HA2	1:F:533:SER:HB3	1.86	0.57
1:F:593:SER:OG	1:F:658:PHE:HE1	1.85	0.57
1:A:369:THR:O	1:A:373:PRO:HD2	2.04	0.57
1:C:1:MET:O	1:C:3:LYS:N	2.37	0.57
1:D:228:GLN:NE2	1:D:230:LEU:H	2.01	0.57
1:E:24:GLY:O	1:E:27:ILE:HG22	2.04	0.57
1:E:735:ALA:O	1:E:740:VAL:HG12	2.03	0.57
1:F:341:VAL:O	1:F:344:LEU:HB3	2.04	0.57
1:F:884:PHE:CE1	1:F:897:PRO:HB2	2.40	0.57
1:B:49:TYR:HE1	1:B:121:GLU:HG3	1.67	0.57
1:B:120:GLN:O	1:B:124:ARG:HG3	2.03	0.57
1:B:360:GLN:HG2	1:B:513:PHE:CD1	2.38	0.57
1:B:742:LEU:HA	1:B:745:ILE:HG12	1.86	0.57
1:C:574:ALA:HB3	1:C:627:ALA:HB3	1.86	0.57
1:C:944:ILE:CG2	1:C:973:ILE:HD11	2.34	0.57
1:E:782:PRO:O	1:E:785:LEU:HB2	2.04	0.57
1:E:843:VAL:O	1:E:847:VAL:HB	2.05	0.57
1:B:328:ASP:O	1:B:331:PRO:HD2	2.04	0.57
1:C:635:GLU:HG3	1:C:636:GLU:H	1.69	0.57
1:C:933:THR:HA	1:C:936:LEU:HD12	1.86	0.57
1:C:985:VAL:O	1:C:989:ILE:HG13	2.05	0.57
1:D:360:GLN:HG2	1:D:513:PHE:CG	2.39	0.57
1:D:695:LEU:HD22	1:D:824:MET:SD	2.45	0.57
1:E:404:LEU:HD13	1:E:449:LEU:HD13	1.85	0.57
1:F:162:ILE:O	1:F:165:PRO:HD2	2.05	0.57
1:A:306:ILE:O	1:A:310:ILE:HD13	2.04	0.57
1:A:734:LYS:O	1:A:738:LEU:HB2	2.05	0.57
1:B:1005:VAL:O	1:B:1006:ILE:HG12	2.04	0.57
1:E:33:ASN:O	1:E:391:ASN:HA	2.04	0.57
1:A:684:LEU:HD22	1:A:826:ILE:HD12	1.87	0.57
1:C:774:GLY:O	1:C:779:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:809:GLU:O	1:C:810:TYR:HB3	2.05	0.57
1:D:492:LEU:O	1:D:496:MET:HB2	2.04	0.57
1:A:671:VAL:HG13	1:A:674:LEU:HD11	1.87	0.57
1:B:228:GLN:HA	1:C:780:MET:CE	2.35	0.57
1:E:239:ARG:HG2	1:E:239:ARG:NH1	2.17	0.57
1:C:541:TYR:HA	1:C:544:ILE:CG2	2.33	0.57
1:D:208:GLN:HA	1:D:759:ASN:ND2	2.18	0.57
1:D:423:GLU:CB	1:D:425:LEU:HD13	2.35	0.57
1:B:383:LEU:HD13	1:B:388:PHE:HB2	1.86	0.56
1:E:359:LEU:HD12	1:E:971:ARG:NH1	2.20	0.56
1:F:336:SER:HA	1:F:993:ALA:CB	2.34	0.56
1:C:930:LEU:O	1:C:933:THR:HB	2.05	0.56
1:F:47:VAL:H	1:F:88:MET:HE3	1.71	0.56
1:A:684:LEU:HD21	1:A:826:ILE:HD11	1.83	0.56
1:A:830:PRO:HB3	1:A:839:ALA:HB2	1.86	0.56
1:B:10:ILE:HB	1:C:892:GLU:OE2	2.05	0.56
1:B:544:ILE:HG23	1:B:1019:TRP:HH2	1.70	0.56
1:B:700:ASN:O	1:B:704:MET:HG2	2.06	0.56
1:C:305:ALA:O	1:C:308:GLN:HB3	2.05	0.56
1:D:467:TYR:C	1:D:468:ARG:O	2.42	0.56
1:F:246:PHE:O	1:F:262:LEU:HD23	2.05	0.56
1:F:507:GLU:HG3	1:F:509:LYS:CB	2.34	0.56
1:F:904:VAL:O	1:F:908:VAL:HG23	2.04	0.56
1:B:695:LEU:HD13	1:B:824:MET:CG	2.35	0.56
1:D:193:LEU:HA	1:D:265:VAL:HG23	1.87	0.56
1:D:367:ILE:HD11	1:D:489:THR:HG23	1.87	0.56
1:D:607:SER:HB2	1:D:632:LYS:HB3	1.87	0.56
1:E:35:TYR:CE2	1:E:671:VAL:HG22	2.40	0.56
1:F:809:GLU:O	1:F:810:TYR:HB3	2.05	0.56
1:B:127:ILE:N	1:B:127:ILE:HD12	2.21	0.56
1:C:388:PHE:CZ	1:C:472:ILE:HG12	2.40	0.56
1:D:273:GLN:OE1	1:D:769:ARG:HD2	2.05	0.56
1:D:1011:THR:O	1:D:1015:LEU:HB2	2.05	0.56
1:E:440:GLY:HA3	2:E:2002:LMT:H2O2	1.67	0.56
1:D:943:LEU:HD13	1:D:969:ARG:NH2	2.20	0.56
1:D:1014:VAL:O	1:D:1014:VAL:HG23	2.04	0.56
1:E:28:LEU:O	1:E:28:LEU:HD12	2.06	0.56
1:A:861:LEU:H	1:A:861:LEU:HD22	1.68	0.56
1:A:989:ILE:O	1:A:989:ILE:HG12	2.06	0.56
1:D:300:LEU:HG	1:D:333:VAL:HG21	1.87	0.56
1:D:329:THR:O	1:D:332:VAL:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:713:GLN:O	1:E:715:VAL:N	2.39	0.56
3:E:2001:P9D:H32A	3:E:2001:P9D:O44	2.04	0.56
1:B:363:ARG:HH11	1:B:498:LYS:HD2	1.69	0.56
1:C:280:GLN:HB3	1:C:285:PRO:HA	1.87	0.56
1:E:727:LYS:HG3	1:E:727:LYS:O	2.05	0.56
1:A:169:THR:HG21	1:A:306:ILE:HG22	1.87	0.56
1:A:183:SER:HB2	1:A:769:ARG:O	2.06	0.56
1:B:151:LYS:HA	1:B:154:LEU:HD12	1.86	0.56
1:C:755:SER:O	1:C:756:SER:HB2	2.06	0.56
1:D:703:LEU:HD11	1:D:717:PRO:HD3	1.87	0.56
1:C:410:ILE:HG12	1:C:976:THR:HG22	1.87	0.55
1:A:723:GLU:HB2	1:A:724:PRO:HD2	1.88	0.55
1:B:637:ARG:HG3	1:B:637:ARG:O	2.05	0.55
1:B:947:PHE:HD2	1:B:968:MET:HE2	1.71	0.55
1:C:214:ILE:CD1	1:C:237:LYS:H	2.19	0.55
1:D:208:GLN:HA	1:D:759:ASN:HD21	1.71	0.55
1:D:363:ARG:NH1	1:D:496:MET:O	2.38	0.55
1:E:469:GLN:O	1:E:473:THR:CG2	2.46	0.55
1:E:987:LEU:O	1:E:990:SER:HB2	2.06	0.55
1:F:20:MET:HG3	1:F:374:VAL:HA	1.87	0.55
1:C:929:GLY:HA2	1:C:932:THR:CG2	2.36	0.55
1:D:184:MET:HB3	1:D:770:VAL:HB	1.88	0.55
1:E:47:VAL:HG22	1:E:127:ILE:HG13	1.86	0.55
1:E:191:ALA:C	1:E:193:LEU:H	2.10	0.55
1:F:671:VAL:HG21	1:F:674:LEU:HD22	1.88	0.55
1:B:60:THR:HG23	1:B:119:PRO:HG3	1.87	0.55
1:B:564:LEU:HD23	1:B:565:PRO:HD2	1.89	0.55
1:B:683:PHE:CE1	1:B:825:GLU:HB2	2.42	0.55
1:D:252:LYS:O	1:D:260:VAL:N	2.31	0.55
1:D:847:VAL:HG11	1:D:856:TYR:CE2	2.42	0.55
1:E:127:ILE:HD12	1:E:127:ILE:N	2.22	0.55
1:F:910:GLY:N	1:F:1011:THR:HG21	2.21	0.55
2:A:2003:LMT:H6D	2:A:2003:LMT:O5B	2.06	0.55
1:B:238:THR:OG1	1:B:239:ARG:N	2.40	0.55
1:D:723:GLU:HB2	1:D:724:PRO:HD2	1.86	0.55
1:E:8:ARG:N	1:E:9:PRO:HD3	2.22	0.55
1:E:314:GLU:HG2	1:E:317:MET:HE1	1.88	0.55
1:B:184:MET:HB3	1:B:770:VAL:HG13	1.89	0.55
1:B:542:LEU:O	1:B:546:VAL:HG23	2.07	0.55
1:C:616:ASN:HA	1:C:626:MET:HG2	1.87	0.55
1:E:47:VAL:HG21	1:E:127:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:729:GLU:HB3	1:E:805:THR:HG22	1.88	0.55
1:A:708:GLN:NE2	1:D:809:GLU:HG3	2.21	0.55
1:A:713:GLN:O	1:A:715:VAL:N	2.40	0.55
1:B:740:VAL:HG11	1:B:745:ILE:HD11	1.88	0.55
1:E:365:THR:HG22	1:E:366:LEU:N	2.21	0.55
1:E:541:TYR:O	1:E:1019:TRP:CZ3	2.60	0.55
1:A:987:LEU:CB	1:A:998:GLN:NE2	2.69	0.55
1:B:8:ARG:HG3	1:B:8:ARG:NH1	2.17	0.55
1:D:632:LYS:O	1:D:637:ARG:HD3	2.07	0.55
1:D:808:TRP:HH2	1:F:230:LEU:HD21	1.71	0.55
1:D:984:VAL:HG11	1:D:1005:VAL:HG23	1.87	0.55
1:E:990:SER:OG	1:E:998:GLN:OE1	2.22	0.55
1:F:489:THR:N	1:F:490:PRO:HD2	2.21	0.55
1:F:826:ILE:C	1:F:826:ILE:HD12	2.27	0.55
1:A:329:THR:O	1:A:332:VAL:HG12	2.07	0.55
1:A:861:LEU:CD2	1:A:861:LEU:N	2.70	0.55
1:C:542:LEU:HD11	1:C:1022:LEU:HD11	1.85	0.55
1:D:401:ALA:O	1:D:405:LEU:HB3	2.06	0.55
1:D:582:SER:HB3	1:D:586:ARG:HG2	1.88	0.55
1:F:340:VAL:HA	1:F:343:THR:CG2	2.37	0.55
1:F:485:ALA:HA	1:F:489:THR:HB	1.87	0.55
1:F:535:LEU:O	1:F:538:ARG:HD3	2.07	0.55
1:C:183:SER:HB3	1:C:273:GLN:HA	1.88	0.55
1:C:916:SER:C	1:C:918:ARG:H	2.10	0.55
1:D:228:GLN:HE21	1:D:230:LEU:H	1.55	0.55
1:D:235:ILE:O	1:D:235:ILE:HG13	2.06	0.55
1:D:861:LEU:CD2	1:D:861:LEU:N	2.70	0.55
1:F:399:VAL:O	1:F:402:ILE:HG13	2.07	0.55
1:F:501:GLU:O	1:F:504:ASP:HB2	2.07	0.55
1:F:685:GLN:HE21	1:F:687:GLN:NE2	2.03	0.55
1:A:403:GLY:HA3	1:A:980:PHE:CD1	2.38	0.54
1:D:419:VAL:CG2	1:D:430:ALA:HB1	2.36	0.54
1:E:247:GLU:HG2	1:E:263:LYS:HB3	1.88	0.54
1:E:438:ILE:HG22	1:E:442:LEU:HG	1.89	0.54
1:D:726:TYR:CZ	1:D:806:GLY:HA3	2.42	0.54
1:D:831:ALA:HB3	1:D:834:LEU:HD11	1.90	0.54
1:E:351:VAL:HG21	1:E:406:VAL:CG2	2.36	0.54
1:E:637:ARG:N	1:E:638:PRO:HD3	2.22	0.54
1:A:277:ILE:H	1:A:277:ILE:HD13	1.73	0.54
1:A:535:LEU:HD22	1:A:1025:VAL:HG21	1.90	0.54
1:B:196:TYR:N	1:B:196:TYR:HD1	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ILE:HD12	1:C:728:LEU:HD13	1.89	0.54
1:C:453:PHE:CE2	1:C:474:ILE:HG21	2.41	0.54
1:C:665:ALA:O	1:C:714:ARG:NH1	2.38	0.54
1:D:918:ARG:HH21	1:D:1003:THR:CG2	2.19	0.54
1:E:460:GLY:H	1:E:871:GLN:HE22	1.54	0.54
1:E:753:TRP:HZ2	1:E:785:LEU:HA	1.71	0.54
1:F:918:ARG:HG3	1:F:918:ARG:O	2.06	0.54
1:A:808:TRP:HH2	1:C:230:LEU:HD21	1.72	0.54
1:A:1009:MET:O	1:A:1010:VAL:C	2.45	0.54
1:B:994:GLY:O	1:B:998:GLN:HG3	2.08	0.54
1:D:228:GLN:HE21	1:D:230:LEU:N	2.04	0.54
1:E:681:ASP:OD2	1:E:859:THR:HG23	2.07	0.54
1:F:430:ALA:O	1:F:434:SER:HB2	2.08	0.54
1:B:53:SER:OG	1:B:56:THR:HG23	2.07	0.54
1:D:303:ALA:HB1	1:D:307:ARG:HH21	1.71	0.54
1:E:7:ASP:C	1:E:9:PRO:HD3	2.28	0.54
1:F:137:LEU:HD13	1:F:293:LEU:HD22	1.89	0.54
1:F:696:LEU:O	1:F:700:ASN:ND2	2.40	0.54
1:B:15:ILE:O	1:B:19:ILE:HG23	2.08	0.54
1:B:248:ASN:HD22	1:B:261:ARG:HH21	1.55	0.54
1:C:302:THR:O	1:C:306:ILE:CG2	2.55	0.54
1:D:283:GLY:HA2	1:D:595:ARG:HH11	1.68	0.54
1:D:517:ASN:OD1	1:D:971:ARG:NH2	2.40	0.54
1:D:780:MET:HB3	1:F:228:GLN:HE22	1.69	0.54
1:F:527:TYR:HD1	1:F:1018:PHE:CE1	2.26	0.54
1:F:539:ALA:CB	1:F:542:LEU:HB2	2.34	0.54
1:F:682:LEU:HD12	1:F:858:TRP:CZ3	2.42	0.54
1:A:985:VAL:O	1:A:989:ILE:HG22	2.06	0.54
1:B:64:VAL:HG21	1:B:117:LEU:HB3	1.89	0.54
1:B:363:ARG:NH1	1:B:498:LYS:HD2	2.23	0.54
1:B:925:PHE:CE1	1:B:997:SER:HB3	2.43	0.54
1:C:596:GLU:O	1:C:598:LEU:N	2.31	0.54
1:C:742:LEU:O	1:C:744:ASP:N	2.39	0.54
1:D:488:LEU:HD22	1:D:492:LEU:HG	1.90	0.54
1:E:351:VAL:O	1:E:355:MET:HB2	2.08	0.54
1:F:669:PRO:CG	1:F:861:LEU:HD11	2.37	0.54
1:A:171:GLY:HA3	1:A:302:THR:HG21	1.90	0.54
1:E:56:THR:O	1:E:60:THR:HB	2.08	0.54
1:E:188:LEU:HD12	1:E:266:ALA:HB2	1.90	0.54
1:E:897:PRO:O	1:E:901:MET:HG3	2.08	0.54
1:A:725:GLN:HE21	1:C:235:ILE:HD11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ALA:N	1:B:540:PRO:HD2	2.23	0.54
1:C:36:PRO:O	1:C:38:ILE:HG23	2.07	0.54
1:C:239:ARG:HH11	1:C:239:ARG:CG	1.90	0.54
1:C:649:LYS:NZ	1:C:713:GLN:NE2	2.56	0.54
1:D:985:VAL:N	1:D:986:PRO:HD2	2.23	0.54
1:E:38:ILE:HG22	1:E:462:SER:HB3	1.90	0.54
1:E:244:GLU:H	1:E:244:GLU:CD	2.11	0.54
1:E:954:GLN:HG2	1:E:954:GLN:O	2.07	0.54
1:A:844:GLU:OE1	1:A:866:ARG:NH1	2.41	0.54
1:A:900:VAL:HG21	1:A:942:ILE:HD13	1.89	0.54
1:B:220:GLY:O	1:B:228:GLN:NE2	2.41	0.54
1:C:639:GLY:O	1:C:642:ASN:N	2.41	0.54
1:D:594:MET:HG3	1:D:655:PHE:CZ	2.43	0.54
1:E:281:PHE:HE2	1:E:324:VAL:HG11	1.72	0.54
1:F:1:MET:CE	1:F:486:LEU:HB3	2.38	0.54
1:B:607:SER:HB2	1:B:632:LYS:HB3	1.89	0.53
1:B:1015:LEU:O	1:B:1019:TRP:HD1	1.91	0.53
1:D:17:LEU:HD21	2:D:2003:LMT:H41	1.90	0.53
1:D:940:ASN:HA	1:D:943:LEU:HD12	1.90	0.53
1:E:727:LYS:O	1:E:727:LYS:CG	2.56	0.53
1:F:336:SER:HA	1:F:993:ALA:HB1	1.89	0.53
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.91	0.53
1:B:154:LEU:HD13	1:B:286:ALA:HA	1.90	0.53
1:C:504:ASP:O	1:C:506:GLY:N	2.41	0.53
1:C:574:ALA:HA	1:C:664:PHE:O	2.07	0.53
1:C:958:ILE:HD13	1:C:1029:THR:CG2	2.38	0.53
1:D:17:LEU:HD23	1:D:20:MET:HE3	1.88	0.53
1:D:225:VAL:HG22	1:D:228:GLN:HB2	1.91	0.53
1:F:248:ASN:HA	1:F:261:ARG:HD3	1.91	0.53
1:E:446:ALA:HB2	1:E:482:VAL:HG21	1.90	0.53
1:F:348:ILE:C	1:F:348:ILE:HD12	2.28	0.53
1:F:455:PRO:HG3	1:F:882:VAL:HG21	1.90	0.53
1:A:884:PHE:HB2	1:A:901:MET:HE2	1.89	0.53
1:B:214:ILE:CG2	1:B:237:LYS:H	2.21	0.53
1:D:30:LEU:HD21	1:D:384:ALA:HA	1.90	0.53
1:D:895:SER:HB2	1:D:1030:LEU:CD1	2.38	0.53
1:A:399:VAL:HG11	1:A:987:LEU:HD23	1.90	0.53
1:C:659:LYS:HG3	1:C:660:ASP:H	1.74	0.53
1:D:597:TYR:O	1:D:601:LYS:HB2	2.09	0.53
1:E:989:ILE:O	1:E:989:ILE:CG2	2.55	0.53
1:A:365:THR:O	1:A:369:THR:CG2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:VAL:HA	1:A:1006:ILE:HD11	1.90	0.53
1:B:281:PHE:CZ	1:B:608:SER:HB2	2.44	0.53
1:C:115:THR:HG22	1:C:116:PRO:HD3	1.91	0.53
1:C:171:GLY:HA2	1:C:297:ALA:CB	2.39	0.53
1:C:410:ILE:HD12	1:C:410:ILE:C	2.29	0.53
1:D:155:SER:OG	1:D:179:GLY:HA3	2.09	0.53
1:E:913:LEU:O	1:E:917:MET:HG2	2.09	0.53
1:F:339:GLU:O	1:F:343:THR:HG22	2.09	0.53
1:C:2:SER:HB3	1:C:435:MET:HG3	1.90	0.53
1:C:587:THR:O	1:C:591:VAL:HG23	2.09	0.53
1:D:80:SER:OG	1:D:817:ARG:HG3	2.09	0.53
1:D:907:GLY:O	1:D:1008:GLY:HA2	2.08	0.53
1:A:307:ARG:O	1:A:311:ALA:HB2	2.08	0.53
1:A:791:ARG:HB2	1:A:797:MET:HE1	1.91	0.53
1:B:176:GLN:HB2	3:B:2001:P9D:H40	1.90	0.53
1:B:682:LEU:HD23	1:B:826:ILE:HB	1.90	0.53
1:C:16:ALA:HB1	1:C:374:VAL:HG21	1.91	0.53
1:C:687:GLN:HE22	1:C:855:GLY:N	2.05	0.53
1:C:746:ASN:HA	1:C:749:VAL:HG22	1.90	0.53
1:F:355:MET:CE	1:F:410:ILE:CG2	2.86	0.53
1:A:298:ASN:O	1:A:302:THR:HG23	2.09	0.53
1:B:840:MET:O	1:B:844:GLU:HB2	2.07	0.53
1:C:64:VAL:HG11	1:C:117:LEU:HB2	1.89	0.53
1:C:809:GLU:HG2	1:C:810:TYR:H	1.73	0.53
1:E:216:SER:HB3	1:E:234:ILE:O	2.09	0.53
1:E:910:GLY:CA	1:E:1011:THR:CG2	2.85	0.53
1:F:142:VAL:HG21	1:F:321:MET:CE	2.38	0.53
1:F:596:GLU:C	1:F:598:LEU:H	2.12	0.53
1:A:193:LEU:CD2	1:A:198:LEU:O	2.57	0.53
1:A:528:GLU:OE2	1:A:967:ARG:HD3	2.09	0.53
1:A:1009:MET:O	1:A:1013:THR:HG22	2.08	0.53
1:C:1009:MET:HA	1:C:1009:MET:CE	2.38	0.53
1:D:989:ILE:O	1:D:989:ILE:CG1	2.56	0.53
1:E:949:LYS:O	1:E:953:GLU:HG3	2.09	0.53
1:A:655:PHE:CD2	1:A:658:PHE:HE2	2.26	0.52
1:A:701:LYS:HB3	1:A:701:LYS:NZ	2.24	0.52
1:A:754:GLY:O	1:A:755:SER:HB2	2.08	0.52
1:A:907:GLY:CA	1:A:1012:ALA:HB2	2.38	0.52
1:B:539:ALA:O	1:B:543:LEU:HG	2.08	0.52
1:C:46:GLN:NE2	1:C:89:THR:HG23	2.24	0.52
1:C:253:VAL:CG1	1:C:259:GLN:HB3	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:GLN:OE1	1:C:308:GLN:HA	2.09	0.52
1:D:887:LEU:CD2	1:D:942:ILE:HD11	2.39	0.52
1:D:1009:MET:HA	1:D:1009:MET:HE3	1.89	0.52
1:F:789:TYR:CD1	1:F:799:PRO:HA	2.44	0.52
1:F:791:ARG:HG3	1:F:797:MET:HE1	1.90	0.52
1:A:137:LEU:HD22	1:A:293:LEU:CD1	2.38	0.52
1:A:791:ARG:HB2	1:A:797:MET:HE2	1.91	0.52
1:B:8:ARG:N	1:B:9:PRO:HD3	2.24	0.52
1:B:507:GLU:O	1:B:518:ARG:NH1	2.42	0.52
1:D:156:ASN:HD21	1:D:768:LYS:NZ	2.07	0.52
1:F:683:PHE:HD1	1:F:823:ALA:HB1	1.75	0.52
1:A:137:LEU:HD22	1:A:293:LEU:HD13	1.91	0.52
1:B:281:PHE:CE2	1:B:324:VAL:HG11	2.44	0.52
1:C:593:SER:OG	1:C:658:PHE:HE1	1.93	0.52
1:C:695:LEU:CD2	1:C:824:MET:SD	2.97	0.52
1:D:350:LEU:HG	1:D:982:LEU:O	2.09	0.52
1:D:791:ARG:HE	1:D:797:MET:HE1	1.74	0.52
1:E:348:ILE:HD12	1:E:369:THR:HG23	1.92	0.52
1:E:365:THR:CG2	1:E:366:LEU:N	2.72	0.52
1:E:909:ILE:HG23	1:E:910:GLY:N	2.24	0.52
1:C:545:TYR:CE1	1:C:1023:PHE:HZ	2.27	0.52
1:C:683:PHE:O	1:C:856:TYR:HA	2.10	0.52
1:F:535:LEU:HD12	1:F:963:ILE:HD11	1.90	0.52
1:A:72:ILE:HG22	1:A:106:GLN:HB3	1.90	0.52
1:C:720:MET:O	1:C:721:SER:HB2	2.10	0.52
1:E:545:TYR:O	1:E:548:ILE:HG13	2.09	0.52
1:F:478:MET:HE2	1:F:478:MET:HA	1.92	0.52
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.92	0.52
1:B:228:GLN:HE22	1:C:622:GLN:NE2	1.98	0.52
1:C:420:MET:SD	1:C:427:PRO:HA	2.50	0.52
1:C:596:GLU:C	1:C:598:LEU:H	2.10	0.52
1:C:763:ASP:O	1:C:764:ARG:HB2	2.08	0.52
1:D:343:THR:HG21	1:D:998:GLN:NE2	2.14	0.52
1:D:485:ALA:O	1:D:490:PRO:HD3	2.08	0.52
1:E:569:GLN:O	1:E:571:VAL:N	2.39	0.52
1:F:46:GLN:HA	1:F:88:MET:HE3	1.92	0.52
1:F:61:VAL:CG2	1:F:62:VAL:N	2.72	0.52
1:B:800:PHE:HD2	1:B:804:ALA:HB2	1.74	0.52
1:C:597:TYR:HB3	1:C:654:HIS:CE1	2.45	0.52
1:D:751:ILE:HG21	1:D:772:LEU:HD23	1.91	0.52
1:D:965:ALA:HA	1:D:968:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:GLN:HG2	1:E:768:LYS:HD3	1.92	0.52
1:E:544:ILE:HG23	1:E:1019:TRP:HH2	1.74	0.52
1:E:573:PHE:HD2	1:E:666:PHE:CE1	2.27	0.52
1:A:306:ILE:C	1:A:308:GLN:N	2.60	0.52
1:A:597:TYR:O	1:A:601:LYS:HB2	2.10	0.52
1:B:7:ASP:C	1:B:9:PRO:HD3	2.29	0.52
1:B:281:PHE:CD2	1:B:324:VAL:HG11	2.44	0.52
1:C:572:LEU:HD21	1:C:665:ALA:HB1	1.91	0.52
1:A:791:ARG:CB	1:A:797:MET:HE2	2.40	0.52
1:B:743:ALA:O	1:B:747:SER:HB3	2.10	0.52
1:C:570:GLY:HA3	1:C:634:TRP:CZ3	2.45	0.52
1:D:537:HIS:O	1:D:538:ARG:CB	2.50	0.52
1:D:633:PRO:O	1:D:637:ARG:HG2	2.10	0.52
1:D:990:SER:O	1:D:999:HIS:NE2	2.38	0.52
1:A:637:ARG:N	1:A:638:PRO:CD	2.73	0.52
1:B:907:GLY:HA2	1:B:1012:ALA:HB2	1.91	0.52
1:C:356:TYR:HD1	1:C:365:THR:HG21	1.74	0.52
1:E:501:GLU:HB2	1:E:504:ASP:HB2	1.91	0.52
1:F:150:THR:H	1:F:153:ASP:HB2	1.73	0.52
1:F:436:GLY:HA2	2:F:2001:LMT:O4'	2.10	0.52
1:F:463:THR:HB	1:F:871:GLN:HE22	1.76	0.52
1:A:456:MET:HG3	1:A:875:LEU:HD11	1.92	0.51
1:B:909:ILE:HG23	1:B:910:GLY:N	2.24	0.51
1:E:981:ILE:HD12	1:E:982:LEU:N	2.25	0.51
1:A:406:VAL:O	1:A:410:ILE:HG13	2.11	0.51
1:B:49:TYR:CE1	1:B:121:GLU:HG3	2.44	0.51
1:C:519:MET:SD	1:C:519:MET:C	2.88	0.51
1:C:524:THR:CG2	1:C:970:LEU:HD12	2.40	0.51
1:D:189:ASP:HB3	1:D:192:LYS:HB2	1.92	0.51
1:D:754:GLY:O	1:D:755:SER:O	2.28	0.51
1:E:344:LEU:CD2	1:E:402:ILE:HG13	2.41	0.51
1:A:753:TRP:HD1	1:A:779:ARG:HB3	1.74	0.51
1:B:351:VAL:HG21	1:B:406:VAL:HG22	1.93	0.51
1:F:314:GLU:H	1:F:315:PRO:HD2	1.75	0.51
1:F:634:TRP:HB3	1:F:637:ARG:NH2	2.25	0.51
1:F:738:LEU:HD13	1:F:802:ALA:HB1	1.92	0.51
1:C:944:ILE:CG2	1:C:973:ILE:CD1	2.87	0.51
1:D:543:LEU:HA	1:D:546:VAL:HG23	1.92	0.51
1:E:900:VAL:HG11	1:E:942:ILE:HG13	1.91	0.51
1:A:443:VAL:O	1:A:447:MET:HB2	2.11	0.51
1:B:556:PHE:O	1:B:559:ILE:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:GLY:O	1:B:792:ASN:HB2	2.11	0.51
1:C:578:THR:HG21	1:C:587:THR:HA	1.93	0.51
1:D:115:THR:HA	1:D:118:LEU:HD22	1.90	0.51
1:D:231:ASN:HB3	1:E:582:SER:O	2.10	0.51
1:D:910:GLY:HA3	1:D:1011:THR:OG1	2.11	0.51
1:E:564:LEU:HD23	1:E:565:PRO:HD2	1.91	0.51
1:A:121:GLU:CD	1:A:121:GLU:H	2.11	0.51
1:A:958:ILE:O	1:A:961:ALA:HB3	2.11	0.51
1:C:80:SER:HA	1:C:89:THR:O	2.11	0.51
1:D:2:SER:O	1:D:6:ILE:HG13	2.10	0.51
1:E:456:MET:HG3	1:E:467:TYR:HB3	1.93	0.51
1:F:471:SER:O	1:F:475:VAL:HG13	2.11	0.51
1:A:388:PHE:CE1	1:A:469:GLN:HG2	2.46	0.51
1:B:967:ARG:HH11	1:B:967:ARG:CG	2.07	0.51
1:C:1:MET:H3	2:C:2001:LMT:H6D	1.76	0.51
1:C:150:THR:HG23	1:C:153:ASP:H	1.75	0.51
1:C:156:ASN:HD22	1:C:182:TYR:H	1.59	0.51
1:C:971:ARG:HB3	1:C:972:PRO:CD	2.41	0.51
1:D:332:VAL:O	1:D:336:SER:HB2	2.11	0.51
1:D:572:LEU:HB3	1:D:629:ILE:HB	1.92	0.51
1:D:632:LYS:HB2	1:D:633:PRO:HD2	1.93	0.51
1:D:713:GLN:O	1:D:715:VAL:N	2.43	0.51
1:F:150:THR:OG1	1:F:152:GLU:HG2	2.10	0.51
1:F:418:ARG:NH2	1:F:437:GLN:HE22	1.96	0.51
1:D:193:LEU:HB2	1:D:265:VAL:HG22	1.92	0.51
1:D:367:ILE:HG12	1:D:413:VAL:HG21	1.92	0.51
1:D:483:ILE:C	1:D:483:ILE:HD12	2.30	0.51
1:E:572:LEU:HD23	1:E:666:PHE:O	2.10	0.51
1:F:452:VAL:HG22	1:F:883:VAL:CG2	2.40	0.51
1:B:419:VAL:O	1:B:423:GLU:HB2	2.11	0.51
1:C:139:VAL:HA	1:C:290:ALA:HA	1.91	0.51
1:E:728:LEU:HD21	1:E:730:ILE:HD11	1.93	0.51
1:F:646:GLU:OE2	1:F:646:GLU:HA	2.10	0.51
1:A:749:VAL:CG2	1:A:753:TRP:HZ3	2.08	0.51
1:A:887:LEU:HD21	1:A:942:ILE:HD12	1.92	0.51
1:C:330:THR:N	1:C:331:PRO:HD2	2.25	0.51
1:C:616:ASN:HD21	1:C:619:GLY:H	1.59	0.51
1:D:80:SER:HA	1:D:89:THR:O	2.11	0.51
1:D:356:TYR:HE1	1:D:513:PHE:CZ	2.25	0.51
1:D:472:ILE:H	1:D:475:VAL:CG1	2.23	0.51
1:E:187:TRP:O	1:E:266:ALA:HB1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:917:MET:O	1:E:919:GLY:N	2.44	0.51
1:E:1005:VAL:O	1:E:1006:ILE:HG12	2.11	0.51
1:F:324:VAL:HG22	1:F:325:TYR:H	1.76	0.51
1:F:355:MET:SD	1:F:368:PRO:HB2	2.50	0.51
1:A:163:GLN:NE2	1:A:175:PHE:HE1	2.09	0.50
1:A:228:GLN:HB2	1:B:780:MET:HE1	1.93	0.50
1:B:199:THR:HG22	1:B:201:GLY:H	1.76	0.50
1:C:916:SER:O	1:C:918:ARG:N	2.43	0.50
1:D:225:VAL:H	1:E:780:MET:HE1	1.76	0.50
1:E:14:VAL:O	1:E:18:VAL:HG12	2.11	0.50
1:F:416:VAL:O	1:F:416:VAL:CG1	2.59	0.50
1:F:472:ILE:HD12	1:F:473:THR:H	1.75	0.50
1:F:682:LEU:CD1	1:F:843:VAL:HG11	2.41	0.50
1:A:705:LEU:HD13	1:A:846:ILE:HD12	1.92	0.50
1:B:448:VAL:O	1:B:452:VAL:HG23	2.11	0.50
1:C:39:ALA:HB2	1:C:673:GLU:HB3	1.93	0.50
1:C:428:ARG:NH1	1:C:432:ARG:HD3	2.26	0.50
1:C:666:PHE:CD2	1:C:716:ARG:NH2	2.79	0.50
1:C:1009:MET:HA	1:C:1009:MET:HE3	1.92	0.50
1:D:705:LEU:HD13	1:D:846:ILE:HG23	1.92	0.50
1:D:904:VAL:HG22	1:D:934:ILE:HB	1.94	0.50
1:E:746:ASN:CA	1:E:749:VAL:HG23	2.38	0.50
2:E:2002:LMT:O2'	2:E:2002:LMT:H11	2.10	0.50
1:F:194:ASN:N	1:F:194:ASN:HD22	2.09	0.50
1:F:355:MET:HE2	1:F:410:ILE:HG22	1.93	0.50
1:F:563:PHE:O	1:F:923:ASP:HB2	2.11	0.50
1:A:962:ALA:O	1:A:965:ALA:HB3	2.12	0.50
1:C:463:THR:CB	1:C:871:GLN:HE22	2.23	0.50
1:C:578:THR:O	1:C:623:SER:HB2	2.11	0.50
1:D:780:MET:HE3	1:F:220:GLY:CA	2.36	0.50
1:F:924:VAL:HA	1:F:927:GLN:HE21	1.75	0.50
1:A:853:GLY:HA2	1:C:316:PHE:CE2	2.47	0.50
1:B:929:GLY:O	1:B:932:THR:HB	2.12	0.50
1:C:469:GLN:O	1:C:473:THR:HG22	2.12	0.50
1:C:986:PRO:O	1:C:990:SER:HB3	2.11	0.50
1:D:61:VAL:HA	1:D:118:LEU:HD12	1.92	0.50
1:E:965:ALA:HA	1:E:968:MET:HE3	1.92	0.50
1:F:61:VAL:HG22	1:F:62:VAL:N	2.27	0.50
1:F:355:MET:CE	1:F:410:ILE:HG22	2.41	0.50
1:F:713:GLN:HG2	1:F:714:ARG:HB2	1.92	0.50
1:A:759:ASN:O	1:A:770:VAL:CG1	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LEU:HD13	1:B:928:VAL:HG12	1.94	0.50
1:B:718:ASN:HB2	1:B:827:LEU:HD11	1.92	0.50
1:B:791:ARG:CG	1:B:791:ARG:NH1	2.69	0.50
1:D:936:LEU:HD23	1:D:936:LEU:O	2.11	0.50
1:F:602:GLU:OE2	1:F:650:ARG:NH1	2.45	0.50
1:F:966:CYS:SG	1:F:1021:PRO:HG2	2.52	0.50
1:B:142:VAL:HG22	1:B:323:VAL:HG12	1.94	0.50
1:D:224:ALA:HB1	1:E:780:MET:HE1	1.94	0.50
1:D:532:ALA:O	1:D:536:LYS:HB2	2.12	0.50
1:D:896:ILE:N	1:D:897:PRO:HD2	2.26	0.50
1:E:197:GLN:CB	1:E:797:MET:SD	3.00	0.50
1:E:631:LEU:N	1:E:631:LEU:CD2	2.71	0.50
1:F:453:PHE:O	1:F:471:SER:OG	2.29	0.50
1:F:578:THR:HG21	1:F:587:THR:HA	1.91	0.50
1:B:555:MET:HE2	1:B:913:LEU:HD12	1.92	0.50
1:D:559:ILE:HD11	1:D:916:SER:HB2	1.93	0.50
1:E:52:ALA:HB1	1:E:56:THR:OG1	2.12	0.50
1:F:648:ALA:HB1	1:F:714:ARG:HH12	1.76	0.50
1:F:773:GLN:HG2	1:F:779:ARG:NH1	2.25	0.50
1:B:222:LEU:HD13	1:B:223:PRO:HA	1.93	0.50
1:B:336:SER:O	1:B:340:VAL:HG23	2.12	0.50
1:C:343:THR:HG21	1:C:998:GLN:OE1	2.11	0.50
1:C:347:ALA:HB1	1:C:402:ILE:HD11	1.94	0.50
1:D:791:ARG:HB2	1:D:797:MET:CE	2.42	0.50
1:E:753:TRP:CH2	1:E:785:LEU:HD22	2.46	0.50
1:F:359:LEU:CD1	1:F:365:THR:HA	2.39	0.50
1:F:985:VAL:CG2	1:F:986:PRO:HD3	2.38	0.50
1:A:138:MET:CE	1:A:325:TYR:CD1	2.95	0.50
1:A:871:GLN:O	1:A:872:ALA:HB2	2.12	0.50
1:B:356:TYR:HE1	1:B:362:PHE:CZ	2.29	0.50
1:C:158:ILE:HA	1:C:162:ILE:HD12	1.92	0.50
1:C:332:VAL:O	1:C:336:SER:HB2	2.12	0.50
1:C:592:ASP:O	1:C:596:GLU:HG2	2.11	0.50
1:C:987:LEU:HD13	1:C:1001:ILE:HG23	1.93	0.50
1:D:162:ILE:O	1:D:166:LEU:HB2	2.12	0.50
1:D:456:MET:HG2	1:D:467:TYR:HB3	1.94	0.50
1:E:344:LEU:CD2	1:E:402:ILE:CG1	2.89	0.50
1:F:561:THR:O	1:F:837:GLY:HA3	2.12	0.50
1:F:564:LEU:HD23	1:F:671:VAL:HG22	1.93	0.50
1:A:354:VAL:HG21	1:A:979:ALA:HA	1.93	0.49
1:A:363:ARG:O	1:A:367:ILE:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:GLY:H	1:A:694:VAL:HG23	1.76	0.49
1:A:914:ALA:HB2	1:A:1007:GLY:HA3	1.94	0.49
1:B:28:LEU:O	1:B:29:SER:HB3	2.12	0.49
1:B:156:ASN:ND2	1:B:182:TYR:H	1.99	0.49
1:D:192:LYS:HD3	1:D:264:ASP:O	2.11	0.49
1:E:247:GLU:HG3	1:E:268:VAL:HG11	1.94	0.49
1:F:105:VAL:CG1	1:F:109:ASN:HD21	2.25	0.49
1:F:434:SER:O	1:F:438:ILE:HG12	2.11	0.49
1:F:695:LEU:CD2	1:F:824:MET:SD	3.00	0.49
1:A:61:VAL:HA	1:A:118:LEU:HD12	1.94	0.49
1:B:741:SER:HB3	1:B:744:ASP:HB2	1.94	0.49
1:B:1018:PHE:O	1:B:1021:PRO:HG2	2.12	0.49
1:C:150:THR:OG1	1:C:151:LYS:N	2.45	0.49
1:C:366:LEU:O	1:C:369:THR:HB	2.12	0.49
1:C:434:SER:O	1:C:438:ILE:HG12	2.11	0.49
1:C:563:PHE:CD2	1:C:564:LEU:HD22	2.47	0.49
1:C:638:PRO:HD2	1:C:642:ASN:ND2	2.24	0.49
1:C:673:GLU:H	1:C:673:GLU:CD	2.14	0.49
1:E:1006:ILE:CA	1:E:1009:MET:HB2	2.27	0.49
1:F:194:ASN:HD22	1:F:194:ASN:H	1.60	0.49
1:F:898:PHE:O	1:F:902:LEU:HD22	2.12	0.49
1:A:555:MET:HA	1:A:555:MET:HE3	1.95	0.49
1:A:632:LYS:O	1:A:637:ARG:HD3	2.12	0.49
1:A:910:GLY:CA	1:A:1011:THR:HG21	2.40	0.49
1:B:551:GLY:O	1:B:555:MET:HB2	2.12	0.49
1:C:246:PHE:O	1:C:262:LEU:HD23	2.12	0.49
1:C:724:PRO:HA	1:C:810:TYR:CB	2.39	0.49
1:D:366:LEU:O	1:D:370:ILE:HG13	2.12	0.49
1:F:552:MET:HB2	1:F:909:ILE:HG23	1.94	0.49
1:A:151:LYS:NZ	1:A:151:LYS:HB3	2.28	0.49
1:C:545:TYR:CE1	1:C:906:LEU:HD11	2.47	0.49
1:C:816:GLU:OE1	1:C:824:MET:HA	2.13	0.49
1:D:716:ARG:HB2	1:D:717:PRO:HD2	1.94	0.49
1:D:835:SER:O	1:D:838:ASP:HB2	2.12	0.49
1:E:879:SER:O	1:E:883:VAL:HG12	2.12	0.49
1:F:326:PRO:HB3	1:F:610:PHE:HB2	1.93	0.49
1:A:228:GLN:HB2	1:B:780:MET:CE	2.42	0.49
1:B:214:ILE:HG23	1:B:237:LYS:N	2.27	0.49
1:B:407:ASP:OD2	1:B:939:LYS:NZ	2.41	0.49
1:C:229:GLN:HA	1:C:229:GLN:NE2	2.27	0.49
1:C:340:VAL:CA	1:C:343:THR:HG23	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:PHE:HA	1:D:290:ALA:O	2.12	0.49
1:D:705:LEU:HD13	1:D:846:ILE:CG2	2.43	0.49
1:D:713:GLN:HG2	1:D:714:ARG:CG	2.41	0.49
1:D:948:ALA:HB1	1:D:1024:TYR:CE2	2.47	0.49
1:E:429:GLU:HA	1:E:432:ARG:HG3	1.93	0.49
1:E:430:ALA:O	1:E:434:SER:HB2	2.13	0.49
1:F:682:LEU:HD13	1:F:843:VAL:HG11	1.94	0.49
1:F:843:VAL:O	1:F:847:VAL:HB	2.11	0.49
1:A:577:GLN:HA	1:A:577:GLN:HE21	1.77	0.49
1:A:683:PHE:CD1	1:A:818:TYR:CD1	3.01	0.49
1:B:95:GLU:HA	1:B:95:GLU:OE2	2.12	0.49
1:B:159:VAL:HG11	1:B:181:GLN:HG3	1.94	0.49
1:B:190:PRO:HG3	1:B:788:TRP:CZ2	2.47	0.49
1:B:335:ALA:O	1:B:339:GLU:HB2	2.13	0.49
1:C:45:VAL:HG22	1:C:129:VAL:HG22	1.93	0.49
1:D:871:GLN:O	1:D:872:ALA:CB	2.60	0.49
1:E:228:GLN:HA	1:F:780:MET:CE	2.42	0.49
1:E:247:GLU:HG3	1:E:268:VAL:HG13	1.93	0.49
1:F:188:LEU:HD23	1:F:266:ALA:HB2	1.95	0.49
1:F:969:ARG:O	1:F:972:PRO:HD2	2.12	0.49
1:A:549:VAL:O	1:A:553:ILE:HG12	2.13	0.49
2:A:2001:LMT:H6D	1:C:29:SER:OG	2.12	0.49
1:B:139:VAL:HG11	3:B:2001:P9D:C7	2.42	0.49
1:B:280:GLN:NE2	1:B:588:GLN:OE1	2.45	0.49
1:C:1:MET:N	2:C:2001:LMT:H6D	2.28	0.49
1:C:23:GLY:HA3	1:C:377:LEU:O	2.13	0.49
1:C:214:ILE:HD13	1:C:237:LYS:H	1.76	0.49
1:C:742:LEU:C	1:C:744:ASP:H	2.15	0.49
1:C:836:SER:O	1:C:840:MET:HB2	2.12	0.49
1:D:210:GLN:NE2	1:D:249:ILE:HA	2.27	0.49
1:D:275:TYR:O	1:F:222:LEU:HD12	2.13	0.49
1:D:355:MET:HE1	1:D:369:THR:HG22	1.93	0.49
1:D:580:PRO:HB3	1:D:723:GLU:HB3	1.94	0.49
1:E:712:LEU:HD21	1:E:842:ALA:HB3	1.93	0.49
1:F:659:LYS:CG	1:F:660:ASP:H	2.24	0.49
1:F:774:GLY:O	1:F:779:ARG:NH1	2.45	0.49
1:F:944:ILE:CG2	1:F:973:ILE:CD1	2.90	0.49
1:A:537:HIS:O	1:A:538:ARG:HB2	2.13	0.49
1:B:139:VAL:HG21	3:B:2001:P9D:N10	2.28	0.49
1:C:362:PHE:C	1:C:364:ALA:H	2.14	0.49
1:C:730:ILE:HD12	1:C:730:ILE:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:VAL:HG23	1:D:334:SER:N	2.27	0.49
1:D:969:ARG:O	1:D:972:PRO:HG2	2.12	0.49
1:E:53:SER:O	1:E:54:ALA:C	2.50	0.49
1:E:527:TYR:OH	1:E:966:CYS:HB3	2.13	0.49
1:F:753:TRP:HZ2	1:F:785:LEU:HA	1.77	0.49
1:A:306:ILE:O	1:A:307:ARG:C	2.50	0.49
1:B:740:VAL:HG13	1:B:745:ILE:HD11	1.95	0.49
1:C:563:PHE:HB2	1:C:865:GLU:HG3	1.95	0.49
1:C:958:ILE:HD13	1:C:1029:THR:HG22	1.95	0.49
1:D:786:SER:C	1:D:788:TRP:H	2.15	0.49
1:D:934:ILE:HD12	1:D:934:ILE:C	2.32	0.49
1:E:904:VAL:HB	1:E:905:PRO:CD	2.40	0.49
1:F:355:MET:HE2	1:F:410:ILE:CG2	2.43	0.49
1:A:472:ILE:HG13	1:A:473:THR:N	2.27	0.49
1:A:587:THR:O	1:A:591:VAL:HG23	2.11	0.49
1:A:1011:THR:O	1:A:1015:LEU:HB2	2.13	0.49
1:B:298:ASN:O	1:B:302:THR:HG23	2.13	0.49
1:B:383:LEU:HD13	1:B:388:PHE:CB	2.43	0.49
1:C:175:PHE:C	1:C:175:PHE:CD1	2.87	0.49
1:C:443:VAL:HG12	1:C:890:LEU:HD21	1.94	0.49
1:C:789:TYR:HB3	1:C:797:MET:HG3	1.93	0.49
1:D:129:VAL:HG23	1:E:113:LEU:HD21	1.95	0.49
1:E:541:TYR:O	1:E:1019:TRP:HZ3	1.95	0.49
1:A:352:PHE:HD1	1:A:369:THR:HG21	1.77	0.48
1:A:925:PHE:O	1:A:1001:ILE:HD12	2.13	0.48
1:B:261:ARG:HH22	1:B:263:LYS:HE3	1.78	0.48
1:B:298:ASN:HD22	1:B:300:LEU:H	1.61	0.48
1:B:573:PHE:CE2	1:B:668:PRO:HB3	2.48	0.48
1:C:573:PHE:O	1:C:665:ALA:HA	2.13	0.48
1:C:914:ALA:O	1:C:918:ARG:HB3	2.13	0.48
1:D:555:MET:SD	1:D:913:LEU:HD12	2.53	0.48
1:D:700:ASN:O	1:D:701:LYS:C	2.50	0.48
1:E:791:ARG:NH1	1:E:791:ARG:CG	2.64	0.48
1:E:906:LEU:HD23	1:E:1015:LEU:HB3	1.95	0.48
1:F:451:ALA:HB1	1:F:882:VAL:HG12	1.94	0.48
1:F:699:ARG:HG2	1:F:824:MET:SD	2.53	0.48
1:E:965:ALA:O	1:E:968:MET:HB3	2.12	0.48
1:B:152:GLU:CD	1:B:152:GLU:H	2.15	0.48
1:B:472:ILE:HD12	2:B:2003:LMT:H82	1.96	0.48
1:D:713:GLN:O	1:D:714:ARG:C	2.51	0.48
1:F:575:GLN:O	1:F:663:VAL:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:694:VAL:O	1:F:697:GLN:HB2	2.12	0.48
1:A:756:SER:O	1:A:771:TYR:HA	2.14	0.48
1:A:928:VAL:HG12	1:A:1001:ILE:HD11	1.94	0.48
1:B:655:PHE:HD1	1:B:658:PHE:CE1	2.32	0.48
1:C:910:GLY:HA3	1:C:1011:THR:CB	2.42	0.48
1:E:278:ASN:HB3	1:E:613:THR:HG22	1.95	0.48
1:E:970:LEU:O	1:E:974:VAL:HG23	2.14	0.48
1:F:930:LEU:O	1:F:933:THR:HB	2.14	0.48
1:A:455:PRO:HG3	1:A:879:SER:HA	1.96	0.48
1:A:1018:PHE:O	1:A:1021:PRO:HD2	2.13	0.48
1:B:108:GLN:HE22	1:C:109:ASN:HA	1.79	0.48
1:B:169:THR:HB	1:B:172:VAL:HG21	1.94	0.48
1:B:442:LEU:HA	1:B:445:ILE:HG23	1.94	0.48
1:C:150:THR:N	1:C:153:ASP:HB2	2.28	0.48
1:C:969:ARG:O	1:C:973:ILE:HD12	2.13	0.48
1:D:950:GLU:O	1:D:953:GLU:HG3	2.14	0.48
2:D:2002:LMT:O5B	2:D:2002:LMT:O3'	2.20	0.48
1:F:239:ARG:NH1	1:F:239:ARG:CG	2.64	0.48
1:A:303:ALA:CB	1:A:330:THR:HG21	2.43	0.48
1:B:156:ASN:HD21	1:B:768:LYS:HZ3	1.61	0.48
1:D:411:VAL:CG1	1:D:442:LEU:HD11	2.44	0.48
1:D:703:LEU:CD1	1:D:717:PRO:HD3	2.43	0.48
1:E:1014:VAL:O	1:E:1014:VAL:HG13	2.13	0.48
1:F:671:VAL:CG2	1:F:674:LEU:HD22	2.43	0.48
1:A:451:ALA:HB1	1:A:882:VAL:HG12	1.91	0.48
1:A:918:ARG:HB3	1:A:920:LEU:HD22	1.96	0.48
1:B:185:ARG:HB2	1:B:269:GLY:O	2.14	0.48
1:B:352:PHE:CE1	1:B:365:THR:HG21	2.49	0.48
1:B:429:GLU:OE2	1:B:429:GLU:HA	2.13	0.48
1:B:456:MET:HE2	1:B:471:SER:HB2	1.95	0.48
1:C:547:VAL:O	1:C:550:ALA:HB3	2.13	0.48
1:C:646:GLU:O	1:C:647:LEU:C	2.52	0.48
1:C:755:SER:HB3	1:C:771:TYR:CD1	2.49	0.48
1:D:678:THR:HG22	1:D:679:GLY:N	2.26	0.48
1:D:734:LYS:O	1:D:738:LEU:HB2	2.13	0.48
1:E:62:VAL:O	1:E:66:GLU:HB2	2.14	0.48
1:E:910:GLY:HA3	1:E:1011:THR:HG23	1.96	0.48
1:F:634:TRP:HE3	1:F:634:TRP:N	2.10	0.48
1:A:904:VAL:CB	1:A:905:PRO:HD3	2.44	0.48
1:A:913:LEU:HB3	1:A:917:MET:HE2	1.95	0.48
1:A:1014:VAL:O	1:A:1014:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:TRP:O	1:C:266:ALA:CB	2.57	0.48
1:D:298:ASN:HD22	1:D:301:ASP:H	1.60	0.48
1:D:443:VAL:O	1:D:447:MET:HB2	2.13	0.48
1:E:38:ILE:HA	1:E:465:VAL:HG11	1.96	0.48
1:F:372:VAL:O	1:F:376:LEU:HB2	2.13	0.48
1:F:606:VAL:HG12	1:F:607:SER:N	2.27	0.48
1:F:1011:THR:O	1:F:1015:LEU:HB2	2.14	0.48
1:B:13:TRP:O	1:B:16:ALA:HB3	2.13	0.48
1:B:248:ASN:ND2	1:B:261:ARG:HH21	2.12	0.48
1:B:323:VAL:O	1:B:323:VAL:CG2	2.61	0.48
1:C:46:GLN:NE2	1:C:89:THR:CG2	2.76	0.48
1:C:415:ASN:O	1:C:419:VAL:HG23	2.14	0.48
1:C:483:ILE:HD11	2:C:2001:LMT:H61	1.96	0.48
1:D:887:LEU:HD22	1:D:942:ILE:CD1	2.43	0.48
1:D:906:LEU:O	1:D:1011:THR:HB	2.14	0.48
1:E:727:LYS:HD3	1:E:809:GLU:OE1	2.14	0.48
1:E:896:ILE:N	1:E:897:PRO:HD2	2.29	0.48
1:B:438:ILE:O	1:B:439:GLN:C	2.53	0.48
1:B:598:LEU:HD22	1:B:629:ILE:HD12	1.95	0.48
1:D:966:CYS:SG	1:D:1021:PRO:CG	3.02	0.48
1:E:447:MET:HE2	2:E:2002:LMT:H72	1.93	0.48
1:E:749:VAL:HA	1:E:753:TRP:HD1	1.77	0.48
1:F:605:SER:OG	1:F:647:LEU:HD22	2.13	0.48
1:A:367:ILE:HD11	1:A:413:VAL:HG23	1.93	0.47
1:A:705:LEU:HD11	1:A:846:ILE:HG23	1.93	0.47
1:A:935:GLY:O	1:A:938:ALA:HB3	2.14	0.47
1:B:438:ILE:HG23	1:B:442:LEU:HG	1.95	0.47
1:B:584:ALA:HB2	1:B:622:GLN:HG2	1.96	0.47
1:C:425:LEU:HD22	1:C:429:GLU:HB3	1.94	0.47
1:C:649:LYS:HZ3	1:C:713:GLN:NE2	2.11	0.47
1:C:659:LYS:HZ2	1:C:661:ALA:HB2	1.79	0.47
1:D:219:LEU:HD22	1:E:726:TYR:HB2	1.96	0.47
1:E:760:ASP:HB3	1:E:767:VAL:CG2	2.43	0.47
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.95	0.47
1:F:310:ILE:HG12	1:F:325:TYR:OH	2.14	0.47
2:F:2001:LMT:H6E	2:F:2001:LMT:H1B	1.95	0.47
1:A:149:MET:SD	1:A:321:MET:CE	3.02	0.47
1:A:337:ILE:HD12	1:A:338:HIS:N	2.28	0.47
1:A:479:ALA:O	1:A:483:ILE:HG23	2.14	0.47
1:B:989:ILE:O	1:B:989:ILE:HG22	2.14	0.47
1:C:840:MET:HG3	1:C:858:TRP:CH2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:GLN:HA	1:F:780:MET:HE1	1.95	0.47
1:E:967:ARG:HH11	1:E:967:ARG:CG	2.22	0.47
1:F:298:ASN:HB3	1:F:301:ASP:HB2	1.95	0.47
1:F:606:VAL:HG13	1:F:607:SER:H	1.79	0.47
1:F:726:TYR:OH	1:F:782:PRO:HB3	2.13	0.47
1:F:766:ARG:HH11	1:F:766:ARG:CG	2.27	0.47
1:F:779:ARG:HH11	1:F:779:ARG:CG	2.21	0.47
1:A:166:LEU:HD12	1:A:166:LEU:HA	1.78	0.47
1:B:375:VAL:HG11	1:B:405:LEU:HD11	1.94	0.47
1:B:655:PHE:CD1	1:B:658:PHE:HE1	2.33	0.47
1:C:47:VAL:HG11	1:C:127:ILE:HG13	1.95	0.47
1:C:792:ASN:HD22	1:C:794:LYS:HB2	1.78	0.47
1:C:845:GLU:C	1:C:847:VAL:H	2.17	0.47
1:D:388:PHE:CE2	1:D:472:ILE:HG12	2.42	0.47
1:D:872:ALA:HA	1:D:875:LEU:HB3	1.96	0.47
1:F:466:ILE:O	1:F:467:TYR:C	2.51	0.47
1:A:151:LYS:NZ	1:A:151:LYS:CB	2.78	0.47
1:A:872:ALA:O	1:A:875:LEU:O	2.33	0.47
1:D:845:GLU:O	1:D:848:LYS:CG	2.57	0.47
1:D:881:LEU:HD12	1:F:21:LEU:HD22	1.96	0.47
1:E:445:ILE:C	1:E:445:ILE:HD12	2.34	0.47
1:E:583:SER:HA	1:E:622:GLN:NE2	2.26	0.47
1:E:680:PHE:CZ	1:E:828:GLY:HA3	2.50	0.47
1:E:924:VAL:HG23	1:E:925:PHE:HD2	1.80	0.47
1:F:30:LEU:HD12	1:F:30:LEU:HA	1.73	0.47
1:F:416:VAL:O	1:F:420:MET:HB2	2.14	0.47
1:F:485:ALA:O	1:F:490:PRO:HD3	2.14	0.47
1:B:228:GLN:NE2	1:B:231:ASN:HB2	2.30	0.47
1:C:239:ARG:NH1	1:C:239:ARG:CG	2.57	0.47
1:C:355:MET:CE	1:C:410:ILE:CG2	2.93	0.47
1:C:957:GLY:O	1:C:959:VAL:N	2.47	0.47
1:E:356:TYR:CE1	1:E:362:PHE:CE1	3.03	0.47
1:E:361:ASN:OD1	1:E:363:ARG:HG3	2.14	0.47
1:E:457:ALA:O	1:E:468:ARG:NH1	2.46	0.47
1:E:507:GLU:C	1:E:509:LYS:H	2.17	0.47
1:E:632:LYS:HB2	1:E:633:PRO:HD2	1.97	0.47
1:E:682:LEU:HD13	1:E:856:TYR:HD1	1.78	0.47
1:F:139:VAL:HG23	1:F:327:TYR:HB3	1.97	0.47
1:F:809:GLU:O	1:F:810:TYR:CB	2.62	0.47
1:A:577:GLN:HA	1:A:577:GLN:NE2	2.30	0.47
1:A:580:PRO:HB3	1:A:723:GLU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLN:O	1:C:391:ASN:HB2	2.14	0.47
1:C:427:PRO:HG3	1:C:499:PRO:HG3	1.95	0.47
1:D:579:PRO:O	1:D:582:SER:OG	2.30	0.47
1:D:866:ARG:HA	1:D:866:ARG:NE	2.23	0.47
1:E:111:LEU:O	1:E:111:LEU:HD22	2.14	0.47
1:A:184:MET:HB3	1:A:770:VAL:HB	1.96	0.47
1:A:233:THR:HG22	1:A:235:ILE:HG22	1.96	0.47
1:B:199:THR:HG22	1:B:201:GLY:N	2.30	0.47
1:B:753:TRP:CE2	1:B:785:LEU:HD13	2.49	0.47
1:B:847:VAL:HG11	1:B:856:TYR:CE2	2.49	0.47
1:B:868:SER:HA	1:B:871:GLN:HE21	1.80	0.47
1:C:61:VAL:CG2	1:C:62:VAL:N	2.68	0.47
1:C:213:GLN:HB2	1:C:239:ARG:HG3	1.97	0.47
1:C:424:GLY:HA3	1:C:502:LYS:HB3	1.96	0.47
1:C:929:GLY:HA2	1:C:932:THR:HG23	1.96	0.47
1:C:971:ARG:HB3	1:C:972:PRO:HD3	1.96	0.47
1:D:225:VAL:CG2	1:D:228:GLN:HB2	2.44	0.47
1:D:410:ILE:O	1:D:411:VAL:C	2.52	0.47
1:D:577:GLN:HE21	1:D:577:GLN:CA	2.23	0.47
1:E:314:GLU:N	1:E:315:PRO:HD2	2.29	0.47
1:E:671:VAL:O	1:E:671:VAL:HG12	2.14	0.47
1:F:727:LYS:HG2	1:F:807:LYS:HE3	1.95	0.47
1:F:929:GLY:HA2	1:F:932:THR:HG23	1.97	0.47
1:F:959:VAL:HG22	1:F:1025:VAL:HG11	1.96	0.47
1:B:391:ASN:HD21	1:B:469:GLN:NE2	2.12	0.47
1:B:1013:THR:O	1:B:1017:ILE:HG12	2.14	0.47
1:C:162:ILE:O	1:C:165:PRO:HD2	2.15	0.47
1:C:167:SER:HB2	1:C:175:PHE:CE2	2.48	0.47
1:E:542:LEU:O	1:E:545:TYR:HB3	2.15	0.47
1:E:586:ARG:O	1:E:589:VAL:HG12	2.15	0.47
1:F:447:MET:CE	1:F:886:CYS:HB3	2.45	0.47
1:A:350:LEU:O	1:A:354:VAL:HG13	2.15	0.47
1:A:527:TYR:O	1:A:531:VAL:HG23	2.14	0.47
1:A:578:THR:HG21	1:A:587:THR:HA	1.96	0.47
1:A:776:PRO:O	1:A:780:MET:HG2	2.15	0.47
1:B:428:ARG:O	1:B:432:ARG:HG2	2.15	0.47
1:C:17:LEU:HD23	1:C:20:MET:CE	2.45	0.47
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.97	0.47
1:C:281:PHE:O	1:C:282:ASN:HB2	2.14	0.47
1:C:420:MET:HE2	1:C:500:ILE:CG2	2.45	0.47
1:D:343:THR:CG2	1:D:998:GLN:HE22	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:577:GLN:HA	1:D:577:GLN:NE2	2.30	0.47
1:D:892:GLU:OE1	1:F:8:ARG:HG2	2.15	0.47
1:E:896:ILE:N	1:E:897:PRO:CD	2.78	0.47
1:F:57:VAL:CG1	1:F:82:SER:HB3	2.37	0.47
1:F:1006:ILE:O	1:F:1010:VAL:HG23	2.15	0.47
1:A:849:GLN:HG3	1:A:849:GLN:O	2.15	0.47
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.95	0.47
1:B:951:LEU:HD11	1:B:968:MET:CE	2.45	0.47
1:B:987:LEU:HD23	1:B:1001:ILE:HG13	1.97	0.47
1:C:480:LEU:O	1:C:484:VAL:HG13	2.15	0.47
1:C:843:VAL:HA	1:C:846:ILE:HG23	1.96	0.47
1:D:472:ILE:N	1:D:475:VAL:HG13	2.24	0.47
1:D:483:ILE:HD12	1:D:483:ILE:O	2.15	0.47
1:D:598:LEU:O	1:D:602:GLU:HB2	2.14	0.47
1:D:725:GLN:HE21	1:F:235:ILE:HD11	1.80	0.47
1:E:164:ASP:OD1	1:F:67:GLN:HG3	2.15	0.47
1:E:281:PHE:CD2	1:E:324:VAL:HG11	2.50	0.47
1:F:779:ARG:HG2	1:F:779:ARG:NH1	2.28	0.47
1:A:222:LEU:HA	1:A:223:PRO:C	2.35	0.46
1:A:878:LEU:HD11	1:C:25:LEU:CD1	2.45	0.46
1:A:985:VAL:N	1:A:1006:ILE:HD11	2.30	0.46
1:B:233:THR:HG23	1:C:725:GLN:HG2	1.97	0.46
1:B:359:LEU:HG	1:B:417:GLU:HG2	1.96	0.46
1:B:537:HIS:O	1:B:540:PRO:HG2	2.14	0.46
1:B:900:VAL:O	1:B:903:VAL:HG13	2.15	0.46
1:D:651:ALA:O	1:D:655:PHE:CD1	2.69	0.46
1:E:414:GLU:HG3	1:E:415:ASN:N	2.29	0.46
1:F:376:LEU:HA	1:F:376:LEU:HD12	1.48	0.46
1:A:255:PRO:C	1:A:257:GLY:H	2.19	0.46
1:A:789:TYR:CE1	1:A:799:PRO:HG3	2.51	0.46
1:C:188:LEU:HD23	1:C:266:ALA:HB2	1.97	0.46
1:C:713:GLN:O	1:C:714:ARG:HB2	2.14	0.46
1:D:419:VAL:HG23	1:D:430:ALA:CB	2.43	0.46
1:E:46:GLN:NE2	1:E:89:THR:OG1	2.47	0.46
1:E:298:ASN:HD21	1:E:300:LEU:HB2	1.80	0.46
1:E:572:LEU:HG	1:E:644:VAL:HG13	1.98	0.46
1:E:572:LEU:O	1:E:629:ILE:HG12	2.15	0.46
1:F:281:PHE:O	1:F:282:ASN:HB2	2.15	0.46
1:F:355:MET:CE	1:F:410:ILE:HG21	2.44	0.46
1:F:452:VAL:HG12	1:F:931:LEU:HD13	1.97	0.46
1:A:958:ILE:HG21	1:A:1028:SER:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:O	1:B:3:LYS:N	2.48	0.46
1:B:598:LEU:HA	1:B:602:GLU:HB2	1.96	0.46
1:B:599:LEU:O	1:B:603:SER:HB3	2.15	0.46
3:B:2001:P9D:C25	3:B:2001:P9D:H37	2.44	0.46
1:D:155:SER:HA	1:D:287:SER:OG	2.15	0.46
1:D:411:VAL:HG11	1:D:442:LEU:CD1	2.46	0.46
1:E:145:THR:HG21	1:E:322:LYS:HD2	1.98	0.46
1:F:30:LEU:HD11	1:F:384:ALA:HA	1.97	0.46
1:F:142:VAL:HG21	1:F:321:MET:HE2	1.96	0.46
1:F:145:THR:N	1:F:320:GLY:O	2.47	0.46
1:C:524:THR:HG22	1:C:970:LEU:HD12	1.97	0.46
1:C:791:ARG:HA	1:C:797:MET:CE	2.46	0.46
1:E:539:ALA:N	1:E:540:PRO:HD2	2.30	0.46
1:F:13:TRP:O	1:F:17:LEU:HG	2.15	0.46
1:F:355:MET:HE1	1:F:410:ILE:CG2	2.46	0.46
1:F:555:MET:HE2	1:F:913:LEU:HG	1.97	0.46
1:A:568:ASP:OD2	1:A:644:VAL:HG12	2.16	0.46
1:A:695:LEU:HD22	1:A:824:MET:CE	2.46	0.46
1:B:315:PRO:HB2	1:B:316:PHE:CD1	2.49	0.46
1:B:574:ALA:HB3	1:B:627:ALA:HB3	1.98	0.46
1:B:903:VAL:HG11	1:B:941:ALA:HB2	1.96	0.46
1:C:367:ILE:HG23	1:C:492:LEU:CD1	2.46	0.46
1:C:659:LYS:HZ3	1:C:661:ALA:HB2	1.79	0.46
1:C:701:LYS:O	1:C:705:LEU:HD12	2.16	0.46
1:D:63:GLN:O	1:D:67:GLN:HG3	2.15	0.46
1:D:253:VAL:HA	1:D:259:GLN:HA	1.98	0.46
1:D:616:ASN:HB2	1:D:624:SER:HB2	1.98	0.46
1:E:49:TYR:HE2	1:E:60:THR:HG21	1.81	0.46
1:E:199:THR:HG22	1:E:201:GLY:H	1.79	0.46
1:E:631:LEU:CD1	1:E:644:VAL:HG22	2.44	0.46
1:F:987:LEU:HA	1:F:998:GLN:HE21	1.81	0.46
1:B:449:LEU:O	1:B:453:PHE:HD2	1.98	0.46
1:C:176:GLN:HE22	1:C:620:ARG:NH2	2.14	0.46
1:E:340:VAL:HG22	1:E:399:VAL:CG2	2.45	0.46
1:F:156:ASN:HD22	1:F:181:GLN:HA	1.79	0.46
1:F:910:GLY:H	1:F:1011:THR:HG21	1.81	0.46
1:A:228:GLN:NE2	1:A:229:GLN:H	2.14	0.46
1:A:680:PHE:HB2	1:A:858:TRP:HZ3	1.81	0.46
1:B:158:ILE:HG12	1:B:162:ILE:HD12	1.96	0.46
1:B:420:MET:SD	1:B:427:PRO:HA	2.55	0.46
1:E:151:LYS:O	1:E:154:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:ILE:H	1:F:127:ILE:HD12	1.81	0.46
1:F:641:GLU:O	1:F:650:ARG:NH2	2.49	0.46
1:F:912:LEU:HD23	1:F:926:PHE:CZ	2.51	0.46
1:A:163:GLN:NE2	1:A:175:PHE:CE1	2.84	0.46
1:A:193:LEU:HD23	1:A:198:LEU:O	2.15	0.46
1:A:672:LEU:O	1:A:674:LEU:N	2.49	0.46
1:A:747:SER:O	1:A:751:ILE:HG13	2.15	0.46
1:C:324:VAL:C	1:C:326:PRO:HD2	2.35	0.46
1:C:337:ILE:HA	1:C:340:VAL:HG12	1.97	0.46
1:C:535:LEU:HD12	1:C:963:ILE:CD1	2.45	0.46
1:D:159:VAL:HG11	1:D:181:GLN:HG2	1.98	0.46
1:E:298:ASN:ND2	1:E:301:ASP:H	2.14	0.46
1:F:739:GLY:O	1:F:741:SER:N	2.49	0.46
1:A:108:GLN:HE21	1:B:112:GLN:HE21	1.64	0.46
1:A:716:ARG:CZ	1:A:827:LEU:CD1	2.94	0.46
1:C:250:LEU:O	1:C:250:LEU:HD12	2.15	0.46
1:C:329:THR:HG21	1:C:672:LEU:HD13	1.96	0.46
1:E:357:LEU:O	1:E:360:GLN:NE2	2.49	0.46
1:E:584:ALA:HB2	1:E:622:GLN:HG2	1.98	0.46
1:E:895:SER:C	1:E:897:PRO:HD2	2.36	0.46
1:A:382:VAL:HG21	1:A:476:SER:OG	2.16	0.46
1:A:388:PHE:HD1	1:A:469:GLN:HE21	1.64	0.46
1:A:812:SER:HA	1:A:813:PRO:HD2	1.68	0.46
1:A:956:LYS:O	1:A:957:GLY:C	2.54	0.46
2:A:2001:LMT:O3'	2:A:2001:LMT:H2B	2.16	0.46
1:B:234:ILE:O	1:B:234:ILE:HG12	2.16	0.46
1:B:660:ASP:O	1:B:661:ALA:HB2	2.16	0.46
1:C:143:VAL:HG22	1:C:144:SER:H	1.80	0.46
1:C:560:PRO:HG2	1:C:921:SER:CB	2.44	0.46
1:C:573:PHE:CE2	1:C:668:PRO:HG3	2.51	0.46
1:C:682:LEU:HD21	1:C:856:TYR:HB2	1.97	0.46
1:D:910:GLY:HA3	1:D:1011:THR:HG1	1.80	0.46
1:E:36:PRO:HG3	1:E:469:GLN:HG3	1.98	0.46
1:E:698:ALA:HB2	1:E:851:PRO:HG2	1.97	0.46
1:F:903:VAL:HG11	1:F:941:ALA:HB2	1.97	0.46
1:A:162:ILE:HG22	1:A:166:LEU:HD22	1.97	0.45
1:A:616:ASN:HD22	1:A:624:SER:CB	2.29	0.45
1:A:842:ALA:O	1:A:846:ILE:HG12	2.16	0.45
1:B:2:SER:O	1:B:6:ILE:N	2.40	0.45
1:B:509:LYS:O	1:B:510:GLY:O	2.33	0.45
1:D:883:VAL:O	1:D:887:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:GLU:O	1:F:249:ILE:N	2.49	0.45
1:F:480:LEU:O	1:F:484:VAL:HG13	2.15	0.45
1:A:228:GLN:CB	1:B:780:MET:HE1	2.45	0.45
1:B:315:PRO:HB2	1:B:316:PHE:HD1	1.80	0.45
1:B:383:LEU:HD21	1:B:473:THR:HA	1.99	0.45
1:B:716:ARG:HB2	1:B:717:PRO:HD2	1.98	0.45
1:C:36:PRO:HG2	1:C:38:ILE:HG22	1.98	0.45
1:C:469:GLN:HA	1:C:472:ILE:HD11	1.97	0.45
1:C:542:LEU:O	1:C:545:TYR:HB3	2.17	0.45
1:C:913:LEU:O	1:C:916:SER:N	2.49	0.45
1:E:48:SER:HA	1:E:87:SER:HA	1.98	0.45
1:E:492:LEU:HD22	1:E:496:MET:CE	2.45	0.45
1:F:374:VAL:CG1	1:F:484:VAL:HG11	2.47	0.45
1:F:498:LYS:HA	1:F:498:LYS:HD3	1.43	0.45
1:A:359:LEU:O	1:A:361:ASN:HB2	2.15	0.45
1:A:467:TYR:C	1:A:468:ARG:O	2.53	0.45
1:A:876:TYR:O	1:A:880:LEU:HD13	2.15	0.45
1:A:895:SER:O	1:A:898:PHE:HB2	2.17	0.45
1:B:193:LEU:CD1	1:B:265:VAL:CG2	2.88	0.45
1:B:354:VAL:CG1	1:B:978:LEU:HD22	2.45	0.45
1:C:261:ARG:NH1	1:C:261:ARG:CG	2.67	0.45
1:D:134:LYS:HE2	1:D:675:GLY:HA2	1.97	0.45
1:D:361:ASN:C	1:D:362:PHE:O	2.54	0.45
1:F:685:GLN:NE2	1:F:687:GLN:HE21	2.10	0.45
1:A:139:VAL:HA	1:A:289:ILE:O	2.16	0.45
1:A:139:VAL:O	1:A:326:PRO:HD2	2.16	0.45
1:A:485:ALA:HA	1:A:489:THR:OG1	2.17	0.45
1:A:516:PHE:O	1:A:519:MET:HB2	2.17	0.45
1:A:789:TYR:HE1	1:A:799:PRO:HG3	1.81	0.45
1:C:186:ILE:HD13	1:C:262:LEU:HD21	1.97	0.45
1:C:667:ALA:O	1:C:678:THR:HB	2.17	0.45
1:D:222:LEU:HG	1:E:622:GLN:OE1	2.17	0.45
1:D:568:ASP:HB3	1:D:634:TRP:HH2	1.76	0.45
1:E:4:PHE:CD2	1:E:4:PHE:C	2.89	0.45
1:E:197:GLN:HB2	1:E:797:MET:SD	2.56	0.45
1:E:367:ILE:HB	1:E:368:PRO:CD	2.46	0.45
1:E:584:ALA:O	1:E:588:GLN:HB2	2.17	0.45
1:E:610:PHE:CD2	3:E:2001:P9D:H18	2.51	0.45
1:E:831:ALA:HB3	1:E:834:LEU:HD13	1.99	0.45
1:F:20:MET:HG3	1:F:374:VAL:HG23	1.99	0.45
1:F:151:LYS:HB2	1:F:152:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:ILE:HG22	1:A:827:LEU:N	2.30	0.45
1:A:951:LEU:O	1:A:956:LYS:HB2	2.17	0.45
1:A:1005:VAL:HG23	1:A:1006:ILE:N	2.31	0.45
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.66	0.45
1:B:456:MET:HG2	1:B:471:SER:HB2	1.99	0.45
1:C:410:ILE:HG13	1:C:411:VAL:N	2.31	0.45
1:C:738:LEU:HD22	1:C:798:VAL:HG23	1.98	0.45
1:D:66:GLU:OE1	1:D:820:GLY:HA2	2.17	0.45
1:A:33:ASN:O	1:A:391:ASN:HA	2.16	0.45
1:A:933:THR:HG23	1:A:1009:MET:HE3	1.99	0.45
1:B:47:VAL:CG2	1:B:127:ILE:HG13	2.46	0.45
1:B:156:ASN:HD21	1:B:768:LYS:HZ2	1.62	0.45
1:B:282:ASN:HA	1:B:595:ARG:HD2	1.98	0.45
1:B:498:LYS:HA	1:B:498:LYS:HE3	1.98	0.45
1:C:99:ASP:HB3	1:C:102:ILE:HG13	1.97	0.45
1:C:909:ILE:HG13	1:C:910:GLY:N	2.32	0.45
1:D:133:VAL:HG23	1:D:293:LEU:O	2.16	0.45
1:E:925:PHE:O	1:E:1001:ILE:CG2	2.65	0.45
1:F:357:LEU:HD22	1:F:516:PHE:CE2	2.52	0.45
1:F:606:VAL:CG1	1:F:607:SER:H	2.29	0.45
1:A:5:PHE:CE2	1:A:487:ILE:HG12	2.51	0.45
1:A:449:LEU:C	1:A:449:LEU:HD13	2.37	0.45
1:A:572:LEU:HD12	1:A:666:PHE:O	2.17	0.45
1:A:709:ASN:HA	1:A:710:PRO:HD3	1.90	0.45
1:A:971:ARG:N	1:A:972:PRO:HD2	2.32	0.45
1:B:986:PRO:O	1:B:990:SER:N	2.50	0.45
1:C:597:TYR:CB	1:C:654:HIS:CE1	2.99	0.45
1:C:729:GLU:C	1:C:730:ILE:HD12	2.37	0.45
1:C:910:GLY:HA3	1:C:1011:THR:HB	1.99	0.45
1:C:995:SER:HA	1:C:998:GLN:HB2	1.99	0.45
1:D:1009:MET:O	1:D:1013:THR:HG22	2.16	0.45
1:E:169:THR:HB	1:E:172:VAL:HG21	1.99	0.45
1:E:188:LEU:HD23	1:E:200:PRO:HB3	1.99	0.45
1:E:694:VAL:O	1:E:697:GLN:HG2	2.16	0.45
1:E:761:PHE:CE2	1:E:763:ASP:HB2	2.52	0.45
1:E:907:GLY:HA2	1:E:1012:ALA:HB2	1.99	0.45
1:A:372:VAL:HG22	1:A:405:LEU:CD2	2.47	0.45
1:A:404:LEU:HD22	1:A:936:LEU:HD12	1.99	0.45
1:A:563:PHE:CE2	1:A:564:LEU:HD12	2.52	0.45
1:A:711:ALA:O	1:A:831:ALA:N	2.43	0.45
1:A:783:ASP:OD1	1:A:783:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLU:H	1:B:121:GLU:CD	2.20	0.45
1:B:160:SER:HA	1:B:766:ARG:HH21	1.81	0.45
1:C:156:ASN:HD21	1:C:768:LYS:NZ	2.15	0.45
1:C:344:LEU:HA	1:C:399:VAL:HG22	1.98	0.45
1:C:753:TRP:HD1	1:C:779:ARG:HB3	1.81	0.45
1:C:810:TYR:HD2	1:C:810:TYR:O	1.99	0.45
1:C:880:LEU:CD1	1:C:934:ILE:HD13	2.47	0.45
1:C:907:GLY:O	1:C:1008:GLY:HA2	2.17	0.45
1:D:745:ILE:O	1:D:749:VAL:HG23	2.17	0.45
1:D:747:SER:O	1:D:751:ILE:HG13	2.16	0.45
1:D:884:PHE:HB2	1:D:901:MET:HE2	1.98	0.45
1:E:879:SER:O	1:E:883:VAL:CG1	2.64	0.45
1:F:61:VAL:HG22	1:F:62:VAL:H	1.82	0.45
1:F:401:ALA:HA	1:F:404:LEU:HD12	1.99	0.45
1:F:573:PHE:HB2	1:F:666:PHE:CE1	2.52	0.45
1:F:683:PHE:O	1:F:856:TYR:HA	2.17	0.45
1:C:324:VAL:O	1:C:326:PRO:HD2	2.17	0.45
1:D:157:TYR:O	1:D:158:ILE:C	2.55	0.45
1:D:400:LEU:HD23	1:D:932:THR:HG21	1.99	0.45
1:D:441:ALA:O	1:D:445:ILE:HG12	2.17	0.45
1:D:634:TRP:CD1	1:D:634:TRP:N	2.85	0.45
1:D:692:HIS:O	1:D:692:HIS:CG	2.70	0.45
1:D:749:VAL:HG13	1:D:753:TRP:CE3	2.52	0.45
1:D:965:ALA:HA	1:D:968:MET:HE3	1.99	0.45
1:E:971:ARG:N	1:E:972:PRO:HD2	2.32	0.45
1:F:395:MET:HA	1:F:395:MET:CE	2.47	0.45
1:B:120:GLN:HG3	1:B:124:ARG:HD2	1.99	0.45
1:B:244:GLU:O	1:B:246:PHE:N	2.49	0.45
1:B:298:ASN:HD21	1:B:300:LEU:HB2	1.81	0.45
1:B:614:GLY:HA2	1:B:621:GLY:O	2.17	0.45
1:C:20:MET:HG3	1:C:374:VAL:HG23	1.99	0.45
1:D:885:LEU:HB3	1:F:14:VAL:HG13	1.99	0.45
1:E:375:VAL:CB	1:E:405:LEU:HD11	2.47	0.45
1:F:105:VAL:HG12	1:F:109:ASN:HD21	1.81	0.45
1:F:213:GLN:HB2	1:F:239:ARG:HG3	1.97	0.45
1:F:391:ASN:H	1:F:394:THR:HG22	1.80	0.45
1:F:493:CYS:O	1:F:497:LEU:HB2	2.17	0.45
1:F:826:ILE:HD12	1:F:826:ILE:O	2.16	0.45
1:A:377:LEU:CD1	2:A:2002:LMT:H101	2.41	0.44
1:B:181:GLN:OE1	1:B:768:LYS:HG2	2.18	0.44
1:C:30:LEU:HD11	1:C:384:ALA:HA	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ILE:HG22	1:C:73:ASP:N	2.32	0.44
1:C:99:ASP:HB3	1:C:102:ILE:CG1	2.47	0.44
1:C:503:GLY:O	1:C:505:HIS:N	2.49	0.44
1:C:507:GLU:CG	1:C:509:LYS:HB2	2.47	0.44
1:C:655:PHE:HD1	1:C:658:PHE:HE2	1.65	0.44
1:C:746:ASN:C	1:C:748:THR:H	2.20	0.44
1:D:161:ASN:O	1:D:165:PRO:CG	2.65	0.44
1:D:324:VAL:CG2	1:D:325:TYR:N	2.81	0.44
1:E:751:ILE:HG21	1:E:772:LEU:HD23	1.99	0.44
1:E:908:VAL:O	1:E:911:ALA:HB3	2.17	0.44
1:F:458:PHE:HB2	2:F:2002:LMT:H21	1.99	0.44
1:F:669:PRO:HG3	1:F:861:LEU:HD11	1.98	0.44
1:F:912:LEU:CD2	1:F:926:PHE:HZ	2.30	0.44
1:A:595:ARG:HD2	1:A:599:LEU:HD22	1.99	0.44
1:B:129:VAL:HB	1:C:112:GLN:NE2	2.31	0.44
1:B:185:ARG:HA	1:B:185:ARG:HD3	1.60	0.44
1:C:115:THR:HG22	1:C:116:PRO:CD	2.47	0.44
1:C:342:LYS:HE3	1:C:346:GLU:OE2	2.17	0.44
1:C:596:GLU:C	1:C:598:LEU:N	2.70	0.44
1:E:972:PRO:O	1:E:976:THR:HG22	2.17	0.44
1:F:56:THR:O	1:F:59:ASP:N	2.50	0.44
1:F:408:ASP:HB3	1:F:442:LEU:HD22	1.99	0.44
1:A:984:VAL:HG11	1:A:1005:VAL:HG22	2.00	0.44
1:B:47:VAL:HG21	1:B:127:ILE:HG13	1.98	0.44
1:B:298:ASN:ND2	1:B:300:LEU:H	2.15	0.44
1:B:316:PHE:CD1	1:B:316:PHE:N	2.85	0.44
1:C:527:TYR:O	1:C:531:VAL:HG23	2.17	0.44
1:D:136:PHE:CD1	1:D:290:ALA:HB1	2.52	0.44
1:D:799:PRO:HB2	1:D:801:ASN:OD1	2.17	0.44
1:D:1020:VAL:HB	1:D:1021:PRO:HD3	1.97	0.44
1:E:579:PRO:HA	1:E:580:PRO:HD2	1.69	0.44
1:F:584:ALA:N	1:F:622:GLN:HE21	2.15	0.44
1:A:365:THR:O	1:A:368:PRO:HD2	2.17	0.44
1:A:650:ARG:HH11	1:A:650:ARG:HB2	1.83	0.44
1:A:984:VAL:HG11	1:A:1005:VAL:CG2	2.47	0.44
1:B:193:LEU:HA	1:B:265:VAL:HG23	1.99	0.44
1:B:655:PHE:CD1	1:B:658:PHE:CE1	3.06	0.44
1:C:291:ILE:HD11	1:C:306:ILE:HD13	1.99	0.44
1:C:343:THR:HG21	1:C:998:GLN:CD	2.36	0.44
1:C:396:PHE:CE1	1:C:998:GLN:HG2	2.53	0.44
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:742:LEU:HA	1:D:745:ILE:HG13	1.99	0.44
1:E:743:ALA:O	1:E:747:SER:HB3	2.18	0.44
1:F:846:ILE:O	1:F:846:ILE:CG1	2.66	0.44
1:F:894:TRP:C	1:F:897:PRO:HD2	2.38	0.44
1:A:69:MET:O	1:A:70:ASN:O	2.36	0.44
1:B:27:ILE:HG12	1:B:380:PHE:CG	2.52	0.44
1:B:361:ASN:OD1	1:B:363:ARG:N	2.49	0.44
1:B:371:ALA:O	1:B:375:VAL:HG23	2.17	0.44
1:B:969:ARG:O	1:B:972:PRO:HD2	2.18	0.44
1:C:283:GLY:HA2	1:C:595:ARG:CZ	2.47	0.44
1:C:858:TRP:CE3	1:C:862:SER:HB3	2.53	0.44
1:D:758:VAL:HG22	1:D:770:VAL:HG22	1.99	0.44
1:D:881:LEU:O	1:D:881:LEU:HD13	2.18	0.44
1:D:930:LEU:O	1:D:934:ILE:HG23	2.16	0.44
1:D:937:SER:HB3	1:D:1009:MET:CE	2.45	0.44
1:E:917:MET:C	1:E:919:GLY:H	2.21	0.44
2:E:2002:LMT:O6B	2:E:2002:LMT:H1B	2.18	0.44
1:F:15:ILE:HG13	1:F:16:ALA:N	2.33	0.44
1:A:372:VAL:H	1:A:373:PRO:HD2	1.83	0.44
1:A:716:ARG:CZ	1:A:827:LEU:HD12	2.48	0.44
1:A:896:ILE:CD1	1:A:949:LYS:HD3	2.48	0.44
1:B:28:LEU:O	1:B:28:LEU:CD1	2.62	0.44
1:B:281:PHE:CE2	1:B:324:VAL:HG21	2.52	0.44
1:B:282:ASN:O	1:B:284:SER:N	2.40	0.44
1:B:541:TYR:O	1:B:542:LEU:C	2.52	0.44
1:B:542:LEU:O	1:B:545:TYR:HB3	2.17	0.44
1:B:545:TYR:O	1:B:548:ILE:HG13	2.17	0.44
1:B:572:LEU:HD23	1:B:666:PHE:O	2.17	0.44
1:C:593:SER:HB2	1:C:597:TYR:CE1	2.52	0.44
1:C:634:TRP:HE3	1:C:637:ARG:HH21	1.66	0.44
1:D:189:ASP:CB	1:D:192:LYS:HD2	2.46	0.44
1:D:713:GLN:CG	1:D:714:ARG:N	2.80	0.44
1:D:966:CYS:HG	1:D:1021:PRO:HG3	1.83	0.44
1:E:17:LEU:HD13	1:E:17:LEU:HA	1.56	0.44
1:A:569:GLN:N	1:A:634:TRP:HH2	2.14	0.44
1:A:713:GLN:O	1:A:714:ARG:C	2.56	0.44
1:B:420:MET:HG3	1:B:425:LEU:O	2.18	0.44
1:C:641:GLU:O	1:C:650:ARG:NH2	2.51	0.44
1:C:840:MET:O	1:C:844:GLU:HG2	2.18	0.44
1:C:1016:ALA:C	1:C:1018:PHE:N	2.71	0.44
1:E:81:GLU:HG3	1:E:814:LYS:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:ASP:HB2	1:E:276:SER:OG	2.16	0.44
1:E:337:ILE:O	1:E:341:VAL:HG13	2.18	0.44
1:E:541:TYR:HA	1:E:544:ILE:CG2	2.45	0.44
1:E:784:ASP:HA	1:E:787:LYS:HG3	2.00	0.44
1:F:720:MET:O	1:F:721:SER:HB2	2.17	0.44
1:A:194:ASN:ND2	1:A:797:MET:HG3	2.33	0.44
1:A:243:ALA:O	1:A:247:GLU:HG3	2.18	0.44
1:A:250:LEU:HB2	1:A:261:ARG:NH1	2.32	0.44
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.73	0.44
1:B:672:LEU:O	1:B:674:LEU:N	2.51	0.44
1:C:181:GLN:OE1	1:C:766:ARG:NH1	2.50	0.44
1:C:635:GLU:HG3	1:C:636:GLU:N	2.32	0.44
1:D:23:GLY:HA3	1:D:377:LEU:O	2.17	0.44
1:D:197:GLN:HB3	1:D:797:MET:HE3	2.00	0.44
1:D:454:LEU:HD12	2:D:2001:LMT:H101	2.00	0.44
1:D:467:TYR:OH	1:D:927:GLN:NE2	2.50	0.44
1:E:951:LEU:HD11	1:E:968:MET:CE	2.44	0.44
1:F:189:ASP:OD2	1:F:192:LYS:HG3	2.17	0.44
1:F:306:ILE:HG13	1:F:307:ARG:N	2.30	0.44
1:F:516:PHE:O	1:F:519:MET:HG3	2.18	0.44
1:F:844:GLU:H	1:F:844:GLU:HG2	1.69	0.44
1:F:944:ILE:HG23	1:F:973:ILE:CD1	2.43	0.44
1:A:273:GLN:HG3	1:A:771:TYR:HE2	1.81	0.44
1:A:566:ASP:OD2	1:A:566:ASP:N	2.51	0.44
1:A:1013:THR:C	1:A:1015:LEU:H	2.21	0.44
1:B:215:SER:HB3	1:C:750:SER:CB	2.45	0.44
1:B:377:LEU:HA	1:B:377:LEU:HD23	1.46	0.44
1:B:776:PRO:O	1:B:780:MET:HG2	2.18	0.44
1:B:784:ASP:HA	1:B:787:LYS:HG3	1.99	0.44
1:C:115:THR:O	1:C:118:LEU:HB2	2.18	0.44
1:C:702:PHE:HZ	1:C:843:VAL:HG13	1.83	0.44
1:D:218:GLN:O	1:D:234:ILE:HD12	2.17	0.44
1:D:222:LEU:HA	1:D:223:PRO:C	2.38	0.44
1:D:243:ALA:O	1:D:247:GLU:HG3	2.18	0.44
1:D:755:SER:HA	1:D:773:GLN:HB2	2.00	0.44
1:F:527:TYR:O	1:F:531:VAL:HG23	2.18	0.44
1:A:228:GLN:HE21	1:A:229:GLN:H	1.65	0.43
1:A:535:LEU:HD13	1:A:959:VAL:HG13	1.99	0.43
1:B:460:GLY:H	1:B:871:GLN:NE2	2.15	0.43
1:B:791:ARG:NH1	1:B:791:ARG:HB2	2.32	0.43
1:C:34:GLN:O	1:C:392:THR:OG1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:PRO:HB2	1:C:122:VAL:HG23	1.99	0.43
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.53	0.43
1:C:466:ILE:HD12	1:C:466:ILE:HG21	1.72	0.43
1:C:702:PHE:CZ	1:C:843:VAL:HG13	2.53	0.43
1:C:738:LEU:CD1	1:C:802:ALA:HB1	2.48	0.43
1:D:399:VAL:HG11	1:D:987:LEU:HD23	1.99	0.43
1:E:545:TYR:HB2	1:E:1019:TRP:CZ3	2.53	0.43
1:E:951:LEU:HD13	1:E:964:GLU:HB3	2.00	0.43
1:F:187:TRP:O	1:F:266:ALA:HB1	2.18	0.43
1:F:555:MET:CE	1:F:913:LEU:HG	2.48	0.43
1:F:593:SER:O	1:F:597:TYR:HD1	2.01	0.43
1:A:691:GLY:H	1:A:694:VAL:HG21	1.82	0.43
1:A:784:ASP:O	1:A:787:LYS:HB3	2.18	0.43
1:B:196:TYR:CD2	1:B:260:VAL:HG11	2.53	0.43
1:B:789:TYR:CZ	1:B:799:PRO:HB3	2.53	0.43
1:B:949:LYS:O	1:B:953:GLU:HG3	2.18	0.43
1:C:866:ARG:HA	1:C:866:ARG:HE	1.83	0.43
1:E:190:PRO:HG3	1:E:788:TRP:CZ2	2.54	0.43
1:E:356:TYR:HE1	1:E:362:PHE:CD1	2.36	0.43
1:F:634:TRP:N	1:F:634:TRP:CE3	2.76	0.43
1:F:912:LEU:HD23	1:F:926:PHE:HZ	1.82	0.43
1:A:908:VAL:HG12	1:A:912:LEU:CD1	2.48	0.43
1:B:454:LEU:O	1:B:455:PRO:C	2.56	0.43
1:B:637:ARG:O	1:B:637:ARG:CG	2.66	0.43
1:C:124:ARG:O	1:C:124:ARG:HG2	2.17	0.43
1:C:526:GLY:O	1:C:529:ARG:O	2.36	0.43
1:C:754:GLY:O	1:C:773:GLN:HG3	2.18	0.43
1:C:835:SER:O	1:C:838:ASP:HB2	2.18	0.43
1:D:119:PRO:HG2	1:D:122:VAL:HG21	2.00	0.43
1:E:156:ASN:ND2	1:E:182:TYR:N	2.34	0.43
1:E:246:PHE:O	1:E:262:LEU:HD23	2.18	0.43
1:E:282:ASN:HA	1:E:595:ARG:HD2	2.00	0.43
1:E:338:HIS:C	1:E:340:VAL:H	2.22	0.43
1:E:352:PHE:CD2	1:E:352:PHE:C	2.91	0.43
1:E:536:LYS:HB2	1:E:537:HIS:CD2	2.53	0.43
1:E:924:VAL:HG23	1:E:925:PHE:CD2	2.52	0.43
1:F:978:LEU:O	1:F:982:LEU:HB2	2.18	0.43
1:F:1019:TRP:CD1	1:F:1022:LEU:HD12	2.54	0.43
1:A:149:MET:SD	1:A:321:MET:HE2	2.58	0.43
1:A:554:TRP:CZ2	1:A:558:ARG:HD3	2.54	0.43
1:A:896:ILE:N	1:A:897:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLN:HE21	1:B:123:GLN:HB3	1.62	0.43
1:B:352:PHE:C	1:B:352:PHE:CD2	2.92	0.43
1:B:355:MET:O	1:B:359:LEU:HB2	2.17	0.43
1:B:425:LEU:HB3	1:B:429:GLU:HB3	2.01	0.43
1:C:379:THR:HG21	1:C:477:ALA:HB2	2.00	0.43
1:C:577:GLN:NE2	1:C:720:MET:HG2	2.34	0.43
1:C:584:ALA:N	1:C:622:GLN:HE21	2.16	0.43
1:C:598:LEU:CD2	1:C:609:VAL:HG21	2.45	0.43
1:C:690:VAL:CG2	1:C:694:VAL:HG21	2.41	0.43
1:C:856:TYR:CD2	1:C:856:TYR:N	2.85	0.43
1:D:918:ARG:HE	1:D:1003:THR:CG2	2.20	0.43
1:E:539:ALA:O	1:E:540:PRO:C	2.56	0.43
1:E:971:ARG:O	1:E:975:MET:HG3	2.17	0.43
1:F:789:TYR:HD1	1:F:799:PRO:HA	1.81	0.43
1:F:791:ARG:HG3	1:F:797:MET:CE	2.47	0.43
1:F:913:LEU:O	1:F:914:ALA:C	2.53	0.43
1:A:555:MET:HA	1:A:555:MET:CE	2.49	0.43
1:B:557:THR:O	1:B:558:ARG:CG	2.64	0.43
1:B:947:PHE:CD2	1:B:968:MET:HE2	2.53	0.43
1:C:498:LYS:HA	1:C:499:PRO:HD3	1.80	0.43
1:C:696:LEU:HD23	1:C:696:LEU:HA	1.88	0.43
1:C:910:GLY:H	1:C:1011:THR:HG21	1.83	0.43
1:D:277:ILE:H	1:D:277:ILE:HD13	1.84	0.43
1:E:84:SER:C	1:E:86:GLY:H	2.22	0.43
1:E:191:ALA:C	1:E:193:LEU:N	2.71	0.43
1:F:194:ASN:C	1:F:196:TYR:N	2.68	0.43
1:F:216:SER:HB2	1:F:234:ILE:O	2.17	0.43
1:F:308:GLN:OE1	1:F:308:GLN:HA	2.19	0.43
1:A:155:SER:OG	1:A:179:GLY:HA3	2.18	0.43
1:A:228:GLN:HE21	1:A:229:GLN:N	2.16	0.43
1:A:1005:VAL:O	1:A:1006:ILE:C	2.57	0.43
1:C:439:GLN:CD	2:C:2001:LMT:H3'	2.39	0.43
1:D:150:THR:O	1:D:154:LEU:HG	2.19	0.43
1:D:435:MET:O	1:D:439:GLN:HB2	2.19	0.43
1:E:396:PHE:CD2	1:E:925:PHE:HE1	2.36	0.43
1:E:641:GLU:OE1	1:E:642:ASN:ND2	2.52	0.43
1:F:20:MET:CG	1:F:374:VAL:HA	2.48	0.43
1:F:46:GLN:HA	1:F:88:MET:CE	2.49	0.43
1:F:48:SER:HA	1:F:87:SER:HA	2.00	0.43
1:F:189:ASP:OD1	1:F:190:PRO:HD2	2.17	0.43
1:F:367:ILE:HG12	1:F:496:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:O	1:A:125:GLN:HG2	2.18	0.43
1:A:175:PHE:HA	1:A:290:ALA:O	2.18	0.43
1:A:188:LEU:CD1	1:A:772:LEU:CD1	2.96	0.43
1:A:400:LEU:HD23	1:A:932:THR:HG21	2.00	0.43
1:A:572:LEU:HB3	1:A:629:ILE:HB	1.99	0.43
1:B:812:SER:HA	1:B:813:PRO:HD3	1.89	0.43
1:C:791:ARG:HA	1:C:797:MET:HE3	1.99	0.43
1:C:910:GLY:N	1:C:1011:THR:HG21	2.33	0.43
1:E:800:PHE:O	1:E:802:ALA:N	2.52	0.43
1:F:68:GLN:O	1:F:110:LYS:CD	2.66	0.43
1:F:105:VAL:HG12	1:F:109:ASN:ND2	2.33	0.43
1:B:509:LYS:HE3	1:B:509:LYS:HB3	1.90	0.43
1:B:913:LEU:O	1:B:917:MET:HG2	2.18	0.43
1:C:453:PHE:CZ	1:C:932:THR:HB	2.51	0.43
1:C:498:LYS:HA	1:C:498:LYS:HD3	1.71	0.43
1:C:956:LYS:HB2	1:C:961:ALA:HB2	2.00	0.43
1:D:411:VAL:HG11	1:D:442:LEU:HD11	2.00	0.43
1:D:762:ILE:HG22	1:D:763:ASP:N	2.34	0.43
1:E:49:TYR:HE1	1:E:121:GLU:HG3	1.83	0.43
1:E:652:GLN:NE2	1:E:652:GLN:CA	2.68	0.43
1:E:653:MET:O	1:E:654:HIS:C	2.57	0.43
1:E:751:ILE:O	1:E:773:GLN:HA	2.18	0.43
1:E:791:ARG:HG2	1:E:792:ASN:N	2.32	0.43
1:F:354:VAL:HG21	1:F:982:LEU:HG	2.00	0.43
1:A:254:ASN:ND2	1:A:258:SER:OG	2.52	0.43
1:A:753:TRP:CD1	1:A:779:ARG:HB3	2.52	0.43
1:B:280:GLN:HB2	1:B:284:SER:O	2.19	0.43
1:B:370:ILE:O	1:B:373:PRO:HD2	2.18	0.43
1:C:1:MET:N	2:C:2001:LMT:C6'	2.81	0.43
1:C:421:ALA:O	1:C:423:GLU:N	2.51	0.43
1:C:486:LEU:HD23	2:C:2001:LMT:H12	2.01	0.43
1:D:108:GLN:NE2	1:E:113:LEU:HD13	2.34	0.43
1:D:567:GLU:OE1	1:D:996:GLY:N	2.50	0.43
1:D:791:ARG:HB2	1:D:797:MET:HE2	2.01	0.43
1:D:984:VAL:O	1:D:985:VAL:C	2.57	0.43
1:D:992:GLY:H	1:D:995:SER:HB2	1.83	0.43
1:D:1009:MET:HA	1:D:1009:MET:CE	2.49	0.43
1:E:176:GLN:HG2	1:E:290:ALA:HB3	1.99	0.43
1:E:190:PRO:HG3	1:E:788:TRP:CE2	2.54	0.43
1:E:429:GLU:O	1:E:432:ARG:N	2.52	0.43
1:E:713:GLN:C	1:E:715:VAL:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:910:GLY:HA2	1:E:1011:THR:HG21	1.99	0.43
1:F:724:PRO:HA	1:F:810:TYR:HB3	2.01	0.43
1:A:228:GLN:CG	1:B:780:MET:HE1	2.49	0.43
1:A:723:GLU:CB	1:A:724:PRO:HD2	2.49	0.43
1:A:989:ILE:O	1:A:989:ILE:CG1	2.67	0.43
1:B:20:MET:SD	1:B:374:VAL:HG22	2.59	0.43
1:B:745:ILE:HD12	1:B:803:PHE:CE1	2.54	0.43
1:C:355:MET:HE3	1:C:410:ILE:HG22	2.00	0.43
1:C:859:THR:HG23	1:C:860:GLY:N	2.34	0.43
1:D:52:ALA:HB1	1:D:56:THR:HB	2.01	0.43
1:D:194:ASN:O	1:D:194:ASN:ND2	2.52	0.43
1:D:225:VAL:HG22	1:E:780:MET:HE2	2.01	0.43
1:D:454:LEU:HD23	1:D:454:LEU:HA	1.78	0.43
1:D:585:GLU:OE2	1:F:227:GLY:HA2	2.18	0.43
1:D:780:MET:HE2	1:F:220:GLY:HA2	1.84	0.43
1:E:356:TYR:HE2	1:E:513:PHE:CZ	2.37	0.43
1:F:277:ILE:HD12	1:F:615:PHE:HB2	2.01	0.43
1:F:428:ARG:HG2	1:F:428:ARG:NH1	2.34	0.43
1:F:447:MET:HE1	1:F:886:CYS:HB3	2.00	0.43
1:F:535:LEU:HD12	1:F:963:ILE:CD1	2.48	0.43
1:F:572:LEU:HD13	1:F:644:VAL:HG22	2.01	0.43
1:F:604:SER:HB2	1:F:642:ASN:OD1	2.19	0.43
1:A:725:GLN:NE2	1:C:235:ILE:HD11	2.32	0.42
1:A:831:ALA:O	1:A:832:PRO:C	2.56	0.42
1:A:875:LEU:HG	1:A:876:TYR:H	1.85	0.42
1:A:966:CYS:HG	1:A:1021:PRO:HG3	1.80	0.42
1:B:454:LEU:HD23	1:B:454:LEU:HA	1.84	0.42
1:B:548:ILE:C	1:B:548:ILE:HD12	2.39	0.42
1:C:641:GLU:HA	1:C:646:GLU:HG2	2.00	0.42
1:C:758:VAL:O	1:C:759:ASN:HB3	2.18	0.42
1:C:929:GLY:O	1:C:932:THR:HG23	2.19	0.42
1:D:9:PRO:HD2	1:E:892:GLU:OE1	2.19	0.42
1:D:406:VAL:O	1:D:410:ILE:HG13	2.18	0.42
1:D:647:LEU:C	1:D:647:LEU:CD2	2.87	0.42
1:E:56:THR:O	1:E:60:THR:HG22	2.19	0.42
1:E:105:VAL:HA	1:E:108:GLN:HG3	2.01	0.42
1:E:420:MET:SD	1:E:427:PRO:HA	2.58	0.42
1:F:388:PHE:CE2	1:F:472:ILE:HG12	2.53	0.42
1:F:851:PRO:O	1:F:852:LYS:C	2.57	0.42
1:A:330:THR:O	1:A:331:PRO:C	2.57	0.42
1:B:298:ASN:HD22	1:B:300:LEU:N	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:ARG:HG2	1:B:432:ARG:H	1.44	0.42
1:B:703:LEU:HD23	1:B:715:VAL:HG12	2.01	0.42
1:B:781:ASN:O	1:B:782:PRO:C	2.56	0.42
1:B:954:GLN:O	1:B:954:GLN:HG2	2.19	0.42
1:C:391:ASN:OD1	1:C:394:THR:HG23	2.19	0.42
1:D:182:TYR:HA	1:D:271:GLY:O	2.19	0.42
1:D:196:TYR:CD2	1:D:196:TYR:N	2.86	0.42
1:D:831:ALA:HB3	1:D:834:LEU:HD12	2.01	0.42
1:E:248:ASN:HD22	1:E:248:ASN:HA	1.71	0.42
1:E:344:LEU:CD2	1:E:402:ILE:HG12	2.49	0.42
1:E:527:TYR:CD1	1:E:970:LEU:HD13	2.54	0.42
1:E:684:LEU:O	1:E:823:ALA:HA	2.18	0.42
1:A:115:THR:N	1:A:116:PRO:HD2	2.33	0.42
1:B:533:SER:O	1:B:536:LYS:HB2	2.19	0.42
1:C:635:GLU:CG	1:C:636:GLU:H	2.32	0.42
1:D:701:LYS:O	1:D:702:PHE:C	2.55	0.42
1:D:763:ASP:C	1:D:765:GLY:N	2.72	0.42
1:D:1018:PHE:O	1:D:1021:PRO:HD2	2.18	0.42
1:E:160:SER:HA	1:E:766:ARG:HH21	1.84	0.42
1:E:468:ARG:O	1:E:469:GLN:C	2.57	0.42
1:E:568:ASP:OD1	1:E:644:VAL:CG2	2.63	0.42
1:F:187:TRP:HA	1:F:773:GLN:O	2.19	0.42
1:F:489:THR:N	1:F:490:PRO:CD	2.82	0.42
1:F:577:GLN:HE22	1:F:624:SER:HB3	1.84	0.42
1:F:631:LEU:HD11	1:F:644:VAL:CG2	2.46	0.42
1:F:683:PHE:CZ	1:F:825:GLU:HB2	2.54	0.42
1:F:907:GLY:O	1:F:1008:GLY:HA2	2.19	0.42
1:A:653:MET:O	1:A:656:PHE:HB3	2.19	0.42
1:B:49:TYR:HE2	1:B:60:THR:HG21	1.84	0.42
1:B:143:VAL:CG2	1:B:284:SER:HB3	2.49	0.42
1:B:184:MET:HB2	1:B:761:PHE:CD1	2.54	0.42
1:B:188:LEU:HD23	1:B:200:PRO:HB3	2.02	0.42
1:C:158:ILE:CG2	1:C:159:VAL:N	2.82	0.42
1:D:14:VAL:HG13	1:E:885:LEU:HB3	2.01	0.42
1:D:368:PRO:O	1:D:371:ALA:HB3	2.19	0.42
1:D:552:MET:O	1:D:553:ILE:C	2.57	0.42
1:E:68:GLN:HG2	1:E:114:ALA:HB2	2.01	0.42
1:A:344:LEU:O	1:A:348:ILE:HG22	2.20	0.42
1:B:31:PRO:HB3	1:B:296:GLY:HA2	2.00	0.42
1:C:83:ASN:HB2	1:C:85:ASP:OD1	2.19	0.42
1:C:402:ILE:HA	1:C:405:LEU:CD1	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:VAL:O	1:C:415:ASN:HB2	2.19	0.42
1:D:166:LEU:HA	1:D:166:LEU:HD12	1.75	0.42
1:D:637:ARG:N	1:D:638:PRO:HD3	2.34	0.42
1:D:1024:TYR:O	1:D:1026:ALA:O	2.38	0.42
1:E:146:ASP:OD2	1:E:146:ASP:C	2.58	0.42
1:E:235:ILE:HD12	1:F:53:SER:HB2	2.02	0.42
1:E:723:GLU:CB	1:E:724:PRO:HD2	2.43	0.42
1:E:901:MET:O	1:E:904:VAL:HG23	2.18	0.42
1:F:203:VAL:O	1:F:204:SER:C	2.58	0.42
1:F:594:MET:HG3	1:F:595:ARG:N	2.34	0.42
1:F:766:ARG:HB3	1:F:768:LYS:HE2	2.00	0.42
1:A:655:PHE:HB3	1:A:663:VAL:HB	2.01	0.42
1:B:222:LEU:HD21	1:C:584:ALA:HB2	2.00	0.42
1:B:250:LEU:HD23	1:B:261:ARG:HD2	2.02	0.42
1:B:391:ASN:O	1:B:395:MET:HG2	2.19	0.42
1:C:189:ASP:HB3	1:C:192:LYS:HB2	2.01	0.42
1:C:452:VAL:HG11	1:C:934:ILE:HG13	2.01	0.42
1:E:184:MET:HE3	1:E:269:GLY:C	2.39	0.42
1:E:214:ILE:HG23	1:E:237:LYS:O	2.19	0.42
1:E:891:TYR:HA	1:E:949:LYS:HE2	2.01	0.42
1:F:535:LEU:HD13	1:F:959:VAL:HG13	2.00	0.42
1:F:687:GLN:HE22	1:F:855:GLY:HA3	1.84	0.42
1:F:782:PRO:O	1:F:785:LEU:CG	2.67	0.42
1:F:894:TRP:O	1:F:897:PRO:HD2	2.20	0.42
1:A:213:GLN:HG2	1:B:56:THR:HB	2.01	0.42
1:A:755:SER:HA	1:A:773:GLN:HB2	2.01	0.42
1:A:887:LEU:HD21	1:A:942:ILE:CD1	2.49	0.42
1:A:910:GLY:CA	1:A:1011:THR:CG2	2.97	0.42
1:B:165:PRO:HG2	1:B:313:LEU:HD11	2.01	0.42
1:B:742:LEU:HA	1:B:745:ILE:CG1	2.48	0.42
1:B:953:GLU:C	1:B:955:GLY:N	2.72	0.42
1:C:354:VAL:CG2	1:C:982:LEU:HG	2.49	0.42
1:C:944:ILE:HD11	1:C:1020:VAL:HB	2.00	0.42
1:C:1016:ALA:O	1:C:1018:PHE:N	2.53	0.42
1:D:47:VAL:HB	1:D:127:ILE:HG12	2.02	0.42
1:D:197:GLN:HB3	1:D:797:MET:CE	2.50	0.42
1:D:871:GLN:NE2	2:D:2001:LMT:O3B	2.52	0.42
1:D:927:GLN:HE21	1:D:927:GLN:HB2	1.53	0.42
1:D:957:GLY:O	1:D:959:VAL:N	2.52	0.42
1:D:981:ILE:CG2	1:D:1009:MET:HB3	2.49	0.42
1:E:542:LEU:HD21	1:E:1022:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:987:LEU:HD23	1:E:1001:ILE:HG13	2.01	0.42
1:E:1015:LEU:O	1:E:1019:TRP:HD1	2.03	0.42
1:F:567:GLU:OE2	1:F:996:GLY:N	2.53	0.42
1:F:866:ARG:HA	1:F:866:ARG:HE	1.85	0.42
1:F:939:LYS:HD3	1:F:940:ASN:N	2.35	0.42
1:A:906:LEU:HB3	1:A:1015:LEU:HD23	2.01	0.42
1:B:250:LEU:H	1:B:250:LEU:HG	1.71	0.42
1:B:316:PHE:HD1	1:B:316:PHE:N	2.17	0.42
1:B:471:SER:O	1:B:475:VAL:CG1	2.66	0.42
1:B:773:GLN:HG2	1:B:774:GLY:N	2.34	0.42
1:C:67:GLN:HA	1:C:70:ASN:ND2	2.35	0.42
1:C:314:GLU:N	1:C:315:PRO:HD2	2.35	0.42
1:C:847:VAL:HG22	1:C:850:LEU:CD2	2.50	0.42
1:C:943:LEU:HD12	1:C:943:LEU:HA	1.76	0.42
1:D:82:SER:HB2	1:D:815:LEU:HB2	2.01	0.42
1:D:725:GLN:HG2	1:F:233:THR:HB	2.01	0.42
1:E:493:CYS:HA	1:E:497:LEU:HD22	2.02	0.42
1:A:229:GLN:HE22	1:B:586:ARG:HD2	1.83	0.42
1:B:628:PHE:N	1:B:628:PHE:CD2	2.88	0.42
1:C:351:VAL:O	1:C:352:PHE:C	2.56	0.42
1:C:671:VAL:HB	1:C:674:LEU:HD13	2.01	0.42
1:C:847:VAL:HA	1:C:850:LEU:HD22	2.01	0.42
1:D:7:ASP:OD2	1:D:432:ARG:NH2	2.44	0.42
1:D:40:PRO:HA	1:D:96:GLN:HE22	1.84	0.42
1:D:333:VAL:CG2	1:D:334:SER:N	2.83	0.42
1:D:587:THR:O	1:D:591:VAL:HG23	2.20	0.42
1:E:995:SER:O	1:E:999:HIS:CD2	2.73	0.42
1:F:845:GLU:C	1:F:847:VAL:H	2.24	0.42
1:A:82:SER:HB2	1:A:815:LEU:HB2	2.01	0.42
1:A:142:VAL:HG23	1:A:154:LEU:HB3	2.01	0.42
1:A:468:ARG:O	1:A:469:GLN:CB	2.53	0.42
1:A:695:LEU:HB3	1:A:824:MET:HE1	2.02	0.42
1:A:985:VAL:CA	1:A:1006:ILE:HD11	2.50	0.42
1:B:38:ILE:HG21	1:B:674:LEU:HD11	2.01	0.42
1:B:621:GLY:O	1:B:624:SER:HB2	2.20	0.42
1:C:121:GLU:O	1:C:125:GLN:HB2	2.19	0.42
1:D:127:ILE:O	1:E:113:LEU:HG	2.20	0.42
1:D:188:LEU:O	1:D:775:ARG:HG2	2.19	0.42
1:D:987:LEU:HA	1:D:990:SER:HB2	2.02	0.42
1:E:908:VAL:HB	1:E:930:LEU:HD11	2.02	0.42
1:F:483:ILE:HG23	1:F:487:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:727:LYS:O	1:F:806:GLY:HA2	2.20	0.42
1:F:761:PHE:O	1:F:761:PHE:CG	2.72	0.42
1:F:766:ARG:HB3	1:F:768:LYS:HE3	2.00	0.42
1:A:372:VAL:O	1:A:373:PRO:C	2.57	0.41
1:A:372:VAL:N	1:A:373:PRO:HD2	2.35	0.41
1:A:884:PHE:HB2	1:A:901:MET:HE1	2.00	0.41
1:B:726:TYR:CZ	1:B:806:GLY:HA3	2.55	0.41
1:B:987:LEU:HG	1:B:998:GLN:HB3	2.02	0.41
1:C:576:VAL:HG22	1:C:663:VAL:HG22	2.01	0.41
1:C:680:PHE:CE2	1:C:828:GLY:O	2.73	0.41
1:D:573:PHE:HE2	1:D:676:ASN:HB2	1.84	0.41
1:D:909:ILE:H	1:D:909:ILE:HG13	1.66	0.41
1:E:308:GLN:NE2	1:E:312:ASN:ND2	2.59	0.41
1:E:759:ASN:HD22	1:E:759:ASN:HA	1.57	0.41
1:E:951:LEU:HB3	1:E:956:LYS:HD2	2.02	0.41
1:F:488:LEU:O	1:F:492:LEU:HG	2.20	0.41
1:F:577:GLN:NE2	1:F:624:SER:HB3	2.35	0.41
1:F:779:ARG:NH1	1:F:779:ARG:CG	2.78	0.41
1:A:213:GLN:HB2	1:A:213:GLN:HE21	1.74	0.41
1:A:749:VAL:HG12	1:C:216:SER:HA	2.01	0.41
1:B:28:LEU:O	1:B:29:SER:CB	2.68	0.41
1:B:542:LEU:HD23	1:B:542:LEU:HA	1.74	0.41
1:B:759:ASN:HD22	1:B:759:ASN:HA	1.62	0.41
1:C:406:VAL:O	1:C:410:ILE:HG23	2.21	0.41
1:C:639:GLY:O	1:C:640:GLY:C	2.58	0.41
1:C:896:ILE:O	1:C:900:VAL:HG13	2.20	0.41
1:D:985:VAL:O	1:D:987:LEU:N	2.53	0.41
1:E:144:SER:O	1:E:285:PRO:HD2	2.20	0.41
1:E:535:LEU:HD22	1:E:1025:VAL:CG2	2.46	0.41
1:F:143:VAL:HG23	1:F:285:PRO:O	2.19	0.41
1:A:578:THR:HG22	1:A:590:VAL:HG21	2.02	0.41
1:A:936:LEU:HD23	1:A:936:LEU:O	2.20	0.41
1:B:631:LEU:N	1:B:631:LEU:HD23	2.35	0.41
1:B:887:LEU:HB2	1:B:897:PRO:HB3	2.02	0.41
3:B:2001:P9D:O13	3:B:2001:P9D:S8	2.76	0.41
1:C:46:GLN:HA	1:C:88:MET:CE	2.49	0.41
1:C:573:PHE:HE2	1:C:668:PRO:HG3	1.84	0.41
1:C:653:MET:C	1:C:655:PHE:H	2.24	0.41
1:C:721:SER:HB3	1:C:722:ASP:H	1.69	0.41
1:C:916:SER:C	1:C:918:ARG:N	2.73	0.41
1:D:220:GLY:HA3	1:D:231:ASN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:LYS:HD3	1:D:237:LYS:HA	1.84	0.41
1:D:330:THR:N	1:D:331:PRO:HD2	2.34	0.41
1:D:357:LEU:HD11	1:D:516:PHE:CE1	2.55	0.41
1:D:599:LEU:HD12	1:D:599:LEU:HA	1.87	0.41
1:D:766:ARG:O	1:D:768:LYS:HG3	2.21	0.41
1:D:783:ASP:C	1:D:785:LEU:N	2.73	0.41
1:E:13:TRP:O	1:E:16:ALA:HB3	2.20	0.41
1:E:33:ASN:O	1:E:391:ASN:CB	2.68	0.41
1:E:314:GLU:HA	1:E:317:MET:HE2	2.02	0.41
1:E:591:VAL:O	1:E:594:MET:HB3	2.19	0.41
1:F:102:ILE:O	1:F:106:GLN:HG3	2.20	0.41
1:F:402:ILE:CA	1:F:405:LEU:HD13	2.40	0.41
1:F:502:LYS:H	1:F:502:LYS:HG3	1.45	0.41
1:A:72:ILE:CG1	1:A:75:LEU:HD12	2.50	0.41
1:A:340:VAL:O	1:A:341:VAL:C	2.58	0.41
1:A:780:MET:SD	1:C:225:VAL:HG22	2.60	0.41
1:A:871:GLN:O	1:A:872:ALA:CB	2.69	0.41
1:B:156:ASN:ND2	1:B:768:LYS:HZ3	2.17	0.41
1:B:394:THR:HA	1:B:473:THR:HG21	2.02	0.41
1:C:913:LEU:O	1:C:914:ALA:C	2.57	0.41
1:D:228:GLN:NE2	1:D:230:LEU:N	2.65	0.41
1:E:163:GLN:HG3	1:E:175:PHE:CE1	2.55	0.41
1:E:361:ASN:OD1	1:E:362:PHE:N	2.53	0.41
1:E:728:LEU:HD23	1:E:728:LEU:C	2.40	0.41
1:F:150:THR:N	1:F:153:ASP:HB2	2.33	0.41
1:F:573:PHE:HB2	1:F:666:PHE:CD1	2.55	0.41
1:F:596:GLU:C	1:F:598:LEU:N	2.74	0.41
1:F:927:GLN:O	1:F:928:VAL:C	2.56	0.41
1:A:324:VAL:O	1:A:326:PRO:HD3	2.20	0.41
1:A:324:VAL:CG2	1:A:325:TYR:N	2.83	0.41
1:B:357:LEU:O	1:B:357:LEU:HG	2.20	0.41
1:B:501:GLU:HB2	1:B:504:ASP:HB2	2.02	0.41
1:C:142:VAL:HG21	1:C:321:MET:HE3	1.97	0.41
1:C:845:GLU:C	1:C:847:VAL:N	2.74	0.41
1:D:382:VAL:HG21	1:D:476:SER:OG	2.21	0.41
1:D:776:PRO:O	1:D:780:MET:HG2	2.21	0.41
1:D:884:PHE:HB2	1:D:901:MET:HE1	2.03	0.41
1:E:400:LEU:HA	1:E:400:LEU:HD23	1.82	0.41
1:E:791:ARG:CB	1:E:791:ARG:CZ	2.97	0.41
1:F:526:GLY:O	1:F:529:ARG:O	2.38	0.41
1:F:952:HIS:HD2	1:F:956:LYS:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HG23	1:B:113:LEU:HD21	2.03	0.41
1:A:197:GLN:HB3	1:A:797:MET:HE3	2.02	0.41
1:A:666:PHE:CD2	1:A:666:PHE:N	2.88	0.41
1:B:572:LEU:HB3	1:B:629:ILE:HB	2.02	0.41
1:B:775:ARG:O	1:B:778:ALA:HB3	2.20	0.41
1:B:903:VAL:O	1:B:906:LEU:HB2	2.20	0.41
1:B:943:LEU:HA	1:B:943:LEU:HD23	1.74	0.41
1:C:186:ILE:HG12	1:C:268:VAL:HG22	2.01	0.41
1:C:561:THR:O	1:C:837:GLY:HA3	2.20	0.41
1:C:652:GLN:HE22	1:C:664:PHE:HA	1.85	0.41
1:D:352:PHE:CD2	1:D:352:PHE:C	2.94	0.41
1:E:8:ARG:N	1:E:9:PRO:CD	2.84	0.41
1:F:142:VAL:HG21	1:F:321:MET:HE3	2.02	0.41
1:F:158:ILE:HA	1:F:162:ILE:HD12	2.03	0.41
1:F:459:PHE:CE1	2:F:2002:LMT:O3'	2.64	0.41
1:F:726:TYR:CE2	1:F:806:GLY:HA3	2.55	0.41
1:F:903:VAL:CG2	1:F:1020:VAL:HG22	2.46	0.41
1:A:452:VAL:HG13	1:A:931:LEU:HD22	2.03	0.41
1:A:910:GLY:HA3	1:A:1011:THR:OG1	2.20	0.41
1:B:601:LYS:HE2	1:B:601:LYS:HB3	1.89	0.41
1:B:713:GLN:HG2	1:B:714:ARG:N	2.34	0.41
1:C:419:VAL:O	1:C:423:GLU:HG3	2.20	0.41
1:C:535:LEU:HD12	1:C:963:ILE:HD11	2.03	0.41
1:D:133:VAL:HG21	1:D:293:LEU:HD23	2.02	0.41
1:D:367:ILE:HD13	1:D:489:THR:HG23	2.01	0.41
1:E:229:GLN:HG2	1:F:586:ARG:NH2	2.36	0.41
1:E:455:PRO:HG2	1:E:879:SER:CB	2.36	0.41
1:F:498:LYS:HD3	1:F:499:PRO:HD3	2.02	0.41
1:F:856:TYR:CD2	1:F:856:TYR:O	2.74	0.41
1:A:437:GLN:H	1:A:437:GLN:HG2	1.43	0.41
1:A:756:SER:N	1:A:772:LEU:O	2.54	0.41
1:B:566:ASP:HB3	1:B:645:PHE:CZ	2.55	0.41
1:B:749:VAL:HA	1:B:753:TRP:HD1	1.86	0.41
1:C:76:ARG:HB3	1:C:93:THR:HG22	2.02	0.41
1:C:175:PHE:C	1:C:175:PHE:HD1	2.23	0.41
1:C:400:LEU:HD23	1:C:400:LEU:HA	1.67	0.41
1:C:509:LYS:HB3	1:C:509:LYS:HE3	1.54	0.41
1:C:683:PHE:HD1	1:C:823:ALA:HB1	1.85	0.41
1:C:957:GLY:O	1:C:960:GLU:N	2.54	0.41
1:D:137:LEU:O	1:D:329:THR:HB	2.21	0.41
1:D:523:THR:O	1:D:526:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:756:SER:O	1:D:771:TYR:HA	2.19	0.41
1:D:1023:PHE:O	1:D:1026:ALA:O	2.38	0.41
1:F:699:ARG:HD2	1:F:699:ARG:O	2.20	0.41
1:F:729:GLU:CB	1:F:805:THR:HB	2.49	0.41
1:A:47:VAL:HG22	1:A:48:SER:N	2.36	0.41
1:A:333:VAL:O	1:A:337:ILE:HG13	2.21	0.41
1:A:453:PHE:O	1:A:456:MET:HB2	2.21	0.41
1:A:787:LYS:HE2	1:A:787:LYS:HB2	1.80	0.41
1:A:896:ILE:HD13	1:A:949:LYS:HD3	2.02	0.41
1:B:47:VAL:HG22	1:B:127:ILE:HG23	2.03	0.41
1:B:234:ILE:O	1:B:234:ILE:CG1	2.68	0.41
1:B:340:VAL:O	1:B:344:LEU:HG	2.21	0.41
1:B:970:LEU:O	1:B:974:VAL:HG23	2.21	0.41
1:C:40:PRO:CD	1:C:96:GLN:NE2	2.77	0.41
1:C:367:ILE:HD11	1:C:496:MET:HB2	2.02	0.41
1:C:682:LEU:O	1:C:825:GLU:HA	2.21	0.41
1:D:190:PRO:HB2	1:D:787:LYS:O	2.20	0.41
1:D:895:SER:CB	1:D:1030:LEU:CD1	2.99	0.41
1:D:970:LEU:HD22	1:D:974:VAL:HG23	2.03	0.41
1:E:273:GLN:HE21	1:E:273:GLN:HB3	1.58	0.41
1:E:325:TYR:HA	1:E:326:PRO:HD2	1.84	0.41
1:E:588:GLN:O	1:E:591:VAL:HG22	2.21	0.41
1:E:612:VAL:CG1	1:E:615:PHE:HB3	2.51	0.41
1:F:186:ILE:HG12	1:F:268:VAL:HG22	2.03	0.41
1:F:219:LEU:HG	1:F:234:ILE:HD11	2.02	0.41
1:F:392:THR:HG22	1:F:396:PHE:CZ	2.56	0.41
1:F:417:GLU:C	1:F:419:VAL:H	2.24	0.41
1:F:753:TRP:CZ2	1:F:785:LEU:HB2	2.55	0.41
1:A:367:ILE:CD1	1:A:413:VAL:CG2	2.91	0.41
1:A:583:SER:O	1:A:586:ARG:HB3	2.21	0.41
1:A:616:ASN:HB3	1:A:618:ALA:H	1.86	0.41
1:B:882:VAL:O	1:B:883:VAL:C	2.59	0.41
1:B:896:ILE:N	1:B:897:PRO:CD	2.84	0.41
1:C:167:SER:CB	1:C:175:PHE:HE2	2.31	0.41
1:C:597:TYR:HB2	1:C:654:HIS:HE1	1.86	0.41
1:C:966:CYS:SG	1:C:1021:PRO:HG3	2.60	0.41
1:C:978:LEU:HD23	1:C:978:LEU:HA	1.59	0.41
1:D:156:ASN:HD21	1:D:768:LYS:HZ3	1.68	0.41
1:D:513:PHE:O	1:D:516:PHE:HB3	2.21	0.41
1:D:610:PHE:HB3	1:D:628:PHE:HB2	2.04	0.41
1:E:350:LEU:O	1:E:354:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:766:ARG:H	1:E:766:ARG:HG3	1.60	0.41
1:F:395:MET:HA	1:F:395:MET:HE2	2.02	0.41
1:F:513:PHE:HD1	1:F:513:PHE:HA	1.77	0.41
1:A:119:PRO:HG2	1:A:122:VAL:CG2	2.46	0.40
1:A:124:ARG:NH2	1:A:757:TYR:O	2.54	0.40
1:A:138:MET:CE	1:A:325:TYR:HD1	2.33	0.40
1:A:691:GLY:C	1:A:693:GLU:N	2.73	0.40
1:B:480:LEU:HD23	1:B:480:LEU:HA	1.70	0.40
1:C:57:VAL:HG21	1:C:86:GLY:O	2.21	0.40
1:C:583:SER:OG	1:C:586:ARG:HG2	2.21	0.40
1:C:779:ARG:HH11	1:C:779:ARG:HG2	1.86	0.40
1:D:480:LEU:HA	1:D:480:LEU:HD23	1.84	0.40
1:D:786:SER:O	1:D:788:TRP:N	2.54	0.40
1:D:874:ALA:C	1:D:875:LEU:O	2.59	0.40
1:E:110:LYS:HD3	1:E:110:LYS:HA	1.77	0.40
1:E:250:LEU:HD23	1:E:261:ARG:CD	2.51	0.40
1:E:310:ILE:CG2	1:E:323:VAL:HG21	2.51	0.40
1:F:336:SER:HA	1:F:993:ALA:HB3	2.03	0.40
1:A:483:ILE:HG13	1:A:484:VAL:N	2.36	0.40
1:A:529:ARG:O	1:A:532:ALA:HB3	2.21	0.40
1:B:552:MET:SD	1:B:908:VAL:CG2	3.09	0.40
1:B:831:ALA:O	1:B:832:PRO:C	2.59	0.40
1:D:195:SER:HB2	1:D:196:TYR:CD2	2.56	0.40
1:D:324:VAL:O	1:D:326:PRO:HD3	2.21	0.40
1:D:658:PHE:C	1:D:660:ASP:H	2.24	0.40
1:E:53:SER:O	1:E:56:THR:N	2.53	0.40
1:F:115:THR:HB	1:F:116:PRO:HD3	2.03	0.40
1:F:185:ARG:HB2	1:F:269:GLY:O	2.20	0.40
1:F:366:LEU:O	1:F:370:ILE:HG12	2.21	0.40
1:F:407:ASP:O	1:F:408:ASP:C	2.58	0.40
1:F:597:TYR:HB2	1:F:654:HIS:NE2	2.36	0.40
1:A:57:VAL:CG1	1:A:82:SER:HB3	2.51	0.40
1:A:609:VAL:HG22	1:A:629:ILE:HG23	2.04	0.40
1:B:438:ILE:CG2	1:B:442:LEU:HG	2.52	0.40
1:B:775:ARG:HG3	1:B:777:ASP:OD2	2.22	0.40
1:B:904:VAL:O	1:B:908:VAL:HG13	2.21	0.40
1:C:339:GLU:O	1:C:343:THR:HG22	2.21	0.40
1:C:351:VAL:HG12	1:C:352:PHE:N	2.35	0.40
1:C:374:VAL:CG1	1:C:484:VAL:HG11	2.52	0.40
1:D:70:ASN:O	1:D:110:LYS:HE2	2.22	0.40
1:E:909:ILE:CG2	1:E:910:GLY:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:325:TYR:N	1:F:326:PRO:HD3	2.37	0.40
1:F:943:LEU:HD12	1:F:943:LEU:HA	1.67	0.40
1:B:139:VAL:HG21	3:B:2001:P9D:HN10	1.85	0.40
1:B:230:LEU:HD21	1:C:808:TRP:HZ2	1.85	0.40
1:B:386:PHE:CE1	2:B:2003:LMT:H81	2.56	0.40
1:B:963:ILE:O	1:B:966:CYS:O	2.39	0.40
1:C:67:GLN:HE21	1:C:67:GLN:HB3	1.74	0.40
1:C:230:LEU:HG	1:C:231:ASN:N	2.37	0.40
1:C:350:LEU:HB3	1:C:982:LEU:HD12	2.03	0.40
1:C:448:VAL:CG1	1:C:887:LEU:HD21	2.51	0.40
1:C:616:ASN:ND2	1:C:619:GLY:O	2.54	0.40
1:D:43:ILE:CD1	1:D:131:LYS:HB3	2.51	0.40
1:D:194:ASN:ND2	1:D:797:MET:HG3	2.36	0.40
1:D:563:PHE:O	1:D:564:LEU:HB2	2.21	0.40
1:D:709:ASN:HD22	1:D:846:ILE:CD1	2.31	0.40
1:D:987:LEU:CB	1:D:998:GLN:HE21	2.33	0.40
1:E:501:GLU:HB2	1:E:504:ASP:CB	2.51	0.40
1:E:840:MET:HG2	1:E:858:TRP:CZ2	2.55	0.40
1:F:313:LEU:O	1:F:317:MET:HG2	2.22	0.40
1:F:836:SER:O	1:F:840:MET:HB2	2.21	0.40
1:A:633:PRO:HD2	1:A:636:GLU:OE1	2.22	0.40
1:A:773:GLN:HG2	1:A:774:GLY:N	2.36	0.40
1:A:972:PRO:HG2	1:A:973:ILE:H	1.86	0.40
1:B:445:ILE:C	1:B:445:ILE:HD13	2.41	0.40
1:B:555:MET:HE1	1:B:913:LEU:HD12	2.02	0.40
1:B:595:ARG:O	1:B:596:GLU:C	2.60	0.40
1:B:789:TYR:CE1	1:B:799:PRO:HB3	2.56	0.40
1:C:489:THR:N	1:C:490:PRO:HD2	2.36	0.40
1:C:588:GLN:HG2	1:C:613:THR:HG21	2.02	0.40
1:C:686:ASP:OD1	1:C:686:ASP:N	2.55	0.40
1:C:872:ALA:O	1:C:873:PRO:C	2.60	0.40
1:D:167:SER:OG	1:E:70:ASN:HB2	2.22	0.40
1:D:365:THR:O	1:D:369:THR:HG23	2.21	0.40
1:D:522:SER:O	1:D:525:HIS:HB2	2.22	0.40
1:D:984:VAL:HG11	1:D:1005:VAL:HG21	1.98	0.40
1:E:152:GLU:CD	1:E:152:GLU:H	2.25	0.40
1:E:210:GLN:NE2	1:E:249:ILE:HB	2.37	0.40
1:E:274:ASP:OD2	1:E:275:TYR:N	2.54	0.40
1:E:963:ILE:O	1:E:966:CYS:O	2.40	0.40
1:F:2:SER:HB3	1:F:435:MET:HG3	2.03	0.40
1:F:41:PRO:HB3	1:F:100:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:PRO:HA	1:F:193:LEU:HB2	2.04	0.40
1:F:310:ILE:HD12	1:F:311:ALA:N	2.37	0.40
1:F:347:ALA:O	1:F:348:ILE:C	2.60	0.40
1:F:534:ILE:HG12	1:F:541:TYR:CE2	2.56	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	1014/1052 (96%)	861 (85%)	122 (12%)	31 (3%)	4	23
1	B	1028/1052 (98%)	874 (85%)	127 (12%)	27 (3%)	5	28
1	C	1028/1052 (98%)	844 (82%)	129 (12%)	55 (5%)	2	12
1	D	1015/1052 (96%)	846 (83%)	130 (13%)	39 (4%)	3	19
1	E	1028/1052 (98%)	865 (84%)	127 (12%)	36 (4%)	3	21
1	F	1031/1052 (98%)	862 (84%)	125 (12%)	44 (4%)	2	17
All	All	6144/6312 (97%)	5152 (84%)	760 (12%)	232 (4%)	3	19

All (232) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	MET
1	A	70	ASN
1	A	498	LYS
1	A	673	GLU
1	A	714	ARG
1	A	738	LEU
1	A	872	ALA
1	A	956	LYS

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Mol	Chain	Res	Type
1	A	958	ILE
1	B	29	SER
1	B	228	GLN
1	B	248	ASN
1	B	509	LYS
1	B	558	ARG
1	B	625	GLY
1	B	673	GLU
1	B	793	ASP
1	B	967	ARG
1	B	1006	ILE
1	C	2	SER
1	C	255	PRO
1	C	270	LEU
1	C	422	GLU
1	C	504	ASP
1	C	505	HIS
1	C	638	PRO
1	C	640	GLY
1	C	659	LYS
1	C	673	GLU
1	C	714	ARG
1	C	721	SER
1	C	805	THR
1	C	914	ALA
1	C	917	MET
1	C	920	LEU
1	C	958	ILE
1	D	69	MET
1	D	70	ASN
1	D	282	ASN
1	D	538	ARG
1	D	603	SER
1	D	714	ARG
1	D	755	SER
1	D	870	SER
1	D	872	ALA
1	D	957	GLY
1	D	958	ILE
1	E	29	SER
1	E	192	LYS
1	E	228	GLN

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Mol	Chain	Res	Type
1	E	248	ASN
1	E	249	ILE
1	E	558	ARG
1	E	563	PHE
1	E	625	GLY
1	E	714	ARG
1	E	967	ARG
1	E	1006	ILE
1	F	505	HIS
1	F	538	ARG
1	F	540	PRO
1	F	638	PRO
1	F	640	GLY
1	F	659	LYS
1	F	690	VAL
1	F	740	VAL
1	A	3	LYS
1	A	256	ASP
1	A	363	ARG
1	A	440	GLY
1	A	787	LYS
1	A	839	ALA
1	A	947	PHE
1	A	957	GLY
1	B	2	SER
1	B	238	THR
1	B	245	GLN
1	B	249	ILE
1	B	510	GLY
1	B	661	ALA
1	B	705	LEU
1	C	238	THR
1	C	363	ARG
1	C	424	GLY
1	C	597	TYR
1	C	743	ALA
1	C	756	SER
1	C	808	TRP
1	D	568	ASP
1	D	644	VAL
1	D	658	PHE
1	D	673	GLU

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Mol	Chain	Res	Type
1	D	764	ARG
1	D	946	GLU
1	D	956	LYS
1	D	1027	VAL
1	E	510	GLY
1	E	555	MET
1	E	673	GLU
1	E	801	ASN
1	E	918	ARG
1	F	158	ILE
1	F	195	SER
1	F	251	LEU
1	F	258	SER
1	F	364	ALA
1	F	418	ARG
1	F	495	THR
1	F	618	ALA
1	F	721	SER
1	F	804	ALA
1	F	1030	LEU
1	A	468	ARG
1	A	569	GLN
1	A	838	ASP
1	A	1014	VAL
1	B	181	GLN
1	B	660	ASP
1	C	147	GLY
1	C	499	PRO
1	C	502	LYS
1	C	568	ASP
1	C	705	LEU
1	C	755	SER
1	C	804	ALA
1	C	1010	VAL
1	D	158	ILE
1	D	363	ARG
1	D	498	LYS
1	D	738	LEU
1	D	779	ARG
1	D	787	LYS
1	E	339	GLU
1	E	463	THR

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Mol	Chain	Res	Type
1	E	580	PRO
1	E	647	LEU
1	E	807	LYS
1	E	993	ALA
1	F	248	ASN
1	F	363	ARG
1	F	429	GLU
1	F	670	SER
1	F	759	ASN
1	A	538	ARG
1	A	564	LEU
1	A	650	ARG
1	B	495	THR
1	B	954	GLN
1	B	1014	VAL
1	C	115	THR
1	C	283	GLY
1	C	557	THR
1	C	633	PRO
1	C	742	LEU
1	D	2	SER
1	D	361	ASN
1	D	564	LEU
1	D	569	GLN
1	E	85	ASP
1	E	133	VAL
1	E	687	GLN
1	E	717	PRO
1	E	793	ASP
1	E	1014	VAL
1	F	238	THR
1	F	507	GLU
1	F	636	GLU
1	F	742	LEU
1	F	843	VAL
1	A	76	ARG
1	A	219	LEU
1	A	1027	VAL
1	B	216	SER
1	B	669	PRO
1	C	191	ALA
1	C	339	GLU

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Mol	Chain	Res	Type
1	C	598	LEU
1	C	872	ALA
1	C	913	LEU
1	D	438	ILE
1	D	846	ILE
1	D	951	LEU
1	D	1015	LEU
1	E	191	ALA
1	E	594	MET
1	E	715	VAL
1	F	240	LEU
1	F	663	VAL
1	F	902	LEU
1	A	315	PRO
1	B	51	GLY
1	C	221	GLY
1	C	663	VAL
1	C	739	GLY
1	C	832	PRO
1	D	553	ILE
1	E	163	GLN
1	F	50	PRO
1	F	147	GLY
1	F	204	SER
1	F	249	ILE
1	F	662	MET
1	A	374	VAL
1	A	851	PRO
1	B	745	ILE
1	C	851	PRO
1	D	539	ALA
1	D	724	PRO
1	F	57	VAL
1	F	236	GLY
1	C	580	PRO
1	C	690	VAL
1	C	717	PRO
1	C	830	PRO
1	E	283	GLY
1	E	570	GLY
1	F	633	PRO
1	F	851	PRO

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Mol	Chain	Res	Type
1	A	438	ILE
1	C	62	VAL
1	C	249	ILE
1	C	549	VAL
1	D	869	GLY
1	D	1014	VAL
1	F	739	GLY
1	B	283	GLY
1	C	795	GLY
1	D	315	PRO
1	F	872	ALA
1	E	830	PRO
1	E	873	PRO
1	F	506	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	833/860 (97%)	696 (84%)	137 (16%)	2 10
1	B	841/860 (98%)	703 (84%)	138 (16%)	2 10
1	C	841/860 (98%)	699 (83%)	142 (17%)	2 9
1	D	834/860 (97%)	696 (84%)	138 (16%)	2 10
1	E	841/860 (98%)	697 (83%)	144 (17%)	2 9
1	F	844/860 (98%)	693 (82%)	151 (18%)	2 8
All	All	5034/5160 (98%)	4184 (83%)	850 (17%)	2 9

All (850) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	21	LEU
1	A	25	LEU
1	A	26	SER

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Mol	Chain	Res	Type
1	A	32	VAL
1	A	49	TYR
1	A	57	VAL
1	A	69	MET
1	A	72	ILE
1	A	88	MET
1	A	92	VAL
1	A	112	GLN
1	A	130	THR
1	A	143	VAL
1	A	145	THR
1	A	160	SER
1	A	181	GLN
1	A	194	ASN
1	A	213	GLN
1	A	214	ILE
1	A	216	SER
1	A	219	LEU
1	A	230	LEU
1	A	235	ILE
1	A	253	VAL
1	A	256	ASP
1	A	259	GLN
1	A	265	VAL
1	A	277	ILE
1	A	285	PRO
1	A	287	SER
1	A	289	ILE
1	A	295	THR
1	A	302	THR
1	A	306	ILE
1	A	310	ILE
1	A	329	THR
1	A	334	SER
1	A	336	SER
1	A	343	THR
1	A	348	ILE
1	A	350	LEU
1	A	353	LEU
1	A	366	LEU
1	A	367	ILE
1	A	369	THR

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Mol	Chain	Res	Type
1	A	377	LEU
1	A	382	VAL
1	A	414	GLU
1	A	417	GLU
1	A	425	LEU
1	A	427	PRO
1	A	432	ARG
1	A	437	GLN
1	A	438	ILE
1	A	442	LEU
1	A	463	THR
1	A	466	ILE
1	A	472	ILE
1	A	475	VAL
1	A	483	ILE
1	A	488	LEU
1	A	497	LEU
1	A	512	PHE
1	A	513	PHE
1	A	521	LEU
1	A	522	SER
1	A	555	MET
1	A	556	PHE
1	A	566	ASP
1	A	569	GLN
1	A	595	ARG
1	A	599	LEU
1	A	612	VAL
1	A	624	SER
1	A	637	ARG
1	A	641	GLU
1	A	643	SER
1	A	647	LEU
1	A	649	LYS
1	A	653	MET
1	A	658	PHE
1	A	678	THR
1	A	682	LEU
1	A	684	LEU
1	A	685	GLN
1	A	686	ASP
1	A	695	LEU

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Mol	Chain	Res	Type
1	A	697	GLN
1	A	703	LEU
1	A	705	LEU
1	A	714	ARG
1	A	715	VAL
1	A	736	SER
1	A	744	ASP
1	A	747	SER
1	A	755	SER
1	A	758	VAL
1	A	760	ASP
1	A	770	VAL
1	A	783	ASP
1	A	786	SER
1	A	800	PHE
1	A	805	THR
1	A	809	GLU
1	A	810	TYR
1	A	815	LEU
1	A	817	ARG
1	A	821	VAL
1	A	829	GLU
1	A	834	LEU
1	A	845	GLU
1	A	861	LEU
1	A	864	GLU
1	A	865	GLU
1	A	870	SER
1	A	885	LEU
1	A	896	ILE
1	A	900	VAL
1	A	913	LEU
1	A	916	SER
1	A	918	ARG
1	A	920	LEU
1	A	928	VAL
1	A	932	THR
1	A	934	ILE
1	A	952	HIS
1	A	958	ILE
1	A	964	GLU
1	A	970	LEU

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Mol	Chain	Res	Type
1	A	982	LEU
1	A	987	LEU
1	A	989	ILE
1	A	1013	THR
1	A	1022	LEU
1	A	1027	VAL
1	A	1030	LEU
1	B	11	PHE
1	B	17	LEU
1	B	18	VAL
1	B	19	ILE
1	B	21	LEU
1	B	27	ILE
1	B	46	GLN
1	B	47	VAL
1	B	48	SER
1	B	49	TYR
1	B	53	SER
1	B	56	THR
1	B	60	THR
1	B	61	VAL
1	B	75	LEU
1	B	84	SER
1	B	88	MET
1	B	89	THR
1	B	90	ILE
1	B	91	THR
1	B	93	THR
1	B	95	GLU
1	B	105	VAL
1	B	130	THR
1	B	134	LYS
1	B	139	VAL
1	B	167	SER
1	B	182	TYR
1	B	184	MET
1	B	188	LEU
1	B	194	ASN
1	B	196	TYR
1	B	197	GLN
1	B	214	ILE
1	B	216	SER

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Mol	Chain	Res	Type
1	B	219	LEU
1	B	222	LEU
1	B	225	VAL
1	B	233	THR
1	B	234	ILE
1	B	235	ILE
1	B	238	THR
1	B	239	ARG
1	B	250	LEU
1	B	253	VAL
1	B	259	GLN
1	B	263	LYS
1	B	268	VAL
1	B	273	GLN
1	B	284	SER
1	B	291	ILE
1	B	292	LYS
1	B	295	THR
1	B	298	ASN
1	B	316	PHE
1	B	348	ILE
1	B	350	LEU
1	B	354	VAL
1	B	362	PHE
1	B	365	THR
1	B	376	LEU
1	B	383	LEU
1	B	402	ILE
1	B	405	LEU
1	B	406	VAL
1	B	414	GLU
1	B	417	GLU
1	B	420	MET
1	B	426	SER
1	B	432	ARG
1	B	437	GLN
1	B	438	ILE
1	B	445	ILE
1	B	456	MET
1	B	463	THR
1	B	473	THR
1	B	475	VAL

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Mol	Chain	Res	Type
1	B	486	LEU
1	B	497	LEU
1	B	498	LYS
1	B	519	MET
1	B	544	ILE
1	B	548	ILE
1	B	557	THR
1	B	572	LEU
1	B	589	VAL
1	B	593	SER
1	B	599	LEU
1	B	610	PHE
1	B	611	THR
1	B	613	THR
1	B	628	PHE
1	B	635	GLU
1	B	641	GLU
1	B	649	LYS
1	B	652	GLN
1	B	662	MET
1	B	676	ASN
1	B	678	THR
1	B	684	LEU
1	B	695	LEU
1	B	696	LEU
1	B	704	MET
1	B	716	ARG
1	B	721	SER
1	B	746	ASN
1	B	747	SER
1	B	749	VAL
1	B	759	ASN
1	B	762	ILE
1	B	775	ARG
1	B	781	ASN
1	B	783	ASP
1	B	784	ASP
1	B	791	ARG
1	B	800	PHE
1	B	817	ARG
1	B	824	MET
1	B	836	SER

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Mol	Chain	Res	Type
1	B	847	VAL
1	B	852	LYS
1	B	880	LEU
1	B	883	VAL
1	B	893	SER
1	B	933	THR
1	B	934	ILE
1	B	936	LEU
1	B	937	SER
1	B	954	GLN
1	B	967	ARG
1	B	969	ARG
1	B	973	ILE
1	B	991	THR
1	B	1001	ILE
1	B	1005	VAL
1	B	1006	ILE
1	B	1022	LEU
1	B	1030	LEU
1	C	10	ILE
1	C	11	PHE
1	C	15	ILE
1	C	30	LEU
1	C	46	GLN
1	C	47	VAL
1	C	53	SER
1	C	58	GLN
1	C	63	GLN
1	C	65	ILE
1	C	67	GLN
1	C	78	ILE
1	C	82	SER
1	C	88	MET
1	C	90	ILE
1	C	91	THR
1	C	96	GLN
1	C	118	LEU
1	C	120	GLN
1	C	124	ARG
1	C	128	ARG
1	C	146	ASP
1	C	149	MET

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Mol	Chain	Res	Type
1	C	153	ASP
1	C	158	ILE
1	C	175	PHE
1	C	183	SER
1	C	194	ASN
1	C	199	THR
1	C	214	ILE
1	C	235	ILE
1	C	238	THR
1	C	239	ARG
1	C	253	VAL
1	C	254	ASN
1	C	259	GLN
1	C	261	ARG
1	C	264	ASP
1	C	265	VAL
1	C	300	LEU
1	C	306	ILE
1	C	323	VAL
1	C	334	SER
1	C	337	ILE
1	C	343	THR
1	C	348	ILE
1	C	357	LEU
1	C	374	VAL
1	C	376	LEU
1	C	379	THR
1	C	392	THR
1	C	405	LEU
1	C	410	ILE
1	C	447	MET
1	C	452	VAL
1	C	463	THR
1	C	466	ILE
1	C	472	ILE
1	C	481	SER
1	C	484	VAL
1	C	486	LEU
1	C	488	LEU
1	C	504	ASP
1	C	505	HIS
1	C	508	HIS

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Mol	Chain	Res	Type
1	C	509	LYS
1	C	513	PHE
1	C	519	MET
1	C	523	THR
1	C	524	THR
1	C	537	HIS
1	C	538	ARG
1	C	544	ILE
1	C	558	ARG
1	C	559	ILE
1	C	564	LEU
1	C	579	PRO
1	C	582	SER
1	C	587	THR
1	C	592	ASP
1	C	595	ARG
1	C	599	LEU
1	C	604	SER
1	C	613	THR
1	C	616	ASN
1	C	634	TRP
1	C	636	GLU
1	C	641	GLU
1	C	642	ASN
1	C	645	PHE
1	C	646	GLU
1	C	647	LEU
1	C	660	ASP
1	C	666	PHE
1	C	671	VAL
1	C	672	LEU
1	C	678	THR
1	C	696	LEU
1	C	699	ARG
1	C	712	LEU
1	C	720	MET
1	C	738	LEU
1	C	744	ASP
1	C	745	ILE
1	C	762	ILE
1	C	764	ARG
1	C	767	VAL

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Mol	Chain	Res	Type
1	C	768	LYS
1	C	779	ARG
1	C	783	ASP
1	C	797	MET
1	C	800	PHE
1	C	808	TRP
1	C	810	TYR
1	C	815	LEU
1	C	844	GLU
1	C	846	ILE
1	C	847	VAL
1	C	850	LEU
1	C	856	TYR
1	C	859	THR
1	C	866	ARG
1	C	867	LEU
1	C	880	LEU
1	C	896	ILE
1	C	900	VAL
1	C	902	LEU
1	C	906	LEU
1	C	930	LEU
1	C	932	THR
1	C	934	ILE
1	C	937	SER
1	C	942	ILE
1	C	943	LEU
1	C	944	ILE
1	C	968	MET
1	C	969	ARG
1	C	974	VAL
1	C	985	VAL
1	C	995	SER
1	C	1009	MET
1	C	1015	LEU
1	D	11	PHE
1	D	21	LEU
1	D	25	LEU
1	D	26	SER
1	D	28	LEU
1	D	32	VAL
1	D	48	SER

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Mol	Chain	Res	Type
1	D	49	TYR
1	D	55	GLU
1	D	57	VAL
1	D	58	GLN
1	D	64	VAL
1	D	72	ILE
1	D	79	SER
1	D	88	MET
1	D	92	VAL
1	D	112	GLN
1	D	118	LEU
1	D	130	THR
1	D	143	VAL
1	D	145	THR
1	D	153	ASP
1	D	160	SER
1	D	170	LYS
1	D	172	VAL
1	D	177	VAL
1	D	181	GLN
1	D	194	ASN
1	D	196	TYR
1	D	205	SER
1	D	210	GLN
1	D	214	ILE
1	D	230	LEU
1	D	235	ILE
1	D	250	LEU
1	D	253	VAL
1	D	259	GLN
1	D	276	SER
1	D	277	ILE
1	D	304	LYS
1	D	306	ILE
1	D	310	ILE
1	D	324	VAL
1	D	329	THR
1	D	343	THR
1	D	348	ILE
1	D	350	LEU
1	D	353	LEU
1	D	354	VAL

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Mol	Chain	Res	Type
1	D	367	ILE
1	D	369	THR
1	D	377	LEU
1	D	382	VAL
1	D	392	THR
1	D	393	LEU
1	D	395	MET
1	D	400	LEU
1	D	405	LEU
1	D	411	VAL
1	D	414	GLU
1	D	417	GLU
1	D	425	LEU
1	D	438	ILE
1	D	442	LEU
1	D	463	THR
1	D	466	ILE
1	D	471	SER
1	D	472	ILE
1	D	475	VAL
1	D	483	ILE
1	D	488	LEU
1	D	497	LEU
1	D	512	PHE
1	D	515	TRP
1	D	521	LEU
1	D	523	THR
1	D	538	ARG
1	D	543	LEU
1	D	555	MET
1	D	556	PHE
1	D	566	ASP
1	D	569	GLN
1	D	575	GLN
1	D	577	GLN
1	D	599	LEU
1	D	608	SER
1	D	620	ARG
1	D	626	MET
1	D	637	ARG
1	D	641	GLU
1	D	646	GLU

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Mol	Chain	Res	Type
1	D	647	LEU
1	D	649	LYS
1	D	653	MET
1	D	670	SER
1	D	671	VAL
1	D	678	THR
1	D	682	LEU
1	D	687	GLN
1	D	696	LEU
1	D	697	GLN
1	D	699	ARG
1	D	705	LEU
1	D	714	ARG
1	D	716	ARG
1	D	722	ASP
1	D	732	ASP
1	D	744	ASP
1	D	760	ASP
1	D	770	VAL
1	D	780	MET
1	D	800	PHE
1	D	805	THR
1	D	809	GLU
1	D	816	GLU
1	D	821	VAL
1	D	827	LEU
1	D	845	GLU
1	D	861	LEU
1	D	865	GLU
1	D	878	LEU
1	D	879	SER
1	D	885	LEU
1	D	896	ILE
1	D	900	VAL
1	D	903	VAL
1	D	909	ILE
1	D	913	LEU
1	D	918	ARG
1	D	920	LEU
1	D	928	VAL
1	D	932	THR
1	D	934	ILE

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Mol	Chain	Res	Type
1	D	958	ILE
1	D	989	ILE
1	D	1009	MET
1	D	1013	THR
1	D	1027	VAL
1	E	2	SER
1	E	3	LYS
1	E	4	PHE
1	E	11	PHE
1	E	17	LEU
1	E	18	VAL
1	E	20	MET
1	E	21	LEU
1	E	27	ILE
1	E	47	VAL
1	E	49	TYR
1	E	58	GLN
1	E	60	THR
1	E	61	VAL
1	E	63	GLN
1	E	78	ILE
1	E	88	MET
1	E	90	ILE
1	E	111	LEU
1	E	113	LEU
1	E	120	GLN
1	E	124	ARG
1	E	139	VAL
1	E	150	THR
1	E	160	SER
1	E	188	LEU
1	E	194	ASN
1	E	197	GLN
1	E	205	SER
1	E	212	VAL
1	E	213	GLN
1	E	214	ILE
1	E	216	SER
1	E	218	GLN
1	E	219	LEU
1	E	229	GLN
1	E	234	ILE

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Mol	Chain	Res	Type
1	E	239	ARG
1	E	248	ASN
1	E	250	LEU
1	E	253	VAL
1	E	263	LYS
1	E	268	VAL
1	E	284	SER
1	E	289	ILE
1	E	298	ASN
1	E	302	THR
1	E	329	THR
1	E	332	VAL
1	E	334	SER
1	E	336	SER
1	E	348	ILE
1	E	354	VAL
1	E	359	LEU
1	E	362	PHE
1	E	365	THR
1	E	383	LEU
1	E	402	ILE
1	E	405	LEU
1	E	414	GLU
1	E	420	MET
1	E	426	SER
1	E	434	SER
1	E	445	ILE
1	E	463	THR
1	E	473	THR
1	E	486	LEU
1	E	497	LEU
1	E	498	LYS
1	E	508	HIS
1	E	544	ILE
1	E	556	PHE
1	E	557	THR
1	E	564	LEU
1	E	572	LEU
1	E	585	GLU
1	E	586	ARG
1	E	598	LEU
1	E	601	LYS

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Mol	Chain	Res	Type
1	E	610	PHE
1	E	611	THR
1	E	613	THR
1	E	629	ILE
1	E	631	LEU
1	E	632	LYS
1	E	635	GLU
1	E	641	GLU
1	E	649	LYS
1	E	650	ARG
1	E	652	GLN
1	E	662	MET
1	E	678	THR
1	E	682	LEU
1	E	684	LEU
1	E	696	LEU
1	E	714	ARG
1	E	716	ARG
1	E	728	LEU
1	E	733	GLU
1	E	742	LEU
1	E	746	ASN
1	E	749	VAL
1	E	759	ASN
1	E	762	ILE
1	E	766	ARG
1	E	767	VAL
1	E	775	ARG
1	E	784	ASP
1	E	790	VAL
1	E	791	ARG
1	E	797	MET
1	E	800	PHE
1	E	803	PHE
1	E	805	THR
1	E	810	TYR
1	E	838	ASP
1	E	844	GLU
1	E	852	LYS
1	E	856	TYR
1	E	862	SER
1	E	866	ARG

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Mol	Chain	Res	Type
1	E	883	VAL
1	E	893	SER
1	E	908	VAL
1	E	916	SER
1	E	924	VAL
1	E	933	THR
1	E	934	ILE
1	E	936	LEU
1	E	954	GLN
1	E	958	ILE
1	E	964	GLU
1	E	968	MET
1	E	969	ARG
1	E	985	VAL
1	E	986	PRO
1	E	990	SER
1	E	995	SER
1	E	1001	ILE
1	E	1005	VAL
1	E	1006	ILE
1	E	1015	LEU
1	E	1022	LEU
1	E	1030	LEU
1	F	11	PHE
1	F	15	ILE
1	F	30	LEU
1	F	38	ILE
1	F	46	GLN
1	F	47	VAL
1	F	53	SER
1	F	60	THR
1	F	63	GLN
1	F	65	ILE
1	F	67	GLN
1	F	77	TYR
1	F	82	SER
1	F	88	MET
1	F	96	GLN
1	F	118	LEU
1	F	124	ARG
1	F	128	ARG
1	F	131	LYS

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Mol	Chain	Res	Type
1	F	146	ASP
1	F	150	THR
1	F	153	ASP
1	F	194	ASN
1	F	199	THR
1	F	214	ILE
1	F	222	LEU
1	F	235	ILE
1	F	238	THR
1	F	239	ARG
1	F	250	LEU
1	F	251	LEU
1	F	253	VAL
1	F	259	GLN
1	F	261	ARG
1	F	264	ASP
1	F	265	VAL
1	F	280	GLN
1	F	289	ILE
1	F	295	THR
1	F	300	LEU
1	F	306	ILE
1	F	319	GLN
1	F	323	VAL
1	F	334	SER
1	F	343	THR
1	F	349	LEU
1	F	355	MET
1	F	357	LEU
1	F	369	THR
1	F	374	VAL
1	F	376	LEU
1	F	379	THR
1	F	404	LEU
1	F	405	LEU
1	F	410	ILE
1	F	423	GLU
1	F	425	LEU
1	F	426	SER
1	F	434	SER
1	F	437	GLN
1	F	439	GLN

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Mol	Chain	Res	Type
1	F	463	THR
1	F	466	ILE
1	F	471	SER
1	F	472	ILE
1	F	473	THR
1	F	475	VAL
1	F	481	SER
1	F	484	VAL
1	F	486	LEU
1	F	498	LYS
1	F	502	LYS
1	F	505	HIS
1	F	508	HIS
1	F	513	PHE
1	F	523	THR
1	F	537	HIS
1	F	538	ARG
1	F	544	ILE
1	F	564	LEU
1	F	594	MET
1	F	595	ARG
1	F	598	LEU
1	F	599	LEU
1	F	601	LYS
1	F	602	GLU
1	F	604	SER
1	F	634	TRP
1	F	641	GLU
1	F	644	VAL
1	F	645	PHE
1	F	646	GLU
1	F	654	HIS
1	F	659	LYS
1	F	666	PHE
1	F	670	SER
1	F	671	VAL
1	F	678	THR
1	F	682	LEU
1	F	685	GLN
1	F	693	GLU
1	F	696	LEU
1	F	699	ARG

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Mol	Chain	Res	Type
1	F	712	LEU
1	F	720	MET
1	F	732	ASP
1	F	733	GLU
1	F	738	LEU
1	F	744	ASP
1	F	745	ILE
1	F	760	ASP
1	F	762	ILE
1	F	766	ARG
1	F	767	VAL
1	F	768	LYS
1	F	779	ARG
1	F	793	ASP
1	F	794	LYS
1	F	800	PHE
1	F	801	ASN
1	F	803	PHE
1	F	808	TRP
1	F	810	TYR
1	F	821	VAL
1	F	824	MET
1	F	840	MET
1	F	844	GLU
1	F	846	ILE
1	F	847	VAL
1	F	856	TYR
1	F	859	THR
1	F	866	ARG
1	F	867	LEU
1	F	880	LEU
1	F	900	VAL
1	F	902	LEU
1	F	903	VAL
1	F	906	LEU
1	F	909	ILE
1	F	918	ARG
1	F	920	LEU
1	F	921	SER
1	F	930	LEU
1	F	932	THR
1	F	934	ILE

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Mol	Chain	Res	Type
1	F	939	LYS
1	F	942	ILE
1	F	943	LEU
1	F	945	VAL
1	F	970	LEU
1	F	1022	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (167) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	63	GLN
1	A	67	GLN
1	A	70	ASN
1	A	106	GLN
1	A	125	GLN
1	A	156	ASN
1	A	163	GLN
1	A	194	ASN
1	A	208	GLN
1	A	210	GLN
1	A	229	GLN
1	A	231	ASN
1	A	298	ASN
1	A	361	ASN
1	A	575	GLN
1	A	577	GLN
1	A	616	ASN
1	A	642	ASN
1	A	654	HIS
1	A	692	HIS
1	A	708	GLN
1	A	725	GLN
1	A	849	GLN
1	A	927	GLN
1	A	954	GLN
1	A	998	GLN
1	B	46	GLN
1	B	67	GLN
1	B	112	GLN
1	B	123	GLN
1	B	156	ASN

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Mol	Chain	Res	Type
1	B	163	GLN
1	B	197	GLN
1	B	210	GLN
1	B	228	GLN
1	B	248	ASN
1	B	278	ASN
1	B	298	ASN
1	B	312	ASN
1	B	415	ASN
1	B	437	GLN
1	B	469	GLN
1	B	505	HIS
1	B	622	GLN
1	B	652	GLN
1	B	676	ASN
1	B	687	GLN
1	B	725	GLN
1	B	746	ASN
1	B	759	ASN
1	B	849	GLN
1	B	871	GLN
1	B	927	GLN
1	C	34	GLN
1	C	67	GLN
1	C	83	ASN
1	C	96	GLN
1	C	112	GLN
1	C	120	GLN
1	C	156	ASN
1	C	176	GLN
1	C	210	GLN
1	C	228	GLN
1	C	229	GLN
1	C	241	GLN
1	C	280	GLN
1	C	360	GLN
1	C	437	GLN
1	C	517	ASN
1	C	569	GLN
1	C	577	GLN
1	C	616	ASN
1	C	622	GLN

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Mol	Chain	Res	Type
1	C	642	ASN
1	C	687	GLN
1	C	713	GLN
1	C	718	ASN
1	C	725	GLN
1	C	871	GLN
1	C	927	GLN
1	C	952	HIS
1	C	998	GLN
1	D	67	GLN
1	D	96	GLN
1	D	106	GLN
1	D	108	GLN
1	D	120	GLN
1	D	125	GLN
1	D	156	ASN
1	D	181	GLN
1	D	194	ASN
1	D	208	GLN
1	D	210	GLN
1	D	213	GLN
1	D	228	GLN
1	D	231	ASN
1	D	298	ASN
1	D	308	GLN
1	D	312	ASN
1	D	361	ASN
1	D	415	ASN
1	D	575	GLN
1	D	622	GLN
1	D	642	ASN
1	D	700	ASN
1	D	759	ASN
1	D	871	GLN
1	D	927	GLN
1	D	954	GLN
1	D	998	GLN
1	E	46	GLN
1	E	67	GLN
1	E	104	GLN
1	E	108	GLN
1	E	120	GLN

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Mol	Chain	Res	Type
1	E	156	ASN
1	E	197	GLN
1	E	210	GLN
1	E	248	ASN
1	E	259	GLN
1	E	273	GLN
1	E	278	ASN
1	E	280	GLN
1	E	298	ASN
1	E	308	GLN
1	E	437	GLN
1	E	469	GLN
1	E	537	HIS
1	E	622	GLN
1	E	652	GLN
1	E	676	ASN
1	E	746	ASN
1	E	849	GLN
1	E	871	GLN
1	E	927	GLN
1	F	34	GLN
1	F	46	GLN
1	F	83	ASN
1	F	109	ASN
1	F	112	GLN
1	F	120	GLN
1	F	156	ASN
1	F	176	GLN
1	F	194	ASN
1	F	210	GLN
1	F	218	GLN
1	F	231	ASN
1	F	241	GLN
1	F	280	GLN
1	F	415	ASN
1	F	437	GLN
1	F	439	GLN
1	F	517	ASN
1	F	569	GLN
1	F	577	GLN
1	F	622	GLN
1	F	685	GLN

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Mol	Chain	Res	Type
1	F	700	ASN
1	F	708	GLN
1	F	725	GLN
1	F	746	ASN
1	F	781	ASN
1	F	871	GLN
1	F	927	GLN
1	F	952	HIS
1	F	998	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

17 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	2002	-	36,36,36	0.66	1 (2%)	47,47,47	1.35	4 (8%)
2	LMT	A	2001	-	36,36,36	0.76	1 (2%)	47,47,47	1.25	5 (10%)
3	P9D	B	2001	-	49,53,53	1.95	12 (24%)	52,77,77	2.15	14 (26%)
2	LMT	F	2001	-	36,36,36	0.82	1 (2%)	47,47,47	2.00	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LMT	B	2002	-	36,36,36	0.77	1 (2%)	47,47,47	1.77	11 (23%)
2	LMT	A	2003	-	36,36,36	0.69	1 (2%)	47,47,47	1.64	11 (23%)
2	LMT	C	2001	-	36,36,36	0.71	1 (2%)	47,47,47	1.32	5 (10%)
2	LMT	D	2003	-	36,36,36	0.81	1 (2%)	47,47,47	1.38	6 (12%)
2	LMT	E	2002	-	36,36,36	0.97	1 (2%)	47,47,47	1.47	9 (19%)
2	LMT	B	2004	-	36,36,36	0.48	0	47,47,47	1.02	3 (6%)
2	LMT	B	2003	-	36,36,36	0.83	1 (2%)	47,47,47	1.61	10 (21%)
2	LMT	E	2003	-	36,36,36	0.76	1 (2%)	47,47,47	1.51	5 (10%)
2	LMT	D	2001	-	36,36,36	0.94	2 (5%)	47,47,47	1.47	7 (14%)
2	LMT	F	2002	-	36,36,36	0.85	1 (2%)	47,47,47	1.36	5 (10%)
2	LMT	E	2004	-	36,36,36	0.69	1 (2%)	47,47,47	1.11	3 (6%)
2	LMT	A	2002	-	36,36,36	0.85	1 (2%)	47,47,47	1.74	15 (31%)
3	P9D	E	2001	-	49,53,53	2.01	9 (18%)	52,77,77	1.71	8 (15%)

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	2002	-	-	9/21/61/61	0/2/2/2
2	LMT	A	2001	-	-	14/21/61/61	0/2/2/2
3	P9D	B	2001	-	-	19/35/49/49	0/5/5/5
2	LMT	F	2001	-	-	12/21/61/61	0/2/2/2
2	LMT	B	2002	-	-	12/21/61/61	0/2/2/2
2	LMT	A	2003	-	-	11/21/61/61	0/2/2/2
2	LMT	C	2001	-	-	14/21/61/61	0/2/2/2
2	LMT	D	2003	-	-	7/21/61/61	0/2/2/2
2	LMT	E	2002	-	-	10/21/61/61	0/2/2/2
2	LMT	B	2004	-	-	9/21/61/61	0/2/2/2
2	LMT	B	2003	-	-	8/21/61/61	0/2/2/2
2	LMT	E	2003	-	-	14/21/61/61	0/2/2/2
2	LMT	D	2001	-	-	16/21/61/61	0/2/2/2
2	LMT	F	2002	-	-	12/21/61/61	0/2/2/2
2	LMT	E	2004	-	-	10/21/61/61	0/2/2/2
2	LMT	A	2002	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	P9D	E	2001	-	-	18/35/49/49	1/5/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2001	P9D	O34-C38	6.54	1.46	1.35
3	B	2001	P9D	N30-N29	5.50	1.41	1.32
3	B	2001	P9D	O34-C38	5.48	1.44	1.35
3	E	2001	P9D	N30-N29	4.95	1.40	1.32
3	E	2001	P9D	N31-N30	4.38	1.41	1.35
3	E	2001	P9D	C15-N16	4.19	1.44	1.38
3	E	2001	P9D	C22-C21	4.16	1.49	1.38
3	B	2001	P9D	C15-N16	4.03	1.44	1.38
3	B	2001	P9D	C22-C21	3.82	1.48	1.38
3	B	2001	P9D	C9-S8	-3.71	1.64	1.70
3	B	2001	P9D	N28-N29	3.70	1.40	1.35
3	E	2001	P9D	C17-N16	3.67	1.45	1.38
3	E	2001	P9D	N28-N29	3.57	1.40	1.35
3	B	2001	P9D	N31-N30	3.42	1.40	1.35
3	E	2001	P9D	C9-S8	-3.40	1.65	1.70
2	D	2003	LMT	O1'-C1'	3.34	1.45	1.40
2	E	2002	LMT	O1'-C1'	3.32	1.45	1.40
2	A	2001	LMT	O1'-C1'	3.29	1.45	1.40
2	D	2001	LMT	O1'-C1'	3.15	1.45	1.40
2	B	2003	LMT	O1'-C1'	3.08	1.45	1.40
2	E	2004	LMT	O1'-C1'	3.01	1.45	1.40
2	F	2002	LMT	O1'-C1'	2.98	1.45	1.40
2	F	2001	LMT	O1'-C1'	2.88	1.45	1.40
2	A	2002	LMT	O1'-C1'	2.84	1.44	1.40
3	B	2001	P9D	C17-N16	2.77	1.43	1.38
2	A	2003	LMT	O1'-C1'	2.72	1.44	1.40
2	C	2001	LMT	O1'-C1'	2.66	1.44	1.40
2	E	2003	LMT	O1'-C1'	2.55	1.44	1.40
3	B	2001	P9D	C43-N42	-2.37	1.47	1.51
3	B	2001	P9D	C21-N24	2.25	1.42	1.37
3	E	2001	P9D	C21-N24	2.21	1.42	1.37
3	B	2001	P9D	C18-C12	-2.19	1.38	1.43
2	B	2002	LMT	O1'-C1'	2.18	1.43	1.40
2	D	2002	LMT	O1'-C1'	2.12	1.43	1.40
3	B	2001	P9D	C15-N19	2.06	1.37	1.33
2	D	2001	LMT	O1B-C1B	2.06	1.47	1.41

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2001	P9D	C9-C4-C2	-6.65	120.64	129.11
2	B	2003	LMT	C1B-O5B-C5B	5.84	125.12	113.72
3	E	2001	P9D	C9-C4-C2	-5.63	121.94	129.11
3	B	2001	P9D	N28-C27-N31	5.55	117.45	111.45
2	F	2001	LMT	C3'-C4'-C5'	-5.13	99.55	110.93
2	E	2003	LMT	C1B-O5B-C5B	5.05	123.58	113.72
2	B	2002	LMT	O5B-C5B-C4B	4.65	118.08	109.70
2	F	2001	LMT	C1-O1'-C1'	4.53	121.42	113.68
3	E	2001	P9D	C32-N24-C21	-4.49	105.62	119.33
2	E	2002	LMT	C1'-O5'-C5'	4.38	122.28	113.72
3	B	2001	P9D	C37-N24-C21	-4.32	107.26	119.71
2	D	2003	LMT	O1'-C1'-C2'	4.31	114.82	108.27
3	B	2001	P9D	C26-C25-C22	-4.24	114.81	126.73
3	B	2001	P9D	N31-N30-N29	-4.21	106.80	109.54
2	F	2001	LMT	O5B-C5B-C6B	4.10	116.61	106.44
2	A	2002	LMT	C1'-O5'-C5'	4.09	121.70	113.72
3	E	2001	P9D	N28-C27-N31	4.02	115.80	111.45
2	F	2002	LMT	C2'-C3'-C4'	3.96	118.66	109.68
2	B	2002	LMT	C1'-O5'-C5'	3.96	121.45	113.72
2	B	2003	LMT	O5B-C5B-C4B	3.96	116.83	109.70
2	D	2001	LMT	C1B-O5B-C5B	3.92	121.38	113.72
2	A	2002	LMT	C2'-C3'-C4'	-3.88	100.86	109.68
2	D	2002	LMT	C1B-O5B-C5B	3.88	121.29	113.72
2	F	2002	LMT	C1'-C2'-C3'	3.87	118.14	110.01
2	F	2001	LMT	O5'-C5'-C4'	-3.86	101.74	109.72
2	A	2003	LMT	O1'-C1'-C2'	3.85	114.12	108.27
2	F	2001	LMT	O1B-C4'-C5'	3.82	119.48	109.48
2	B	2002	LMT	C2'-C3'-C4'	3.78	118.25	109.68
2	F	2001	LMT	C1'-C2'-C3'	3.77	117.94	110.01
2	B	2002	LMT	C3B-C4B-C5B	3.72	116.97	110.23
3	B	2001	P9D	O34-C38-N39	3.68	117.00	111.01
2	A	2002	LMT	O1B-C4'-C3'	3.63	116.45	107.23
2	D	2002	LMT	O5'-C5'-C4'	3.60	117.17	109.72
2	E	2003	LMT	C3B-C4B-C5B	3.57	116.71	110.23
2	A	2003	LMT	O1B-C1B-C2B	3.56	116.86	108.09
2	D	2001	LMT	O1B-C1B-C2B	3.43	116.53	108.09
2	E	2003	LMT	O1B-C4'-C3'	3.39	115.85	107.23
2	A	2003	LMT	O5B-C5B-C4B	3.39	115.80	109.70
2	A	2003	LMT	C1B-O5B-C5B	3.38	120.33	113.72
2	A	2003	LMT	C4B-C3B-C2B	-3.34	104.96	110.83
3	B	2001	P9D	C7-N10-C11	-3.30	118.86	126.58
2	B	2002	LMT	C1'-C2'-C3'	3.29	116.94	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2001	LMT	C2'-C3'-C4'	3.27	117.11	109.68
2	D	2001	LMT	C1'-O5'-C5'	3.26	120.09	113.72
2	A	2002	LMT	C3B-C4B-C5B	3.20	116.04	110.23
3	E	2001	P9D	C17-N16-C20	3.20	121.31	117.34
2	E	2002	LMT	O1B-C1B-C2B	3.15	115.84	108.09
3	E	2001	P9D	N28-N29-N30	-3.14	107.50	109.54
2	A	2001	LMT	C3B-C4B-C5B	3.14	115.93	110.23
2	E	2003	LMT	O5B-C5B-C4B	3.12	115.32	109.70
2	F	2002	LMT	C1B-O1B-C4'	3.11	125.36	117.98
2	A	2001	LMT	C1'-O5'-C5'	3.10	119.77	113.72
2	F	2001	LMT	O1B-C1B-C2B	3.08	115.67	108.09
2	E	2002	LMT	O5'-C5'-C6'	3.06	114.03	106.44
2	A	2003	LMT	O2B-C2B-C3B	3.06	117.58	110.38
2	F	2001	LMT	C6'-C5'-C4'	3.06	121.97	113.38
2	C	2001	LMT	C1B-O5B-C5B	3.05	119.68	113.72
3	B	2001	P9D	O23-C20-C22	-3.04	118.51	124.96
2	A	2003	LMT	O5'-C1'-C2'	-3.04	104.13	110.37
2	E	2003	LMT	C1'-O5'-C5'	3.01	119.61	113.72
2	F	2001	LMT	O2'-C2'-C3'	-2.97	103.36	110.38
3	B	2001	P9D	C17-N16-C20	2.93	120.97	117.34
2	B	2003	LMT	O1'-C1'-C2'	2.92	112.71	108.27
2	F	2002	LMT	O1B-C4'-C3'	2.91	114.63	107.23
2	B	2002	LMT	O5'-C5'-C4'	2.91	115.74	109.72
2	B	2003	LMT	O1B-C4'-C3'	2.88	114.55	107.23
2	B	2002	LMT	C1B-O1B-C4'	-2.87	111.18	117.98
2	D	2003	LMT	C1B-O5B-C5B	2.86	119.31	113.72
2	E	2004	LMT	O3B-C3B-C2B	-2.84	103.69	110.38
2	E	2004	LMT	O5B-C5B-C6B	2.82	113.42	106.44
2	A	2002	LMT	O5B-C5B-C6B	2.80	113.39	106.44
2	A	2002	LMT	O5B-C5B-C4B	2.80	114.74	109.70
2	B	2002	LMT	C3'-C4'-C5'	2.79	117.11	110.93
3	B	2001	P9D	C35-C36-C37	-2.76	107.13	110.75
2	D	2003	LMT	C3B-C4B-C5B	2.75	115.22	110.23
2	F	2001	LMT	O1'-C1'-C2'	2.74	112.43	108.27
2	F	2001	LMT	C1B-O5B-C5B	2.73	119.04	113.72
2	B	2002	LMT	C1B-O5B-C5B	2.71	119.00	113.72
2	F	2001	LMT	O5'-C5'-C6'	2.70	113.13	106.44
2	D	2001	LMT	O5'-C1'-O1'	2.67	116.34	110.04
2	B	2003	LMT	O1B-C1B-C2B	2.65	114.60	108.09
2	E	2004	LMT	O1'-C1'-C2'	2.63	112.27	108.27
2	C	2001	LMT	O5'-C1'-C2'	-2.63	104.97	110.37
2	A	2002	LMT	O2'-C2'-C3'	-2.61	104.23	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	LMT	O1'-C1'-C2'	2.57	112.18	108.27
2	D	2001	LMT	O5B-C5B-C6B	2.56	112.79	106.44
2	D	2002	LMT	C1'-O5'-C5'	2.56	118.71	113.72
2	B	2003	LMT	C4B-C3B-C2B	-2.55	106.35	110.83
2	A	2002	LMT	C1B-O5B-C5B	2.55	118.70	113.72
2	A	2002	LMT	O1B-C4'-C5'	2.47	115.94	109.48
2	B	2003	LMT	C3'-C4'-C5'	-2.46	105.47	110.93
2	E	2002	LMT	O1B-C4'-C5'	2.44	115.87	109.48
2	D	2003	LMT	O5'-C5'-C6'	2.43	112.45	106.44
2	D	2001	LMT	O5'-C5'-C6'	2.42	112.44	106.44
2	E	2002	LMT	O5'-C5'-C4'	2.40	114.69	109.72
2	A	2002	LMT	C1B-O1B-C4'	2.40	123.67	117.98
2	A	2001	LMT	C1B-O1B-C4'	-2.39	112.31	117.98
2	E	2002	LMT	C1-O1'-C1'	2.37	117.73	113.68
2	C	2001	LMT	O2'-C2'-C3'	-2.37	104.79	110.38
2	E	2002	LMT	O3'-C3'-C4'	-2.35	103.91	109.94
2	A	2003	LMT	O1B-C4'-C5'	2.34	115.62	109.48
3	E	2001	P9D	N31-N30-N29	-2.34	108.02	109.54
3	B	2001	P9D	O23-C20-N16	2.33	122.44	118.40
2	A	2002	LMT	O5'-C5'-C4'	2.33	114.55	109.72
2	B	2003	LMT	C1B-O1B-C4'	-2.33	112.46	117.98
3	B	2001	P9D	C36-C37-N24	-2.32	105.96	110.67
3	E	2001	P9D	C26-C25-C22	-2.31	120.23	126.73
2	B	2004	LMT	O1'-C1'-C2'	2.31	111.78	108.27
2	A	2002	LMT	C4B-C3B-C2B	2.30	114.86	110.83
2	D	2002	LMT	O5B-C5B-C6B	2.29	112.12	106.44
2	A	2003	LMT	O5B-C1B-C2B	-2.28	105.68	110.37
2	A	2003	LMT	C1B-O1B-C4'	-2.28	112.57	117.98
2	A	2001	LMT	C4B-C3B-C2B	2.28	114.83	110.83
2	F	2002	LMT	O2'-C2'-C3'	-2.27	105.03	110.38
2	E	2002	LMT	O5B-C5B-C4B	2.27	113.78	109.70
2	B	2003	LMT	C1-O1'-C1'	2.23	117.48	113.68
2	B	2002	LMT	O1B-C1B-C2B	2.21	113.52	108.09
2	A	2002	LMT	O5'-C1'-O1'	2.21	115.26	110.04
2	A	2003	LMT	C6B-C5B-C4B	-2.20	107.61	113.02
3	B	2001	P9D	O34-C38-O44	-2.20	121.31	124.55
2	D	2001	LMT	O5'-C5'-C4'	2.19	114.26	109.72
2	C	2001	LMT	O1B-C1B-C2B	2.19	113.48	108.09
2	B	2002	LMT	O5'-C1'-O1'	2.17	115.18	110.04
3	B	2001	P9D	O44-C38-N39	-2.15	121.69	124.93
2	B	2004	LMT	C1B-C2B-C3B	-2.14	105.51	110.01
2	D	2003	LMT	O4'-C4B-C3B	-2.13	105.36	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2001	LMT	O2B-C2B-C3B	2.13	115.39	110.38
2	B	2004	LMT	O3B-C3B-C4B	2.12	115.38	110.38
2	D	2003	LMT	C1-O1'-C1'	2.09	117.26	113.68
3	E	2001	P9D	C37-N24-C21	-2.08	113.72	119.71
2	A	2002	LMT	O1B-C1B-O5B	2.08	116.17	110.69
2	A	2002	LMT	O5'-C1'-C2'	2.07	114.63	110.37
2	E	2002	LMT	O4'-C4B-C5B	2.05	114.38	109.32
2	B	2003	LMT	O5'-C5'-C6'	2.01	111.41	106.44

There are no chirality outliers.

All (208) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	LMT	O5'-C1'-O1'-C1
2	A	2002	LMT	C3'-C4'-O1B-C1B
2	B	2004	LMT	C2-C1-O1'-C1'
2	D	2001	LMT	C2'-C1'-O1'-C1
2	D	2001	LMT	O5'-C1'-O1'-C1
2	D	2003	LMT	C2-C1-O1'-C1'
2	E	2002	LMT	O5'-C1'-O1'-C1
2	E	2003	LMT	C2'-C1'-O1'-C1
2	F	2001	LMT	C2B-C1B-O1B-C4'
2	F	2001	LMT	C2'-C1'-O1'-C1
3	B	2001	P9D	N10-C11-C12-C18
3	B	2001	P9D	O13-C11-C12-C18
3	B	2001	P9D	N19-C21-N24-C37
3	B	2001	P9D	C32-C33-O34-C38
3	B	2001	P9D	N39-C40-C41-N42
3	B	2001	P9D	C45-C43-N42-C41
3	B	2001	P9D	C45-C43-N42-C48
3	B	2001	P9D	C45-C43-N42-C49
3	B	2001	P9D	N42-C43-C45-O46
3	B	2001	P9D	N42-C43-C45-O47
3	E	2001	P9D	O13-C11-C12-C14
3	E	2001	P9D	N39-C38-O34-C33
3	E	2001	P9D	O44-C38-O34-C33
3	E	2001	P9D	O34-C38-N39-C40
3	E	2001	P9D	O44-C38-N39-C40
3	E	2001	P9D	C40-C41-N42-C43
3	E	2001	P9D	C40-C41-N42-C48
3	E	2001	P9D	C40-C41-N42-C49
3	E	2001	P9D	C45-C43-N42-C41

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Mol	Chain	Res	Type	Atoms
3	E	2001	P9D	C45-C43-N42-C48
3	E	2001	P9D	C45-C43-N42-C49
3	E	2001	P9D	N42-C43-C45-O46
3	E	2001	P9D	N42-C43-C45-O47
2	F	2002	LMT	C3'-C4'-O1B-C1B
2	D	2002	LMT	O5B-C1B-O1B-C4'
2	D	2001	LMT	C2B-C1B-O1B-C4'
2	C	2001	LMT	O5B-C1B-O1B-C4'
2	F	2001	LMT	O5B-C1B-O1B-C4'
2	F	2002	LMT	O5B-C1B-O1B-C4'
2	A	2001	LMT	C4'-C5'-C6'-O6'
2	D	2001	LMT	O5'-C5'-C6'-O6'
2	A	2002	LMT	O5B-C5B-C6B-O6B
2	D	2001	LMT	O5B-C5B-C6B-O6B
2	B	2002	LMT	O5B-C5B-C6B-O6B
2	E	2003	LMT	C4B-C5B-C6B-O6B
2	F	2002	LMT	C4'-C5'-C6'-O6'
2	A	2003	LMT	O5B-C5B-C6B-O6B
2	B	2003	LMT	O5B-C5B-C6B-O6B
2	A	2001	LMT	O5'-C5'-C6'-O6'
2	B	2002	LMT	C4B-C5B-C6B-O6B
2	D	2001	LMT	C4'-C5'-C6'-O6'
2	A	2002	LMT	O5'-C1'-O1'-C1
2	B	2002	LMT	O5'-C1'-O1'-C1
2	C	2001	LMT	O5'-C1'-O1'-C1
2	E	2003	LMT	O5'-C1'-O1'-C1
2	F	2002	LMT	O5'-C1'-O1'-C1
2	F	2002	LMT	O5'-C5'-C6'-O6'
2	A	2001	LMT	O5B-C5B-C6B-O6B
2	C	2001	LMT	C4B-C5B-C6B-O6B
2	F	2001	LMT	C4'-C5'-C6'-O6'
2	A	2002	LMT	C4B-C5B-C6B-O6B
2	E	2003	LMT	C4'-C5'-C6'-O6'
2	A	2001	LMT	C2'-C1'-O1'-C1
2	A	2002	LMT	C2'-C1'-O1'-C1
2	B	2002	LMT	C2'-C1'-O1'-C1
2	C	2001	LMT	C2'-C1'-O1'-C1
2	F	2002	LMT	C2'-C1'-O1'-C1
2	C	2001	LMT	O5B-C5B-C6B-O6B
2	E	2003	LMT	O5B-C5B-C6B-O6B
2	A	2001	LMT	C4B-C5B-C6B-O6B
2	A	2003	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
2	B	2003	LMT	C4B-C5B-C6B-O6B
2	D	2001	LMT	C4B-C5B-C6B-O6B
2	F	2001	LMT	O5'-C5'-C6'-O6'
2	B	2004	LMT	O1'-C1-C2-C3
2	E	2002	LMT	O5'-C5'-C6'-O6'
2	E	2003	LMT	O5'-C5'-C6'-O6'
3	B	2001	P9D	C40-C41-N42-C49
2	F	2001	LMT	O5'-C1'-O1'-C1
2	C	2001	LMT	O5'-C5'-C6'-O6'
2	B	2002	LMT	C2B-C1B-O1B-C4'
2	E	2004	LMT	C4B-C5B-C6B-O6B
2	D	2002	LMT	C1-C2-C3-C4
2	E	2002	LMT	C11-C10-C9-C8
2	A	2002	LMT	C1-C2-C3-C4
2	B	2003	LMT	C7-C8-C9-C10
2	F	2002	LMT	C6-C7-C8-C9
2	D	2003	LMT	C4-C5-C6-C7
2	E	2003	LMT	C2-C1-O1'-C1'
2	A	2001	LMT	C2-C3-C4-C5
2	B	2004	LMT	C4-C5-C6-C7
2	E	2004	LMT	C11-C10-C9-C8
2	B	2004	LMT	C1-C2-C3-C4
2	A	2002	LMT	C3-C4-C5-C6
2	F	2002	LMT	C11-C10-C9-C8
2	C	2001	LMT	C1-C2-C3-C4
2	C	2001	LMT	C7-C8-C9-C10
2	B	2004	LMT	C2-C3-C4-C5
2	D	2001	LMT	C3'-C4'-O1B-C1B
2	E	2003	LMT	C3-C4-C5-C6
2	F	2001	LMT	C1-C2-C3-C4
2	B	2004	LMT	C11-C10-C9-C8
2	E	2002	LMT	C7-C8-C9-C10
2	B	2004	LMT	C7-C8-C9-C10
2	F	2002	LMT	C2-C3-C4-C5
2	F	2001	LMT	C5-C6-C7-C8
2	B	2002	LMT	C6-C7-C8-C9
2	E	2004	LMT	C2-C3-C4-C5
2	A	2002	LMT	C11-C10-C9-C8
2	D	2001	LMT	C2-C3-C4-C5
2	D	2003	LMT	C2-C3-C4-C5
2	E	2003	LMT	C2-C3-C4-C5
2	E	2004	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
2	D	2001	LMT	C7-C8-C9-C10
3	B	2001	P9D	C12-C11-N10-C7
2	E	2004	LMT	O1'-C1-C2-C3
2	F	2001	LMT	C3'-C4'-O1B-C1B
2	D	2002	LMT	O5'-C5'-C6'-O6'
2	A	2003	LMT	C1-C2-C3-C4
2	C	2001	LMT	C2B-C1B-O1B-C4'
2	F	2002	LMT	O5B-C5B-C6B-O6B
3	B	2001	P9D	O13-C11-N10-C7
2	E	2002	LMT	C4-C5-C6-C7
2	C	2001	LMT	C5-C6-C7-C8
2	D	2002	LMT	C2-C3-C4-C5
2	D	2002	LMT	C5'-C4'-O1B-C1B
2	D	2002	LMT	C11-C10-C9-C8
2	A	2001	LMT	C7-C8-C9-C10
2	D	2002	LMT	C3'-C4'-O1B-C1B
2	B	2004	LMT	C3-C4-C5-C6
2	A	2003	LMT	C4'-C5'-C6'-O6'
2	D	2001	LMT	C5'-C4'-O1B-C1B
2	C	2001	LMT	C3'-C4'-O1B-C1B
3	E	2001	P9D	N19-C21-N24-C32
3	B	2001	P9D	O13-C11-C12-C14
2	B	2002	LMT	C4'-C5'-C6'-O6'
2	A	2001	LMT	C11-C10-C9-C8
2	A	2003	LMT	C11-C10-C9-C8
2	C	2001	LMT	C2-C3-C4-C5
2	A	2002	LMT	C9-C10-C11-C12
2	C	2001	LMT	C5'-C4'-O1B-C1B
2	A	2001	LMT	C5-C6-C7-C8
2	D	2001	LMT	O1'-C1-C2-C3
2	D	2003	LMT	C9-C10-C11-C12
2	D	2001	LMT	C4-C5-C6-C7
2	F	2002	LMT	C9-C10-C11-C12
2	F	2002	LMT	O1'-C1-C2-C3
2	B	2002	LMT	O5B-C1B-O1B-C4'
2	B	2003	LMT	C2-C1-O1'-C1'
2	D	2001	LMT	C2-C1-O1'-C1'
2	A	2002	LMT	C2-C3-C4-C5
2	A	2002	LMT	C7-C8-C9-C10
3	B	2001	P9D	N10-C11-C12-C14
3	E	2001	P9D	N10-C11-C12-C14
2	A	2001	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	E	2002	LMT	C9-C10-C11-C12
2	E	2003	LMT	C9-C10-C11-C12
2	E	2004	LMT	C5-C6-C7-C8
2	E	2003	LMT	C11-C10-C9-C8
2	E	2004	LMT	C9-C10-C11-C12
2	D	2001	LMT	C9-C10-C11-C12
2	D	2003	LMT	O5'-C5'-C6'-O6'
2	E	2002	LMT	C2'-C1'-O1'-C1
2	E	2003	LMT	O1'-C1-C2-C3
3	B	2001	P9D	N39-C38-O34-C33
2	F	2001	LMT	C5'-C4'-O1B-C1B
3	E	2001	P9D	C32-C33-O34-C38
2	A	2003	LMT	C7-C8-C9-C10
2	E	2002	LMT	C5-C6-C7-C8
3	E	2001	P9D	C41-C40-N39-C38
2	A	2002	LMT	C4'-C5'-C6'-O6'
2	D	2003	LMT	C6-C7-C8-C9
2	E	2004	LMT	C3-C4-C5-C6
2	E	2003	LMT	C1-C2-C3-C4
2	E	2002	LMT	C3-C4-C5-C6
2	A	2003	LMT	C5-C6-C7-C8
2	C	2001	LMT	C3-C4-C5-C6
2	D	2001	LMT	C1-C2-C3-C4
2	B	2002	LMT	C3-C4-C5-C6
2	D	2002	LMT	O1'-C1-C2-C3
2	B	2002	LMT	C2-C3-C4-C5
3	B	2001	P9D	O44-C38-O34-C33
2	E	2004	LMT	C4-C5-C6-C7
2	F	2001	LMT	C2-C3-C4-C5
2	F	2001	LMT	C4-C5-C6-C7
3	B	2001	P9D	C40-C41-N42-C43
2	A	2001	LMT	C2B-C1B-O1B-C4'
2	A	2003	LMT	O5'-C5'-C6'-O6'
2	B	2003	LMT	C11-C10-C9-C8
2	E	2004	LMT	C2-C1-O1'-C1'
2	B	2003	LMT	C4-C5-C6-C7
2	A	2003	LMT	O5'-C1'-O1'-C1
2	E	2002	LMT	C2B-C1B-O1B-C4'
2	B	2002	LMT	C5-C6-C7-C8
2	A	2001	LMT	C4-C5-C6-C7
2	B	2003	LMT	C3-C4-C5-C6
2	B	2003	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
2	B	2002	LMT	C7-C8-C9-C10
2	E	2003	LMT	C4-C5-C6-C7
2	D	2002	LMT	C2-C1-O1'-C1'
2	A	2003	LMT	C9-C10-C11-C12
2	A	2003	LMT	C3-C4-C5-C6
2	B	2004	LMT	C6-C7-C8-C9
3	E	2001	P9D	C35-C33-O34-C38
2	D	2003	LMT	C5-C6-C7-C8
2	A	2001	LMT	O5B-C1B-O1B-C4'
3	B	2001	P9D	C22-C21-N24-C37
2	A	2002	LMT	C5-C6-C7-C8

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2001	P9D	C32-C33-C35-C36-C37-N24

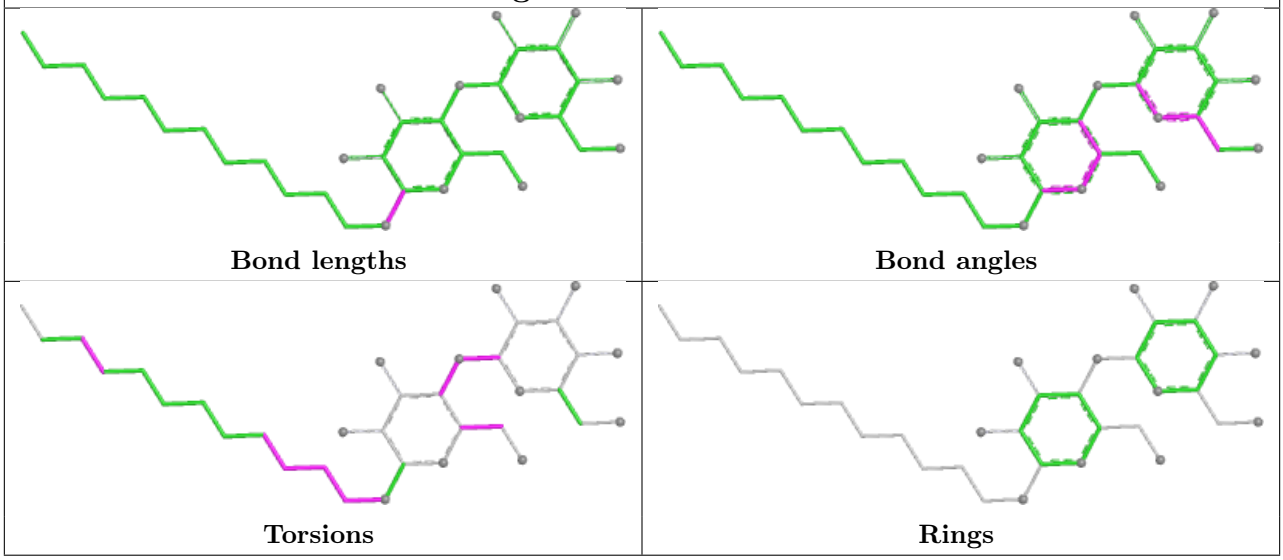
16 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2002	LMT	1	0
2	A	2001	LMT	2	0
3	B	2001	P9D	8	0
2	F	2001	LMT	4	0
2	B	2002	LMT	2	0
2	A	2003	LMT	2	0
2	C	2001	LMT	6	0
2	D	2003	LMT	2	0
2	E	2002	LMT	9	0
2	B	2004	LMT	1	0
2	B	2003	LMT	2	0
2	E	2003	LMT	1	0
2	D	2001	LMT	2	0
2	F	2002	LMT	3	0
2	A	2002	LMT	2	0
3	E	2001	P9D	8	0

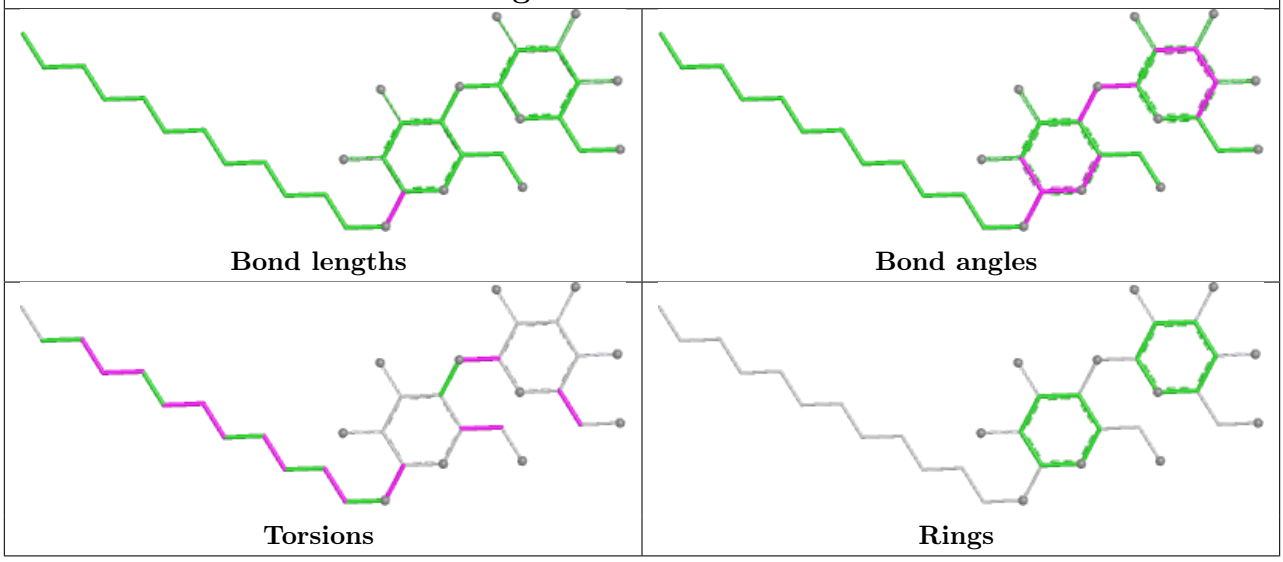
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

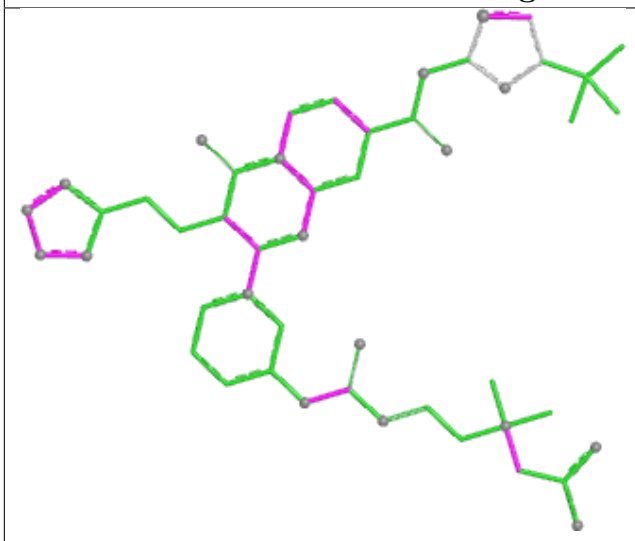
Ligand LMT D 2002



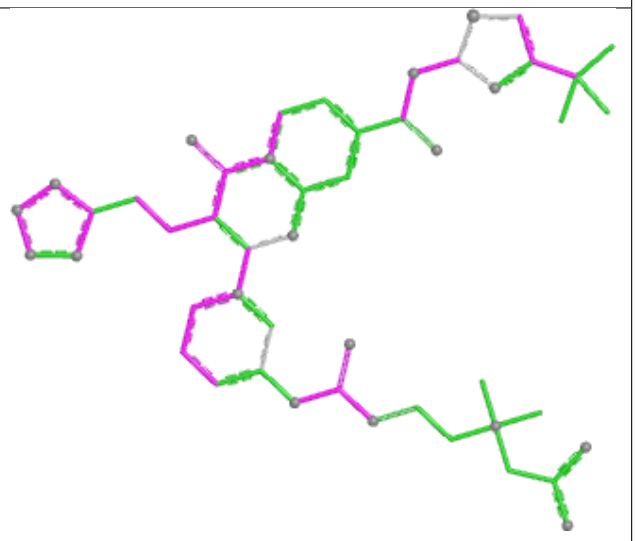
Ligand LMT A 2001



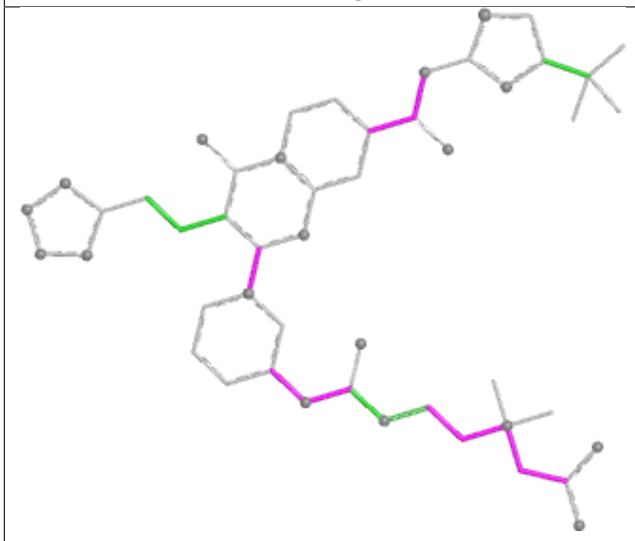
Ligand P9D B 2001



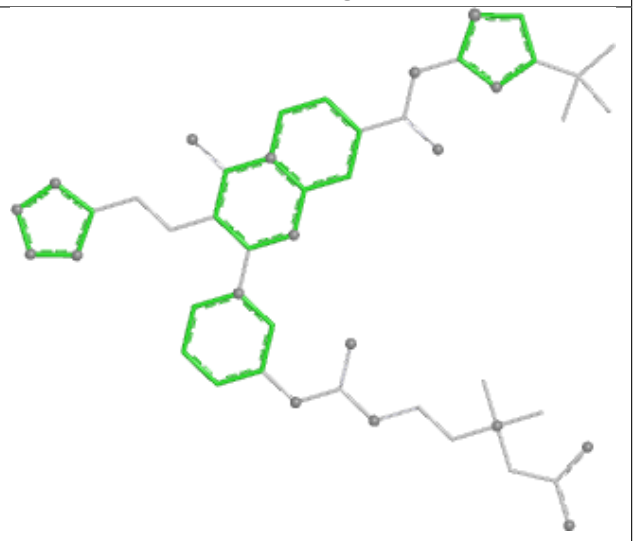
Bond lengths



Bond angles

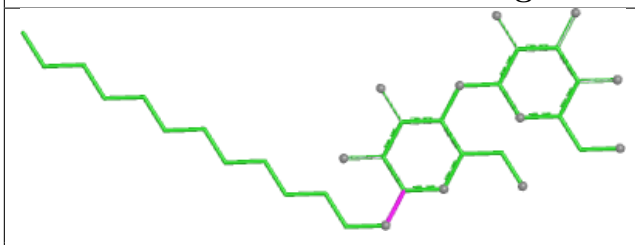


Torsions



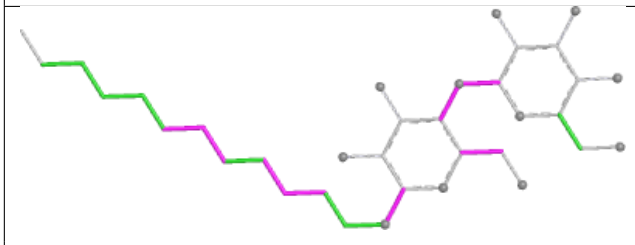
Rings

Ligand LMT F 2001

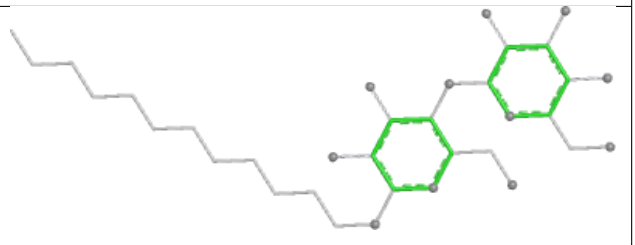


Bond lengths

Bond angles

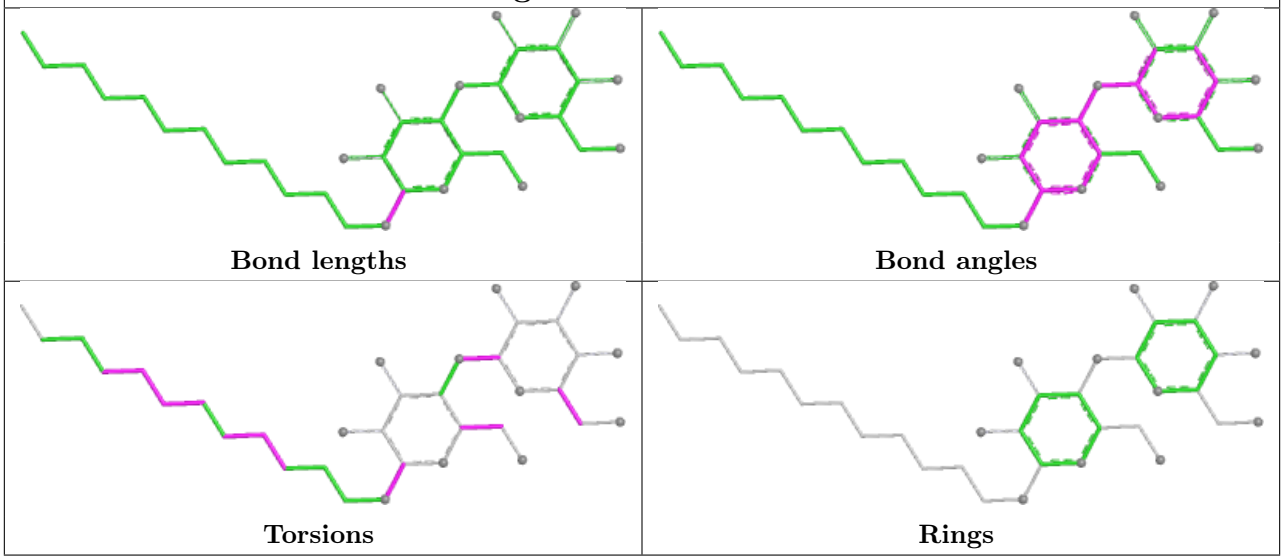


Torsions

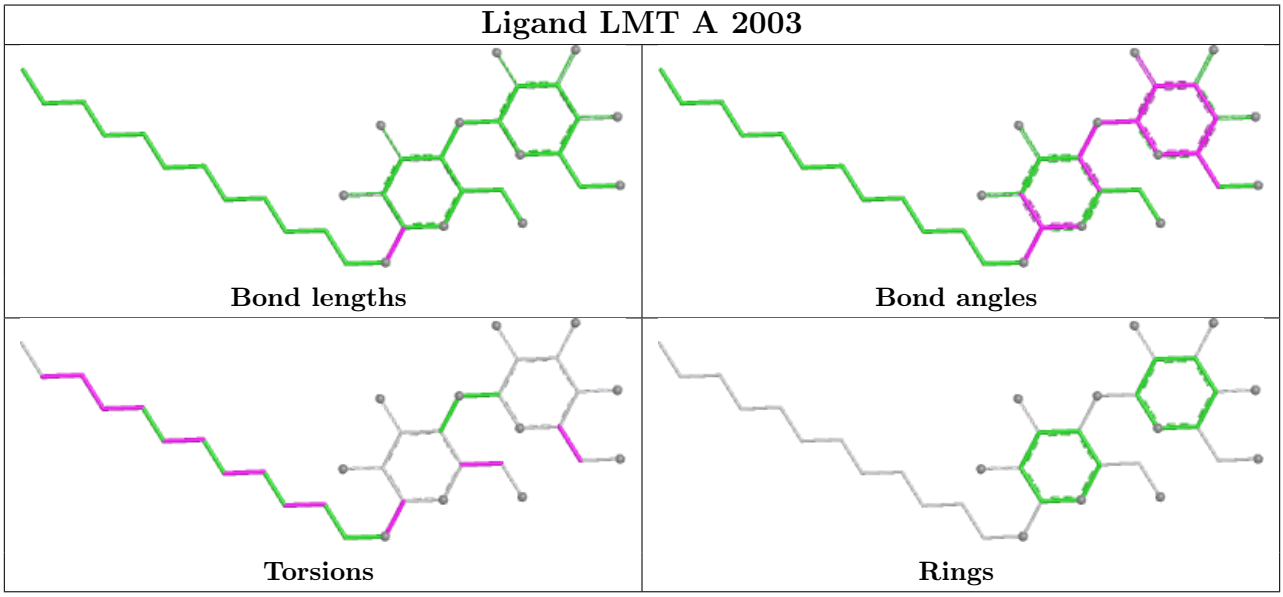


Rings

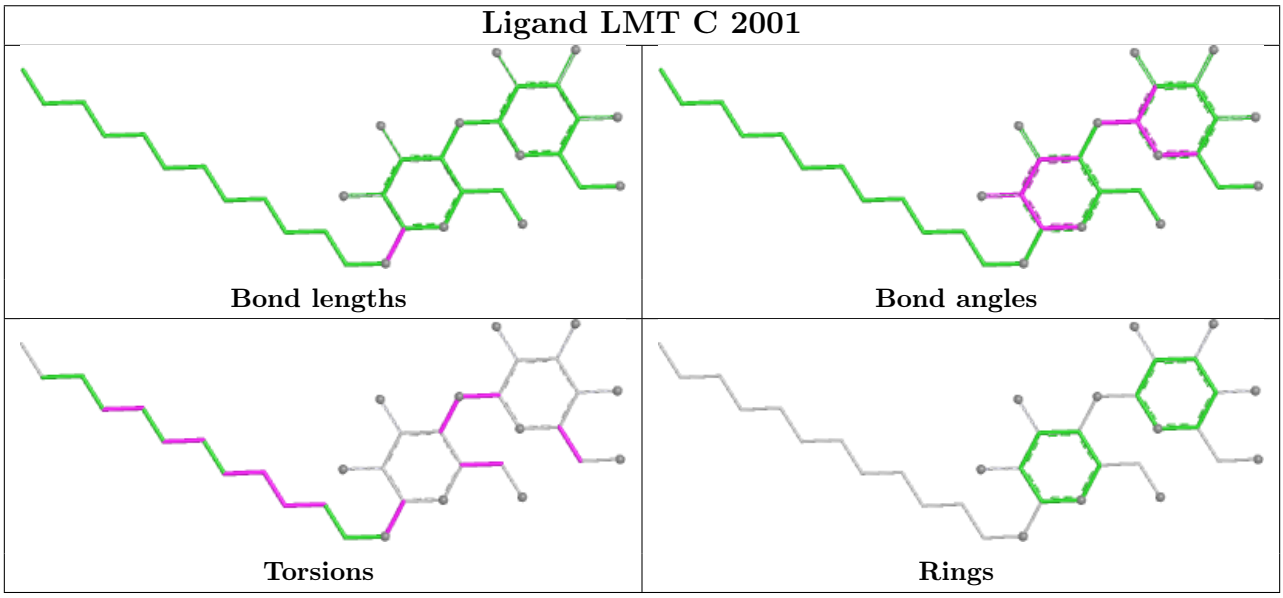
Ligand LMT B 2002



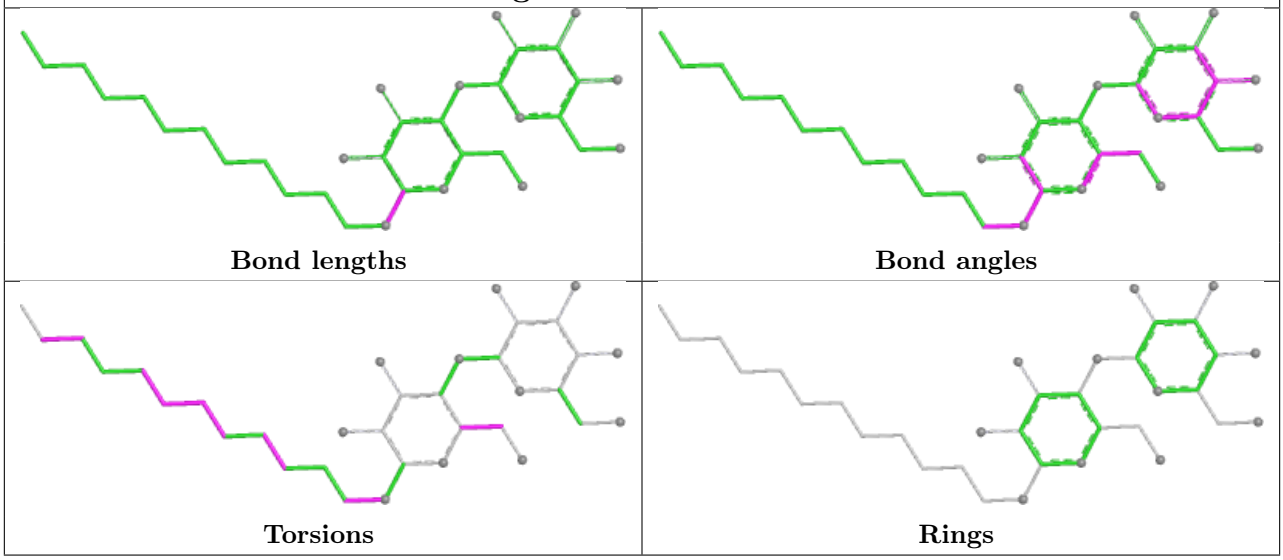
Ligand LMT A 2003



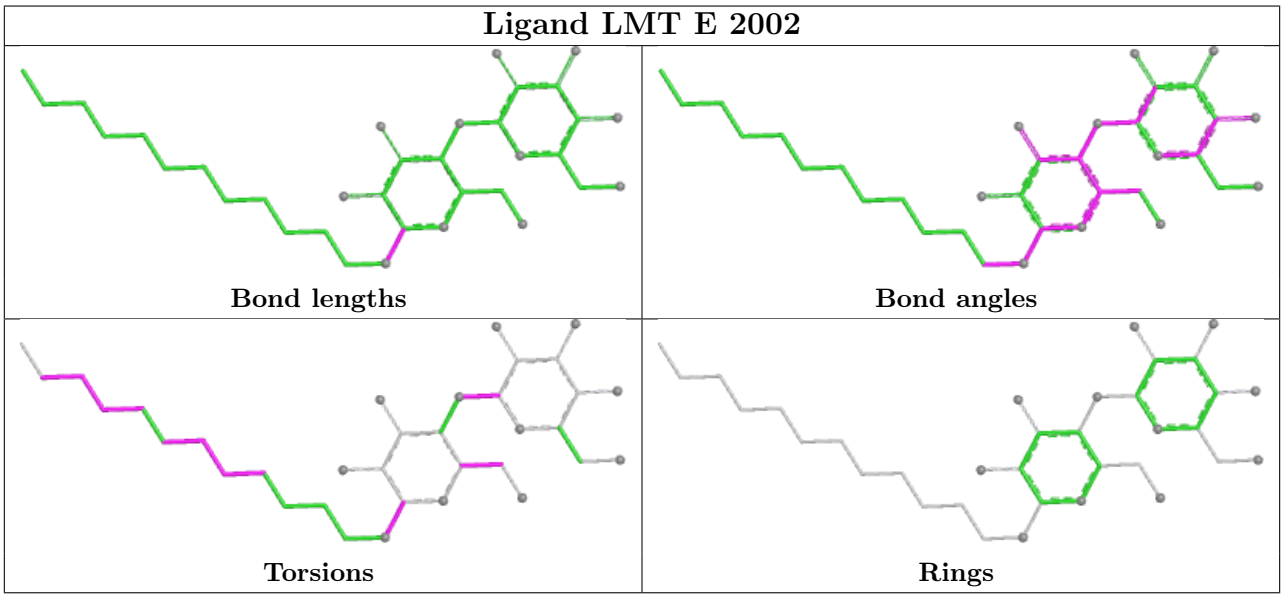
Ligand LMT C 2001



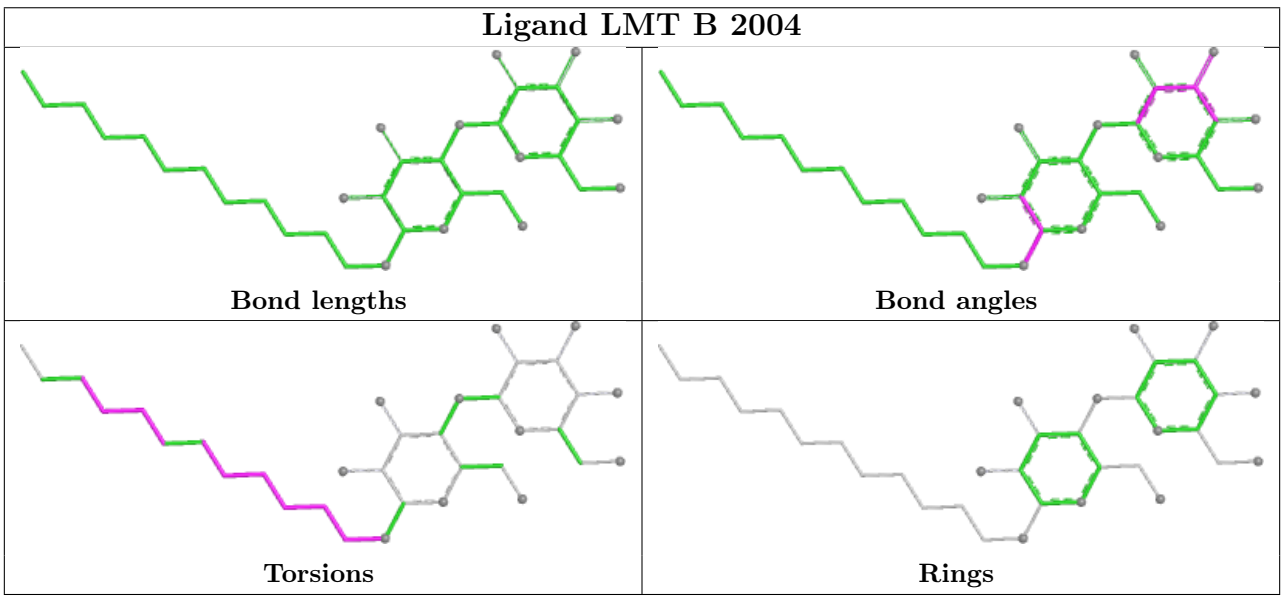
Ligand LMT D 2003



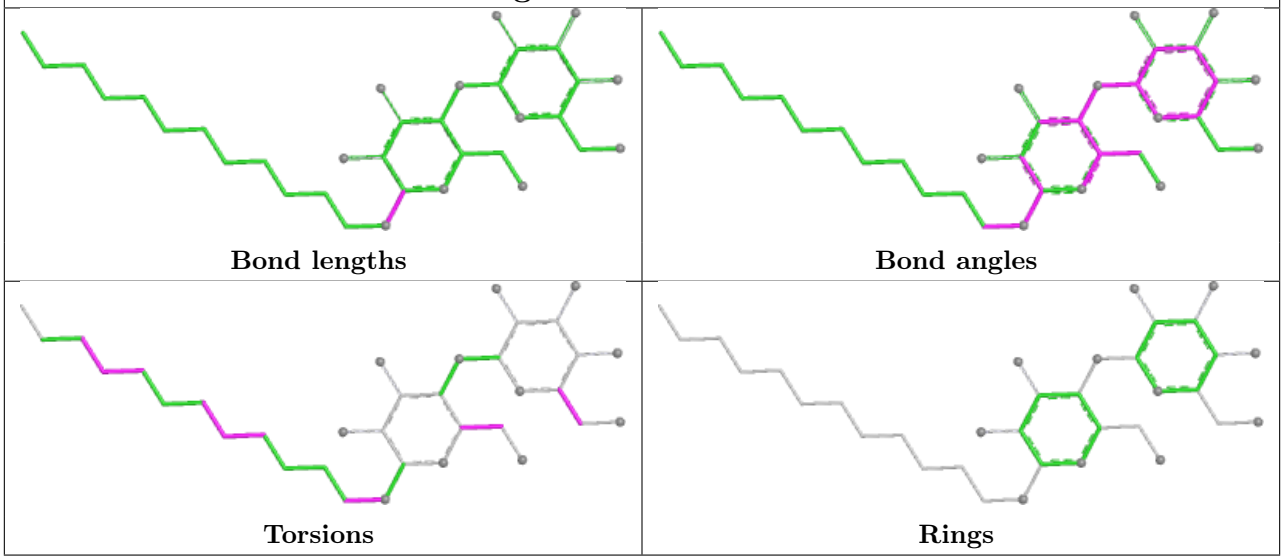
Ligand LMT E 2002



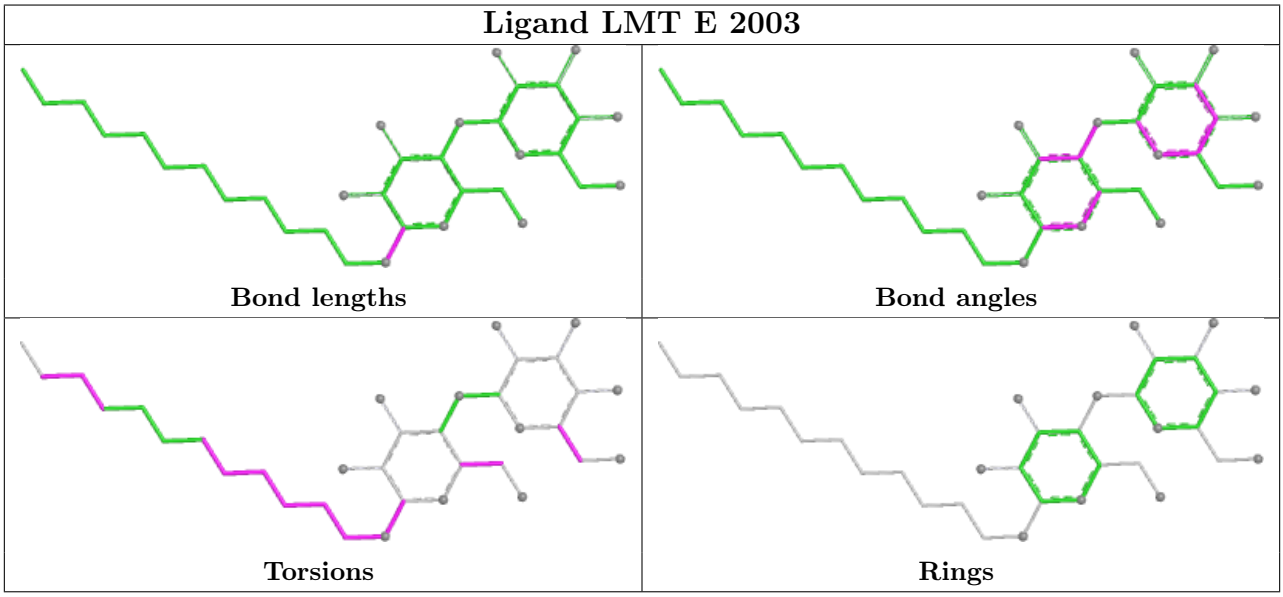
Ligand LMT B 2004



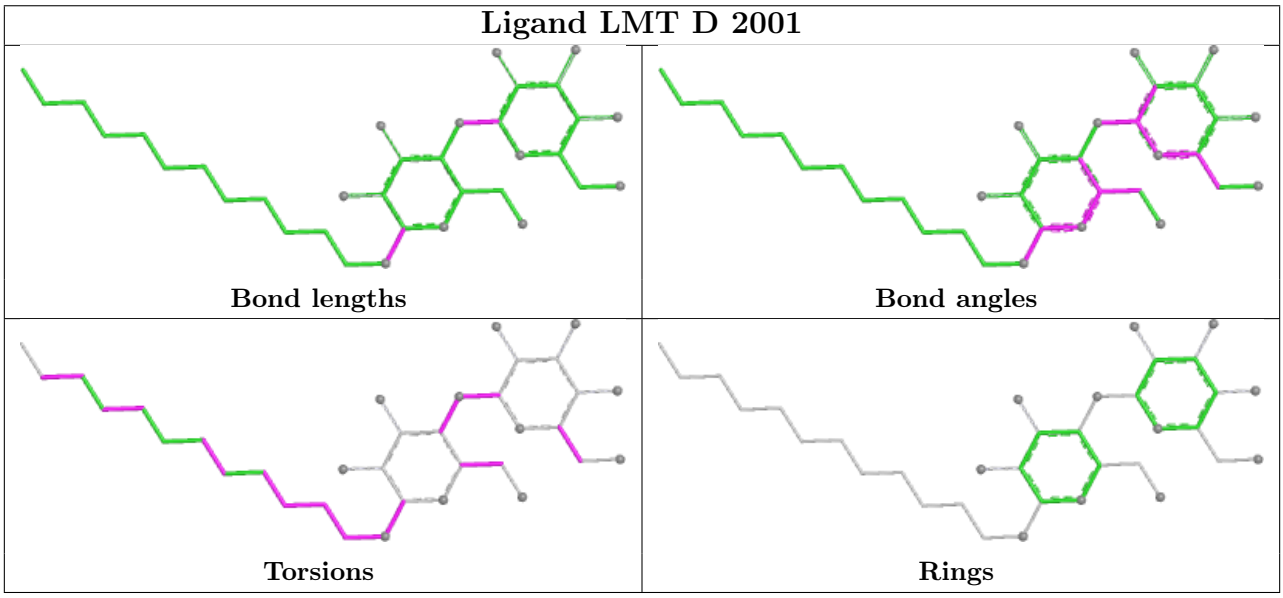
Ligand LMT B 2003



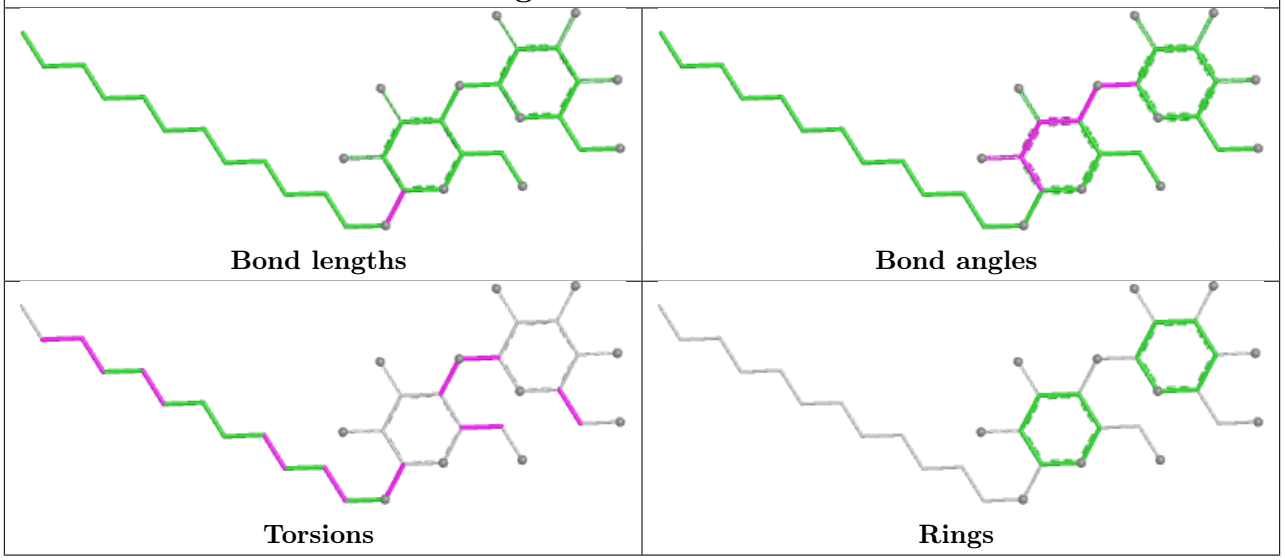
Ligand LMT E 2003



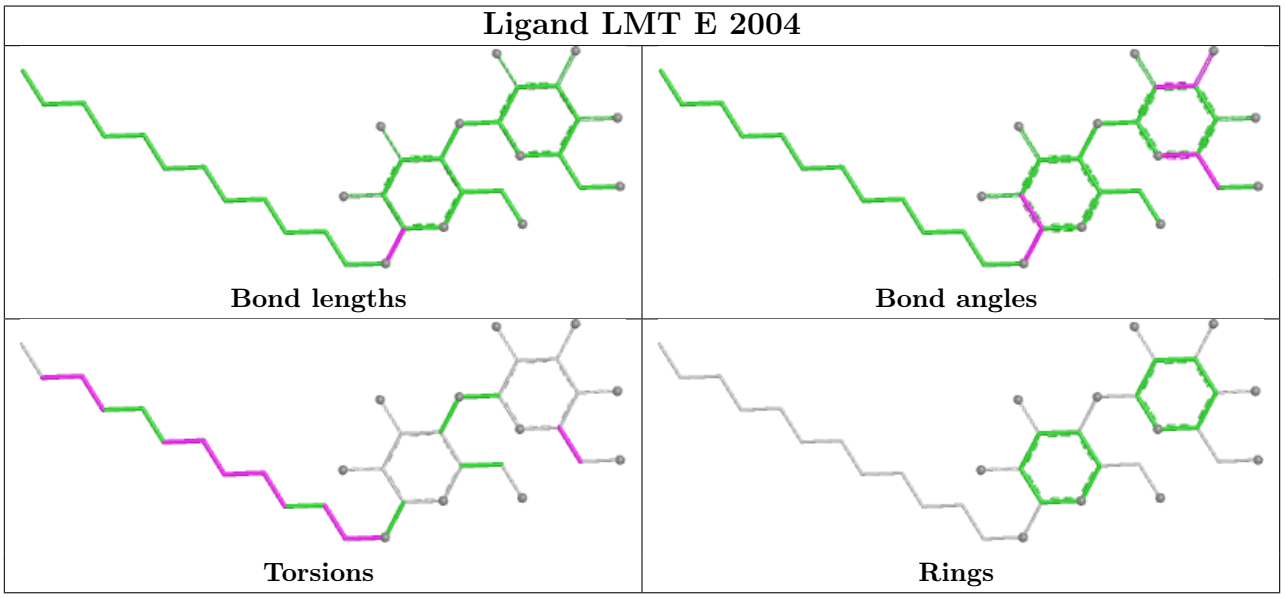
Ligand LMT D 2001



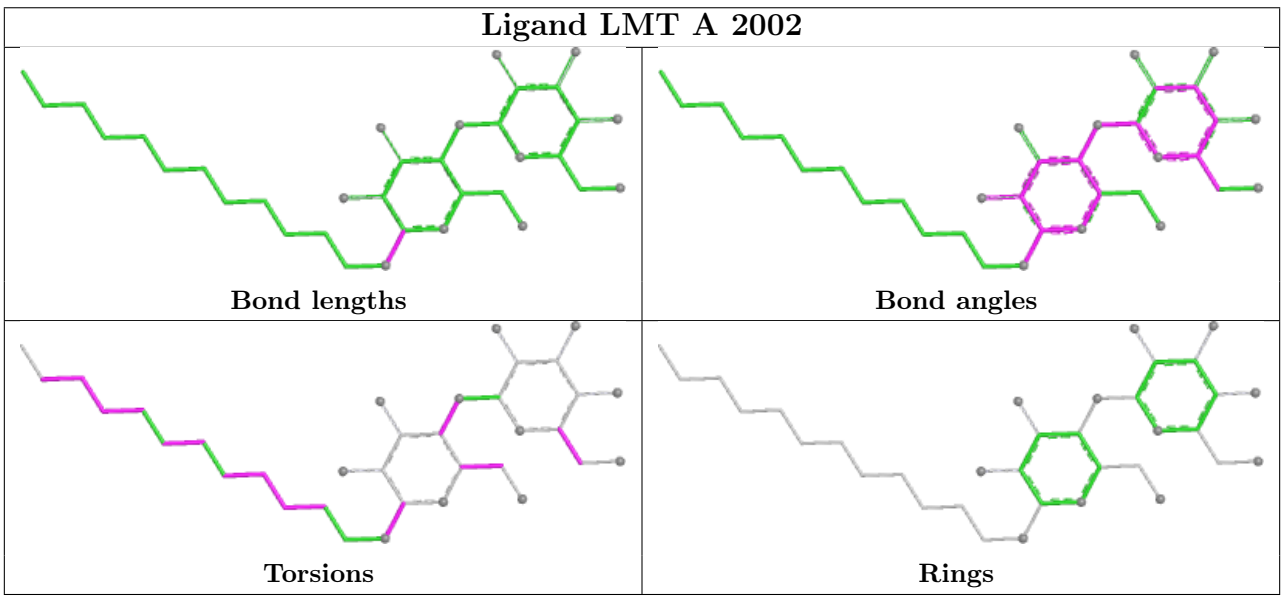
Ligand LMT F 2002



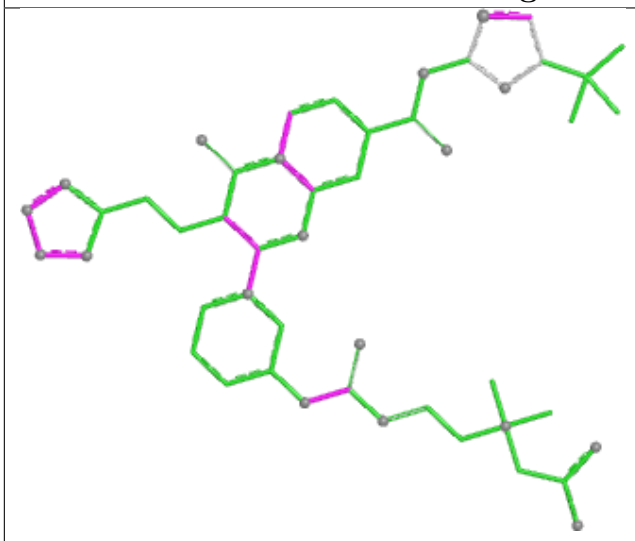
Ligand LMT E 2004



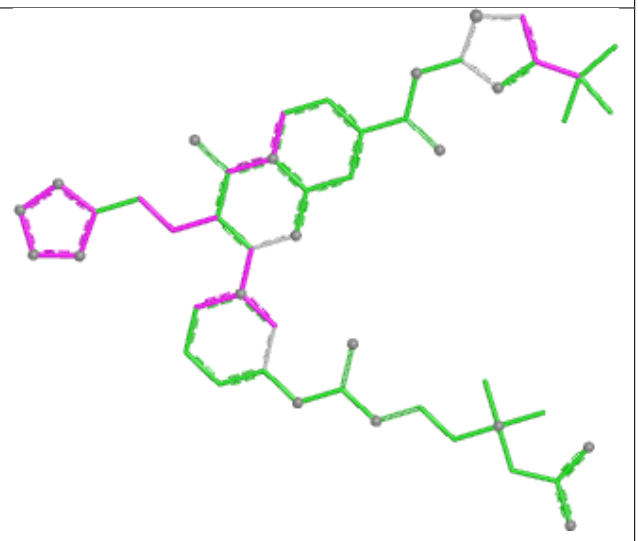
Ligand LMT A 2002



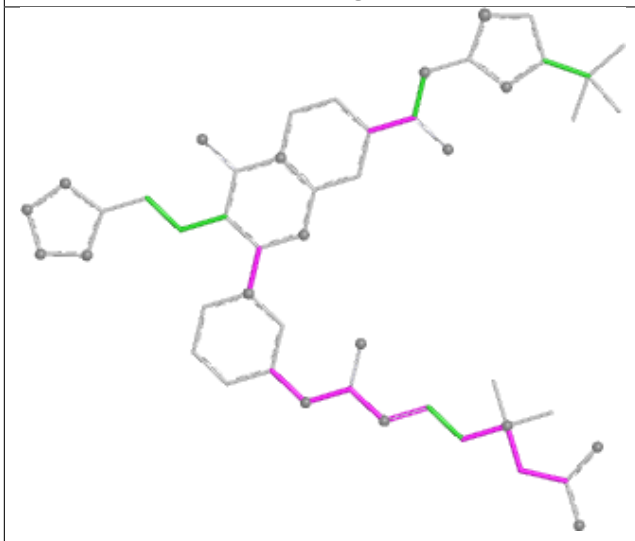
Ligand P9D E 2001



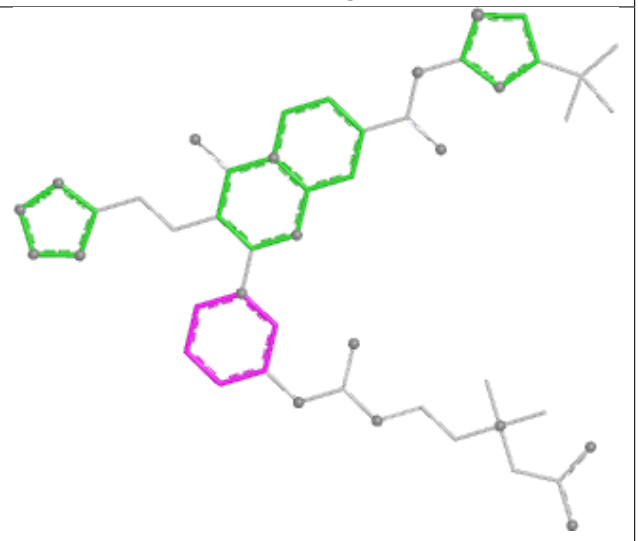
Bond lengths



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	1018/1052 (96%)	-0.36	6 (0%)	89	84	39, 75, 112, 164	0
1	B	1030/1052 (97%)	-0.40	6 (0%)	89	84	40, 73, 113, 152	0
1	C	1030/1052 (97%)	-0.23	28 (2%)	54	38	43, 87, 143, 201	0
1	D	1019/1052 (96%)	-0.37	11 (1%)	80	70	47, 78, 117, 160	0
1	E	1030/1052 (97%)	-0.28	13 (1%)	77	66	46, 78, 124, 162	0
1	F	1033/1052 (98%)	-0.26	15 (1%)	73	61	45, 79, 129, 264	0
All	All	6160/6312 (97%)	-0.32	79 (1%)	77	66	39, 78, 124, 264	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	253	VAL	5.6
1	F	259	GLN	4.8
1	F	742	LEU	4.3
1	C	600	GLU	4.0
1	C	256	ASP	3.8
1	D	954	GLN	3.8
1	F	741	SER	3.8
1	A	954	GLN	3.7
1	C	733	GLU	3.4
1	F	641	GLU	3.4
1	C	601	LYS	3.3
1	D	1031	PHE	3.3
1	C	738	LEU	3.2
1	F	753	TRP	3.2
1	C	731	ASP	3.1
1	C	511	GLY	3.0
1	C	753	TRP	3.0
1	E	676	ASN	3.0
1	C	721	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	260	VAL	2.9
1	C	800	PHE	2.9
1	A	870	SER	2.9
1	C	505	HIS	2.8
1	F	254	ASN	2.8
1	C	853	GLY	2.8
1	A	513	PHE	2.8
1	C	508	HIS	2.8
1	D	790	VAL	2.8
1	C	257	GLY	2.8
1	B	259	GLN	2.8
1	F	800	PHE	2.8
1	C	778	ALA	2.7
1	E	1030	LEU	2.7
1	B	261	ARG	2.7
1	C	638	PRO	2.7
1	E	601	LYS	2.7
1	D	955	GLY	2.6
1	C	676	ASN	2.6
1	A	537	HIS	2.6
1	C	792	ASN	2.5
1	E	675	GLY	2.5
1	C	732	ASP	2.5
1	A	688	ALA	2.4
1	B	257	GLY	2.4
1	F	660	ASP	2.4
1	C	748	THR	2.4
1	E	600	GLU	2.4
1	E	708	GLN	2.4
1	C	785	LEU	2.4
1	C	741	SER	2.3
1	E	710	PRO	2.3
1	E	197	GLN	2.3
1	E	260	VAL	2.3
1	C	597	TYR	2.2
1	F	656	PHE	2.2
1	D	641	GLU	2.2
1	E	834	LEU	2.2
1	B	835	SER	2.2
1	C	801	ASN	2.2
1	F	991	THR	2.2
1	A	687	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	259	GLN	2.1
1	F	256	ASP	2.1
1	E	258	SER	2.1
1	C	512	PHE	2.1
1	E	704	MET	2.1
1	D	785	LEU	2.1
1	F	670	SER	2.1
1	C	642	ASN	2.0
1	D	638	PRO	2.0
1	D	536	LYS	2.0
1	D	640	GLY	2.0
1	F	501	GLU	2.0
1	C	509	LYS	2.0
1	D	267	ASP	2.0
1	D	537	HIS	2.0
1	E	198	LEU	2.0
1	F	502	LYS	2.0
1	B	253	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LMT	D	2001	35/35	0.79	0.44	47,65,79,89	35
2	LMT	F	2001	35/35	0.84	0.28	82,104,126,139	0
2	LMT	A	2001	35/35	0.85	0.34	43,66,94,103	35
2	LMT	F	2002	35/35	0.85	0.34	76,118,147,148	0
2	LMT	C	2001	35/35	0.88	0.34	80,105,146,151	0

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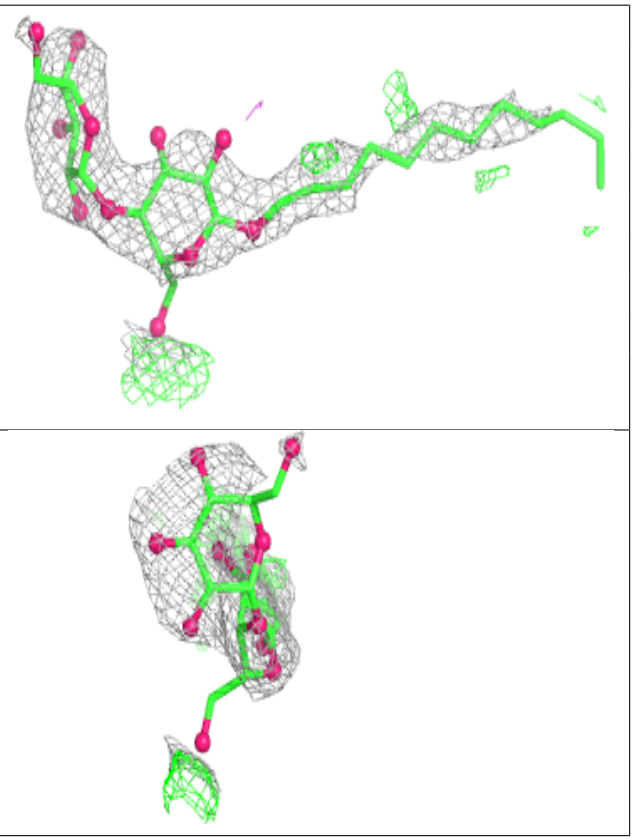
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LMT	E	2002	35/35	0.90	0.25	67,106,124,132	0
2	LMT	E	2003	35/35	0.90	0.38	67,94,108,124	0
2	LMT	B	2002	35/35	0.90	0.23	63,106,135,137	0
2	LMT	D	2003	35/35	0.90	0.25	70,98,134,144	0
2	LMT	A	2002	35/35	0.91	0.26	60,86,132,142	0
2	LMT	A	2003	35/35	0.91	0.23	64,90,115,120	0
2	LMT	D	2002	35/35	0.93	0.31	69,111,137,144	0
2	LMT	B	2003	35/35	0.93	0.28	71,82,104,111	0
3	P9D	E	2001	49/49	0.93	0.27	60,78,108,123	0
3	P9D	B	2001	49/49	0.94	0.24	53,71,85,108	0
2	LMT	B	2004	35/35	0.94	0.23	62,69,78,84	0
2	LMT	E	2004	35/35	0.95	0.32	67,74,100,103	0

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

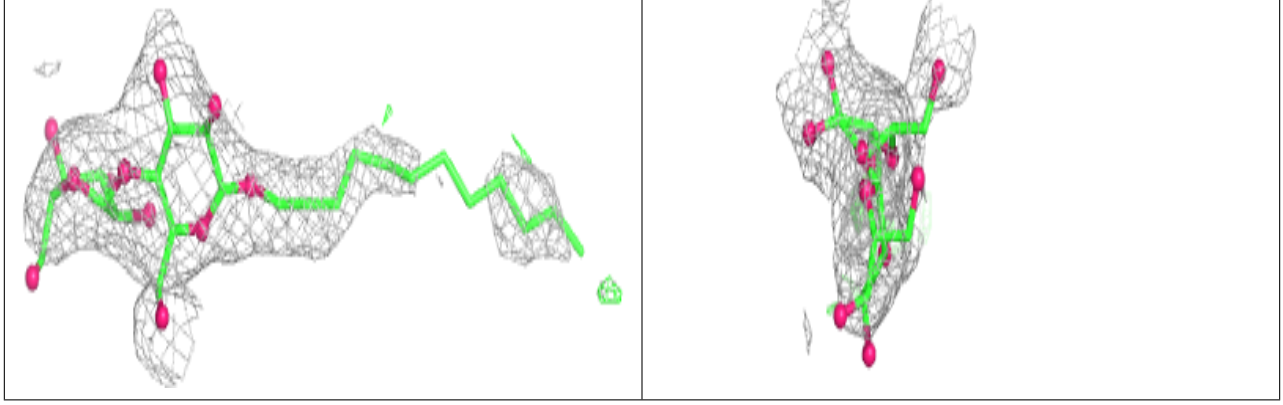
Electron density around LMT D 2001:

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



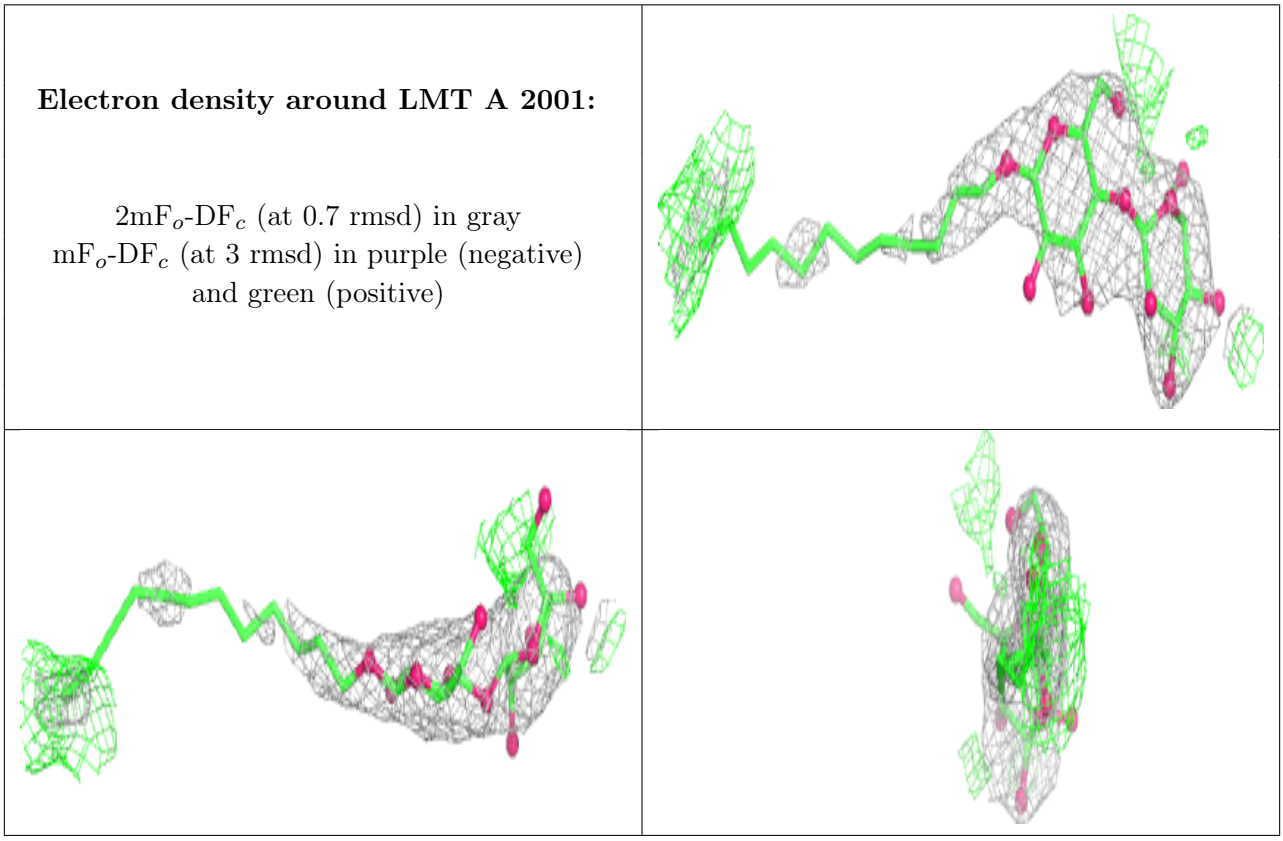
Electron density around LMT F 2001:

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



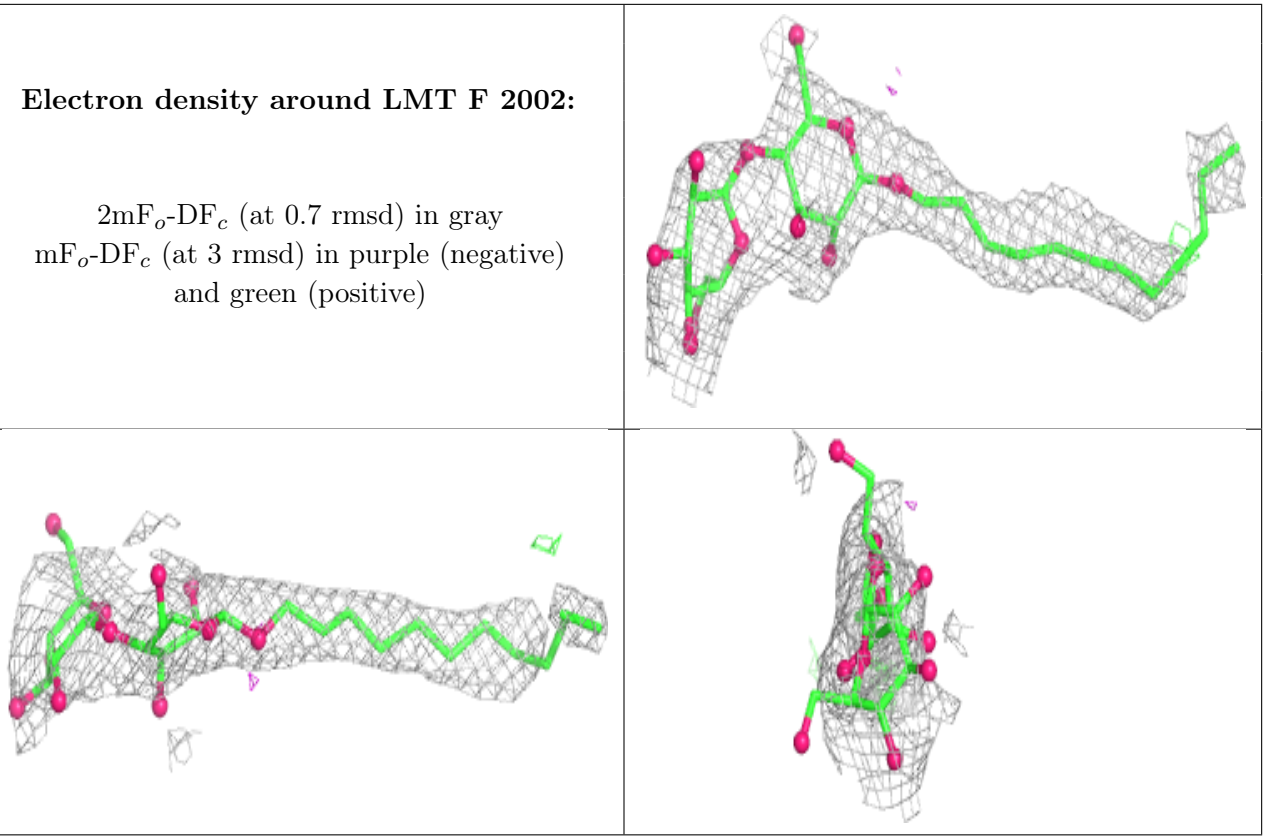
Electron density around LMT A 2001:

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



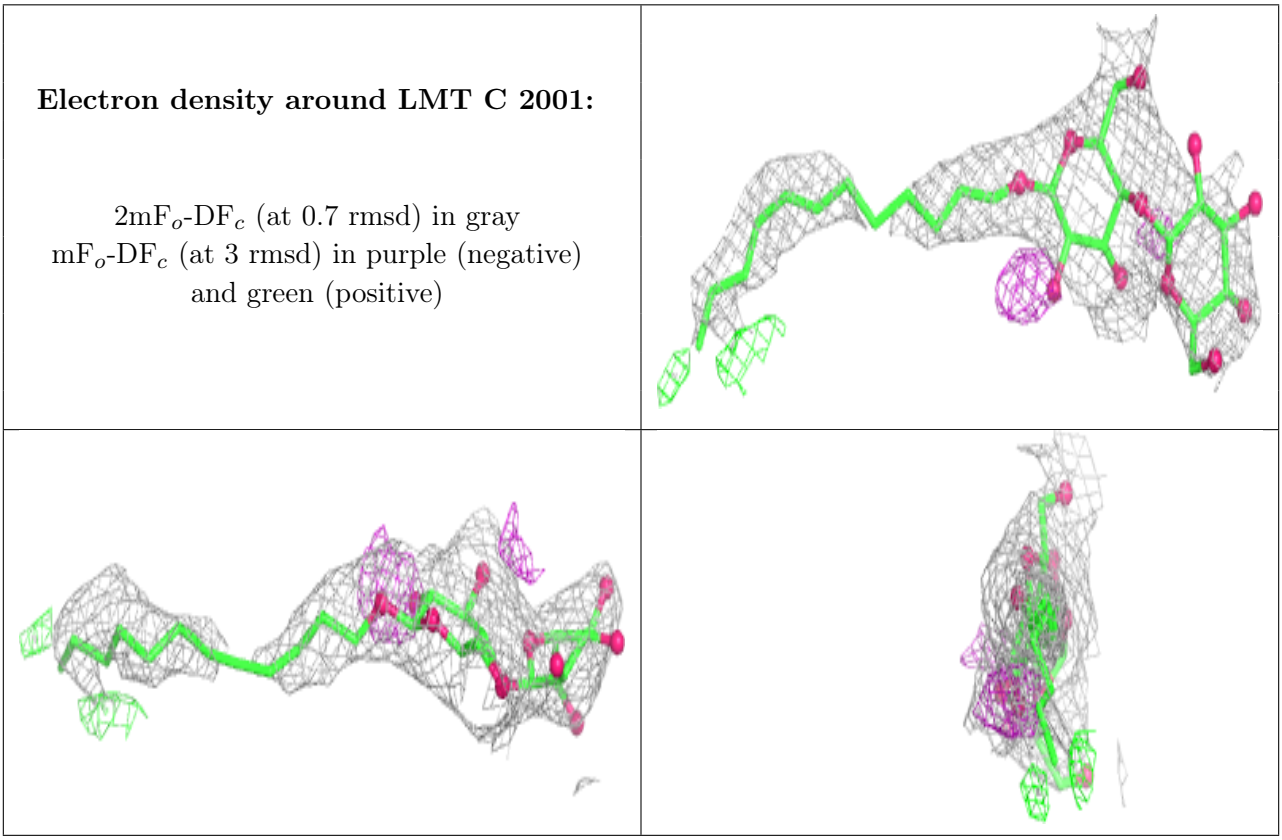
Electron density around LMT F 2002:

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



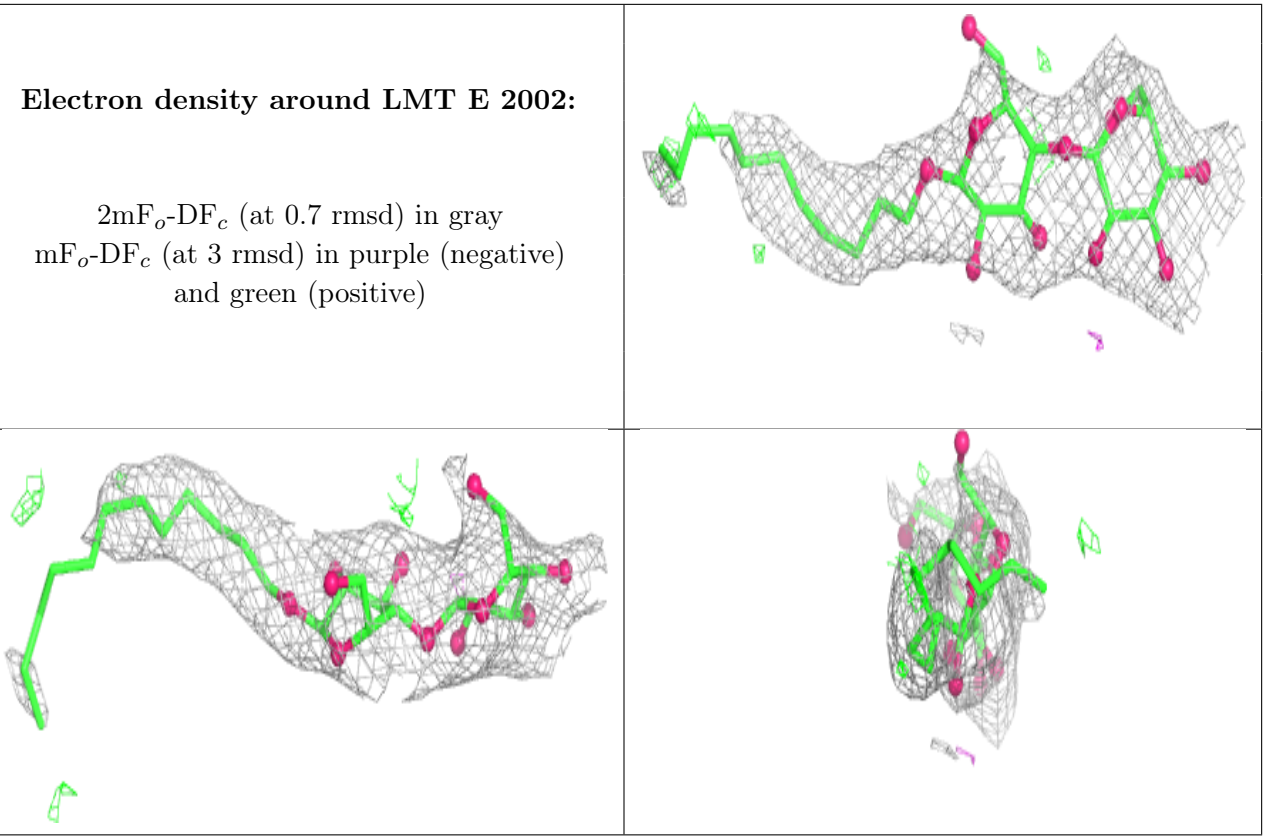
Electron density around LMT C 2001:

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



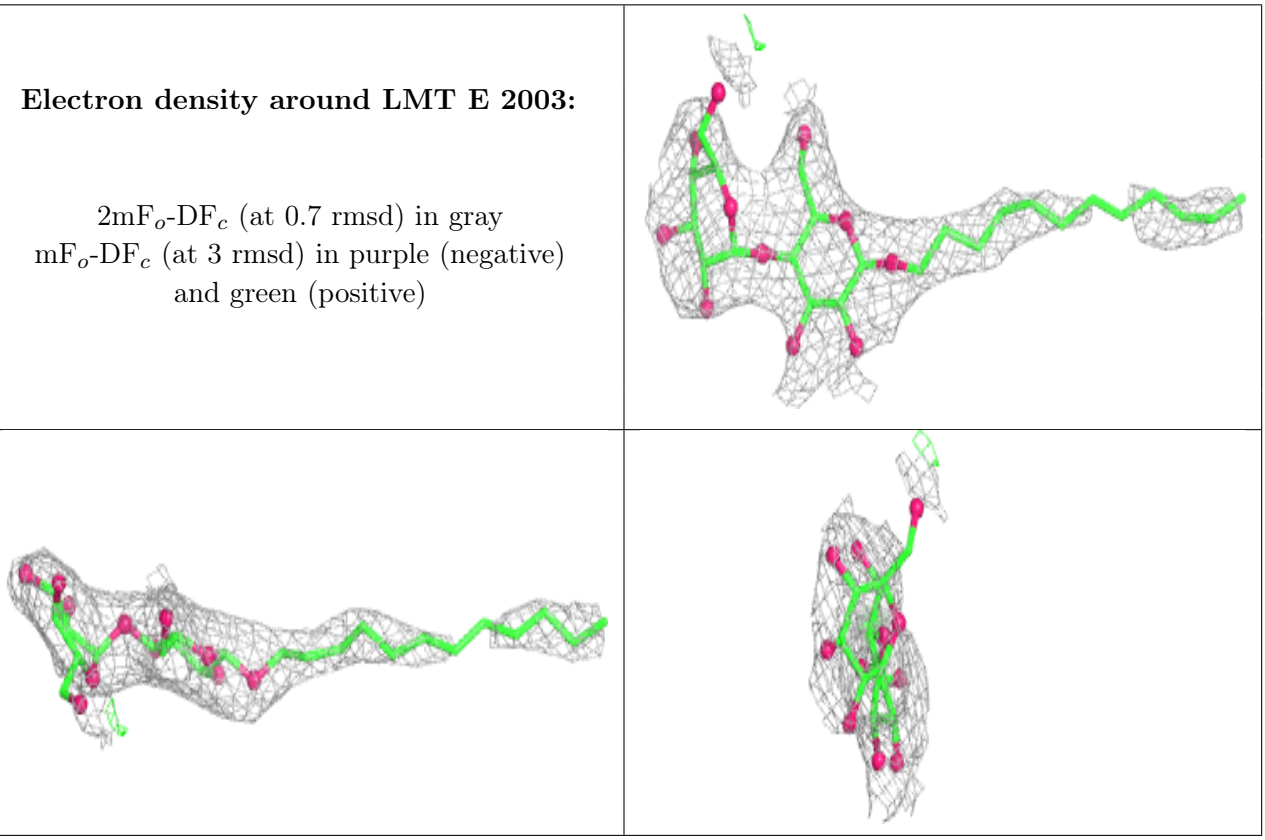
Electron density around LMT E 2002:

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



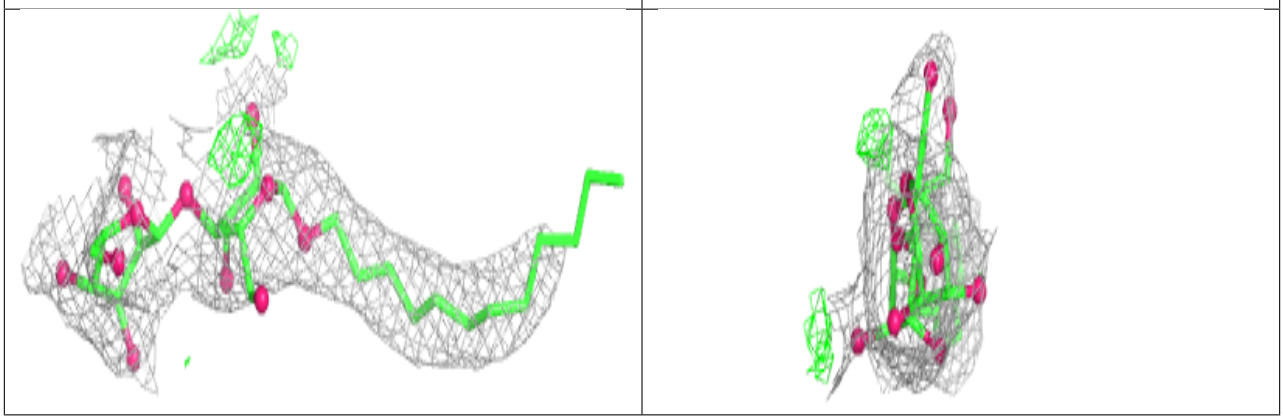
Electron density around LMT E 2003:

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



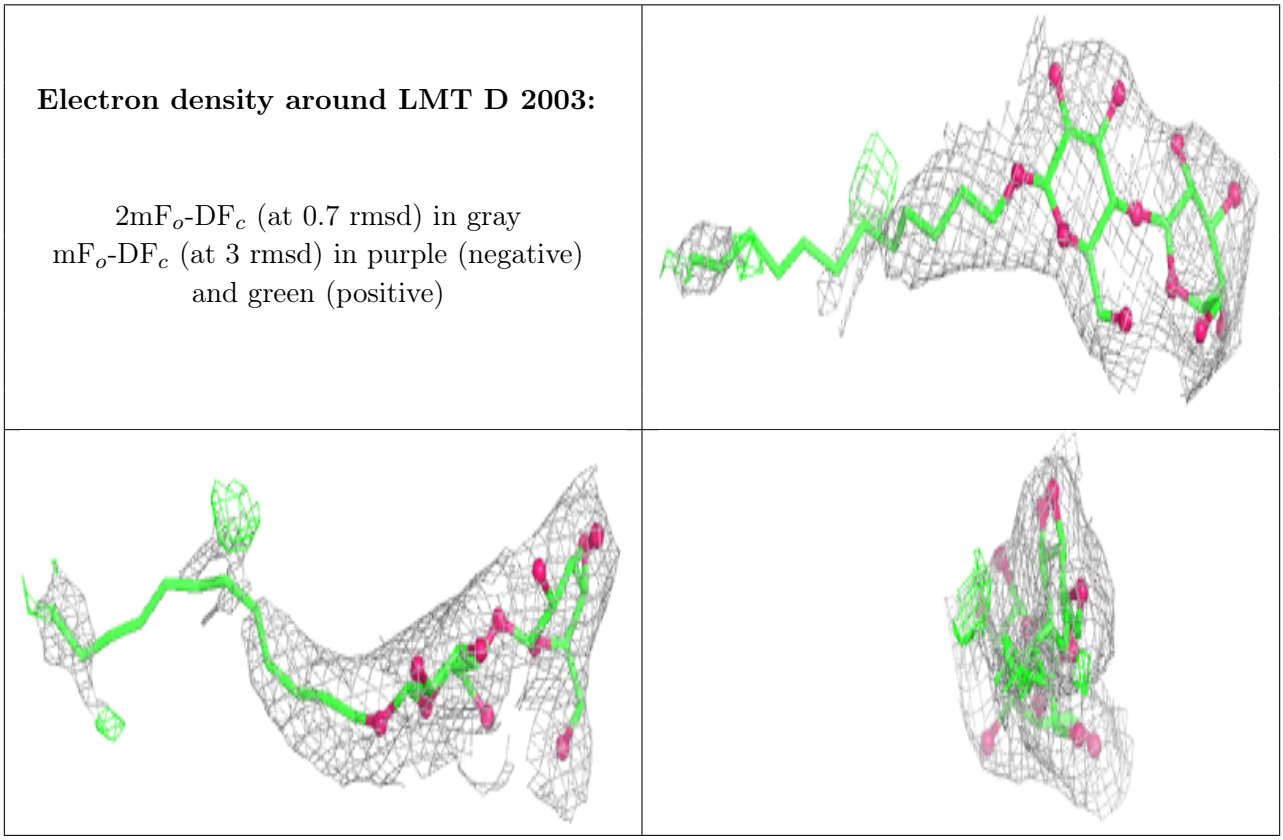
Electron density around LMT B 2002:

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



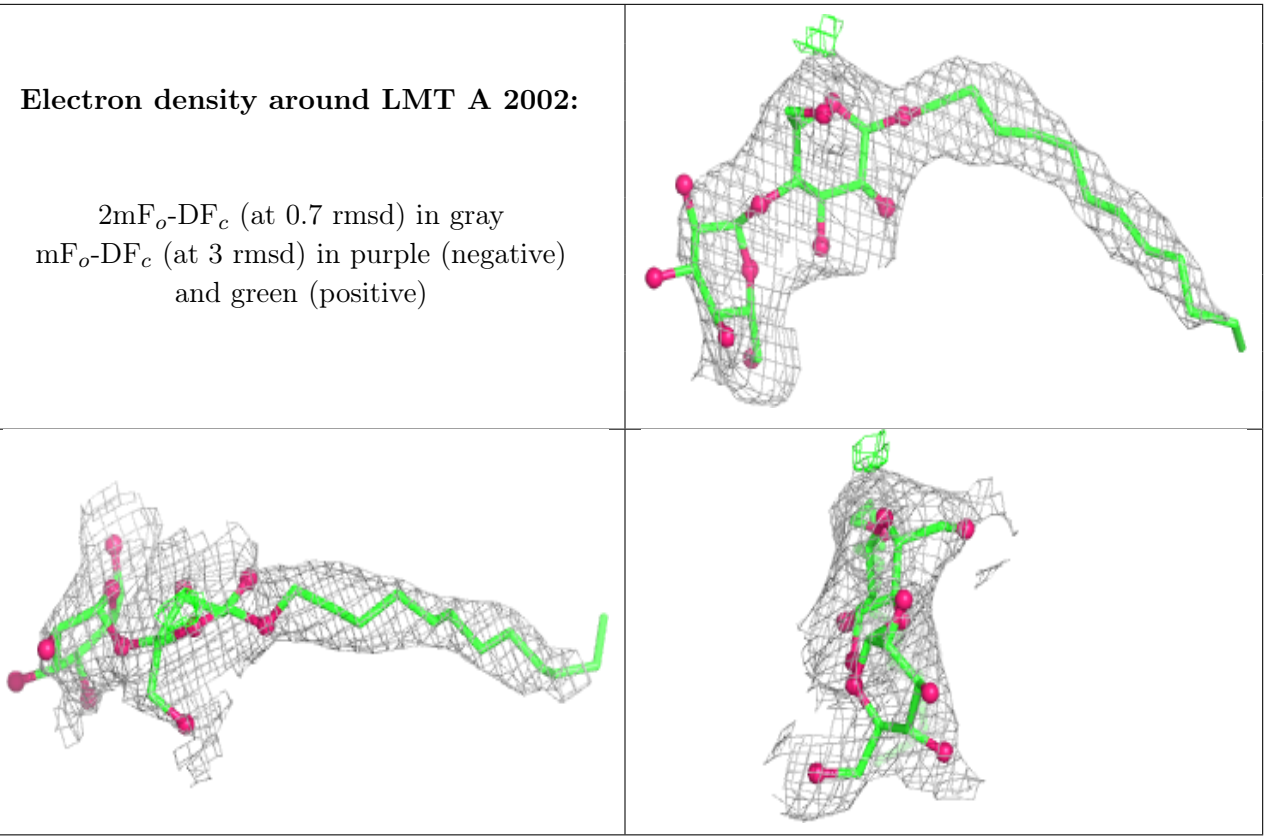
Electron density around LMT D 2003:

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



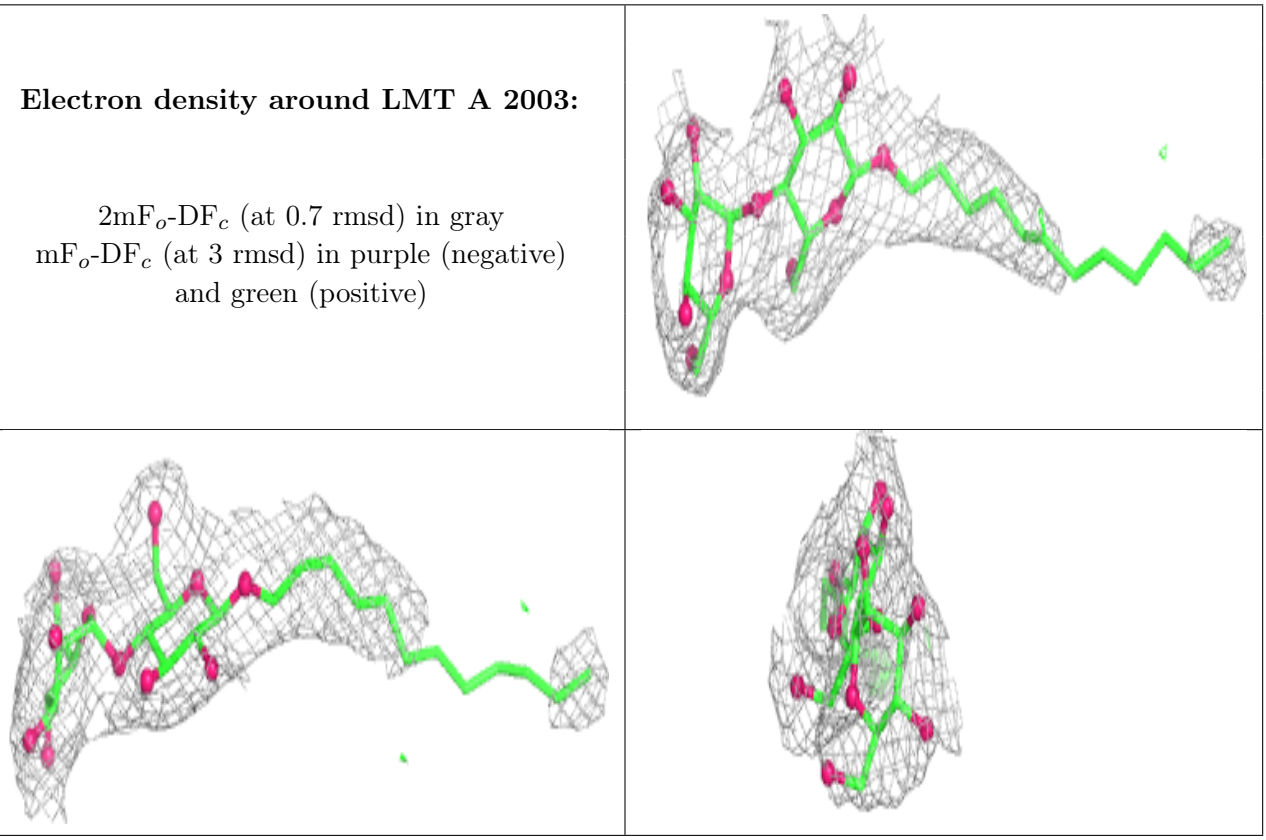
Electron density around LMT A 2002:

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



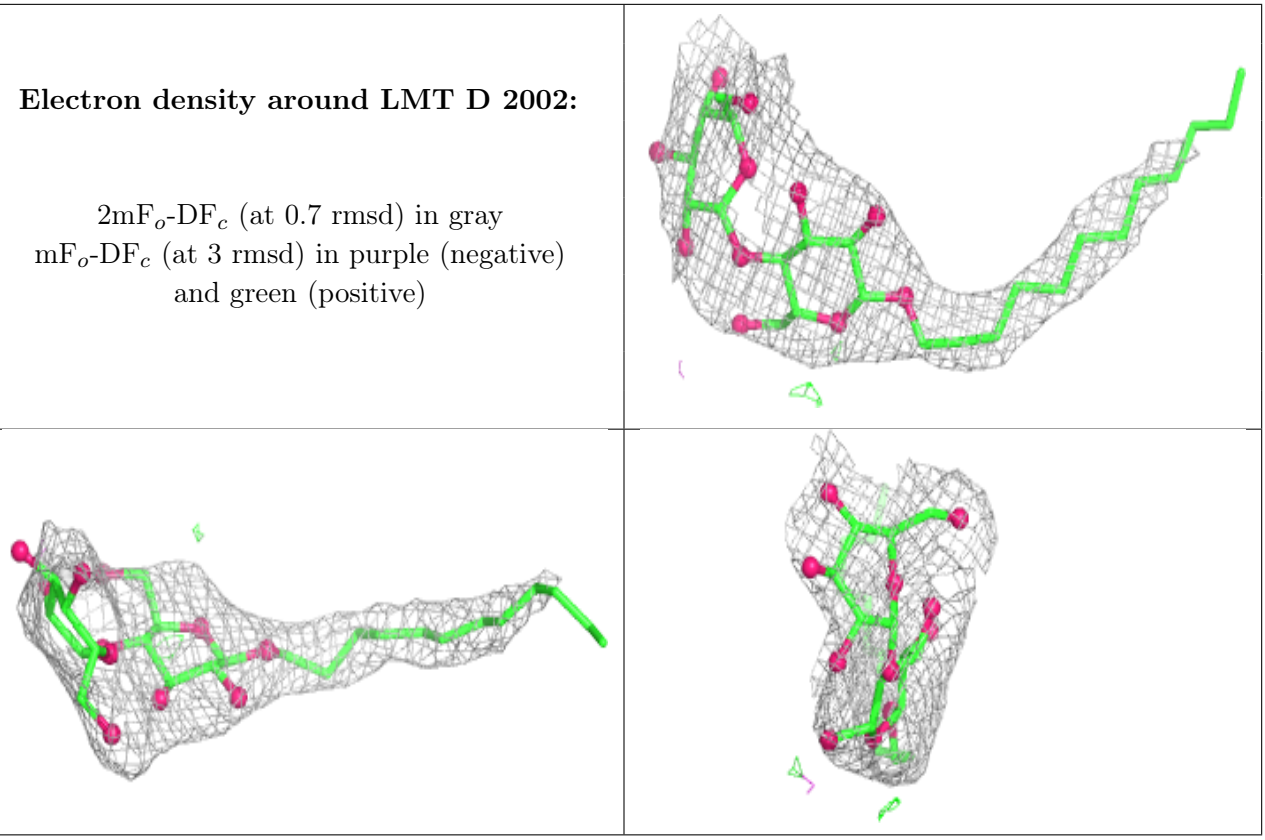
Electron density around LMT A 2003:

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



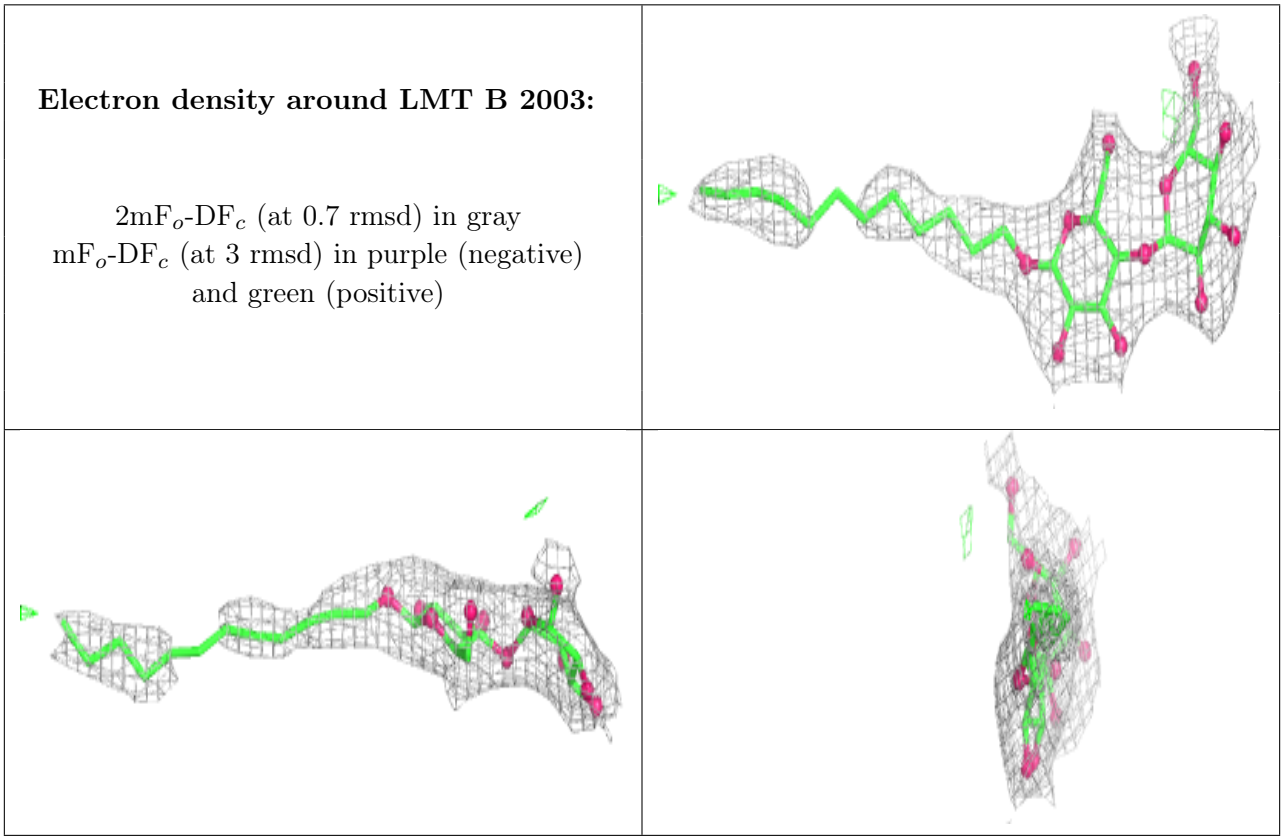
Electron density around LMT D 2002:

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



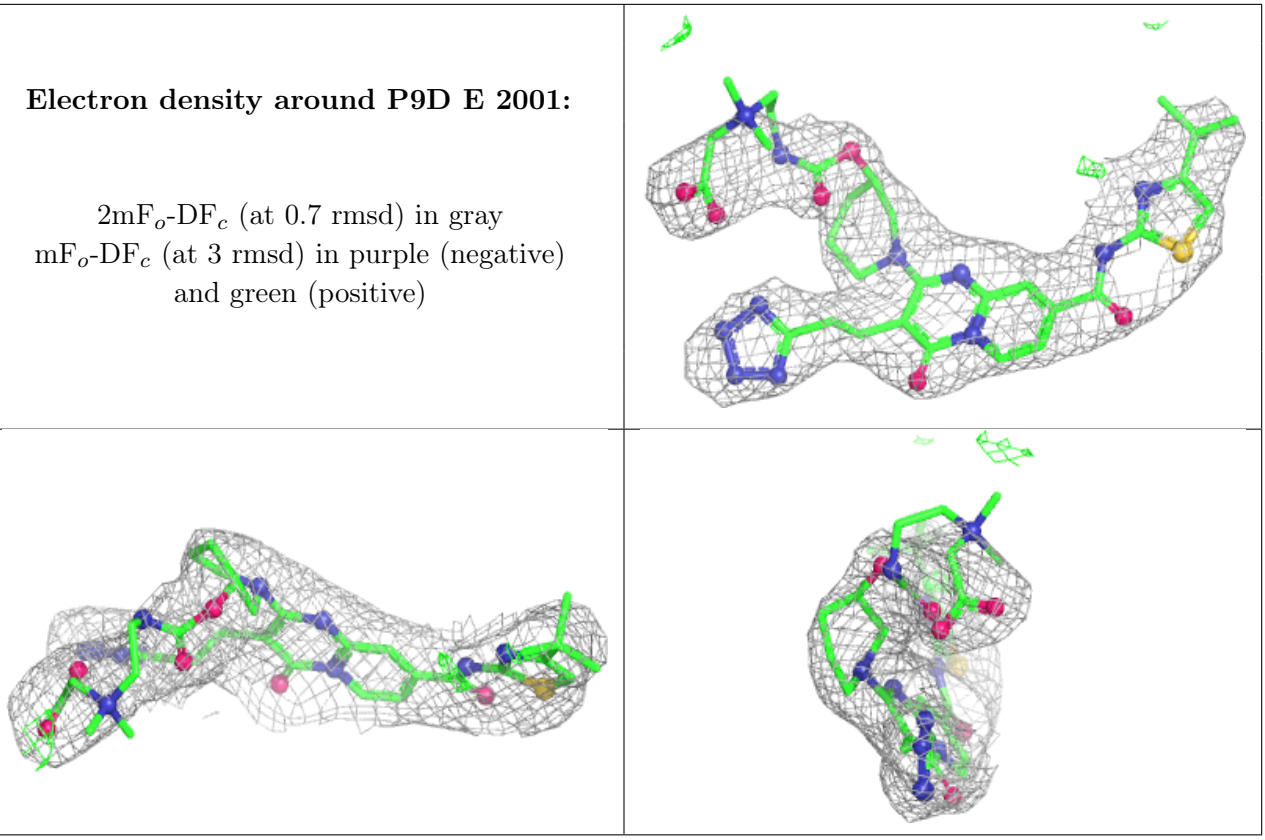
Electron density around LMT B 2003:

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



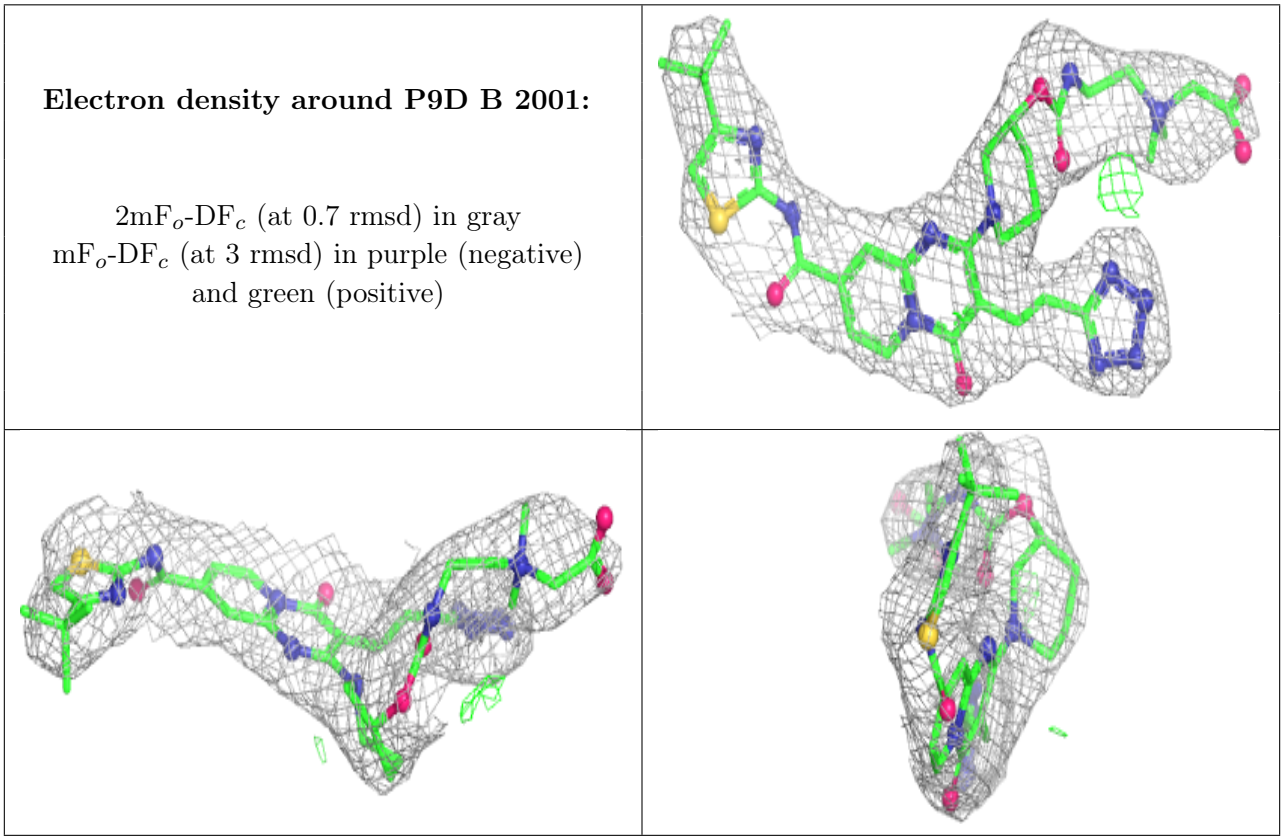
Electron density around P9D E 2001:

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



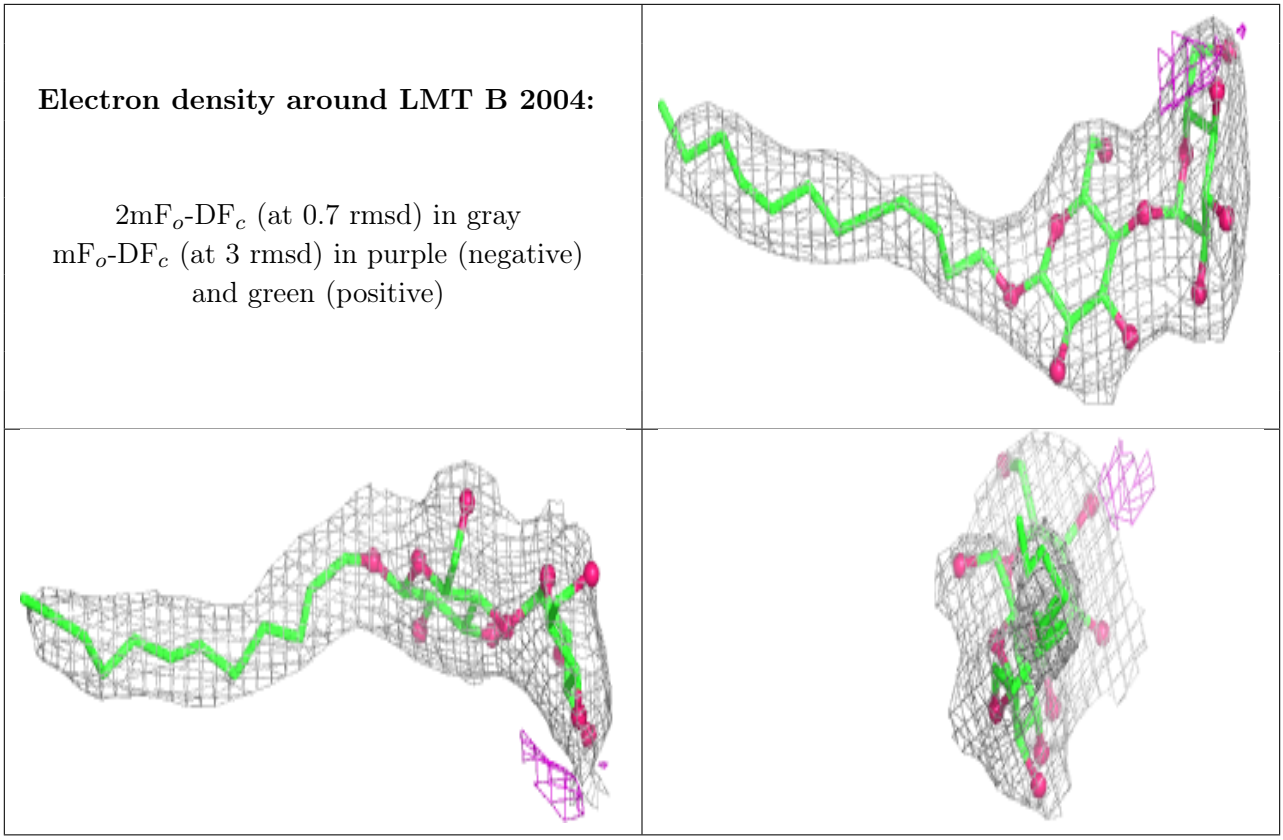
Electron density around P9D B 2001:

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



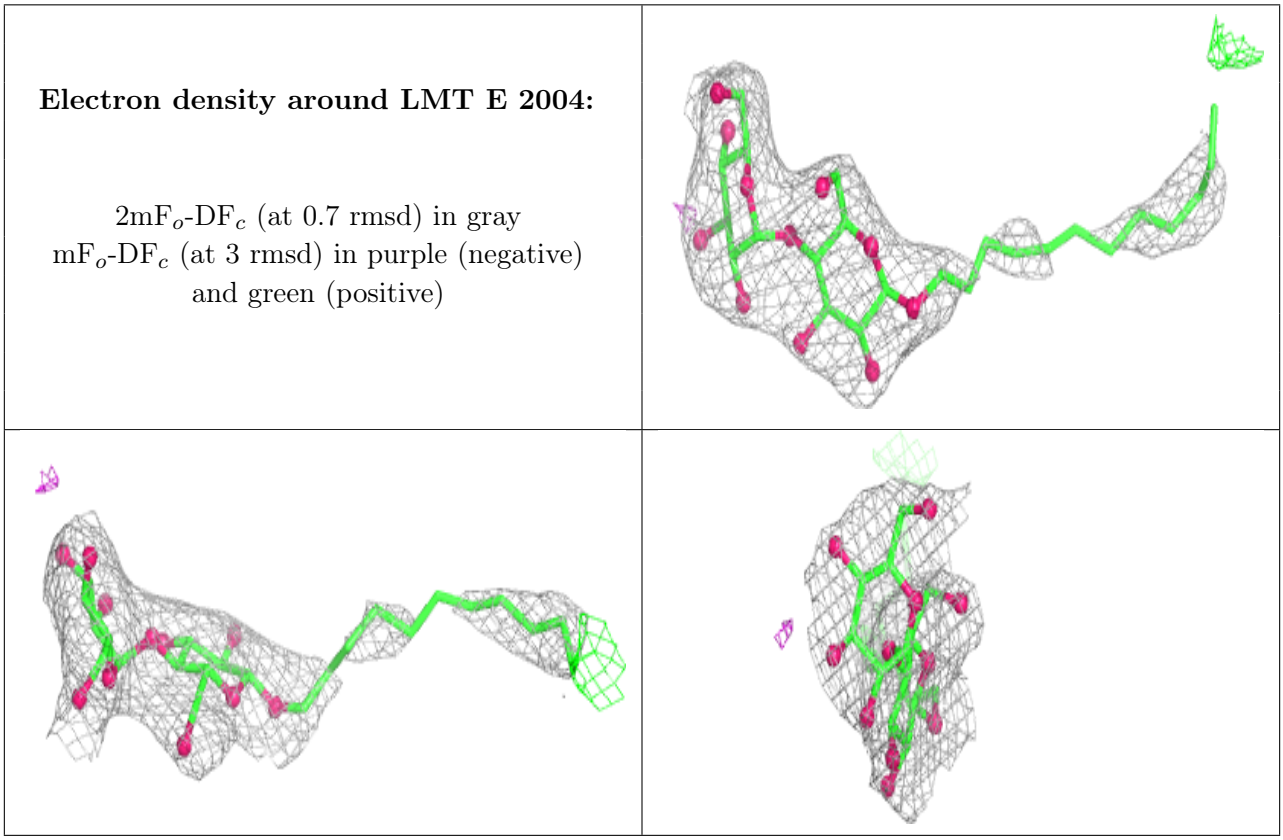
Electron density around LMT B 2004:

$2mF_o$-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 2004:

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



6.5 Other polymers (i)

There are no such residues in this entry.