



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:16 PM UTC

PDB ID : 3W9J / pdb_00003w9j
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

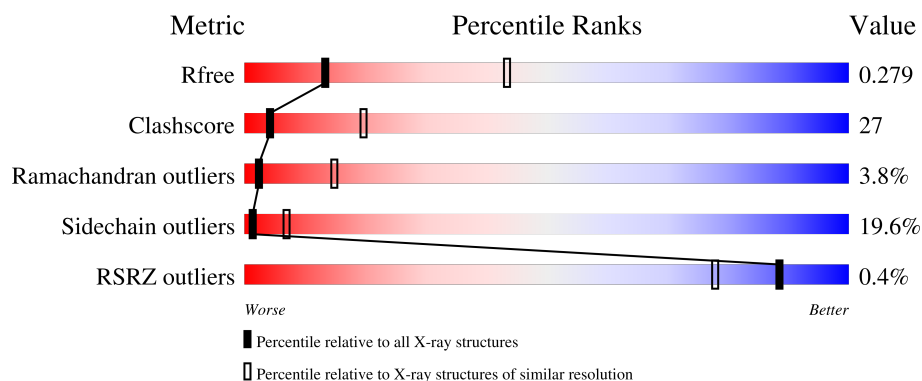
1 Overall quality at a glance

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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1052	48% 38% 9% ..
1	B	1052	48% 39% 10% ..
1	C	1052	% 44% 41% 12% ..
1	D	1052	45% 41% 10% ..
1	E	1052	45% 39% 12% ..

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Mol	Chain	Length	Quality of chain
1	F	1052	% 45% 40% 11% ..

2 Entry composition

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:

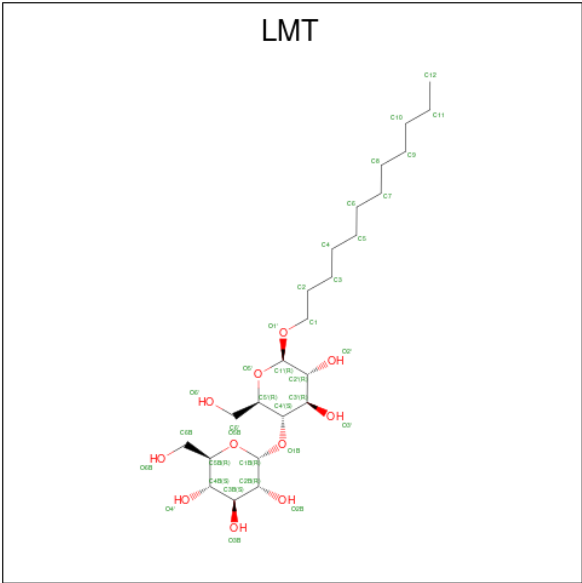
Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	expression tag	UNP P52002
A	1048	HIS	-	expression tag	UNP P52002
A	1049	HIS	-	expression tag	UNP P52002
A	1050	HIS	-	expression tag	UNP P52002
A	1051	HIS	-	expression tag	UNP P52002
A	1052	HIS	-	expression tag	UNP P52002
B	1047	HIS	-	expression 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 (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



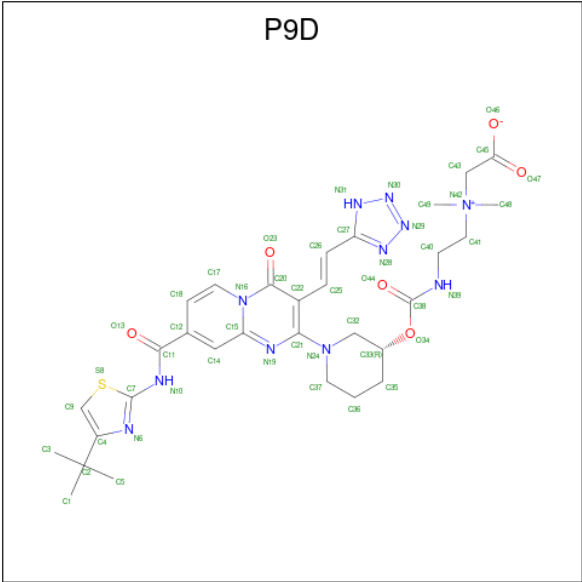
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	A	1	Total	C	O	0	0
			35	24	11		

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

- 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 (CCD ID: P9D) (formula: C₃₁H₃₉N₁₁O₆S).

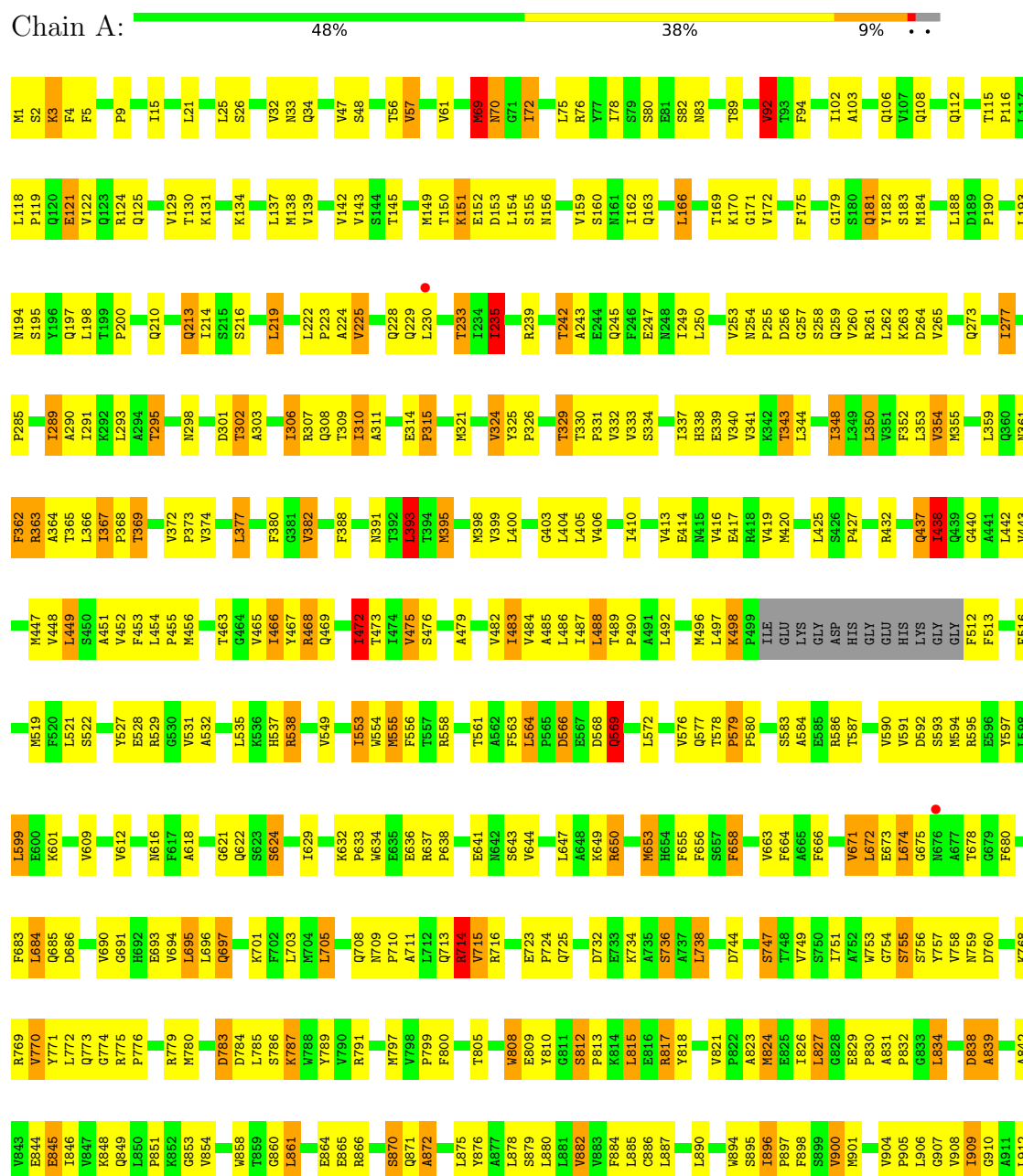


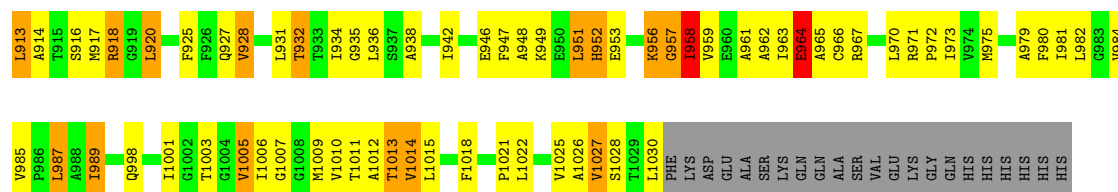
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			49	31	11	6	1		
3	E	1	Total	C	N	O	S	0	0
			49	31	11	6	1		

3 Residue-property plots

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.

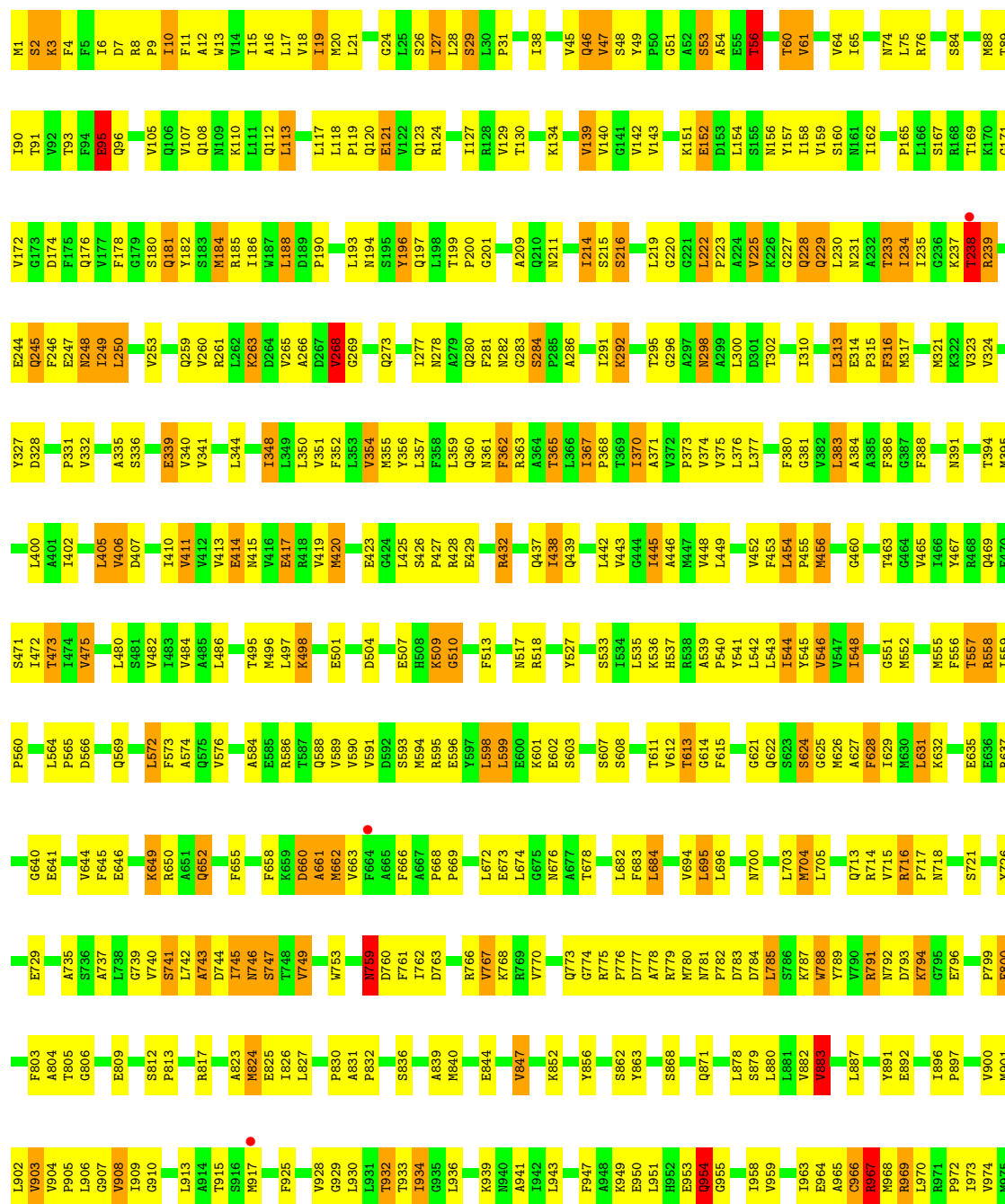
• Molecule 1: Multidrug resistance protein MexB

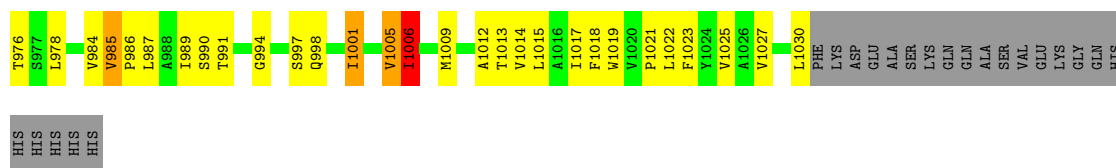




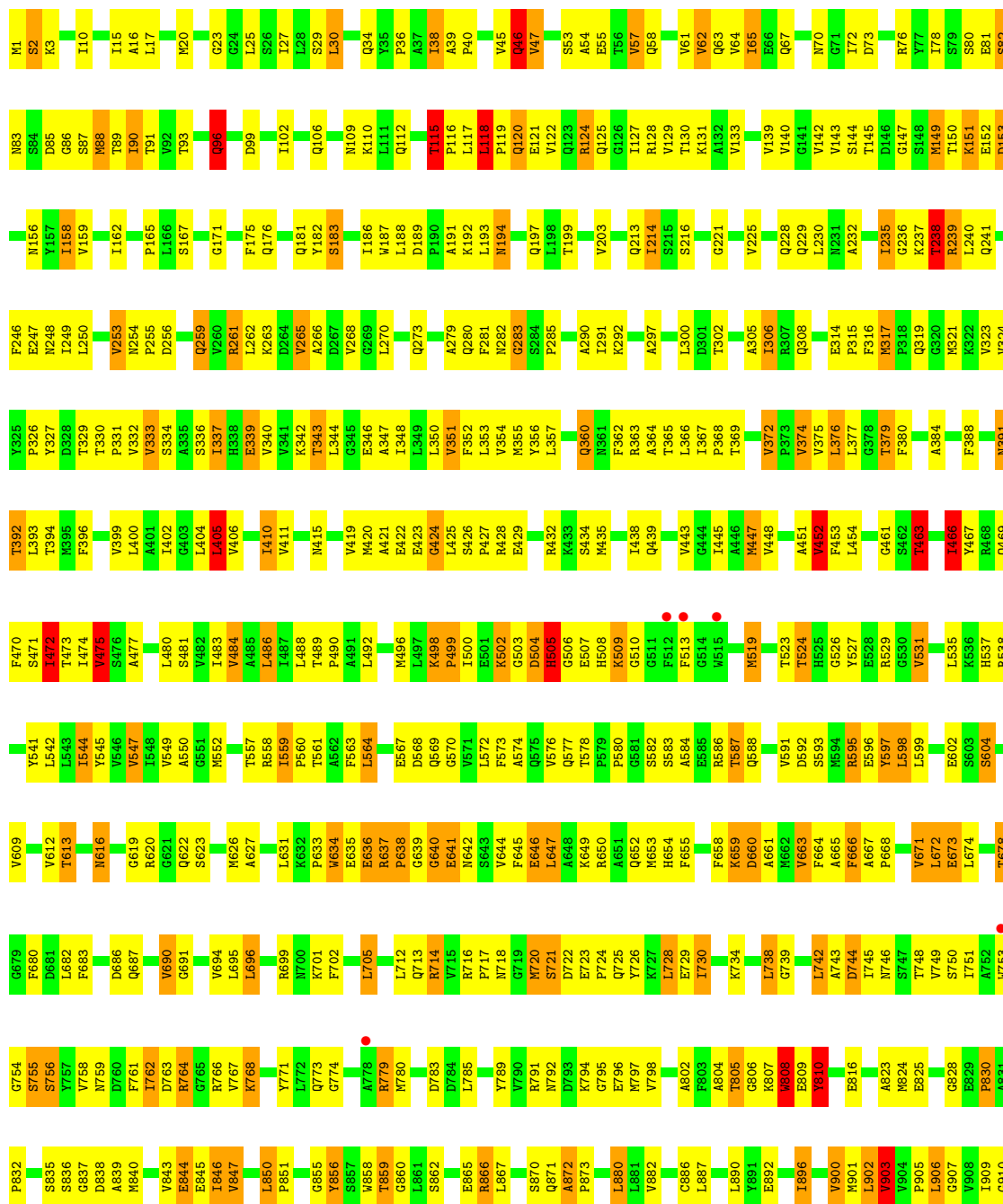
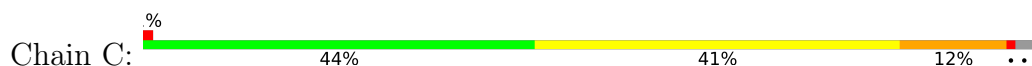
Molecule 1: Multidrug resistance protein MexB

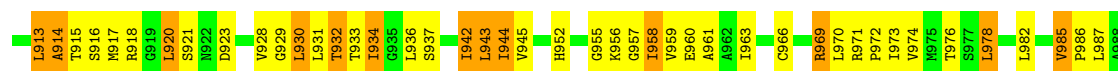
Chain B: 48% 39% 10% ..





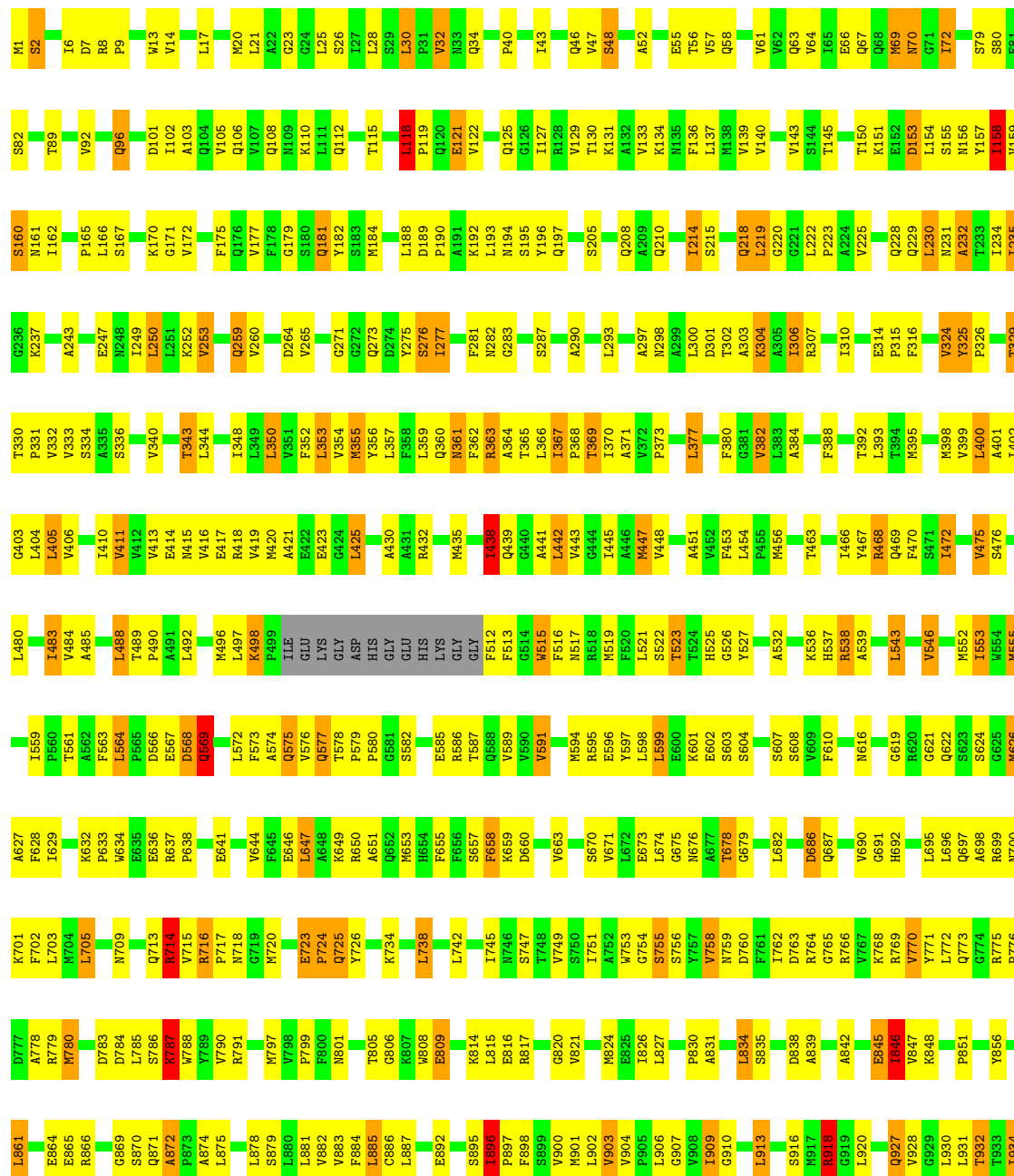
• Molecule 1: Multidrug resistance protein MexB

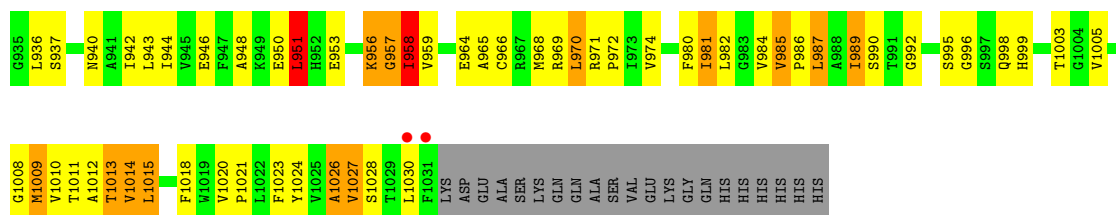




• Molecule 1: Multidrug resistance protein MexB

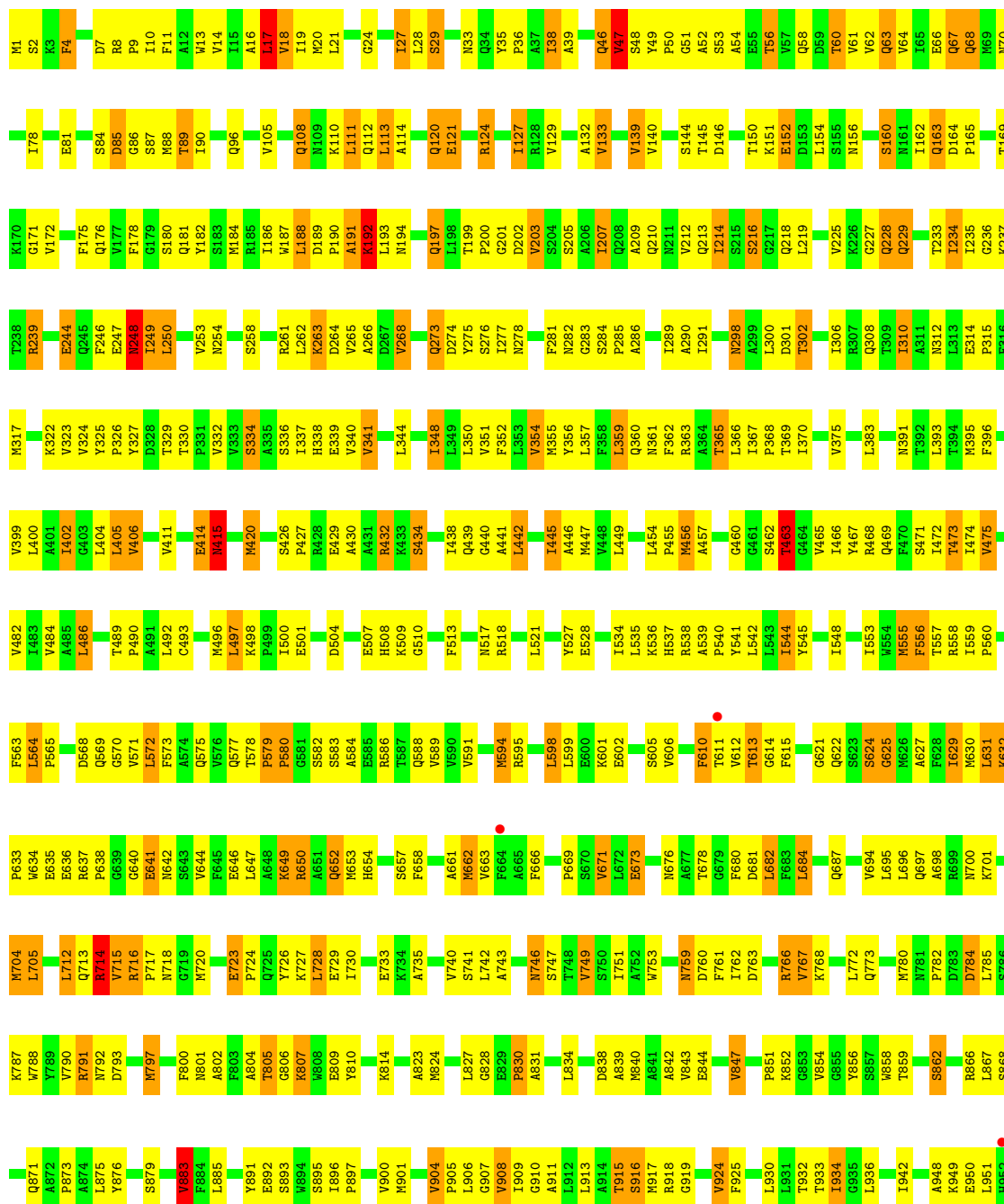
Chain D: 45% 41% 10% ••

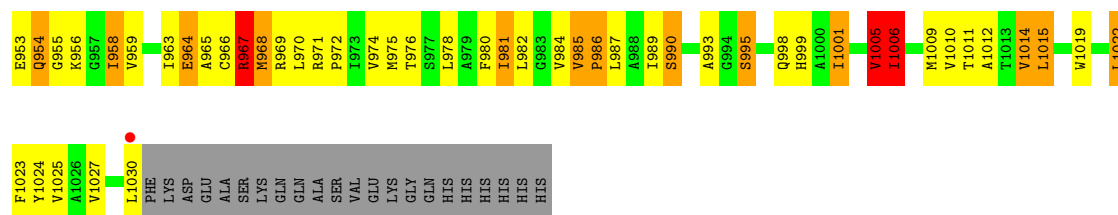




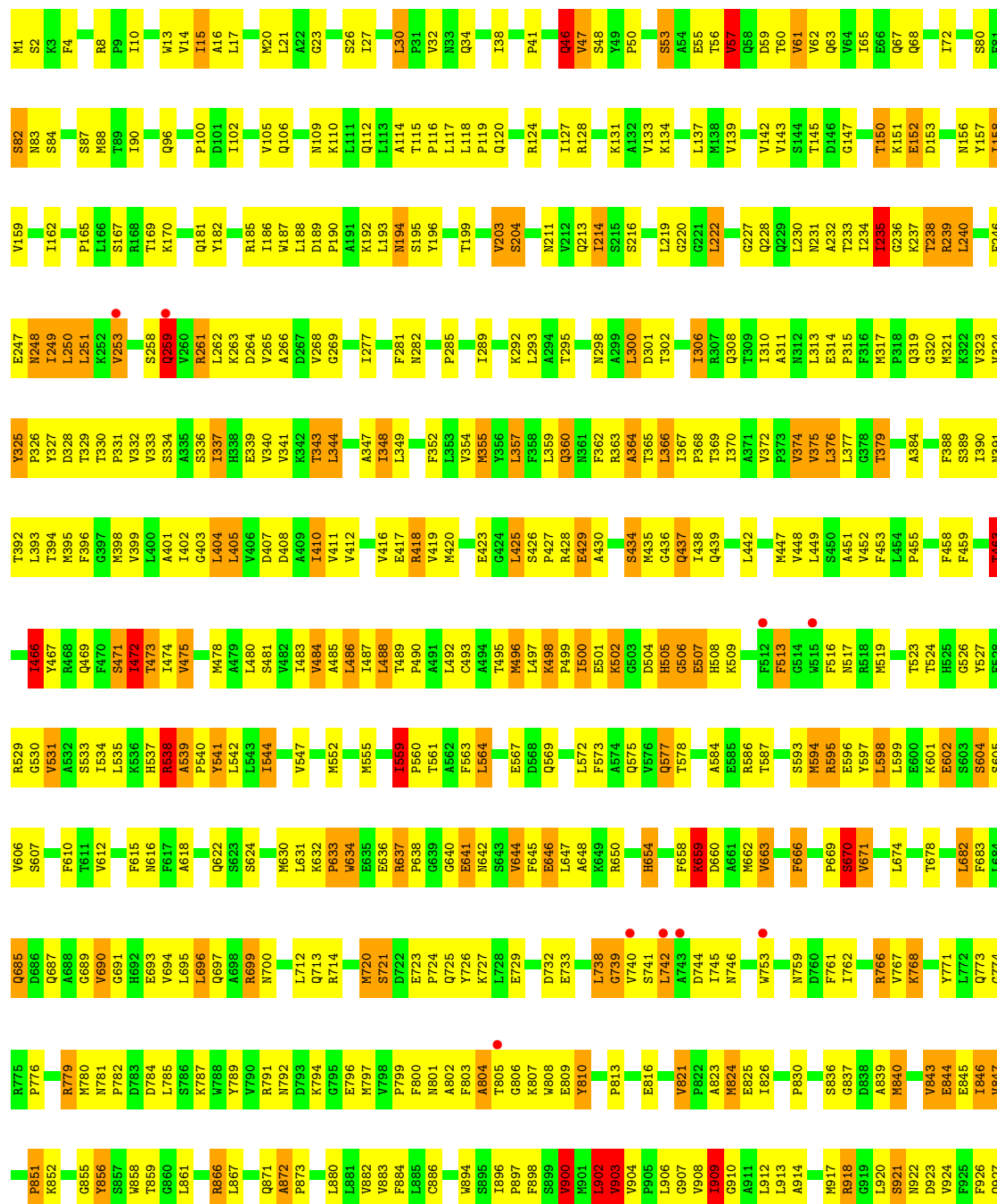
• Molecule 1: Multidrug resistance protein MexB

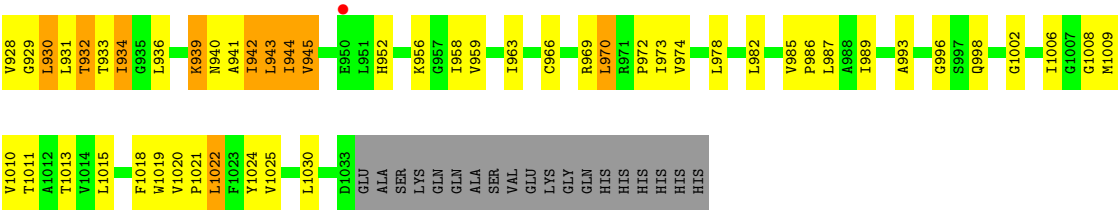
Chain E: 45% 39% 12% ..





• Molecule 1: Multidrug resistance protein MexB





4 Data and refinement statistics

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) 97.3 (42.19-3.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.87%)	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)	0.29 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, P9D

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	0.76	2/7880 (0.0%)	1.16	31/10712 (0.3%)
1	B	0.76	0/7971	1.15	26/10833 (0.2%)
1	C	0.71	0/7971	1.16	31/10833 (0.3%)
1	D	0.73	1/7892 (0.0%)	1.14	30/10728 (0.3%)
1	E	0.74	0/7971	1.14	28/10833 (0.3%)
1	F	0.73	0/8000	1.16	31/10871 (0.3%)
All	All	0.74	3/47685 (0.0%)	1.15	177/64810 (0.3%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	GLN	C-N	8.33	1.44	1.33
1	A	498	LYS	CA-C	6.07	1.60	1.52
1	D	498	LYS	CA-C	5.41	1.59	1.52

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	812	SER	CA-C-N	10.18	130.45	119.87
1	A	812	SER	C-N-CA	10.18	130.45	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	723	GLU	N-CA-C	9.19	118.70	108.14
1	A	675	GLY	N-CA-C	-9.01	102.30	111.85
1	F	325	TYR	CA-C-N	8.46	128.59	119.28
1	F	325	TYR	C-N-CA	8.46	128.59	119.28
1	C	531	VAL	N-CA-C	-8.44	102.31	110.42
1	A	870	SER	N-CA-C	8.16	120.31	110.19
1	D	716	ARG	N-CA-C	8.11	115.28	108.07
1	B	180	SER	N-CA-C	8.01	118.83	108.34
1	C	559	ILE	N-CA-C	7.84	116.63	108.95
1	E	180	SER	N-CA-C	7.82	118.86	108.07
1	E	741	SER	N-CA-C	7.67	121.90	112.54
1	F	46	GLN	N-CA-C	7.62	122.19	108.69
1	C	393	LEU	N-CA-C	7.58	119.18	111.07
1	B	496	MET	N-CA-C	7.50	121.87	112.87
1	F	472	ILE	CB-CA-C	-7.49	102.20	112.02
1	B	759	ASN	N-CA-C	7.47	120.09	108.96
1	D	621	GLY	N-CA-C	-7.27	103.27	111.63
1	A	674	LEU	N-CA-C	7.22	119.11	110.44
1	B	118	LEU	CA-C-N	7.21	127.26	119.90
1	B	118	LEU	C-N-CA	7.21	127.26	119.90
1	E	46	GLN	N-CA-C	7.20	121.44	108.48
1	F	474	ILE	N-CA-C	7.08	117.69	110.82
1	C	232	ALA	N-CA-C	7.02	119.19	108.52
1	D	325	TYR	CA-C-N	6.86	126.55	119.56
1	D	325	TYR	C-N-CA	6.86	126.55	119.56
1	F	539	ALA	CA-C-N	6.86	143.45	127.00
1	F	539	ALA	C-N-CA	6.86	143.45	127.00
1	F	531	VAL	N-CA-C	-6.85	104.09	110.53
1	F	903	VAL	CA-C-N	6.82	124.54	120.24
1	F	903	VAL	C-N-CA	6.82	124.54	120.24
1	E	579	PRO	CA-C-N	6.76	128.29	119.84
1	E	579	PRO	C-N-CA	6.76	128.29	119.84
1	A	621	GLY	N-CA-C	-6.74	100.91	110.75
1	E	454	LEU	CA-C-N	-6.71	112.79	119.56
1	E	454	LEU	C-N-CA	-6.71	112.79	119.56
1	B	54	ALA	N-CA-C	-6.70	103.90	111.07
1	F	559	ILE	N-CA-C	6.68	115.50	108.95
1	F	637	ARG	CA-C-N	6.66	128.16	119.84
1	F	637	ARG	C-N-CA	6.66	128.16	119.84
1	E	411	VAL	N-CA-CB	6.64	117.88	110.51
1	F	900	VAL	CB-CA-C	6.58	116.85	111.06
1	E	606	VAL	N-CA-C	6.55	117.87	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	30	LEU	CA-C-N	6.54	126.49	119.76
1	D	30	LEU	C-N-CA	6.54	126.49	119.76
1	A	498	LYS	N-CA-C	6.51	124.20	109.81
1	F	1002	GLY	N-CA-C	6.50	120.53	112.73
1	A	362	PHE	N-CA-C	-6.50	101.52	110.35
1	D	421	ALA	N-CA-C	-6.49	105.66	113.97
1	D	218	GLN	CB-CA-C	6.45	124.74	112.43
1	D	896	ILE	N-CA-CB	6.43	114.55	110.50
1	C	1002	GLY	N-CA-C	6.43	121.98	113.37
1	C	463	THR	N-CA-C	-6.42	104.19	111.07
1	E	286	ALA	N-CA-C	6.42	118.82	109.07
1	C	118	LEU	CA-C-N	6.39	127.82	119.84
1	C	118	LEU	C-N-CA	6.39	127.82	119.84
1	E	883	VAL	N-CA-CB	6.38	118.02	110.55
1	F	539	ALA	C-N-CD	-6.32	106.69	120.60
1	E	624	SER	N-CA-C	6.32	121.58	113.18
1	C	46	GLN	N-CA-C	6.21	118.52	108.34
1	C	903	VAL	N-CA-C	6.20	118.80	111.05
1	F	83	ASN	N-CA-C	6.19	119.11	109.52
1	E	538	ARG	N-CA-C	6.18	117.89	111.03
1	A	83	ASN	N-CA-C	6.15	120.07	110.17
1	B	788	TRP	N-CA-C	6.14	118.95	109.07
1	E	432	ARG	N-CA-C	-6.14	104.51	111.14
1	F	232	ALA	N-CA-C	6.12	118.47	108.55
1	B	694	VAL	CB-CA-C	-6.11	104.02	112.02
1	C	637	ARG	CA-C-N	6.05	127.40	119.84
1	C	637	ARG	C-N-CA	6.05	127.40	119.84
1	F	466	ILE	N-CA-CB	6.05	117.48	110.65
1	C	466	ILE	N-CA-CB	6.04	118.30	110.57
1	A	438	ILE	N-CA-C	6.03	121.89	109.34
1	C	256	ASP	N-CA-C	6.03	119.29	109.59
1	C	472	ILE	N-CA-CB	6.00	117.17	110.62
1	F	781	ASN	N-CA-C	6.00	115.21	108.25
1	F	463	THR	N-CA-C	-5.96	103.96	111.11
1	D	718	ASN	N-CA-C	-5.94	106.67	112.97
1	A	579	PRO	CA-C-N	-5.89	113.69	119.76
1	A	579	PRO	C-N-CA	-5.89	113.69	119.76
1	B	569	GLN	N-CA-C	-5.85	103.22	110.41
1	F	821	VAL	CB-CA-C	5.83	115.05	109.33
1	F	472	ILE	N-CA-CB	5.81	118.00	110.57
1	B	46	GLN	N-CA-C	5.76	118.60	108.75
1	B	966	CYS	N-CA-C	-5.76	102.52	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	391	ASN	N-CA-C	5.76	116.69	108.74
1	B	411	VAL	N-CA-CB	5.76	118.37	110.54
1	B	741	SER	N-CA-C	5.74	118.48	111.82
1	F	375	VAL	N-CA-C	-5.70	106.15	111.45
1	F	300	LEU	N-CA-C	5.70	117.58	111.36
1	A	808	TRP	N-CA-C	5.69	118.70	110.28
1	E	627	ALA	N-CA-C	5.68	118.72	109.06
1	D	1026	ALA	N-CA-C	-5.67	103.04	110.53
1	E	17	LEU	N-CA-C	5.64	117.88	111.11
1	B	809	GLU	N-CA-C	-5.63	100.73	109.24
1	A	465	VAL	CB-CA-C	-5.62	104.69	111.88
1	A	823	ALA	N-CA-C	5.61	115.51	108.45
1	F	235	ILE	N-CA-C	5.58	115.30	106.32
1	B	74	ASN	N-CA-C	5.57	119.66	112.86
1	A	472	ILE	N-CA-CB	5.57	120.42	111.23
1	A	952	HIS	N-CA-C	-5.56	103.81	111.81
1	C	333	VAL	N-CA-C	-5.55	105.69	110.74
1	D	232	ALA	N-CA-C	5.54	117.41	108.32
1	F	771	TYR	N-CA-C	5.54	117.42	108.34
1	B	779	ARG	N-CA-C	5.50	116.90	110.41
1	D	498	LYS	N-CA-C	5.49	121.95	109.81
1	E	904	VAL	CB-CA-C	-5.48	108.49	113.70
1	E	981	ILE	N-CA-CB	5.48	116.59	110.51
1	E	904	VAL	O-C-N	5.47	123.92	120.42
1	E	474	ILE	N-CA-C	5.47	115.72	110.74
1	D	118	LEU	CA-C-N	5.46	126.66	119.84
1	D	118	LEU	C-N-CA	5.46	126.66	119.84
1	D	353	LEU	N-CA-C	5.45	116.91	110.97
1	A	696	LEU	O-C-N	-5.45	115.94	122.15
1	D	438	ILE	N-CA-C	5.44	120.66	109.34
1	A	92	VAL	CB-CA-C	5.44	118.93	111.31
1	A	894	TRP	CB-CA-C	-5.43	104.49	111.50
1	F	259	GLN	N-CA-C	5.43	117.33	109.07
1	C	498	LYS	CA-C-N	5.43	126.63	119.84
1	C	498	LYS	C-N-CA	5.43	126.63	119.84
1	D	276	SER	N-CA-C	5.41	116.87	110.97
1	D	219	LEU	N-CA-C	-5.40	104.35	111.96
1	E	663	VAL	N-CA-C	5.39	114.56	106.42
1	C	604	SER	N-CA-C	-5.36	105.51	111.36
1	C	475	VAL	N-CA-CB	5.33	117.78	110.54
1	E	1005	VAL	N-CA-C	-5.33	102.72	109.80
1	C	470	PHE	N-CA-C	-5.31	105.06	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	723	GLU	CA-C-N	5.31	126.14	119.98
1	E	723	GLU	C-N-CA	5.31	126.14	119.98
1	C	96	GLN	N-CA-C	5.30	119.23	112.87
1	D	578	THR	CA-C-N	5.29	125.83	120.38
1	D	578	THR	C-N-CA	5.29	125.83	120.38
1	A	309	THR	N-CA-C	-5.27	104.45	112.04
1	D	663	VAL	N-CA-C	5.26	115.43	107.75
1	E	415	ASN	N-CA-C	5.25	116.69	111.07
1	B	883	VAL	N-CA-CB	5.25	116.34	110.51
1	A	89	THR	CB-CA-C	-5.25	102.96	110.62
1	B	624	SER	N-CA-C	5.25	121.22	114.56
1	D	468	ARG	N-CA-C	-5.24	99.63	110.80
1	E	291	ILE	N-CA-C	5.24	116.52	108.71
1	C	955	GLY	N-CA-C	5.24	119.18	113.58
1	A	242	THR	N-CA-C	5.21	117.11	109.24
1	D	674	LEU	N-CA-C	5.20	117.54	110.88
1	C	810	TYR	N-CA-C	5.20	121.86	110.80
1	F	541	TYR	N-CA-C	5.19	117.61	111.33
1	C	87	SER	N-CA-C	5.18	116.98	110.24
1	F	909	ILE	N-CA-CB	5.17	116.25	110.51
1	A	235	ILE	CB-CA-C	5.16	117.21	110.96
1	A	579	PRO	N-CA-C	5.16	117.00	110.70
1	C	405	LEU	CA-CB-CG	5.14	134.30	116.30
1	D	918	ARG	N-CA-C	-5.14	106.25	112.88
1	D	8	ARG	CA-C-N	5.13	124.63	119.19
1	D	8	ARG	C-N-CA	5.13	124.63	119.19
1	A	775	ARG	CA-C-N	5.12	126.24	119.84
1	A	775	ARG	C-N-CA	5.12	126.24	119.84
1	B	107	VAL	N-CA-C	5.10	115.71	110.36
1	E	47	VAL	CB-CA-C	-5.09	101.69	110.30
1	C	279	ALA	N-CA-C	5.08	116.80	109.07
1	E	904	VAL	N-CA-CB	5.08	113.92	110.52
1	B	95	GLU	N-CA-C	5.07	117.39	110.24
1	B	56	THR	N-CA-CB	5.07	117.57	110.12
1	A	553	ILE	CB-CA-C	-5.06	105.41	112.04
1	C	510	GLY	N-CA-C	5.06	117.19	112.08
1	B	268	VAL	N-CA-C	5.06	115.93	107.18
1	D	32	VAL	CB-CA-C	5.05	117.94	110.77
1	C	360	GLN	N-CA-C	5.05	118.41	111.54
1	A	393	LEU	CA-CB-CG	-5.04	98.65	116.30
1	B	465	VAL	N-CA-C	-5.04	105.58	110.42
1	C	452	VAL	CB-CA-C	-5.04	104.10	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	964	GLU	N-CA-C	-5.03	104.89	111.02
1	D	46	GLN	N-CA-C	5.03	116.77	108.13
1	F	577	GLN	N-CA-C	5.03	116.42	109.54
1	A	134	LYS	N-CA-C	5.02	116.75	111.28
1	B	454	LEU	CA-C-N	-5.01	113.77	119.28
1	B	454	LEU	C-N-CA	-5.01	113.77	119.28
1	B	743	ALA	N-CA-C	-5.01	105.90	111.36

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

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	403	0
1	B	7812	0	7944	427	0
1	C	7812	0	7944	500	0
1	D	7735	0	7873	443	0
1	E	7812	0	7944	448	0
1	F	7840	0	7970	459	0
2	A	105	0	138	5	0
2	B	105	0	138	5	0
2	C	35	0	46	6	0
2	D	105	0	138	5	0
2	E	105	0	138	9	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	2597	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 27.

All (2597) 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:C:142:VAL:HG21	1:C:321:MET:HE3	1.16	1.13
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:A:791:ARG:HB2	1:A:797:MET:HE1	1.35	1.08
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:B:555:MET:HE2	1:B:913:LEU:HD12	1.35	1.06
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:D:456:MET:HE2	1:D:931:LEU:HD13	1.38	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:C:420:MET:HE3	1:C:500:ILE:HG22	1.40	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
1:C:355:MET:HE1	1:C:410:ILE:HG22	1.43	0.99
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:492:LEU:HD22	1:E:496:MET:HE3	1.49	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:576:VAL:HG22	1:D:594:MET:HE1	1.55	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:F:142:VAL:HG21	1:F:321:MET:HE3	1.55	0.87
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:E:951:LEU:HD11	1:E:968:MET:HE1	1.58	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:GLN:HB3	1:D:797:MET:HE3	1.59	0.85
1:B:640:GLY:O	1:B:646:GLU:HG3	1.77	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:F:355:MET:HE1	1:F:410:ILE:HG22	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:C:142:VAL:HG21	1:C:321:MET:CE	2.06	0.82
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:D:780:MET:HE1	1:F:220:GLY:HA2	1.61	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:355:MET:HE1	1:F:410:ILE:CG2	2.10	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:F:395:MET:HE2	1:F:395:MET:HA	1.63	0.81
1:C:942:ILE:HA	1:C:945:VAL:HG12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:LEU:HD22	1:A:824:MET:HE3	1.63	0.80
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
1:D:884:PHE:HB2	1:D:901:MET:HE2	1.64	0.80
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:D:791:ARG:HB2	1:D:797:MET:HE1	1.65	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:951:LEU:HD11	1:B:968:MET:HE1	1.65	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:142:VAL:CG2	1:C:321:MET:HE3	2.07	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:780:MET:HE3	1:F:220:GLY:HA2	1.62	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
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: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:D:456:MET:HE2	1:D:931:LEU:CD1	2.15	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:A:576:VAL:CG2	1:A:594:MET:HE1	2.16	0.75
1:B:414:GLU:HG2	1:B:972:PRO:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:224:ALA:HB1	1:B:780:MET:HE1	1.70	0.74
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:C:355:MET:HE1	1:C:410:ILE:CG2	2.18	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:D:576:VAL:CG2	1:D:594:MET:HE1	2.17	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:C:649:LYS:HZ2	1:C:713:GLN:HE21	1.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:410:ILE:C	1:F:410:ILE:HD12	2.15	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: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:D:225:VAL:H	1:E:780:MET:HE2	1.56	0.71
1:B:209:ALA:HB1	1:C:742:LEU:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:619:GLY:HA3	1:D:720:MET:HE3	1.73	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
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:B:156:ASN:HD21	1:B:768:LYS:HZ2	1.39	0.70
1:F:194:ASN:C	1:F:196:TYR:H	2.00	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:B:947:PHE:CD2	1:B:968:MET:HE3	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:652:GLN:HA	1:E:652:GLN:NE2	1.98	0.69
1:A:845:GLU:OE1	1:A:845:GLU:HA	1.92	0.69
1:B:1009:MET:HE2	1:B:1009:MET:HA	1.75	0.69
1:E:447:MET:HE2	2:E:2002:LMT:H72	1.73	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:E:298:ASN:C	1:E:298:ASN:HD22	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:197:GLN:HB3	1:A:797:MET:HE3	1.77	0.67
1:C:156:ASN:ND2	1:C:182:TYR:H	1.93	0.67
3:E:2001:P9D:H37	3:E:2001:P9D:C26	2.25	0.67
1:B:298:ASN:C	1:B:298:ASN:HD22	2.03	0.67
1:C:47:VAL:HG13	1:C:127:ILE:HA	1.76	0.67
1:C:366:LEU:HD12	1:C:496:MET:HE1	1.76	0.67
1:F:1020:VAL:HB	1:F:1021:PRO:HD3	1.77	0.67
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:D:713:GLN:HG2	1:D:714:ARG:N	2.09	0.67
1:E:718:ASN:HB2	1:E:827:LEU:HD13	1.75	0.67
1:A:228:GLN:OE1	1:B:780:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:906:LEU:O	1:C:1011:THR:HG23	1.94	0.66
1:C:1009:MET:HA	1:C:1009:MET:HE3	1.76	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:150:THR:HG22	1:A:153:ASP:CG	2.20	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: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
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: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:B:626:MET:HE2	1:B:628:PHE:CE2	2.30	0.65
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:A:2:SER:O	1:A:3:LYS:HB2	1.97	0.65
1:A:791:ARG:CB	1:A:797:MET:HE1	2.20	0.65
1:C:649:LYS:NZ	1:C:713:GLN:HE21	1.93	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:420:MET:HE3	1:F:500:ILE:HG22	1.79	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:B:228:GLN:HA	1:C:780:MET:HE1	1.79	0.65
1:B:555:MET:HE2	1:B:913:LEU:CD1	2.22	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
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: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:D:1009:MET:HA	1:D:1009:MET:HE3	1.78	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:C:791:ARG:HA	1:C:797:MET:HE3	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:355:MET:HE1	1:D:369:THR:HG22	1.80	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:F:969:ARG:C	1:F:972:PRO:HD2	2.23	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: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: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:C:791:ARG:HG3	1:C:797:MET:HE1	1.80	0.63
1:D:228:GLN:OE1	1:E:780:MET:HE3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:791:ARG:HG3	1:F:797:MET:HE1	1.81	0.62
1:A:225:VAL:HG22	1:B:780:MET:HE2	1.80	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:B:662:MET:HE3	1:B:662:MET:H	1.64	0.62
1:D:1009:MET:O	1:D:1013:THR:CG2	2.47	0.62
1:E:555:MET:HE2	1:E:913:LEU:HD12	1.79	0.62
1:F:46:GLN:HA	1:F:88:MET:HE3	1.81	0.62
1:F:367:ILE:HG12	1:F:496:MET:HE2	1.81	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: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:A:884:PHE:HB2	1:A:901:MET:HE2	1.81	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:655:PHE:HD2	1:A:658:PHE:CE2	2.18	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: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
1:B:456:MET:HE3	1:B:471:SER:HB2	1.80	0.61
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:C:367:ILE:HG12	1:C:496:MET:HE2	1.84	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:E:191:ALA:C	1:E:193:LEU:H	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:596:GLU:C	1:C:598:LEU:H	2.10	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: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:F:826:ILE:C	1:F:826:ILE:HD12	2.27	0.59
1:C:420:MET:HE3	1:C:500:ILE:CG2	2.24	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:228:GLN:HG3	1:F:780:MET:HE1	1.84	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
1:B:902:LEU:O	1:B:905:PRO:HD2	2.03	0.59
1:C:573:PHE:HB2	1:C:666:PHE:CE1	2.37	0.59
1:C:916:SER:C	1:C:918:ARG:H	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1009:MET:O	1:A:1010:VAL:C	2.45	0.59
1:C:909:ILE:HG13	1:C:910:GLY:H	1.68	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: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:7:ASP:C	1:E:9:PRO:HD3	2.28	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
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:D:989:ILE:HG12	1:D:989:ILE:O	2.01	0.58
1:B:323:VAL:HG23	1:B:323:VAL:O	2.02	0.58
1:D:467:TYR:C	1:D:468:ARG:O	2.42	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:E:244:GLU:H	1:E:244:GLU:CD	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:410:ILE:HD12	1:C:410:ILE:C	2.29	0.58
1:D:468:ARG:O	1:D:469:GLN:HB2	2.02	0.58
1:E:1009:MET:HE2	1:E:1009:MET:HA	1.85	0.58
1:F:348:ILE:C	1:F:348:ILE:HD12	2.28	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:B:947:PHE:HD2	1:B:968:MET:HE3	1.66	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:B:965:ALA:HA	1:B:968:MET:HE2	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
1:E:351:VAL:HG21	1:E:406:VAL:HG22	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:596:GLU:C	1:F:598:LEU:H	2.12	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:47:VAL:H	1:C:88:MET:HE2	1.70	0.57
1:C:774:GLY:O	1:C:779:ARG:NH1	2.38	0.57
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:D:576:VAL:HG22	1:D:594:MET:CE	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:483:ILE:C	1:D:483:ILE:HD12	2.30	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:E:806:GLY:O	1:E:807:LYS:HB2	2.04	0.56
1:F:336:SER:HA	1:F:993:ALA:CB	2.34	0.56
1:A:306:ILE:C	1:A:308:GLN:N	2.60	0.56
1:C:420:MET:CE	1:C:500:ILE:HG22	2.26	0.56
1:C:930:LEU:O	1:C:933:THR:HB	2.05	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:7:ASP:C	1:B:9:PRO:HD3	2.29	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: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:A:225:VAL:H	1:B:780:MET:CE	2.19	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:395:MET:HE2	1:E:395:MET:HA	1.88	0.56
1:E:440:GLY:HA3	2:E:2002:LMT:H2O2	1.67	0.56
1:C:519:MET:SD	1:C:519:MET:C	2.88	0.56
1:D:791:ARG:HE	1:D:797:MET:HE1	1.71	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:395:MET:HE2	1:A:395:MET:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:121:GLU:CD	1:A:121:GLU:H	2.11	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:E:314:GLU:HA	1:E:317:MET:HE2	1.88	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:B:840:MET:HE2	1:B:862:SER:OG	2.06	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: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:F:1:MET:HE3	1:F:486:LEU:HB3	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:937:SER:HB3	1:D:1009:MET:HE1	1.88	0.55
1:E:8:ARG:N	1:E:9:PRO:HD3	2.22	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
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:E:653:MET:HE2	1:E:653:MET:HA	1.87	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: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:317:MET:SD	1:C:321:MET:HE2	2.47	0.55
1:D:228:GLN:HE21	1:D:230:LEU:H	1.55	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:F:317:MET:SD	1:F:321:MET:HE2	2.46	0.54
1:A:576:VAL:HG22	1:A:594:MET:HE1	1.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:235:ILE:O	1:D:235:ILE:HG13	2.06	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:B:152:GLU:CD	1:B:152:GLU:H	2.15	0.54
1:B:576:VAL:HG22	1:B:594:MET:HE1	1.88	0.54
1:B:994:GLY:O	1:B:998:GLN:HG3	2.08	0.54
1:C:673:GLU:H	1:C:673:GLU:CD	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:742:LEU:C	1:C:744:ASP:H	2.15	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:53:SER:O	1:E:54:ALA:C	2.50	0.54
1:E:954:GLN:HG2	1:E:954:GLN:O	2.07	0.54
1:F:366:LEU:HD12	1:F:496:MET:HE1	1.89	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:362:PHE:C	1:C:364:ALA:H	2.14	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:A:306:ILE:O	1:A:307:ARG:C	2.50	0.53
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:934:ILE:HD12	1:D:934:ILE:C	2.32	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:175:PHE:C	1:C:175:PHE:CD1	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:VAL:HG22	1:D:228:GLN:HB2	1.91	0.53
1:D:700:ASN:O	1:D:701:LYS:C	2.50	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:455:PRO:HG3	1:F:882:VAL:HG21	1.90	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:786:SER:C	1:D:788:TRP:H	2.15	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:D:713:GLN:O	1:D:714:ARG:C	2.51	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
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: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: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: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:646:GLU:O	1:C:647:LEU:C	2.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:MET:O	1:A:1013:THR:HG22	2.08	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:F:355:MET:CE	1:F:410:ILE:CG2	2.86	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:438:ILE:O	1:B:439:GLN:C	2.53	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
1:C:308:GLN:OE1	1:C:308:GLN:HA	2.09	0.52
1:D:17:LEU:HA	1:D:20:MET:HE3	1.90	0.52
1:D:887:LEU:CD2	1:D:942:ILE:HD11	2.39	0.52
1:F:789:TYR:CD1	1:F:799:PRO:HA	2.44	0.52
1:A:137:LEU:HD22	1:A:293:LEU:CD1	2.38	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:328:ASP:O	1:F:630:MET:HE1	2.09	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:E:348:ILE:HD12	1:E:369:THR:HG23	1.92	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:845:GLU:C	1:C:847:VAL:H	2.17	0.52
1:C:1009:MET:HA	1:C:1009:MET:CE	2.38	0.52
1:E:1:MET:HE3	1:E:486:LEU:HB3	1.91	0.52
1:E:445:ILE:C	1:E:445:ILE:HD12	2.34	0.52
1:E:545:TYR:O	1:E:548:ILE:HG13	2.09	0.52
1:F:466:ILE:O	1:F:467:TYR:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:MET:SD	1:C:427:PRO:HA	2.50	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: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
1:E:181:GLN:HG2	1:E:768:LYS:HD3	1.92	0.52
1:E:507:GLU:C	1:E:509:LYS:H	2.17	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:F:478:MET:HE2	1:F:478:MET:HA	1.92	0.52
1:A:597:TYR:O	1:A:601:LYS:HB2	2.10	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: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:C:720:MET:O	1:C:721:SER:HB2	2.10	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:F:157:TYR:CD2	1:F:321:MET:HE1	2.45	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:D:410:ILE:O	1:D:411:VAL:C	2.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:225:VAL:HG13	1:B:780:MET:HE2	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
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:255:PRO:C	1:A:257:GLY:H	2.19	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:154:LEU:HD23	1:A:321:MET:HE2	1.93	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:A:222:LEU:HA	1:A:223:PRO:C	2.35	0.51
1:B:576:VAL:CG2	1:B:594:MET:HE1	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:355:MET:HE1	1:F:410:ILE:HG21	1.92	0.51
1:F:646:GLU:OE2	1:F:646:GLU:HA	2.10	0.51
1:A:456:MET:HE2	1:A:931:LEU:HD13	1.93	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:324:VAL:C	1:C:326:PRO:HD2	2.35	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
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:149:MET:SD	1:A:321:MET:HE3	2.51	0.50
1:A:163:GLN:NE2	1:A:175:PHE:HE1	2.09	0.50
1:B:199:THR:HG22	1:B:201:GLY:H	1.76	0.50
1:B:314:GLU:HG2	1:B:317:MET:HE2	1.92	0.50
1:C:916:SER:O	1:C:918:ARG:N	2.43	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: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:563:PHE:O	1:F:923:ASP:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:LYS:O	1:A:957:GLY:C	2.54	0.50
1:A:962:ALA:O	1:A:965:ALA:HB3	2.12	0.50
1:B:184:MET:HE2	1:B:268:VAL:HG23	1.92	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:E:365:THR:CG2	1:E:366:LEU:N	2.72	0.50
1:E:895:SER:C	1:E:897:PRO:HD2	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:F:61:VAL:HG22	1:F:62:VAL:N	2.27	0.50
1:F:713:GLN:HG2	1:F:714:ARG:HB2	1.92	0.50
1:A:156:ASN:HD21	1:A:768:LYS:HZ2	1.58	0.50
1:A:467:TYR:C	1:A:468:ARG:O	2.53	0.50
1:A:759:ASN:O	1:A:770:VAL:CG1	2.57	0.50
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:E:555:MET:HE3	1:E:916:SER:CB	2.41	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:361:ASN:C	1:D:362:PHE:O	2.54	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:A:913:LEU:HB3	1:A:917:MET:HE2	1.94	0.50
1:D:559:ILE:HD11	1:D:916:SER:HB2	1.93	0.50
1:E:4:PHE:C	1:E:4:PHE:CD2	2.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:449:LEU:C	1:A:449:LEU:HD13	2.37	0.49
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:C:729:GLU:C	1:C:730:ILE:HD12	2.37	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:121:GLU:H	1:B:121:GLU:CD	2.20	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:157:TYR:O	1:D:158:ILE:C	2.55	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
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:355:MET:HE1	1:A:369:THR:HG22	1.94	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:C:596:GLU:C	1:C:598:LEU:N	2.70	0.49
1:C:746:ASN:C	1:C:748:THR:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:343:THR:HG21	1:C:998:GLN:CD	2.36	0.49
1:C:659:LYS:HZ2	1:C:661:ALA:HB2	1.78	0.49
1:C:730:ILE:HD12	1:C:730:ILE:N	2.28	0.49
1:D:969:ARG:O	1:D:972:PRO:HG2	2.12	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:F:894:TRP:C	1:F:897:PRO:HD2	2.38	0.49
1:F:1009:MET:HA	1:F:1009:MET:HE3	1.94	0.49
1:B:541:TYR:O	1:B:542:LEU:C	2.52	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:E:662:MET:HE3	1:E:662:MET:H	1.78	0.49
1:E:904:VAL:HB	1:E:905:PRO:CD	2.40	0.49
1:E:917:MET:C	1:E:919:GLY:H	2.21	0.49
1:A:151:LYS:HB3	1:A:151:LYS:HZ3	1.78	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:713:GLN:O	1:A:714:ARG:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:MET:CE	1:C:410:ILE:HG22	2.30	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:D:634:TRP:CD1	1:D:634:TRP:H	2.28	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:900:VAL:HG23	1:C:901:MET:HE2	1.95	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: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:A:1013:THR:C	1:A:1015:LEU:H	2.21	0.48
1:B:472:ILE:HD12	2:B:2003:LMT:H82	1.96	0.48
1:F:575:GLN:O	1:F:663:VAL:HA	2.13	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ALA:CB	1:A:330:THR:HG21	2.43	0.48
1:C:150:THR:OG1	1:C:151:LYS:N	2.45	0.48
1:D:380:PHE:CZ	1:D:398:MET:HE3	2.49	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:338:HIS:C	1:E:340:VAL:H	2.22	0.48
1:E:352:PHE:CD2	1:E:352:PHE:C	2.91	0.48
1:E:539:ALA:O	1:E:540:PRO:C	2.56	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:C	1:B:352:PHE:CD2	2.92	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:C:547:VAL:O	1:C:550:ALA:HB3	2.13	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:840:MET:HE2	1:E:862:SER:HB3	1.95	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:F:913:LEU:O	1:F:914:ALA:C	2.53	0.48
1:A:904:VAL:CB	1:A:905:PRO:HD3	2.44	0.48
1:A:1014:VAL:O	1:A:1014:VAL:HG23	2.13	0.48
1:B:548:ILE:C	1:B:548:ILE:HD12	2.39	0.48
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:E:84:SER:C	1:E:86:GLY:H	2.22	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:A:225:VAL:H	1:B:780:MET:HE2	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:222:LEU:HA	1:D:223:PRO:C	2.38	0.48
1:D:647:LEU:C	1:D:647:LEU:CD2	2.87	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:598:LEU:HD22	1:B:629:ILE:HD12	1.95	0.48
1:C:439:GLN:CD	2:C:2001:LMT:H3'	2.39	0.48
1:D:966:CYS:SG	1:D:1021:PRO:CG	3.02	0.48
1:E:653:MET:O	1:E:654:HIS:C	2.57	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:A:1005:VAL:O	1:A:1006:ILE:C	2.57	0.47
1:B:47:VAL:HG23	1:B:88:MET:HE3	1.96	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: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:194:ASN:C	1:F:196:TYR:N	2.68	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
1:C:1016:ALA:C	1:C:1018:PHE:N	2.71	0.47
1:D:984:VAL:O	1:D:985:VAL:C	2.57	0.47
1:E:713:GLN:C	1:E:715:VAL:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:142:VAL:HG21	1:F:321:MET:CE	2.38	0.47
1:A:151:LYS:NZ	1:A:151:LYS:CB	2.78	0.47
1:A:831:ALA:O	1:A:832:PRO:C	2.56	0.47
1:A:872:ALA:O	1:A:875:LEU:O	2.33	0.47
1:B:456:MET:HE3	1:B:471:SER:CA	2.45	0.47
1:D:156:ASN:HD21	1:D:768:LYS:HZ2	1.62	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: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:F:851:PRO:O	1:F:852:LYS:C	2.57	0.47
1:B:228:GLN:NE2	1:B:231:ASN:HB2	2.30	0.47
1:B:781:ASN:O	1:B:782:PRO:C	2.56	0.47
1:C:239:ARG:NH1	1:C:239:ARG:CG	2.57	0.47
1:C:957:GLY:O	1:C:959:VAL:N	2.47	0.47
1:D:333:VAL:HG23	1:D:334:SER:N	2.27	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: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
1:B:317:MET:HE1	1:B:323:VAL:HG13	1.97	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:763:ASP:C	1:D:765:GLY:N	2.72	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:E:468:ARG:O	1:E:469:GLN:C	2.57	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:626:MET:HE2	1:B:628:PHE:CZ	2.49	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:552:MET:O	1:D:553:ILE:C	2.57	0.47
1:D:577:GLN:HE21	1:D:577:GLN:CA	2.23	0.47
1:E:146:ASP:OD2	1:E:146:ASP:C	2.58	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:203:VAL:O	1:F:204:SER:C	2.58	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:A:330:THR:O	1:A:331:PRO:C	2.57	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:C:916:SER:C	1:C:918:ARG:N	2.73	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:B:953:GLU:C	1:B:955:GLY:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:343:THR:CG2	1:D:998:GLN:HE22	2.17	0.47
1:D:577:GLN:HA	1:D:577:GLN:NE2	2.30	0.47
1:D:701:LYS:O	1:D:702:PHE:C	2.55	0.47
1:D:892:GLU:OE1	1:F:8:ARG:HG2	2.15	0.47
1:E:191:ALA:C	1:E:193:LEU:N	2.71	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: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:780:MET:HE2	1:A:780:MET:HA	1.97	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:C:351:VAL:O	1:C:352:PHE:C	2.56	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:789:TYR:CE1	1:A:799:PRO:HG3	2.51	0.46
1:B:228:GLN:CA	1:C:780:MET:HE1	2.43	0.46
1:B:456:MET:HE3	1:B:471:SER:CB	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:452:VAL:HG12	1:F:931:LEU:HD13	1.97	0.46
1:A:372:VAL:O	1:A:373:PRO:C	2.57	0.46
1:A:958:ILE:HG21	1:A:1028:SER:HB3	1.96	0.46
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:145:THR:N	1:F:320:GLY:O	2.47	0.46
1:B:454:LEU:O	1:B:455:PRO:C	2.56	0.46
1:C:524:THR:HG22	1:C:970:LEU:HD12	1.97	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:A:568:ASP:OD2	1:A:644:VAL:HG12	2.16	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:701:LYS:O	1:C:705:LEU:HD12	2.16	0.46
1:D:13:TRP:NE1	2:D:2003:LMT:O2'	2.45	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:A:340:VAL:O	1:A:341:VAL:C	2.58	0.46
1:B:449:LEU:O	1:B:453:PHE:HD2	1.98	0.46
1:C:45:VAL:O	1:C:88:MET:HE1	2.15	0.46
1:C:176:GLN:HE22	1:C:620:ARG:NH2	2.14	0.46
1:C:913:LEU:O	1:C:914:ALA:C	2.57	0.46
1:D:937:SER:HB3	1:D:1009:MET:CE	2.45	0.46
1:E:340:VAL:HG22	1:E:399:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:728:LEU:HD23	1:E:728:LEU:C	2.40	0.46
1:F:156:ASN:HD22	1:F:181:GLN:HA	1.79	0.46
1:F:355:MET:CE	1:F:410:ILE:HG21	2.44	0.46
1:F:596:GLU:C	1:F:598:LEU:N	2.74	0.46
1:F:910:GLY:H	1:F:1011:THR:HG21	1.81	0.46
1:F:927:GLN:O	1:F:928:VAL:C	2.56	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:C:845:GLU:C	1:C:847:VAL:N	2.74	0.46
1:E:151:LYS:O	1:E:154:LEU:HB2	2.16	0.46
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: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:D:352:PHE:CD2	1:D:352:PHE:C	2.94	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:555:MET:HE2	1:A:555:MET:O	2.15	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:C:653:MET:C	1:C:655:PHE:H	2.24	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: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
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:175:PHE:C	1:C:175:PHE:HD1	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:244:GLU:C	1:B:246:PHE:N	2.73	0.45
1:B:509:LYS:O	1:B:510:GLY:O	2.33	0.45
1:C:639:GLY:O	1:C:640:GLY:C	2.58	0.45
1:D:883:VAL:O	1:D:887:LEU:HG	2.17	0.45
1:F:247:GLU:O	1:F:249:ILE:N	2.49	0.45
1:F:379:THR:OG1	1:F:398:MET:HE2	2.17	0.45
1:F:480:LEU:O	1:F:484:VAL:HG13	2.15	0.45
1:F:845:GLU:C	1:F:847:VAL:H	2.24	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:447:MET:HE2	1:C:447:MET:HB3	1.62	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:F:374:VAL:CG1	1:F:484:VAL:HG11	2.47	0.45
1:F:417:GLU:C	1:F:419:VAL:H	2.24	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:PHE:O	1:A:519:MET:HB2	2.17	0.45
1:A:691:GLY:C	1:A:693:GLU:N	2.73	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:D:1026:ALA:C	1:D:1028:SER:H	2.24	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
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:B:831:ALA:O	1:B:832:PRO:C	2.59	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:D:658:PHE:C	1:D:660:ASP:H	2.24	0.45
1:F:412:VAL:HG13	1:F:435:MET:HE1	1.97	0.45
1:A:33:ASN:O	1:A:391:ASN:HA	2.16	0.45
1:B:47:VAL:CG2	1:B:127:ILE:HG13	2.46	0.45
1:B:156:ASN:ND2	1:B:768:LYS:HZ2	2.10	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:662:MET:HE3	1:E:662:MET:N	2.32	0.45
1:E:917:MET:C	1:E:919:GLY:N	2.75	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:380:PHE:CZ	1:A:398:MET:HE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:780:MET:HE3	1:F:220:GLY:CA	2.40	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
1:B:160:SER:HA	1:B:766:ARG:HH21	1.81	0.45
1:B:595:ARG:O	1:B:596:GLU:C	2.60	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:659:LYS:HZ3	1:C:661:ALA:HB2	1.81	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:872:ALA:O	1:C:873:PRO:C	2.60	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: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:347:ALA:O	1:F:348:ILE:C	2.60	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:A:791:ARG:HB2	1:A:797:MET:CE	2.26	0.45
1:B:445:ILE:C	1:B:445:ILE:HD13	2.41	0.45
1:B:882:VAL:O	1:B:883:VAL:C	2.59	0.45
1:C:324:VAL:O	1:C:326:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:971:ARG:N	1:E:972:PRO:HD2	2.32	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:114:ALA:O	1:F:115:THR:C	2.60	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:B:184:MET:HE1	1:B:269:GLY:C	2.42	0.44
1:C:30:LEU:HD11	1:C:384:ALA:HA	1.97	0.44
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: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:152:GLU:CD	1:E:152:GLU:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:355:MET:CE	1:C:410:ILE:CG2	2.93	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:10:ILE:O	1:E:11:PHE:C	2.60	0.44
1:E:298:ASN:C	1:E:298:ASN:ND2	2.71	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:396:PHE:CE1	1:C:998:GLN:HG2	2.53	0.44
1:C:447:MET:HE3	1:C:886:CYS:HB3	2.00	0.44
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.82	0.44
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: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:917:MET:HE2	1:B:917:MET:HA	1.99	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:314:GLU:C	1:D:316:PHE:H	2.26	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
2:E:2002:LMT:O6B	2:E:2002:LMT:H1B	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:ILE:HG13	1:F:16:ALA:N	2.33	0.44
1:A:69:MET:O	1:A:70:ASN:C	2.61	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: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:C:1016:ALA:C	1:C:1018:PHE:H	2.26	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:E:17:LEU:HD13	1:E:17:LEU:HA	1.56	0.44
1:F:917:MET:HE3	1:F:917:MET:HB2	1.83	0.44
1:A:475:VAL:O	1:A:476:SER:C	2.60	0.44
1:A:569:GLN:N	1:A:634:TRP:HH2	2.14	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:E:81:GLU:HG3	1:E:814:LYS:HE2	2.00	0.44
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:E:800:PHE:C	1:E:802:ALA:H	2.26	0.44
1:F:720:MET:O	1:F:721:SER:HB2	2.17	0.44
1:A:156:ASN:HD21	1:A:768:LYS:HZ3	1.61	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:TRP:C	1:D:636:GLU:H	2.26	0.44
1:D:780:MET:HE2	1:F:220:GLY:HA2	1.85	0.44
1:D:783:ASP:C	1:D:785:LEU:N	2.73	0.44
1:F:189:ASP:OD2	1:F:192:LYS:HG3	2.17	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: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: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:E:541:TYR:O	1:E:542:LEU:C	2.61	0.44
1:F:407:ASP:O	1:F:408:ASP:C	2.58	0.44
1:F:417:GLU:C	1:F:419:VAL:N	2.76	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
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:D:626:MET:HE2	1:D:626:MET:HB2	1.92	0.43
1:D:874:ALA:C	1:D:875:LEU:O	2.59	0.43
1:E:438:ILE:O	1:E:439:GLN:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ILE:C	1:A:308:GLN:H	2.26	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:244:GLU:O	1:B:245:GLN:C	2.61	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:D:845:GLU:O	1:D:846:ILE:C	2.60	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: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:D:778:ALA:C	1:D:784:ASP:HB3	2.44	0.43
1:E:49:TYR:O	1:E:50:PRO:C	2.61	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: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:47:VAL:H	1:F:88:MET:HE3	1.82	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: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
1:A:984:VAL:O	1:A:985:VAL:C	2.62	0.43
1:B:123:GLN:HE21	1:B:123:GLN:HB3	1.62	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:B:737:ALA:C	1:B:739:GLY:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:594:MET:HE3	1:B:594:MET:HB2	1.73	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: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:F:839:ALA:O	1:F:840:MET:C	2.62	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:B:298:ASN:C	1:B:298:ASN:ND2	2.72	0.43
1:B:891:TYR:O	1:B:892:GLU:C	2.61	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: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:632:LYS:O	1:F:633:PRO:C	2.61	0.43
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:225:VAL:HG23	1:C:780:MET:HE2	2.00	0.43
1:B:812:SER:HA	1:B:813:PRO:HD3	1.89	0.43
1:C:910:GLY:N	1:C:1011:THR:HG21	2.33	0.43
1:D:281:PHE:C	1:D:283:GLY:H	2.26	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:F:169:THR:O	1:F:170:LYS:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:C	1:A:264:ASP:H	2.26	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:CA	1:E:652:GLN:NE2	2.68	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:46:GLN:HA	1:F:88:MET:CE	2.49	0.43
1:F:354:VAL:HG21	1:F:982:LEU:HG	2.00	0.43
1:F:687:GLN:C	1:F:689:GLY:N	2.76	0.43
1:A:149:MET:HE2	1:A:153:ASP:HB3	2.01	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:992:GLY:H	1:D:995:SER:HB2	1.83	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:910:GLY:HA2	1:E:1011:THR:HG21	1.99	0.43
1:F:410:ILE:C	1:F:410:ILE:CD1	2.85	0.43
1:F:724:PRO:HA	1:F:810:TYR:HB3	2.01	0.43
1:A:723:GLU:CB	1:A:724:PRO:HD2	2.49	0.43
1:A:845:GLU:O	1:A:846:ILE:C	2.61	0.43
1:A:975:MET:HE2	1:A:975:MET:HB3	1.90	0.43
1:A:989:ILE:O	1:A:989:ILE:CG1	2.67	0.43
1:B:4:PHE:CD1	1:B:4:PHE:C	2.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:ASN:O	1:D:194:ASN:ND2	2.52	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: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: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:F:669:PRO:O	1:F:670:SER:C	2.61	0.43
1:A:725:GLN:NE2	1:C:235:ILE:HD11	2.32	0.42
1:A:875:LEU:HG	1:A:876:TYR:H	1.85	0.42
1:B:454:LEU:HD23	1:B:454:LEU:HA	1.84	0.42
1:C:47:VAL:N	1:C:88:MET:HE2	2.34	0.42
1:C:53:SER:O	1:C:54:ALA:C	2.61	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:121:GLU:H	1:D:121:GLU:CD	2.27	0.42
1:D:406:VAL:O	1:D:410:ILE:HG13	2.18	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:A:380:PHE:CE2	1:A:398:MET:HE3	2.53	0.42
1:B:298:ASN:HD22	1:B:300:LEU:N	2.16	0.42
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: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:763:ASP:C	1:D:765:GLY:H	2.28	0.42
1:D:831:ALA:HB3	1:D:834:LEU:HD12	2.01	0.42
1:E:162:ILE:C	1:E:165:PRO:HD2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:VAL:C	1:A:326:PRO:HD3	2.44	0.42
1:A:890:LEU:HD23	1:A:890:LEU:C	2.44	0.42
1:B:533:SER:O	1:B:536:LYS:HB2	2.19	0.42
1:B:953:GLU:C	1:B:955:GLY:H	2.26	0.42
1:C:635:GLU:CG	1:C:636:GLU:H	2.32	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:568:ASP:OD1	1:E:644:VAL:CG2	2.63	0.42
1:E:577:GLN:HE22	1:E:720:MET:HE3	1.83	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:B:211:ASN:O	1:B:211:ASN:CG	2.61	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:E:68:GLN:HG2	1:E:114:ALA:HB2	2.01	0.42
1:E:980:PHE:O	1:E:981:ILE:C	2.61	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
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:194:ASN:C	1:D:194:ASN:HD22	2.26	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: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:447:MET:HE2	1:F:447:MET:HB3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:102:ILE:O	1:D:103:ALA:C	2.63	0.42
1:D:632:LYS:O	1:D:633:PRO:C	2.62	0.42
1:E:214:ILE:HG23	1:E:237:LYS:O	2.19	0.42
1:E:489:THR:O	1:E:490:PRO:C	2.61	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:579:PRO:O	1:A:580:PRO:C	2.62	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: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:515:TRP:CD1	1:D:515:TRP:C	2.98	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
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:195:SER:C	1:A:197:GLN:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ASN:O	1:B:518:ARG:C	2.63	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:184:MET:HA	1:E:184:MET:HE3	2.02	0.42
1:E:493:CYS:HA	1:E:497:LEU:HD22	2.02	0.42
1:F:26:SER:O	1:F:27:ILE:C	2.62	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: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: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: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:587:THR:OG1	1:A:622:GLN:O	2.35	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:61:VAL:O	1:C:62:VAL:C	2.63	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
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:N	1:A:373:PRO:HD2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:800:PHE:C	1:E:802:ALA:N	2.77	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:592:ASP:O	1:A:593:SER:C	2.62	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: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:A:1026:ALA:C	1:A:1028:SER:H	2.27	0.41
1:B:413:VAL:O	1:B:414:GLU:C	2.63	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:649:LYS:HZ2	1:C:713:GLN:NE2	2.07	0.41
1:C:721:SER:HB3	1:C:722:ASP:H	1.69	0.41
1:D:194:ASN:ND2	1:D:194:ASN:C	2.78	0.41
1:D:220:GLY:HA3	1:D:231:ASN:HA	2.02	0.41
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:VAL:HG23	1:E:88:MET:HE3	2.03	0.41
1:E:591:VAL:O	1:E:594:MET:HB3	2.19	0.41
1:F:56:THR:O	1:F:57:VAL:C	2.63	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: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:184:MET:HE1	1:B:269:GLY:CA	2.50	0.41
1:B:394:THR:HA	1:B:473:THR:HG21	2.02	0.41
1:C:587:THR:OG1	1:C:622:GLN:O	2.37	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:462:SER:O	1:E:463:THR:C	2.63	0.41
1:E:555:MET:HE3	1:E:916:SER:HB2	2.02	0.41
1:E:953:GLU:C	1:E:955:GLY:H	2.27	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: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:11:PHE:O	1:B:12:ALA:C	2.62	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:D:303:ALA:O	1:D:304:LYS:C	2.63	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:791:ARG:HB2	1:D:797:MET:CE	2.42	0.41
1:E:400:LEU:HA	1:E:400:LEU:HD23	1.82	0.41
1:E:657:SER:O	1:E:658:PHE:C	2.64	0.41
1:E:791:ARG:CB	1:E:791:ARG:CZ	2.97	0.41
1:E:875:LEU:O	1:E:876:TYR:C	2.63	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
1:A:129:VAL:HG23	1:B:113:LEU:HD21	2.03	0.41
1:A:666:PHE:CD2	1:A:666:PHE:N	2.88	0.41
1:B:157:TYR:CG	1:B:321:MET:HE1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:8:ARG:N	1:E:9:PRO:CD	2.84	0.41
1:E:517:ASN:O	1:E:518:ARG:C	2.62	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:A:946:GLU:C	1:A:948:ALA:N	2.78	0.41
1:B:156:ASN:ND2	1:B:768:LYS:NZ	2.64	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:C:957:GLY:O	1:C:958:ILE:C	2.63	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:352:PHE:CD2	1:F:352:PHE:C	2.98	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:A:951:LEU:C	1:A:953:GLU:H	2.28	0.41
1:A:972:PRO:HA	1:A:975:MET:HE2	2.03	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: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:791:ARG:HA	1:C:797:MET:CE	2.46	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
1:D:756:SER:O	1:D:771:TYR:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1023:PHE:O	1:D:1026:ALA:O	2.38	0.41
1:F:507:GLU:C	1:F:509:LYS:H	2.28	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:340:VAL:O	1:B:344:LEU:HG	2.21	0.41
1:B:442:LEU:O	1:B:443:VAL:C	2.64	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:333:VAL:CG2	1:D:334:SER:N	2.83	0.41
1:D:344:LEU:HD23	1:D:344:LEU:C	2.46	0.41
1:D:369:THR:C	1:D:371:ALA:N	2.78	0.41
1:D:453:PHE:HA	1:D:456:MET:HE3	2.02	0.41
1:D:596:GLU:O	1:D:597:TYR:C	2.64	0.41
1:D:686:ASP:OD1	1:D:686:ASP:C	2.64	0.41
1:D:780:MET:HE3	1:D:780:MET:HA	2.02	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:E:989:ILE:O	1:E:990:SER:C	2.64	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:324:VAL:C	1:F:326:PRO:HD3	2.46	0.41
1:F:392:THR:HG22	1:F:396:PHE:CZ	2.56	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:26:SER:O	1:B:27:ILE:C	2.64	0.41
1:B:896:ILE:N	1:B:897:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:SER:CB	1:C:175:PHE:HE2	2.31	0.41
1:C:329:THR:C	1:C:331:PRO:HD2	2.46	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: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:D:786:SER:C	1:D:788:TRP:N	2.76	0.41
1:D:896:ILE:O	1:D:897:PRO:C	2.64	0.41
1:D:965:ALA:HA	1:D:968:MET:HE3	2.03	0.41
1:E:350:LEU:O	1:E:354:VAL:HG13	2.20	0.41
1:E:634:TRP:C	1:E:636:GLU:H	2.29	0.41
1:E:766:ARG:H	1:E:766:ARG:HG3	1.60	0.41
1:F:513:PHE:HD1	1:F:513:PHE:HA	1.77	0.41
1:A:102:ILE:O	1:A:103:ALA:C	2.64	0.40
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:963:ILE:O	1:A:964:GLU:C	2.64	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:E:110:LYS:HD3	1:E:110:LYS:HA	1.77	0.40
1:E:164:ASP:CG	1:F:67:GLN:HG3	2.46	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:152:GLU:CD	1:F:152:GLU:H	2.29	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: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:519:MET:HE2	1:D:519:MET:HB3	1.94	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:330:THR:O	1:F:331:PRO:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:366:LEU:O	1:F:370:ILE:HG12	2.21	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:A:860:GLY:O	1:A:861:LEU:C	2.64	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:D:150:THR:O	1:D:151:LYS:C	2.64	0.40
1:D:418:ARG:C	1:D:420:MET:N	2.80	0.40
1:E:132:ALA:O	1:E:133:VAL:C	2.64	0.40
1:E:909:ILE:CG2	1:E:910:GLY:N	2.84	0.40
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:45:VAL:O	1:C:88:MET:CE	2.69	0.40
1:C:67:GLN:HE21	1:C:67:GLN:HB3	1.74	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:306:ILE:O	1:D:307:ARG:C	2.65	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:789:TYR:CE1	1:B:799:PRO:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:913:LEU:C	1:C:915:THR:N	2.79	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:D:1009:MET:O	1:D:1010:VAL:C	2.63	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
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:534:ILE:HG12	1:F:541:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	3	18
1	B	1028/1052 (98%)	874 (85%)	127 (12%)	27 (3%)	4	21
1	C	1028/1052 (98%)	844 (82%)	129 (12%)	55 (5%)	1	9
1	D	1015/1052 (96%)	846 (83%)	130 (13%)	39 (4%)	2	15
1	E	1028/1052 (98%)	865 (84%)	127 (12%)	36 (4%)	3	16
1	F	1031/1052 (98%)	862 (84%)	125 (12%)	44 (4%)	2	13
All	All	6144/6312 (97%)	5152 (84%)	760 (12%)	232 (4%)	2	15

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	678 (81%)	155 (19%)	1	8
1	B	841/860 (98%)	676 (80%)	165 (20%)	1	7
1	C	841/860 (98%)	677 (80%)	164 (20%)	1	7
1	D	834/860 (97%)	681 (82%)	153 (18%)	2	8
1	E	841/860 (98%)	660 (78%)	181 (22%)	1	5
1	F	844/860 (98%)	676 (80%)	168 (20%)	1	7
All	All	5034/5160 (98%)	4048 (80%)	986 (20%)	1	7

All (986) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	21	LEU
1	A	25	LEU
1	A	26	SER
1	A	32	VAL
1	A	57	VAL
1	A	69	MET
1	A	72	ILE
1	A	78	ILE
1	A	92	VAL
1	A	112	GLN
1	A	121	GLU
1	A	130	THR
1	A	143	VAL
1	A	145	THR
1	A	151	LYS
1	A	152	GLU
1	A	160	SER
1	A	166	LEU
1	A	170	LYS
1	A	172	VAL
1	A	181	GLN
1	A	213	GLN
1	A	214	ILE
1	A	216	SER
1	A	219	LEU
1	A	225	VAL
1	A	230	LEU
1	A	233	THR
1	A	235	ILE
1	A	253	VAL
1	A	259	GLN
1	A	260	VAL
1	A	265	VAL
1	A	277	ILE
1	A	285	PRO
1	A	289	ILE
1	A	291	ILE
1	A	295	THR
1	A	302	THR
1	A	306	ILE
1	A	310	ILE

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Mol	Chain	Res	Type
1	A	324	VAL
1	A	329	THR
1	A	334	SER
1	A	343	THR
1	A	348	ILE
1	A	350	LEU
1	A	353	LEU
1	A	354	VAL
1	A	366	LEU
1	A	367	ILE
1	A	369	THR
1	A	377	LEU
1	A	382	VAL
1	A	393	LEU
1	A	395	MET
1	A	414	GLU
1	A	417	GLU
1	A	419	VAL
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	449	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	561	THR
1	A	566	ASP
1	A	569	GLN
1	A	599	LEU

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Mol	Chain	Res	Type
1	A	612	VAL
1	A	624	SER
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	671	VAL
1	A	672	LEU
1	A	678	THR
1	A	684	LEU
1	A	685	GLN
1	A	686	ASP
1	A	690	VAL
1	A	695	LEU
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	824	MET
1	A	827	LEU
1	A	829	GLU
1	A	834	LEU
1	A	845	GLU

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Mol	Chain	Res	Type
1	A	861	LEU
1	A	864	GLU
1	A	865	GLU
1	A	870	SER
1	A	882	VAL
1	A	885	LEU
1	A	896	ILE
1	A	900	VAL
1	A	909	ILE
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
1	A	981	ILE
1	A	982	LEU
1	A	987	LEU
1	A	989	ILE
1	A	1005	VAL
1	A	1013	THR
1	A	1022	LEU
1	A	1027	VAL
1	A	1030	LEU
1	B	3	LYS
1	B	10	ILE
1	B	17	LEU
1	B	18	VAL
1	B	19	ILE
1	B	21	LEU
1	B	27	ILE
1	B	45	VAL
1	B	46	GLN
1	B	47	VAL
1	B	48	SER
1	B	53	SER
1	B	56	THR

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Mol	Chain	Res	Type
1	B	60	THR
1	B	61	VAL
1	B	65	ILE
1	B	75	LEU
1	B	84	SER
1	B	89	THR
1	B	90	ILE
1	B	91	THR
1	B	93	THR
1	B	95	GLU
1	B	96	GLN
1	B	105	VAL
1	B	113	LEU
1	B	121	GLU
1	B	130	THR
1	B	134	LYS
1	B	139	VAL
1	B	140	VAL
1	B	152	GLU
1	B	167	SER
1	B	184	MET
1	B	186	ILE
1	B	188	LEU
1	B	194	ASN
1	B	196	TYR
1	B	197	GLN
1	B	214	ILE
1	B	216	SER
1	B	219	LEU
1	B	222	LEU
1	B	225	VAL
1	B	229	GLN
1	B	233	THR
1	B	234	ILE
1	B	235	ILE
1	B	238	THR
1	B	239	ARG
1	B	249	ILE
1	B	250	LEU
1	B	253	VAL
1	B	259	GLN
1	B	263	LYS

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Mol	Chain	Res	Type
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	313	LEU
1	B	316	PHE
1	B	332	VAL
1	B	339	GLU
1	B	341	VAL
1	B	348	ILE
1	B	350	LEU
1	B	354	VAL
1	B	362	PHE
1	B	365	THR
1	B	367	ILE
1	B	370	ILE
1	B	376	LEU
1	B	383	LEU
1	B	402	ILE
1	B	405	LEU
1	B	406	VAL
1	B	410	ILE
1	B	411	VAL
1	B	414	GLU
1	B	415	ASN
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
1	B	484	VAL
1	B	486	LEU
1	B	497	LEU

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Mol	Chain	Res	Type
1	B	498	LYS
1	B	544	ILE
1	B	546	VAL
1	B	548	ILE
1	B	557	THR
1	B	572	LEU
1	B	589	VAL
1	B	590	VAL
1	B	591	VAL
1	B	593	SER
1	B	598	LEU
1	B	599	LEU
1	B	611	THR
1	B	613	THR
1	B	628	PHE
1	B	631	LEU
1	B	635	GLU
1	B	641	GLU
1	B	644	VAL
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	767	VAL
1	B	783	ASP
1	B	785	LEU
1	B	791	ARG
1	B	794	LYS
1	B	800	PHE
1	B	817	ARG

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Mol	Chain	Res	Type
1	B	824	MET
1	B	836	SER
1	B	847	VAL
1	B	852	LYS
1	B	880	LEU
1	B	883	VAL
1	B	903	VAL
1	B	908	VAL
1	B	932	THR
1	B	933	THR
1	B	934	ILE
1	B	936	LEU
1	B	954	GLN
1	B	959	VAL
1	B	964	GLU
1	B	967	ARG
1	B	969	ARG
1	B	973	ILE
1	B	984	VAL
1	B	985	VAL
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	15	ILE
1	C	30	LEU
1	C	38	ILE
1	C	46	GLN
1	C	47	VAL
1	C	55	GLU
1	C	57	VAL
1	C	58	GLN
1	C	63	GLN
1	C	65	ILE
1	C	78	ILE
1	C	81	GLU
1	C	82	SER
1	C	88	MET
1	C	90	ILE

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Mol	Chain	Res	Type
1	C	91	THR
1	C	96	GLN
1	C	110	LYS
1	C	115	THR
1	C	118	LEU
1	C	120	GLN
1	C	124	ARG
1	C	128	ARG
1	C	130	THR
1	C	131	LYS
1	C	145	THR
1	C	149	MET
1	C	151	LYS
1	C	152	GLU
1	C	153	ASP
1	C	158	ILE
1	C	183	SER
1	C	194	ASN
1	C	199	THR
1	C	203	VAL
1	C	214	ILE
1	C	235	ILE
1	C	238	THR
1	C	239	ARG
1	C	240	LEU
1	C	253	VAL
1	C	254	ASN
1	C	259	GLN
1	C	261	ARG
1	C	265	VAL
1	C	300	LEU
1	C	306	ILE
1	C	317	MET
1	C	319	GLN
1	C	323	VAL
1	C	334	SER
1	C	337	ILE
1	C	343	THR
1	C	348	ILE
1	C	351	VAL
1	C	357	LEU
1	C	360	GLN

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Mol	Chain	Res	Type
1	C	372	VAL
1	C	374	VAL
1	C	376	LEU
1	C	379	THR
1	C	392	THR
1	C	404	LEU
1	C	405	LEU
1	C	410	ILE
1	C	445	ILE
1	C	447	MET
1	C	452	VAL
1	C	463	THR
1	C	466	ILE
1	C	472	ILE
1	C	475	VAL
1	C	481	SER
1	C	484	VAL
1	C	486	LEU
1	C	488	LEU
1	C	505	HIS
1	C	508	HIS
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	547	VAL
1	C	558	ARG
1	C	559	ILE
1	C	564	LEU
1	C	582	SER
1	C	587	THR
1	C	595	ARG
1	C	599	LEU
1	C	604	SER
1	C	612	VAL
1	C	613	THR
1	C	616	ASN
1	C	631	LEU

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Mol	Chain	Res	Type
1	C	634	TRP
1	C	636	GLU
1	C	641	GLU
1	C	644	VAL
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	718	ASN
1	C	720	MET
1	C	728	LEU
1	C	730	ILE
1	C	738	LEU
1	C	744	ASP
1	C	745	ILE
1	C	751	ILE
1	C	762	ILE
1	C	764	ARG
1	C	767	VAL
1	C	768	LYS
1	C	779	ARG
1	C	783	ASP
1	C	785	LEU
1	C	808	TRP
1	C	810	TYR
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	870	SER
1	C	880	LEU

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Mol	Chain	Res	Type
1	C	896	ILE
1	C	900	VAL
1	C	902	LEU
1	C	903	VAL
1	C	906	LEU
1	C	920	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	969	ARG
1	C	974	VAL
1	C	978	LEU
1	C	985	VAL
1	C	995	SER
1	C	1009	MET
1	C	1011	THR
1	C	1015	LEU
1	C	1022	LEU
1	D	21	LEU
1	D	25	LEU
1	D	26	SER
1	D	28	LEU
1	D	32	VAL
1	D	48	SER
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	92	VAL
1	D	96	GLN
1	D	112	GLN
1	D	118	LEU
1	D	121	GLU
1	D	130	THR
1	D	140	VAL
1	D	143	VAL

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Mol	Chain	Res	Type
1	D	145	THR
1	D	153	ASP
1	D	158	ILE
1	D	160	SER
1	D	170	LYS
1	D	172	VAL
1	D	177	VAL
1	D	181	GLN
1	D	205	SER
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
1	D	355	MET
1	D	359	LEU
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	402	ILE
1	D	405	LEU
1	D	411	VAL
1	D	414	GLU
1	D	417	GLU

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Mol	Chain	Res	Type
1	D	425	LEU
1	D	438	ILE
1	D	442	LEU
1	D	447	MET
1	D	463	THR
1	D	466	ILE
1	D	472	ILE
1	D	475	VAL
1	D	483	ILE
1	D	484	VAL
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	543	LEU
1	D	546	VAL
1	D	555	MET
1	D	561	THR
1	D	566	ASP
1	D	569	GLN
1	D	575	GLN
1	D	577	GLN
1	D	589	VAL
1	D	591	VAL
1	D	599	LEU
1	D	608	SER
1	D	626	MET
1	D	641	GLU
1	D	646	GLU
1	D	647	LEU
1	D	649	LYS
1	D	650	ARG
1	D	653	MET
1	D	670	SER
1	D	671	VAL
1	D	678	THR
1	D	682	LEU
1	D	686	ASP
1	D	687	GLN
1	D	690	VAL

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Mol	Chain	Res	Type
1	D	696	LEU
1	D	697	GLN
1	D	699	ARG
1	D	705	LEU
1	D	714	ARG
1	D	725	GLN
1	D	758	VAL
1	D	760	ASP
1	D	770	VAL
1	D	780	MET
1	D	787	LYS
1	D	790	VAL
1	D	805	THR
1	D	809	GLU
1	D	816	GLU
1	D	821	VAL
1	D	826	ILE
1	D	827	LEU
1	D	834	LEU
1	D	845	GLU
1	D	846	ILE
1	D	861	LEU
1	D	864	GLU
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	927	GLN
1	D	928	VAL
1	D	932	THR
1	D	934	ILE
1	D	944	ILE
1	D	958	ILE
1	D	964	GLU
1	D	970	LEU

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Mol	Chain	Res	Type
1	D	981	ILE
1	D	985	VAL
1	D	987	LEU
1	D	989	ILE
1	D	1009	MET
1	D	1013	THR
1	D	1027	VAL
1	E	2	SER
1	E	4	PHE
1	E	17	LEU
1	E	18	VAL
1	E	19	ILE
1	E	20	MET
1	E	21	LEU
1	E	27	ILE
1	E	38	ILE
1	E	47	VAL
1	E	56	THR
1	E	58	GLN
1	E	60	THR
1	E	61	VAL
1	E	63	GLN
1	E	64	VAL
1	E	67	GLN
1	E	68	GLN
1	E	78	ILE
1	E	89	THR
1	E	90	ILE
1	E	96	GLN
1	E	108	GLN
1	E	111	LEU
1	E	113	LEU
1	E	120	GLN
1	E	121	GLU
1	E	124	ARG
1	E	127	ILE
1	E	139	VAL
1	E	140	VAL
1	E	150	THR
1	E	152	GLU
1	E	160	SER
1	E	188	LEU

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Mol	Chain	Res	Type
1	E	192	LYS
1	E	194	ASN
1	E	197	GLN
1	E	203	VAL
1	E	205	SER
1	E	207	ILE
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
1	E	239	ARG
1	E	244	GLU
1	E	248	ASN
1	E	250	LEU
1	E	253	VAL
1	E	263	LYS
1	E	268	VAL
1	E	273	GLN
1	E	284	SER
1	E	289	ILE
1	E	298	ASN
1	E	302	THR
1	E	306	ILE
1	E	310	ILE
1	E	329	THR
1	E	332	VAL
1	E	334	SER
1	E	336	SER
1	E	341	VAL
1	E	348	ILE
1	E	354	VAL
1	E	359	LEU
1	E	365	THR
1	E	370	ILE
1	E	383	LEU
1	E	402	ILE
1	E	405	LEU
1	E	406	VAL

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Mol	Chain	Res	Type
1	E	414	GLU
1	E	415	ASN
1	E	420	MET
1	E	426	SER
1	E	434	SER
1	E	442	LEU
1	E	445	ILE
1	E	456	MET
1	E	463	THR
1	E	473	THR
1	E	475	VAL
1	E	484	VAL
1	E	486	LEU
1	E	497	LEU
1	E	498	LYS
1	E	500	ILE
1	E	508	HIS
1	E	521	LEU
1	E	544	ILE
1	E	553	ILE
1	E	556	PHE
1	E	557	THR
1	E	564	LEU
1	E	572	LEU
1	E	575	GLN
1	E	598	LEU
1	E	599	LEU
1	E	601	LYS
1	E	610	PHE
1	E	611	THR
1	E	613	THR
1	E	629	ILE
1	E	630	MET
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	671	VAL

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Mol	Chain	Res	Type
1	E	678	THR
1	E	682	LEU
1	E	684	LEU
1	E	696	LEU
1	E	704	MET
1	E	705	LEU
1	E	712	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	784	ASP
1	E	790	VAL
1	E	791	ARG
1	E	797	MET
1	E	805	THR
1	E	810	TYR
1	E	838	ASP
1	E	844	GLU
1	E	847	VAL
1	E	852	LYS
1	E	854	VAL
1	E	862	SER
1	E	866	ARG
1	E	867	LEU
1	E	883	VAL
1	E	893	SER
1	E	908	VAL
1	E	915	THR
1	E	916	SER
1	E	924	VAL
1	E	932	THR
1	E	933	THR
1	E	934	ILE
1	E	936	LEU

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Mol	Chain	Res	Type
1	E	954	GLN
1	E	958	ILE
1	E	959	VAL
1	E	964	GLU
1	E	967	ARG
1	E	968	MET
1	E	969	ARG
1	E	978	LEU
1	E	984	VAL
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	1010	VAL
1	E	1015	LEU
1	E	1022	LEU
1	E	1030	LEU
1	F	10	ILE
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	55	GLU
1	F	57	VAL
1	F	60	THR
1	F	61	VAL
1	F	63	GLN
1	F	65	ILE
1	F	72	ILE
1	F	82	SER
1	F	96	GLN
1	F	117	LEU
1	F	118	LEU
1	F	124	ARG
1	F	128	ARG
1	F	131	LYS
1	F	134	LYS

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Mol	Chain	Res	Type
1	F	150	THR
1	F	152	GLU
1	F	194	ASN
1	F	199	THR
1	F	203	VAL
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	289	ILE
1	F	295	THR
1	F	300	LEU
1	F	306	ILE
1	F	319	GLN
1	F	323	VAL
1	F	329	THR
1	F	334	SER
1	F	337	ILE
1	F	343	THR
1	F	344	LEU
1	F	348	ILE
1	F	349	LEU
1	F	355	MET
1	F	357	LEU
1	F	360	GLN
1	F	366	LEU
1	F	369	THR
1	F	374	VAL
1	F	376	LEU
1	F	379	THR
1	F	393	LEU
1	F	404	LEU
1	F	405	LEU
1	F	410	ILE

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Mol	Chain	Res	Type
1	F	411	VAL
1	F	423	GLU
1	F	425	LEU
1	F	426	SER
1	F	434	SER
1	F	437	GLN
1	F	439	GLN
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	488	LEU
1	F	496	MET
1	F	498	LYS
1	F	500	ILE
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	547	VAL
1	F	559	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	612	VAL
1	F	634	TRP
1	F	641	GLU
1	F	644	VAL

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Mol	Chain	Res	Type
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
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	762	ILE
1	F	766	ARG
1	F	767	VAL
1	F	768	LYS
1	F	779	ARG
1	F	794	LYS
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

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Mol	Chain	Res	Type
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
1	F	939	LYS
1	F	942	ILE
1	F	943	LEU
1	F	944	ILE
1	F	945	VAL
1	F	958	ILE
1	F	970	LEU
1	F	974	VAL
1	F	1013	THR
1	F	1022	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (182) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	63	GLN
1	A	67	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	254	ASN
1	A	361	ASN
1	A	575	GLN
1	A	577	GLN
1	A	616	ASN
1	A	692	HIS
1	A	697	GLN

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Mol	Chain	Res	Type
1	A	708	GLN
1	A	718	ASN
1	A	725	GLN
1	A	781	ASN
1	A	819	ASN
1	A	849	GLN
1	A	927	GLN
1	A	952	HIS
1	A	954	GLN
1	A	998	GLN
1	B	46	GLN
1	B	67	GLN
1	B	83	ASN
1	B	108	GLN
1	B	112	GLN
1	B	120	GLN
1	B	123	GLN
1	B	156	ASN
1	B	163	GLN
1	B	197	GLN
1	B	210	GLN
1	B	228	GLN
1	B	229	GLN
1	B	245	GLN
1	B	248	ASN
1	B	278	ASN
1	B	298	ASN
1	B	308	GLN
1	B	415	ASN
1	B	469	GLN
1	B	508	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	C	34	GLN
1	C	67	GLN

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Mol	Chain	Res	Type
1	C	68	GLN
1	C	70	ASN
1	C	96	GLN
1	C	112	GLN
1	C	120	GLN
1	C	123	GLN
1	C	125	GLN
1	C	156	ASN
1	C	161	ASN
1	C	176	GLN
1	C	228	GLN
1	C	229	GLN
1	C	241	GLN
1	C	280	GLN
1	C	360	GLN
1	C	415	ASN
1	C	437	GLN
1	C	517	ASN
1	C	569	GLN
1	C	575	GLN
1	C	588	GLN
1	C	616	ASN
1	C	622	GLN
1	C	642	ASN
1	C	687	GLN
1	C	713	GLN
1	C	725	GLN
1	C	849	GLN
1	C	871	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

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Mol	Chain	Res	Type
1	D	213	GLN
1	D	228	GLN
1	D	231	ASN
1	D	254	ASN
1	D	298	ASN
1	D	361	ASN
1	D	415	ASN
1	D	575	GLN
1	D	622	GLN
1	D	676	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
1	E	156	ASN
1	E	161	ASN
1	E	197	GLN
1	E	229	GLN
1	E	245	GLN
1	E	248	ASN
1	E	259	GLN
1	E	273	GLN
1	E	298	ASN
1	E	308	GLN
1	E	312	ASN
1	E	319	GLN
1	E	360	GLN
1	E	469	GLN
1	E	505	HIS
1	E	537	HIS
1	E	622	GLN
1	E	652	GLN
1	E	676	ASN
1	E	687	GLN
1	E	746	ASN

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Mol	Chain	Res	Type
1	E	849	GLN
1	E	871	GLN
1	F	33	ASN
1	F	34	GLN
1	F	46	GLN
1	F	83	ASN
1	F	104	GLN
1	F	109	ASN
1	F	112	GLN
1	F	120	GLN
1	F	125	GLN
1	F	156	ASN
1	F	176	GLN
1	F	194	ASN
1	F	208	GLN
1	F	210	GLN
1	F	218	GLN
1	F	231	ASN
1	F	280	GLN
1	F	360	GLN
1	F	361	ASN
1	F	415	ASN
1	F	437	GLN
1	F	439	GLN
1	F	469	GLN
1	F	575	GLN
1	F	577	GLN
1	F	622	GLN
1	F	685	GLN
1	F	700	ASN
1	F	708	GLN
1	F	713	GLN
1	F	746	ASN
1	F	781	ASN
1	F	849	GLN
1	F	871	GLN
1	F	927	GLN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	2002	-	36,36,36	0.77	1 (2%)	47,47,47	1.77	11 (23%)
2	LMT	D	2002	-	36,36,36	0.66	1 (2%)	47,47,47	1.35	4 (8%)
3	P9D	B	2001	-	53,53,53	2.38	16 (30%)	62,77,77	2.61	22 (35%)
2	LMT	F	2002	-	36,36,36	0.85	1 (2%)	47,47,47	1.36	5 (10%)
2	LMT	A	2001	-	36,36,36	0.76	1 (2%)	47,47,47	1.25	5 (10%)
2	LMT	D	2001	-	36,36,36	0.94	2 (5%)	47,47,47	1.47	7 (14%)
2	LMT	A	2003	-	36,36,36	0.69	1 (2%)	47,47,47	1.64	11 (23%)
2	LMT	E	2002	-	36,36,36	0.97	1 (2%)	47,47,47	1.47	9 (19%)
2	LMT	C	2001	-	36,36,36	0.71	1 (2%)	47,47,47	1.32	5 (10%)
2	LMT	E	2004	-	36,36,36	0.69	1 (2%)	47,47,47	1.11	3 (6%)
2	LMT	D	2003	-	36,36,36	0.81	1 (2%)	47,47,47	1.38	6 (12%)
2	LMT	B	2004	-	36,36,36	0.48	0	47,47,47	1.02	3 (6%)
2	LMT	F	2001	-	36,36,36	0.82	1 (2%)	47,47,47	2.00	13 (27%)
3	P9D	E	2001	-	53,53,53	2.40	15 (28%)	62,77,77	2.36	11 (17%)
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	A	2002	-	36,36,36	0.85	1 (2%)	47,47,47	1.74	15 (31%)

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	B	2002	-	-	12/21/61/61	0/2/2/2
2	LMT	D	2002	-	-	9/21/61/61	0/2/2/2
3	P9D	B	2001	-	-	24/39/49/49	0/5/5/5
2	LMT	F	2002	-	-	12/21/61/61	0/2/2/2
2	LMT	A	2001	-	-	14/21/61/61	0/2/2/2
2	LMT	D	2001	-	-	16/21/61/61	0/2/2/2
2	LMT	A	2003	-	-	11/21/61/61	0/2/2/2
2	LMT	E	2002	-	-	10/21/61/61	0/2/2/2
2	LMT	C	2001	-	-	14/21/61/61	0/2/2/2
2	LMT	E	2004	-	-	10/21/61/61	0/2/2/2
2	LMT	D	2003	-	-	7/21/61/61	0/2/2/2
2	LMT	B	2004	-	-	9/21/61/61	0/2/2/2
2	LMT	F	2001	-	-	12/21/61/61	0/2/2/2
3	P9D	E	2001	-	-	21/39/49/49	1/5/5/5
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	A	2002	-	-	13/21/61/61	0/2/2/2

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	P9D	C7-S8	-8.30	1.62	1.74
3	E	2001	P9D	C7-S8	-7.12	1.64	1.74
3	E	2001	P9D	O34-C38	6.54	1.46	1.35
3	B	2001	P9D	N30-N29	6.05	1.41	1.30
3	E	2001	P9D	C9-C4	5.59	1.41	1.35
3	E	2001	P9D	N30-N29	5.53	1.40	1.30
3	B	2001	P9D	O34-C38	5.48	1.44	1.35
3	E	2001	P9D	N31-N30	5.25	1.41	1.35
3	B	2001	P9D	C9-C4	4.96	1.40	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	N31-N30	4.07	1.40	1.35
3	B	2001	P9D	C15-N16	4.03	1.44	1.38
3	B	2001	P9D	C22-C21	3.82	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2001	P9D	C17-N16	3.67	1.45	1.38
3	B	2001	P9D	C7-N6	3.48	1.36	1.31
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
3	B	2001	P9D	C9-S8	-2.91	1.64	1.71
3	B	2001	P9D	N28-N29	2.90	1.40	1.36
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
3	E	2001	P9D	N28-N29	2.77	1.40	1.36
3	E	2001	P9D	C7-N6	2.73	1.35	1.31
2	A	2003	LMT	O1'-C1'	2.72	1.44	1.40
3	E	2001	P9D	C9-S8	-2.71	1.65	1.71
2	C	2001	LMT	O1'-C1'	2.66	1.44	1.40
3	E	2001	P9D	C26-C27	2.60	1.48	1.45
2	E	2003	LMT	O1'-C1'	2.55	1.44	1.40
3	B	2001	P9D	C11-N10	-2.40	1.32	1.37
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
3	E	2001	P9D	C7-N10	-2.05	1.35	1.38
3	E	2001	P9D	C11-N10	-2.01	1.33	1.37

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	P9D	C9-S8-C7	10.64	96.67	88.40
3	E	2001	P9D	C9-S8-C7	9.26	95.60	88.40
3	B	2001	P9D	N31-C27-N28	6.77	117.45	108.92
3	E	2001	P9D	C4-C9-S8	-6.72	104.42	111.32
3	B	2001	P9D	C4-C9-S8	-6.26	104.90	111.32
3	E	2001	P9D	C9-C4-N6	6.01	119.14	114.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2001	P9D	C7-N6-C4	-5.87	106.28	110.01
2	B	2003	LMT	C1B-O5B-C5B	5.84	125.12	113.72
3	E	2001	P9D	N31-C27-N28	5.46	115.80	108.92
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
3	B	2001	P9D	C9-C4-N6	4.41	117.81	114.13
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	C7-N6-C4	-4.16	107.36	110.01
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
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
3	B	2001	P9D	C27-N28-N29	-3.41	102.52	105.36
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	123.78
2	B	2002	LMT	C1'-C2'-C3'	3.29	116.94	110.01
2	C	2001	LMT	C2'-C3'-C4'	3.27	117.11	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
3	B	2001	P9D	C27-N31-N30	-3.18	103.84	108.48
3	E	2001	P9D	C27-N31-N30	-3.17	103.86	108.48
2	E	2002	LMT	O1B-C1B-C2B	3.15	115.84	108.09
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
3	E	2001	P9D	C26-C27-N28	-3.04	122.13	125.94
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	C26-C27-N28	-2.79	122.44	125.94
3	B	2001	P9D	C12-C11-N10	2.76	121.35	116.07
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
3	B	2001	P9D	C26-C25-C22	-2.65	114.81	125.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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
3	E	2001	P9D	N28-N29-N30	-2.52	107.50	110.50
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	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	B	2001	P9D	S8-C7-N6	-2.32	113.25	115.69
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	P9D	N10-C7-N6	2.17	124.93	121.18
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
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 (216) 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	N6-C7-N10-C11
3	B	2001	P9D	S8-C7-N10-C11
3	B	2001	P9D	C12-C11-N10-C7
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	C25-C26-C27-N28
3	B	2001	P9D	C25-C26-C27-N31
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

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Mol	Chain	Res	Type	Atoms
3	B	2001	P9D	N42-C43-C45-O47
3	E	2001	P9D	O13-C11-C12-C14
3	E	2001	P9D	C25-C26-C27-N28
3	E	2001	P9D	C25-C26-C27-N31
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
2	D	2001	LMT	C7-C8-C9-C10
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
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

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Mol	Chain	Res	Type	Atoms
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
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
3	B	2001	P9D	O13-C11-N10-C7
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

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Mol	Chain	Res	Type	Atoms
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'
2	B	2002	LMT	C7-C8-C9-C10
3	B	2001	P9D	C1-C2-C4-N6
3	E	2001	P9D	C5-C2-C4-N6
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 53 short contacts:

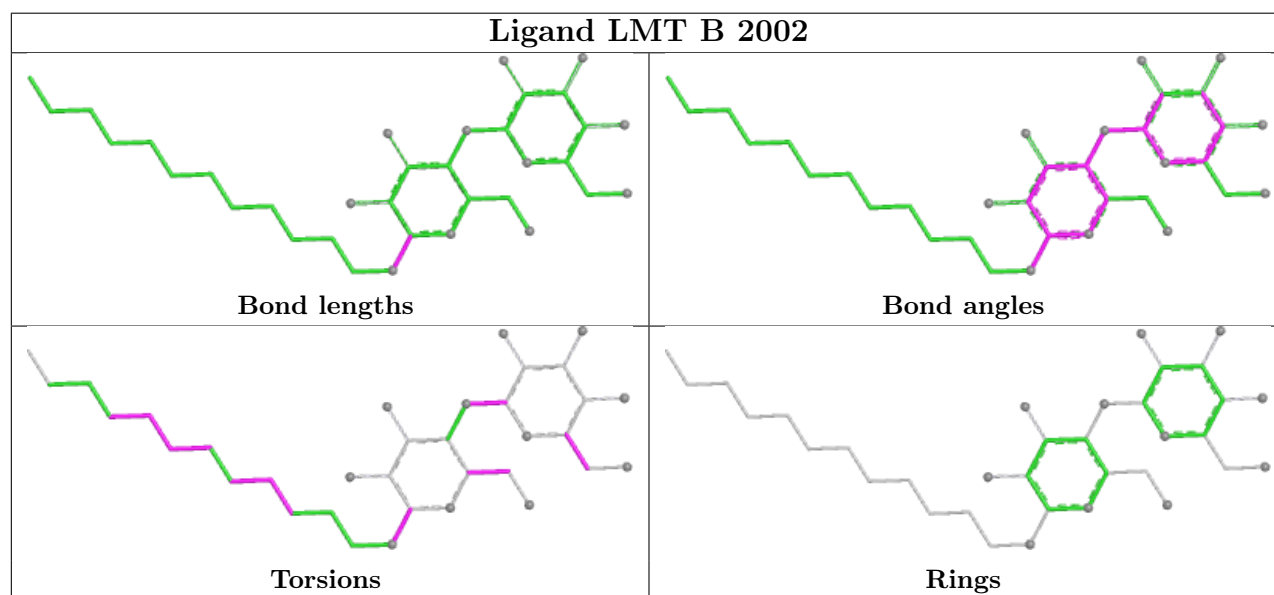
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2002	LMT	2	0
2	D	2002	LMT	1	0
3	B	2001	P9D	8	0
2	F	2002	LMT	3	0
2	A	2001	LMT	2	0
2	D	2001	LMT	2	0
2	A	2003	LMT	1	0
2	E	2002	LMT	8	0
2	C	2001	LMT	6	0

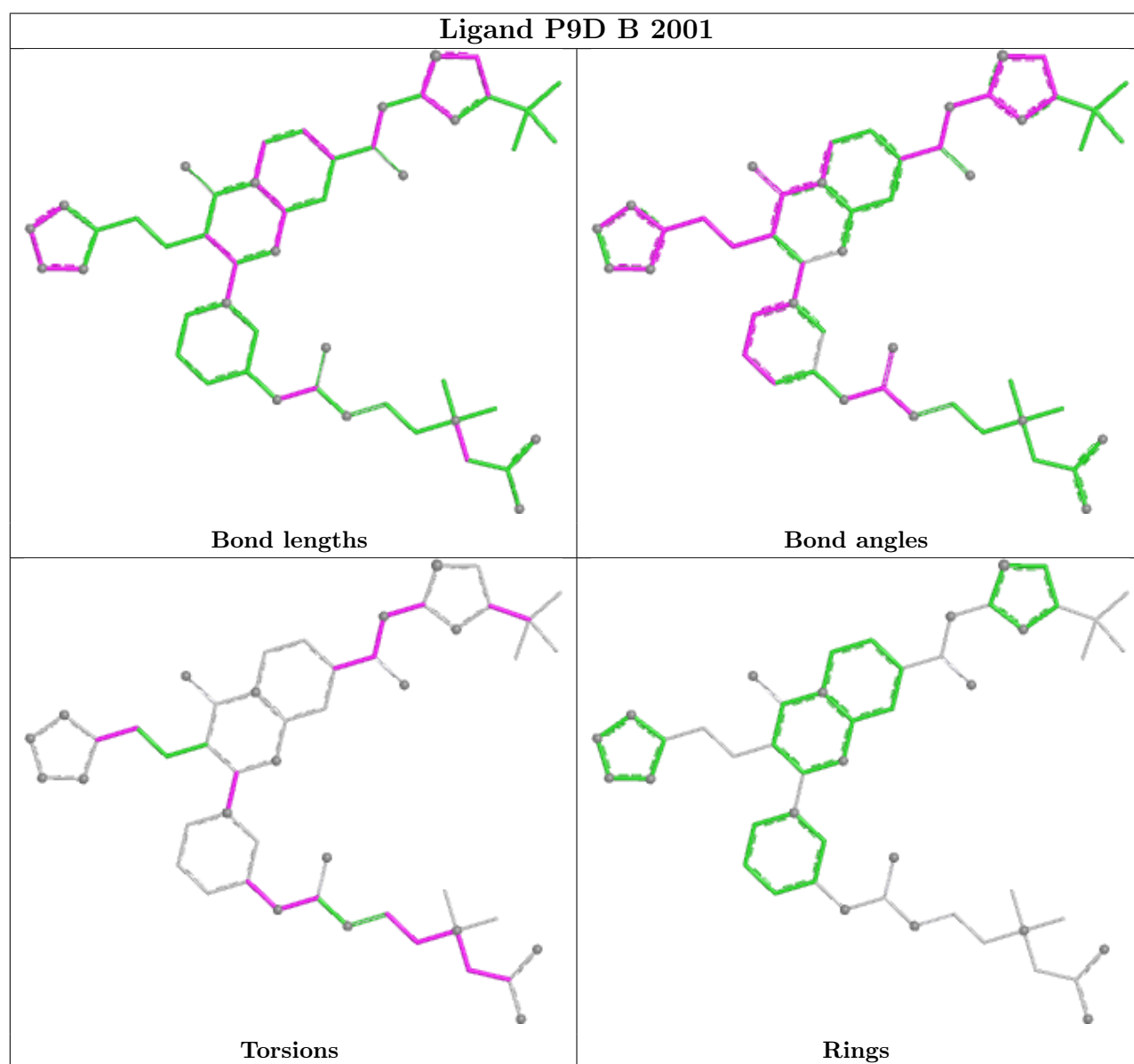
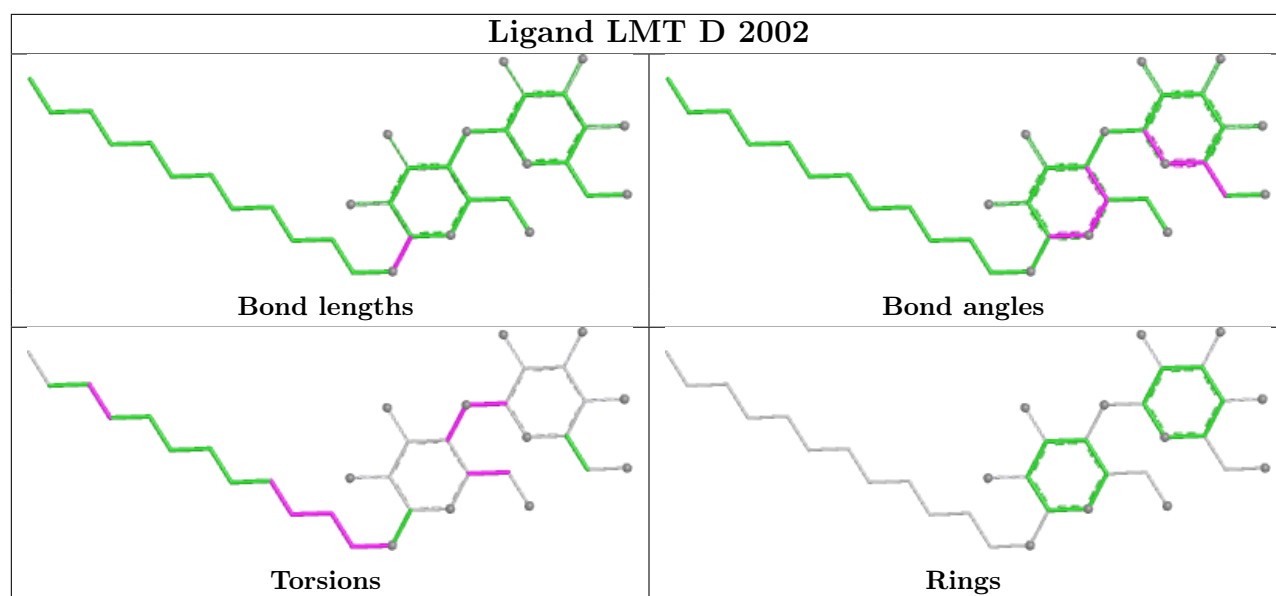
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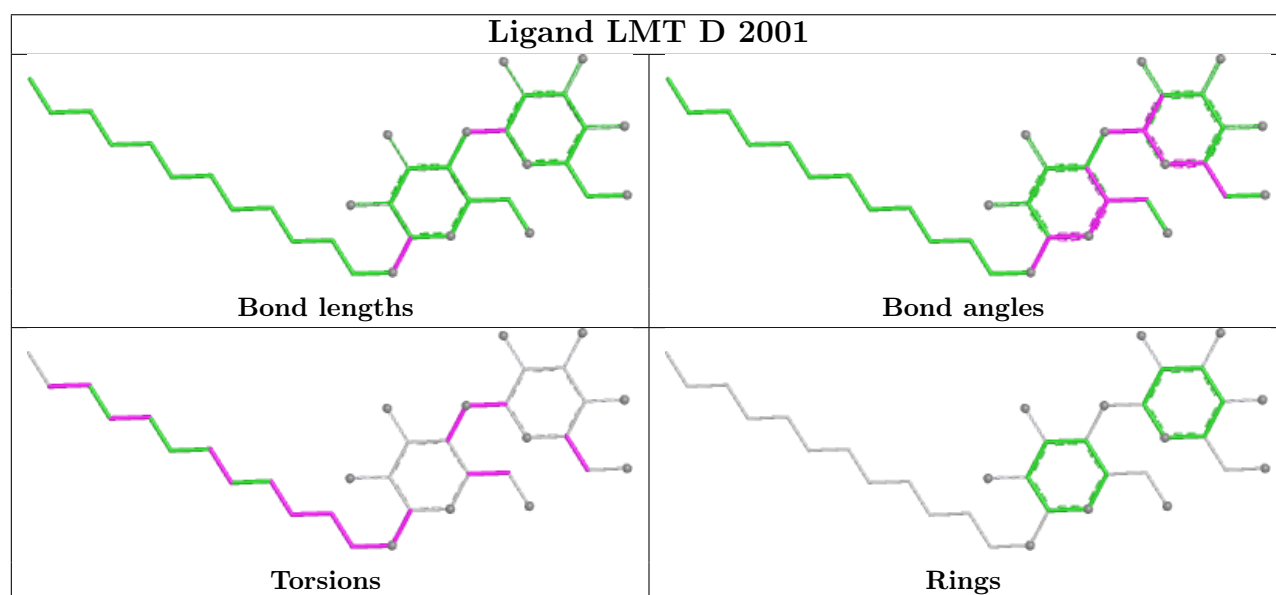
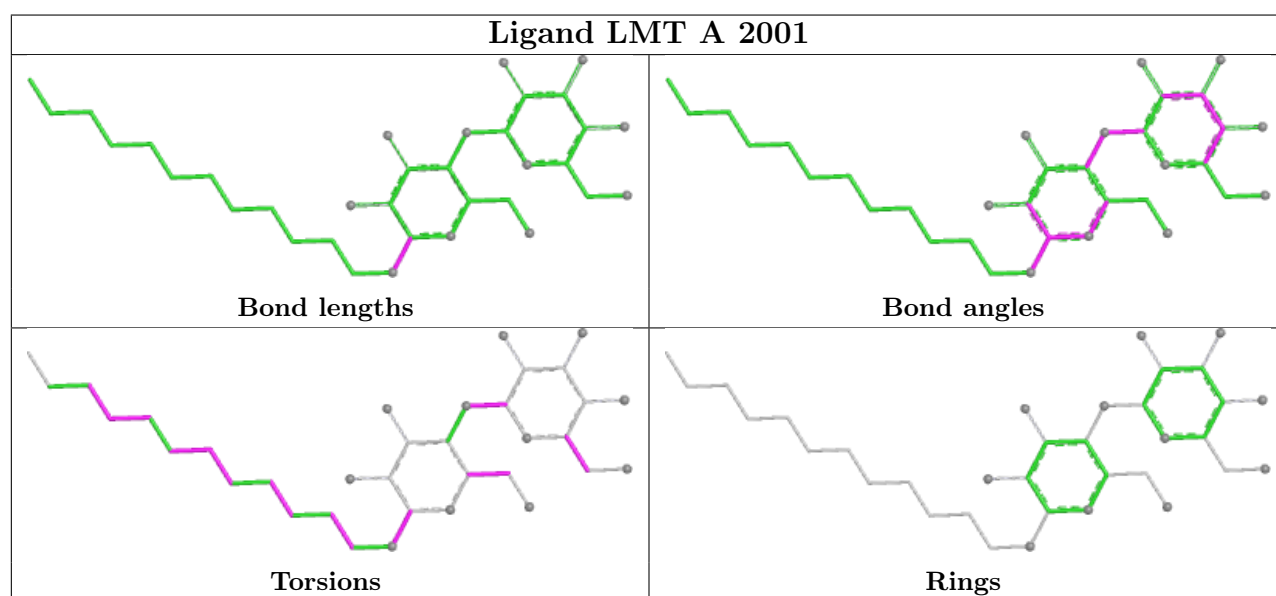
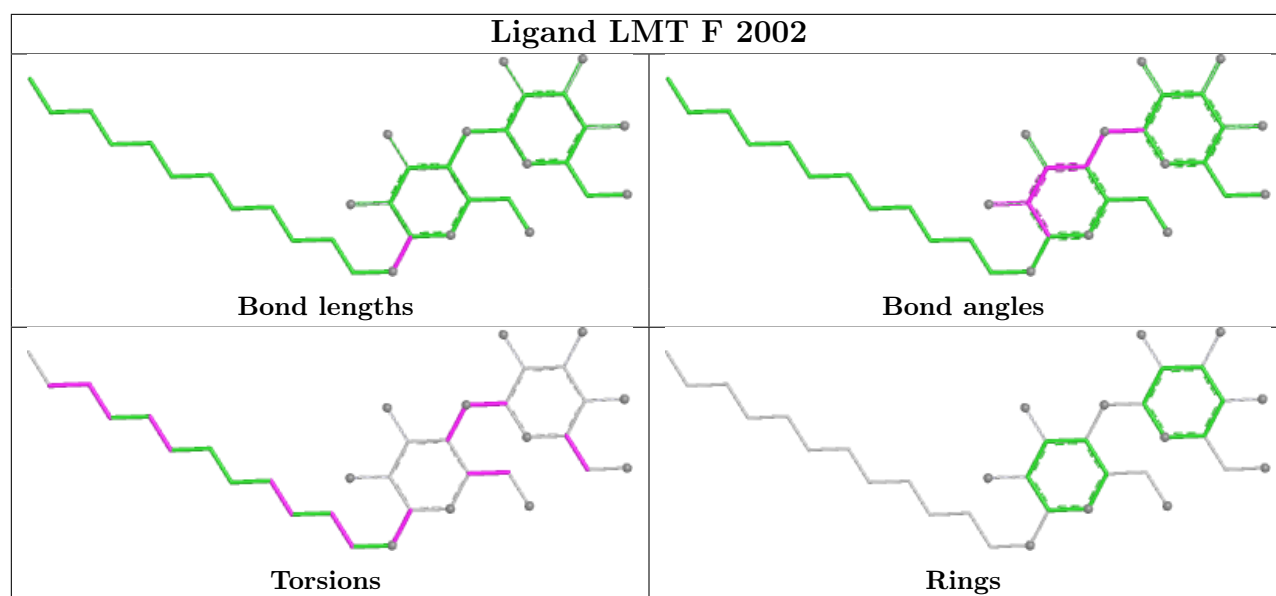
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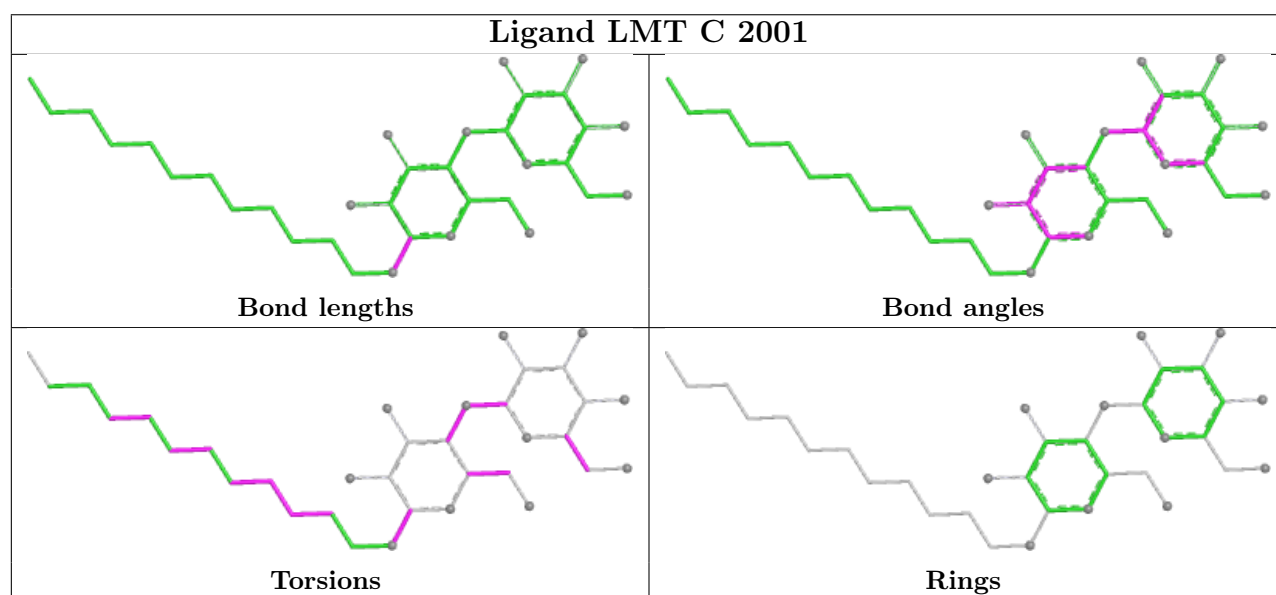
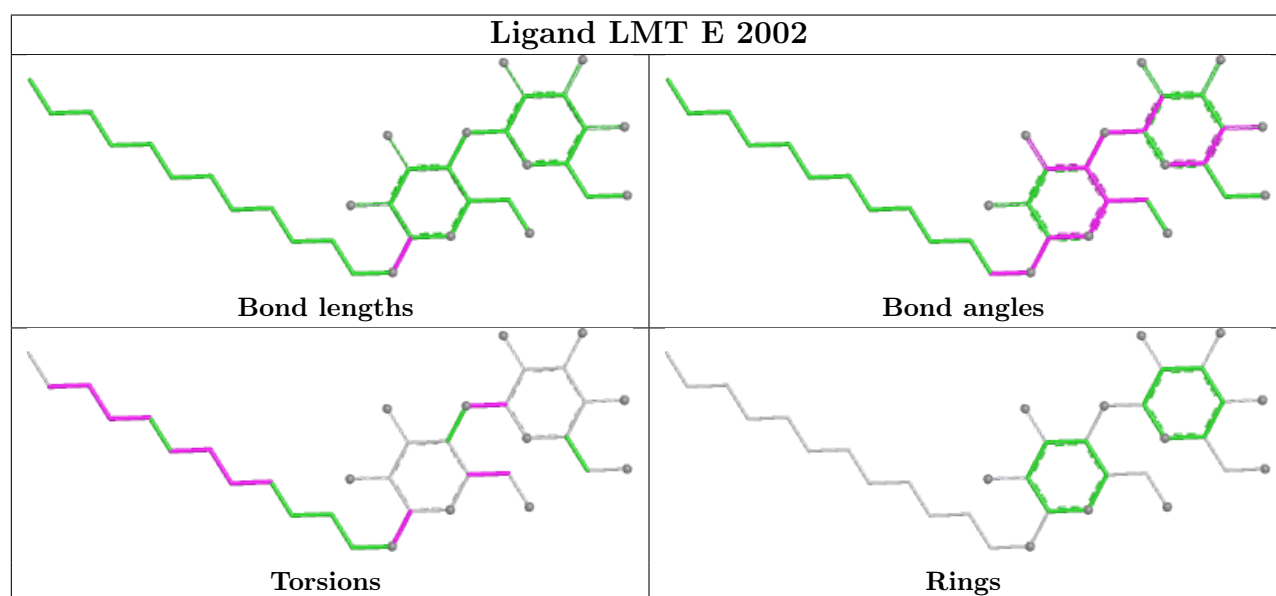
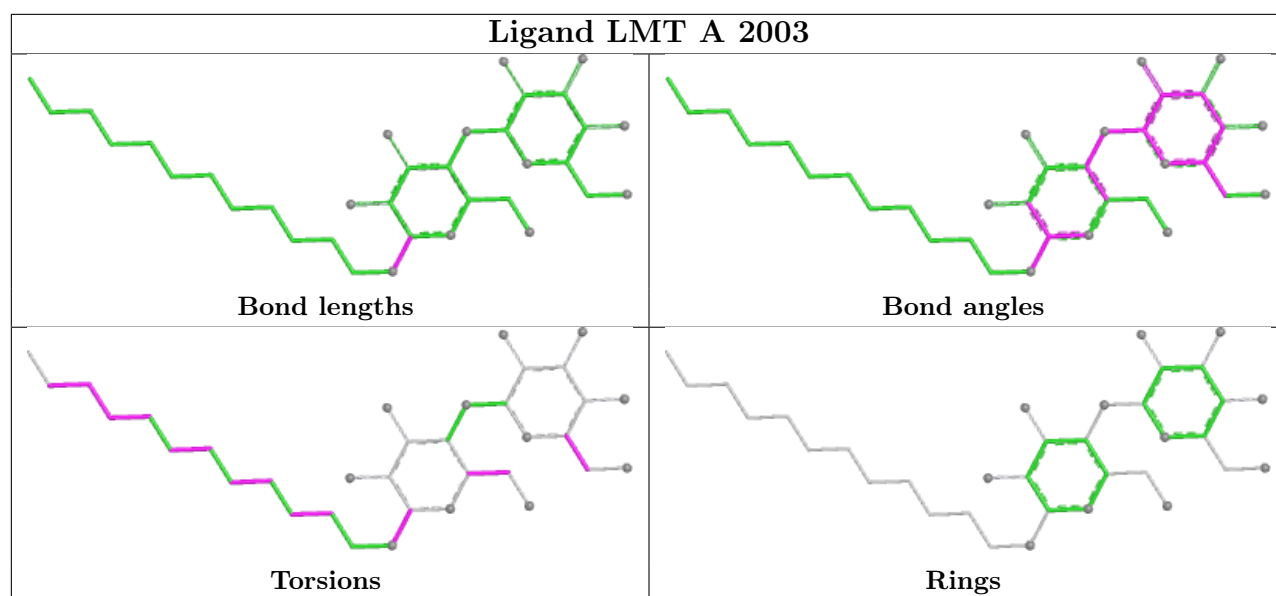
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2003	LMT	2	0
2	B	2004	LMT	1	0
2	F	2001	LMT	4	0
3	E	2001	P9D	8	0
2	B	2003	LMT	2	0
2	E	2003	LMT	1	0
2	A	2002	LMT	2	0

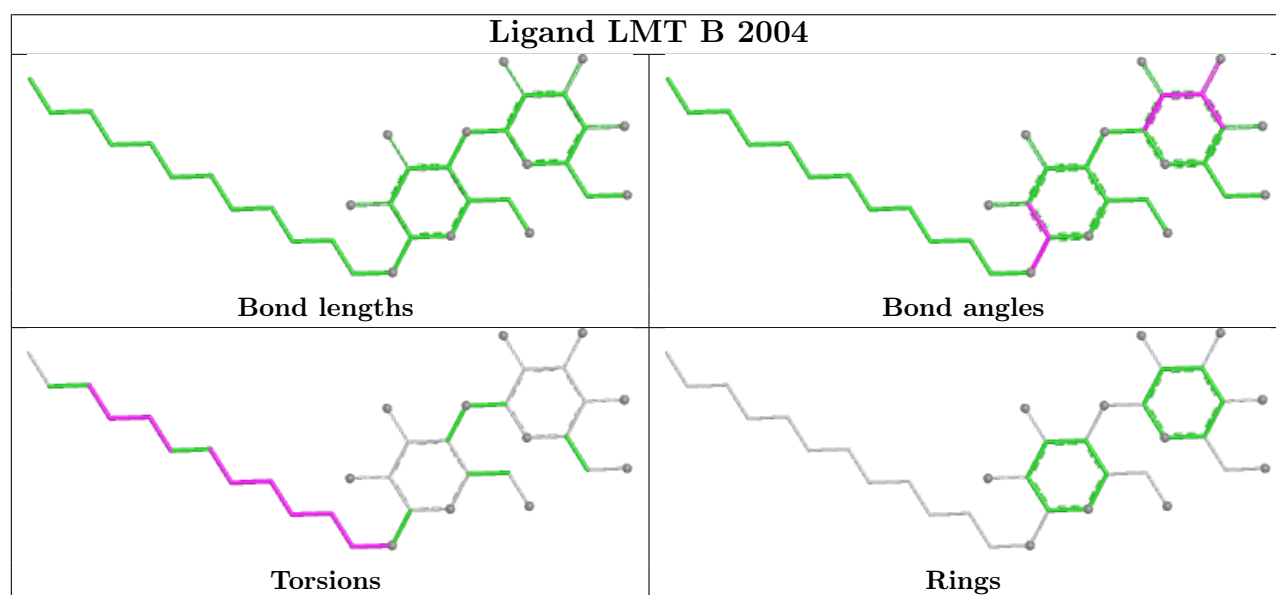
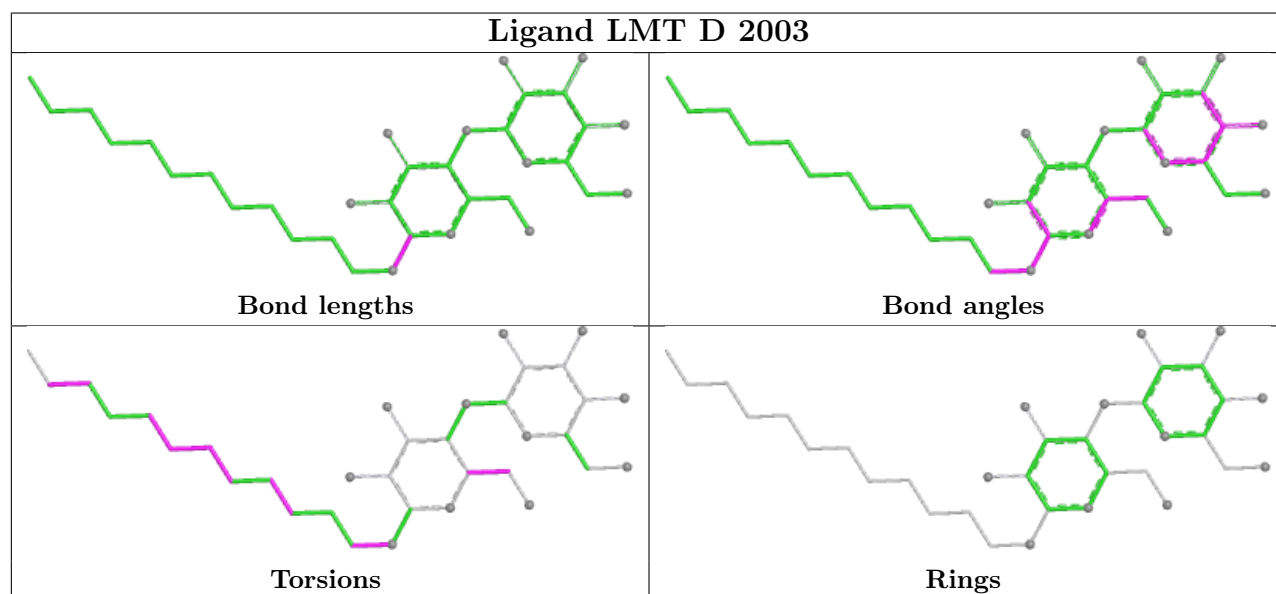
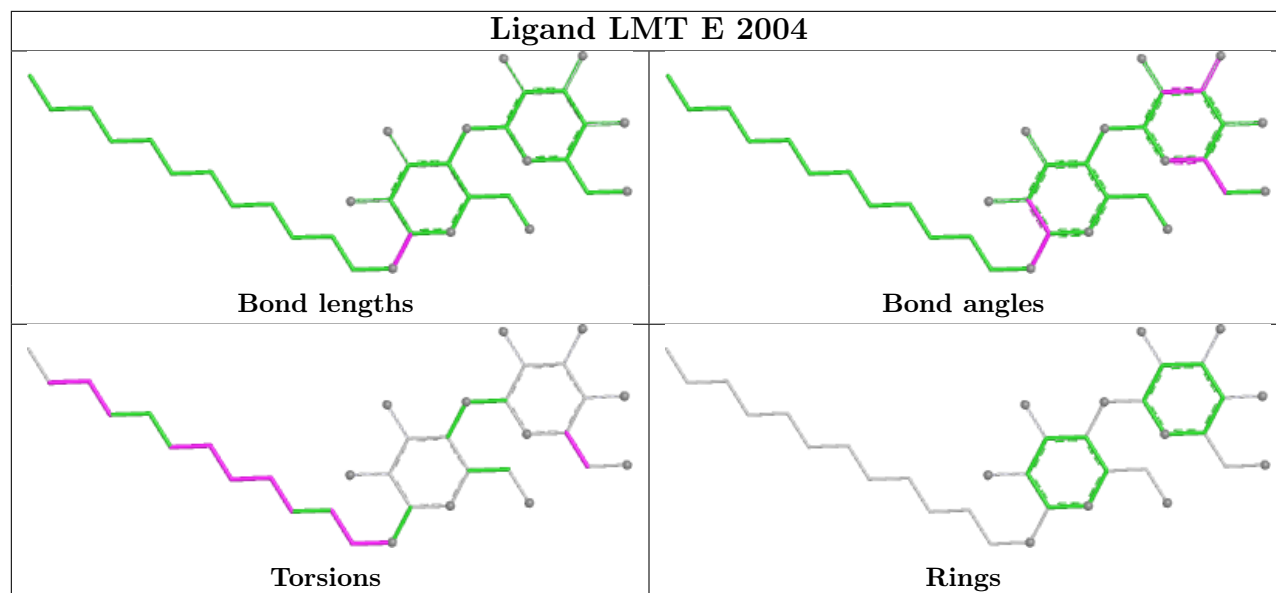
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

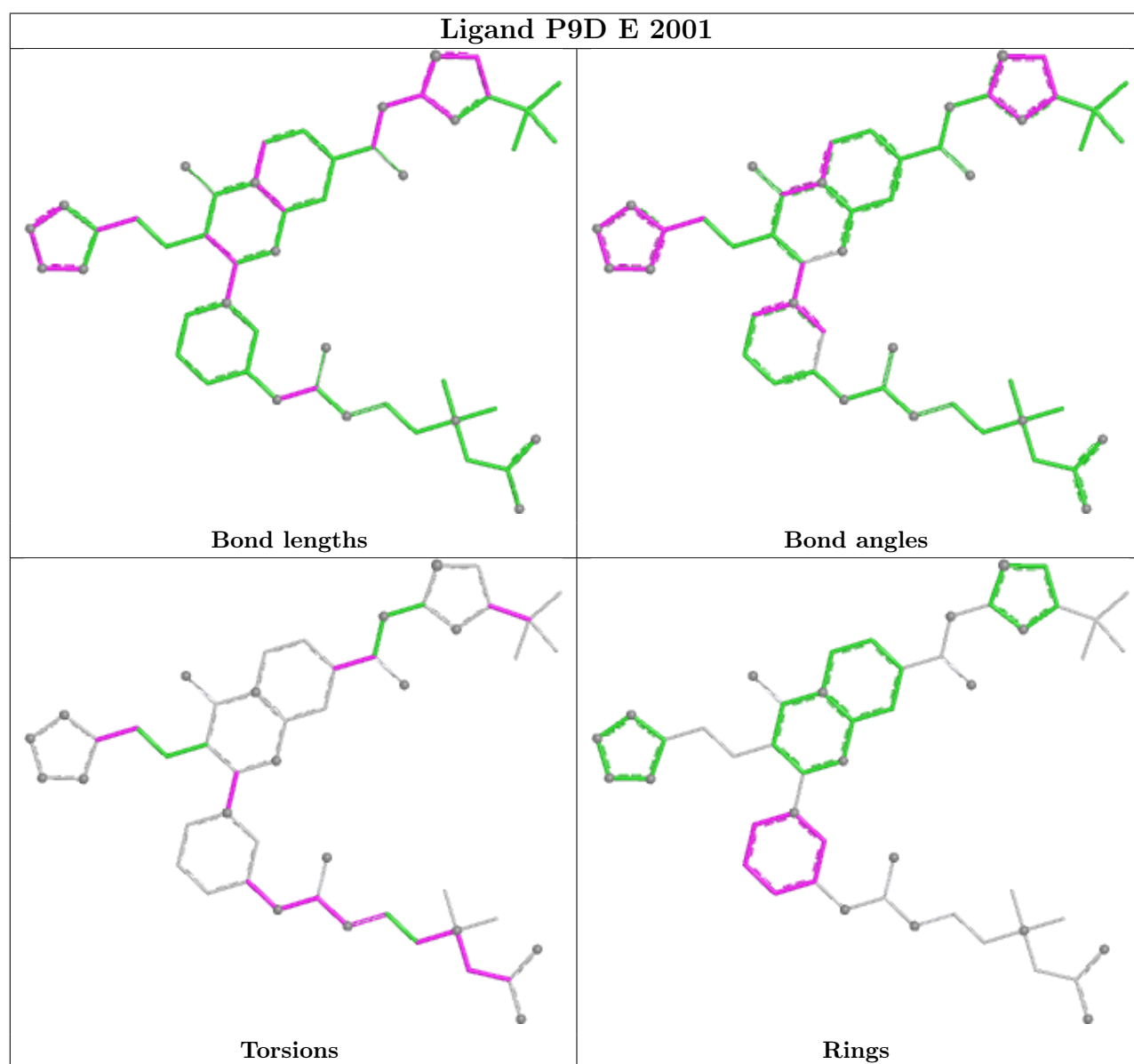
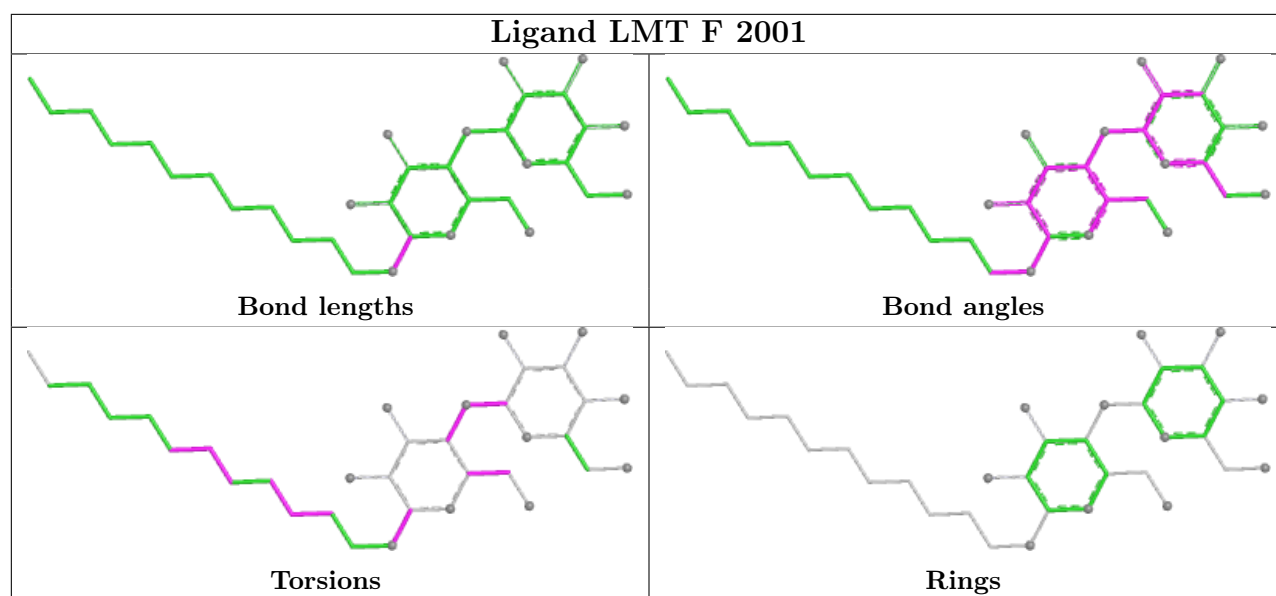


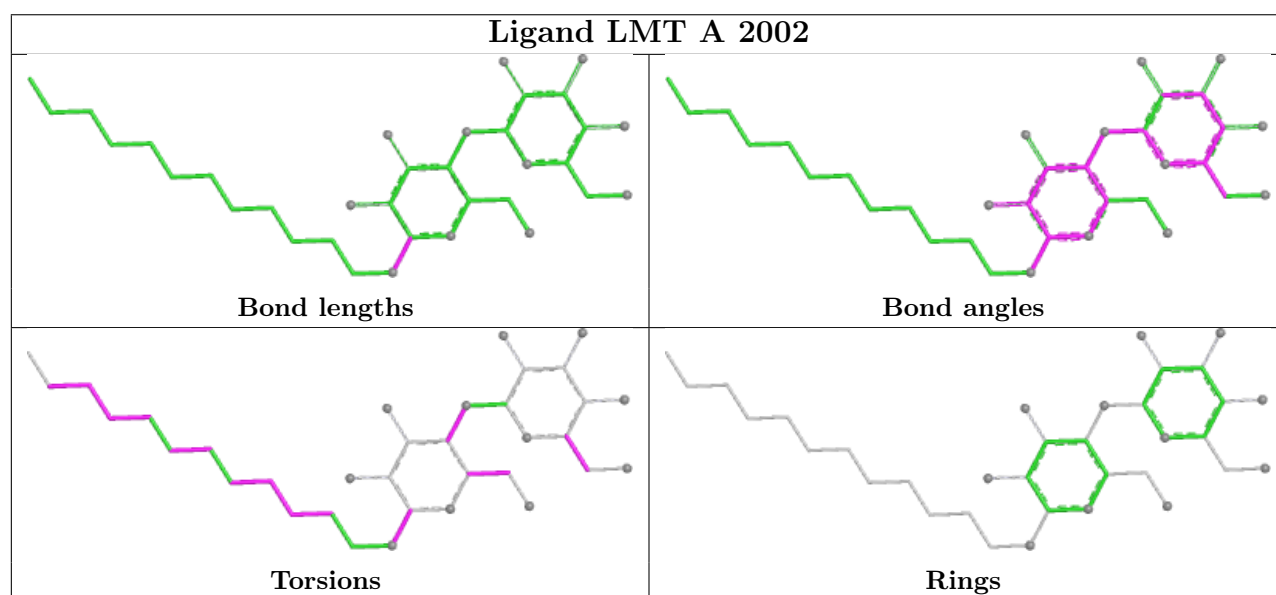
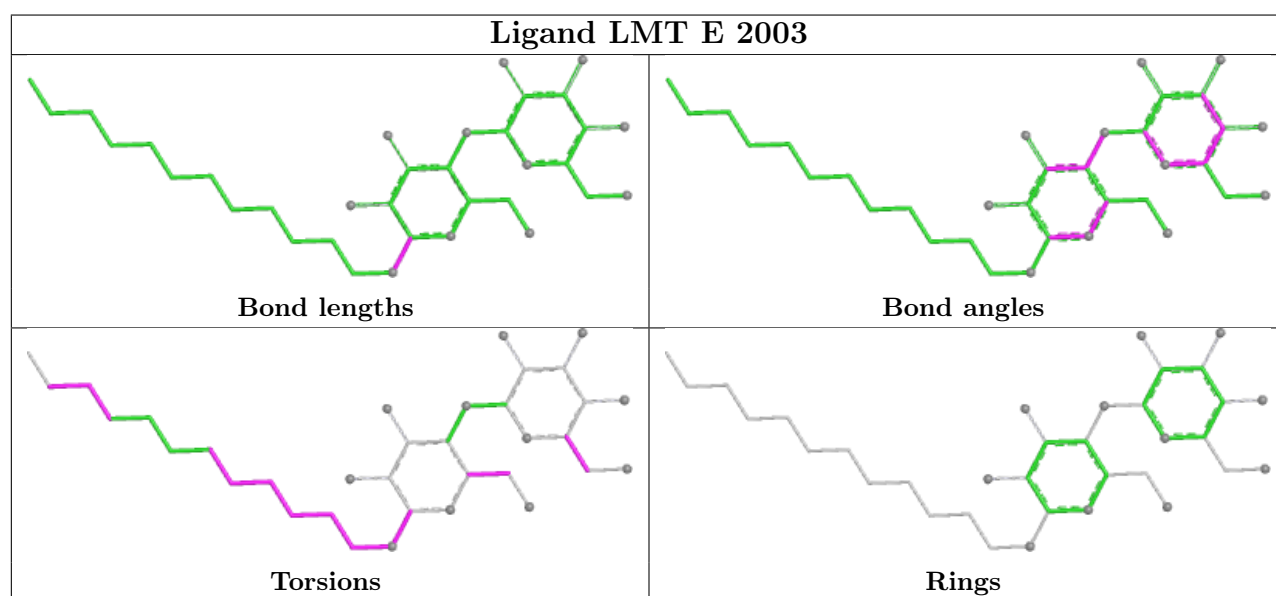
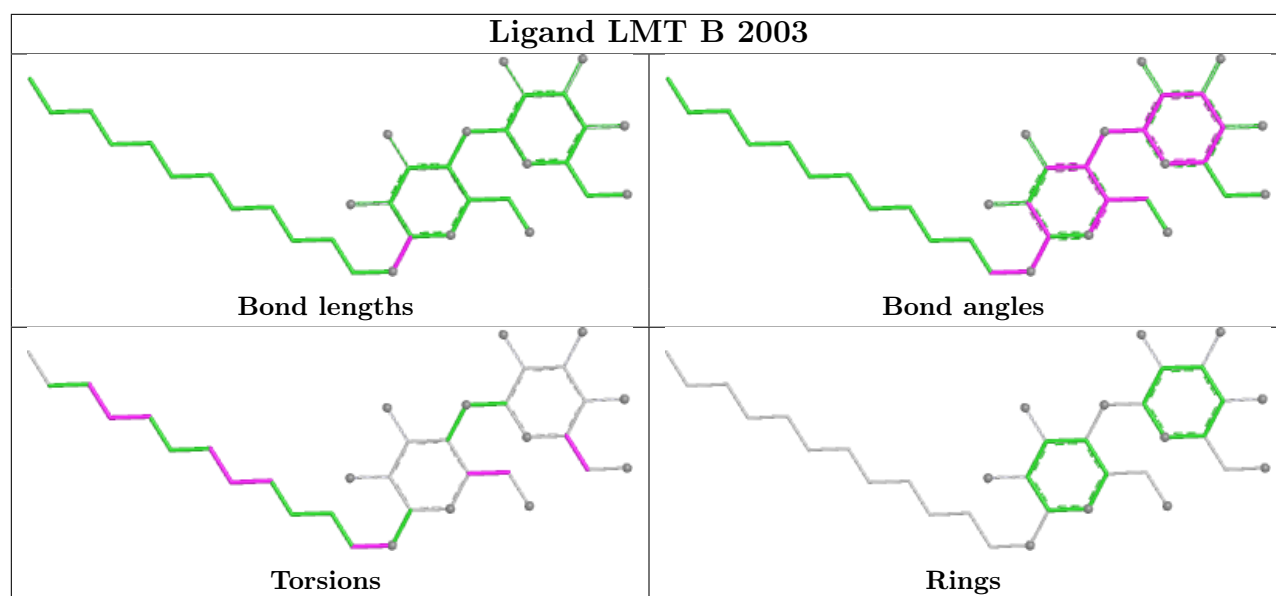












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	1018/1052 (96%)	-0.40	2 (0%)	91 84	39, 75, 112, 164	0
1	B	1030/1052 (97%)	-0.47	3 (0%)	90 81	40, 73, 113, 152	0
1	C	1030/1052 (97%)	-0.23	6 (0%)	85 72	43, 87, 143, 201	0
1	D	1019/1052 (96%)	-0.39	2 (0%)	91 84	47, 78, 117, 160	0
1	E	1030/1052 (97%)	-0.38	4 (0%)	88 78	46, 78, 124, 162	0
1	F	1033/1052 (98%)	-0.29	10 (0%)	79 62	45, 79, 129, 264	0
All	All	6160/6312 (97%)	-0.36	27 (0%)	88 78	39, 78, 124, 264	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1031	PHE	5.8
1	F	740	VAL	4.1
1	F	742	LEU	3.5
1	A	676	ASN	3.3
1	D	1030	LEU	3.1
1	F	515	TRP	3.1
1	B	917	MET	2.9
1	E	664	PHE	2.9
1	C	778	ALA	2.8
1	C	513	PHE	2.8
1	C	515	TRP	2.5
1	C	1029	THR	2.5
1	F	753	TRP	2.5
1	C	753	TRP	2.4
1	C	512	PHE	2.4
1	F	512	PHE	2.4
1	E	1030	LEU	2.3
1	F	253	VAL	2.3
1	B	238	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	805	THR	2.2
1	E	952	HIS	2.1
1	F	259	GLN	2.1
1	A	230	LEU	2.1
1	F	950	GLU	2.1
1	F	743	ALA	2.1
1	B	664	PHE	2.0
1	E	611	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LMT	C	2001	35/35	0.79	0.12	80,105,146,151	0
2	LMT	F	2001	35/35	0.80	0.13	82,104,126,139	0
2	LMT	D	2003	35/35	0.84	0.14	70,98,134,144	0
2	LMT	F	2002	35/35	0.85	0.12	76,118,147,148	0
2	LMT	A	2001	35/35	0.87	0.21	43,66,94,103	35
2	LMT	D	2001	35/35	0.89	0.21	47,65,79,89	35
2	LMT	A	2003	35/35	0.89	0.11	64,90,115,120	0
2	LMT	E	2002	35/35	0.90	0.15	67,106,124,132	0
2	LMT	E	2003	35/35	0.90	0.11	67,94,108,124	0
2	LMT	B	2002	35/35	0.92	0.14	63,106,135,137	0
2	LMT	E	2004	35/35	0.92	0.10	67,74,100,103	0
2	LMT	B	2003	35/35	0.92	0.10	71,82,104,111	0
2	LMT	A	2002	35/35	0.92	0.10	60,86,132,142	0
2	LMT	D	2002	35/35	0.93	0.10	69,111,137,144	0
2	LMT	B	2004	35/35	0.94	0.09	62,69,78,84	0

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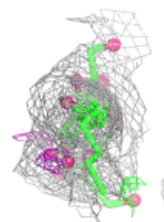
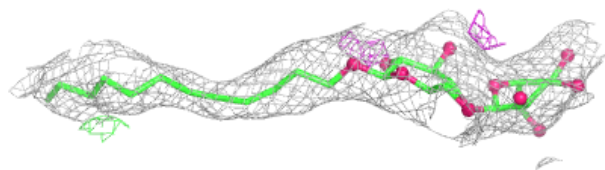
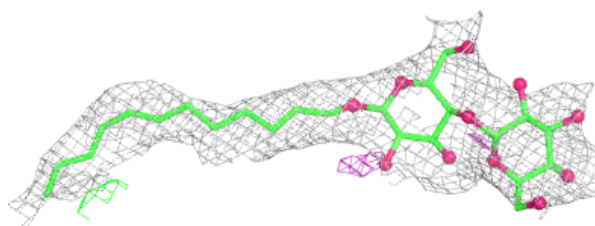
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	P9D	E	2001	49/49	0.94	0.10	60,78,108,123	0
3	P9D	B	2001	49/49	0.95	0.09	53,71,85,108	0

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.

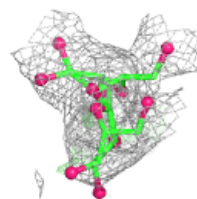
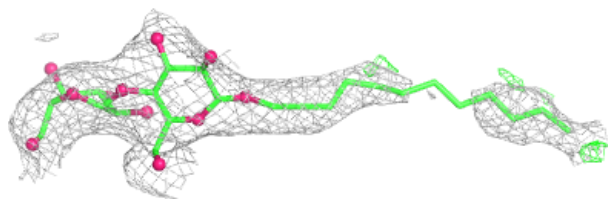
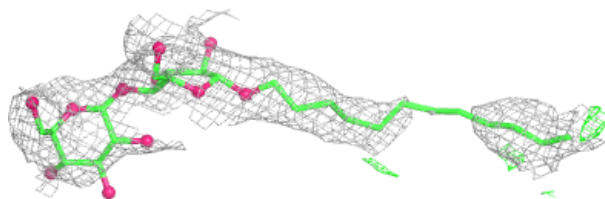
Electron density around LMT C 2001:

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

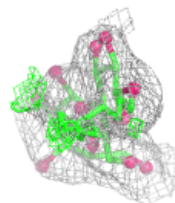
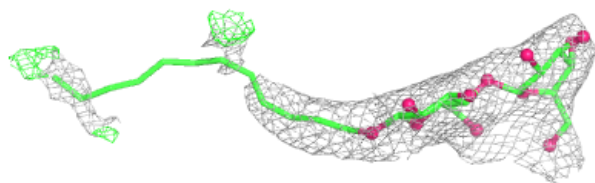
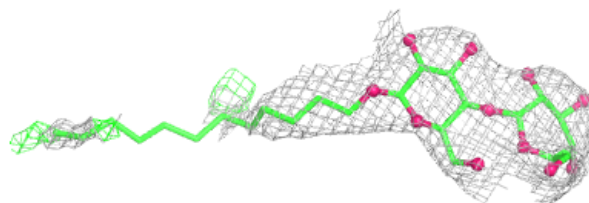


Electron density around LMT F 2001:

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

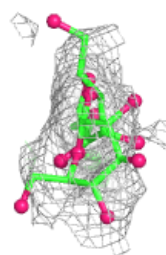
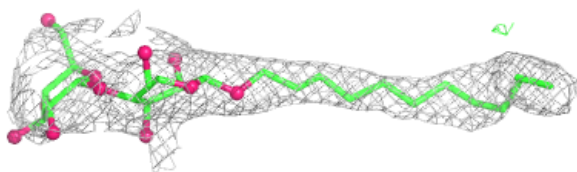
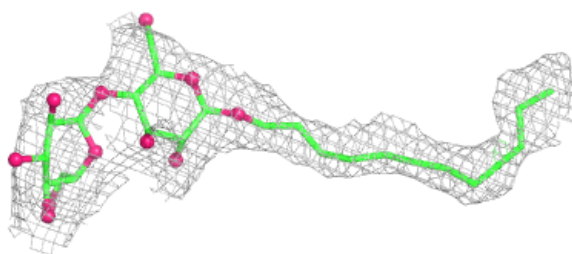
**Electron density around LMT D 2003:**

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

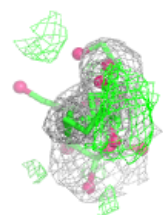
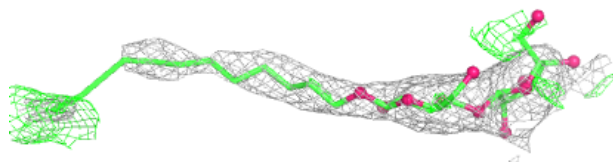
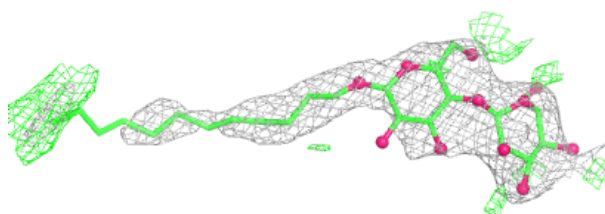


Electron density around LMT F 2002:

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

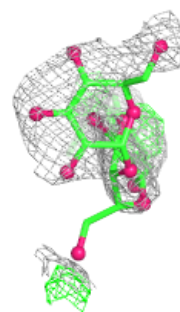
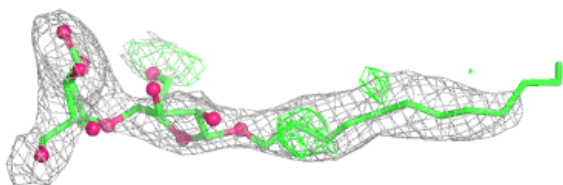
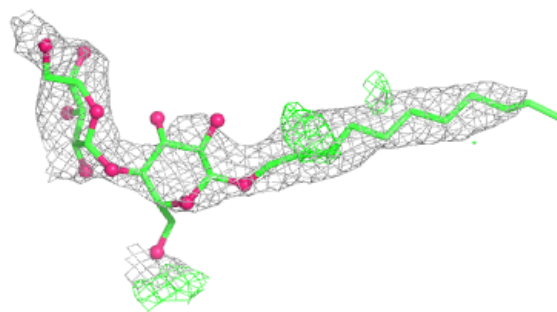
**Electron density around LMT A 2001:**

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

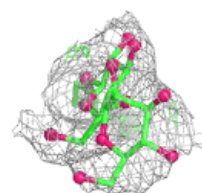
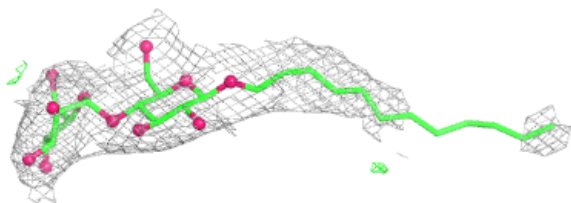
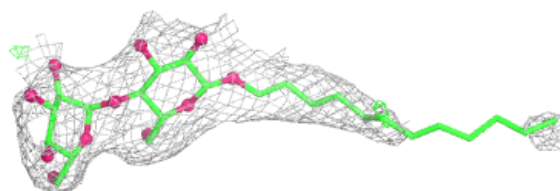


Electron density around LMT D 2001:

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

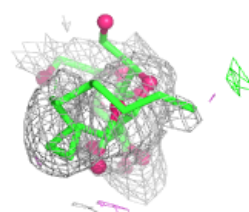
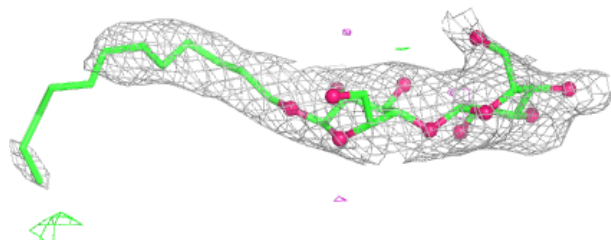
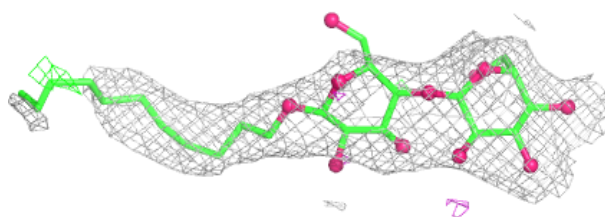
**Electron density around LMT A 2003:**

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

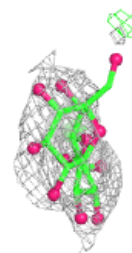
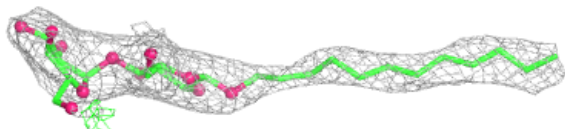
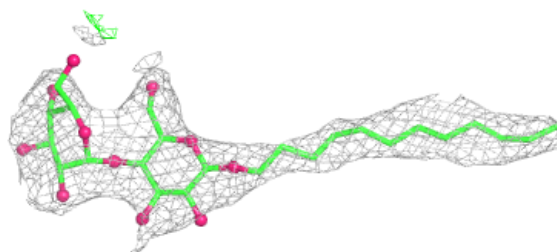


Electron density around LMT E 2002:

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

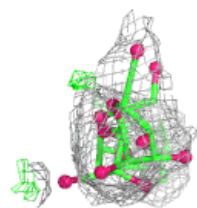
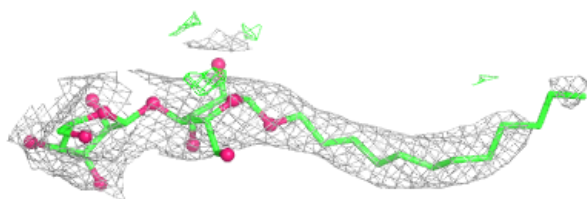
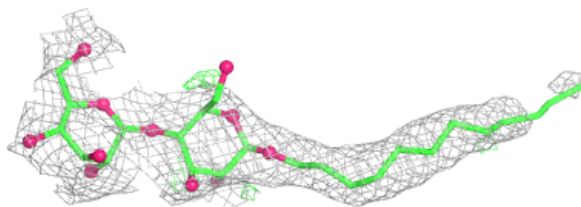
**Electron density around LMT E 2003:**

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

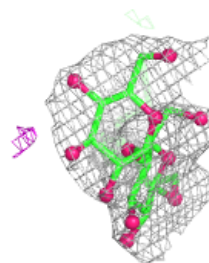
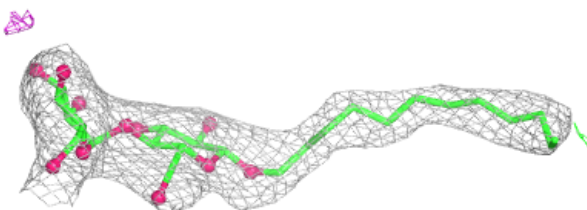
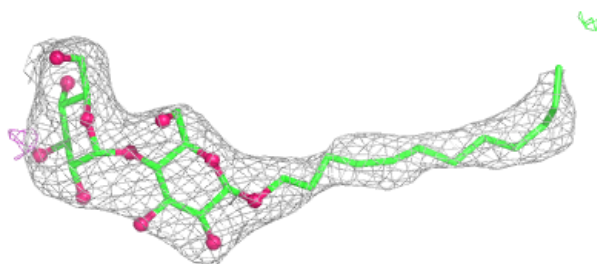


Electron density around LMT B 2002:

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

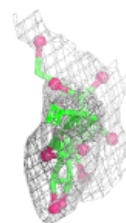
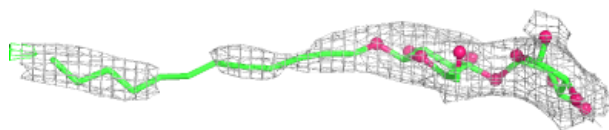
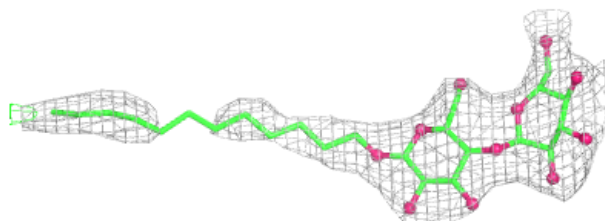
**Electron density around LMT E 2004:**

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

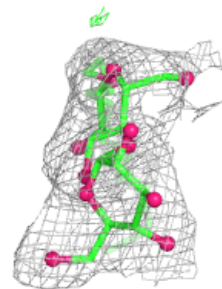
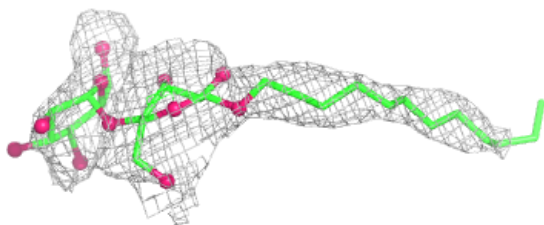
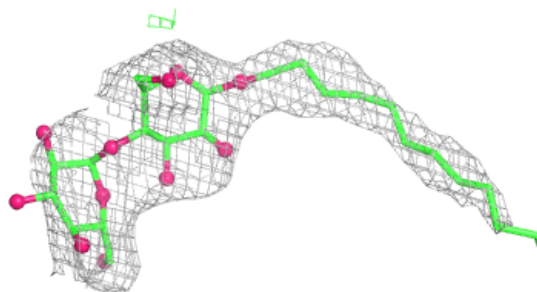


Electron density around LMT B 2003:

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

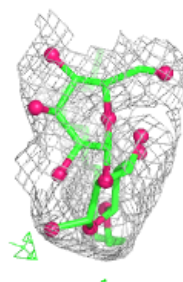
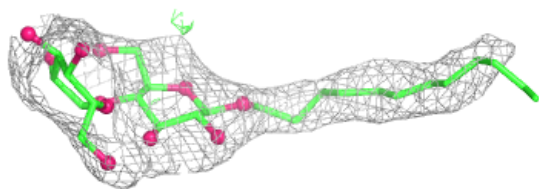
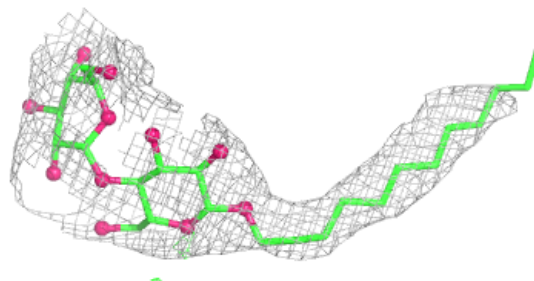
**Electron density around LMT A 2002:**

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

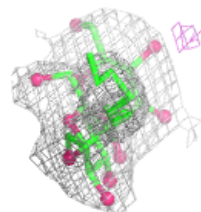
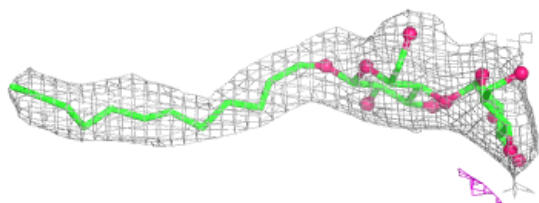
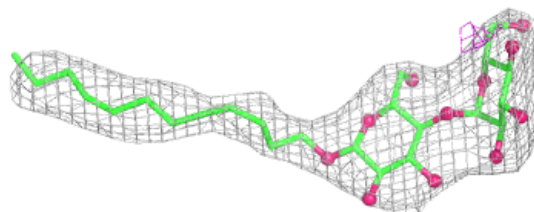


Electron density around LMT D 2002:

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

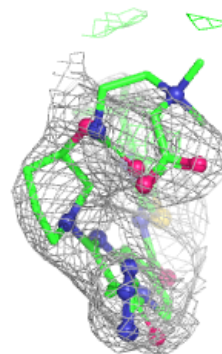
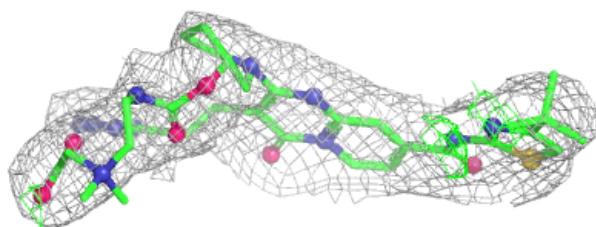
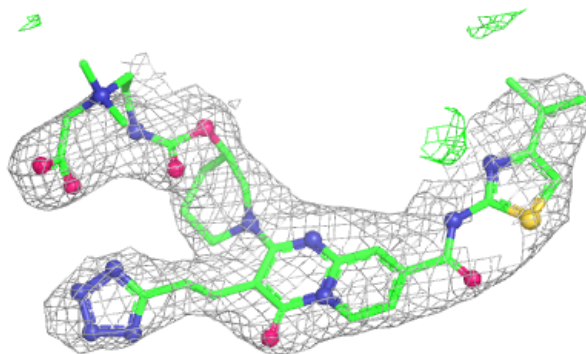
**Electron density around LMT B 2004:**

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

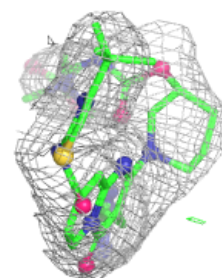
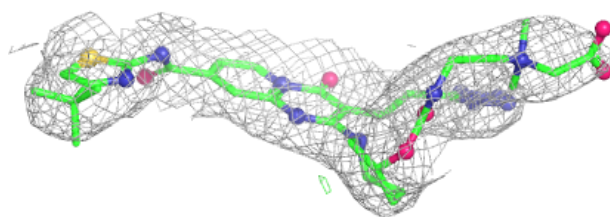
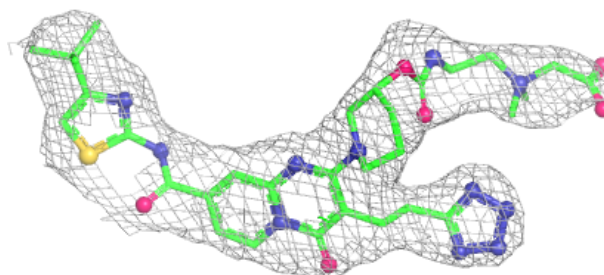


Electron density around P9D E 2001:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.