



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:32 AM UTC

PDB ID : 4ZJO / pdb_00004zjo
Title : Crystal structure of AcrB triple mutant in complex with antibiotic in P21 space group
Authors : Ababou, A.; Koronakis, V.
Deposited on : 2015-04-29
Resolution : 3.60 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

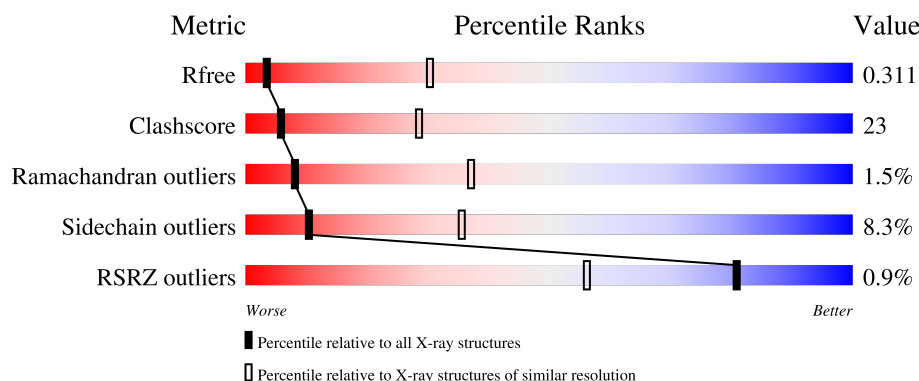
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	1049	51% 42% 7% .
1	B	1049	53% 41% 5% ..
1	C	1049	49% 42% 7% .
1	D	1049	53% 39% 7% .
1	E	1049	51% 43% 5% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	1049	% 52% 41% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LMT	B	1101	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 47876 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 efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	B	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	C	1044	Total	C	N	O	S	0	0	0
			7924	5090	1312	1479	43			
1	D	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7907	5080	1308	1476	43			
1	F	1046	Total	C	N	O	S	0	0	0
			7939	5099	1314	1483	43			

There are 18 discrepancies between the modelled and reference sequences:

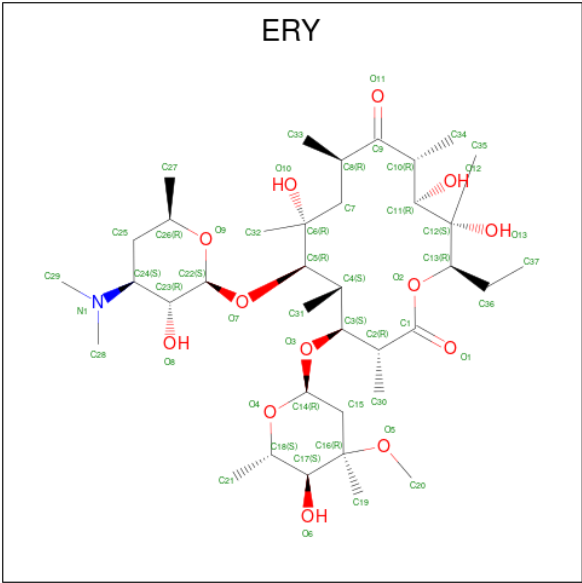
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	ALA	PHE	engineered mutation	UNP P31224
A	617	ALA	PHE	engineered mutation	UNP P31224
A	620	ALA	ARG	engineered mutation	UNP P31224
B	615	ALA	PHE	engineered mutation	UNP P31224
B	617	ALA	PHE	engineered mutation	UNP P31224
B	620	ALA	ARG	engineered mutation	UNP P31224
C	615	ALA	PHE	engineered mutation	UNP P31224
C	617	ALA	PHE	engineered mutation	UNP P31224
C	620	ALA	ARG	engineered mutation	UNP P31224
D	615	ALA	PHE	engineered mutation	UNP P31224
D	617	ALA	PHE	engineered mutation	UNP P31224
D	620	ALA	ARG	engineered mutation	UNP P31224
E	615	ALA	PHE	engineered mutation	UNP P31224
E	617	ALA	PHE	engineered mutation	UNP P31224
E	620	ALA	ARG	engineered mutation	UNP P31224
F	615	ALA	PHE	engineered mutation	UNP P31224
F	617	ALA	PHE	engineered mutation	UNP P31224

Continued on next page...

Continued from previous page...

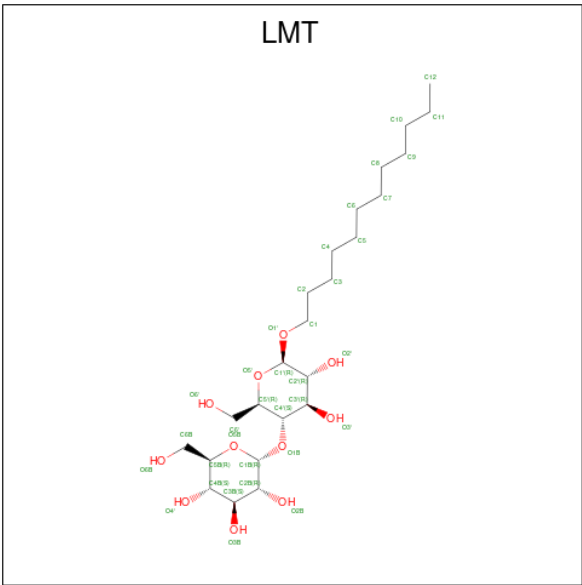
Chain	Residue	Modelled	Actual	Comment	Reference
F	620	ALA	ARG	engineered mutation	UNP P31224

- Molecule 2 is ERYTHROMYCIN A (CCD ID: ERY) (formula: C₃₇H₆₇NO₁₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	51	37	1	13	0	0
2	D	1	51	37	1	13	0	0

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

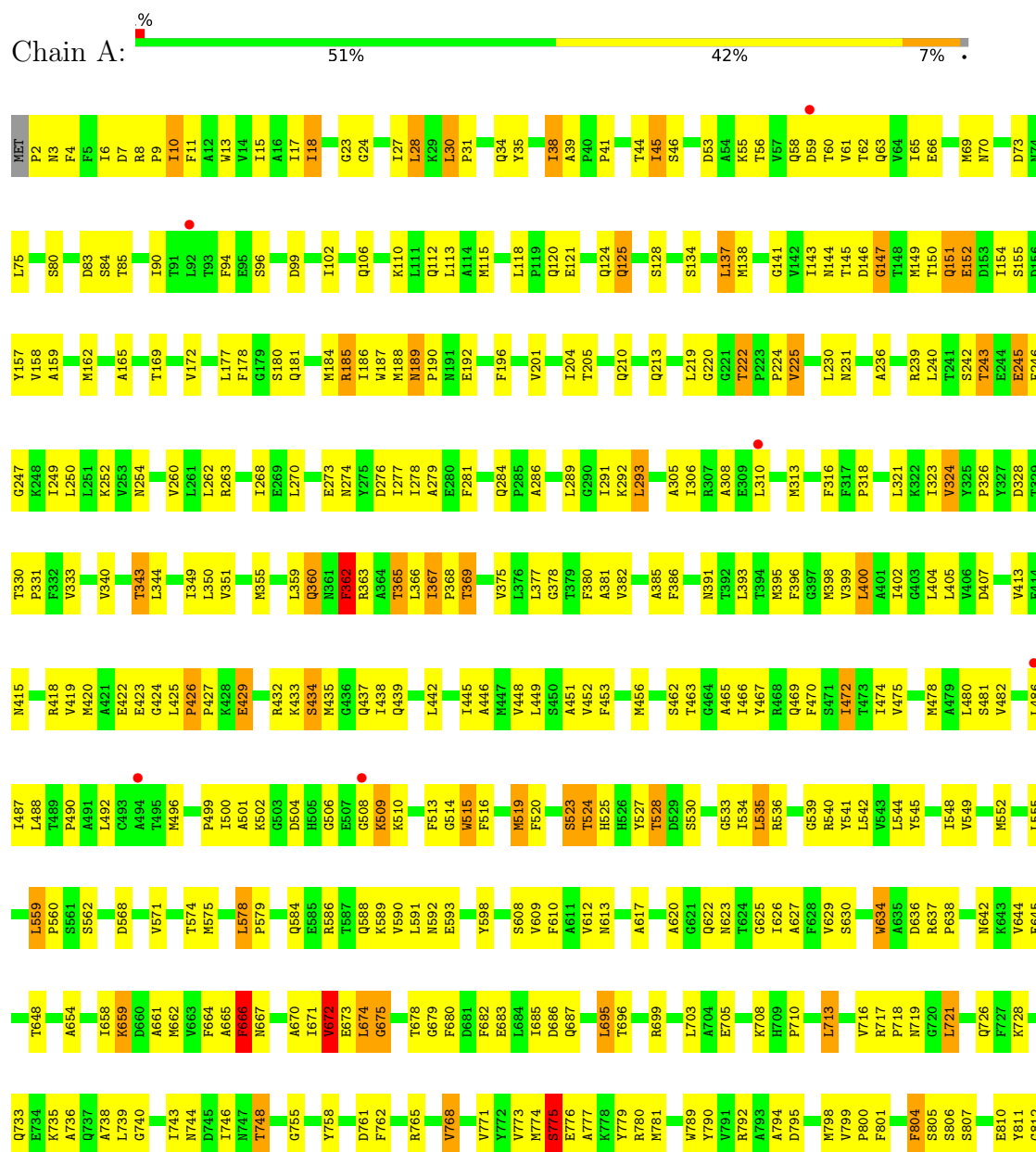
- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

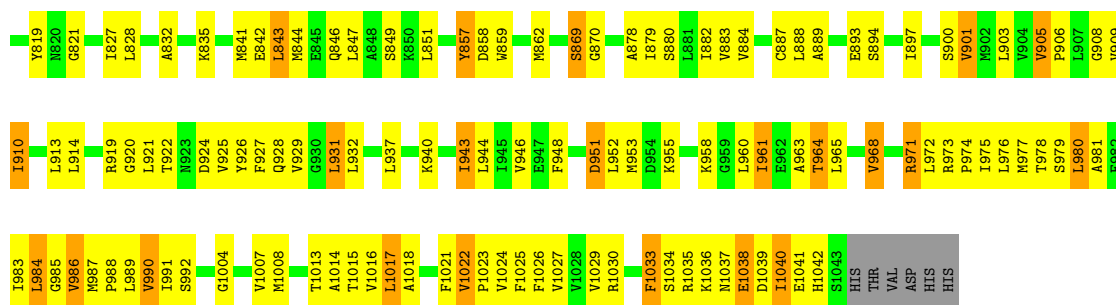
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ni 1 1	0	0
4	C	1	Total Ni 1 1	0	0
4	E	1	Total Ni 1 1	0	0

3 Residue-property plots

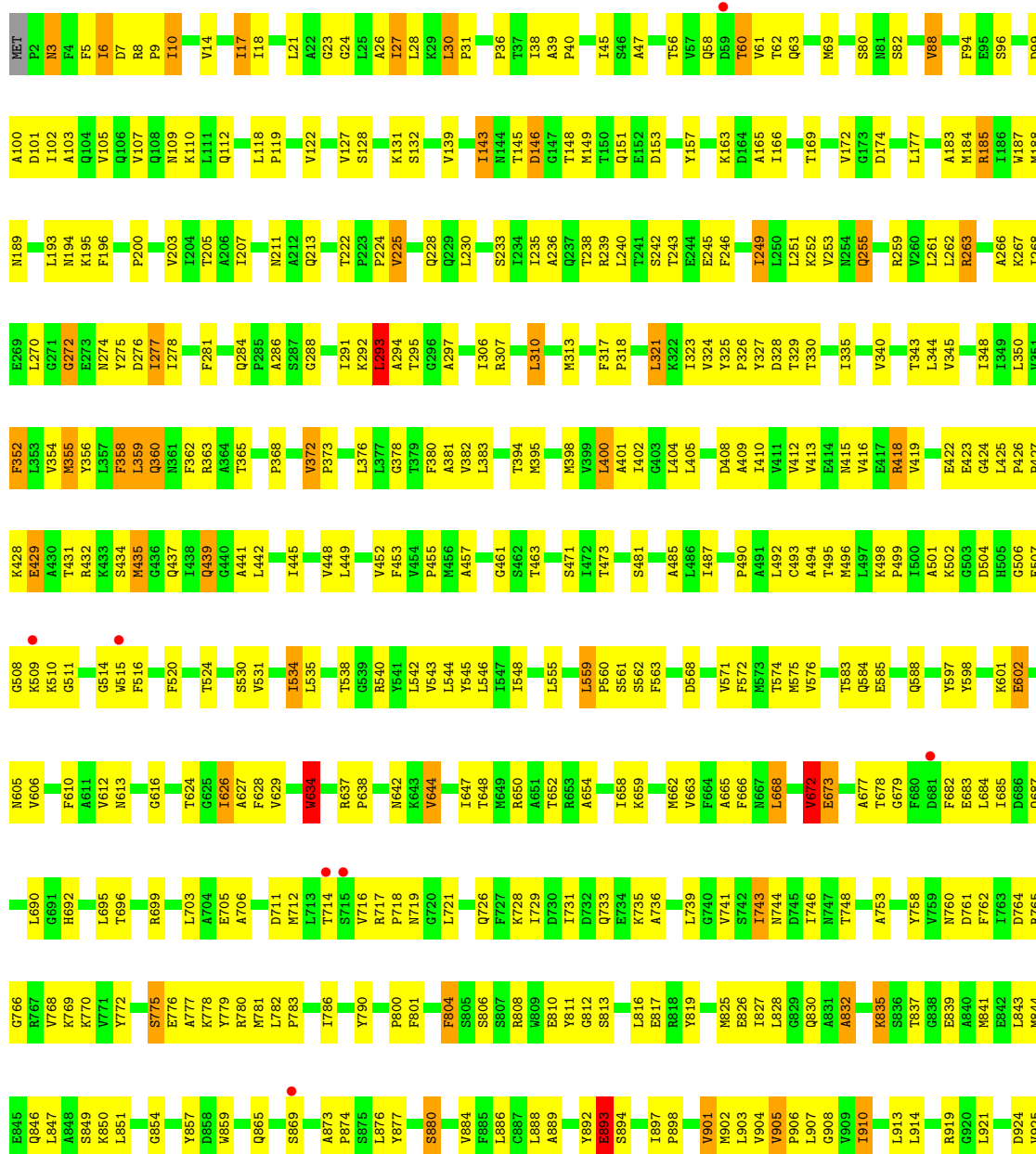
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

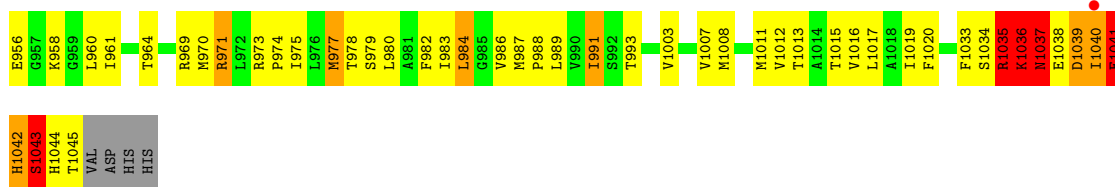




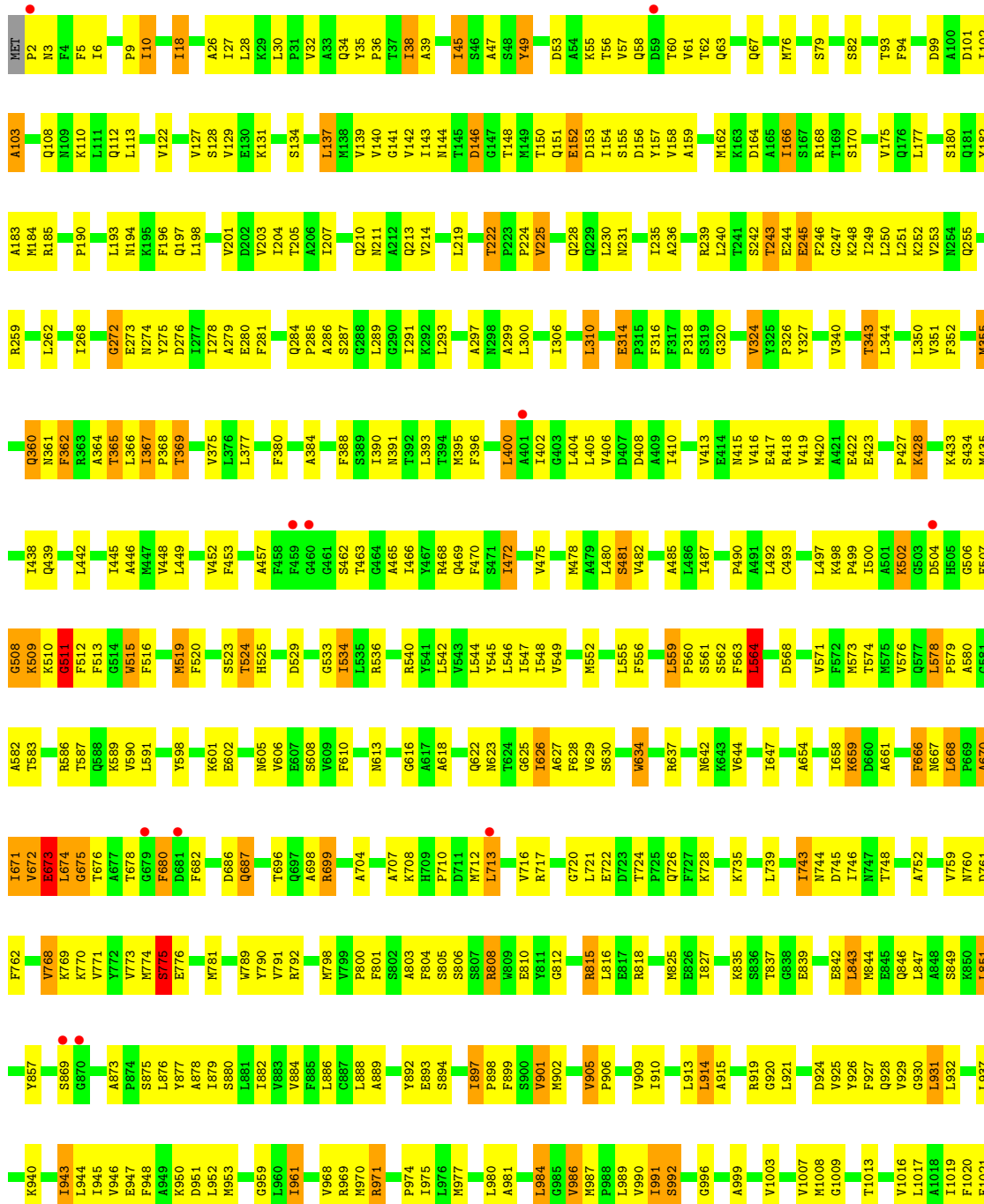
• Molecule 1: Multidrug efflux pump subunit AcrB





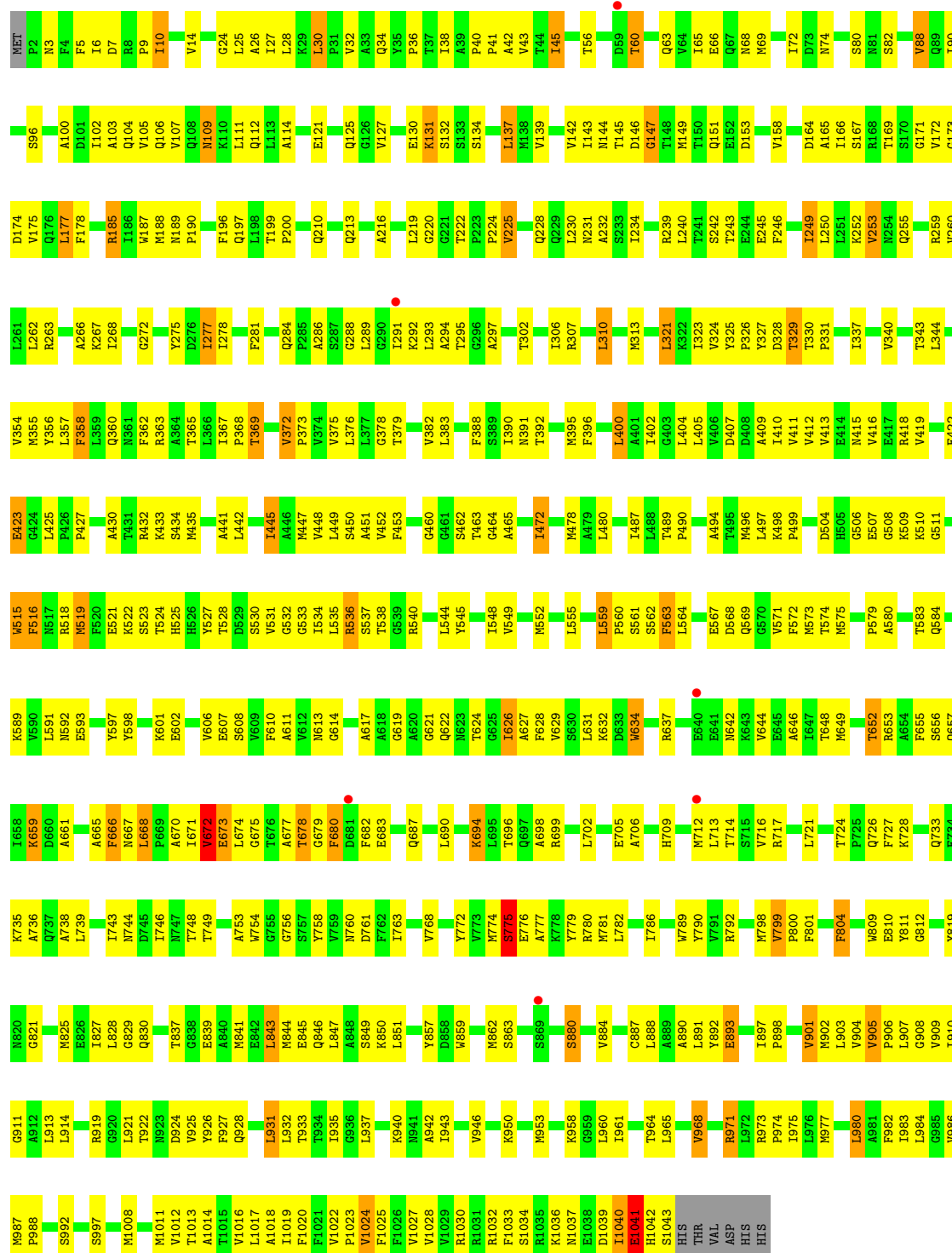


● Molecule 1: Multidrug efflux pump subunit AcrB

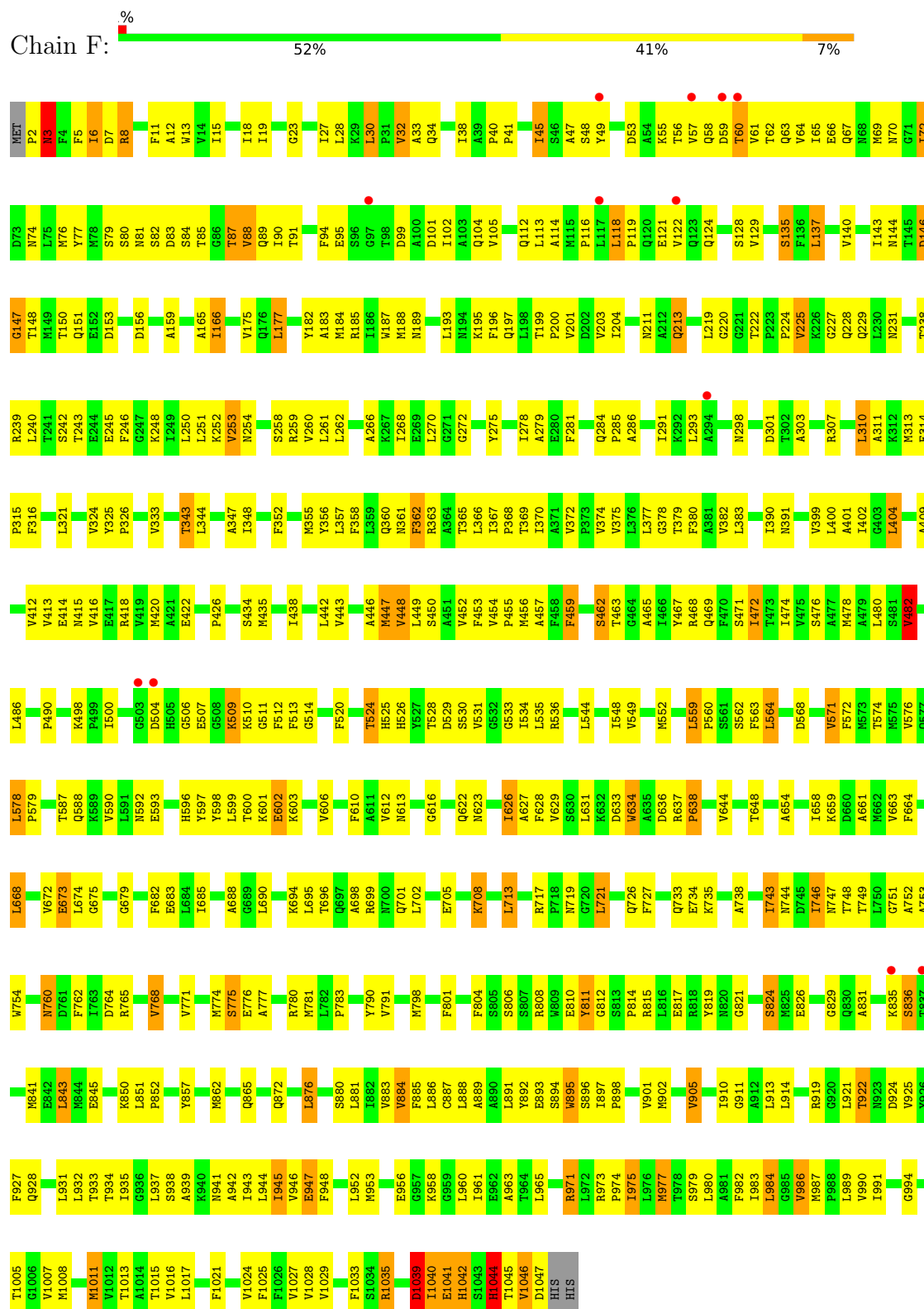




● Molecule 1: Multidrug efflux pump subunit AcrB



- Molecule 1: Multidrug efflux pump subunit AcrB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	151.18Å 156.77Å 218.17Å 90.00° 93.09° 90.00°	Depositor
Resolution (Å)	19.96 – 3.60 19.96 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.96-3.60) 96.5 (19.96-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.238 , 0.307 0.248 , 0.311	Depositor DCC
R_{free} test set	5867 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	101.0	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	47876	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2263e-04.*

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: NI, ERY, LMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.79	2/8056 (0.0%)	1.21	34/10940 (0.3%)
1	B	0.80	1/8056 (0.0%)	1.20	46/10940 (0.4%)
1	C	0.80	1/8074 (0.0%)	1.24	54/10965 (0.5%)
1	D	0.75	2/8056 (0.0%)	1.19	43/10940 (0.4%)
1	E	0.75	2/8056 (0.0%)	1.18	35/10940 (0.3%)
1	F	0.78	3/8089 (0.0%)	1.22	50/10986 (0.5%)
All	All	0.78	11/48387 (0.0%)	1.21	262/65711 (0.4%)

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	B	0	2
1	C	0	1
1	D	0	1
1	F	0	2
All	All	0	7

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	905	VAL	CA-CB	6.70	1.57	1.54
1	C	905	VAL	CA-CB	6.46	1.57	1.54
1	E	905	VAL	CA-CB	6.24	1.57	1.54
1	F	905	VAL	CA-CB	5.84	1.57	1.54
1	A	1022	VAL	CA-CB	5.76	1.57	1.54
1	B	905	VAL	CA-CB	5.58	1.56	1.54
1	A	905	VAL	CA-CB	5.54	1.56	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	426	PRO	CA-C	5.25	1.54	1.51
1	D	1033	PHE	CA-C	5.20	1.59	1.52
1	F	372	VAL	CA-CB	5.06	1.60	1.54
1	E	489	THR	CA-CB	5.04	1.60	1.53

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ALA	CA-C-N	12.29	128.63	119.66
1	A	39	ALA	C-N-CA	12.29	128.63	119.66
1	B	559	LEU	CA-C-N	11.99	132.11	119.76
1	B	559	LEU	C-N-CA	11.99	132.11	119.76
1	F	559	LEU	CA-C-N	11.92	132.04	119.76
1	F	559	LEU	C-N-CA	11.92	132.04	119.76
1	E	559	LEU	CA-C-N	11.30	131.40	119.76
1	E	559	LEU	C-N-CA	11.30	131.40	119.76
1	A	515	TRP	N-CA-C	-11.08	98.97	111.71
1	F	118	LEU	CA-C-N	11.05	131.74	119.92
1	F	118	LEU	C-N-CA	11.05	131.74	119.92
1	F	8	ARG	CA-C-N	10.43	130.19	119.56
1	F	8	ARG	C-N-CA	10.43	130.19	119.56
1	C	8	ARG	CA-C-N	9.77	129.52	119.56
1	C	8	ARG	C-N-CA	9.77	129.52	119.56
1	C	118	LEU	CA-C-N	9.28	129.85	119.92
1	C	118	LEU	C-N-CA	9.28	129.85	119.92
1	B	30	LEU	CA-C-N	9.08	129.15	119.89
1	B	30	LEU	C-N-CA	9.08	129.15	119.89
1	D	559	LEU	CA-C-N	8.66	129.18	119.83
1	D	559	LEU	C-N-CA	8.66	129.18	119.83
1	C	559	LEU	CA-C-N	8.62	128.64	119.76
1	C	559	LEU	C-N-CA	8.62	128.64	119.76
1	B	869	SER	N-CA-C	8.58	121.77	111.82
1	D	1033	PHE	N-CA-C	-8.25	94.45	107.73
1	D	367	ILE	CA-C-N	-8.15	111.33	119.56
1	D	367	ILE	C-N-CA	-8.15	111.33	119.56
1	E	288	GLY	N-CA-C	8.11	123.04	110.96
1	E	1041	GLU	CA-C-N	8.06	136.21	121.70
1	E	1041	GLU	C-N-CA	8.06	136.21	121.70
1	D	38	ILE	N-CA-C	-8.01	105.39	112.12
1	C	1041	GLU	N-CA-C	-7.97	93.83	110.80
1	E	30	LEU	CA-C-N	7.91	127.95	119.89
1	E	30	LEU	C-N-CA	7.91	127.95	119.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	85	THR	N-CA-C	-7.89	103.66	113.20
1	D	49	TYR	CA-C-N	7.86	129.67	119.84
1	D	49	TYR	C-N-CA	7.86	129.67	119.84
1	B	243	THR	N-CA-C	-7.84	102.35	112.23
1	A	30	LEU	CA-C-N	7.64	127.68	119.89
1	A	30	LEU	C-N-CA	7.64	127.68	119.89
1	F	189	ASN	CA-C-N	7.58	127.11	118.85
1	F	189	ASN	C-N-CA	7.58	127.11	118.85
1	A	367	ILE	CA-C-N	-7.54	112.02	119.64
1	A	367	ILE	C-N-CA	-7.54	112.02	119.64
1	F	40	PRO	CA-C-N	7.39	127.97	119.99
1	F	40	PRO	C-N-CA	7.39	127.97	119.99
1	A	675	GLY	N-CA-C	7.33	130.56	113.18
1	B	189	ASN	CA-C-N	7.31	126.82	118.85
1	B	189	ASN	C-N-CA	7.31	126.82	118.85
1	F	30	LEU	CA-C-N	7.28	127.26	119.76
1	F	30	LEU	C-N-CA	7.28	127.26	119.76
1	B	39	ALA	CA-C-N	7.25	124.95	119.66
1	B	39	ALA	C-N-CA	7.25	124.95	119.66
1	A	38	ILE	N-CA-C	-7.23	106.05	112.12
1	F	213	GLN	N-CA-C	-7.21	98.56	110.17
1	C	1041	GLU	CA-C-N	7.09	134.46	121.70
1	C	1041	GLU	C-N-CA	7.09	134.46	121.70
1	C	325	TYR	CA-C-N	7.06	126.69	119.56
1	C	325	TYR	C-N-CA	7.06	126.69	119.56
1	E	709	HIS	CA-C-N	7.00	128.22	120.45
1	E	709	HIS	C-N-CA	7.00	128.22	120.45
1	E	189	ASN	CA-C-N	6.99	126.47	118.85
1	E	189	ASN	C-N-CA	6.99	126.47	118.85
1	C	170	SER	N-CA-C	6.97	120.34	109.96
1	B	1039	ASP	N-CA-C	6.94	118.60	110.41
1	D	515	TRP	N-CA-C	-6.88	103.98	112.38
1	D	214	VAL	N-CA-C	6.84	118.16	108.17
1	F	325	TYR	CA-C-N	6.81	126.44	119.56
1	F	325	TYR	C-N-CA	6.81	126.44	119.56
1	B	893	GLU	N-CA-C	-6.80	96.32	110.80
1	E	799	VAL	CA-C-N	6.78	126.69	119.85
1	E	799	VAL	C-N-CA	6.78	126.69	119.85
1	C	515	TRP	N-CA-C	-6.77	103.90	111.28
1	E	760	ASN	N-CA-C	6.70	118.30	108.86
1	A	717	ARG	CA-C-N	-6.59	113.16	120.14
1	A	717	ARG	C-N-CA	-6.59	113.16	120.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	516	PHE	N-CA-C	6.57	118.52	111.36
1	C	482	VAL	CB-CA-C	-6.54	103.19	112.22
1	D	365	THR	N-CA-C	-6.54	103.99	112.23
1	D	39	ALA	CA-C-N	6.53	124.42	119.66
1	D	39	ALA	C-N-CA	6.53	124.42	119.66
1	D	808	ARG	N-CA-C	6.53	117.19	108.38
1	C	7	ASP	CA-C-N	6.50	129.63	122.74
1	C	7	ASP	C-N-CA	6.50	129.63	122.74
1	D	851	LEU	CA-C-N	6.50	127.96	119.84
1	D	851	LEU	C-N-CA	6.50	127.96	119.84
1	C	667	ASN	N-CA-C	6.45	119.97	109.59
1	F	60	THR	N-CA-C	-6.44	106.05	114.04
1	F	72	ILE	N-CA-C	-6.43	99.32	108.58
1	F	156	ASP	N-CA-C	6.38	118.32	111.36
1	B	132	SER	N-CA-C	6.34	117.49	108.54
1	C	371	ALA	N-CA-C	-6.34	104.36	111.28
1	F	243	THR	N-CA-C	-6.33	104.25	112.23
1	B	832	ALA	CA-C-N	6.27	125.76	119.24
1	B	832	ALA	C-N-CA	6.27	125.76	119.24
1	E	498	LYS	CA-C-N	6.26	126.03	119.76
1	E	498	LYS	C-N-CA	6.26	126.03	119.76
1	E	763	ILE	N-CA-C	6.25	116.65	106.72
1	A	28	LEU	N-CA-C	6.24	118.16	111.36
1	B	40	PRO	O-C-N	6.21	124.17	121.31
1	B	1037	ASN	N-CA-C	6.18	123.97	110.80
1	D	670	ALA	N-CA-C	-6.18	104.09	111.69
1	B	272	GLY	N-CA-C	6.18	119.94	111.54
1	D	687	GLN	N-CA-C	6.18	120.95	113.41
1	F	824	SER	N-CA-C	6.16	118.14	108.96
1	F	482	VAL	CB-CA-C	-6.13	103.76	112.22
1	B	325	TYR	CA-C-N	6.10	125.72	119.56
1	B	325	TYR	C-N-CA	6.10	125.72	119.56
1	D	564	LEU	CA-C-N	6.08	126.56	119.99
1	D	564	LEU	C-N-CA	6.08	126.56	119.99
1	C	676	THR	N-CA-C	-6.07	104.01	112.45
1	F	829	GLY	N-CA-C	6.06	119.42	110.63
1	C	657	GLN	N-CA-C	-6.04	104.62	112.23
1	C	269	GLU	N-CA-C	6.02	118.44	108.99
1	B	288	GLY	N-CA-C	6.01	120.09	110.90
1	A	125	GLN	N-CA-C	-5.99	105.46	112.89
1	C	330	THR	N-CA-C	5.99	120.38	112.35
1	D	897	ILE	N-CA-C	5.99	121.81	108.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	921	LEU	N-CA-C	5.97	118.55	109.95
1	E	325	TYR	CA-C-N	5.95	126.06	119.87
1	E	325	TYR	C-N-CA	5.95	126.06	119.87
1	E	515	TRP	N-CA-C	-5.95	105.13	112.38
1	B	3	ASN	N-CA-C	-5.94	104.89	111.36
1	F	32	VAL	N-CA-C	5.92	116.81	108.17
1	F	921	LEU	N-CA-C	5.90	118.44	109.95
1	F	135	SER	N-CA-C	5.89	118.55	109.07
1	E	674	LEU	N-CA-C	5.88	118.97	109.86
1	D	717	ARG	CA-C-N	-5.88	113.91	120.14
1	D	717	ARG	C-N-CA	-5.88	113.91	120.14
1	B	143	ILE	N-CA-C	5.87	115.69	108.53
1	E	893	GLU	N-CA-C	-5.86	98.33	110.80
1	D	1033	PHE	CA-C-N	5.83	132.20	121.70
1	D	1033	PHE	C-N-CA	5.83	132.20	121.70
1	F	404	LEU	N-CA-C	5.82	118.84	111.69
1	C	390	ILE	CB-CA-C	-5.80	105.65	111.80
1	C	213	GLN	N-CA-C	-5.80	100.83	110.17
1	D	272	GLY	N-CA-C	5.80	119.42	111.54
1	E	532	GLY	N-CA-C	-5.78	105.80	112.73
1	F	872	GLN	N-CA-C	-5.77	106.41	113.50
1	F	895	TRP	N-CA-C	-5.76	106.25	113.28
1	A	807	SER	N-CA-C	5.76	118.44	109.52
1	C	367	ILE	CA-C-N	-5.74	113.76	119.56
1	C	367	ILE	C-N-CA	-5.74	113.76	119.56
1	F	119	PRO	N-CA-C	5.74	120.23	111.34
1	A	487	ILE	CB-CA-C	-5.72	106.84	111.71
1	D	481	SER	N-CA-C	-5.68	105.23	111.82
1	B	6	ILE	N-CA-C	-5.65	103.99	111.05
1	A	513	PHE	N-CA-C	-5.63	106.76	113.97
1	C	768	VAL	N-CA-C	5.63	116.34	109.30
1	D	1033	PHE	O-C-N	-5.63	117.97	123.26
1	B	851	LEU	CA-C-N	5.63	125.58	119.78
1	B	851	LEU	C-N-CA	5.63	125.58	119.78
1	A	365	THR	N-CA-C	-5.63	105.67	112.54
1	D	314	GLU	N-CA-C	5.62	121.27	113.45
1	F	919	ARG	N-CA-C	-5.62	102.45	110.59
1	C	120	GLN	N-CA-C	5.61	119.30	112.23
1	D	519	MET	CB-CG-SD	5.60	129.51	112.70
1	A	84	SER	N-CA-C	-5.60	106.53	113.19
1	A	254	ASN	N-CA-C	5.59	117.75	110.53
1	B	359	LEU	N-CA-C	-5.58	106.37	114.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	511	GLY	N-CA-C	5.57	126.38	113.18
1	A	362	PHE	N-CA-C	5.56	117.02	111.07
1	B	80	SER	N-CA-C	5.56	117.85	109.23
1	C	666	PHE	N-CA-C	5.56	116.71	108.60
1	B	439	GLN	N-CA-C	5.53	117.77	111.02
1	C	150	THR	N-CA-C	5.51	117.19	110.41
1	F	945	ILE	N-CA-C	5.50	115.64	110.30
1	D	673	GLU	N-CA-C	5.49	122.50	110.80
1	B	666	PHE	N-CA-C	5.49	116.61	108.60
1	C	445	ILE	CB-CA-C	-5.49	104.95	111.97
1	B	880	SER	N-CA-C	5.48	117.25	111.28
1	E	134	SER	N-CA-C	-5.48	106.27	113.17
1	C	937	LEU	N-CA-C	5.47	117.04	111.14
1	D	675	GLY	N-CA-C	5.47	126.14	113.18
1	E	519	MET	CB-CG-SD	5.46	129.09	112.70
1	A	519	MET	CB-CG-SD	5.46	129.09	112.70
1	C	1039	ASP	CA-C-N	5.46	131.53	121.70
1	C	1039	ASP	C-N-CA	5.46	131.53	121.70
1	D	103	ALA	N-CA-C	-5.43	105.26	111.07
1	F	633	ASP	CA-C-N	5.43	128.10	120.28
1	F	633	ASP	C-N-CA	5.43	128.10	120.28
1	B	672	VAL	N-CA-C	5.43	120.63	109.34
1	C	83	ASP	N-CA-C	5.42	118.65	109.76
1	D	720	GLY	N-CA-C	-5.40	100.38	113.18
1	D	480	LEU	N-CA-C	5.40	117.25	111.36
1	B	644	VAL	N-CA-C	5.39	116.77	110.62
1	A	472	ILE	N-CA-C	5.38	116.16	110.72
1	F	994	GLY	N-CA-C	-5.37	102.42	110.42
1	B	293	LEU	CA-CB-CG	5.36	135.06	116.30
1	B	330	THR	CA-C-N	-5.36	113.39	119.28
1	B	330	THR	C-N-CA	-5.36	113.39	119.28
1	A	1017	LEU	N-CA-C	-5.36	107.40	114.04
1	B	624	THR	N-CA-C	5.36	118.29	109.72
1	B	782	LEU	CA-C-N	5.36	125.42	119.32
1	B	782	LEU	C-N-CA	5.36	125.42	119.32
1	B	929	VAL	N-CA-C	-5.35	105.16	110.62
1	D	699	ARG	N-CA-C	5.34	117.18	111.36
1	B	143	ILE	CB-CA-C	-5.33	103.12	110.91
1	C	243	THR	N-CA-C	-5.32	105.52	112.23
1	E	672	VAL	N-CA-C	5.31	120.38	109.34
1	F	975	ILE	N-CA-C	-5.31	104.79	110.36
1	F	922	THR	N-CA-C	5.29	117.44	109.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	679	GLY	N-CA-C	5.29	116.53	111.67
1	D	498	LYS	CA-C-N	5.28	125.18	119.85
1	D	498	LYS	C-N-CA	5.28	125.18	119.85
1	D	1033	PHE	CA-C-O	-5.26	115.37	121.26
1	F	529	ASP	N-CA-C	-5.26	104.80	111.11
1	F	634	TRP	N-CA-C	5.25	117.75	111.71
1	F	459	PHE	N-CA-C	5.25	117.64	110.55
1	F	3	ASN	N-CA-C	-5.24	105.65	111.36
1	C	851	LEU	CA-C-N	5.24	125.52	119.92
1	C	851	LEU	C-N-CA	5.24	125.52	119.92
1	B	435	MET	N-CA-C	-5.23	105.58	111.28
1	E	644	VAL	N-CA-C	5.22	116.58	110.62
1	B	629	VAL	N-CA-C	5.22	115.37	107.80
1	E	522	LYS	N-CA-C	-5.21	104.86	111.11
1	B	634	TRP	N-CA-C	5.21	117.70	111.71
1	E	423	GLU	N-CA-C	5.20	120.28	113.88
1	A	905	VAL	CB-CA-C	-5.20	108.76	113.70
1	C	30	LEU	CA-C-N	5.20	125.11	119.76
1	C	30	LEU	C-N-CA	5.20	125.11	119.76
1	C	89	GLN	N-CA-C	5.16	117.48	108.76
1	F	526	HIS	N-CA-C	-5.16	104.92	111.11
1	B	964	THR	N-CA-C	-5.16	105.66	111.28
1	A	535	LEU	N-CA-C	-5.15	106.83	113.01
1	A	851	LEU	CA-C-N	5.15	126.28	119.84
1	A	851	LEU	C-N-CA	5.15	126.28	119.84
1	A	666	PHE	N-CA-C	5.15	116.12	108.60
1	A	795	ASP	N-CA-C	5.15	117.68	111.40
1	D	686	ASP	N-CA-C	5.15	116.69	108.41
1	E	1024	VAL	CB-CA-C	-5.14	105.39	111.97
1	C	81	ASN	N-CA-C	5.13	117.86	109.59
1	C	879	ILE	N-CA-C	5.13	115.27	110.30
1	E	1039	ASP	N-CA-C	5.11	116.50	107.61
1	C	1043	SER	N-CA-C	-5.10	99.94	110.80
1	B	27	ILE	N-CA-C	-5.09	105.58	110.72
1	C	656	SER	N-CA-C	5.09	118.93	111.04
1	F	984	LEU	N-CA-C	5.08	117.72	111.82
1	C	1043	SER	CA-C-N	5.08	130.85	121.70
1	C	1043	SER	C-N-CA	5.08	130.85	121.70
1	E	164	ASP	N-CA-C	5.08	117.94	111.69
1	F	1040	ILE	CA-C-N	5.08	130.84	121.70
1	F	1040	ILE	C-N-CA	5.08	130.84	121.70
1	C	644	VAL	N-CA-C	5.07	116.40	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	19	ILE	N-CA-C	5.07	115.29	110.42
1	C	677	ALA	N-CA-C	5.07	117.97	109.96
1	C	203	VAL	N-CA-C	-5.07	105.56	110.42
1	A	189	ASN	CA-C-N	5.07	124.37	118.85
1	A	189	ASN	C-N-CA	5.07	124.37	118.85
1	E	657	GLN	N-CA-C	5.05	117.91	111.69
1	F	38	ILE	N-CA-C	-5.05	107.88	112.12
1	A	943	ILE	N-CA-C	-5.05	105.47	110.62
1	D	193	LEU	CA-C-N	5.05	127.46	120.29
1	D	193	LEU	C-N-CA	5.05	127.46	120.29
1	C	590	VAL	CB-CA-C	-5.03	105.52	111.81
1	F	40	PRO	O-C-N	5.03	123.62	121.31
1	C	135	SER	N-CA-C	5.03	116.71	108.52
1	A	426	PRO	CA-C-N	5.02	126.12	119.84
1	A	426	PRO	C-N-CA	5.02	126.12	119.84
1	E	445	ILE	N-CA-C	-5.01	105.51	110.62
1	F	122	VAL	N-CA-C	-5.01	105.61	110.42
1	F	374	VAL	CB-CA-C	-5.00	105.29	111.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1033	PHE	Peptide
1	B	1036	LYS	Peptide
1	B	1040	ILE	Peptide
1	C	1036	LYS	Peptide
1	D	1033	PHE	Peptide
1	F	1039	ASP	Peptide
1	F	1041	GLU	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	7907	0	8050	414	0
1	B	7907	0	8050	359	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7924	0	8064	413	1
1	D	7907	0	8050	368	1
1	E	7907	0	8050	363	0
1	F	7939	0	8077	391	0
2	A	51	0	67	9	0
2	D	51	0	67	5	0
3	A	70	0	92	5	0
3	B	35	0	46	5	0
3	C	35	0	46	1	0
3	D	70	0	92	9	0
3	E	35	0	46	3	0
3	F	35	0	46	5	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	47876	0	48843	2233	1

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 23.

All (2233) 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:A:530:SER:OG	3:A:1102:LMT:O2'	1.59	1.15
1:A:427:PRO:HD3	1:A:499:PRO:HB3	1.41	1.03
1:C:831:ALA:HB3	1:C:835:LYS:HG3	1.42	0.98
1:E:340:VAL:HG21	1:E:395:MET:HB3	1.46	0.98
1:A:144:ASN:O	1:A:284:GLN:NE2	2.01	0.94
1:D:196:PHE:O	1:D:252:LYS:NZ	2.01	0.94
1:C:808:ARG:NH1	1:C:810:GLU:OE2	2.00	0.93
1:A:971:ARG:HG2	1:A:974:PRO:HG2	1.50	0.93
1:D:618:ALA:O	1:D:815:ARG:NH2	2.01	0.93
1:F:1040:ILE:HA	1:F:1041:GLU:HB2	1.48	0.92
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.50	0.92
1:E:196:PHE:O	1:E:252:LYS:NZ	2.02	0.92
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.52	0.91
1:D:564:LEU:HB2	1:D:671:ILE:HD11	1.51	0.91
1:C:894:SER:HB3	1:C:897:ILE:HG12	1.53	0.90
1:B:350:LEU:HD13	1:B:984:LEU:HB3	1.53	0.89
1:F:298:ASN:ND2	1:F:301:ASP:OD2	2.05	0.89
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.55	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.55	0.88
1:F:831:ALA:HB3	1:F:835:LYS:HG3	1.53	0.88
1:F:363:ARG:HH21	1:F:498:LYS:HD2	1.36	0.87
1:F:634:TRP:CD1	1:F:634:TRP:H	1.91	0.87
1:E:593:GLU:OE1	1:E:659:LYS:NZ	2.06	0.87
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.08	0.87
1:D:144:ASN:O	1:D:284:GLN:NE2	2.08	0.86
1:F:941:ASN:HD21	1:F:1015:THR:HG22	1.40	0.86
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.08	0.86
1:C:40:PRO:HD2	1:C:674:LEU:HD21	1.55	0.85
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.59	0.85
1:B:196:PHE:O	1:B:252:LYS:NZ	2.10	0.84
1:A:355:MET:HE2	1:A:368:PRO:HG2	1.58	0.84
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.59	0.83
1:A:515:TRP:O	1:A:519:MET:HG3	1.79	0.83
1:C:1039:ASP:HB3	1:C:1040:ILE:HA	1.59	0.83
1:B:668:LEU:HD23	1:B:668:LEU:H	1.42	0.82
1:D:634:TRP:CD1	1:D:634:TRP:H	1.96	0.82
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.60	0.82
1:C:578:LEU:HG	1:C:587:THR:HG22	1.60	0.82
1:E:3:ASN:HA	1:E:6:ILE:HD12	1.62	0.82
1:B:3:ASN:HA	1:B:6:ILE:HD12	1.60	0.81
1:C:634:TRP:CD1	1:C:634:TRP:H	1.94	0.81
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.62	0.81
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.60	0.81
1:B:101:ASP:OD1	1:B:131:LYS:NZ	2.12	0.81
1:A:134:SER:OG	2:A:1101:ERY:H323	1.80	0.81
1:D:228:GLN:NE2	1:D:230:LEU:O	2.14	0.80
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.11	0.80
1:F:383:LEU:HD23	1:F:472:ILE:HD13	1.63	0.80
1:C:210:GLN:HE22	1:C:250:LEU:HB3	1.45	0.80
1:E:415:ASN:OD1	1:E:418:ARG:NH1	2.13	0.80
1:A:579:PRO:HD3	1:A:661:ALA:HB2	1.64	0.80
1:B:383:LEU:HD21	1:B:473:THR:HA	1.64	0.80
1:A:931:LEU:HD13	3:A:1103:LMT:H42	1.62	0.79
1:A:562:SER:HB2	1:A:924:ASP:HB3	1.64	0.79
1:B:56:THR:O	1:B:60:THR:OG1	2.00	0.79
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.63	0.79
1:F:892:TYR:O	1:F:894:SER:N	2.14	0.78
1:D:213:GLN:HG2	1:D:239:ARG:HG2	1.65	0.78
1:D:236:ALA:O	1:E:728:LYS:NZ	2.17	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ILE:HD13	1:C:25:LEU:HD21	1.63	0.78
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.66	0.78
1:D:244:GLU:HG2	1:D:248:LYS:HE2	1.64	0.78
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.66	0.78
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.47	0.78
1:A:696:THR:HG23	1:A:699:ARG:HH12	1.47	0.78
1:E:451:ALA:O	1:E:880:SER:OG	2.01	0.78
1:F:509:LYS:HB3	1:F:514:GLY:HA3	1.64	0.78
1:B:712:MET:HE3	1:B:839:GLU:HB3	1.64	0.77
1:C:222:THR:HA	1:C:224:PRO:HD3	1.67	0.77
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.67	0.77
1:E:680:PHE:HD1	1:E:859:TRP:HZ3	1.31	0.77
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.65	0.77
1:C:428:LYS:HG2	1:C:494:ALA:HB1	1.67	0.77
1:D:225:VAL:HG12	1:E:777:ALA:HB1	1.66	0.77
1:E:634:TRP:H	1:E:634:TRP:CD1	2.03	0.77
1:D:137:LEU:HD22	1:D:293:LEU:HG	1.67	0.77
1:A:634:TRP:CD1	1:A:634:TRP:H	2.03	0.76
1:B:508:GLY:O	1:B:510:LYS:N	2.15	0.76
1:D:800:PRO:HG2	1:D:803:ALA:HB2	1.66	0.76
1:A:637:ARG:NH1	1:A:642:ASN:O	2.18	0.76
1:A:186:ILE:HB	1:A:773:VAL:HG22	1.65	0.76
1:C:274:ASN:ND2	1:C:276:ASP:OD2	2.19	0.76
1:F:462:SER:HB3	1:F:865:GLN:HG2	1.67	0.76
1:D:225:VAL:HG22	1:E:781:MET:HE2	1.65	0.76
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.66	0.75
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.68	0.75
1:D:562:SER:HB2	1:D:924:ASP:HB3	1.68	0.75
1:A:225:VAL:HG12	1:B:777:ALA:HB1	1.68	0.75
1:E:222:THR:HA	1:E:224:PRO:HD3	1.67	0.75
1:D:986:VAL:HG12	1:D:1008:MET:HE3	1.68	0.75
1:B:775:SER:OG	1:B:776:GLU:O	2.05	0.74
1:C:945:ILE:HA	1:C:971:ARG:HH12	1.53	0.74
1:E:7:ASP:OD1	1:E:432:ARG:NH2	2.19	0.74
1:F:683:GLU:HG2	1:F:819:TYR:CD2	2.22	0.74
1:B:511:GLY:HA2	1:B:515:TRP:HE1	1.53	0.74
1:A:545:TYR:OH	1:A:903:LEU:O	2.04	0.74
1:F:610:PHE:HB3	1:F:628:PHE:HB2	1.69	0.74
1:A:34:GLN:HB2	1:A:333:VAL:HG22	1.70	0.74
1:C:418:ARG:O	1:C:422:GLU:HB2	1.88	0.74
1:D:405:LEU:HD22	1:D:481:SER:HB3	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:901:VAL:HG21	1:D:943:ILE:HG13	1.68	0.74
1:E:733:GLN:HE22	1:E:743:ILE:HG21	1.53	0.74
1:B:901:VAL:HG21	1:B:943:ILE:HG13	1.69	0.74
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.69	0.74
1:A:196:PHE:O	1:A:252:LYS:NZ	2.21	0.74
1:C:445:ILE:HG12	1:C:940:LYS:HG3	1.70	0.74
1:B:415:ASN:HD22	1:B:434:SER:HB2	1.53	0.73
1:D:919:ARG:HG2	1:D:920:GLY:H	1.52	0.73
1:D:146:ASP:OD2	1:D:146:ASP:N	2.21	0.73
1:A:38:ILE:HG23	1:A:462:SER:HB2	1.70	0.73
1:B:530:SER:OG	3:B:1101:LMT:O2'	2.06	0.73
1:E:678:THR:HA	1:E:837:THR:OG1	1.89	0.73
1:D:699:ARG:NH1	1:D:825:MET:SD	2.61	0.73
1:C:3:ASN:OD1	1:C:3:ASN:N	2.13	0.73
1:D:781:MET:HE3	1:F:228:GLN:NE2	2.04	0.73
1:B:846:GLN:O	1:B:849:SER:OG	2.07	0.73
1:D:222:THR:HA	1:D:224:PRO:HD3	1.70	0.73
1:B:363:ARG:HD3	1:B:496:MET:O	1.87	0.72
1:B:272:GLY:N	1:B:275:TYR:OH	2.22	0.72
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.69	0.72
1:C:562:SER:HB2	1:C:924:ASP:HB3	1.70	0.72
1:D:362:PHE:O	1:D:366:LEU:HG	1.90	0.72
1:E:919:ARG:HB3	1:E:921:LEU:HD23	1.70	0.72
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.71	0.72
1:F:253:VAL:HG13	1:F:259:ARG:HG2	1.71	0.72
1:F:901:VAL:HG23	1:F:942:ALA:HB3	1.70	0.72
1:C:944:LEU:HB3	1:C:971:ARG:CZ	2.20	0.72
1:E:698:ALA:HB1	1:E:851:LEU:HD13	1.71	0.72
1:C:520:PHE:O	1:C:524:THR:HG22	1.90	0.71
1:C:971:ARG:CZ	1:C:971:ARG:HB3	2.18	0.71
1:B:808:ARG:NH1	1:B:810:GLU:OE2	2.23	0.71
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.71	0.71
1:E:682:PHE:CZ	1:E:857:TYR:HB2	2.26	0.71
1:C:944:LEU:HB3	1:C:971:ARG:NE	2.05	0.71
1:E:250:LEU:HD21	1:E:253:VAL:HG22	1.73	0.71
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.72	0.71
1:E:562:SER:OG	1:E:563:PHE:N	2.21	0.71
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.73	0.71
1:D:9:PRO:HG2	1:D:10:ILE:HD12	1.71	0.71
1:A:928:GLN:HG2	3:A:1103:LMT:H21	1.73	0.71
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:ALA:HA	1:C:586:ARG:NH2	2.06	0.70
1:E:262:LEU:HG	1:E:268:ILE:HD11	1.73	0.70
1:C:356:TYR:C	1:C:358:PHE:H	1.96	0.70
1:E:668:LEU:HD23	1:E:668:LEU:H	1.55	0.70
1:E:448:VAL:HG13	1:E:884:VAL:HG22	1.73	0.70
1:B:383:LEU:HD11	1:B:473:THR:HG23	1.71	0.70
1:C:144:ASN:O	1:C:284:GLN:NE2	2.23	0.70
1:A:424:GLY:HA3	1:A:502:LYS:HB3	1.72	0.70
1:A:781:MET:HE2	1:C:225:VAL:HG22	1.73	0.70
1:D:134:SER:HB2	2:D:1101:ERY:O10	1.90	0.70
1:A:70:ASN:O	1:A:110:LYS:NZ	2.25	0.70
1:A:274:ASN:ND2	1:A:276:ASP:OD2	2.25	0.70
1:B:355:MET:HE1	1:B:410:ILE:HG12	1.74	0.70
1:E:441:ALA:O	1:E:445:ILE:HG23	1.91	0.70
1:C:775:SER:OG	1:C:776:GLU:O	2.10	0.70
1:D:580:ALA:HB1	1:D:724:THR:HG22	1.74	0.70
1:F:808:ARG:NH1	1:F:810:GLU:OE2	2.25	0.69
1:A:644:VAL:HG11	1:A:667:ASN:HB2	1.74	0.69
1:E:575:MET:HE3	1:E:617:ALA:HB3	1.72	0.69
1:F:943:ILE:O	1:F:947:GLU:HB3	1.91	0.69
1:C:366:LEU:O	1:C:370:ILE:HG13	1.92	0.69
1:D:516:PHE:HA	1:D:519:MET:HE2	1.74	0.69
1:D:846:GLN:O	1:D:849:SER:OG	2.08	0.69
1:E:652:THR:HG23	1:E:665:ALA:HB3	1.74	0.69
1:B:634:TRP:H	1:B:634:TRP:CD1	2.08	0.69
1:C:242:SER:HB2	1:C:245:GLU:HG3	1.72	0.69
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.28	0.69
1:A:974:PRO:HA	1:A:977:MET:HE3	1.74	0.69
1:B:236:ALA:O	1:C:728:LYS:NZ	2.19	0.69
1:B:452:VAL:HG23	1:B:453:PHE:CD2	2.27	0.69
1:C:453:PHE:O	1:C:471:SER:OG	2.11	0.69
1:D:262:LEU:HG	1:D:268:ILE:HD11	1.75	0.69
1:D:886:LEU:HD13	1:F:18:ILE:HG13	1.74	0.69
1:C:159:ALA:HB2	1:C:177:LEU:HD11	1.75	0.69
1:F:32:VAL:HG22	1:F:390:ILE:HB	1.74	0.69
1:B:24:GLY:O	1:B:27:ILE:HG22	1.93	0.68
1:C:171:GLY:HA3	1:C:302:THR:OG1	1.92	0.68
1:D:139:VAL:HB	1:D:327:TYR:HB3	1.74	0.68
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.74	0.68
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.74	0.68
1:B:238:THR:OG1	1:C:728:LYS:NZ	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:LEU:H	1:B:668:LEU:CD2	2.07	0.68
1:E:174:ASP:HB3	1:E:292:LYS:HB2	1.76	0.68
1:F:45:ILE:HD12	1:F:90:ILE:HB	1.75	0.68
1:F:418:ARG:O	1:F:422:GLU:HB2	1.94	0.68
1:A:687:GLN:HG2	1:C:316:PHE:CD1	2.29	0.68
1:F:937:LEU:HD22	1:F:1011:MET:HE2	1.74	0.68
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.76	0.68
1:F:530:SER:OG	3:F:1101:LMT:O2'	2.12	0.68
1:D:536:ARG:NH1	3:D:1102:LMT:O3B	2.27	0.68
1:A:986:VAL:HG21	1:A:1007:VAL:HG11	1.76	0.68
1:C:702:LEU:HD12	1:C:851:LEU:HD11	1.76	0.68
1:D:586:ARG:O	1:D:589:LYS:HB3	1.94	0.68
1:B:7:ASP:OD2	1:B:432:ARG:NH2	2.25	0.67
1:C:318:PRO:HG2	1:C:321:LEU:HB2	1.75	0.67
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.74	0.67
1:F:719:ASN:HB3	1:F:826:GLU:HB3	1.76	0.67
1:A:775:SER:OG	1:A:776:GLU:O	2.11	0.67
1:D:26:ALA:O	1:D:30:LEU:HB2	1.94	0.67
1:E:143:ILE:HG22	1:E:286:ALA:HB2	1.77	0.67
1:F:250:LEU:HD11	1:F:259:ARG:HB3	1.74	0.67
1:E:213:GLN:HG2	1:E:239:ARG:HG3	1.77	0.67
1:D:668:LEU:H	1:D:668:LEU:HD23	1.59	0.67
1:F:81:ASN:OD1	1:F:815:ARG:NH2	2.28	0.67
1:F:753:ALA:O	1:F:775:SER:HB3	1.93	0.67
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.76	0.67
1:E:327:TYR:HD1	1:E:628:PHE:HZ	1.43	0.67
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.75	0.67
1:A:343:THR:HG21	1:A:989:LEU:HD21	1.76	0.67
1:A:419:VAL:HG11	1:A:433:LYS:HG2	1.77	0.67
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.30	0.67
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.77	0.67
1:D:164:ASP:HB3	1:D:168:ARG:HH21	1.60	0.67
1:D:198:LEU:HD23	1:D:792:ARG:HH21	1.60	0.67
1:F:876:LEU:HD22	1:F:932:LEU:HD11	1.75	0.67
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.75	0.66
1:A:73:ASP:OD2	1:C:131:LYS:NZ	2.27	0.66
1:E:242:SER:HB2	1:E:245:GLU:HG3	1.77	0.66
1:F:910:ILE:O	1:F:914:LEU:HB2	1.94	0.66
1:A:699:ARG:HD2	1:A:718:PRO:HB3	1.77	0.66
1:E:516:PHE:HA	1:E:519:MET:HE2	1.77	0.66
1:F:953:MET:HE2	1:F:963:ALA:HB3	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:THR:HG23	1:A:268:ILE:HG22	1.77	0.66
1:F:99:ASP:HB3	1:F:102:ILE:HB	1.76	0.66
1:A:225:VAL:HG22	1:B:781:MET:HE2	1.76	0.66
1:B:696:THR:HG23	1:B:699:ARG:NH1	2.11	0.66
1:C:979:SER:HA	1:C:1011:MET:HE3	1.78	0.66
1:E:971:ARG:O	1:E:975:ILE:HG12	1.96	0.66
1:D:60:THR:HG23	1:D:61:VAL:HG23	1.76	0.66
1:C:83:ASP:HB2	1:C:87:THR:O	1.95	0.66
1:D:108:GLN:NE2	1:E:109:ASN:HB2	2.11	0.66
1:D:355:MET:HB3	1:D:365:THR:OG1	1.96	0.65
1:E:104:GLN:HB2	1:E:131:LYS:HE3	1.78	0.65
1:A:222:THR:HG23	1:B:275:TYR:HB2	1.79	0.65
1:A:733:GLN:HE22	1:A:743:ILE:HG21	1.61	0.65
1:A:888:LEU:HD13	1:A:901:VAL:HG13	1.78	0.65
1:B:434:SER:HA	1:B:437:GLN:HB2	1.77	0.65
1:B:597:TYR:HE1	1:B:601:LYS:HD2	1.59	0.65
1:E:508:GLY:O	1:E:510:LYS:N	2.30	0.65
1:B:82:SER:HA	1:B:88:VAL:HG22	1.78	0.65
1:D:38:ILE:HG23	1:D:462:SER:HB2	1.78	0.65
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.31	0.65
1:E:239:ARG:HH12	1:E:761:ASP:HB2	1.61	0.65
1:A:588:GLN:NE2	1:A:592:ASN:OD1	2.28	0.65
1:C:465:ALA:HA	1:C:468:ARG:HH11	1.61	0.65
1:F:937:LEU:HD11	1:F:982:PHE:HE2	1.61	0.65
1:F:941:ASN:ND2	1:F:1015:THR:HG22	2.11	0.65
1:C:654:ALA:O	1:C:658:ILE:HG12	1.96	0.65
1:E:580:ALA:HB1	1:E:724:THR:HG22	1.77	0.65
1:F:578:LEU:HG	1:F:587:THR:HG22	1.77	0.65
1:A:80:SER:HB3	1:A:90:ILE:HG12	1.77	0.65
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.79	0.65
1:E:775:SER:OG	1:E:776:GLU:O	2.15	0.65
1:F:196:PHE:O	1:F:252:LYS:NZ	2.28	0.65
1:C:455:PRO:HG3	1:C:883:VAL:HG21	1.78	0.65
1:C:945:ILE:HG13	1:C:971:ARG:HH22	1.61	0.65
1:F:211:ASN:HD22	1:F:760:ASN:HD21	1.44	0.65
1:F:262:LEU:HG	1:F:268:ILE:HD11	1.78	0.65
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.78	0.65
1:D:680:PHE:HE1	1:D:844:MET:HG3	1.62	0.65
1:E:983:ILE:HG23	1:E:1008:MET:HE2	1.78	0.65
1:F:443:VAL:O	1:F:447:MET:HB3	1.96	0.65
1:B:362:PHE:O	1:B:365:THR:HG22	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:832:ALA:HB3	1:B:835:LYS:HB2	1.79	0.65
1:D:360:GLN:NE2	1:D:513:PHE:HB3	2.11	0.65
1:C:82:SER:HB2	1:C:816:LEU:HB2	1.78	0.64
1:F:137:LEU:HD11	1:F:303:ALA:HB2	1.79	0.64
1:B:188:MET:HE1	1:B:200:PRO:HG3	1.77	0.64
1:B:919:ARG:HB3	1:B:921:LEU:HD23	1.79	0.64
1:C:1019:ILE:HG13	1:C:1020:PHE:CD1	2.33	0.64
1:F:455:PRO:HG3	1:F:883:VAL:HG21	1.78	0.64
1:A:222:THR:HA	1:A:224:PRO:HD3	1.79	0.64
1:A:740:GLY:O	1:A:794:ALA:N	2.29	0.64
1:B:696:THR:HG23	1:B:699:ARG:HH12	1.61	0.64
1:C:196:PHE:O	1:C:252:LYS:NZ	2.27	0.64
1:C:713:LEU:HD11	1:C:843:LEU:HD12	1.79	0.64
1:E:6:ILE:HG23	1:E:494:ALA:HB2	1.80	0.64
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.78	0.64
1:F:1041:GLU:HB3	1:F:1042:HIS:HB3	1.79	0.64
1:A:948:PHE:O	1:A:952:LEU:HG	1.98	0.64
1:F:937:LEU:HD13	1:F:1011:MET:HG2	1.79	0.64
1:D:243:THR:HG23	1:D:268:ILE:HG22	1.79	0.64
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.80	0.64
1:F:600:THR:O	1:F:603:LYS:HG3	1.98	0.64
1:F:690:LEU:O	1:F:694:LYS:HB2	1.97	0.64
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.77	0.64
1:B:185:ARG:HG2	1:B:187:TRP:CZ2	2.32	0.64
1:D:735:LYS:O	1:D:739:LEU:HG	1.97	0.64
1:D:971:ARG:HH21	1:D:975:ILE:HD11	1.63	0.64
1:A:141:GLY:HA3	1:A:324:VAL:HG12	1.79	0.64
1:C:360:GLN:OE1	1:C:517:ASN:ND2	2.24	0.64
1:E:165:ALA:HB3	1:E:313:MET:CE	2.26	0.64
1:E:442:LEU:O	1:E:445:ILE:HG13	1.97	0.64
1:A:913:LEU:HD23	1:A:927:PHE:HZ	1.63	0.64
1:C:56:THR:O	1:C:60:THR:OG1	2.12	0.64
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.80	0.63
1:A:420:MET:HE3	1:A:500:ILE:HG13	1.80	0.63
1:A:427:PRO:CD	1:A:499:PRO:HB3	2.22	0.63
1:A:544:LEU:O	1:A:548:ILE:HG13	1.98	0.63
1:B:143:ILE:HG22	1:B:286:ALA:HB2	1.78	0.63
1:B:597:TYR:CE1	1:B:601:LYS:HD2	2.33	0.63
1:B:703:LEU:HD21	1:B:718:PRO:HD3	1.78	0.63
1:C:66:GLU:OE1	1:C:821:GLY:HA2	1.98	0.63
1:C:897:ILE:O	1:C:901:VAL:HG12	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:VAL:HG23	1:F:82:SER:HB3	1.80	0.63
1:F:597:TYR:HE1	1:F:601:LYS:HD2	1.62	0.63
2:A:1101:ERY:O10	2:A:1101:ERY:O1	2.16	0.63
1:B:26:ALA:O	1:B:30:LEU:HB2	1.98	0.63
1:B:545:TYR:CE2	1:B:1025:PHE:HZ	2.16	0.63
1:A:112:GLN:HG3	1:B:112:GLN:OE1	1.98	0.63
1:C:597:TYR:HE1	1:C:601:LYS:HD2	1.63	0.63
1:E:240:LEU:HB2	1:E:246:PHE:CE1	2.33	0.63
1:F:188:MET:HA	1:F:266:ALA:HB2	1.78	0.63
1:F:463:THR:HG23	1:F:925:VAL:HG22	1.81	0.63
1:B:910:ILE:O	1:B:914:LEU:HB2	1.98	0.63
1:D:637:ARG:HB3	1:D:642:ASN:HB3	1.78	0.63
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.79	0.63
1:A:520:PHE:O	1:A:524:THR:HG22	1.99	0.63
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.80	0.63
1:E:508:GLY:HA2	1:E:518:ARG:HH21	1.63	0.63
1:A:400:LEU:HD23	1:A:929:VAL:HG12	1.80	0.63
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.81	0.63
1:D:1013:THR:O	1:D:1017:LEU:HB2	1.99	0.63
1:D:775:SER:OG	1:D:776:GLU:O	2.16	0.63
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.80	0.63
1:C:588:GLN:NE2	1:C:592:ASN:OD1	2.32	0.63
1:D:682:PHE:HB3	1:D:827:ILE:HB	1.80	0.63
1:E:228:GLN:NE2	1:E:230:LEU:O	2.30	0.63
1:E:801:PHE:HD1	1:E:804:PHE:HE2	1.44	0.63
1:B:14:VAL:HG13	1:C:886:LEU:HD12	1.81	0.63
1:C:30:LEU:HD23	1:C:390:ILE:HD11	1.80	0.63
1:D:108:GLN:O	1:D:112:GLN:HG2	1.98	0.63
1:D:637:ARG:NH1	1:D:642:ASN:O	2.30	0.63
1:E:682:PHE:HB3	1:E:827:ILE:HB	1.80	0.62
1:F:6:ILE:CG2	1:F:12:ALA:HB2	2.28	0.62
1:F:27:ILE:HA	1:F:30:LEU:HD22	1.80	0.62
1:F:195:LYS:HB3	1:F:196:PHE:HD1	1.64	0.62
1:F:382:VAL:HG21	1:F:476:SER:HB2	1.80	0.62
1:A:549:VAL:O	1:A:552:MET:HE2	1.98	0.62
1:C:372:VAL:HG22	1:C:405:LEU:HD11	1.81	0.62
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.79	0.62
1:B:544:LEU:O	1:B:548:ILE:HG13	1.99	0.62
1:B:783:PRO:O	1:B:786:ILE:HG12	1.99	0.62
1:C:800:PRO:HG2	1:C:803:ALA:HB2	1.82	0.62
1:F:66:GLU:OE1	1:F:821:GLY:HA2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:455:PRO:HG2	1:F:880:SER:HA	1.82	0.62
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.81	0.62
1:B:637:ARG:HB3	1:B:642:ASN:HB3	1.81	0.62
1:C:841:MET:O	1:C:845:GLU:HG2	2.00	0.62
1:D:680:PHE:CE1	1:D:844:MET:HG3	2.35	0.62
1:F:777:ALA:O	1:F:781:MET:HE3	2.00	0.62
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.22	0.62
1:B:455:PRO:HG2	1:B:880:SER:OG	1.98	0.62
1:C:228:GLN:NE2	1:C:230:LEU:O	2.33	0.62
1:C:688:ALA:O	1:C:690:LEU:N	2.32	0.62
1:D:278:ILE:HG13	1:D:613:ASN:HB3	1.81	0.62
1:E:655:PHE:HA	1:E:659:LYS:HD3	1.81	0.62
1:A:45:ILE:HD12	1:A:90:ILE:HB	1.81	0.62
1:D:672:VAL:HB	1:D:673:GLU:CD	2.25	0.62
1:C:801:PHE:HA	1:C:804:PHE:CE2	2.34	0.62
1:E:294:ALA:HB3	1:E:297:ALA:HB2	1.82	0.62
1:A:219:LEU:HD13	1:B:783:PRO:HG3	1.82	0.62
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.33	0.62
1:F:947:GLU:HG3	1:F:948:PHE:CD1	2.35	0.62
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.82	0.61
1:A:705:GLU:HB3	1:A:847:LEU:HD22	1.81	0.61
1:A:919:ARG:NH2	1:A:990:VAL:O	2.29	0.61
1:A:1035:ARG:HG2	1:A:1036:LYS:H	1.65	0.61
1:B:654:ALA:O	1:B:658:ILE:HG12	2.00	0.61
1:F:343:THR:HG21	1:F:989:LEU:HD23	1.82	0.61
1:F:952:LEU:O	1:F:956:GLU:HB2	1.99	0.61
1:A:53:ASP:OD1	1:A:56:THR:OG1	2.15	0.61
1:B:240:LEU:HB2	1:B:246:PHE:CE1	2.35	0.61
1:D:582:ALA:HA	1:D:586:ARG:NH2	2.15	0.61
1:B:637:ARG:HA	1:B:642:ASN:HD22	1.65	0.61
1:D:201:VAL:HA	1:D:204:ILE:HD12	1.80	0.61
1:E:534:ILE:HG22	3:E:1101:LMT:H5'	1.83	0.61
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.83	0.61
1:C:404:LEU:HB3	1:C:478:MET:SD	2.40	0.61
1:F:188:MET:HE1	1:F:200:PRO:HG3	1.81	0.61
1:F:947:GLU:HG3	1:F:948:PHE:HD1	1.63	0.61
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.01	0.61
1:D:141:GLY:HA3	1:D:324:VAL:HG12	1.82	0.61
1:F:165:ALA:HB3	1:F:313:MET:HE1	1.82	0.61
1:A:240:LEU:HB2	1:A:246:PHE:HE1	1.66	0.61
1:B:753:ALA:O	1:B:775:SER:HB3	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:ARG:HG2	1:A:977:MET:HE2	1.82	0.61
1:B:658:ILE:O	1:B:659:LYS:HD2	2.01	0.61
1:D:888:LEU:HD13	1:D:901:VAL:HG13	1.82	0.61
1:E:519:MET:O	1:E:523:SER:OG	2.14	0.61
1:F:448:VAL:HG21	1:F:939:ALA:HB1	1.83	0.61
1:F:452:VAL:O	1:F:455:PRO:HD2	2.00	0.61
1:A:672:VAL:O	1:A:674:LEU:N	2.33	0.61
1:B:262:LEU:HG	1:B:268:ILE:HD11	1.81	0.61
1:C:3:ASN:O	1:C:6:ILE:N	2.33	0.61
1:D:251:LEU:HD11	1:D:262:LEU:HA	1.83	0.61
1:E:272:GLY:N	1:E:275:TYR:OH	2.29	0.61
1:F:973:ARG:HG2	1:F:977:MET:HE2	1.83	0.61
1:A:35:TYR:HB3	1:A:38:ILE:HD11	1.83	0.61
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.83	0.61
1:A:777:ALA:HB1	1:C:225:VAL:HG12	1.83	0.61
1:C:905:VAL:HG13	1:C:935:ILE:HG12	1.83	0.61
1:D:1034:SER:O	1:D:1034:SER:OG	2.13	0.61
1:A:150:THR:OG1	1:A:152:GLU:HG2	2.01	0.60
1:A:549:VAL:O	1:A:552:MET:HB3	2.01	0.60
1:B:174:ASP:HB3	1:B:292:LYS:HB2	1.82	0.60
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.83	0.60
1:E:187:TRP:HE3	1:E:775:SER:O	1.85	0.60
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.31	0.60
1:F:482:VAL:O	1:F:486:LEU:HG	2.00	0.60
1:B:9:PRO:HB3	1:B:495:THR:HG21	1.84	0.60
1:C:27:ILE:HA	1:C:30:LEU:HD22	1.83	0.60
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.83	0.60
1:C:574:THR:HG21	1:C:598:TYR:HE2	1.66	0.60
1:D:190:PRO:HG3	1:D:789:TRP:CZ2	2.36	0.60
1:D:281:PHE:CE1	1:D:608:SER:HB2	2.36	0.60
1:D:991:ILE:HG22	1:D:992:SER:H	1.66	0.60
1:F:363:ARG:HE	1:F:498:LYS:HB2	1.65	0.60
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.83	0.60
1:A:380:PHE:CE2	1:A:398:MET:HE3	2.36	0.60
1:E:682:PHE:CD2	1:E:827:ILE:HD12	2.37	0.60
1:F:382:VAL:HG11	1:F:476:SER:HB3	1.84	0.60
1:F:685:ILE:HD11	1:F:819:TYR:HD2	1.66	0.60
1:A:654:ALA:O	1:A:658:ILE:HG12	2.01	0.60
1:B:441:ALA:O	1:B:445:ILE:HG23	2.02	0.60
1:E:32:VAL:HG12	1:E:390:ILE:HB	1.81	0.60
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:952:LEU:O	1:C:956:GLU:HB2	2.01	0.60
1:A:744:ASN:O	1:A:748:THR:HG23	2.01	0.60
1:A:1026:PHE:CZ	1:A:1030:ARG:HG3	2.37	0.60
1:F:987:MET:HG3	1:F:1008:MET:HE1	1.82	0.60
1:B:983:ILE:HG23	1:B:1008:MET:HE2	1.83	0.60
1:C:135:SER:HB3	1:C:673:GLU:HA	1.82	0.60
1:C:155:SER:HB3	1:C:180:SER:H	1.67	0.60
1:C:973:ARG:HG2	1:C:977:MET:HE2	1.84	0.60
1:F:696:THR:HG23	1:F:699:ARG:HH12	1.67	0.60
1:C:698:ALA:O	1:C:701:GLN:HB3	2.02	0.60
1:E:9:PRO:HG2	1:E:10:ILE:HD12	1.83	0.60
1:F:83:ASP:HB2	1:F:87:THR:O	2.01	0.60
1:C:574:THR:HG23	1:C:627:ALA:HB3	1.84	0.60
1:C:945:ILE:HA	1:C:971:ARG:NH1	2.16	0.60
1:D:574:THR:HG23	1:D:627:ALA:HB3	1.84	0.60
1:D:658:ILE:HG13	1:D:659:LYS:HE2	1.84	0.60
1:E:26:ALA:O	1:E:30:LEU:HB2	2.01	0.60
1:E:901:VAL:HG23	1:E:942:ALA:HB3	1.82	0.60
1:A:144:ASN:ND2	1:A:146:ASP:OD2	2.35	0.60
1:A:960:LEU:HD21	1:A:1027:VAL:HG13	1.84	0.60
1:C:228:GLN:NE2	1:C:230:LEU:H	2.00	0.60
1:C:982:PHE:HD2	1:C:1011:MET:HG2	1.66	0.60
1:F:151:GLN:HE22	1:F:278:ILE:HA	1.66	0.60
1:F:764:ASP:OD1	1:F:765:ARG:HG3	2.02	0.60
1:A:185:ARG:HB3	1:A:187:TRP:NE1	2.17	0.59
1:A:1018:ALA:O	1:A:1022:VAL:HG23	2.02	0.59
1:B:139:VAL:O	1:B:326:PRO:HD2	2.01	0.59
1:B:195:LYS:HB3	1:B:196:PHE:HD1	1.67	0.59
1:D:32:VAL:HB	1:D:300:LEU:HD22	1.84	0.59
1:D:35:TYR:HB3	1:D:38:ILE:HD11	1.84	0.59
1:B:1037:ASN:N	1:B:1038:GLU:HB3	2.17	0.59
1:C:65:ILE:HG23	1:C:111:LEU:HD23	1.83	0.59
1:C:244:GLU:HG2	1:C:248:LYS:HE3	1.84	0.59
1:D:540:ARG:NH2	3:D:1102:LMT:O6B	2.35	0.59
1:D:544:LEU:HA	1:D:547:ILE:HD12	1.84	0.59
1:D:790:TYR:HB3	1:D:798:MET:HB3	1.85	0.59
1:D:925:VAL:O	1:D:928:GLN:N	2.35	0.59
1:E:355:MET:HE1	1:E:410:ILE:HG12	1.84	0.59
1:A:901:VAL:HG21	1:A:943:ILE:HG13	1.83	0.59
1:E:613:ASN:HD22	1:E:614:GLY:N	2.01	0.59
1:B:726:GLN:CD	1:B:812:GLY:HA3	2.27	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:HD12	1:C:101:ASP:HB3	1.83	0.59
1:B:733:GLN:HE22	1:B:743:ILE:HG21	1.67	0.59
1:C:465:ALA:HA	1:C:468:ARG:NH1	2.18	0.59
1:C:744:ASN:O	1:C:748:THR:HG23	2.02	0.59
1:D:578:LEU:HD21	1:D:590:VAL:HG21	1.84	0.59
1:F:284:GLN:HG3	1:F:285:PRO:HD2	1.85	0.59
1:F:356:TYR:HA	1:F:365:THR:HG21	1.84	0.59
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.38	0.59
1:A:736:ALA:HB1	1:A:746:ILE:HD11	1.84	0.59
1:E:1016:VAL:HG13	3:E:1101:LMT:H112	1.84	0.59
1:F:885:PHE:HD2	1:F:886:LEU:HD22	1.66	0.59
1:A:758:TYR:OH	1:A:761:ASP:OD1	2.16	0.59
1:D:166:ILE:HD11	1:D:310:LEU:HD13	1.85	0.59
1:D:781:MET:HB3	1:F:228:GLN:NE2	2.17	0.59
1:D:971:ARG:CZ	1:D:971:ARG:HB3	2.32	0.59
1:B:344:LEU:HD13	1:B:376:LEU:HD13	1.84	0.59
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.38	0.59
1:E:56:THR:O	1:E:60:THR:OG1	2.18	0.59
1:F:144:ASN:OD1	1:F:148:THR:HA	2.02	0.59
1:A:593:GLU:OE2	1:A:659:LYS:NZ	2.35	0.59
1:D:375:VAL:HG21	1:D:481:SER:HA	1.85	0.59
1:F:412:VAL:HG13	1:F:435:MET:HE1	1.83	0.59
1:B:340:VAL:HG11	1:B:395:MET:HE3	1.84	0.59
1:C:586:ARG:O	1:C:589:LYS:HB2	2.03	0.59
1:D:159:ALA:HB2	1:D:177:LEU:HD11	1.85	0.59
1:F:344:LEU:O	1:F:348:ILE:HG13	2.02	0.59
1:F:979:SER:CB	1:F:1015:THR:HG21	2.33	0.59
1:A:38:ILE:CG2	1:A:462:SER:HB2	2.33	0.58
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.84	0.58
1:D:519:MET:O	1:D:523:SER:OG	2.18	0.58
1:F:324:VAL:HG23	1:F:326:PRO:HD3	1.84	0.58
1:A:983:ILE:HG23	1:A:1008:MET:HE2	1.85	0.58
1:C:943:ILE:O	1:C:947:GLU:HB3	2.03	0.58
1:E:327:TYR:HD1	1:E:628:PHE:CZ	2.21	0.58
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.84	0.58
1:E:1032:ARG:NE	1:E:1032:ARG:HA	2.17	0.58
1:A:375:VAL:HG21	1:A:481:SER:HA	1.83	0.58
1:A:900:SER:HB3	1:A:1029:VAL:HG21	1.85	0.58
1:E:531:VAL:O	1:E:534:ILE:HG13	2.03	0.58
1:A:1016:VAL:HG13	3:A:1102:LMT:H112	1.85	0.58
1:B:1033:PHE:CD1	1:B:1034:SER:HB3	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:530:SER:HG	3:F:1101:LMT:H2O2	1.48	0.58
1:B:501:ALA:O	1:B:504:ASP:HB2	2.04	0.58
1:C:272:GLY:N	1:C:275:TYR:OH	2.28	0.58
1:D:36:PRO:O	1:D:38:ILE:HG13	2.04	0.58
1:D:144:ASN:HA	1:D:320:GLY:O	2.03	0.58
1:E:911:GLY:HA3	1:E:1013:THR:OG1	2.03	0.58
1:A:112:GLN:OE1	1:A:115:MET:HG3	2.03	0.58
1:B:562:SER:HB3	1:B:924:ASP:HB3	1.85	0.58
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.85	0.58
1:C:568:ASP:O	1:C:634:TRP:HH2	1.87	0.58
1:C:682:PHE:HE2	1:C:702:LEU:HD11	1.69	0.58
1:E:705:GLU:HB3	1:E:847:LEU:HD22	1.83	0.58
1:A:23:GLY:HA2	1:A:381:ALA:HB2	1.86	0.58
1:A:210:GLN:HE22	1:A:250:LEU:HB3	1.68	0.58
1:A:869:SER:OG	1:A:870:GLY:N	2.35	0.58
1:B:979:SER:OG	1:B:1015:THR:HG21	2.03	0.58
1:C:203:VAL:O	1:C:207:ILE:HG13	2.03	0.58
1:D:38:ILE:CG2	1:D:462:SER:HB2	2.34	0.58
1:D:102:ILE:HD12	1:F:101:ASP:HB3	1.86	0.58
1:F:195:LYS:HZ1	1:F:196:PHE:HE1	1.52	0.58
1:A:18:ILE:HG13	1:B:886:LEU:HD23	1.85	0.58
1:A:186:ILE:HD11	1:A:246:PHE:HD2	1.69	0.58
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.85	0.58
1:D:563:PHE:HD2	1:D:671:ILE:HD13	1.69	0.58
1:D:698:ALA:HB1	1:D:851:LEU:HD13	1.86	0.58
1:F:379:THR:HG23	1:F:476:SER:OG	2.04	0.58
1:F:775:SER:OG	1:F:776:GLU:O	2.20	0.58
1:A:878:ALA:O	1:A:882:ILE:HG12	2.03	0.58
1:B:99:ASP:HB3	1:B:102:ILE:HB	1.86	0.58
1:B:442:LEU:O	1:B:445:ILE:HG13	2.04	0.58
1:C:332:PHE:HD1	1:C:634:TRP:CZ2	2.22	0.58
1:D:101:ASP:OD1	1:D:131:LYS:HE2	2.03	0.58
1:A:575:MET:CG	1:A:664:PHE:HB2	2.33	0.57
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.85	0.57
1:C:356:TYR:C	1:C:358:PHE:N	2.62	0.57
1:E:888:LEU:HD21	1:E:943:ILE:HD11	1.85	0.57
1:B:163:LYS:HD2	1:B:177:LEU:HG	1.85	0.57
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.86	0.57
1:C:683:GLU:HB3	1:C:858:ASP:HB3	1.86	0.57
1:C:740:GLY:O	1:C:794:ALA:N	2.36	0.57
1:D:170:SER:OG	1:E:74:ASN:N	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:SER:O	1:D:438:ILE:HG12	2.04	0.57
1:E:1032:ARG:HA	1:E:1032:ARG:HE	1.68	0.57
1:F:242:SER:HB2	1:F:245:GLU:HG3	1.86	0.57
1:B:47:ALA:HB2	1:B:127:VAL:HG13	1.85	0.57
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.39	0.57
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.84	0.57
1:C:253:VAL:HG22	1:C:259:ARG:HG2	1.86	0.57
1:C:746:ILE:HG13	1:C:747:ASN:N	2.19	0.57
1:F:453:PHE:O	1:F:471:SER:OG	2.19	0.57
1:A:971:ARG:C	1:A:974:PRO:HD2	2.29	0.57
1:C:311:ALA:HA	1:C:314:GLU:CD	2.30	0.57
1:C:730:ASP:OD2	1:C:808:ARG:NH2	2.36	0.57
1:C:947:GLU:HG3	1:C:948:PHE:N	2.19	0.57
1:D:351:VAL:HG22	1:D:981:ALA:HB1	1.85	0.57
1:E:375:VAL:O	1:E:379:THR:OG1	2.22	0.57
1:F:562:SER:HB2	1:F:924:ASP:HB3	1.86	0.57
1:E:574:THR:HG23	1:E:627:ALA:HB3	1.85	0.57
1:F:435:MET:HE3	1:F:490:PRO:HB3	1.87	0.57
1:B:404:LEU:HD21	1:B:449:LEU:HD22	1.85	0.57
1:E:24:GLY:O	1:E:27:ILE:HG22	2.03	0.57
1:E:1013:THR:O	1:E:1017:LEU:HB2	2.04	0.57
1:A:728:LYS:NZ	1:C:236:ALA:O	2.30	0.57
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.40	0.57
1:C:388:PHE:CE2	1:C:472:ILE:HG21	2.39	0.57
1:D:790:TYR:HD1	1:D:800:PRO:HA	1.69	0.57
1:D:910:ILE:O	1:D:914:LEU:HB2	2.05	0.57
1:E:173:GLY:O	1:F:70:ASN:ND2	2.35	0.57
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.70	0.57
1:A:960:LEU:O	1:A:964:THR:HG23	2.05	0.57
2:A:1101:ERY:H352	2:A:1101:ERY:H71	1.87	0.57
1:A:146:ASP:OD2	1:A:146:ASP:N	2.37	0.57
1:A:368:PRO:HG3	1:A:413:VAL:HG21	1.87	0.57
1:C:47:ALA:HB3	1:C:88:VAL:HG13	1.86	0.57
1:C:587:THR:HG21	1:C:622:GLN:O	2.05	0.57
1:D:878:ALA:O	1:D:882:ILE:HG12	2.03	0.57
1:F:140:VAL:HG23	1:F:291:ILE:HD13	1.87	0.57
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.40	0.57
1:B:907:LEU:HG	1:B:1017:LEU:HD23	1.87	0.57
1:C:66:GLU:OE2	1:C:80:SER:OG	2.14	0.57
1:D:3:ASN:O	1:D:6:ILE:N	2.37	0.57
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:361:ASN:HD21	1:F:498:LYS:HD3	1.70	0.57
1:F:746:ILE:HG22	1:F:791:VAL:HG21	1.87	0.57
1:D:744:ASN:O	1:D:748:THR:HG23	2.05	0.56
1:E:210:GLN:HG2	1:F:733:GLN:NE2	2.19	0.56
1:E:355:MET:CE	1:E:410:ILE:HG12	2.34	0.56
1:D:49:TYR:HB3	1:D:57:VAL:HG22	1.86	0.56
1:D:728:LYS:HB2	1:D:810:GLU:CD	2.31	0.56
1:E:158:VAL:HG11	1:E:177:LEU:HD21	1.85	0.56
1:A:187:TRP:HE3	1:A:775:SER:O	1.88	0.56
1:B:45:ILE:HD11	1:B:69:MET:HE2	1.87	0.56
1:B:188:MET:HA	1:B:266:ALA:HB2	1.87	0.56
1:B:535:LEU:HD22	1:B:1027:VAL:HG11	1.87	0.56
1:D:113:LEU:HD11	1:F:128:SER:HB3	1.87	0.56
1:D:253:VAL:HG12	1:D:259:ARG:HG2	1.87	0.56
1:E:1041:GLU:HB3	1:E:1042:HIS:HB2	1.86	0.56
1:F:434:SER:O	1:F:438:ILE:HG12	2.05	0.56
1:F:894:SER:HG	1:F:896:SER:HG	1.52	0.56
1:F:1039:ASP:HB3	1:F:1040:ILE:HA	1.86	0.56
1:B:764:ASP:OD1	1:B:765:ARG:HG3	2.05	0.56
1:D:157:TYR:CZ	1:D:318:PRO:HD3	2.41	0.56
1:D:544:LEU:O	1:D:548:ILE:HG13	2.05	0.56
1:E:460:GLY:O	1:E:463:THR:OG1	2.23	0.56
1:E:683:GLU:HG2	1:E:819:TYR:CD2	2.40	0.56
1:F:574:THR:HG23	1:F:627:ALA:HB3	1.87	0.56
1:F:925:VAL:O	1:F:928:GLN:N	2.38	0.56
1:A:482:VAL:O	1:A:486:LEU:HG	2.06	0.56
1:A:888:LEU:HD13	1:A:901:VAL:CG1	2.36	0.56
1:B:183:ALA:O	1:B:270:LEU:HD12	2.05	0.56
1:B:971:ARG:HB3	1:B:971:ARG:CZ	2.34	0.56
1:C:752:ALA:O	1:C:774:MET:HA	2.06	0.56
1:E:908:GLY:HA2	1:E:1014:ALA:HB2	1.87	0.56
1:F:698:ALA:O	1:F:701:GLN:HB3	2.06	0.56
1:A:637:ARG:HB3	1:A:642:ASN:HB3	1.88	0.56
1:C:3:ASN:HA	1:C:6:ILE:HB	1.88	0.56
1:D:393:LEU:HB3	1:D:470:PHE:CE1	2.41	0.56
1:D:844:MET:HA	1:D:844:MET:HE2	1.87	0.56
1:E:545:TYR:CE2	1:E:1025:PHE:HZ	2.22	0.56
1:E:606:VAL:HA	1:E:631:LEU:HD23	1.88	0.56
1:F:53:ASP:OD1	1:F:56:THR:OG1	2.18	0.56
1:B:974:PRO:HA	1:B:977:MET:HE3	1.88	0.56
1:D:194:ASN:CG	1:D:790:TYR:HD2	2.14	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ASN:O	1:D:760:ASN:ND2	2.39	0.56
1:E:324:VAL:HG13	1:E:326:PRO:HD3	1.86	0.56
1:F:654:ALA:O	1:F:658:ILE:HG12	2.05	0.56
1:A:719:ASN:HB2	1:A:828:LEU:HG	1.88	0.56
1:A:953:MET:HE2	1:A:963:ALA:HB3	1.87	0.56
1:A:1040:ILE:HG23	1:A:1041:GLU:H	1.70	0.56
1:E:537:SER:OG	1:E:540:ARG:NH2	2.39	0.56
1:E:559:LEU:HD21	1:E:922:THR:HA	1.87	0.56
1:E:607:GLU:HA	1:E:632:LYS:HE2	1.87	0.56
1:E:680:PHE:CD1	1:E:859:TRP:HZ3	2.17	0.56
1:F:2:PRO:O	1:F:5:PHE:HB3	2.06	0.56
1:F:817:GLU:HB2	1:F:824:SER:O	2.06	0.56
1:F:1016:VAL:HG13	3:F:1101:LMT:H112	1.86	0.56
1:A:462:SER:O	1:A:466:ILE:HG12	2.06	0.56
1:A:897:ILE:HA	1:A:1029:VAL:HG11	1.86	0.56
1:D:235:ILE:O	1:E:728:LYS:HD2	2.06	0.56
1:D:435:MET:O	1:D:439:GLN:HB2	2.06	0.56
1:E:445:ILE:HD12	1:E:449:LEU:HD12	1.88	0.56
1:E:1018:ALA:O	1:E:1022:VAL:HG23	2.06	0.56
1:D:948:PHE:O	1:D:952:LEU:HG	2.05	0.56
1:D:959:GLY:HA2	1:D:1039:ASP:HA	1.87	0.56
1:E:690:LEU:HD22	1:E:694:LYS:HG2	1.87	0.56
1:F:599:LEU:O	1:F:603:LYS:HG2	2.06	0.56
1:B:146:ASP:HB2	1:B:148:THR:OG1	2.06	0.55
1:B:652:THR:CG2	1:B:665:ALA:H	2.20	0.55
1:C:453:PHE:HB3	1:C:471:SER:HA	1.87	0.55
1:F:504:ASP:C	1:F:506:GLY:H	2.13	0.55
1:A:519:MET:O	1:A:523:SER:OG	2.21	0.55
1:B:616:GLY:HA2	1:B:626:ILE:HD13	1.89	0.55
1:B:847:LEU:O	1:B:850:LYS:HB2	2.05	0.55
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.88	0.55
1:A:423:GLU:HB2	1:A:425:LEU:HD12	1.89	0.55
1:B:1013:THR:O	1:B:1017:LEU:HB2	2.06	0.55
1:D:913:LEU:HD23	1:D:927:PHE:HZ	1.71	0.55
1:F:74:ASN:O	1:F:94:PHE:HD2	1.90	0.55
1:A:617:ALA:HA	2:A:1101:ERY:H353	1.88	0.55
1:B:172:VAL:HG13	1:B:291:ILE:HG23	1.87	0.55
1:B:685:ILE:HD11	1:B:819:TYR:CD2	2.41	0.55
1:C:860:THR:HA	1:C:864:TYR:HB2	1.87	0.55
1:D:293:LEU:HD22	1:D:297:ALA:HB3	1.89	0.55
1:E:337:ILE:HA	1:E:395:MET:HE2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.87	0.55
1:A:846:GLN:O	1:A:849:SER:OG	2.19	0.55
1:C:110:LYS:O	1:C:113:LEU:HB2	2.06	0.55
1:C:600:THR:O	1:C:603:LYS:HG3	2.06	0.55
1:E:281:PHE:HD1	1:E:610:PHE:HD1	1.55	0.55
1:E:354:VAL:HG22	1:E:980:LEU:HD23	1.89	0.55
1:E:591:LEU:HD13	1:E:611:ALA:HB1	1.88	0.55
1:E:1019:ILE:HG13	1:E:1020:PHE:CD1	2.41	0.55
1:A:946:VAL:HG13	1:A:1026:PHE:CD1	2.42	0.55
1:B:119:PRO:HG2	1:B:122:VAL:HB	1.89	0.55
1:B:555:LEU:HB3	1:B:913:LEU:HB3	1.88	0.55
1:D:583:THR:OG1	1:D:586:ARG:HG3	2.06	0.55
1:E:281:PHE:CE1	1:E:608:SER:HB2	2.42	0.55
1:E:1019:ILE:HG13	1:E:1020:PHE:HD1	1.71	0.55
1:A:155:SER:HB3	1:A:180:SER:H	1.71	0.55
1:A:584:GLN:HB2	1:A:622:GLN:HG2	1.87	0.55
1:C:65:ILE:HD11	1:C:118:LEU:HD11	1.89	0.55
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.41	0.55
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.87	0.55
1:F:219:LEU:O	1:F:231:ASN:ND2	2.38	0.55
1:A:976:LEU:O	1:A:980:LEU:HB2	2.06	0.55
1:A:1033:PHE:HD2	1:A:1034:SER:N	2.04	0.55
1:C:278:ILE:HG13	1:C:613:ASN:HB3	1.88	0.55
1:C:671:ILE:HG21	1:C:674:LEU:HD12	1.88	0.55
1:C:1034:SER:OG	1:C:1038:GLU:O	2.22	0.55
1:E:712:MET:HE3	1:E:839:GLU:HB3	1.88	0.55
1:E:909:VAL:HA	1:E:931:LEU:HD21	1.89	0.55
1:F:947:GLU:HG3	1:F:948:PHE:N	2.21	0.55
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.89	0.55
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.88	0.55
1:B:744:ASN:O	1:B:748:THR:HG23	2.06	0.55
1:C:36:PRO:O	1:C:38:ILE:HG13	2.07	0.55
1:C:463:THR:HG23	1:C:925:VAL:HG22	1.89	0.55
1:C:971:ARG:NH2	1:C:975:ILE:HD11	2.22	0.55
1:D:400:LEU:HD11	1:D:1007:VAL:HG21	1.89	0.55
1:E:199:THR:HG21	1:E:792:ARG:H	1.72	0.55
1:E:388:PHE:CE2	1:E:472:ILE:HG21	2.42	0.55
1:F:144:ASN:O	1:F:284:GLN:NE2	2.40	0.55
1:B:985:GLY:O	1:B:988:PRO:HD2	2.07	0.55
1:C:941:ASN:ND2	1:C:1015:THR:HG22	2.22	0.55
1:D:175:VAL:HG11	1:D:289:LEU:HD22	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:LYS:HE3	1:E:260:VAL:HG21	1.89	0.55
1:E:544:LEU:O	1:E:548:ILE:HG13	2.07	0.55
1:F:197:GLN:HA	1:F:798:MET:SD	2.47	0.55
1:F:644:VAL:O	1:F:648:THR:HG23	2.06	0.55
1:F:892:TYR:C	1:F:894:SER:H	2.14	0.55
1:B:448:VAL:HG13	1:B:884:VAL:HG22	1.89	0.54
1:C:735:LYS:O	1:C:739:LEU:HG	2.06	0.54
1:C:743:ILE:H	1:C:743:ILE:HD12	1.73	0.54
1:D:393:LEU:HD22	1:D:470:PHE:HE1	1.72	0.54
1:E:702:LEU:HD11	1:E:847:LEU:HB3	1.88	0.54
1:F:705:GLU:HA	1:F:708:LYS:NZ	2.22	0.54
1:A:230:LEU:HG	1:A:231:ASN:N	2.21	0.54
1:B:235:ILE:O	1:C:728:LYS:HD2	2.07	0.54
1:D:45:ILE:HA	1:D:128:SER:O	2.06	0.54
1:F:590:VAL:O	1:F:593:GLU:HB2	2.07	0.54
1:B:743:ILE:HA	1:B:746:ILE:HD12	1.89	0.54
1:D:583:THR:HG21	1:F:229:GLN:HA	1.88	0.54
1:D:888:LEU:HD22	1:D:901:VAL:HG11	1.89	0.54
1:E:396:PHE:HD1	1:E:926:TYR:HE2	1.55	0.54
1:F:559:LEU:HD23	1:F:560:PRO:CD	2.37	0.54
1:F:1021:PHE:HB3	1:F:1025:PHE:CE1	2.43	0.54
1:E:82:SER:HA	1:E:88:VAL:HG22	1.88	0.54
1:F:358:PHE:CD2	1:F:977:MET:HG3	2.41	0.54
1:D:687:GLN:HG2	1:F:316:PHE:CD1	2.42	0.54
1:D:969:ARG:NH1	1:D:970:MET:HB3	2.23	0.54
1:F:356:TYR:C	1:F:358:PHE:H	2.14	0.54
1:C:307:ARG:NH2	1:C:314:GLU:OE2	2.38	0.54
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.89	0.54
1:D:158:VAL:HA	1:D:162:MET:HE2	1.89	0.54
1:F:166:ILE:HG22	1:F:175:VAL:HG21	1.90	0.54
1:F:905:VAL:HG13	1:F:935:ILE:HG12	1.90	0.54
1:B:531:VAL:O	1:B:534:ILE:HG13	2.08	0.54
1:C:200:PRO:HB2	1:C:749:THR:HG22	1.89	0.54
1:C:671:ILE:HD13	1:C:674:LEU:HD12	1.90	0.54
1:D:420:MET:HB3	1:D:500:ILE:HB	1.90	0.54
1:A:6:ILE:HD11	1:A:432:ARG:HE	1.73	0.54
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.89	0.54
1:A:685:ILE:HD11	1:A:819:TYR:HD2	1.72	0.54
1:B:492:LEU:O	1:B:496:MET:HG2	2.08	0.54
1:D:137:LEU:HD23	1:D:291:ILE:HG22	1.89	0.54
1:F:121:GLU:O	1:F:124:GLN:HG2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:PHE:HB3	1:B:628:PHE:HB3	1.90	0.54
1:B:711:ASP:OD2	1:F:850:LYS:NZ	2.40	0.54
1:F:159:ALA:HB2	1:F:177:LEU:HD11	1.88	0.54
1:F:841:MET:O	1:F:845:GLU:HG2	2.08	0.54
1:C:356:TYR:HA	1:C:365:THR:HG21	1.89	0.54
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.89	0.54
1:E:391:ASN:O	1:E:395:MET:HG2	2.07	0.54
1:E:680:PHE:HB2	1:E:863:SER:OG	2.07	0.54
1:E:776:GLU:HB3	1:E:779:TYR:CD1	2.43	0.54
1:F:775:SER:OG	1:F:780:ARG:HG2	2.08	0.54
1:A:159:ALA:HB2	1:A:177:LEU:HD11	1.89	0.53
1:A:685:ILE:HD11	1:A:819:TYR:CD2	2.43	0.53
1:B:932:LEU:HD23	1:B:935:ILE:HD12	1.90	0.53
1:C:356:TYR:O	1:C:358:PHE:N	2.41	0.53
1:F:187:TRP:HE3	1:F:775:SER:O	1.91	0.53
1:F:188:MET:HA	1:F:266:ALA:CB	2.37	0.53
1:F:559:LEU:HD23	1:F:560:PRO:HD2	1.89	0.53
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.90	0.53
1:A:913:LEU:HD23	1:A:927:PHE:CZ	2.44	0.53
1:B:187:TRP:HE3	1:B:775:SER:O	1.91	0.53
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.08	0.53
1:E:680:PHE:HE2	1:E:829:GLY:HA3	1.73	0.53
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.91	0.53
1:C:58:GLN:HA	1:C:62:THR:HB	1.88	0.53
1:C:75:LEU:HD11	1:C:92:LEU:HD12	1.90	0.53
1:C:414:GLU:HG3	1:C:977:MET:HE1	1.90	0.53
1:C:456:MET:HB3	1:C:876:LEU:HD21	1.89	0.53
1:C:913:LEU:HD23	1:C:927:PHE:HZ	1.72	0.53
1:D:61:VAL:HG21	1:D:122:VAL:HG21	1.89	0.53
1:E:447:MET:HB3	1:E:887:CYS:SG	2.48	0.53
1:F:113:LEU:O	1:F:116:PRO:HD2	2.07	0.53
1:F:195:LYS:NZ	1:F:196:PHE:HE1	2.06	0.53
1:F:272:GLY:N	1:F:275:TYR:OH	2.34	0.53
3:F:1101:LMT:H2O1	3:F:1101:LMT:H3O2	1.56	0.53
1:A:801:PHE:HA	1:A:804:PHE:CE2	2.44	0.53
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.08	0.53
1:B:327:TYR:HB2	1:B:628:PHE:HE2	1.74	0.53
1:C:591:LEU:HD11	1:C:625:GLY:HA3	1.89	0.53
1:C:644:VAL:HG11	1:C:667:ASN:HB2	1.91	0.53
1:D:587:THR:OG1	1:D:622:GLN:O	2.19	0.53
1:D:676:THR:O	3:D:1103:LMT:O6B	2.14	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:TYR:CD1	1:E:628:PHE:HZ	2.24	0.53
1:F:913:LEU:HD23	1:F:927:PHE:HZ	1.73	0.53
1:A:41:PRO:HD3	1:A:96:SER:HA	1.91	0.53
1:B:5:PHE:CE1	1:B:487:ILE:HG12	2.44	0.53
1:B:485:ALA:O	1:B:490:PRO:HD3	2.08	0.53
1:D:155:SER:HB3	1:D:180:SER:H	1.73	0.53
1:D:156:ASP:OD2	1:D:769:LYS:NZ	2.32	0.53
1:D:366:LEU:HA	1:D:369:THR:HB	1.91	0.53
1:E:102:ILE:O	1:E:106:GLN:HG3	2.09	0.53
1:E:549:VAL:O	1:E:552:MET:HB3	2.08	0.53
1:F:971:ARG:C	1:F:974:PRO:HD2	2.33	0.53
1:A:418:ARG:NH2	1:A:948:PHE:HE2	2.06	0.53
1:B:166:ILE:HD11	1:B:310:LEU:CD1	2.39	0.53
1:C:293:LEU:HD11	1:C:297:ALA:O	2.07	0.53
1:D:32:VAL:HG22	1:D:390:ILE:HB	1.89	0.53
1:D:712:MET:SD	1:D:835:LYS:HE2	2.49	0.53
1:E:743:ILE:H	1:E:743:ILE:HD12	1.74	0.53
1:B:23:GLY:HA2	1:B:381:ALA:HB2	1.90	0.53
1:B:352:PHE:C	1:B:352:PHE:CD2	2.87	0.53
1:B:950:LYS:HZ1	1:B:1030:ARG:CZ	2.21	0.53
1:E:144:ASN:ND2	1:E:149:MET:HE3	2.24	0.53
1:E:225:VAL:HG12	1:F:777:ALA:HB1	1.91	0.53
1:E:589:LYS:O	1:E:592:ASN:HB2	2.08	0.53
1:F:979:SER:OG	1:F:1015:THR:HG21	2.08	0.53
1:C:960:LEU:O	1:C:964:THR:HG23	2.08	0.53
1:D:99:ASP:HB3	1:D:102:ILE:HB	1.91	0.53
1:D:781:MET:HE3	1:F:228:GLN:HE21	1.72	0.53
1:E:407:ASP:O	1:E:411:VAL:HG23	2.08	0.53
1:F:184:MET:HB2	1:F:762:PHE:CE2	2.44	0.53
1:B:682:PHE:HB3	1:B:827:ILE:HB	1.91	0.53
1:E:38:ILE:HG22	1:E:462:SER:HB3	1.91	0.53
1:E:213:GLN:HE21	1:E:239:ARG:HG3	1.72	0.53
1:F:446:ALA:HA	1:F:478:MET:HE2	1.90	0.53
1:F:960:LEU:HD21	1:F:1027:VAL:HA	1.91	0.53
1:A:568:ASP:CG	1:A:637:ARG:HH22	2.17	0.53
1:D:274:ASN:ND2	1:D:276:ASP:OD2	2.38	0.53
1:F:636:ASP:C	1:F:638:PRO:HD3	2.33	0.53
1:F:727:PHE:CE1	1:F:783:PRO:HB3	2.43	0.53
1:A:533:GLY:O	1:A:536:ARG:HB2	2.08	0.52
1:C:53:ASP:OD1	1:C:56:THR:OG1	2.08	0.52
1:C:686:ASP:HB3	1:C:823:PRO:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:696:THR:HA	1:D:699:ARG:NH1	2.25	0.52
1:E:568:ASP:O	1:E:634:TRP:HZ3	1.92	0.52
1:F:188:MET:HB3	1:F:193:LEU:HD11	1.92	0.52
1:F:414:GLU:HG2	1:F:973:ARG:NH1	2.24	0.52
1:F:456:MET:HB3	1:F:876:LEU:HD21	1.90	0.52
1:F:616:GLY:HA2	1:F:626:ILE:HD12	1.89	0.52
1:A:648:THR:HB	1:A:665:ALA:O	2.09	0.52
1:A:937:LEU:O	1:A:940:LYS:HB3	2.08	0.52
1:B:892:TYR:O	1:B:893:GLU:HB2	2.08	0.52
1:C:841:MET:HG2	1:C:859:TRP:CH2	2.44	0.52
1:D:272:GLY:N	1:D:275:TYR:OH	2.40	0.52
1:D:400:LEU:HD23	1:D:929:VAL:HG12	1.90	0.52
1:E:910:ILE:O	1:E:914:LEU:HB2	2.09	0.52
1:A:575:MET:HE3	1:A:666:PHE:CZ	2.44	0.52
1:A:857:TYR:HE2	1:C:312:LYS:NZ	2.08	0.52
1:C:427:PRO:HD3	1:C:499:PRO:HB3	1.91	0.52
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.44	0.52
1:D:728:LYS:HG2	1:D:808:ARG:CZ	2.39	0.52
1:E:726:GLN:CD	1:E:812:GLY:HA3	2.34	0.52
1:F:576:VAL:HG22	1:F:663:VAL:HG13	1.91	0.52
1:F:587:THR:OG1	1:F:613:ASN:ND2	2.38	0.52
1:A:781:MET:HE1	1:C:225:VAL:H	1.75	0.52
1:E:441:ALA:HA	1:E:891:LEU:HD21	1.90	0.52
1:F:463:THR:HG22	1:F:467:TYR:CZ	2.44	0.52
1:B:165:ALA:HB3	1:B:313:MET:CE	2.40	0.52
1:B:778:LYS:HG3	1:B:779:TYR:CE1	2.45	0.52
1:B:971:ARG:O	1:B:975:ILE:HG12	2.10	0.52
1:C:699:ARG:HD3	1:C:825:MET:SD	2.48	0.52
1:D:47:ALA:HB2	1:D:127:VAL:HG13	1.91	0.52
1:D:545:TYR:HB2	1:D:1021:PHE:CE2	2.44	0.52
1:E:521:GLU:HA	1:E:524:THR:HG22	1.91	0.52
1:E:968:VAL:HG21	1:E:1023:PRO:HG3	1.91	0.52
1:F:343:THR:HG21	1:F:989:LEU:CD2	2.39	0.52
1:F:588:GLN:NE2	1:F:592:ASN:OD1	2.43	0.52
1:F:937:LEU:HD11	1:F:982:PHE:CE2	2.45	0.52
1:A:318:PRO:HD2	1:A:321:LEU:HG	1.91	0.52
1:B:9:PRO:HG2	1:B:10:ILE:HD12	1.92	0.52
1:B:344:LEU:O	1:B:348:ILE:HG13	2.08	0.52
1:E:375:VAL:HG13	1:E:480:LEU:HB3	1.91	0.52
1:F:77:TYR:HB2	1:F:819:TYR:CE1	2.45	0.52
1:F:412:VAL:O	1:F:416:VAL:HG23	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:568:ASP:OD1	1:F:637:ARG:NH1	2.41	0.52
1:F:1040:ILE:CA	1:F:1041:GLU:HB2	2.31	0.52
1:A:901:VAL:HG21	1:A:943:ILE:CG1	2.40	0.52
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.44	0.52
1:C:841:MET:HE3	1:C:859:TRP:CE2	2.44	0.52
1:D:184:MET:HB3	1:D:771:VAL:HG13	1.92	0.52
1:E:974:PRO:HA	1:E:977:MET:HE3	1.92	0.52
1:A:138:MET:HE2	1:A:328:ASP:OD1	2.10	0.52
1:B:185:ARG:HD2	1:B:772:TYR:HB2	1.92	0.52
1:B:228:GLN:OE1	1:C:781:MET:HB3	2.09	0.52
1:B:544:LEU:HD23	1:B:1021:PHE:CZ	2.45	0.52
1:C:5:PHE:CD2	1:C:6:ILE:HG12	2.45	0.52
1:C:354:VAL:HG23	1:C:984:LEU:HD12	1.90	0.52
1:C:382:VAL:HG21	1:C:476:SER:HB2	1.91	0.52
1:C:531:VAL:O	1:C:534:ILE:HG13	2.09	0.52
1:C:610:PHE:O	1:C:627:ALA:HA	2.10	0.52
1:C:1036:LYS:O	1:C:1037:ASN:ND2	2.39	0.52
1:D:146:ASP:HB2	1:D:148:THR:HG23	1.91	0.52
1:E:185:ARG:HB3	1:E:187:TRP:NE1	2.25	0.52
1:E:375:VAL:HG13	1:E:480:LEU:CB	2.40	0.52
1:E:534:ILE:CD1	1:E:1024:VAL:HG22	2.40	0.52
1:E:678:THR:HA	1:E:837:THR:HG1	1.74	0.52
1:E:564:LEU:HD13	1:E:671:ILE:HD12	1.92	0.52
1:F:13:TRP:CH2	1:F:370:ILE:HD13	2.45	0.52
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.45	0.52
1:F:183:ALA:O	1:F:270:LEU:HD12	2.10	0.52
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.92	0.52
1:A:743:ILE:H	1:A:743:ILE:HD12	1.75	0.52
1:A:910:ILE:O	1:A:914:LEU:HB2	2.10	0.52
1:B:363:ARG:HD2	1:B:498:LYS:HG3	1.92	0.52
1:B:418:ARG:HD3	1:B:970:MET:HB2	1.91	0.52
1:D:768:VAL:HG12	1:E:63:GLN:OE1	2.09	0.52
1:E:579:PRO:HD3	1:E:661:ALA:HB2	1.92	0.52
1:F:982:PHE:HD2	1:F:1011:MET:HG2	1.74	0.52
1:A:391:ASN:O	1:A:395:MET:HG2	2.10	0.51
1:A:897:ILE:HD11	1:A:1030:ARG:HD3	1.92	0.51
1:B:185:ARG:HH11	1:B:772:TYR:HB3	1.76	0.51
1:C:453:PHE:HD2	1:C:456:MET:CE	2.23	0.51
1:C:743:ILE:HA	1:C:746:ILE:HG23	1.92	0.51
1:F:64:VAL:HG12	1:F:114:ALA:HB1	1.91	0.51
1:F:143:ILE:O	1:F:321:LEU:HD22	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:447:MET:SD	1:F:887:CYS:HB3	2.50	0.51
1:F:549:VAL:O	1:F:552:MET:HB3	2.10	0.51
1:B:766:GLY:O	1:C:59:ASP:HB2	2.10	0.51
1:C:153:ASP:OD2	1:C:182:TYR:OH	2.28	0.51
1:D:672:VAL:HB	1:D:673:GLU:OE2	2.10	0.51
1:A:775:SER:HB3	1:A:780:ARG:HD3	1.92	0.51
1:B:602:GLU:HB3	1:B:606:VAL:HG23	1.92	0.51
1:D:242:SER:OG	1:D:245:GLU:HG2	2.10	0.51
1:D:418:ARG:CZ	1:D:970:MET:HE2	2.41	0.51
1:E:363:ARG:HD3	1:E:496:MET:O	2.11	0.51
1:E:423:GLU:OE1	1:E:433:LYS:HE3	2.11	0.51
1:F:34:GLN:HB2	1:F:333:VAL:CG2	2.38	0.51
1:A:112:GLN:HG3	1:B:112:GLN:CD	2.36	0.51
1:A:574:THR:HG21	1:A:598:TYR:CE2	2.46	0.51
1:A:575:MET:HG3	1:A:664:PHE:HB2	1.92	0.51
1:A:953:MET:HE1	1:A:1026:PHE:HE2	1.76	0.51
1:B:418:ARG:CZ	1:B:418:ARG:HB3	2.40	0.51
1:B:431:THR:HG21	1:B:494:ALA:HB2	1.92	0.51
1:C:925:VAL:O	1:C:928:GLN:N	2.43	0.51
1:D:400:LEU:HD21	1:D:930:GLY:HA2	1.93	0.51
1:E:166:ILE:O	1:E:169:THR:HB	2.11	0.51
1:E:562:SER:HB3	1:E:924:ASP:HB3	1.91	0.51
1:A:9:PRO:HG2	1:A:10:ILE:HD12	1.93	0.51
1:A:85:THR:HG21	1:A:620:ALA:HB3	1.92	0.51
1:A:429:GLU:H	1:A:429:GLU:CD	2.18	0.51
1:B:242:SER:HB2	1:B:245:GLU:HG3	1.93	0.51
1:B:946:VAL:HG13	1:B:1026:PHE:CD1	2.45	0.51
1:C:412:VAL:HG13	1:C:435:MET:HE1	1.91	0.51
1:C:945:ILE:CG1	1:C:971:ARG:HH22	2.24	0.51
1:D:400:LEU:CD2	1:D:929:VAL:HG12	2.40	0.51
1:F:534:ILE:HG22	3:F:1101:LMT:H5'	1.92	0.51
1:F:702:LEU:HD12	1:F:851:LEU:HD11	1.93	0.51
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.93	0.51
1:A:359:LEU:C	1:A:360:GLN:HG2	2.34	0.51
1:B:58:GLN:HA	1:B:62:THR:HB	1.92	0.51
1:C:669:PRO:HD3	1:C:677:ALA:O	2.11	0.51
1:C:751:GLY:O	1:C:754:TRP:N	2.44	0.51
1:C:971:ARG:HG2	1:C:974:PRO:HG3	1.93	0.51
1:D:219:LEU:O	1:D:231:ASN:ND2	2.43	0.51
1:E:754:TRP:CZ2	1:E:786:ILE:HD13	2.46	0.51
1:E:960:LEU:HD21	1:E:1027:VAL:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:ASN:HD22	1:F:435:MET:HG3	1.75	0.51
1:D:408:ASP:OD2	1:D:940:LYS:NZ	2.40	0.51
1:D:699:ARG:NH2	1:D:722:GLU:OE1	2.44	0.51
1:F:560:PRO:HB2	1:F:836:SER:OG	2.11	0.51
1:F:801:PHE:CD1	1:F:804:PHE:HE2	2.29	0.51
1:A:377:LEU:O	1:A:380:PHE:HB2	2.10	0.51
1:A:426:PRO:HB2	1:A:429:GLU:OE2	2.11	0.51
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.92	0.51
1:D:156:ASP:CG	1:D:769:LYS:HZ3	2.19	0.51
1:D:946:VAL:HG13	1:D:1026:PHE:CD1	2.46	0.51
1:D:987:MET:HA	1:D:1008:MET:HE1	1.93	0.51
1:F:378:GLY:O	1:F:382:VAL:HG23	2.10	0.51
1:F:948:PHE:CE1	1:F:971:ARG:HD3	2.45	0.51
1:A:404:LEU:HD21	1:A:449:LEU:HD22	1.92	0.51
1:B:423:GLU:O	1:B:502:LYS:HD2	2.10	0.51
1:B:758:TYR:HE1	1:B:770:LYS:HG2	1.76	0.51
1:C:382:VAL:HG11	1:C:476:SER:HB3	1.93	0.51
1:D:634:TRP:CD1	1:D:634:TRP:N	2.74	0.51
1:E:80:SER:HB3	1:E:90:ILE:HG12	1.92	0.51
1:E:291:ILE:HG21	1:E:306:ILE:HD11	1.92	0.51
1:E:340:VAL:O	1:E:344:LEU:HG	2.11	0.51
1:F:254:ASN:HB2	1:F:258:SER:O	2.10	0.51
1:F:598:TYR:CE2	1:F:629:VAL:HG21	2.46	0.51
1:F:898:PRO:O	1:F:902:MET:HG2	2.11	0.51
1:A:220:GLY:HA3	1:A:230:LEU:O	2.11	0.50
1:A:683:GLU:HG2	1:A:819:TYR:CD2	2.46	0.50
1:A:987:MET:HA	1:A:1008:MET:HE1	1.93	0.50
1:A:1036:LYS:HA	1:A:1038:GLU:HG2	1.93	0.50
1:C:380:PHE:HA	1:C:383:LEU:HD12	1.93	0.50
1:D:520:PHE:O	1:D:524:THR:HG22	2.10	0.50
1:D:533:GLY:O	1:D:536:ARG:HB2	2.10	0.50
1:E:165:ALA:HB3	1:E:313:MET:HE3	1.91	0.50
1:B:270:LEU:HD11	1:B:762:PHE:HZ	1.76	0.50
1:B:419:VAL:HG21	1:B:434:SER:HB3	1.93	0.50
1:C:1040:ILE:O	1:C:1041:GLU:HG3	2.11	0.50
1:D:350:LEU:HD13	1:D:984:LEU:HB3	1.93	0.50
1:E:1041:GLU:HB3	1:E:1042:HIS:CB	2.41	0.50
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.93	0.50
1:D:728:LYS:HB2	1:D:810:GLU:OE1	2.10	0.50
1:D:1040:ILE:HG12	1:D:1041:GLU:H	1.75	0.50
1:F:140:VAL:HG11	1:F:310:LEU:HD21	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:THR:OG1	1:D:152:GLU:HG2	2.11	0.50
1:D:888:LEU:HB2	1:D:898:PRO:HB3	1.93	0.50
1:E:356:TYR:C	1:E:358:PHE:H	2.19	0.50
1:F:222:THR:HA	1:F:224:PRO:HD3	1.93	0.50
1:F:971:ARG:HB3	1:F:971:ARG:NH1	2.26	0.50
1:A:316:PHE:CG	1:B:687:GLN:HG2	2.46	0.50
1:A:330:THR:HB	1:A:331:PRO:HD3	1.93	0.50
1:A:420:MET:HB3	1:A:500:ILE:HB	1.92	0.50
1:A:1033:PHE:CD2	1:A:1034:SER:N	2.80	0.50
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.46	0.50
1:C:298:ASN:ND2	1:C:301:ASP:OD2	2.41	0.50
1:F:58:GLN:HA	1:F:62:THR:HB	1.93	0.50
1:A:17:ILE:HG22	1:B:886:LEU:HD21	1.93	0.50
1:A:857:TYR:H	1:A:857:TYR:HD2	1.59	0.50
1:C:1043:SER:HB2	1:C:1044:HIS:HB3	1.93	0.50
1:E:36:PRO:HD3	1:E:391:ASN:OD1	2.11	0.50
1:E:72:ILE:HD13	1:E:107:VAL:HG22	1.94	0.50
1:E:897:ILE:N	1:E:898:PRO:HD2	2.26	0.50
1:F:559:LEU:HD21	1:F:922:THR:HA	1.93	0.50
1:B:583:THR:HG22	1:B:585:GLU:H	1.76	0.50
1:C:1043:SER:CB	1:C:1044:HIS:HB3	2.41	0.50
1:D:368:PRO:HG3	1:D:413:VAL:HG21	1.92	0.50
1:D:393:LEU:HD11	1:D:466:ILE:HD12	1.94	0.50
1:F:743:ILE:H	1:F:743:ILE:HD12	1.75	0.50
1:A:145:THR:C	1:A:147:GLY:H	2.20	0.50
1:C:757:SER:O	1:C:772:TYR:HA	2.11	0.50
1:C:876:LEU:HD22	1:C:932:LEU:HD11	1.94	0.50
1:D:108:GLN:OE1	1:D:129:VAL:HB	2.12	0.50
1:D:457:ALA:HA	1:D:468:ARG:HA	1.93	0.50
1:D:974:PRO:HA	1:D:977:MET:HE3	1.94	0.50
1:E:362:PHE:O	1:E:365:THR:HG22	2.11	0.50
1:E:412:VAL:O	1:E:416:VAL:HG23	2.12	0.50
1:F:801:PHE:HA	1:F:804:PHE:CE2	2.47	0.50
1:B:149:MET:HB2	1:B:153:ASP:HB2	1.94	0.50
1:C:284:GLN:HG3	1:C:285:PRO:HD2	1.94	0.50
1:C:479:ALA:O	1:C:482:VAL:HG23	2.11	0.50
1:C:574:THR:HG21	1:C:598:TYR:CE2	2.45	0.50
1:D:418:ARG:NE	1:D:970:MET:HE2	2.27	0.50
1:D:419:VAL:HG11	1:D:433:LYS:HG2	1.94	0.50
1:E:507:GLU:HG2	1:E:518:ARG:HA	1.94	0.50
1:E:525:HIS:HA	1:E:528:THR:HG22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:530:SER:OG	3:E:1101:LMT:O2'	2.12	0.50
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.92	0.49
1:B:682:PHE:CD2	1:B:827:ILE:HD12	2.47	0.49
1:C:465:ALA:O	1:C:469:GLN:HG2	2.12	0.49
1:D:58:GLN:HA	1:D:62:THR:HB	1.93	0.49
1:E:225:VAL:HG13	1:F:781:MET:SD	2.51	0.49
1:E:355:MET:SD	1:E:368:PRO:HG2	2.51	0.49
1:E:841:MET:O	1:E:845:GLU:HG3	2.12	0.49
1:F:531:VAL:O	1:F:534:ILE:HG13	2.12	0.49
1:A:17:ILE:CG2	1:B:886:LEU:HD21	2.43	0.49
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.94	0.49
1:A:728:LYS:HB2	1:A:810:GLU:OE1	2.13	0.49
1:B:151:GLN:OE1	1:B:278:ILE:HA	2.12	0.49
1:E:102:ILE:O	1:E:105:VAL:HG12	2.12	0.49
1:E:219:LEU:HD12	1:E:232:ALA:HB3	1.94	0.49
1:E:404:LEU:HD21	1:E:449:LEU:HD22	1.94	0.49
1:E:699:ARG:NH1	1:E:825:MET:HE1	2.27	0.49
1:F:61:VAL:HA	1:F:118:LEU:CD2	2.42	0.49
1:F:187:TRP:HA	1:F:774:MET:O	2.12	0.49
1:B:903:LEU:HB3	1:B:1025:PHE:CZ	2.47	0.49
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.95	0.49
1:D:375:VAL:HB	1:D:405:LEU:HD13	1.95	0.49
1:D:712:MET:HE3	1:D:839:GLU:HB3	1.94	0.49
1:D:928:GLN:HE22	3:D:1103:LMT:H12	1.77	0.49
1:E:415:ASN:O	1:E:419:VAL:HG23	2.12	0.49
1:F:380:PHE:O	1:F:383:LEU:HB2	2.12	0.49
1:A:841:MET:HE3	1:A:859:TRP:CZ2	2.48	0.49
1:B:3:ASN:HD21	1:B:432:ARG:HD3	1.75	0.49
1:B:356:TYR:C	1:B:358:PHE:H	2.21	0.49
1:B:424:GLY:HA3	1:B:502:LYS:HB2	1.95	0.49
1:B:435:MET:HG3	1:B:490:PRO:HB3	1.94	0.49
1:C:120:GLN:HA	1:C:123:GLN:HB2	1.94	0.49
1:C:407:ASP:O	1:C:411:VAL:HG23	2.12	0.49
1:D:743:ILE:HG23	1:D:746:ILE:HD12	1.94	0.49
1:E:713:LEU:HD11	1:E:843:LEU:HD12	1.93	0.49
1:A:252:LYS:HE3	1:A:260:VAL:HG21	1.93	0.49
1:A:682:PHE:HB3	1:A:827:ILE:HB	1.94	0.49
1:A:776:GLU:HB3	1:A:779:TYR:CD1	2.47	0.49
1:C:242:SER:CB	1:C:245:GLU:HG3	2.41	0.49
1:C:568:ASP:O	1:C:634:TRP:CH2	2.66	0.49
1:C:764:ASP:OD1	1:C:765:ARG:HG3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:ARG:HD2	1:D:761:ASP:O	2.12	0.49
1:A:35:TYR:HE1	1:A:670:ALA:HB1	1.76	0.49
1:A:435:MET:HG3	1:A:490:PRO:HB3	1.95	0.49
1:A:671:ILE:HG22	1:A:674:LEU:HB3	1.93	0.49
1:C:242:SER:HB2	1:C:245:GLU:H	1.77	0.49
1:C:434:SER:O	1:C:438:ILE:HG12	2.13	0.49
1:C:455:PRO:HG2	1:C:880:SER:HA	1.94	0.49
1:C:948:PHE:O	1:C:952:LEU:HG	2.12	0.49
1:D:598:TYR:HB3	1:D:606:VAL:HG11	1.93	0.49
1:D:752:ALA:O	1:D:774:MET:HA	2.12	0.49
1:E:137:LEU:HD12	1:E:329:THR:HG22	1.94	0.49
1:E:736:ALA:HB1	1:E:746:ILE:HD11	1.94	0.49
1:F:571:VAL:N	1:F:631:LEU:HD12	2.27	0.49
1:F:990:VAL:HG13	1:F:1005:THR:OG1	2.13	0.49
1:C:897:ILE:HD12	1:C:946:VAL:CG1	2.43	0.49
1:E:121:GLU:O	1:E:125:GLN:HB2	2.13	0.49
1:A:1037:ASN:HA	1:A:1038:GLU:HB2	1.94	0.49
1:C:108:GLN:HB3	1:C:129:VAL:HG11	1.94	0.49
1:D:225:VAL:HG13	1:E:781:MET:SD	2.53	0.49
1:E:234:ILE:HD11	1:F:754:TRP:CE3	2.47	0.49
1:F:33:ALA:O	1:F:391:ASN:HA	2.13	0.49
1:E:653:ARG:O	1:E:656:SER:OG	2.25	0.49
1:F:11:PHE:O	1:F:15:ILE:HG13	2.13	0.49
1:F:15:ILE:O	1:F:19:ILE:HG13	2.13	0.49
1:F:897:ILE:O	1:F:901:VAL:HG12	2.12	0.49
1:A:6:ILE:HG22	1:A:490:PRO:HB2	1.94	0.49
1:A:137:LEU:HD22	1:A:293:LEU:HG	1.94	0.49
1:A:680:PHE:HD1	1:A:859:TRP:HZ3	1.60	0.49
1:B:946:VAL:HG13	1:B:1026:PHE:CE1	2.47	0.49
1:C:378:GLY:O	1:C:382:VAL:HG23	2.12	0.49
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.94	0.49
1:D:164:ASP:HB3	1:D:168:ARG:NH2	2.25	0.49
1:F:49:TYR:HD1	1:F:57:VAL:HG12	1.78	0.49
1:F:563:PHE:CD2	1:F:564:LEU:HB2	2.48	0.49
1:A:679:GLY:O	1:A:862:MET:HE2	2.13	0.48
1:A:790:TYR:CE1	1:A:800:PRO:HB3	2.48	0.48
1:B:184:MET:HA	1:B:184:MET:HE3	1.93	0.48
1:B:455:PRO:O	1:B:876:LEU:HD13	2.13	0.48
1:C:150:THR:O	1:C:154:ILE:HG13	2.13	0.48
1:C:254:ASN:HB2	1:C:258:SER:O	2.13	0.48
1:D:583:THR:HA	1:D:622:GLN:OE1	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:PHE:HA	1:A:249:ILE:HG13	1.95	0.48
1:A:350:LEU:HD13	1:A:984:LEU:O	2.13	0.48
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.95	0.48
1:A:979:SER:OG	1:A:1015:THR:HG21	2.13	0.48
1:B:10:ILE:HB	1:C:893:GLU:OE1	2.13	0.48
1:B:1024:VAL:O	1:B:1028:VAL:HG23	2.13	0.48
1:C:456:MET:HE3	1:C:467:TYR:O	2.13	0.48
1:C:832:ALA:O	1:C:835:LYS:HB2	2.13	0.48
1:D:986:VAL:HG21	1:D:1007:VAL:HG11	1.94	0.48
1:E:1016:VAL:O	1:E:1016:VAL:HG12	2.13	0.48
1:F:184:MET:HA	1:F:184:MET:HE3	1.95	0.48
1:A:3:ASN:O	1:A:4:PHE:C	2.56	0.48
1:A:404:LEU:HD12	1:A:937:LEU:CD2	2.42	0.48
1:B:58:GLN:O	1:B:63:GLN:HG3	2.13	0.48
1:B:790:TYR:HD1	1:B:800:PRO:HA	1.78	0.48
1:C:211:ASN:OD1	1:C:240:LEU:N	2.42	0.48
1:C:910:ILE:O	1:C:914:LEU:HB2	2.12	0.48
1:E:567:GLU:HG3	1:E:670:ALA:HB2	1.94	0.48
1:A:281:PHE:CZ	1:A:608:SER:HB2	2.48	0.48
1:A:420:MET:HB2	1:A:500:ILE:HD12	1.96	0.48
1:A:792:ARG:HB2	1:A:798:MET:SD	2.53	0.48
1:B:678:THR:HA	1:B:837:THR:OG1	2.13	0.48
1:B:695:LEU:HD22	1:B:825:MET:SD	2.53	0.48
1:C:549:VAL:O	1:C:552:MET:HE2	2.13	0.48
1:C:913:LEU:HD23	1:C:927:PHE:CZ	2.47	0.48
1:D:197:GLN:HA	1:D:798:MET:SD	2.53	0.48
1:D:391:ASN:O	1:D:395:MET:HG2	2.13	0.48
1:D:893:GLU:OE1	1:F:8:ARG:HB3	2.13	0.48
1:F:58:GLN:O	1:F:62:THR:HB	2.14	0.48
1:A:187:TRP:HA	1:A:774:MET:O	2.13	0.48
1:A:636:ASP:O	1:A:638:PRO:HD3	2.13	0.48
1:B:416:VAL:HG21	1:B:493:CYS:SG	2.54	0.48
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.47	0.48
1:D:1019:ILE:HG13	1:D:1020:PHE:CD1	2.48	0.48
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.95	0.48
1:A:378:GLY:O	1:A:381:ALA:HB3	2.14	0.48
1:B:7:ASP:O	1:B:8:ARG:HG3	2.13	0.48
1:B:211:ASN:ND2	1:B:760:ASN:HD22	2.11	0.48
1:B:762:PHE:HE2	1:B:770:LYS:O	1.97	0.48
1:B:801:PHE:HA	1:B:804:PHE:CE2	2.48	0.48
1:D:94:PHE:CZ	1:D:103:ALA:HB1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:GLU:HB3	1:D:423:GLU:HG3	1.95	0.48
1:D:946:VAL:HG13	1:D:1026:PHE:CE1	2.48	0.48
1:E:696:THR:HG23	1:E:699:ARG:NH1	2.24	0.48
1:E:753:ALA:O	1:E:775:SER:HB3	2.13	0.48
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.95	0.48
1:A:382:VAL:O	1:A:386:PHE:HD1	1.97	0.48
1:A:1038:GLU:HB3	1:A:1039:ASP:C	2.38	0.48
1:B:27:ILE:HD13	1:B:380:PHE:CD1	2.48	0.48
1:D:27:ILE:HD11	1:D:380:PHE:CD1	2.49	0.48
1:F:746:ILE:HG22	1:F:791:VAL:HG11	1.95	0.48
1:A:591:LEU:HD11	1:A:625:GLY:HA3	1.96	0.48
1:A:919:ARG:HG2	1:A:920:GLY:H	1.79	0.48
1:B:644:VAL:O	1:B:648:THR:HG23	2.13	0.48
1:D:247:GLY:C	1:D:249:ILE:H	2.22	0.48
1:D:801:PHE:HA	1:D:804:PHE:CE2	2.49	0.48
1:E:682:PHE:HZ	1:E:857:TYR:HB2	1.73	0.48
1:E:690:LEU:HD13	1:E:694:LYS:HB3	1.96	0.48
1:F:366:LEU:O	1:F:370:ILE:HG13	2.13	0.48
1:F:412:VAL:HG23	1:F:442:LEU:HD21	1.96	0.48
1:A:888:LEU:HD22	1:A:901:VAL:HG11	1.95	0.48
1:B:291:ILE:HG21	1:B:306:ILE:CD1	2.43	0.48
1:B:765:ARG:HH21	1:B:769:LYS:HZ1	1.62	0.48
1:C:201:VAL:HG22	1:C:748:THR:OG1	2.13	0.48
1:D:55:LYS:NZ	1:F:238:THR:HG23	2.29	0.48
1:D:449:LEU:HB3	1:D:478:MET:SD	2.54	0.48
1:D:475:VAL:HA	1:D:478:MET:HE2	1.96	0.48
1:E:281:PHE:CZ	1:E:324:VAL:HG21	2.49	0.48
1:E:545:TYR:OH	1:E:903:LEU:O	2.26	0.48
1:F:744:ASN:O	1:F:748:THR:HG23	2.13	0.48
1:F:983:ILE:O	1:F:987:MET:HB2	2.14	0.48
1:A:610:PHE:O	1:A:627:ALA:HA	2.13	0.48
1:A:728:LYS:HB2	1:A:810:GLU:CD	2.39	0.48
1:B:139:VAL:HB	1:B:327:TYR:HB3	1.96	0.48
1:B:588:GLN:HB2	1:B:613:ASN:HD22	1.78	0.48
1:C:751:GLY:O	1:C:753:ALA:N	2.47	0.48
1:F:409:ALA:O	1:F:413:VAL:HG23	2.13	0.48
1:F:548:ILE:O	1:F:910:ILE:HD13	2.13	0.48
1:F:1025:PHE:O	1:F:1029:VAL:HG23	2.13	0.48
1:A:686:ASP:HB2	1:A:695:LEU:HD12	1.96	0.47
1:A:726:GLN:OE1	1:A:812:GLY:HA3	2.13	0.47
1:B:898:PRO:O	1:B:902:MET:HG3	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:GLN:HE21	1:C:230:LEU:H	1.62	0.47
1:C:987:MET:HE2	1:C:987:MET:HB3	1.61	0.47
1:D:913:LEU:HD23	1:D:927:PHE:CZ	2.48	0.47
1:E:733:GLN:NE2	1:E:743:ILE:HG21	2.26	0.47
1:F:456:MET:HB2	1:F:876:LEU:HD11	1.95	0.47
1:A:242:SER:HG	1:A:245:GLU:HG2	1.79	0.47
1:A:442:LEU:O	1:A:445:ILE:HG13	2.13	0.47
1:B:146:ASP:OD2	1:B:146:ASP:N	2.46	0.47
1:B:412:VAL:O	1:B:416:VAL:HG23	2.14	0.47
1:B:1040:ILE:HG23	1:B:1041:GLU:N	2.29	0.47
1:C:58:GLN:OE1	1:C:816:LEU:HB3	2.14	0.47
1:C:247:GLY:C	1:C:249:ILE:H	2.22	0.47
1:D:316:PHE:CG	1:E:687:GLN:HG2	2.49	0.47
1:F:65:ILE:HG23	1:F:69:MET:HE3	1.95	0.47
1:F:150:THR:N	1:F:153:ASP:OD1	2.42	0.47
1:F:201:VAL:HA	1:F:204:ILE:HD12	1.96	0.47
1:F:251:LEU:HD11	1:F:262:LEU:HA	1.96	0.47
1:F:453:PHE:CE1	1:F:474:ILE:HG21	2.49	0.47
1:F:525:HIS:HA	1:F:528:THR:HG22	1.95	0.47
1:A:781:MET:CE	1:C:225:VAL:H	2.28	0.47
1:A:844:MET:HA	1:A:844:MET:HE2	1.94	0.47
1:A:905:VAL:O	1:A:909:VAL:HG23	2.14	0.47
1:C:388:PHE:HE2	1:C:472:ILE:HG13	1.78	0.47
1:B:971:ARG:HB3	1:B:971:ARG:NH1	2.29	0.47
1:C:78:MET:HG3	1:C:92:LEU:HD13	1.96	0.47
1:D:781:MET:HB3	1:F:228:GLN:HE22	1.78	0.47
1:E:38:ILE:HG23	1:E:465:ALA:HB3	1.94	0.47
1:E:756:GLY:CA	1:E:774:MET:HG3	2.45	0.47
1:F:6:ILE:HG21	1:F:12:ALA:HB2	1.94	0.47
1:F:520:PHE:O	1:F:524:THR:HG22	2.13	0.47
1:F:610:PHE:O	1:F:628:PHE:N	2.32	0.47
1:A:279:ALA:HB3	1:A:286:ALA:O	2.14	0.47
1:A:448:VAL:O	1:A:451:ALA:HB3	2.15	0.47
1:A:509:LYS:HG2	1:A:510:LYS:HG3	1.95	0.47
1:C:244:GLU:CG	1:C:248:LYS:HE3	2.45	0.47
1:C:340:VAL:HG11	1:C:395:MET:CB	2.42	0.47
1:C:412:VAL:CG1	1:C:435:MET:HE1	2.45	0.47
1:D:53:ASP:OD1	1:D:56:THR:OG1	2.25	0.47
1:F:5:PHE:CZ	1:F:8:ARG:HD2	2.49	0.47
1:F:187:TRP:HB3	1:F:776:GLU:HG2	1.96	0.47
1:F:447:MET:HG3	1:F:448:VAL:N	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:559:LEU:CD2	1:F:922:THR:HA	2.45	0.47
1:F:971:ARG:HG2	1:F:974:PRO:HG3	1.96	0.47
1:A:149:MET:HE2	1:A:154:ILE:HG12	1.97	0.47
1:A:465:ALA:O	1:A:469:GLN:HG2	2.14	0.47
1:B:344:LEU:HD23	1:B:402:ILE:HD11	1.96	0.47
1:B:409:ALA:O	1:B:413:VAL:HG23	2.15	0.47
1:B:415:ASN:O	1:B:419:VAL:HG23	2.15	0.47
1:C:137:LEU:O	1:C:329:THR:HG23	2.14	0.47
1:C:197:GLN:HA	1:C:798:MET:SD	2.54	0.47
1:C:1042:HIS:O	1:C:1043:SER:HB3	2.13	0.47
1:D:462:SER:O	1:D:466:ILE:HG12	2.15	0.47
1:E:45:ILE:HD11	1:E:69:MET:HE2	1.95	0.47
1:E:913:LEU:HD23	1:E:927:PHE:HZ	1.79	0.47
1:F:352:PHE:HA	1:F:355:MET:CE	2.45	0.47
1:F:509:LYS:HG2	1:F:513:PHE:HB2	1.96	0.47
1:F:705:GLU:HA	1:F:708:LYS:HZ2	1.79	0.47
1:A:44:THR:HA	1:A:90:ILE:O	2.15	0.47
1:A:134:SER:OG	2:A:1101:ERY:C32	2.56	0.47
1:A:418:ARG:O	1:A:422:GLU:HB2	2.14	0.47
1:A:527:TYR:CD2	1:A:972:LEU:HG	2.49	0.47
1:A:574:THR:CG2	1:A:627:ALA:HB3	2.44	0.47
1:A:739:LEU:HD12	1:A:799:VAL:HG11	1.97	0.47
1:B:82:SER:HB2	1:B:816:LEU:HB2	1.95	0.47
1:B:145:THR:O	1:B:284:GLN:NE2	2.46	0.47
1:B:555:LEU:HA	1:B:555:LEU:HD23	1.56	0.47
1:B:950:LYS:HZ1	1:B:1030:ARG:NH2	2.12	0.47
1:B:953:MET:HE1	1:B:1026:PHE:CE2	2.50	0.47
1:C:45:ILE:HD11	1:C:69:MET:HE3	1.96	0.47
1:C:55:LYS:HB3	1:C:55:LYS:HE2	1.70	0.47
1:C:108:GLN:O	1:C:112:GLN:HB2	2.14	0.47
1:C:370:ILE:O	1:C:374:VAL:HG23	2.15	0.47
1:C:568:ASP:HB2	1:C:643:LYS:HG3	1.96	0.47
1:C:932:LEU:O	1:C:933:THR:C	2.57	0.47
1:D:30:LEU:HD11	1:D:384:ALA:HA	1.97	0.47
1:D:34:GLN:OE1	1:D:670:ALA:HB1	2.15	0.47
1:D:183:ALA:HB2	1:D:273:GLU:HG3	1.97	0.47
1:D:225:VAL:H	1:E:781:MET:HE1	1.80	0.47
1:D:388:PHE:HE1	1:D:469:GLN:HE22	1.61	0.47
1:D:790:TYR:HE1	1:D:800:PRO:HB3	1.79	0.47
1:E:197:GLN:HA	1:E:798:MET:SD	2.55	0.47
1:E:391:ASN:C	1:E:395:MET:HG2	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:960:LEU:O	1:E:964:THR:HG23	2.15	0.47
1:E:992:SER:O	1:E:997:SER:HB2	2.14	0.47
1:F:185:ARG:HB3	1:F:187:TRP:NE1	2.30	0.47
1:F:365:THR:O	1:F:368:PRO:HD2	2.14	0.47
1:F:504:ASP:C	1:F:506:GLY:N	2.70	0.47
1:F:597:TYR:CE1	1:F:601:LYS:HD2	2.46	0.47
1:A:190:PRO:HD3	1:A:779:TYR:CD1	2.50	0.47
1:A:535:LEU:HD22	1:A:1027:VAL:HG21	1.95	0.47
1:A:658:ILE:HG13	1:A:659:LYS:HE2	1.96	0.47
3:A:1102:LMT:H6E	3:A:1102:LMT:O5B	2.15	0.47
1:B:463:THR:HG22	1:B:563:PHE:HE2	1.80	0.47
1:C:404:LEU:HG	1:C:449:LEU:HD13	1.96	0.47
1:C:944:LEU:HB3	1:C:971:ARG:NH2	2.29	0.47
1:C:971:ARG:HB3	1:C:971:ARG:NH1	2.30	0.47
2:D:1101:ERY:H251	2:D:1101:ERY:H283	1.67	0.47
1:E:430:ALA:O	1:E:433:LYS:HB3	2.14	0.47
1:E:844:MET:HE2	1:E:844:MET:HA	1.97	0.47
1:F:362:PHE:O	1:F:366:LEU:HG	2.14	0.47
1:F:751:GLY:O	1:F:753:ALA:N	2.48	0.47
1:F:1035:ARG:HD3	1:F:1035:ARG:HA	1.74	0.47
1:A:781:MET:SD	1:C:225:VAL:HG13	2.55	0.47
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.55	0.47
1:B:222:THR:HA	1:B:224:PRO:HD3	1.96	0.47
1:B:1016:VAL:HG13	3:B:1101:LMT:H102	1.96	0.47
1:C:187:TRP:HE3	1:C:775:SER:O	1.98	0.47
1:D:246:PHE:O	1:D:262:LEU:HD23	2.15	0.47
1:E:575:MET:HA	1:E:626:ILE:HG13	1.97	0.47
1:F:5:PHE:CE1	1:F:8:ARG:HD2	2.49	0.47
1:F:752:ALA:O	1:F:774:MET:HA	2.15	0.47
1:A:181:GLN:HB3	1:A:273:GLU:OE1	2.15	0.47
1:A:929:VAL:O	1:A:932:LEU:HB2	2.15	0.47
1:B:801:PHE:CD1	1:B:804:PHE:HE2	2.33	0.47
1:C:140:VAL:HG23	1:C:291:ILE:HD13	1.97	0.47
1:C:194:ASN:HA	1:C:798:MET:HE2	1.97	0.47
1:C:452:VAL:O	1:C:455:PRO:HD2	2.15	0.47
1:E:575:MET:HE2	1:E:575:MET:HB2	1.65	0.47
1:E:602:GLU:HB3	1:E:606:VAL:HG23	1.97	0.47
1:E:909:VAL:HG13	1:E:931:LEU:HD11	1.96	0.47
1:F:986:VAL:HG21	1:F:1007:VAL:HG11	1.96	0.47
1:F:1024:VAL:O	1:F:1028:VAL:HG23	2.15	0.47
1:A:165:ALA:HB3	1:A:313:MET:HE1	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ARG:HB2	1:A:541:TYR:CD1	2.49	0.46
1:B:7:ASP:C	1:B:8:ARG:HG3	2.40	0.46
1:B:169:THR:HG21	1:B:306:ILE:HG13	1.97	0.46
1:B:506:GLY:C	1:B:508:GLY:H	2.22	0.46
1:B:937:LEU:HA	1:B:937:LEU:HD23	1.49	0.46
1:C:49:TYR:HD1	1:C:57:VAL:HG12	1.81	0.46
1:D:417:GLU:OE1	1:D:497:LEU:HD11	2.15	0.46
1:D:555:LEU:HD13	1:D:913:LEU:HB2	1.97	0.46
1:D:573:MET:HG2	1:D:628:PHE:HD1	1.80	0.46
1:E:32:VAL:HA	1:E:390:ILE:O	2.15	0.46
1:E:142:VAL:HG12	1:E:321:LEU:HD11	1.96	0.46
1:E:330:THR:HB	1:E:331:PRO:HD3	1.97	0.46
1:F:3:ASN:C	1:F:5:PHE:N	2.71	0.46
1:F:881:LEU:HD21	1:F:905:VAL:HG11	1.98	0.46
1:A:4:PHE:O	1:A:8:ARG:HD2	2.15	0.46
1:A:154:ILE:O	1:A:157:TYR:N	2.49	0.46
1:A:328:ASP:O	1:A:331:PRO:HD2	2.15	0.46
1:A:453:PHE:CE2	1:A:474:ILE:HG21	2.50	0.46
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.97	0.46
1:A:1036:LYS:C	1:A:1038:GLU:HG2	2.41	0.46
1:B:277:ILE:HA	1:B:613:ASN:O	2.15	0.46
1:B:817:GLU:OE1	1:B:826:GLU:HB2	2.15	0.46
1:C:112:GLN:O	1:C:115:MET:HB2	2.15	0.46
1:C:182:TYR:O	1:C:769:LYS:HD3	2.14	0.46
1:C:426:PRO:HD2	1:C:429:GLU:CB	2.46	0.46
1:C:668:LEU:H	1:C:668:LEU:HG	1.46	0.46
1:D:182:TYR:HB2	1:D:769:LYS:NZ	2.30	0.46
1:D:971:ARG:HB3	1:D:971:ARG:NH1	2.29	0.46
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.80	0.46
1:E:801:PHE:HA	1:E:804:PHE:CE2	2.50	0.46
1:F:356:TYR:C	1:F:358:PHE:N	2.74	0.46
1:F:664:PHE:HD2	1:F:717:ARG:CD	2.28	0.46
1:A:236:ALA:O	1:B:728:LYS:NZ	2.46	0.46
1:A:434:SER:O	1:A:438:ILE:HG12	2.15	0.46
1:B:652:THR:HG22	1:B:665:ALA:H	1.80	0.46
1:B:974:PRO:HA	1:B:977:MET:CE	2.44	0.46
1:D:961:ILE:H	1:D:961:ILE:HG13	1.12	0.46
1:B:36:PRO:O	1:B:38:ILE:HG13	2.15	0.46
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.98	0.46
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.30	0.46
1:C:672:VAL:HG23	1:C:673:GLU:OE2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:931:LEU:HD13	3:D:1103:LMT:H81	1.98	0.46
1:E:40:PRO:HA	1:E:41:PRO:HD3	1.68	0.46
1:E:675:GLY:HA3	1:E:862:MET:SD	2.56	0.46
1:F:760:ASN:O	1:F:771:VAL:HB	2.14	0.46
1:A:423:GLU:OE2	1:A:433:LYS:HE2	2.15	0.46
1:A:844:MET:HE2	1:A:847:LEU:HD12	1.98	0.46
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.97	0.46
1:B:511:GLY:O	1:B:515:TRP:NE1	2.49	0.46
1:C:119:PRO:O	1:C:123:GLN:HG3	2.15	0.46
1:C:907:LEU:HG	1:C:1017:LEU:HD23	1.97	0.46
1:C:1040:ILE:HG12	1:C:1041:GLU:N	2.26	0.46
2:D:1101:ERY:H272	2:D:1101:ERY:H292	1.98	0.46
1:F:27:ILE:HA	1:F:30:LEU:CD2	2.46	0.46
1:F:452:VAL:HG13	1:F:884:VAL:CG2	2.46	0.46
1:F:664:PHE:HE2	1:F:717:ARG:HB3	1.80	0.46
1:F:932:LEU:O	1:F:933:THR:C	2.59	0.46
1:A:721:LEU:HA	1:A:721:LEU:HD12	1.81	0.46
1:A:736:ALA:HB2	1:A:804:PHE:HB2	1.98	0.46
1:A:1040:ILE:HG23	1:A:1041:GLU:N	2.30	0.46
1:C:101:ASP:OD1	1:C:131:LYS:NZ	2.29	0.46
1:E:172:VAL:HG22	1:E:306:ILE:HD11	1.98	0.46
1:F:311:ALA:HA	1:F:314:GLU:HG3	1.98	0.46
1:F:524:THR:O	1:F:528:THR:HG22	2.16	0.46
1:A:83:ASP:HB3	1:A:85:THR:H	1.80	0.46
1:B:143:ILE:HG21	1:B:281:PHE:CD2	2.51	0.46
1:B:203:VAL:HG12	1:B:207:ILE:HD11	1.97	0.46
1:C:341:VAL:O	1:C:344:LEU:HB3	2.16	0.46
1:D:416:VAL:HG21	1:D:493:CYS:SG	2.56	0.46
1:D:673:GLU:HB2	2:D:1101:ERY:H213	1.97	0.46
1:D:1024:VAL:O	1:D:1028:VAL:HG23	2.16	0.46
1:E:10:ILE:HG12	1:F:895:TRP:HB2	1.98	0.46
1:E:744:ASN:O	1:E:748:THR:HG23	2.16	0.46
1:E:904:VAL:O	1:E:907:LEU:HB2	2.16	0.46
1:E:982:PHE:HD2	1:E:1011:MET:HE2	1.81	0.46
1:A:545:TYR:CE2	1:A:1025:PHE:HZ	2.34	0.46
1:B:188:MET:HA	1:B:266:ALA:CB	2.46	0.46
1:C:222:THR:HA	1:C:224:PRO:CD	2.43	0.46
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.46	0.46
1:C:434:SER:O	1:C:437:GLN:HB2	2.15	0.46
1:C:457:ALA:HB2	1:C:471:SER:OG	2.15	0.46
1:C:898:PRO:HA	1:C:901:VAL:HG12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.98	0.46
1:D:453:PHE:CE2	1:D:932:LEU:HB3	2.51	0.46
1:D:971:ARG:NH2	1:D:975:ILE:HD11	2.31	0.46
3:D:1103:LMT:H112	3:D:1103:LMT:H82	1.79	0.46
1:E:634:TRP:CD1	1:E:634:TRP:N	2.79	0.46
1:E:652:THR:CG2	1:E:665:ALA:H	2.28	0.46
1:A:504:ASP:C	1:A:506:GLY:H	2.24	0.46
1:B:344:LEU:HD11	1:B:398:MET:CE	2.46	0.46
1:B:1033:PHE:CE1	1:B:1034:SER:HB3	2.51	0.46
1:C:398:MET:O	1:C:402:ILE:HG13	2.16	0.46
1:C:844:MET:HE3	1:C:844:MET:HB3	1.79	0.46
1:D:573:MET:HB2	1:D:666:PHE:HE1	1.81	0.46
1:E:289:LEU:HD23	1:E:289:LEU:HA	1.52	0.46
1:E:904:VAL:HG21	1:E:942:ALA:HB2	1.98	0.46
1:F:578:LEU:HB3	1:F:579:PRO:HD2	1.98	0.46
1:F:987:MET:HB3	1:F:987:MET:HE2	1.58	0.46
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.51	0.46
1:B:195:LYS:HB3	1:B:196:PHE:CD1	2.51	0.46
1:B:576:VAL:HG22	1:B:663:VAL:HG22	1.98	0.46
1:B:683:GLU:HG2	1:B:819:TYR:CG	2.51	0.46
1:B:1026:PHE:O	1:B:1030:ARG:HB2	2.16	0.46
1:C:3:ASN:C	1:C:6:ILE:H	2.23	0.46
1:C:187:TRP:HA	1:C:774:MET:O	2.16	0.46
1:D:568:ASP:O	1:D:634:TRP:HZ3	1.98	0.46
1:D:897:ILE:HG12	1:D:1030:ARG:HD3	1.97	0.46
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.98	0.46
1:D:919:ARG:HD3	1:D:921:LEU:HD23	1.98	0.46
1:F:452:VAL:C	1:F:455:PRO:HD2	2.41	0.46
1:F:572:PHE:CE1	1:F:648:THR:HG22	2.51	0.46
1:B:194:ASN:CG	1:B:790:TYR:HD2	2.24	0.45
1:B:405:LEU:HD22	1:B:481:SER:HB3	1.96	0.45
1:C:310:LEU:O	1:C:314:GLU:HG3	2.16	0.45
1:C:969:ARG:HH11	1:C:970:MET:HB3	1.81	0.45
1:D:225:VAL:H	1:E:781:MET:CE	2.29	0.45
1:D:573:MET:HG2	1:D:628:PHE:CD1	2.51	0.45
1:D:610:PHE:O	1:D:627:ALA:HA	2.16	0.45
1:E:418:ARG:O	1:E:422:GLU:HB2	2.15	0.45
1:E:425:LEU:HD12	1:E:430:ALA:HA	1.98	0.45
1:E:847:LEU:O	1:E:850:LYS:HB2	2.16	0.45
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.97	0.45
1:F:281:PHE:CE1	1:F:324:VAL:HG21	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:894:SER:HB3	1:F:897:ILE:HG12	1.98	0.45
1:A:2:PRO:O	1:A:6:ILE:HG23	2.16	0.45
1:A:467:TYR:HE1	1:A:925:VAL:HG22	1.81	0.45
1:A:535:LEU:HD23	1:A:535:LEU:HA	1.67	0.45
1:A:857:TYR:CD2	1:A:857:TYR:N	2.85	0.45
1:A:1008:MET:HB2	1:A:1008:MET:HE3	1.72	0.45
1:B:270:LEU:HD12	1:B:270:LEU:HA	1.78	0.45
1:B:520:PHE:O	1:B:524:THR:HG22	2.16	0.45
1:C:11:PHE:O	1:C:11:PHE:HD2	1.99	0.45
1:C:246:PHE:O	1:C:262:LEU:HD23	2.15	0.45
1:C:406:VAL:O	1:C:407:ASP:C	2.59	0.45
1:D:255:GLN:H	1:D:255:GLN:CD	2.24	0.45
1:D:415:ASN:HB3	1:D:434:SER:HB2	1.98	0.45
1:D:442:LEU:HA	1:D:442:LEU:HD23	1.67	0.45
1:D:485:ALA:O	1:D:490:PRO:HD3	2.16	0.45
1:E:728:LYS:HB2	1:E:810:GLU:OE1	2.15	0.45
1:F:195:LYS:HB3	1:F:196:PHE:CD1	2.48	0.45
1:A:404:LEU:HD12	1:A:937:LEU:HD21	1.98	0.45
1:A:452:VAL:HA	1:A:880:SER:OG	2.15	0.45
1:A:708:LYS:C	1:A:710:PRO:HD3	2.42	0.45
1:A:926:TYR:H	1:A:926:TYR:HD1	1.64	0.45
1:A:985:GLY:O	1:A:988:PRO:HD2	2.17	0.45
1:C:165:ALA:HB3	1:C:313:MET:CE	2.46	0.45
1:C:382:VAL:O	1:C:386:PHE:HD2	1.99	0.45
1:C:563:PHE:HB2	1:C:866:GLU:HB2	1.97	0.45
1:C:658:ILE:HG13	1:C:658:ILE:O	2.17	0.45
1:D:708:LYS:C	1:D:710:PRO:HD3	2.42	0.45
1:D:919:ARG:HG2	1:D:920:GLY:N	2.26	0.45
1:E:358:PHE:CD1	1:E:977:MET:HG2	2.51	0.45
1:A:172:VAL:CG2	1:A:306:ILE:HD11	2.46	0.45
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.51	0.45
1:B:294:ALA:HB3	1:B:297:ALA:HB2	1.97	0.45
1:B:844:MET:HE2	1:B:844:MET:HA	1.99	0.45
1:B:957:GLY:O	1:B:1041:GLU:HA	2.16	0.45
1:C:138:MET:HE3	1:C:138:MET:HB2	1.67	0.45
1:D:310:LEU:O	1:D:314:GLU:HG3	2.17	0.45
1:E:105:VAL:HB	1:F:105:VAL:HG13	1.99	0.45
1:E:199:THR:HG23	1:E:798:MET:HE1	1.97	0.45
1:E:515:TRP:O	1:E:519:MET:HG3	2.16	0.45
1:F:3:ASN:OD1	1:F:3:ASN:N	2.49	0.45
1:F:459:PHE:CE1	1:F:876:LEU:HG	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:701:GLN:HE22	1:F:852:PRO:HD3	1.81	0.45
1:A:801:PHE:CD1	1:A:804:PHE:HE2	2.35	0.45
1:A:965:LEU:HA	1:A:965:LEU:HD23	1.64	0.45
1:C:280:GLU:HG3	1:C:285:PRO:HA	1.98	0.45
1:C:686:ASP:OD1	1:C:690:LEU:HB2	2.17	0.45
1:D:542:LEU:O	1:D:546:LEU:HG	2.16	0.45
1:D:654:ALA:O	1:D:658:ILE:HG12	2.17	0.45
1:D:947:GLU:O	1:D:951:ASP:HB2	2.17	0.45
1:D:999:ALA:O	1:D:1003:VAL:HG23	2.16	0.45
1:E:66:GLU:OE1	1:E:821:GLY:HA2	2.17	0.45
1:F:84:SER:HB3	1:F:814:PRO:HA	1.98	0.45
1:A:242:SER:OG	1:A:245:GLU:HG2	2.16	0.45
1:D:112:GLN:NE2	1:E:112:GLN:HB3	2.32	0.45
1:D:375:VAL:HG11	1:D:405:LEU:HD22	1.98	0.45
1:D:876:LEU:HD23	1:D:879:ILE:HD12	1.98	0.45
1:D:996:GLY:O	1:D:999:ALA:N	2.49	0.45
1:E:14:VAL:HG13	1:F:886:LEU:HD12	1.98	0.45
1:F:510:LYS:O	1:F:512:PHE:N	2.46	0.45
1:A:584:GLN:N	1:A:622:GLN:HB3	2.31	0.45
1:A:775:SER:OG	1:A:780:ARG:HG2	2.16	0.45
1:A:986:VAL:HG12	1:A:1008:MET:HE3	1.99	0.45
2:A:1101:ERY:H321	2:A:1101:ERY:H8	1.64	0.45
1:B:255:GLN:H	1:B:255:GLN:HG3	1.29	0.45
1:B:888:LEU:HD23	1:B:888:LEU:HA	1.75	0.45
1:B:950:LYS:NZ	1:B:1030:ARG:NH2	2.64	0.45
1:C:156:ASP:CG	1:C:769:LYS:HZ3	2.24	0.45
1:C:443:VAL:HG12	1:C:891:LEU:CD2	2.46	0.45
1:C:987:MET:O	1:C:991:ILE:HG22	2.17	0.45
1:D:899:PHE:HD2	1:D:902:MET:HE2	1.80	0.45
1:D:932:LEU:HD23	1:D:932:LEU:HA	1.75	0.45
1:D:991:ILE:HG22	1:D:992:SER:N	2.29	0.45
1:E:533:GLY:O	1:E:536:ARG:HB2	2.17	0.45
1:E:619:GLY:O	1:E:624:THR:HG21	2.17	0.45
1:E:758:TYR:HB2	1:E:772:TYR:CE1	2.51	0.45
1:A:889:ALA:HA	1:A:894:SER:O	2.17	0.45
1:B:729:ILE:HG22	1:B:731:ILE:HD13	1.99	0.45
1:C:240:LEU:HD11	1:C:249:ILE:HD11	1.98	0.45
1:C:682:PHE:CZ	1:C:857:TYR:HB2	2.52	0.45
1:C:789:TRP:O	1:C:801:PHE:HD2	1.98	0.45
1:C:941:ASN:HD21	1:C:1015:THR:HG22	1.81	0.45
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:LEU:HD22	1:D:245:GLU:OE1	2.17	0.45
1:D:889:ALA:HA	1:D:894:SER:O	2.17	0.45
1:E:219:LEU:HD11	1:F:727:PHE:CD1	2.51	0.45
1:E:983:ILE:HD13	1:E:1012:VAL:HG22	1.99	0.45
1:F:664:PHE:HD2	1:F:717:ARG:HD3	1.82	0.45
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.46	0.45
1:A:703:LEU:HD21	1:A:718:PRO:HD3	1.99	0.45
1:C:987:MET:HG3	1:C:1008:MET:HE1	1.99	0.45
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.82	0.45
1:D:925:VAL:HG12	1:D:926:TYR:N	2.30	0.45
1:E:230:LEU:HG	1:E:231:ASN:N	2.31	0.45
1:F:363:ARG:NH2	1:F:498:LYS:HD2	2.18	0.45
1:F:659:LYS:HA	1:F:659:LYS:HD3	1.84	0.45
1:B:69:MET:HE1	1:B:107:VAL:HG13	1.99	0.45
1:B:143:ILE:O	1:B:321:LEU:HA	2.16	0.45
1:C:844:MET:HA	1:C:847:LEU:HD22	1.98	0.45
1:D:875:SER:O	1:D:879:ILE:HG13	2.17	0.45
1:E:166:ILE:HD11	1:E:310:LEU:CD1	2.48	0.45
1:E:344:LEU:HD23	1:E:402:ILE:HD11	1.99	0.45
1:E:355:MET:HE3	1:E:355:MET:HB2	1.68	0.45
1:E:448:VAL:HA	1:E:451:ALA:HB3	1.99	0.45
1:E:1024:VAL:O	1:E:1028:VAL:HG23	2.17	0.45
1:F:314:GLU:HB2	1:F:315:PRO:HD3	1.99	0.45
1:F:578:LEU:CG	1:F:587:THR:HG22	2.47	0.45
1:F:664:PHE:CD2	1:F:717:ARG:HD3	2.52	0.45
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.76	0.44
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.66	0.44
1:B:699:ARG:HE	1:B:703:LEU:HD11	1.82	0.44
1:B:931:LEU:HD23	1:B:931:LEU:HA	1.73	0.44
1:C:11:PHE:O	1:C:15:ILE:HG13	2.17	0.44
1:C:227:GLY:O	1:C:229:GLN:HG3	2.17	0.44
1:D:58:GLN:O	1:D:63:GLN:HG3	2.17	0.44
1:D:343:THR:HG21	1:D:989:LEU:HD21	1.99	0.44
1:D:406:VAL:O	1:D:410:ILE:HG13	2.16	0.44
1:D:1008:MET:HE3	1:D:1008:MET:HB2	1.76	0.44
1:F:901:VAL:HG23	1:F:942:ALA:CB	2.43	0.44
1:A:500:ILE:HG22	1:A:501:ALA:O	2.17	0.44
1:A:1038:GLU:HA	1:A:1039:ASP:HB3	1.99	0.44
1:C:216:ALA:HB1	1:C:234:ILE:HG22	1.99	0.44
1:C:926:TYR:HD2	1:C:1003:VAL:HG22	1.82	0.44
1:D:316:PHE:CD1	1:E:687:GLN:HG2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:759:VAL:HG12	1:D:760:ASN:HB2	1.99	0.44
1:D:839:GLU:O	1:D:842:GLU:HB3	2.17	0.44
1:E:680:PHE:CZ	1:E:844:MET:HG3	2.52	0.44
1:A:541:TYR:CD1	1:A:541:TYR:N	2.85	0.44
1:B:324:VAL:HG13	1:B:326:PRO:HD3	2.00	0.44
1:B:534:ILE:HG22	3:B:1101:LMT:H5'	1.99	0.44
1:B:685:ILE:HD11	1:B:819:TYR:HD2	1.80	0.44
1:C:185:ARG:HB3	1:C:187:TRP:NE1	2.32	0.44
1:C:394:THR:O	1:C:398:MET:HG3	2.18	0.44
1:C:425:LEU:HA	1:C:425:LEU:HD23	1.80	0.44
1:F:69:MET:HA	1:F:72:ILE:HD11	1.99	0.44
1:F:375:VAL:HG13	1:F:480:LEU:HB2	2.00	0.44
1:A:7:ASP:O	1:A:8:ARG:HG3	2.17	0.44
1:A:80:SER:CB	1:A:90:ILE:HG12	2.46	0.44
1:A:158:VAL:HA	1:A:162:MET:HE2	2.00	0.44
1:A:359:LEU:O	1:A:360:GLN:C	2.61	0.44
1:A:609:VAL:HG13	1:A:629:VAL:HG22	1.99	0.44
1:B:461:GLY:HA2	1:B:865:GLN:HE21	1.82	0.44
1:C:858:ASP:OD2	1:C:859:TRP:N	2.51	0.44
1:C:1016:VAL:HG12	1:C:1016:VAL:O	2.18	0.44
1:D:67:GLN:NE2	1:F:768:VAL:HG13	2.31	0.44
1:D:678:THR:HA	1:D:837:THR:OG1	2.18	0.44
1:F:743:ILE:O	1:F:746:ILE:HG13	2.18	0.44
1:A:426:PRO:O	1:A:429:GLU:HG2	2.18	0.44
1:A:544:LEU:HA	1:A:544:LEU:HD12	1.83	0.44
1:A:623:ASN:OD1	1:A:623:ASN:N	2.48	0.44
1:B:281:PHE:HZ	1:B:324:VAL:HG21	1.80	0.44
1:B:418:ARG:HD2	1:B:422:GLU:OE1	2.17	0.44
1:B:605:ASN:HD22	1:B:647:ILE:HD11	1.83	0.44
1:B:741:VAL:HG21	1:B:804:PHE:CE1	2.53	0.44
1:D:568:ASP:OD1	1:D:637:ARG:NH1	2.42	0.44
1:D:579:PRO:HD3	1:D:661:ALA:HB2	1.98	0.44
1:E:378:GLY:O	1:E:382:VAL:HG23	2.17	0.44
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.74	0.44
1:B:652:THR:HG23	1:B:665:ALA:HB3	1.99	0.44
1:B:690:LEU:HD11	1:B:854:GLY:HA3	2.00	0.44
1:C:31:PRO:HB2	1:C:389:SER:CB	2.47	0.44
1:C:403:GLY:O	1:C:406:VAL:HG22	2.17	0.44
1:D:781:MET:HE1	1:F:225:VAL:H	1.81	0.44
1:E:375:VAL:HG11	1:E:405:LEU:HD22	1.98	0.44
1:E:404:LEU:HD12	1:E:937:LEU:HD21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:573:MET:HG3	1:E:666:PHE:HE1	1.81	0.44
1:E:706:ALA:HB1	1:E:716:VAL:HG11	2.00	0.44
1:A:801:PHE:O	1:A:805:SER:OG	2.30	0.44
1:A:893:GLU:CD	1:C:8:ARG:HB3	2.43	0.44
1:A:960:LEU:H	1:A:1039:ASP:HA	1.82	0.44
1:A:1038:GLU:HA	1:A:1039:ASP:CB	2.47	0.44
2:A:1101:ERY:H18	2:A:1101:ERY:H5	1.99	0.44
1:B:575:MET:HE2	1:B:575:MET:HB2	1.67	0.44
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.99	0.44
1:C:549:VAL:O	1:C:552:MET:HB3	2.18	0.44
1:C:649:MET:HE1	1:C:653:ARG:NH2	2.33	0.44
1:D:463:THR:HG22	1:D:563:PHE:CE1	2.53	0.44
1:D:502:LYS:H	1:D:502:LYS:HG2	1.47	0.44
1:E:111:LEU:HD11	1:E:127:VAL:HB	1.99	0.44
1:E:845:GLU:HG3	1:E:859:TRP:HZ2	1.82	0.44
1:E:903:LEU:O	1:E:906:PRO:HD2	2.18	0.44
1:F:1039:ASP:OD2	1:F:1041:GLU:HG3	2.18	0.44
1:B:274:ASN:HD21	1:B:276:ASP:CG	2.22	0.44
1:B:559:LEU:HG	1:B:560:PRO:HD2	2.00	0.44
1:B:904:VAL:HG13	1:B:907:LEU:HD22	2.00	0.44
1:B:959:GLY:HA2	1:B:1040:ILE:HG22	1.98	0.44
1:C:376:LEU:HD22	1:C:398:MET:HE3	1.99	0.44
1:C:443:VAL:HG12	1:C:891:LEU:HD21	2.00	0.44
1:C:582:ALA:HB3	1:C:623:ASN:HB3	1.99	0.44
1:C:587:THR:OG1	1:C:613:ASN:ND2	2.50	0.44
1:D:153:ASP:OD2	1:D:182:TYR:OH	2.35	0.44
1:E:637:ARG:HB3	1:E:642:ASN:HB3	2.00	0.44
1:E:727:PHE:HD1	1:E:809:TRP:CE2	2.36	0.44
1:F:279:ALA:HB2	1:F:612:VAL:HG22	2.00	0.44
1:F:944:LEU:HD13	1:F:975:ILE:HG12	2.00	0.44
1:E:555:LEU:HB3	1:E:913:LEU:HB3	2.00	0.44
1:E:846:GLN:O	1:E:849:SER:OG	2.35	0.44
1:E:973:ARG:HG2	1:E:977:MET:HE2	2.00	0.44
1:F:664:PHE:CE2	1:F:717:ARG:HB3	2.53	0.44
1:A:201:VAL:HA	1:A:204:ILE:HD12	2.00	0.43
1:B:228:GLN:O	1:C:583:THR:HG21	2.17	0.43
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.81	0.43
1:C:983:ILE:HD13	1:C:1012:VAL:HG22	2.00	0.43
1:D:549:VAL:O	1:D:552:MET:HB3	2.18	0.43
1:E:932:LEU:HD23	1:E:932:LEU:HA	1.77	0.43
1:F:688:ALA:HB3	1:F:690:LEU:HG	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:751:GLY:O	1:F:754:TRP:N	2.51	0.43
1:A:937:LEU:HD23	1:A:937:LEU:HA	1.85	0.43
1:A:1034:SER:OG	1:A:1035:ARG:N	2.51	0.43
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.98	0.43
1:B:335:ILE:HG21	1:B:995:ALA:HB3	2.00	0.43
1:B:969:ARG:NH1	1:B:970:MET:HB3	2.32	0.43
1:C:190:PRO:HB3	1:C:789:TRP:CZ3	2.53	0.43
1:C:728:LYS:HG2	1:C:808:ARG:CZ	2.49	0.43
1:C:865:GLN:O	1:C:868:LEU:HB3	2.18	0.43
1:D:201:VAL:HG21	1:D:745:ASP:OD2	2.18	0.43
1:D:428:LYS:H	1:D:428:LYS:HG2	1.24	0.43
1:D:573:MET:HE2	1:D:666:PHE:CE1	2.53	0.43
1:E:43:VAL:HG11	1:E:104:GLN:HG3	2.00	0.43
1:E:190:PRO:HG3	1:E:779:TYR:HB3	2.00	0.43
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.56	0.43
1:F:143:ILE:HG22	1:F:286:ALA:HB2	2.01	0.43
1:F:404:LEU:HG	1:F:449:LEU:HD13	2.01	0.43
1:F:572:PHE:CD1	1:F:648:THR:HG22	2.53	0.43
1:B:572:PHE:CD1	1:B:648:THR:HG22	2.53	0.43
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.46	0.43
1:C:894:SER:HG	1:C:896:SER:HG	1.64	0.43
1:D:622:GLN:NE2	1:F:220:GLY:O	2.49	0.43
1:D:894:SER:HB3	1:D:897:ILE:HB	2.00	0.43
1:E:34:GLN:O	1:E:392:THR:OG1	2.35	0.43
1:E:42:ALA:HB3	1:E:132:SER:HB3	2.00	0.43
1:E:167:SER:CB	1:E:175:VAL:HG21	2.46	0.43
1:E:743:ILE:HA	1:E:746:ILE:HD12	2.00	0.43
1:E:931:LEU:O	1:E:935:ILE:HG13	2.18	0.43
1:A:762:PHE:O	1:A:768:VAL:HA	2.17	0.43
1:A:841:MET:HE3	1:A:859:TRP:CE2	2.52	0.43
1:B:426:PRO:HG2	1:B:429:GLU:HB2	1.99	0.43
1:C:156:ASP:OD2	1:C:182:TYR:HB2	2.18	0.43
1:C:409:ALA:O	1:C:413:VAL:HG23	2.18	0.43
1:C:775:SER:HB2	1:C:789:TRP:CH2	2.53	0.43
1:C:940:LYS:NZ	1:C:978:THR:HG21	2.33	0.43
1:D:210:GLN:OE1	1:D:250:LEU:HB3	2.18	0.43
1:D:492:LEU:HA	1:D:492:LEU:HD23	1.65	0.43
1:E:901:VAL:HG21	1:E:943:ILE:HG13	2.00	0.43
1:E:987:MET:HB3	1:E:988:PRO:HD3	1.99	0.43
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.73	0.43
1:B:61:VAL:HG22	1:B:118:LEU:HD22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:THR:HG22	1:B:584:GLN:N	2.33	0.43
1:B:873:ALA:N	1:B:874:PRO:HD2	2.32	0.43
1:C:72:ILE:HD12	1:C:75:LEU:HD22	1.99	0.43
1:C:351:VAL:HG12	1:C:355:MET:HE2	1.99	0.43
1:D:563:PHE:CD2	1:D:671:ILE:HD13	2.52	0.43
1:E:188:MET:HA	1:E:266:ALA:HB2	2.00	0.43
1:E:508:GLY:HA2	1:E:518:ARG:NH2	2.32	0.43
1:E:597:TYR:CE1	1:E:601:LYS:HD2	2.53	0.43
1:E:887:CYS:O	1:E:890:ALA:HB3	2.19	0.43
1:E:1041:GLU:OE1	1:E:1042:HIS:HB2	2.18	0.43
1:F:65:ILE:CG2	1:F:90:ILE:HD12	2.49	0.43
1:F:80:SER:CB	1:F:90:ILE:HG12	2.49	0.43
1:F:457:ALA:HB2	1:F:471:SER:OG	2.18	0.43
1:F:587:THR:HG21	1:F:622:GLN:O	2.18	0.43
1:F:623:ASN:OD1	1:F:623:ASN:N	2.49	0.43
1:A:169:THR:HG21	1:A:306:ILE:HG13	2.01	0.43
1:A:185:ARG:HB3	1:A:187:TRP:HE1	1.82	0.43
1:A:350:LEU:HD22	1:A:984:LEU:HD13	2.00	0.43
1:B:684:LEU:HD12	1:B:684:LEU:HA	1.84	0.43
1:B:948:PHE:CE2	1:B:971:ARG:HD2	2.54	0.43
1:C:201:VAL:HA	1:C:204:ILE:HD12	2.00	0.43
1:C:664:PHE:CD2	1:C:717:ARG:HD2	2.54	0.43
1:C:673:GLU:H	1:C:673:GLU:CD	2.26	0.43
1:D:76:MET:HB2	1:D:93:THR:O	2.18	0.43
1:D:404:LEU:HD12	1:D:937:LEU:HD21	1.99	0.43
1:D:625:GLY:O	1:D:626:ILE:HD12	2.18	0.43
1:D:726:GLN:CD	1:D:812:GLY:HA3	2.43	0.43
1:D:1016:VAL:O	1:D:1016:VAL:HG12	2.19	0.43
1:E:568:ASP:O	1:E:634:TRP:CZ3	2.69	0.43
1:F:509:LYS:HB3	1:F:514:GLY:CA	2.42	0.43
1:F:953:MET:HB2	1:F:953:MET:HE3	1.74	0.43
1:A:46:SER:HB2	1:A:128:SER:OG	2.18	0.43
1:A:102:ILE:CD1	1:C:101:ASP:HB3	2.47	0.43
1:A:184:MET:HG2	1:A:246:PHE:CE2	2.54	0.43
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.64	0.43
1:B:514:GLY:C	1:B:516:PHE:H	2.27	0.43
1:B:978:THR:O	1:B:981:ALA:N	2.52	0.43
1:C:124:GLN:HG3	1:C:125:GLN:N	2.34	0.43
1:C:897:ILE:HD12	1:C:946:VAL:HG11	2.01	0.43
1:D:79:SER:HA	1:D:818:ARG:O	2.19	0.43
1:D:388:PHE:CE2	1:D:472:ILE:HG21	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:902:MET:O	1:E:905:VAL:HG23	2.19	0.43
1:E:950:LYS:NZ	1:E:1030:ARG:HE	2.17	0.43
1:F:146:ASP:OD2	1:F:147:GLY:N	2.52	0.43
1:F:352:PHE:HA	1:F:355:MET:HE2	1.99	0.43
1:F:746:ILE:HG13	1:F:747:ASN:N	2.33	0.43
1:A:393:LEU:HD11	1:A:466:ILE:HD12	2.01	0.43
1:A:685:ILE:HD12	1:A:858:ASP:HB2	2.01	0.43
1:A:961:ILE:H	1:A:961:ILE:HG13	1.20	0.43
1:B:61:VAL:HG21	1:B:122:VAL:HG21	2.00	0.43
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.54	0.43
1:B:187:TRP:HB3	1:B:776:GLU:HA	2.01	0.43
1:B:249:ILE:HG12	1:B:262:LEU:HB2	2.01	0.43
1:B:925:VAL:O	1:B:928:GLN:N	2.52	0.43
1:C:344:LEU:HA	1:C:399:VAL:HG22	2.01	0.43
1:C:552:MET:HE2	1:C:552:MET:HB3	1.88	0.43
1:D:352:PHE:CD2	1:D:352:PHE:C	2.97	0.43
1:D:465:ALA:O	1:D:469:GLN:HG2	2.18	0.43
1:D:556:PHE:HZ	3:D:1103:LMT:H52	1.84	0.43
1:E:200:PRO:HB2	1:E:749:THR:HG22	2.01	0.43
1:E:965:LEU:HD23	1:E:965:LEU:HA	1.80	0.43
1:F:248:LYS:HA	1:F:261:LEU:HD13	2.00	0.43
1:F:610:PHE:N	1:F:628:PHE:O	2.46	0.43
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.77	0.43
1:A:636:ASP:C	1:A:638:PRO:HD3	2.44	0.43
1:B:568:ASP:OD1	1:B:644:VAL:HG23	2.19	0.43
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.99	0.43
1:B:987:MET:HB3	1:B:988:PRO:HD3	2.01	0.43
1:C:435:MET:O	1:C:439:GLN:HB2	2.19	0.43
1:C:462:SER:HB3	1:C:865:GLN:HG2	2.00	0.43
1:D:108:GLN:HE21	1:E:109:ASN:HB2	1.81	0.43
1:D:182:TYR:HB2	1:D:769:LYS:HZ3	1.84	0.43
1:D:344:LEU:HD22	1:D:402:ILE:CD1	2.43	0.43
1:D:423:GLU:C	1:D:502:LYS:HB3	2.44	0.43
1:E:43:VAL:HG13	1:E:130:GLU:O	2.18	0.43
1:E:409:ALA:O	1:E:413:VAL:HG23	2.19	0.43
1:A:362:PHE:O	1:A:365:THR:HG22	2.19	0.43
1:A:396:PHE:CD1	1:A:926:TYR:HE2	2.37	0.43
1:A:699:ARG:HE	1:A:718:PRO:HG3	1.84	0.43
1:A:857:TYR:HD2	1:A:857:TYR:N	2.16	0.43
1:C:568:ASP:OD1	1:C:637:ARG:NH1	2.49	0.43
1:D:362:PHE:O	1:D:365:THR:HG22	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:MET:HB3	1:D:552:MET:HE2	1.97	0.43
1:E:68:ASN:CB	1:E:114:ALA:HB2	2.49	0.43
1:E:327:TYR:CD1	1:E:628:PHE:CZ	3.04	0.43
1:E:739:LEU:HD12	1:E:799:VAL:HG11	2.00	0.43
1:E:781:MET:HB2	1:E:782:LEU:HG	2.01	0.43
1:E:950:LYS:HZ1	1:E:1030:ARG:NH2	2.17	0.43
1:F:401:ALA:O	1:F:404:LEU:N	2.52	0.43
1:F:735:LYS:O	1:F:738:ALA:HB3	2.19	0.43
1:A:85:THR:HG21	1:A:620:ALA:CB	2.48	0.42
1:A:366:LEU:HA	1:A:369:THR:HB	2.01	0.42
1:A:672:VAL:C	1:A:674:LEU:H	2.27	0.42
1:B:101:ASP:N	1:B:131:LYS:HZ3	2.17	0.42
1:B:398:MET:HB3	1:B:398:MET:HE3	1.55	0.42
1:C:57:VAL:HG23	1:C:82:SER:HB3	2.00	0.42
1:C:331:PRO:O	1:C:335:ILE:HG22	2.19	0.42
1:D:203:VAL:O	1:D:207:ILE:HG13	2.20	0.42
1:D:239:ARG:NH1	1:D:761:ASP:O	2.52	0.42
1:D:324:VAL:HG13	1:D:326:PRO:HD3	2.00	0.42
1:D:559:LEU:HA	1:D:560:PRO:HD2	1.66	0.42
1:D:909:VAL:HG22	1:D:931:LEU:HD21	2.01	0.42
1:E:400:LEU:HD13	1:E:400:LEU:HA	1.63	0.42
1:F:151:GLN:HE22	1:F:278:ILE:HG22	1.84	0.42
1:A:56:THR:O	1:A:60:THR:HG22	2.19	0.42
1:A:382:VAL:O	1:A:385:ALA:HB3	2.19	0.42
1:B:378:GLY:O	1:B:382:VAL:HG23	2.19	0.42
1:B:616:GLY:CA	1:B:626:ILE:HD13	2.48	0.42
1:B:1035:ARG:O	1:B:1037:ASN:HB2	2.19	0.42
1:B:1040:ILE:HG12	1:B:1041:GLU:H	1.83	0.42
1:C:157:TYR:O	1:C:161:ASN:HB2	2.18	0.42
1:C:674:LEU:HA	1:C:674:LEU:HD23	1.75	0.42
1:C:953:MET:HE3	1:C:953:MET:HB2	1.57	0.42
1:D:5:PHE:CE1	1:D:487:ILE:HG12	2.54	0.42
1:D:605:ASN:HD22	1:D:647:ILE:HD11	1.84	0.42
1:D:876:LEU:HD23	1:D:876:LEU:HA	1.84	0.42
1:E:416:VAL:HG11	1:E:497:LEU:HD23	2.01	0.42
1:F:446:ALA:HA	1:F:478:MET:CE	2.49	0.42
1:A:240:LEU:HD12	1:A:246:PHE:CE1	2.54	0.42
1:A:246:PHE:O	1:A:262:LEU:HB3	2.20	0.42
1:A:586:ARG:O	1:A:589:LYS:HB3	2.19	0.42
1:B:368:PRO:HG3	1:B:413:VAL:HG21	2.01	0.42
1:B:717:ARG:HD2	1:B:828:LEU:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:TYR:HE1	1:B:800:PRO:HB3	1.84	0.42
1:B:931:LEU:O	1:B:935:ILE:HG13	2.20	0.42
1:B:953:MET:HB2	1:B:953:MET:HE3	1.50	0.42
1:C:423:GLU:OE1	1:C:433:LYS:HE2	2.19	0.42
1:D:360:GLN:HE21	1:D:360:GLN:HB3	1.39	0.42
1:D:544:LEU:O	1:D:547:ILE:HB	2.19	0.42
1:E:30:LEU:HD12	1:E:30:LEU:HA	1.77	0.42
1:F:177:LEU:HA	1:F:177:LEU:HD23	1.74	0.42
1:F:913:LEU:HD23	1:F:927:PHE:CZ	2.54	0.42
1:F:979:SER:HB3	1:F:1015:THR:HG21	1.99	0.42
1:A:75:LEU:HD21	1:C:168:ARG:HD3	2.02	0.42
1:A:151:GLN:HG3	1:A:152:GLU:N	2.30	0.42
1:A:480:LEU:HA	1:A:480:LEU:HD23	1.85	0.42
1:A:679:GLY:C	1:A:862:MET:HE2	2.44	0.42
1:A:1017:LEU:O	1:A:1021:PHE:HD1	2.02	0.42
1:B:310:LEU:HD23	1:B:323:ILE:HG21	2.01	0.42
1:B:574:THR:HG21	1:B:598:TYR:HE2	1.84	0.42
1:B:1036:LYS:O	1:B:1038:GLU:HA	2.20	0.42
1:C:343:THR:HG21	1:C:989:LEU:HD23	2.01	0.42
1:C:450:SER:O	1:C:454:VAL:HG23	2.20	0.42
1:C:599:LEU:O	1:C:603:LYS:HG2	2.20	0.42
1:D:293:LEU:HD11	1:D:299:ALA:HA	2.02	0.42
1:E:145:THR:O	1:E:284:GLN:NE2	2.53	0.42
1:E:210:GLN:HG2	1:F:733:GLN:HE21	1.84	0.42
1:E:572:PHE:CE1	1:E:648:THR:HG22	2.55	0.42
1:E:735:LYS:O	1:E:738:ALA:HB3	2.19	0.42
1:F:135:SER:HB3	1:F:673:GLU:HB3	2.01	0.42
1:F:375:VAL:HA	1:F:480:LEU:HD13	2.01	0.42
1:F:568:ASP:CG	1:F:637:ARG:HH12	2.25	0.42
1:F:889:ALA:HB2	1:F:898:PRO:HG2	2.01	0.42
1:B:225:VAL:HG12	1:C:777:ALA:HB1	2.01	0.42
1:B:428:LYS:HG2	1:B:494:ALA:HB1	2.01	0.42
1:B:781:MET:HE3	1:B:781:MET:HB3	1.90	0.42
1:B:903:LEU:HD13	1:B:1025:PHE:CD2	2.54	0.42
1:B:919:ARG:NH2	1:B:921:LEU:HD21	2.35	0.42
1:B:1030:ARG:HH11	1:B:1030:ARG:HD2	1.70	0.42
1:C:80:SER:HB3	1:C:90:ILE:HG23	2.02	0.42
1:C:189:ASN:OD1	1:C:190:PRO:HD2	2.19	0.42
1:C:703:LEU:CD1	1:C:718:PRO:HD3	2.49	0.42
1:C:860:THR:CA	1:C:864:TYR:HB2	2.50	0.42
2:D:1101:ERY:H71	2:D:1101:ERY:H4	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:PRO:HD3	1:E:391:ASN:CG	2.44	0.42
1:E:145:THR:C	1:E:147:GLY:H	2.26	0.42
1:E:572:PHE:CD1	1:E:648:THR:HG22	2.54	0.42
1:E:679:GLY:HA2	1:E:830:GLN:HA	2.00	0.42
1:F:450:SER:O	1:F:454:VAL:HG23	2.19	0.42
1:F:726:GLN:NE2	1:F:812:GLY:HA3	2.35	0.42
1:F:1040:ILE:HG22	1:F:1044:HIS:HB2	2.00	0.42
1:A:65:ILE:O	1:A:69:MET:HG2	2.20	0.42
1:A:363:ARG:O	1:A:496:MET:HE2	2.19	0.42
1:A:475:VAL:HA	1:A:478:MET:HE2	2.02	0.42
1:B:261:LEU:HD12	1:B:263:ARG:NH2	2.35	0.42
1:B:435:MET:O	1:B:439:GLN:HG3	2.19	0.42
1:C:524:THR:O	1:C:528:THR:HG22	2.19	0.42
1:C:694:LYS:HE3	1:C:694:LYS:H	1.85	0.42
1:C:714:THR:OG1	1:C:832:ALA:HA	2.20	0.42
1:C:888:LEU:HD23	1:C:888:LEU:HA	1.80	0.42
1:D:110:LYS:HD3	1:D:110:LYS:HA	1.76	0.42
1:D:228:GLN:OE1	1:E:781:MET:HE3	2.19	0.42
1:E:950:LYS:NZ	1:E:1030:ARG:HH21	2.18	0.42
1:F:45:ILE:O	1:F:89:GLN:HA	2.20	0.42
1:F:658:ILE:O	1:F:658:ILE:HG13	2.19	0.42
1:F:721:LEU:HD12	1:F:721:LEU:HA	1.83	0.42
1:F:851:LEU:HB3	1:F:852:PRO:HD2	2.02	0.42
1:B:157:TYR:CZ	1:B:318:PRO:HD3	2.55	0.42
1:B:224:PRO:HA	1:C:781:MET:HE1	2.01	0.42
1:B:905:VAL:HB	1:B:906:PRO:HD3	2.02	0.42
1:C:415:ASN:O	1:C:419:VAL:HG23	2.19	0.42
1:C:559:LEU:HA	1:C:560:PRO:HD2	1.70	0.42
1:D:377:LEU:O	1:D:380:PHE:HB2	2.19	0.42
1:D:525:HIS:NE2	1:D:529:ASP:OD2	2.53	0.42
1:D:582:ALA:HB3	1:D:623:ASN:HB3	2.01	0.42
1:D:598:TYR:CE2	1:D:629:VAL:HG21	2.55	0.42
1:D:781:MET:HE2	1:F:225:VAL:HG22	2.00	0.42
1:E:445:ILE:HG21	1:E:940:LYS:HD2	2.01	0.42
1:F:227:GLY:O	1:F:229:GLN:HG3	2.19	0.42
1:F:382:VAL:HG11	1:F:476:SER:CB	2.49	0.42
1:F:898:PRO:HA	1:F:901:VAL:HG12	2.01	0.42
1:F:965:LEU:HD23	1:F:965:LEU:HA	1.79	0.42
1:A:59:ASP:HB3	1:C:763:ILE:CD1	2.48	0.42
1:A:842:GLU:HG2	1:A:846:GLN:OE1	2.20	0.42
1:B:540:ARG:HH22	3:B:1101:LMT:H6'1	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:MET:HA	1:B:662:MET:HE3	2.01	0.42
1:B:889:ALA:HA	1:B:894:SER:O	2.20	0.42
1:C:34:GLN:HB2	1:C:333:VAL:CG2	2.49	0.42
1:C:1033:PHE:O	1:C:1035:ARG:N	2.51	0.42
1:D:82:SER:HB2	1:D:816:LEU:HB2	2.00	0.42
1:D:279:ALA:HB3	1:D:286:ALA:O	2.19	0.42
1:D:534:ILE:HD11	1:D:1024:VAL:HG22	2.01	0.42
1:D:644:VAL:HG11	1:D:667:ASN:HB2	2.02	0.42
1:E:65:ILE:O	1:E:69:MET:HG2	2.19	0.42
1:E:383:LEU:HD23	1:E:383:LEU:HA	1.83	0.42
1:E:925:VAL:O	1:E:928:GLN:N	2.53	0.42
1:E:1041:GLU:HB3	1:E:1042:HIS:CA	2.50	0.42
1:F:211:ASN:CG	1:F:240:LEU:HG	2.44	0.42
1:F:361:ASN:ND2	1:F:498:LYS:HD3	2.34	0.42
1:F:602:GLU:HB3	1:F:606:VAL:HG23	2.01	0.42
1:F:675:GLY:HA3	1:F:862:MET:HG2	2.01	0.42
1:A:178:PHE:HA	1:A:277:ILE:HG21	2.01	0.42
1:A:324:VAL:HG13	1:A:326:PRO:HD3	2.01	0.42
1:A:426:PRO:HD2	1:A:429:GLU:HG3	2.01	0.42
1:A:790:TYR:HB3	1:A:798:MET:HB3	2.00	0.42
1:D:38:ILE:HG22	1:D:674:LEU:HD13	2.02	0.42
1:D:576:VAL:HG21	1:D:591:LEU:HD23	2.02	0.42
1:D:991:ILE:CG2	1:D:992:SER:H	2.28	0.42
1:E:190:PRO:HB3	1:E:789:TRP:CD2	2.55	0.42
1:E:277:ILE:H	1:E:277:ILE:HG13	1.56	0.42
1:E:527:TYR:OH	1:E:968:VAL:HG22	2.20	0.42
1:E:583:THR:HG22	1:E:584:GLN:N	2.35	0.42
1:E:672:VAL:H	1:E:672:VAL:HG22	1.54	0.42
1:F:571:VAL:HG12	1:F:668:LEU:HD11	2.01	0.42
1:F:948:PHE:CD1	1:F:971:ARG:HD3	2.54	0.42
1:A:58:GLN:HA	1:A:62:THR:HB	2.01	0.42
1:A:121:GLU:O	1:A:125:GLN:HB2	2.20	0.42
1:A:475:VAL:O	1:A:478:MET:HB3	2.20	0.42
1:A:971:ARG:O	1:A:975:ILE:HG12	2.20	0.42
1:B:345:VAL:HA	1:B:348:ILE:HD12	2.01	0.42
1:B:735:LYS:O	1:B:739:LEU:HG	2.20	0.42
1:B:950:LYS:HE2	1:B:950:LYS:HB2	1.81	0.42
1:B:961:ILE:O	1:B:965:LEU:HG	2.20	0.42
1:C:26:ALA:HB1	1:C:384:ALA:HB2	2.02	0.42
1:C:129:VAL:C	1:C:130:GLU:HG3	2.45	0.42
1:C:559:LEU:HD23	1:C:560:PRO:CD	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:902:MET:O	1:D:905:VAL:HG23	2.20	0.42
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.49	0.42
1:E:376:LEU:HD23	1:E:376:LEU:HA	1.91	0.42
1:E:584:GLN:HB2	1:E:622:GLN:HG2	2.01	0.42
1:F:11:PHE:O	1:F:11:PHE:HD2	2.02	0.42
1:F:76:MET:HG3	1:F:95:GLU:CD	2.45	0.42
1:F:344:LEU:HD22	1:F:402:ILE:HD11	2.01	0.42
1:F:344:LEU:HD13	1:F:402:ILE:HD11	2.01	0.42
1:F:412:VAL:CG1	1:F:435:MET:HE1	2.50	0.42
1:F:668:LEU:H	1:F:668:LEU:HG	1.26	0.42
1:F:911:GLY:HA2	1:F:1013:THR:HG21	2.02	0.42
1:F:945:ILE:HA	1:F:971:ARG:HH22	1.85	0.42
1:A:11:PHE:CE1	1:A:15:ILE:HD11	2.55	0.41
1:A:120:GLN:O	1:A:124:GLN:HG2	2.20	0.41
1:A:407:ASP:OD1	1:A:978:THR:HG21	2.19	0.41
1:A:622:GLN:HE21	1:C:222:THR:CG2	2.33	0.41
1:A:775:SER:OG	1:A:776:GLU:N	2.53	0.41
1:A:921:LEU:HA	1:A:921:LEU:HD13	1.86	0.41
1:A:951:ASP:O	1:A:955:LYS:HB2	2.19	0.41
1:A:990:VAL:HG22	1:A:1004:GLY:HA3	2.01	0.41
1:A:1040:ILE:O	1:A:1041:GLU:HG3	2.19	0.41
1:B:401:ALA:O	1:B:405:LEU:HG	2.20	0.41
1:B:692:HIS:NE2	1:B:813:SER:HB2	2.35	0.41
1:C:13:TRP:O	1:C:17:ILE:HG13	2.19	0.41
1:C:158:VAL:HG22	1:C:162:MET:CE	2.50	0.41
1:C:188:MET:HA	1:C:266:ALA:CB	2.49	0.41
1:C:363:ARG:HH21	1:C:498:LYS:HD2	1.85	0.41
1:D:442:LEU:O	1:D:445:ILE:HG13	2.20	0.41
1:D:515:TRP:O	1:D:519:MET:HG3	2.19	0.41
1:D:573:MET:HB2	1:D:666:PHE:CE1	2.55	0.41
1:E:555:LEU:HD23	1:E:555:LEU:HA	1.66	0.41
1:E:572:PHE:HA	1:E:668:LEU:CD2	2.50	0.41
1:E:758:TYR:HB2	1:E:772:TYR:HE1	1.84	0.41
1:E:937:LEU:HA	1:E:937:LEU:HD23	1.56	0.41
1:F:452:VAL:HG13	1:F:884:VAL:HG23	2.02	0.41
1:F:682:PHE:CZ	1:F:857:TYR:HB2	2.55	0.41
1:F:811:TYR:HD1	1:F:811:TYR:HA	1.72	0.41
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.51	0.41
1:B:510:LYS:HA	1:B:510:LYS:HD3	1.87	0.41
1:B:699:ARG:HH11	1:B:825:MET:HE1	1.84	0.41
1:D:659:LYS:HA	1:D:659:LYS:HD3	1.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:950:LYS:HZ3	1:D:1030:ARG:CZ	2.33	0.41
1:D:1036:LYS:HB2	1:D:1036:LYS:HE2	1.59	0.41
1:E:5:PHE:CE1	1:E:487:ILE:HG12	2.56	0.41
1:E:104:GLN:CB	1:E:131:LYS:HE3	2.48	0.41
1:E:453:PHE:HZ	1:E:933:THR:HA	1.85	0.41
1:E:478:MET:HE3	1:E:478:MET:HB3	1.82	0.41
1:F:465:ALA:HA	1:F:468:ARG:HH11	1.85	0.41
1:B:17:ILE:HD13	1:B:17:ILE:HG21	1.80	0.41
1:B:239:ARG:NH1	1:B:761:ASP:HB2	2.35	0.41
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.85	0.41
1:B:950:LYS:HZ1	1:B:1030:ARG:NE	2.19	0.41
1:C:31:PRO:HB2	1:C:389:SER:HB3	2.00	0.41
1:C:48:SER:O	1:C:122:VAL:HA	2.20	0.41
1:C:869:SER:HG	1:C:928:GLN:HE22	1.67	0.41
1:D:616:GLY:HA2	1:D:626:ILE:HD13	2.02	0.41
1:D:791:VAL:HG21	1:D:804:PHE:HZ	1.86	0.41
1:E:354:VAL:O	1:E:358:PHE:HB2	2.21	0.41
1:E:950:LYS:HA	1:E:953:MET:HE3	2.02	0.41
1:F:55:LYS:HB3	1:F:55:LYS:HE2	1.77	0.41
1:F:153:ASP:OD2	1:F:182:TYR:OH	2.37	0.41
1:F:211:ASN:ND2	1:F:760:ASN:HD21	2.15	0.41
1:F:892:TYR:C	1:F:894:SER:N	2.75	0.41
1:A:435:MET:O	1:A:439:GLN:HB2	2.20	0.41
1:A:451:ALA:HB1	1:A:883:VAL:HG12	2.02	0.41
1:B:99:ASP:O	1:B:100:ALA:C	2.64	0.41
1:B:317:PHE:CE2	1:B:323:ILE:HD13	2.55	0.41
1:B:894:SER:HB2	1:B:897:ILE:HD12	2.01	0.41
1:B:966:ASP:O	1:B:969:ARG:HB3	2.21	0.41
1:C:40:PRO:HB2	1:C:94:PHE:O	2.20	0.41
1:C:398:MET:HE3	1:C:398:MET:HB3	1.80	0.41
1:C:696:THR:HG23	1:C:699:ARG:HH12	1.85	0.41
1:D:273:GLU:OE2	1:D:770:LYS:HD2	2.20	0.41
1:D:504:ASP:C	1:D:506:GLY:H	2.27	0.41
1:E:535:LEU:HA	1:E:535:LEU:HD23	1.85	0.41
1:E:717:ARG:HE	1:E:828:LEU:HD12	1.84	0.41
1:A:188:MET:HE3	1:A:188:MET:HB2	1.94	0.41
1:A:225:VAL:HG13	1:B:781:MET:SD	2.60	0.41
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.86	0.41
1:A:1033:PHE:HD2	1:A:1034:SER:H	1.66	0.41
1:B:400:LEU:HD12	1:B:933:THR:HG21	2.02	0.41
1:B:647:ILE:HG12	1:B:650:ARG:NH1	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:TYR:HD2	1:B:877:TYR:HA	1.73	0.41
1:C:393:LEU:CD1	1:C:469:GLN:HG3	2.46	0.41
1:C:563:PHE:CD2	1:C:564:LEU:HB2	2.55	0.41
1:D:2:PRO:HG2	1:D:3:ASN:H	1.85	0.41
1:D:142:VAL:HG21	1:D:158:VAL:HG22	2.02	0.41
1:D:154:ILE:HG22	1:D:287:SER:HB3	2.03	0.41
1:D:280:GLU:HG2	1:D:285:PRO:HA	2.02	0.41
1:D:396:PHE:HE1	1:D:999:ALA:HB1	1.85	0.41
1:D:847:LEU:HD23	1:D:847:LEU:HA	1.83	0.41
1:D:892:TYR:OH	1:D:946:VAL:HB	2.20	0.41
1:E:621:GLY:O	1:E:624:THR:HG22	2.21	0.41
1:E:971:ARG:C	1:E:974:PRO:HD2	2.45	0.41
1:F:196:PHE:CD2	1:F:260:VAL:HG13	2.55	0.41
1:A:158:VAL:HG22	1:A:162:MET:CE	2.50	0.41
1:A:467:TYR:CE1	1:A:925:VAL:HG22	2.56	0.41
1:A:527:TYR:CE2	1:A:968:VAL:HG13	2.56	0.41
1:B:228:GLN:HE21	1:B:230:LEU:H	1.68	0.41
1:B:542:LEU:HD23	1:B:542:LEU:HA	1.85	0.41
1:C:34:GLN:HB2	1:C:333:VAL:HG13	2.01	0.41
1:C:597:TYR:CD2	1:C:655:PHE:HZ	2.38	0.41
1:C:623:ASN:OD1	1:C:623:ASN:N	2.43	0.41
1:C:678:THR:O	1:C:830:GLN:HG2	2.21	0.41
1:C:731:ILE:HG21	1:C:746:ILE:HD13	2.03	0.41
1:D:361:ASN:HB3	1:D:364:ALA:HB3	2.03	0.41
1:D:393:LEU:HD12	1:D:469:GLN:HG3	2.02	0.41
1:D:801:PHE:O	1:D:805:SER:OG	2.34	0.41
1:D:873:ALA:HB2	3:D:1103:LMT:H21	2.03	0.41
1:E:220:GLY:HA3	1:E:230:LEU:O	2.20	0.41
1:E:527:TYR:OH	1:E:1019:ILE:O	2.29	0.41
1:E:559:LEU:HD23	1:E:560:PRO:CD	2.50	0.41
1:E:888:LEU:HD23	1:E:888:LEU:HA	1.74	0.41
1:F:250:LEU:CD1	1:F:259:ARG:HB3	2.46	0.41
1:F:344:LEU:HA	1:F:399:VAL:HG22	2.02	0.41
1:F:559:LEU:HA	1:F:560:PRO:HD2	1.56	0.41
1:A:24:GLY:O	1:A:27:ILE:HB	2.21	0.41
1:A:55:LYS:HE2	1:A:55:LYS:HB3	1.78	0.41
1:A:141:GLY:O	1:A:323:ILE:HG23	2.20	0.41
1:B:775:SER:OG	1:B:780:ARG:HG2	2.20	0.41
1:D:94:PHE:CE2	1:D:103:ALA:HB1	2.56	0.41
1:D:953:MET:HE3	1:D:953:MET:HB2	1.59	0.41
1:D:1034:SER:O	1:D:1035:ARG:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:942:ALA:O	1:E:946:VAL:HG23	2.21	0.41
1:F:533:GLY:O	1:F:536:ARG:HB2	2.21	0.41
1:A:66:GLU:OE1	1:A:821:GLY:HA2	2.21	0.41
1:A:514:GLY:C	1:A:516:PHE:N	2.76	0.41
1:A:925:VAL:HG12	1:A:926:TYR:N	2.35	0.41
1:B:188:MET:HB3	1:B:193:LEU:HD11	2.03	0.41
1:B:950:LYS:NZ	1:B:1030:ARG:HH21	2.18	0.41
1:C:270:LEU:HD11	1:C:762:PHE:HZ	1.86	0.41
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.89	0.41
1:C:465:ALA:O	1:C:468:ARG:HB3	2.20	0.41
1:D:18:ILE:HG21	1:D:18:ILE:HD13	1.83	0.41
1:D:687:GLN:HG2	1:F:316:PHE:CE1	2.56	0.41
1:E:139:VAL:O	1:E:326:PRO:HD2	2.21	0.41
1:E:369:THR:O	1:E:373:PRO:CD	2.69	0.41
1:E:448:VAL:O	1:E:452:VAL:HG13	2.20	0.41
1:E:504:ASP:C	1:E:506:GLY:H	2.29	0.41
1:E:598:TYR:CE2	1:E:629:VAL:HG21	2.56	0.41
1:F:23:GLY:HA3	1:F:377:LEU:HB3	2.02	0.41
1:F:1039:ASP:HB3	1:F:1041:GLU:HB2	2.03	0.41
1:F:1045:THR:O	1:F:1046:VAL:HB	2.21	0.41
1:A:224:PRO:CB	1:B:781:MET:HE1	2.51	0.41
1:A:246:PHE:O	1:A:262:LEU:HD23	2.21	0.41
1:A:278:ILE:CG1	1:A:613:ASN:HB3	2.47	0.41
1:A:292:LYS:NZ	2:A:1101:ERY:O11	2.53	0.41
1:A:488:LEU:HD12	1:A:488:LEU:HA	1.76	0.41
1:A:508:GLY:O	1:A:509:LYS:C	2.64	0.41
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.60	0.41
1:A:659:LYS:HD3	1:A:659:LYS:HA	1.51	0.41
1:A:735:LYS:O	1:A:738:ALA:HB3	2.20	0.41
1:A:755:GLY:C	1:A:774:MET:HE3	2.46	0.41
1:A:953:MET:HE3	1:A:953:MET:HB2	1.88	0.41
1:B:211:ASN:OD1	1:B:239:ARG:HA	2.21	0.41
1:B:562:SER:OG	1:B:563:PHE:N	2.53	0.41
1:C:154:ILE:HG22	1:C:287:SER:HB3	2.03	0.41
1:C:431:THR:HG21	1:C:490:PRO:O	2.21	0.41
1:C:578:LEU:CG	1:C:587:THR:HG22	2.42	0.41
1:C:610:PHE:HB3	1:C:628:PHE:HB2	2.02	0.41
1:C:682:PHE:CE1	1:C:857:TYR:HB2	2.55	0.41
1:D:140:VAL:HB	1:D:289:LEU:HB2	2.02	0.41
1:D:143:ILE:HG22	1:D:286:ALA:CB	2.51	0.41
1:D:166:ILE:HD13	1:D:166:ILE:HA	1.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:743:ILE:H	1:D:743:ILE:HD12	1.86	0.41
1:E:435:MET:SD	1:E:490:PRO:HB3	2.61	0.41
1:E:450:SER:HB3	1:E:478:MET:HE1	2.02	0.41
1:E:646:ALA:O	1:E:649:MET:HB3	2.21	0.41
1:E:717:ARG:NE	1:E:828:LEU:HD12	2.36	0.41
1:E:790:TYR:CE1	1:E:800:PRO:HB3	2.56	0.41
1:E:932:LEU:HD23	1:E:935:ILE:HD12	2.02	0.41
1:F:199:THR:HG22	1:F:790:TYR:O	2.21	0.41
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.55	0.41
1:F:469:GLN:O	1:F:472:ILE:HG22	2.21	0.41
1:F:578:LEU:HD22	1:F:661:ALA:HB3	2.03	0.41
1:A:99:ASP:HB3	1:A:102:ILE:HB	2.03	0.41
1:A:247:GLY:C	1:A:249:ILE:H	2.29	0.41
1:A:305:ALA:O	1:A:308:ALA:HB3	2.20	0.41
1:A:344:LEU:HD11	1:A:398:MET:CB	2.51	0.41
1:A:944:LEU:HB3	1:A:971:ARG:CZ	2.51	0.41
1:A:1041:GLU:HB3	1:A:1042:HIS:H	1.68	0.41
1:B:213:GLN:HE22	1:B:238:THR:HG23	1.85	0.41
1:B:394:THR:O	1:B:473:THR:HG21	2.20	0.41
1:B:457:ALA:HB2	1:B:471:SER:OG	2.19	0.41
1:B:919:ARG:HH21	1:B:921:LEU:HD21	1.86	0.41
1:C:380:PHE:CD2	1:C:383:LEU:HD12	2.56	0.41
1:C:926:TYR:CD2	1:C:1003:VAL:HG22	2.55	0.41
1:C:937:LEU:HD23	1:C:937:LEU:HA	1.64	0.41
1:C:940:LYS:O	1:C:943:ILE:HB	2.21	0.41
1:C:987:MET:HB3	1:C:988:PRO:HD3	2.03	0.41
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.56	0.41
1:D:944:LEU:HA	1:D:944:LEU:HD23	1.65	0.41
1:E:775:SER:OG	1:E:780:ARG:HG2	2.21	0.41
1:E:987:MET:HE2	1:E:988:PRO:HD3	2.02	0.41
1:F:5:PHE:O	1:F:7:ASP:N	2.49	0.41
1:F:199:THR:HB	1:F:749:THR:HG21	2.03	0.41
1:A:186:ILE:HB	1:A:773:VAL:CG2	2.44	0.40
1:A:367:ILE:HG12	1:A:492:LEU:HB3	2.04	0.40
1:A:448:VAL:HG22	1:A:887:CYS:HB3	2.02	0.40
1:A:525:HIS:HA	1:A:528:THR:HG22	2.03	0.40
1:A:539:GLY:O	1:A:542:LEU:HB2	2.21	0.40
1:A:672:VAL:C	1:A:674:LEU:N	2.79	0.40
1:A:910:ILE:O	1:A:910:ILE:HG13	2.20	0.40
1:B:362:PHE:HA	1:B:365:THR:HG22	2.03	0.40
1:B:679:GLY:HA2	1:B:830:GLN:HA	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:841:MET:HG2	1:B:859:TRP:CH2	2.57	0.40
1:B:932:LEU:HD23	1:B:932:LEU:HA	1.78	0.40
1:C:882:ILE:O	1:C:886:LEU:HD23	2.21	0.40
1:D:510:LYS:O	1:D:512:PHE:N	2.54	0.40
1:D:915:ALA:HB2	1:D:1009:GLY:HA3	2.03	0.40
1:E:171:GLY:HA3	1:E:302:THR:OG1	2.21	0.40
1:E:363:ARG:O	1:E:367:ILE:HG13	2.20	0.40
1:E:396:PHE:HD1	1:E:926:TYR:CE2	2.34	0.40
1:E:911:GLY:HA2	1:E:1013:THR:HG21	2.03	0.40
1:F:79:SER:O	1:F:91:THR:HB	2.21	0.40
1:F:420:MET:HB3	1:F:500:ILE:HB	2.02	0.40
1:F:443:VAL:HG12	1:F:891:LEU:HD21	2.03	0.40
1:F:713:LEU:HD21	1:F:843:LEU:HD12	2.03	0.40
1:A:534:ILE:CD1	1:A:1024:VAL:HG22	2.52	0.40
1:B:418:ARG:O	1:B:422:GLU:HB2	2.21	0.40
1:B:542:LEU:O	1:B:546:LEU:HG	2.22	0.40
1:B:719:ASN:HB2	1:B:828:LEU:HG	2.03	0.40
1:B:948:PHE:CZ	1:B:971:ARG:HD2	2.55	0.40
1:B:1016:VAL:HG13	3:B:1101:LMT:C10	2.51	0.40
1:C:143:ILE:O	1:C:321:LEU:HD22	2.21	0.40
1:C:182:TYR:HD1	1:C:182:TYR:HA	1.65	0.40
1:C:775:SER:OG	1:C:780:ARG:HG2	2.22	0.40
1:C:892:TYR:C	1:C:894:SER:N	2.78	0.40
1:C:930:GLY:HA2	1:C:1007:VAL:HG23	2.02	0.40
1:D:452:VAL:HA	1:D:880:SER:OG	2.22	0.40
1:E:448:VAL:HG13	1:E:884:VAL:CG2	2.47	0.40
1:F:544:LEU:HD23	1:F:1021:PHE:CZ	2.57	0.40
1:A:375:VAL:HG13	1:A:480:LEU:CB	2.51	0.40
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.82	0.40
1:B:354:VAL:O	1:B:358:PHE:HB2	2.21	0.40
1:B:359:LEU:C	1:B:360:GLN:HG2	2.45	0.40
1:B:419:VAL:HG12	1:B:425:LEU:HD12	2.02	0.40
1:B:434:SER:C	1:B:437:GLN:H	2.30	0.40
1:B:540:ARG:O	1:B:543:VAL:HB	2.22	0.40
1:B:736:ALA:HB1	1:B:741:VAL:HG23	2.03	0.40
1:B:938:SER:OG	1:B:1014:ALA:HB1	2.20	0.40
1:C:102:ILE:HD12	1:C:102:ILE:HG23	1.84	0.40
1:C:120:GLN:O	1:C:123:GLN:HB2	2.22	0.40
1:C:509:LYS:HD2	1:C:509:LYS:HA	1.79	0.40
1:C:536:ARG:NH2	3:C:1101:LMT:O3B	2.55	0.40
1:C:555:LEU:HD23	1:C:555:LEU:HA	1.79	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:971:ARG:C	1:C:974:PRO:HD2	2.46	0.40
1:D:61:VAL:CG2	1:D:122:VAL:HG21	2.51	0.40
1:D:507:GLU:O	1:D:508:GLY:O	2.38	0.40
1:D:574:THR:HG21	1:D:598:TYR:CE2	2.56	0.40
1:D:877:TYR:CE1	3:D:1103:LMT:H91	2.57	0.40
1:E:103:ALA:HA	1:E:106:GLN:OE1	2.21	0.40
1:E:775:SER:HB3	1:E:780:ARG:HD3	2.03	0.40
1:E:1041:GLU:HB3	1:E:1042:HIS:C	2.46	0.40
1:F:63:GLN:O	1:F:67:GLN:HG3	2.22	0.40
1:F:415:ASN:ND2	1:F:434:SER:HB2	2.36	0.40
1:F:888:LEU:HD21	1:F:943:ILE:HD11	2.02	0.40
1:A:13:TRP:O	1:A:17:ILE:HG13	2.21	0.40
1:A:30:LEU:HA	1:A:31:PRO:HD3	1.86	0.40
1:A:63:GLN:OE1	1:C:768:VAL:HG12	2.21	0.40
1:A:134:SER:HG	2:A:1101:ERY:H323	1.81	0.40
1:A:351:VAL:O	1:A:355:MET:HG2	2.21	0.40
1:A:402:ILE:HD13	1:A:402:ILE:HG21	1.81	0.40
1:B:736:ALA:HB1	1:B:746:ILE:HD11	2.03	0.40
1:B:987:MET:HB3	1:B:987:MET:HE2	1.65	0.40
1:C:104:GLN:HG3	1:C:105:VAL:N	2.35	0.40
1:C:388:PHE:HE2	1:C:472:ILE:CG1	2.34	0.40
1:C:659:LYS:HD3	1:C:659:LYS:HA	1.27	0.40
1:C:1041:GLU:HB3	1:C:1042:HIS:CA	2.52	0.40
1:D:573:MET:O	1:D:666:PHE:HD1	2.05	0.40
1:D:704:ALA:O	1:D:707:ALA:HB3	2.22	0.40
1:E:100:ALA:C	1:E:131:LYS:HZ1	2.30	0.40
1:E:907:LEU:HG	1:E:1017:LEU:HD23	2.03	0.40
1:F:535:LEU:HD23	1:F:535:LEU:HA	1.63	0.40
1:F:931:LEU:O	1:F:934:THR:HB	2.21	0.40
1:F:1021:PHE:HD2	1:F:1025:PHE:CZ	2.39	0.40
1:F:1041:GLU:HB3	1:F:1042:HIS:CB	2.50	0.40
1:B:196:PHE:CD1	1:B:196:PHE:N	2.90	0.40
1:B:233:SER:HB2	1:C:726:GLN:HG2	2.02	0.40
1:B:278:ILE:HG13	1:B:613:ASN:HB3	2.04	0.40
1:B:743:ILE:HA	1:B:746:ILE:CD1	2.50	0.40
1:C:162:MET:HA	1:C:313:MET:HE1	2.03	0.40
1:C:196:PHE:CD2	1:C:260:VAL:HG13	2.56	0.40
1:D:448:VAL:HG13	1:D:884:VAL:HG22	2.03	0.40
1:D:509:LYS:C	1:D:511:GLY:H	2.29	0.40
1:D:888:LEU:CD1	1:D:901:VAL:HG13	2.48	0.40
1:E:463:THR:OG1	1:E:464:GLY:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:TRP:HH2	1:F:370:ILE:HD13	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:HIS:NE2	1:D:525:HIS:NE2[1_556]	2.02	0.18

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1040/1049 (99%)	951 (91%)	75 (7%)	14 (1%)	9	39
1	B	1040/1049 (99%)	957 (92%)	70 (7%)	13 (1%)	9	39
1	C	1042/1049 (99%)	954 (92%)	72 (7%)	16 (2%)	8	37
1	D	1040/1049 (99%)	946 (91%)	79 (8%)	15 (1%)	9	38
1	E	1040/1049 (99%)	960 (92%)	63 (6%)	17 (2%)	7	36
1	F	1044/1049 (100%)	945 (90%)	83 (8%)	16 (2%)	8	37
All	All	6246/6294 (99%)	5713 (92%)	442 (7%)	91 (2%)	8	37

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	LYS
1	A	673	GLU
1	A	675	GLY
1	A	991	ILE
1	A	1040	ILE
1	B	509	LYS
1	B	677	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	893	GLU
1	B	1038	GLU
1	B	1040	ILE
1	C	1035	ARG
1	C	1036	LYS
1	C	1043	SER
1	D	508	GLY
1	D	511	GLY
1	D	673	GLU
1	D	675	GLY
1	D	992	SER
1	D	1034	SER
1	D	1040	ILE
1	E	509	LYS
1	E	672	VAL
1	E	677	ALA
1	F	511	GLY
1	F	893	GLU
1	A	147	GLY
1	A	869	SER
1	B	672	VAL
1	B	673	GLU
1	B	1037	ASN
1	B	1041	GLU
1	C	146	ASP
1	C	360	GLN
1	C	689	GLY
1	C	1041	GLU
1	D	509	LYS
1	D	991	ILE
1	D	1037	ASN
1	D	1039	ASP
1	E	893	GLU
1	E	1034	SER
1	E	1037	ASN
1	F	146	ASP
1	F	1033	PHE
1	F	1042	HIS
1	F	1046	VAL
1	B	263	ARG
1	B	507	GLU
1	C	893	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1037	ASN
1	E	147	GLY
1	E	673	GLU
1	E	1033	PHE
1	F	360	GLN
1	F	836	SER
1	A	992	SER
1	A	1038	GLU
1	C	357	LEU
1	C	407	ASP
1	C	1042	HIS
1	D	869	SER
1	D	1042	HIS
1	E	775	SER
1	E	1041	GLU
1	F	147	GLY
1	A	775	SER
1	C	775	SER
1	D	775	SER
1	E	263	ARG
1	E	892	TYR
1	F	357	LEU
1	F	507	GLU
1	F	509	LYS
1	F	1044	HIS
1	A	263	ARG
1	A	765	ARG
1	C	765	ARG
1	D	1038	GLU
1	E	146	ASP
1	E	357	LEU
1	E	511	GLY
1	E	1040	ILE
1	F	1039	ASP
1	C	6	ILE
1	F	638	PRO
1	A	672	VAL
1	B	638	PRO
1	A	910	ILE
1	B	910	ILE
1	C	638	PRO
1	F	6	ILE

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	845/852 (99%)	773 (92%)	72 (8%)	10	35
1	B	845/852 (99%)	779 (92%)	66 (8%)	11	38
1	C	847/852 (99%)	773 (91%)	74 (9%)	9	34
1	D	845/852 (99%)	777 (92%)	68 (8%)	11	37
1	E	845/852 (99%)	773 (92%)	72 (8%)	10	35
1	F	849/852 (100%)	780 (92%)	69 (8%)	11	36
All	All	5076/5112 (99%)	4655 (92%)	421 (8%)	10	35

All (421) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	18	ILE
1	A	28	LEU
1	A	45	ILE
1	A	137	LEU
1	A	151	GLN
1	A	152	GLU
1	A	185	ARG
1	A	205	THR
1	A	222	THR
1	A	225	VAL
1	A	243	THR
1	A	245	GLU
1	A	293	LEU
1	A	310	LEU
1	A	324	VAL
1	A	343	THR
1	A	349	ILE
1	A	360	GLN
1	A	362	PHE
1	A	369	THR
1	A	400	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	415	ASN
1	A	429	GLU
1	A	434	SER
1	A	437	GLN
1	A	456	MET
1	A	463	THR
1	A	472	ILE
1	A	523	SER
1	A	524	THR
1	A	528	THR
1	A	559	LEU
1	A	571	VAL
1	A	578	LEU
1	A	612	VAL
1	A	626	ILE
1	A	630	SER
1	A	634	TRP
1	A	645	GLU
1	A	659	LYS
1	A	662	MET
1	A	666	PHE
1	A	672	VAL
1	A	674	LEU
1	A	678	THR
1	A	695	LEU
1	A	713	LEU
1	A	716	VAL
1	A	721	LEU
1	A	748	THR
1	A	768	VAL
1	A	775	SER
1	A	804	PHE
1	A	806	SER
1	A	811	TYR
1	A	843	LEU
1	A	857	TYR
1	A	884	VAL
1	A	901	VAL
1	A	922	THR
1	A	931	LEU
1	A	951	ASP
1	A	958	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	961	ILE
1	A	964	THR
1	A	968	VAL
1	A	971	ARG
1	A	980	LEU
1	A	984	LEU
1	A	986	VAL
1	A	990	VAL
1	B	10	ILE
1	B	17	ILE
1	B	18	ILE
1	B	21	LEU
1	B	28	LEU
1	B	60	THR
1	B	88	VAL
1	B	96	SER
1	B	105	VAL
1	B	109	ASN
1	B	128	SER
1	B	146	ASP
1	B	185	ARG
1	B	205	THR
1	B	225	VAL
1	B	249	ILE
1	B	253	VAL
1	B	255	GLN
1	B	259	ARG
1	B	267	LYS
1	B	277	ILE
1	B	293	LEU
1	B	295	THR
1	B	310	LEU
1	B	321	LEU
1	B	329	THR
1	B	343	THR
1	B	352	PHE
1	B	355	MET
1	B	358	PHE
1	B	360	GLN
1	B	372	VAL
1	B	400	LEU
1	B	418	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	429	GLU
1	B	534	ILE
1	B	538	THR
1	B	561	SER
1	B	571	VAL
1	B	602	GLU
1	B	612	VAL
1	B	626	ILE
1	B	634	TRP
1	B	668	LEU
1	B	672	VAL
1	B	673	GLU
1	B	714	THR
1	B	721	LEU
1	B	743	ILE
1	B	768	VAL
1	B	775	SER
1	B	804	PHE
1	B	806	SER
1	B	811	TYR
1	B	835	LYS
1	B	843	LEU
1	B	901	VAL
1	B	931	LEU
1	B	958	LYS
1	B	968	VAL
1	B	980	LEU
1	B	984	LEU
1	B	986	VAL
1	B	1024	VAL
1	B	1035	ARG
1	B	1041	GLU
1	C	3	ASN
1	C	27	ILE
1	C	28	LEU
1	C	45	ILE
1	C	48	SER
1	C	59	ASP
1	C	60	THR
1	C	87	THR
1	C	88	VAL
1	C	102	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	104	GLN
1	C	137	LEU
1	C	166	ILE
1	C	177	LEU
1	C	182	TYR
1	C	185	ARG
1	C	203	VAL
1	C	225	VAL
1	C	243	THR
1	C	253	VAL
1	C	280	GLU
1	C	293	LEU
1	C	310	LEU
1	C	343	THR
1	C	415	ASN
1	C	429	GLU
1	C	439	GLN
1	C	462	SER
1	C	463	THR
1	C	472	ILE
1	C	482	VAL
1	C	524	THR
1	C	534	ILE
1	C	561	SER
1	C	564	LEU
1	C	571	VAL
1	C	578	LEU
1	C	602	GLU
1	C	623	ASN
1	C	626	ILE
1	C	634	TRP
1	C	659	LYS
1	C	668	LEU
1	C	673	GLU
1	C	694	LYS
1	C	695	LEU
1	C	708	LYS
1	C	713	LEU
1	C	716	VAL
1	C	721	LEU
1	C	746	ILE
1	C	768	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	775	SER
1	C	837	THR
1	C	843	LEU
1	C	847	LEU
1	C	865	GLN
1	C	876	LEU
1	C	897	ILE
1	C	938	SER
1	C	947	GLU
1	C	958	LYS
1	C	961	ILE
1	C	971	ARG
1	C	977	MET
1	C	980	LEU
1	C	984	LEU
1	C	986	VAL
1	C	991	ILE
1	C	993	THR
1	C	1035	ARG
1	C	1037	ASN
1	C	1040	ILE
1	C	1045	THR
1	D	10	ILE
1	D	18	ILE
1	D	28	LEU
1	D	45	ILE
1	D	137	LEU
1	D	146	ASP
1	D	151	GLN
1	D	152	GLU
1	D	166	ILE
1	D	185	ARG
1	D	205	THR
1	D	222	THR
1	D	225	VAL
1	D	243	THR
1	D	245	GLU
1	D	310	LEU
1	D	324	VAL
1	D	343	THR
1	D	355	MET
1	D	360	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	362	PHE
1	D	369	THR
1	D	400	LEU
1	D	428	LYS
1	D	472	ILE
1	D	502	LYS
1	D	524	THR
1	D	534	ILE
1	D	561	SER
1	D	564	LEU
1	D	571	VAL
1	D	578	LEU
1	D	601	LYS
1	D	602	GLU
1	D	626	ILE
1	D	630	SER
1	D	634	TRP
1	D	659	LYS
1	D	666	PHE
1	D	668	LEU
1	D	671	ILE
1	D	672	VAL
1	D	674	LEU
1	D	680	PHE
1	D	713	LEU
1	D	716	VAL
1	D	721	LEU
1	D	743	ILE
1	D	768	VAL
1	D	773	VAL
1	D	775	SER
1	D	806	SER
1	D	815	ARG
1	D	843	LEU
1	D	857	TYR
1	D	901	VAL
1	D	914	LEU
1	D	931	LEU
1	D	943	ILE
1	D	945	ILE
1	D	961	ILE
1	D	968	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	971	ARG
1	D	980	LEU
1	D	984	LEU
1	D	986	VAL
1	D	990	VAL
1	D	1036	LYS
1	E	10	ILE
1	E	25	LEU
1	E	28	LEU
1	E	45	ILE
1	E	60	THR
1	E	88	VAL
1	E	96	SER
1	E	109	ASN
1	E	131	LYS
1	E	137	LEU
1	E	151	GLN
1	E	177	LEU
1	E	185	ARG
1	E	225	VAL
1	E	243	THR
1	E	249	ILE
1	E	253	VAL
1	E	255	GLN
1	E	259	ARG
1	E	267	LYS
1	E	277	ILE
1	E	293	LEU
1	E	295	THR
1	E	310	LEU
1	E	321	LEU
1	E	323	ILE
1	E	329	THR
1	E	343	THR
1	E	358	PHE
1	E	360	GLN
1	E	369	THR
1	E	372	VAL
1	E	400	LEU
1	E	472	ILE
1	E	536	ARG
1	E	538	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	561	SER
1	E	563	PHE
1	E	569	GLN
1	E	571	VAL
1	E	626	ILE
1	E	634	TRP
1	E	652	THR
1	E	659	LYS
1	E	666	PHE
1	E	667	ASN
1	E	668	LEU
1	E	672	VAL
1	E	673	GLU
1	E	678	THR
1	E	680	PHE
1	E	694	LYS
1	E	714	THR
1	E	721	LEU
1	E	768	VAL
1	E	775	SER
1	E	804	PHE
1	E	811	TYR
1	E	843	LEU
1	E	880	SER
1	E	901	VAL
1	E	931	LEU
1	E	958	LYS
1	E	961	ILE
1	E	968	VAL
1	E	971	ARG
1	E	980	LEU
1	E	984	LEU
1	E	986	VAL
1	E	1036	LYS
1	E	1040	ILE
1	E	1043	SER
1	F	3	ASN
1	F	28	LEU
1	F	45	ILE
1	F	48	SER
1	F	59	ASP
1	F	60	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	87	THR
1	F	88	VAL
1	F	104	GLN
1	F	112	GLN
1	F	129	VAL
1	F	137	LEU
1	F	166	ILE
1	F	177	LEU
1	F	203	VAL
1	F	225	VAL
1	F	253	VAL
1	F	293	LEU
1	F	307	ARG
1	F	310	LEU
1	F	343	THR
1	F	362	PHE
1	F	369	THR
1	F	400	LEU
1	F	447	MET
1	F	448	VAL
1	F	462	SER
1	F	472	ILE
1	F	482	VAL
1	F	524	THR
1	F	564	LEU
1	F	571	VAL
1	F	578	LEU
1	F	596	HIS
1	F	602	GLU
1	F	626	ILE
1	F	668	LEU
1	F	672	VAL
1	F	673	GLU
1	F	674	LEU
1	F	695	LEU
1	F	708	LYS
1	F	713	LEU
1	F	721	LEU
1	F	734	GLU
1	F	743	ILE
1	F	746	ILE
1	F	760	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	768	VAL
1	F	775	SER
1	F	806	SER
1	F	811	TYR
1	F	843	LEU
1	F	876	LEU
1	F	884	VAL
1	F	938	SER
1	F	947	GLU
1	F	958	LYS
1	F	961	ILE
1	F	971	ARG
1	F	977	MET
1	F	980	LEU
1	F	984	LEU
1	F	986	VAL
1	F	991	ILE
1	F	1011	MET
1	F	1035	ARG
1	F	1044	HIS
1	F	1047	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	70	ASN
1	A	81	ASN
1	A	151	GLN
1	A	298	ASN
1	A	439	GLN
1	A	588	GLN
1	A	592	ASN
1	A	667	ASN
1	B	284	GLN
1	B	415	ASN
1	B	525	HIS
1	B	526	HIS
1	B	737	GLN
1	B	760	ASN
1	B	865	GLN
1	B	1042	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	161	ASN
1	C	181	GLN
1	C	194	ASN
1	C	231	ASN
1	C	274	ASN
1	C	657	GLN
1	C	846	GLN
1	C	928	GLN
1	D	74	ASN
1	D	123	GLN
1	D	360	GLN
1	D	469	GLN
1	E	81	ASN
1	E	104	GLN
1	E	125	GLN
1	E	213	GLN
1	E	517	ASN
1	E	569	GLN
1	E	604	ASN
1	E	613	ASN
1	E	744	ASN
1	F	151	GLN
1	F	197	GLN
1	F	228	GLN
1	F	525	HIS
1	F	588	GLN
1	F	592	ASN
1	F	709	HIS
1	F	726	GLN
1	F	760	ASN
1	F	846	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

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$
3	LMT	F	1101	-	36,36,36	1.82	9 (25%)	47,47,47	1.37	8 (17%)
3	LMT	C	1101	-	36,36,36	1.77	10 (27%)	47,47,47	1.52	8 (17%)
2	ERY	D	1101	-	53,53,53	1.41	6 (11%)	82,82,82	2.05	23 (28%)
2	ERY	A	1101	-	53,53,53	1.30	4 (7%)	82,82,82	2.07	25 (30%)
3	LMT	D	1102	-	36,36,36	1.85	11 (30%)	47,47,47	1.01	2 (4%)
3	LMT	E	1101	-	36,36,36	1.85	9 (25%)	47,47,47	1.32	6 (12%)
3	LMT	A	1102	-	36,36,36	1.79	9 (25%)	47,47,47	1.16	5 (10%)
3	LMT	D	1103	-	36,36,36	1.77	9 (25%)	47,47,47	1.56	9 (19%)
3	LMT	A	1103	-	36,36,36	1.90	9 (25%)	47,47,47	1.47	9 (19%)
3	LMT	B	1101	-	36,36,36	1.87	9 (25%)	47,47,47	1.89	11 (23%)

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
3	LMT	F	1101	-	-	9/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	10/21/61/61	0/2/2/2
2	ERY	D	1101	-	-	12/72/107/107	0/3/3/3
2	ERY	A	1101	-	-	38/72/107/107	0/3/3/3
3	LMT	D	1102	-	-	15/21/61/61	0/2/2/2
3	LMT	E	1101	-	-	10/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	1102	-	-	8/21/61/61	0/2/2/2
3	LMT	D	1103	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	13/21/61/61	0/2/2/2
3	LMT	B	1101	-	1/1/10/10	11/21/61/61	0/2/2/2

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	ERY	O2-C1	5.49	1.46	1.34
2	D	1101	ERY	O2-C1	5.37	1.46	1.34
3	A	1103	LMT	O5'-C5'	5.07	1.56	1.44
3	B	1101	LMT	O1'-C1'	4.35	1.47	1.40
3	E	1101	LMT	O1'-C1'	4.34	1.47	1.40
3	D	1102	LMT	O1'-C1'	4.30	1.47	1.40
3	D	1103	LMT	O5B-C1B	4.21	1.52	1.41
3	A	1102	LMT	O5'-C5'	4.12	1.54	1.44
3	F	1101	LMT	O1'-C1'	4.04	1.46	1.40
3	F	1101	LMT	O5'-C5'	3.97	1.54	1.44
3	C	1101	LMT	O1'-C1'	3.89	1.46	1.40
3	E	1101	LMT	O5'-C5'	3.83	1.53	1.44
3	D	1103	LMT	O5'-C5'	3.82	1.53	1.44
3	C	1101	LMT	O5'-C5'	3.82	1.53	1.44
3	A	1103	LMT	O5B-C1B	3.81	1.51	1.41
3	B	1101	LMT	O5'-C5'	3.70	1.53	1.44
3	D	1103	LMT	O1'-C1'	3.69	1.46	1.40
3	D	1102	LMT	O5B-C1B	3.63	1.51	1.41
3	A	1103	LMT	O5'-C1'	3.62	1.51	1.41
3	B	1101	LMT	O5B-C1B	3.61	1.51	1.41
3	F	1101	LMT	O5'-C1'	3.61	1.51	1.41
3	A	1103	LMT	O1'-C1'	3.56	1.46	1.40
3	A	1102	LMT	O5B-C1B	3.54	1.51	1.41
3	B	1101	LMT	O5'-C1'	3.46	1.50	1.41
3	A	1102	LMT	O1'-C1'	3.45	1.45	1.40
3	A	1103	LMT	O3B-C3B	3.38	1.51	1.43
3	D	1102	LMT	C6'-C5'	-3.38	1.40	1.51
3	E	1101	LMT	O5'-C1'	3.36	1.50	1.41
3	C	1101	LMT	O5'-C1'	3.34	1.50	1.41
3	C	1101	LMT	O5B-C1B	3.32	1.50	1.41
3	D	1102	LMT	O5'-C5'	3.29	1.52	1.44
3	F	1101	LMT	C6'-C5'	-3.25	1.40	1.51
3	D	1102	LMT	O5'-C1'	3.22	1.50	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1101	LMT	O5B-C1B	3.20	1.50	1.41
3	B	1101	LMT	O3B-C3B	3.19	1.50	1.43
3	D	1102	LMT	O3B-C3B	3.18	1.50	1.43
3	D	1103	LMT	C6'-C5'	-3.17	1.41	1.51
3	D	1103	LMT	O5'-C1'	3.15	1.49	1.41
3	E	1101	LMT	C3'-C2'	-3.14	1.44	1.52
3	A	1103	LMT	C6'-C5'	-3.08	1.41	1.51
3	C	1101	LMT	C6'-C5'	-3.02	1.41	1.51
3	A	1102	LMT	C6'-C5'	-2.97	1.41	1.51
3	F	1101	LMT	O5B-C1B	2.94	1.49	1.41
3	A	1102	LMT	O3B-C3B	2.93	1.50	1.43
3	A	1102	LMT	O5'-C1'	2.91	1.49	1.41
3	E	1101	LMT	C6'-C5'	-2.85	1.42	1.51
3	E	1101	LMT	O3B-C3B	2.83	1.50	1.43
3	B	1101	LMT	C6'-C5'	-2.83	1.42	1.51
3	D	1103	LMT	O3B-C3B	2.82	1.49	1.43
3	F	1101	LMT	O3B-C3B	2.65	1.49	1.43
3	B	1101	LMT	O3'-C3'	2.52	1.49	1.43
3	B	1101	LMT	C5-C4	2.51	1.64	1.51
2	D	1101	ERY	O11-C9	2.48	1.25	1.21
2	D	1101	ERY	C25-C26	2.48	1.56	1.52
3	E	1101	LMT	C5-C4	2.46	1.64	1.51
3	C	1101	LMT	C3B-C2B	-2.45	1.46	1.52
3	C	1101	LMT	O2'-C2'	2.42	1.48	1.43
3	F	1101	LMT	C3'-C2'	-2.42	1.46	1.52
3	D	1102	LMT	O2'-C2'	2.40	1.48	1.43
2	A	1101	ERY	C25-C26	2.37	1.56	1.52
3	E	1101	LMT	C3B-C2B	-2.36	1.46	1.52
3	B	1101	LMT	O2'-C2'	2.35	1.48	1.43
3	A	1103	LMT	O3'-C3'	2.32	1.48	1.43
3	D	1102	LMT	C3B-C2B	-2.30	1.46	1.52
3	A	1103	LMT	O2'-C2'	2.29	1.48	1.43
3	A	1102	LMT	C5-C4	2.29	1.63	1.51
3	A	1102	LMT	O2'-C2'	2.28	1.48	1.43
3	D	1103	LMT	O3'-C3'	2.28	1.48	1.43
3	D	1103	LMT	O2'-C2'	2.27	1.48	1.43
3	D	1102	LMT	O3'-C3'	2.24	1.48	1.43
3	F	1101	LMT	O2'-C2'	2.22	1.48	1.43
3	D	1102	LMT	C5-C4	2.22	1.62	1.51
2	A	1101	ERY	O11-C9	2.22	1.25	1.21
3	C	1101	LMT	C3'-C2'	-2.18	1.46	1.52
3	C	1101	LMT	O3'-C3'	2.17	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1101	LMT	C5-C4	2.16	1.62	1.51
2	A	1101	ERY	O6-C17	2.15	1.47	1.42
3	A	1102	LMT	C3'-C2'	-2.15	1.46	1.52
3	D	1102	LMT	C3'-C2'	-2.14	1.46	1.52
3	F	1101	LMT	C5-C4	2.09	1.62	1.51
2	D	1101	ERY	O9-C22	2.09	1.47	1.41
3	D	1103	LMT	C5-C4	2.06	1.62	1.51
3	A	1103	LMT	C5-C4	2.06	1.62	1.51
2	D	1101	ERY	O6-C17	2.03	1.46	1.42
2	D	1101	ERY	C22-C23	2.01	1.58	1.52

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	ERY	O7-C5-C6	6.13	113.71	106.40
2	D	1101	ERY	C20-O5-C16	5.59	128.89	117.51
2	D	1101	ERY	O12-C11-C10	5.53	118.61	110.77
2	A	1101	ERY	C20-O5-C16	5.45	128.60	117.51
3	B	1101	LMT	O5'-C5'-C6'	5.43	119.89	106.44
2	A	1101	ERY	O2-C1-O1	-5.06	114.81	123.95
2	A	1101	ERY	O7-C5-C6	4.83	112.16	106.40
2	A	1101	ERY	O12-C11-C10	4.71	117.46	110.77
3	B	1101	LMT	O1'-C1'-C2'	4.71	115.43	108.27
2	D	1101	ERY	C15-C16-C17	4.61	115.53	107.64
3	D	1103	LMT	C1'-O5'-C5'	-4.33	105.26	113.72
2	D	1101	ERY	C29-N1-C24	4.26	125.41	113.15
3	B	1101	LMT	O5'-C5'-C4'	-4.25	100.94	109.72
2	A	1101	ERY	C15-C16-C17	4.19	114.81	107.64
2	A	1101	ERY	C29-N1-C24	4.18	125.18	113.15
2	A	1101	ERY	C13-O2-C1	-3.99	111.23	118.20
3	A	1103	LMT	C1B-O1B-C4'	-3.92	108.69	117.98
3	C	1101	LMT	C3B-C4B-C5B	3.84	117.20	110.23
3	B	1101	LMT	C4B-C3B-C2B	3.81	117.53	110.83
2	A	1101	ERY	O2-C1-C2	3.79	119.63	111.53
2	D	1101	ERY	C25-C24-N1	-3.78	104.97	115.59
3	A	1103	LMT	C3B-C4B-C5B	3.77	117.07	110.23
3	B	1101	LMT	C1B-O1B-C4'	-3.75	109.08	117.98
2	A	1101	ERY	O3-C3-C4	3.61	112.48	108.23
3	E	1101	LMT	O5'-C5'-C6'	3.56	115.26	106.44
2	A	1101	ERY	O2-C13-C36	3.54	113.95	107.36
3	B	1101	LMT	C1'-O5'-C5'	-3.53	106.83	113.72
2	A	1101	ERY	C19-C16-C15	-3.48	104.57	110.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	ERY	O9-C26-C25	3.46	114.29	109.34
3	F	1101	LMT	C1B-C2B-C3B	3.35	117.06	110.01
3	A	1103	LMT	O5B-C5B-C4B	3.33	115.70	109.70
2	A	1101	ERY	O7-C5-C4	-3.30	106.81	111.58
3	C	1101	LMT	O1'-C1'-C2'	3.26	113.23	108.27
2	A	1101	ERY	O7-C22-C23	3.22	116.02	108.09
3	D	1103	LMT	O5'-C5'-C4'	-3.22	103.07	109.72
3	D	1103	LMT	C1'-C2'-C3'	3.19	116.72	110.01
3	C	1101	LMT	O5B-C5B-C4B	3.18	115.43	109.70
3	E	1101	LMT	O5B-C5B-C4B	3.16	115.39	109.70
3	A	1102	LMT	C1B-C2B-C3B	3.12	116.57	110.01
3	E	1101	LMT	C3B-C4B-C5B	3.08	115.82	110.23
3	C	1101	LMT	O2B-C2B-C1B	-3.02	102.88	110.08
3	D	1103	LMT	C3'-C4'-C5'	-3.01	104.27	110.93
3	F	1101	LMT	C4B-C3B-C2B	2.97	116.05	110.83
2	D	1101	ERY	O13-C12-C11	2.94	114.58	108.88
2	A	1101	ERY	C33-C8-C7	-2.91	104.47	109.88
3	F	1101	LMT	O5B-C5B-C4B	2.88	114.89	109.70
3	B	1101	LMT	O5B-C5B-C4B	2.88	114.89	109.70
3	D	1102	LMT	O1'-C1'-C2'	2.88	112.64	108.27
3	C	1101	LMT	C1B-O5B-C5B	2.87	119.33	113.72
2	D	1101	ERY	C19-C16-C15	-2.86	105.64	110.64
2	D	1101	ERY	C22-O9-C26	2.81	117.24	112.91
3	D	1103	LMT	O1'-C1'-C2'	2.77	112.47	108.27
2	D	1101	ERY	O4-C18-C21	2.76	112.86	106.74
3	E	1101	LMT	C1B-O1B-C4'	-2.74	111.48	117.98
3	A	1102	LMT	C1B-O1B-C4'	-2.72	111.53	117.98
3	C	1101	LMT	O1B-C4'-C3'	2.72	114.15	107.23
3	E	1101	LMT	O1'-C1'-C2'	2.72	112.40	108.27
3	A	1103	LMT	C1'-O5'-C5'	2.71	119.02	113.72
3	D	1103	LMT	O5B-C5B-C4B	2.70	114.57	109.70
2	A	1101	ERY	O10-C6-C32	-2.67	102.30	108.48
3	C	1101	LMT	C1B-O1B-C4'	-2.67	111.66	117.98
3	F	1101	LMT	O4'-C4B-C3B	-2.66	104.10	110.38
3	F	1101	LMT	O4'-C4B-C5B	2.65	115.84	109.32
3	F	1101	LMT	O2B-C2B-C1B	-2.64	103.79	110.08
2	D	1101	ERY	C31-C4-C3	-2.63	106.76	111.40
3	B	1101	LMT	O5B-C1B-C2B	2.62	115.76	110.37
3	A	1102	LMT	O1B-C1B-C2B	2.58	114.44	108.09
2	D	1101	ERY	O3-C3-C4	-2.57	105.21	108.23
2	D	1101	ERY	C26-C25-C24	2.56	114.83	110.46
3	F	1101	LMT	C1-O1'-C1'	2.54	118.03	113.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1101	LMT	O5'-C5'-C6'	2.53	112.70	106.44
3	A	1103	LMT	O5'-C5'-C4'	2.50	114.90	109.72
3	D	1103	LMT	O5B-C5B-C6B	2.46	112.55	106.44
3	A	1103	LMT	C4B-C3B-C2B	2.44	115.11	110.83
2	A	1101	ERY	C33-C8-C9	2.42	115.28	109.43
2	D	1101	ERY	C7-C6-C5	2.42	114.97	110.38
2	D	1101	ERY	C33-C8-C7	-2.40	105.42	109.88
3	A	1102	LMT	C2'-C3'-C4'	2.39	115.11	109.68
3	E	1101	LMT	C1-O1'-C1'	2.38	117.74	113.68
2	D	1101	ERY	O13-C12-C13	-2.38	103.61	107.24
3	D	1103	LMT	O5'-C5'-C6'	2.36	112.30	106.44
2	D	1101	ERY	O10-C6-C5	-2.34	103.28	107.60
3	B	1101	LMT	O2B-C2B-C3B	2.31	115.82	110.38
2	A	1101	ERY	O4-C18-C21	2.28	111.80	106.74
3	B	1101	LMT	O1'-C1-C2	2.28	117.09	109.37
2	A	1101	ERY	C22-O7-C5	2.27	120.13	116.26
2	A	1101	ERY	C35-C12-C13	2.26	114.32	111.26
3	D	1103	LMT	O1B-C4'-C3'	2.25	112.95	107.23
2	D	1101	ERY	C3-C4-C5	-2.24	106.52	111.17
2	D	1101	ERY	C36-C13-C12	-2.23	111.12	115.20
2	D	1101	ERY	C33-C8-C9	2.20	114.73	109.43
2	D	1101	ERY	O7-C22-C23	2.19	113.47	108.09
2	A	1101	ERY	O1-C1-C2	-2.18	118.45	124.11
3	A	1102	LMT	C1'-C2'-C3'	2.17	114.58	110.01
3	A	1103	LMT	C2'-C3'-C4'	-2.17	104.75	109.68
3	F	1101	LMT	O5'-C5'-C6'	2.16	111.78	106.44
2	A	1101	ERY	C7-C6-C5	2.16	114.47	110.38
3	D	1102	LMT	O5B-C1B-C2B	2.15	114.80	110.37
2	A	1101	ERY	O2-C13-C12	2.15	110.66	107.28
2	A	1101	ERY	C30-C2-C3	2.14	117.78	113.00
3	B	1101	LMT	C3B-C4B-C5B	2.13	114.10	110.23
3	A	1103	LMT	O3'-C3'-C2'	2.10	115.33	110.38
2	A	1101	ERY	C35-C12-C11	-2.10	109.51	113.14
3	A	1103	LMT	O1'-C1'-C2'	2.07	111.41	108.27
2	D	1101	ERY	O8-C23-C22	2.01	114.86	110.08
2	A	1101	ERY	C6-C7-C8	-2.00	111.61	115.61

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1101	LMT	C3B

All (137) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	ERY	C9-C10-C11-C12
2	A	1101	ERY	C9-C10-C11-O12
2	A	1101	ERY	C34-C10-C11-C12
2	A	1101	ERY	C34-C10-C11-O12
2	A	1101	ERY	C10-C11-C12-C13
2	A	1101	ERY	C10-C11-C12-C35
2	A	1101	ERY	C10-C11-C12-O13
2	A	1101	ERY	O12-C11-C12-C13
2	A	1101	ERY	O12-C11-C12-C35
2	A	1101	ERY	O12-C11-C12-O13
2	A	1101	ERY	C11-C12-C13-O2
2	A	1101	ERY	C35-C12-C13-C36
2	A	1101	ERY	O13-C12-C13-O2
2	A	1101	ERY	O2-C13-C36-C37
2	A	1101	ERY	C2-C1-O2-C13
2	A	1101	ERY	C32-C6-C7-C8
2	A	1101	ERY	C23-C24-N1-C29
2	A	1101	ERY	C25-C24-N1-C28
2	D	1101	ERY	C6-C7-C8-C33
2	D	1101	ERY	C23-C24-N1-C29
2	D	1101	ERY	C25-C24-N1-C29
3	A	1103	LMT	O5'-C1'-O1'-C1
3	C	1101	LMT	C2-C1-O1'-C1'
3	D	1102	LMT	C2-C1-O1'-C1'
3	D	1103	LMT	O5'-C1'-O1'-C1
3	E	1101	LMT	C2'-C1'-O1'-C1
3	A	1103	LMT	O5'-C5'-C6'-O6'
3	C	1101	LMT	O5B-C5B-C6B-O6B
3	D	1103	LMT	C4B-C5B-C6B-O6B
3	E	1101	LMT	O5'-C5'-C6'-O6'
3	F	1101	LMT	O5'-C5'-C6'-O6'
3	A	1103	LMT	C4'-C5'-C6'-O6'
3	B	1101	LMT	O5B-C5B-C6B-O6B
3	C	1101	LMT	C4B-C5B-C6B-O6B
3	E	1101	LMT	C4'-C5'-C6'-O6'
3	D	1102	LMT	O5B-C5B-C6B-O6B
3	F	1101	LMT	C4'-C5'-C6'-O6'
3	A	1103	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	O5'-C1'-O1'-C1
3	D	1103	LMT	O5B-C5B-C6B-O6B
2	A	1101	ERY	C2-C3-C4-C31
3	D	1102	LMT	C4'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1101	ERY	O4-C14-O3-C3
3	D	1103	LMT	C4-C5-C6-C7
3	B	1101	LMT	O5'-C5'-C6'-O6'
3	A	1103	LMT	C4B-C5B-C6B-O6B
3	B	1101	LMT	C2'-C1'-O1'-C1
3	D	1102	LMT	O5'-C5'-C6'-O6'
3	A	1102	LMT	C4'-C5'-C6'-O6'
3	B	1101	LMT	C4'-C5'-C6'-O6'
3	B	1101	LMT	C4B-C5B-C6B-O6B
3	D	1102	LMT	C4B-C5B-C6B-O6B
3	A	1102	LMT	O5'-C5'-C6'-O6'
2	A	1101	ERY	O2-C1-C2-C3
3	E	1101	LMT	O5'-C1'-O1'-C1
2	A	1101	ERY	C2-C3-C4-C5
2	A	1101	ERY	C25-C24-N1-C29
3	A	1102	LMT	C2'-C1'-O1'-C1
3	C	1101	LMT	C2'-C1'-O1'-C1
3	D	1102	LMT	C2'-C1'-O1'-C1
3	D	1103	LMT	C4'-C5'-C6'-O6'
3	A	1102	LMT	O5'-C1'-O1'-C1
3	C	1101	LMT	O5'-C1'-O1'-C1
2	D	1101	ERY	C2-C1-O2-C13
2	A	1101	ERY	C23-C24-N1-C28
3	D	1102	LMT	C3-C4-C5-C6
3	D	1102	LMT	C11-C10-C9-C8
2	A	1101	ERY	O3-C3-C4-C5
3	D	1103	LMT	C2-C1-O1'-C1'
3	E	1101	LMT	C2-C1-O1'-C1'
3	C	1101	LMT	C1-C2-C3-C4
3	D	1103	LMT	O5'-C5'-C6'-O6'
2	A	1101	ERY	C19-C16-O5-C20
3	D	1102	LMT	C1-C2-C3-C4
3	E	1101	LMT	C1-C2-C3-C4
3	F	1101	LMT	C1-C2-C3-C4
3	A	1103	LMT	C5-C6-C7-C8
3	C	1101	LMT	C3-C4-C5-C6
3	E	1101	LMT	C11-C10-C9-C8
3	B	1101	LMT	O1'-C1-C2-C3
3	D	1103	LMT	C1-C2-C3-C4
3	A	1103	LMT	C7-C8-C9-C10
3	C	1101	LMT	C6-C7-C8-C9
3	E	1101	LMT	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1103	LMT	O5B-C1B-O1B-C4'
3	B	1101	LMT	C2-C3-C4-C5
3	E	1101	LMT	O1'-C1-C2-C3
3	D	1102	LMT	O5'-C1'-O1'-C1
2	A	1101	ERY	O3-C3-C4-C31
3	A	1103	LMT	C9-C10-C11-C12
3	A	1102	LMT	C3-C4-C5-C6
3	D	1103	LMT	C7-C8-C9-C10
3	A	1102	LMT	C6-C7-C8-C9
2	A	1101	ERY	C11-C12-C13-C36
3	F	1101	LMT	C6-C7-C8-C9
3	D	1102	LMT	C4-C5-C6-C7
3	A	1103	LMT	C4-C5-C6-C7
2	A	1101	ERY	O10-C6-C7-C8
3	B	1101	LMT	C4-C5-C6-C7
2	D	1101	ERY	O7-C5-C6-C7
2	D	1101	ERY	C4-C5-C6-O10
2	A	1101	ERY	C4-C5-O7-C22
2	A	1101	ERY	C6-C5-O7-C22
2	A	1101	ERY	C15-C16-O5-C20
2	D	1101	ERY	C15-C16-O5-C20
2	D	1101	ERY	C19-C16-O5-C20
3	A	1103	LMT	C1-C2-C3-C4
3	D	1103	LMT	C11-C10-C9-C8
3	C	1101	LMT	C7-C8-C9-C10
3	D	1102	LMT	C6-C7-C8-C9
2	D	1101	ERY	O2-C13-C36-C37
2	D	1101	ERY	C17-C16-O5-C20
3	D	1102	LMT	O1'-C1-C2-C3
3	A	1102	LMT	C7-C8-C9-C10
2	A	1101	ERY	O1-C1-C2-C3
3	A	1103	LMT	C6-C7-C8-C9
3	C	1101	LMT	O1'-C1-C2-C3
3	F	1101	LMT	O5B-C5B-C6B-O6B
3	D	1102	LMT	C7-C8-C9-C10
2	A	1101	ERY	O1-C1-C2-C30
3	B	1101	LMT	C6-C7-C8-C9
2	A	1101	ERY	C6-C7-C8-C33
2	A	1101	ERY	C12-C13-C36-C37
2	D	1101	ERY	C12-C13-C36-C37
3	E	1101	LMT	C9-C10-C11-C12
3	F	1101	LMT	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

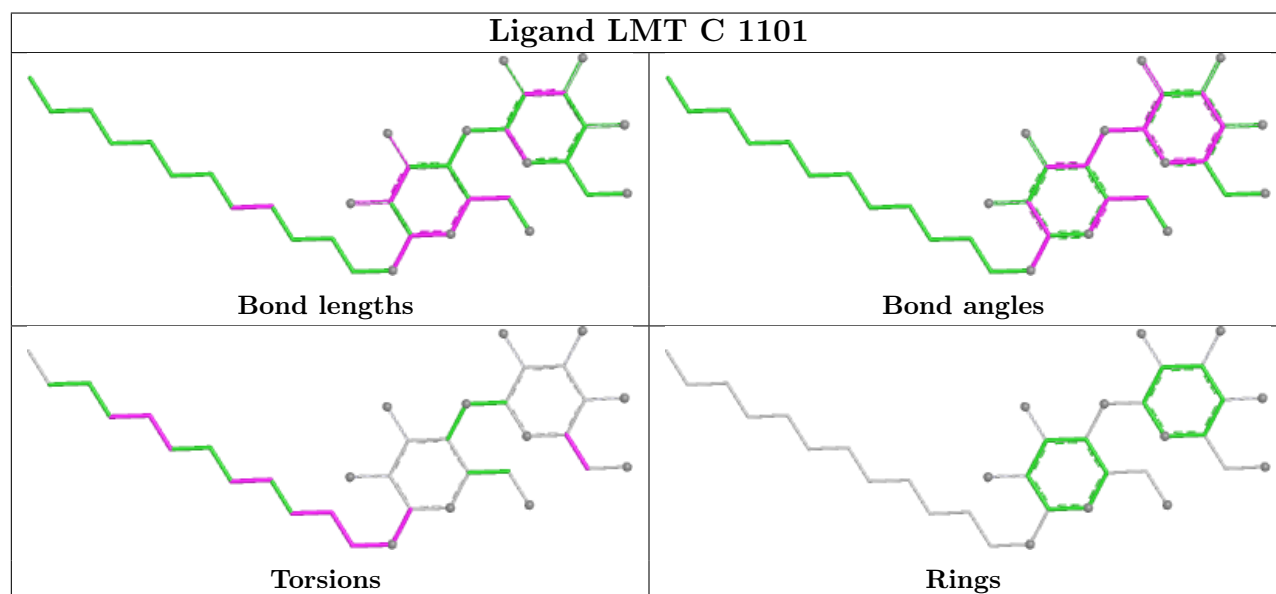
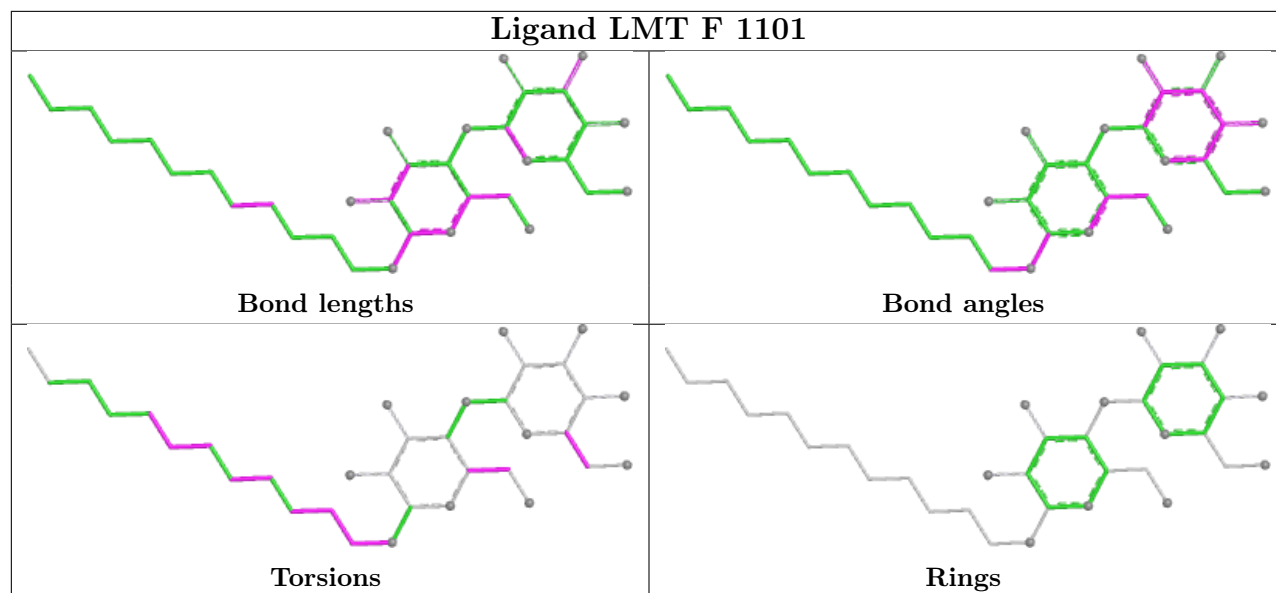
Mol	Chain	Res	Type	Atoms
3	A	1102	LMT	O1'-C1-C2-C3
3	A	1103	LMT	C2B-C1B-O1B-C4'
2	A	1101	ERY	O1-C1-O2-C13
2	A	1101	ERY	C17-C16-O5-C20
3	F	1101	LMT	O1'-C1-C2-C3
3	D	1102	LMT	C2-C3-C4-C5
3	F	1101	LMT	C3-C4-C5-C6
3	F	1101	LMT	C2-C1-O1'-C1'
2	D	1101	ERY	C6-C7-C8-C9
3	D	1103	LMT	C2-C3-C4-C5
3	B	1101	LMT	C9-C10-C11-C12

There are no ring outliers.

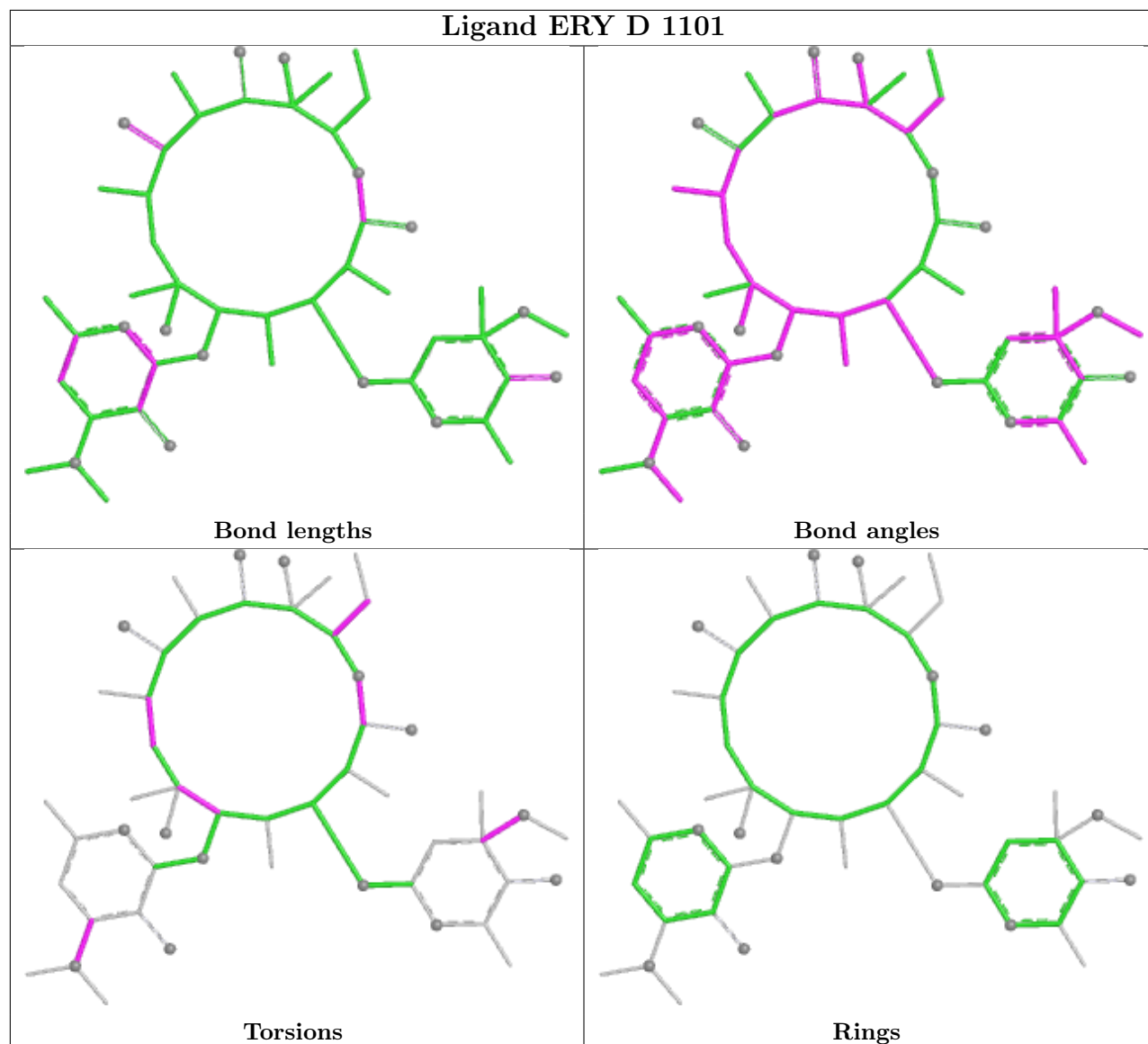
10 monomers are involved in 42 short contacts:

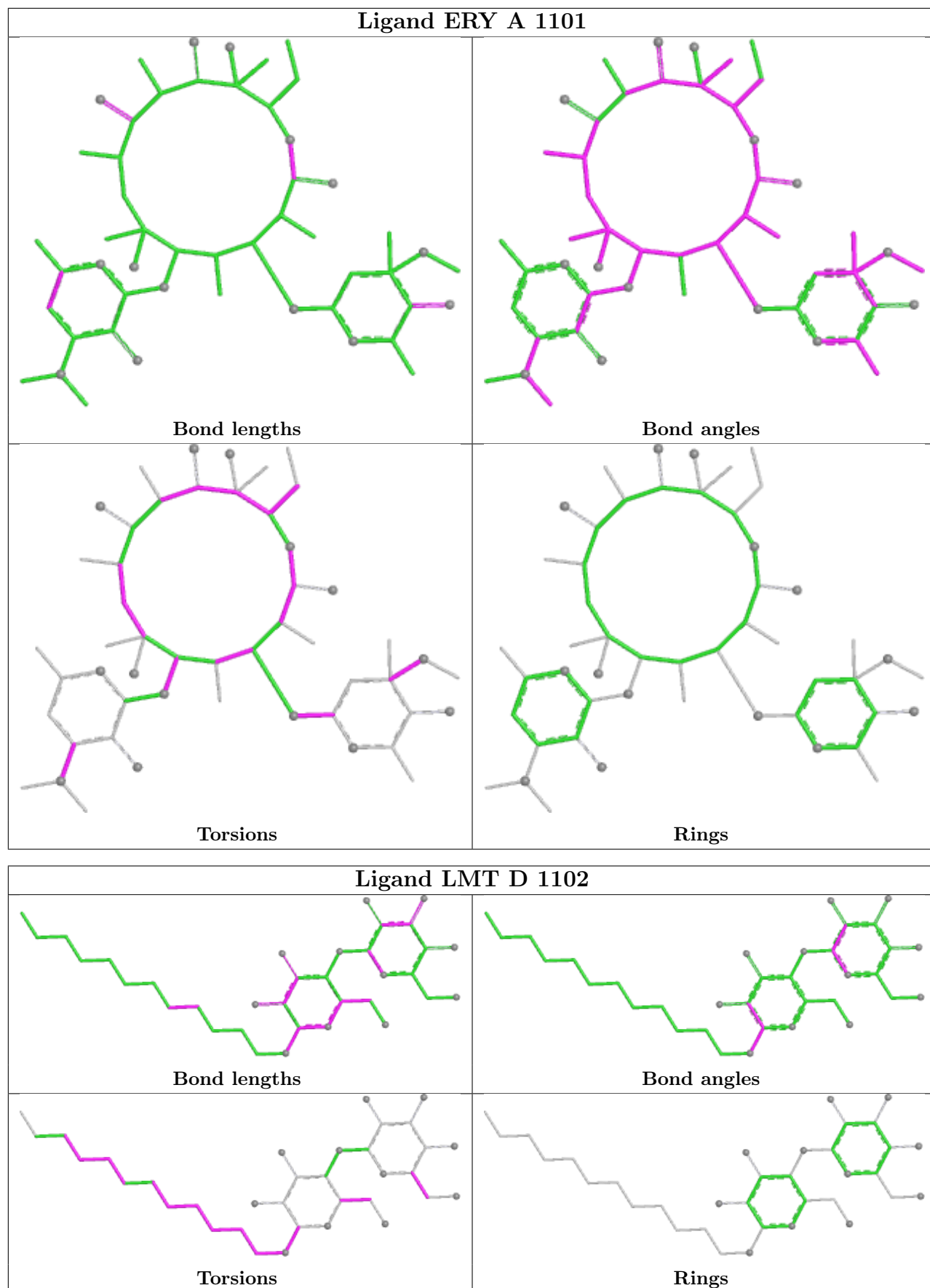
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1101	LMT	5	0
3	C	1101	LMT	1	0
2	D	1101	ERY	5	0
2	A	1101	ERY	9	0
3	D	1102	LMT	2	0
3	E	1101	LMT	3	0
3	A	1102	LMT	3	0
3	D	1103	LMT	7	0
3	A	1103	LMT	2	0
3	B	1101	LMT	5	0

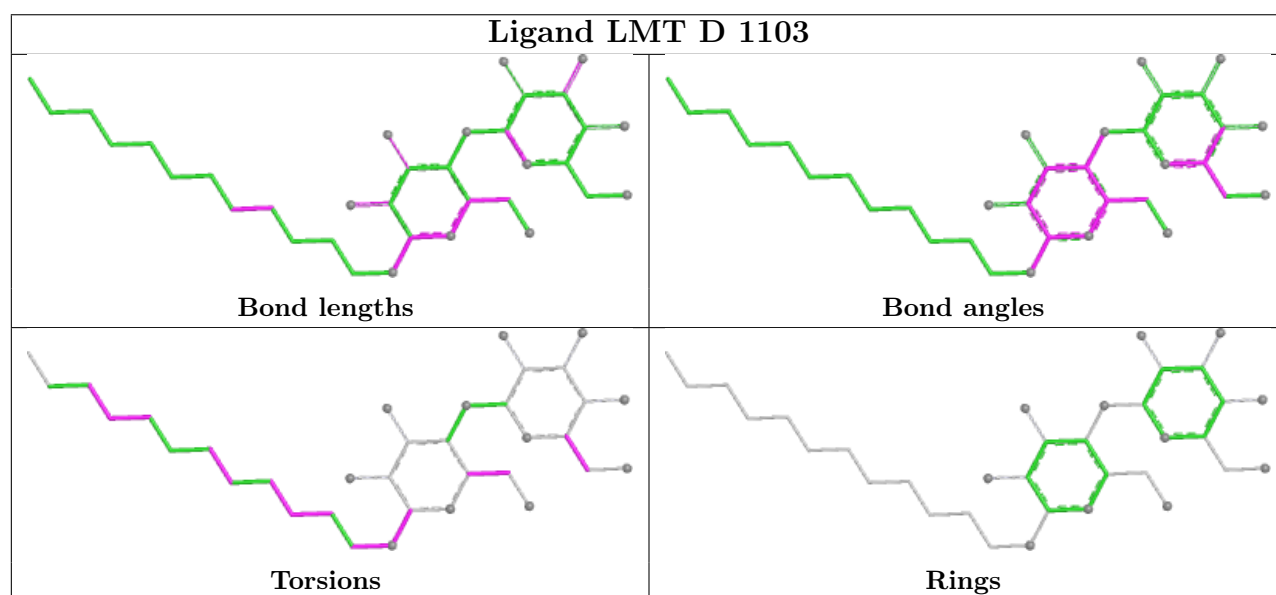
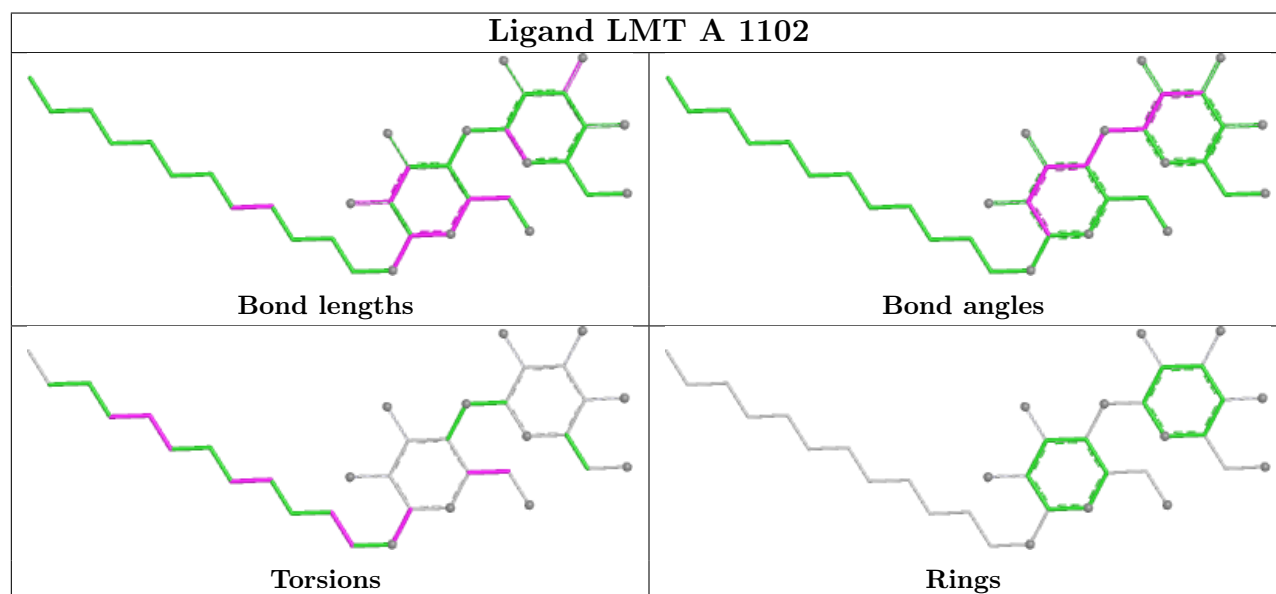
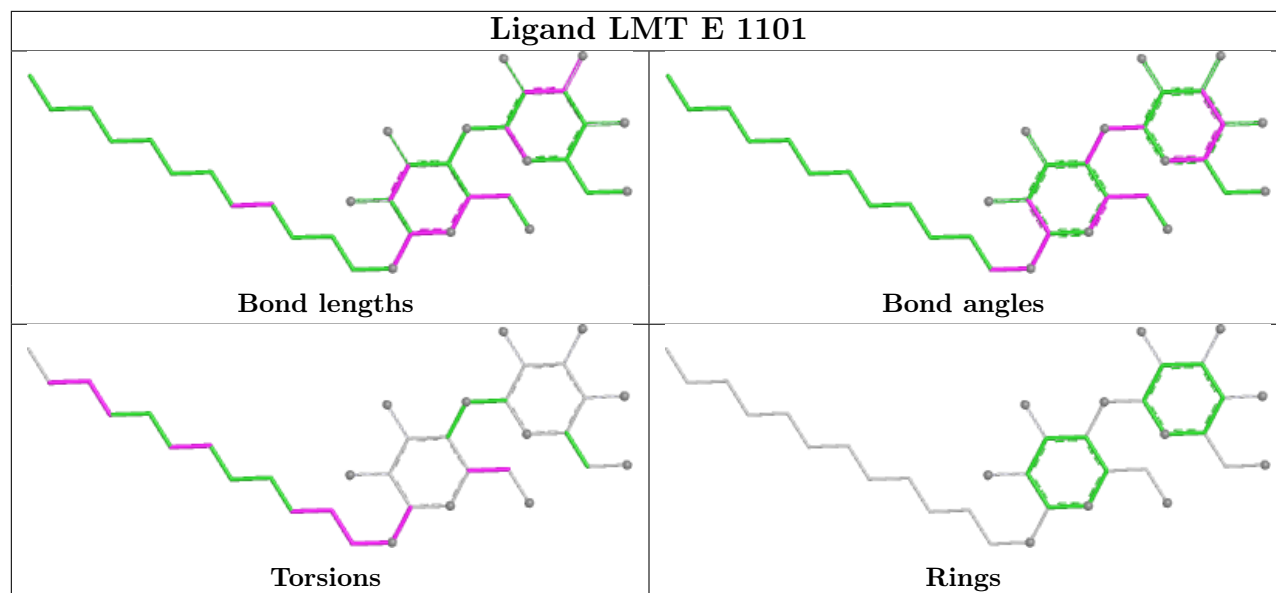
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

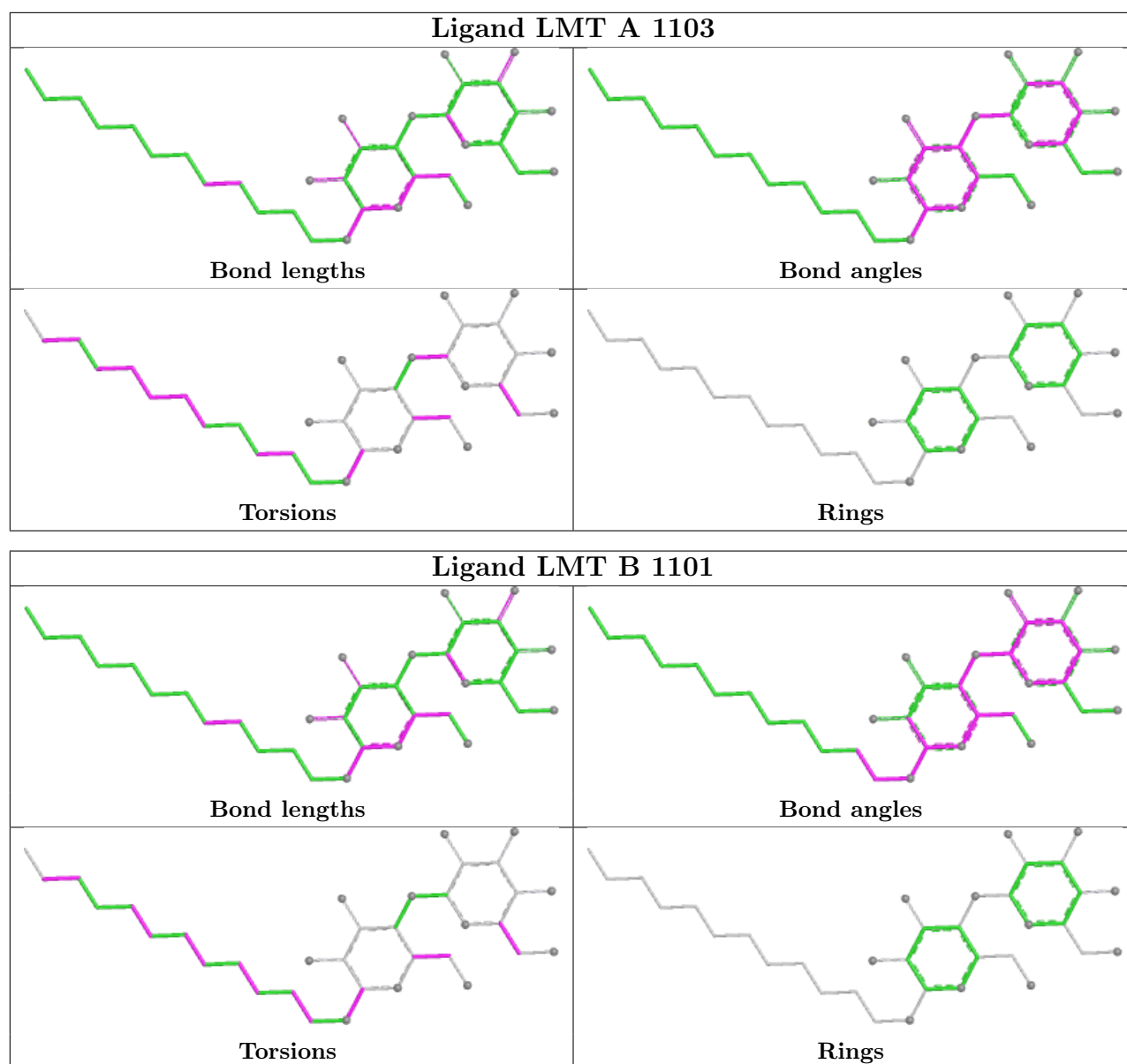


Ligand ERY D 1101









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	1042/1049 (99%)	-0.13	6 (0%)	85 64	49, 83, 120, 150	0
1	B	1042/1049 (99%)	-0.20	7 (0%)	84 61	45, 81, 117, 154	0
1	C	1044/1049 (99%)	-0.10	15 (1%)	73 46	40, 83, 120, 176	0
1	D	1042/1049 (99%)	-0.08	11 (1%)	78 52	43, 94, 130, 161	0
1	E	1042/1049 (99%)	-0.05	6 (0%)	85 64	57, 94, 125, 151	0
1	F	1046/1049 (99%)	-0.03	12 (1%)	78 52	44, 89, 124, 158	0
All	All	6258/6294 (99%)	-0.10	57 (0%)	81 56	40, 87, 124, 176	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	869	SER	5.1
1	E	869	SER	4.0
1	E	291	ILE	3.9
1	C	856	GLY	3.9
1	C	871	ASN	3.8
1	F	294	ALA	3.7
1	C	494	ALA	3.5
1	B	715	SER	3.5
1	A	59	ASP	3.4
1	F	59	ASP	3.3
1	C	127	VAL	3.2
1	D	59	ASP	3.2
1	D	401	ALA	3.0
1	C	97	GLY	2.9
1	F	97	GLY	2.8
1	C	421	ALA	2.8
1	C	822	LEU	2.7
1	B	681	ASP	2.6
1	F	49	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	869	SER	2.6
1	F	504	ASP	2.6
1	B	59	ASP	2.6
1	E	712	MET	2.6
1	B	515	TRP	2.5
1	C	122	VAL	2.5
1	D	681	ASP	2.5
1	A	486	LEU	2.5
1	D	870	GLY	2.5
1	F	835	LYS	2.4
1	D	504	ASP	2.4
1	E	59	ASP	2.4
1	A	310	LEU	2.4
1	A	494	ALA	2.3
1	D	460	GLY	2.3
1	F	117	LEU	2.3
1	C	59	ASP	2.3
1	F	503	GLY	2.3
1	A	92	LEU	2.2
1	C	838	GLY	2.2
1	C	501	ALA	2.2
1	D	459	PHE	2.2
1	C	49	TYR	2.2
1	A	508	GLY	2.2
1	B	714	THR	2.2
1	C	1040	ILE	2.2
1	C	855	VAL	2.1
1	E	640	GLU	2.1
1	F	60	THR	2.1
1	D	679	GLY	2.1
1	C	837	THR	2.1
1	D	713	LEU	2.1
1	F	57	VAL	2.1
1	F	837	THR	2.1
1	B	509	LYS	2.1
1	D	2	PRO	2.0
1	F	122	VAL	2.0
1	E	681	ASP	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

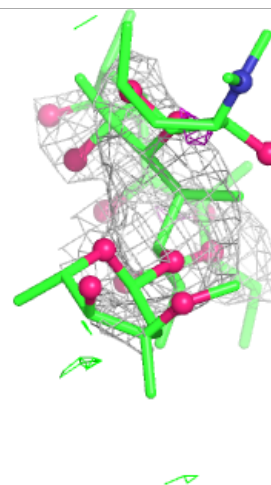
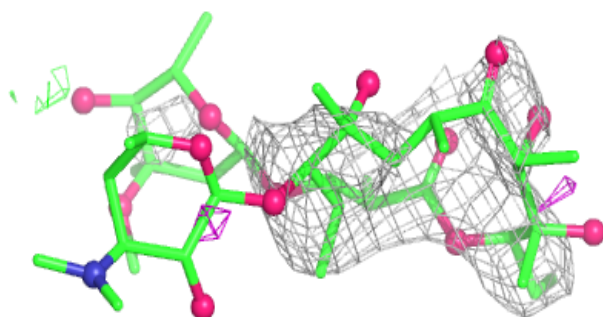
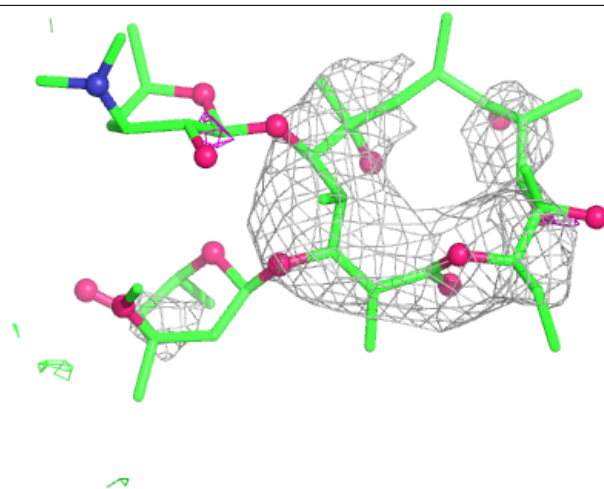
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ERY	D	1101	51/51	0.71	0.19	73,92,103,104	51
3	LMT	D	1103	35/35	0.76	0.14	79,94,108,110	0
2	ERY	A	1101	51/51	0.81	0.14	75,87,97,106	51
3	LMT	F	1101	35/35	0.83	0.10	49,77,91,99	0
3	LMT	B	1101	35/35	0.84	0.10	49,76,101,110	0
3	LMT	A	1103	35/35	0.86	0.11	58,93,104,107	0
3	LMT	D	1102	35/35	0.86	0.08	55,79,93,93	0
3	LMT	E	1101	35/35	0.87	0.11	57,76,88,116	0
3	LMT	C	1101	35/35	0.87	0.10	55,72,93,98	0
3	LMT	A	1102	35/35	0.89	0.08	26,76,84,88	0
4	NI	E	1102	1/1	0.99	0.03	94,94,94,94	0
4	NI	C	1102	1/1	1.00	0.03	62,62,62,62	0
4	NI	A	1104	1/1	1.00	0.03	54,54,54,54	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.

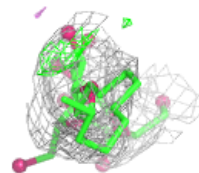
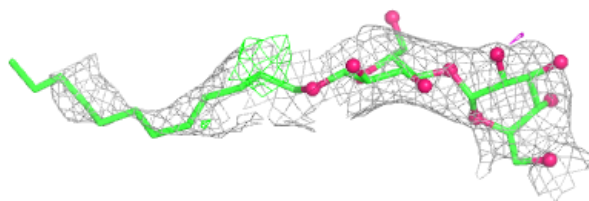
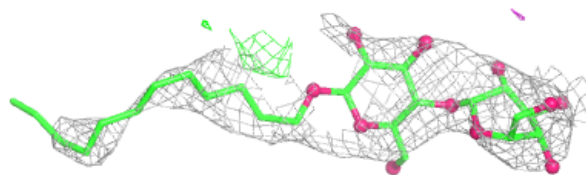
Electron density around ERY D 1101:

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



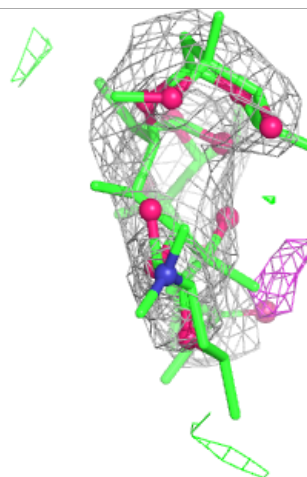
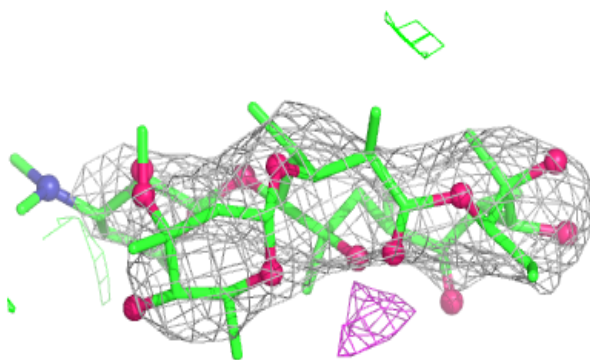
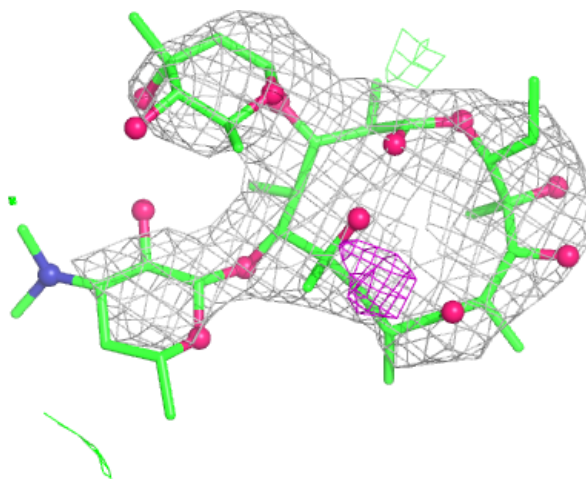
Electron density around LMT D 1103:

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



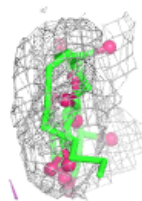
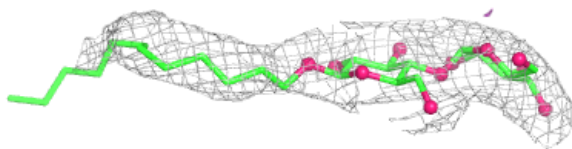
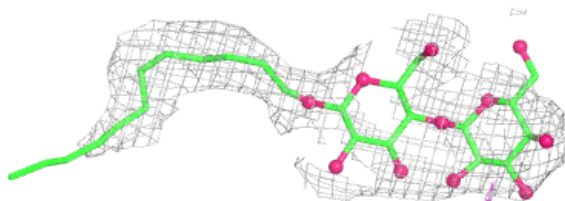
Electron density around ERY A 1101:

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

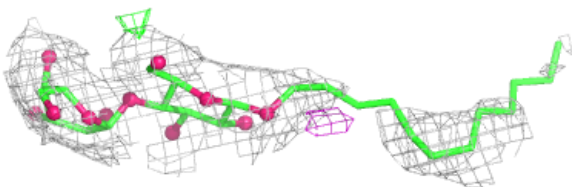
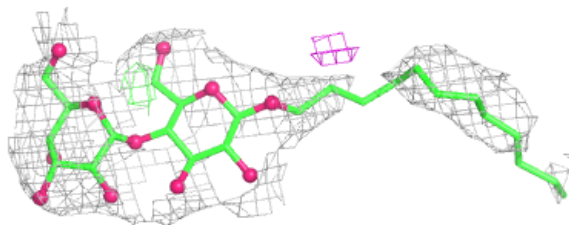


Electron density around LMT F 1101:

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

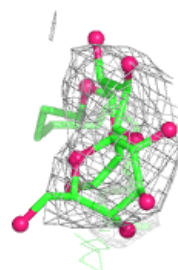
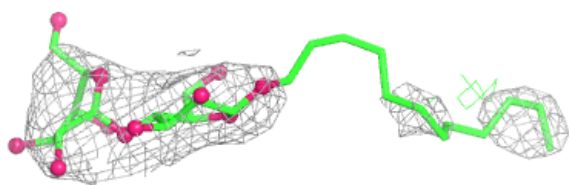
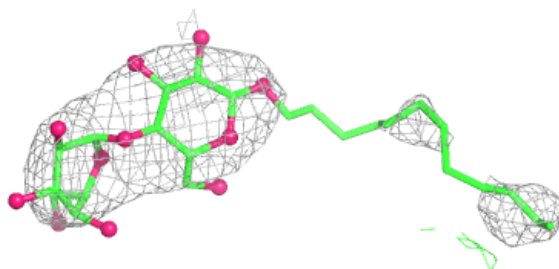
**Electron density around LMT B 1101:**

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

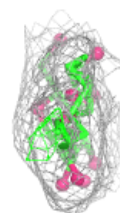
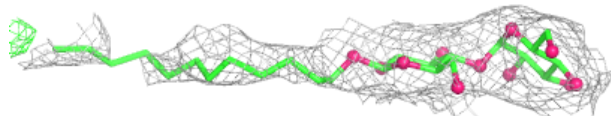
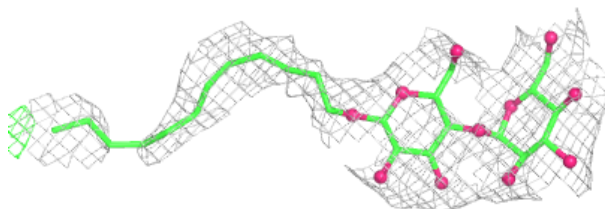


Electron density around LMT A 1103:

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

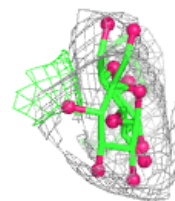
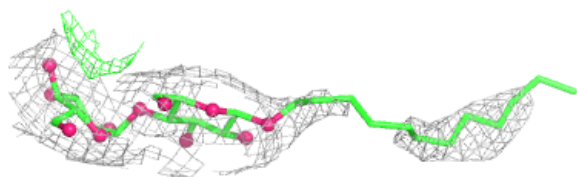
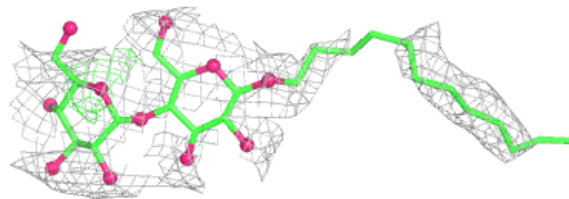
**Electron density around LMT D 1102:**

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

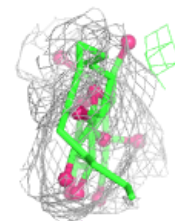
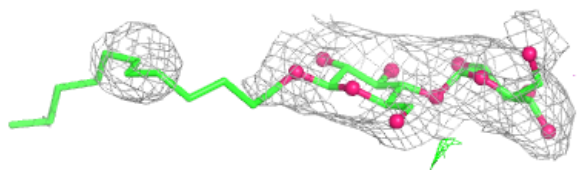
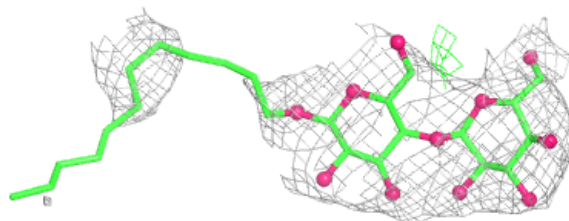


Electron density around LMT E 1101:

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

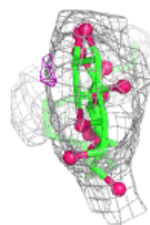
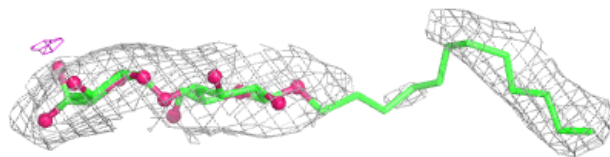
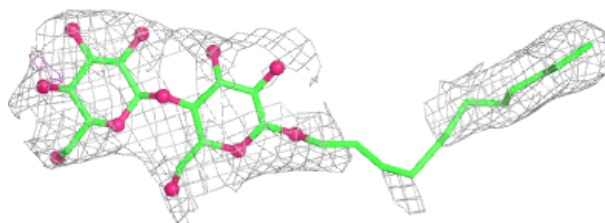
**Electron density around LMT C 1101:**

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



Electron density around LMT A 1102:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.