



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:46 AM UTC

PDB ID : 4I0U / pdb_00004i0u
Title : Improved structure of Thermotoga maritima CorA at 2.7 Å resolution
Authors : Nordin, N.; Guskov, A.; Phua, T.; Sahaf, N.; Xia, Y.; Lu, S.Y.; Eshaghi, H.;
Eshaghi, S.
Deposited on : 2012-11-19
Resolution : 2.70 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

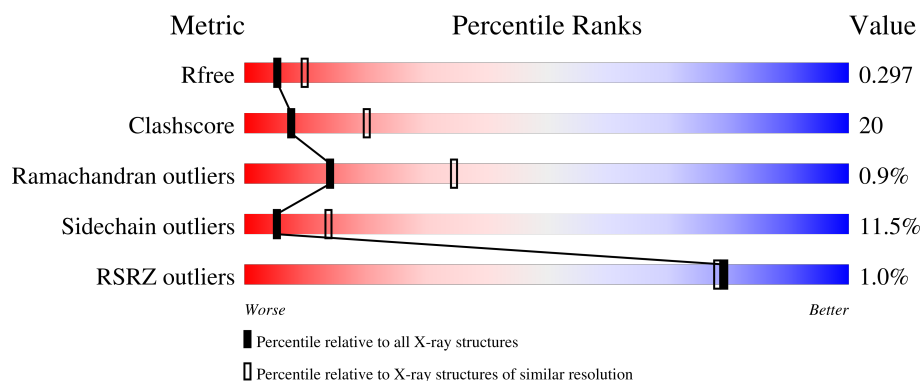
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	351	
1	B	351	
1	C	351	
1	D	351	
1	E	351	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	351	
1	G	351	
1	H	351	
1	I	351	
1	J	351	

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	CL	G	406	-	-	X	-
4	LMT	A	403	-	-	X	-
4	LMT	B	406	-	-	X	-
5	PEG	C	406	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29094 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 Magnesium transport protein CorA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2886	1880	471	525	10			
1	B	348	Total	C	N	O	S	0	0	0
			2895	1885	472	528	10			
1	C	347	Total	C	N	O	S	0	0	0
			2865	1862	469	525	9			
1	D	343	Total	C	N	O	S	0	0	0
			2849	1857	463	519	10			
1	E	345	Total	C	N	O	S	0	1	0
			2844	1850	465	519	10			
1	F	346	Total	C	N	O	S	0	0	0
			2856	1859	466	522	9			
1	G	346	Total	C	N	O	S	0	0	0
			2844	1850	465	519	10			
1	H	343	Total	C	N	O	S	0	0	0
			2826	1838	461	518	9			
1	I	345	Total	C	N	O	S	0	0	0
			2850	1857	462	521	10			
1	J	345	Total	C	N	O	S	0	0	0
			2844	1849	465	520	10			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	3	Total	Mg	0	0
			3	3		
2	C	2	Total	Mg	0	0
			2	2		
2	D	3	Total	Mg	0	0
			3	3		

Continued on next page...

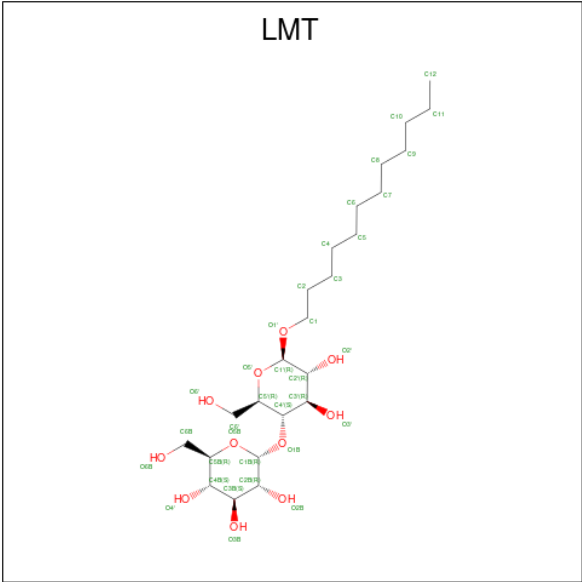
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total 2	Mg 2	0	0
2	F	2	Total 2	Mg 2	0	0
2	G	5	Total 5	Mg 5	0	0
2	I	3	Total 3	Mg 3	0	0
2	J	3	Total 3	Mg 3	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

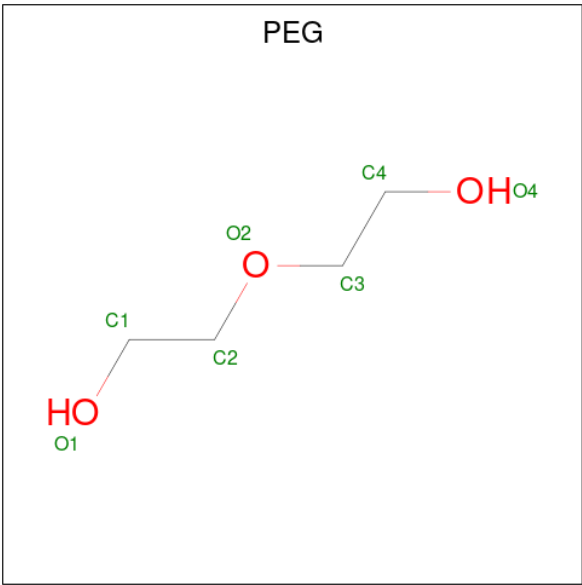
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0
3	B	2	Total 2	Cl 2	0	0
3	C	2	Total 2	Cl 2	0	0
3	D	1	Total 1	Cl 1	0	0
3	E	2	Total 2	Cl 2	0	0
3	F	1	Total 1	Cl 1	0	0
3	G	2	Total 2	Cl 2	0	0
3	H	1	Total 1	Cl 1	0	0
3	J	1	Total 1	Cl 1	0	0

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			32	21	11		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



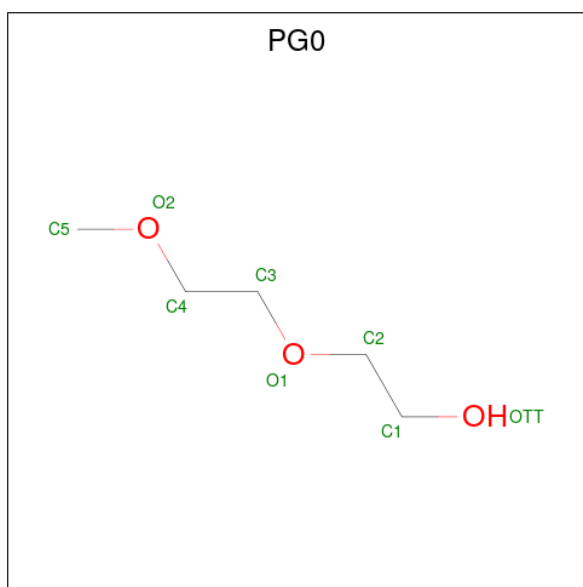
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	F	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	G	1	Total	C	O	0	0
			7	4	3		
5	H	1	Total	C	O	0	0
			7	4	3		
5	I	1	Total	C	O	0	0
			7	4	3		
5	J	1	Total	C	O	0	0
			7	4	3		
5	J	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: C₅H₁₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			8	5	3		

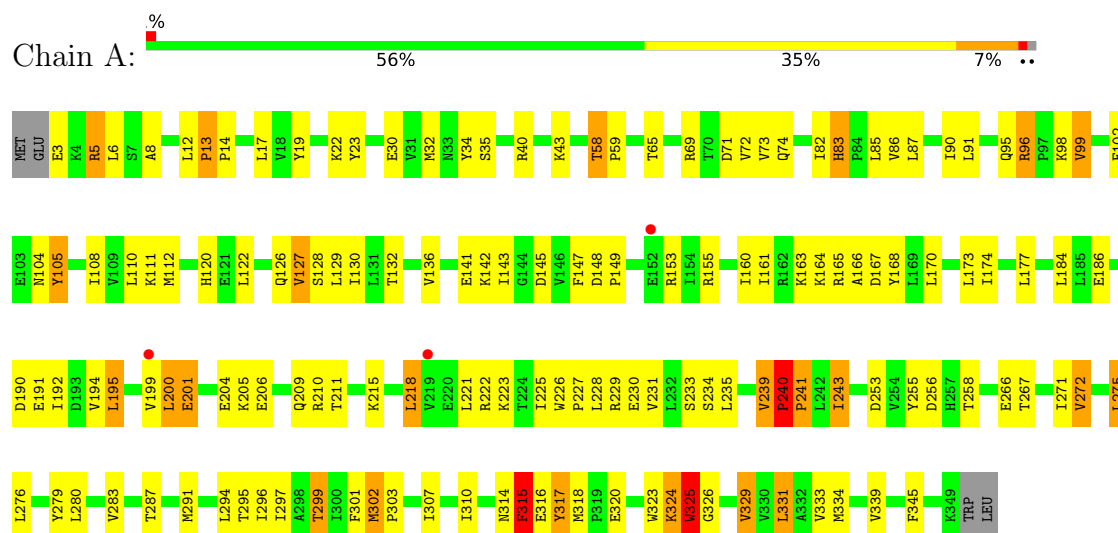
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	20	Total	O	0	0
			20	20		
7	B	28	Total	O	0	0
			28	28		
7	C	27	Total	O	0	0
			27	27		
7	D	25	Total	O	0	0
			25	25		
7	E	27	Total	O	0	0
			27	27		
7	F	20	Total	O	0	0
			20	20		
7	G	35	Total	O	0	0
			35	35		
7	H	15	Total	O	0	0
			15	15		
7	I	21	Total	O	0	0
			21	21		
7	J	23	Total	O	0	0
			23	23		

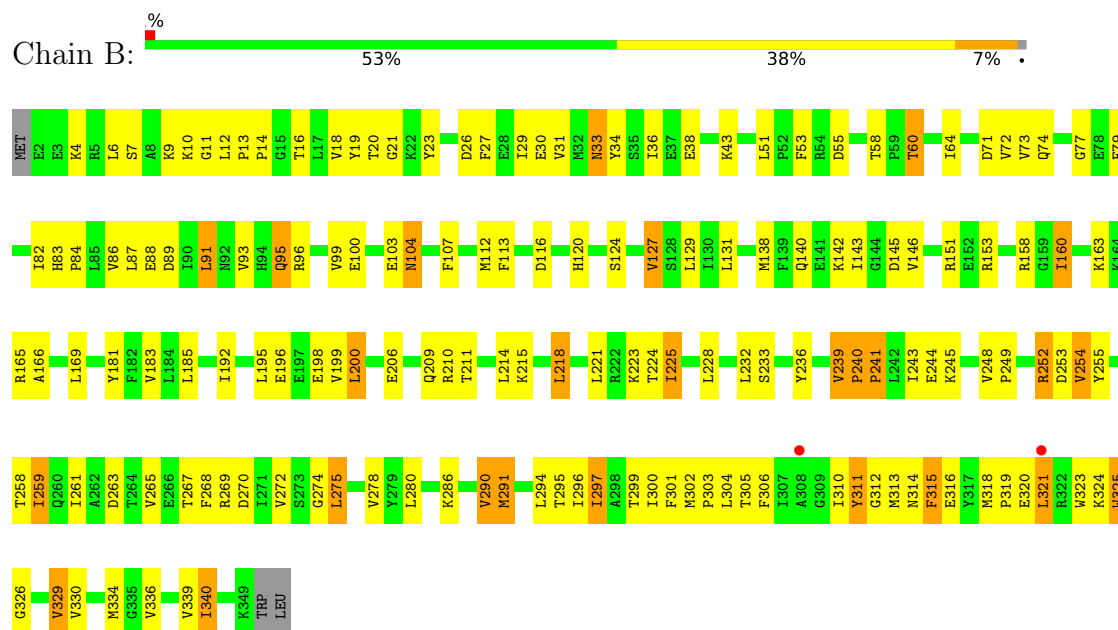
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

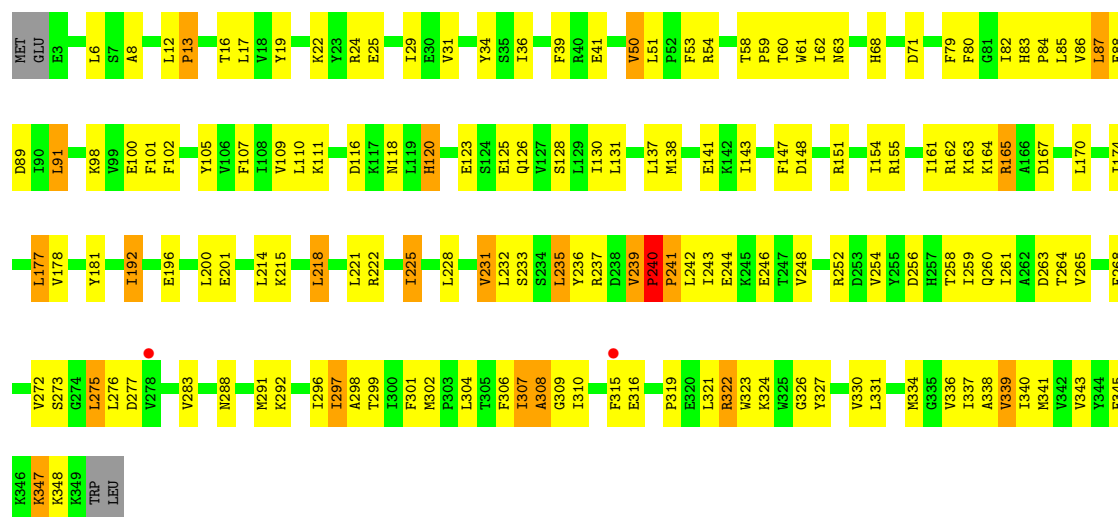
• Molecule 1: Magnesium transport protein CorA



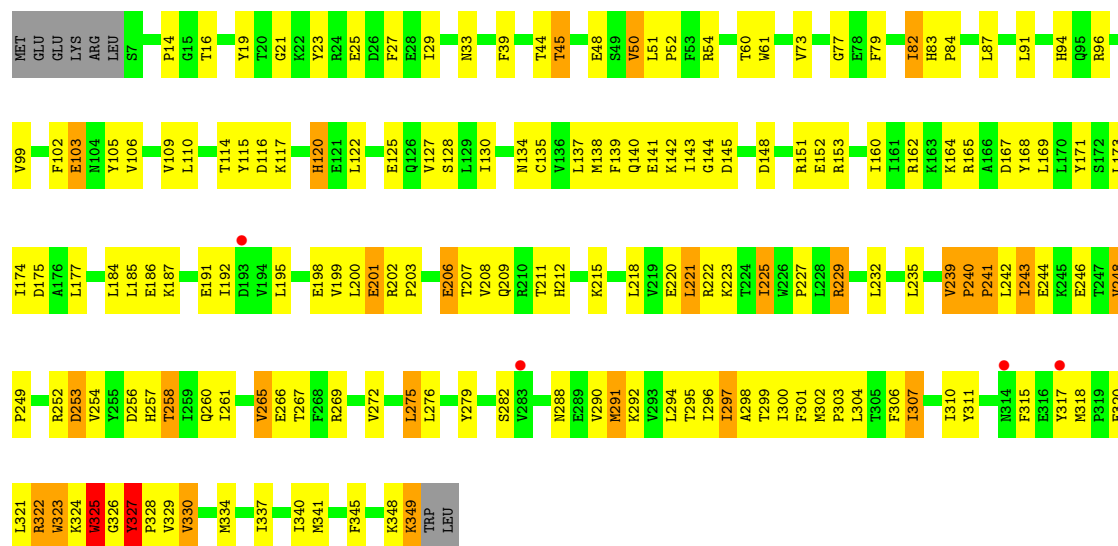
• Molecule 1: Magnesium transport protein CorA



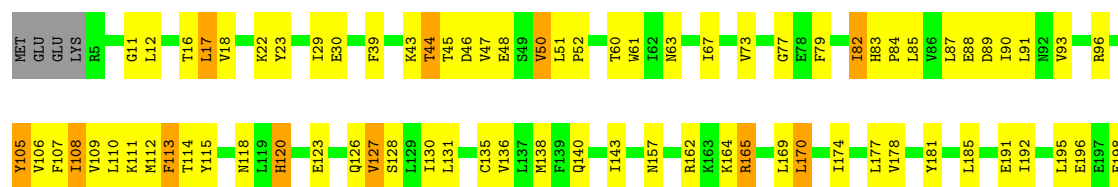
• Molecule 1: Magnesium transport protein CorA

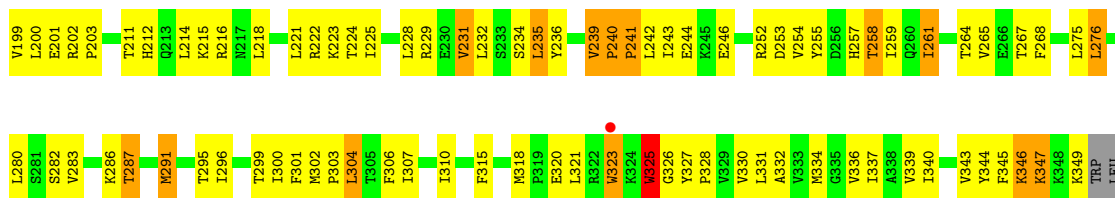


• Molecule 1: Magnesium transport protein CorA



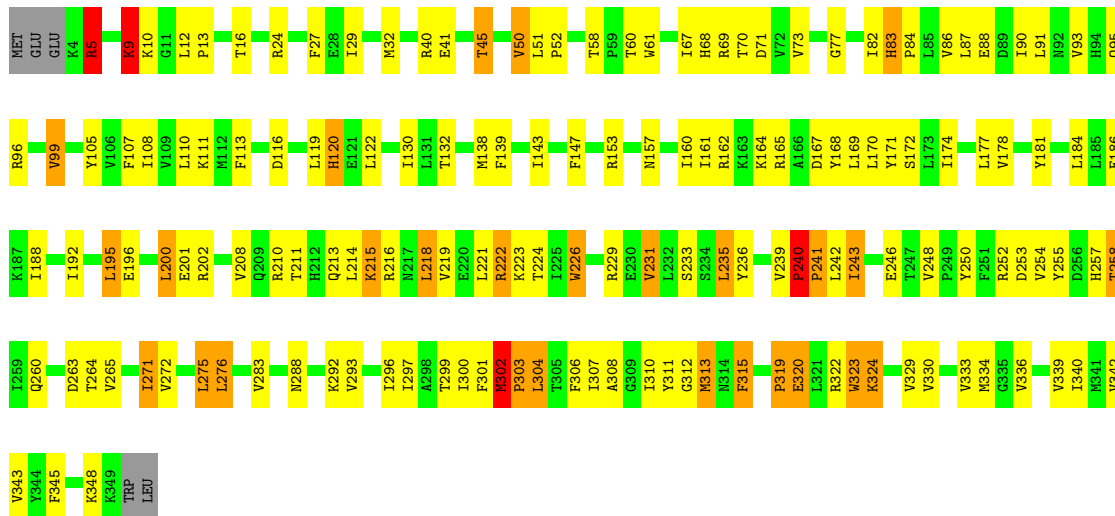
• Molecule 1: Magnesium transport protein CorA





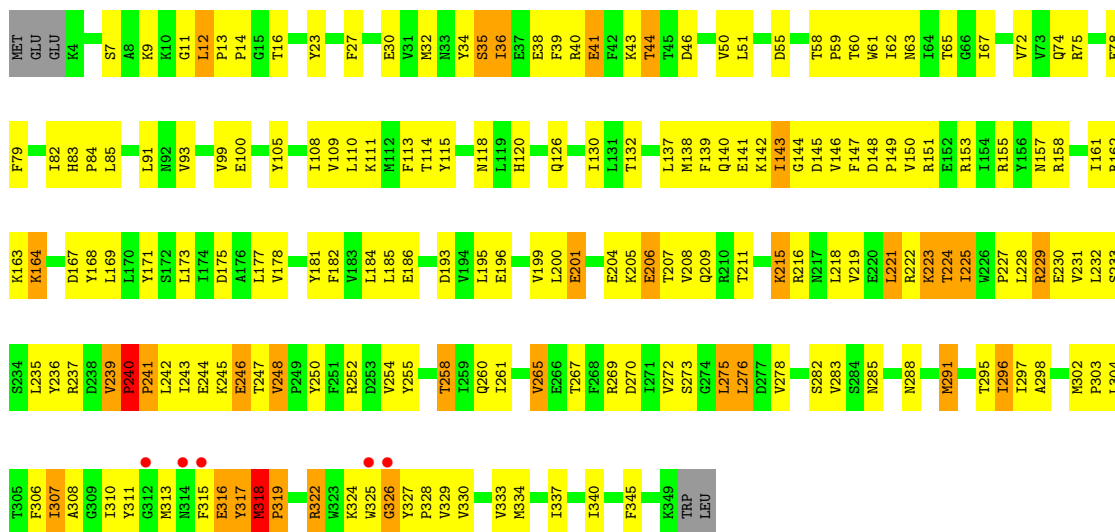
• Molecule 1: Magnesium transport protein CorA

Chain F: 54% 36% 8% ..



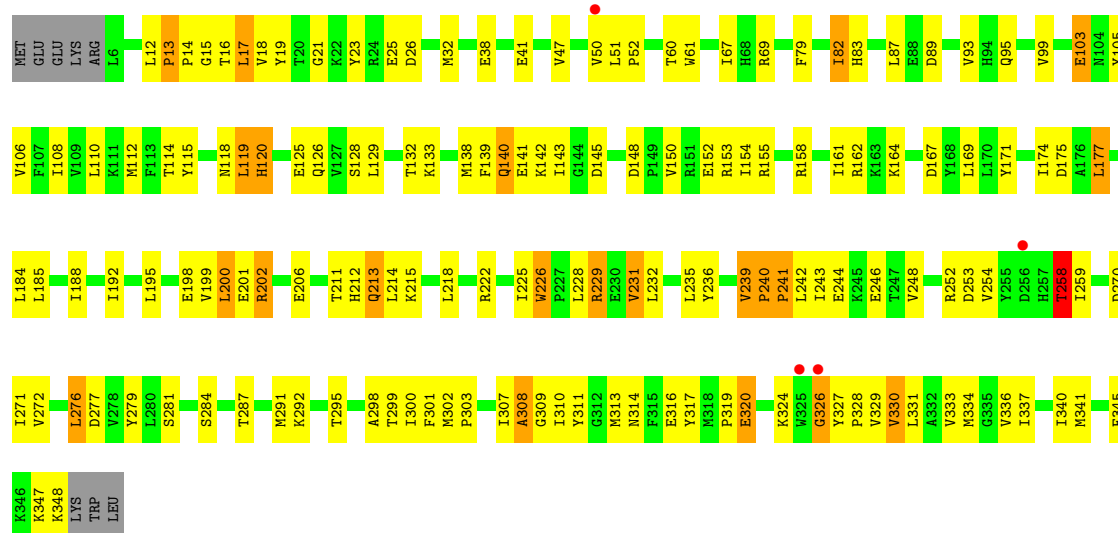
• Molecule 1: Magnesium transport protein CorA

Chain G: 45% 44% 9% ..

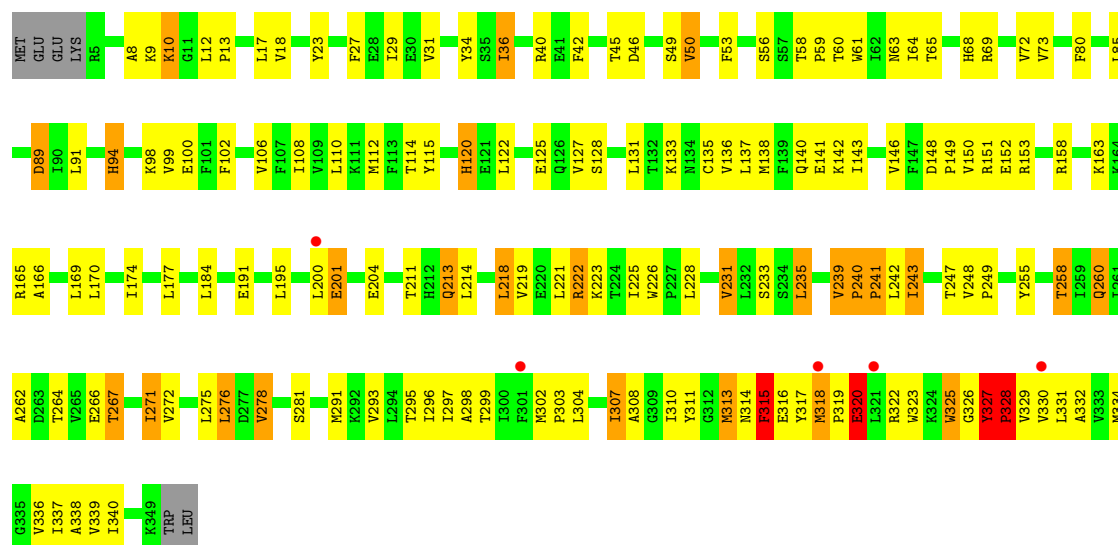


• Molecule 1: Magnesium transport protein CorA

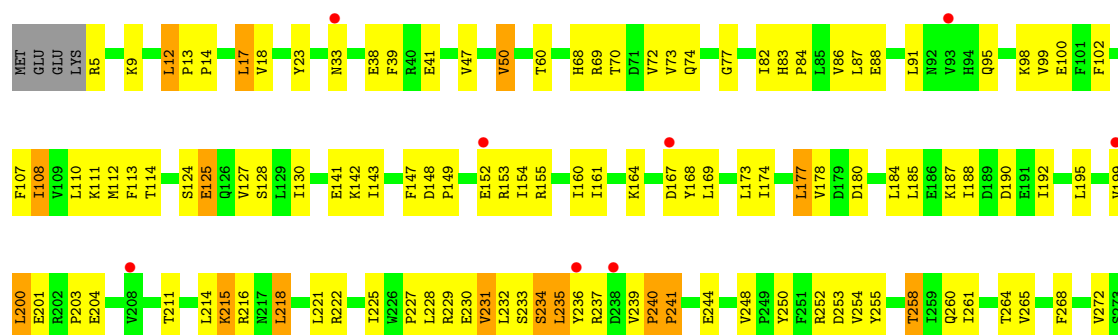
Chain H: 54% 38% 6% ..

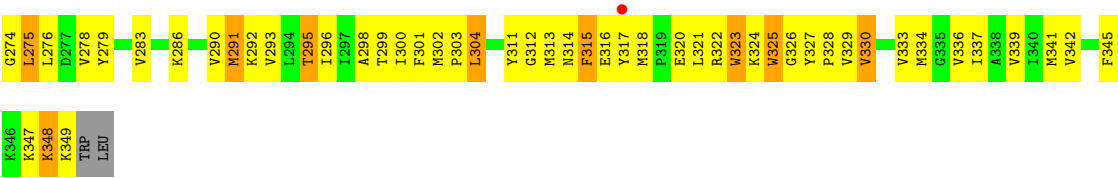


• Molecule 1: Magnesium transport protein CorA



• Molecule 1: Magnesium transport protein CorA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.25Å 151.50Å 143.36Å 90.00° 98.88° 90.00°	Depositor
Resolution (Å)	38.30 – 2.70 38.30 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.5 (38.30-2.70) 90.5 (38.30-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.228 , 0.289 0.242 , 0.297	Depositor DCC
R_{free} test set	6083 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 87.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29094	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, CL, PEG, PG0, MG

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	0.69	2/2950 (0.1%)	1.13	16/3997 (0.4%)
1	B	0.77	1/2959 (0.0%)	1.12	16/4009 (0.4%)
1	C	0.71	2/2925 (0.1%)	1.12	17/3962 (0.4%)
1	D	0.65	1/2913 (0.0%)	1.09	15/3949 (0.4%)
1	E	0.70	1/2907 (0.0%)	1.09	15/3941 (0.4%)
1	F	0.72	2/2918 (0.1%)	1.11	18/3955 (0.5%)
1	G	0.76	1/2905 (0.0%)	1.14	13/3938 (0.3%)
1	H	0.69	0/2887	1.10	19/3915 (0.5%)
1	I	0.69	2/2914 (0.1%)	1.07	19/3952 (0.5%)
1	J	0.70	0/2905	1.08	8/3939 (0.2%)
All	All	0.71	12/29183 (0.0%)	1.11	156/39557 (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	C	0	1
1	D	0	1
1	E	0	2
1	F	0	2
1	G	0	1
1	H	0	1
1	I	0	3
All	All	0	12

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	240	PRO	CA-C	6.88	1.58	1.52
1	A	240	PRO	CA-C	6.55	1.58	1.52
1	E	240	PRO	CA-C	6.52	1.58	1.52
1	G	240	PRO	CA-C	5.88	1.57	1.52
1	C	240	PRO	CA-C	5.87	1.57	1.52
1	C	13	PRO	CA-C	5.86	1.57	1.52
1	F	240	PRO	CA-C	5.81	1.57	1.52
1	I	240	PRO	CA-C	5.34	1.57	1.52
1	I	328	PRO	N-CD	5.30	1.55	1.47
1	B	240	PRO	CA-C	5.18	1.56	1.52
1	F	302	MET	C-N	5.11	1.40	1.34
1	A	13	PRO	CA-C	5.09	1.54	1.51

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	LEU	CA-C-N	10.93	127.64	119.66
1	A	12	LEU	C-N-CA	10.93	127.64	119.66
1	F	323	TRP	N-CA-C	10.29	125.57	112.92
1	A	96	ARG	CA-C-N	9.98	130.04	119.76
1	A	96	ARG	C-N-CA	9.98	130.04	119.76
1	E	240	PRO	N-CA-C	9.82	122.68	110.70
1	B	311	TYR	N-CA-C	9.63	123.45	112.57
1	D	240	PRO	N-CA-C	9.03	121.71	110.70
1	F	240	PRO	N-CA-C	8.89	121.55	110.70
1	G	240	PRO	N-CA-C	8.74	121.36	110.70
1	B	240	PRO	N-CA-C	8.51	121.08	110.70
1	G	248	VAL	CA-C-N	-8.50	109.61	119.05
1	G	248	VAL	C-N-CA	-8.50	109.61	119.05
1	I	320	GLU	N-CA-C	8.37	128.64	110.80
1	D	134	ASN	N-CA-C	8.32	123.15	112.92
1	A	240	PRO	N-CA-C	8.16	120.66	110.70
1	I	315	PHE	N-CA-C	-7.94	93.49	108.17
1	C	308	ALA	N-CA-C	7.89	123.11	113.17
1	I	240	PRO	N-CA-C	7.82	120.25	110.70
1	C	240	PRO	N-CA-C	7.77	120.18	110.70
1	F	226	TRP	CA-C-N	-7.64	110.57	119.05
1	F	226	TRP	C-N-CA	-7.64	110.57	119.05
1	G	316	GLU	N-CA-C	7.58	121.67	110.46
1	E	325	TRP	N-CA-C	-7.55	98.98	111.37
1	D	325	TRP	N-CA-C	-7.27	103.88	112.89
1	B	254	VAL	N-CA-C	-7.21	103.14	111.00
1	F	83	HIS	CA-C-N	7.17	127.49	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	83	HIS	C-N-CA	7.17	127.49	119.32
1	D	326	GLY	N-CA-C	-7.04	101.72	112.84
1	B	104	ASN	N-CA-C	6.96	121.94	113.17
1	B	33	ASN	N-CA-C	-6.89	97.73	109.24
1	C	87	LEU	N-CA-C	-6.88	103.86	111.36
1	A	13	PRO	CA-C-N	6.79	128.32	119.84
1	A	13	PRO	C-N-CA	6.79	128.32	119.84
1	G	318	MET	CA-C-N	6.75	128.27	119.84
1	G	318	MET	C-N-CA	6.75	128.27	119.84
1	H	317	TYR	N-CA-C	6.75	118.32	110.97
1	H	308	ALA	N-CA-C	6.74	121.66	113.17
1	I	89	ASP	N-CA-C	6.74	120.72	112.23
1	E	239	VAL	N-CA-C	6.73	123.42	108.88
1	D	201	GLU	N-CA-C	6.66	121.56	113.17
1	G	239	VAL	N-CA-C	6.56	123.05	108.88
1	A	83	HIS	CA-C-N	6.52	126.75	119.32
1	A	83	HIS	C-N-CA	6.52	126.75	119.32
1	I	327	TYR	CA-C-N	-6.51	111.70	119.84
1	I	327	TYR	C-N-CA	-6.51	111.70	119.84
1	B	239	VAL	CA-C-N	-6.50	113.68	120.38
1	B	239	VAL	C-N-CA	-6.50	113.68	120.38
1	H	239	VAL	N-CA-C	6.48	122.87	108.88
1	D	25	GLU	N-CA-C	6.46	119.57	111.24
1	D	239	VAL	N-CA-C	6.45	122.81	108.88
1	A	105	TYR	N-CA-C	6.38	118.55	108.79
1	A	315	PHE	N-CA-C	-6.38	99.03	108.79
1	D	327	TYR	CA-C-N	-6.35	111.91	119.84
1	D	327	TYR	C-N-CA	-6.35	111.91	119.84
1	H	25	GLU	N-CA-C	6.35	117.89	110.97
1	C	148	ASP	CA-C-N	-6.34	112.47	119.19
1	C	148	ASP	C-N-CA	-6.34	112.47	119.19
1	J	239	VAL	CA-C-N	-6.31	113.88	120.38
1	J	239	VAL	C-N-CA	-6.31	113.88	120.38
1	C	323	TRP	N-CA-C	-6.29	99.02	109.46
1	J	113	PHE	N-CA-C	6.23	119.62	109.59
1	B	239	VAL	N-CA-C	6.23	122.33	108.88
1	J	240	PRO	N-CA-C	6.20	118.27	110.70
1	F	99	VAL	CB-CA-C	-6.20	101.92	110.96
1	H	240	PRO	N-CA-C	6.09	118.13	110.70
1	E	170	LEU	N-CA-C	-6.07	104.58	111.07
1	F	9	LYS	N-CA-C	-6.05	97.24	108.02
1	I	239	VAL	CA-C-N	-6.04	114.16	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	239	VAL	C-N-CA	-6.04	114.16	120.38
1	D	239	VAL	CA-C-N	-6.02	114.18	120.38
1	D	239	VAL	C-N-CA	-6.02	114.18	120.38
1	E	105	TYR	N-CA-C	5.99	117.96	108.79
1	G	11	GLY	N-CA-C	-5.94	107.56	115.40
1	F	302	MET	CA-C-N	-5.94	112.38	118.85
1	F	302	MET	C-N-CA	-5.94	112.38	118.85
1	G	201	GLU	N-CA-C	5.93	120.64	113.17
1	B	263	ASP	N-CA-C	-5.92	104.75	111.14
1	I	318	MET	CA-C-N	5.88	141.10	127.00
1	I	318	MET	C-N-CA	5.88	141.10	127.00
1	F	303	PRO	N-CA-C	-5.84	105.58	113.40
1	H	13	PRO	CA-C-N	5.83	127.13	119.84
1	H	13	PRO	C-N-CA	5.83	127.13	119.84
1	I	239	VAL	N-CA-C	5.80	121.42	108.88
1	A	239	VAL	N-CA-C	5.80	121.41	108.88
1	E	108	ILE	N-CA-C	5.79	116.63	108.17
1	D	330	VAL	N-CA-C	-5.79	104.69	110.30
1	A	318	MET	CA-C-N	5.77	125.14	118.85
1	A	318	MET	C-N-CA	5.77	125.14	118.85
1	C	25	GLU	N-CA-C	5.70	117.30	111.14
1	B	225	ILE	N-CA-C	5.70	118.17	111.05
1	H	83	HIS	CA-C-N	5.69	125.81	119.32
1	H	83	HIS	C-N-CA	5.69	125.81	119.32
1	F	5	ARG	N-CA-C	5.66	119.14	111.17
1	G	35	SER	N-CA-C	-5.65	100.94	108.74
1	E	239	VAL	CA-C-N	-5.64	114.57	120.38
1	E	239	VAL	C-N-CA	-5.64	114.57	120.38
1	H	259	ILE	CB-CA-C	-5.63	104.66	112.04
1	C	165	ARG	N-CA-C	5.62	118.76	109.94
1	E	165	ARG	N-CA-C	5.60	118.54	109.86
1	F	239	VAL	N-CA-C	5.58	120.93	108.88
1	E	261	ILE	CB-CA-C	-5.58	104.61	112.14
1	B	259	ILE	N-CA-C	-5.56	104.94	111.00
1	E	301	PHE	N-CA-C	5.52	119.19	112.23
1	A	201	GLU	N-CA-C	5.52	120.12	113.17
1	J	239	VAL	N-CA-C	5.51	120.79	108.88
1	H	240	PRO	CA-C-N	-5.50	112.96	119.84
1	H	240	PRO	C-N-CA	-5.50	112.96	119.84
1	F	58	THR	CA-C-N	5.49	125.75	119.83
1	F	58	THR	C-N-CA	5.49	125.75	119.83
1	G	225	ILE	N-CA-C	5.48	116.21	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	258	THR	N-CA-C	-5.47	105.47	111.82
1	C	239	VAL	N-CA-C	5.46	120.66	108.88
1	E	11	GLY	N-CA-C	-5.42	108.16	115.36
1	C	91	LEU	N-CA-C	5.41	119.05	112.23
1	D	248	VAL	N-CA-CB	5.40	114.66	110.45
1	H	38	GLU	N-CA-C	5.40	116.19	108.74
1	J	38	GLU	N-CA-C	5.40	116.19	108.74
1	F	119	LEU	N-CA-C	-5.39	101.38	109.15
1	A	166	ALA	N-CA-C	5.36	117.81	111.33
1	I	133	LYS	CB-CA-C	-5.35	109.95	117.23
1	C	71	ASP	N-CA-C	-5.33	105.36	111.07
1	F	239	VAL	CA-C-N	-5.31	114.91	120.38
1	F	239	VAL	C-N-CA	-5.31	114.91	120.38
1	E	113	PHE	N-CA-C	5.31	118.14	109.59
1	I	146	VAL	N-CA-C	-5.31	107.58	112.83
1	I	201	GLU	N-CA-C	5.30	119.91	113.38
1	G	38	GLU	N-CA-C	5.30	117.03	109.14
1	I	318	MET	C-N-CD	-5.29	108.96	120.60
1	C	105	TYR	N-CA-C	5.28	116.86	108.79
1	I	8	ALA	N-CA-C	5.27	117.24	108.02
1	G	326	GLY	N-CA-C	5.24	119.02	112.73
1	J	12	LEU	CA-C-N	5.24	125.78	120.38
1	J	12	LEU	C-N-CA	5.24	125.78	120.38
1	B	38	GLU	N-CA-C	5.21	115.41	108.38
1	E	18	VAL	N-CA-C	5.21	115.77	108.17
1	B	91	LEU	N-CA-C	5.20	117.86	111.82
1	C	259	ILE	N-CA-C	5.20	115.92	110.62
1	C	225	ILE	N-CA-C	5.19	116.66	111.00
1	C	239	VAL	CA-C-N	-5.19	115.04	120.38
1	C	239	VAL	C-N-CA	-5.19	115.04	120.38
1	H	239	VAL	CA-C-N	-5.16	115.06	120.38
1	H	239	VAL	C-N-CA	-5.16	115.06	120.38
1	H	202	ARG	CA-C-N	5.14	126.27	119.84
1	H	202	ARG	C-N-CA	5.14	126.27	119.84
1	D	16	THR	N-CA-C	5.13	117.10	109.25
1	B	321	LEU	N-CA-C	5.07	117.19	111.11
1	I	219	VAL	N-CA-C	5.04	115.27	110.53
1	B	183	VAL	CB-CA-C	-5.03	105.44	111.88
1	E	344	TYR	N-CA-C	-5.03	105.89	112.23
1	H	133	LYS	CB-CA-C	-5.02	110.40	117.23
1	B	93	VAL	N-CA-C	5.02	117.01	112.29
1	I	226	TRP	CA-C-N	-5.02	114.49	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	226	TRP	C-N-CA	-5.02	114.49	119.56
1	C	22	LYS	N-CA-C	5.01	119.44	113.23
1	D	127	VAL	CB-CA-C	-5.00	103.66	110.96

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	ALA	Peptide
1	C	326	GLY	Peptide
1	D	327	TYR	Peptide
1	E	323	TRP	Peptide
1	E	325	TRP	Peptide
1	F	315	PHE	Peptide
1	F	323	TRP	Peptide
1	G	317	TYR	Peptide
1	H	326	GLY	Peptide
1	I	320	GLU	Peptide
1	I	327	TYR	Peptide
1	I	94	HIS	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	2886	0	2938	110	0
1	B	2895	0	2944	129	0
1	C	2865	0	2915	117	0
1	D	2849	0	2895	119	0
1	E	2844	0	2890	121	0
1	F	2856	0	2897	133	0
1	G	2844	0	2882	147	0
1	H	2826	0	2862	106	0
1	I	2850	0	2879	148	0
1	J	2844	0	2882	126	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	5	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
3	A	1	0	0	1	0
3	B	2	0	0	1	0
3	C	2	0	0	1	0
3	D	1	0	0	0	0
3	E	2	0	0	2	0
3	F	1	0	0	1	0
3	G	2	0	0	2	0
3	H	1	0	0	1	0
3	J	1	0	0	1	0
4	A	35	0	46	27	0
4	B	67	0	83	34	0
5	B	28	0	40	5	0
5	C	14	0	20	4	0
5	D	7	0	10	0	0
5	E	28	0	40	1	0
5	F	7	0	10	0	0
5	G	35	0	50	8	0
5	H	7	0	10	0	0
5	I	7	0	10	0	0
5	J	14	0	20	2	0
6	E	8	0	12	0	0
7	A	20	0	0	5	0
7	B	28	0	0	8	0
7	C	27	0	0	4	0
7	D	25	0	0	8	0
7	E	27	0	0	4	0
7	F	20	0	0	2	0
7	G	35	0	0	12	0
7	H	15	0	0	3	0
7	I	21	0	0	4	0
7	J	23	0	0	6	0
All	All	29094	0	29335	1164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1164) 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:G:246:GLU:OE1	5:G:411:PEG:H22	1.24	1.32
4:A:403:LMT:H3B	4:B:406:LMT:C6'	1.59	1.32
1:I:327:TYR:CE1	1:J:318:MET:HE3	1.80	1.15
4:A:403:LMT:C3B	4:B:406:LMT:H6E	1.83	1.08
4:A:403:LMT:H3B	4:B:406:LMT:H6E	1.07	1.06
1:G:246:GLU:OE1	5:G:411:PEG:C2	2.06	1.02
1:F:307:ILE:O	1:F:310:ILE:HG22	1.60	1.00
1:F:307:ILE:CD1	1:F:334:MET:HE3	1.92	1.00
1:F:307:ILE:HD11	1:F:334:MET:CE	1.91	1.00
4:A:403:LMT:H3B	4:B:406:LMT:H6D	1.50	0.93
1:B:323:TRP:HB2	4:B:407:LMT:O4'	1.70	0.92
1:F:307:ILE:HD11	1:F:334:MET:CG	1.98	0.92
1:I:316:GLU:HB2	1:I:318:MET:HG2	1.49	0.92
1:I:326:GLY:HA3	1:I:328:PRO:HD3	1.50	0.92
1:I:330:VAL:O	1:I:334:MET:HG3	1.68	0.92
1:C:256:ASP:OD1	1:E:96[B]:ARG:NH2	2.03	0.91
4:A:403:LMT:C3B	4:B:406:LMT:C6'	2.47	0.91
1:F:301:PHE:HE2	1:I:303:PRO:HG3	1.32	0.91
1:C:316:GLU:HG2	1:E:321:LEU:HB3	1.53	0.90
1:B:43:LYS:HD2	5:B:410:PEG:H11	1.53	0.90
4:A:403:LMT:C3'	4:B:406:LMT:H4'	2.03	0.89
1:A:323:TRP:HB3	1:A:324:LYS:HA	1.54	0.88
1:D:203:PRO:HB2	7:D:521:HOH:O	1.73	0.88
1:G:61:TRP:HB2	1:G:169:LEU:HD21	1.56	0.87
1:G:196:GLU:OE1	1:H:212:HIS:NE2	2.06	0.86
1:F:110:LEU:HD13	1:F:177:LEU:HD22	1.58	0.86
1:D:203:PRO:CB	7:D:521:HOH:O	2.22	0.85
1:E:88:GLU:OE1	7:E:501:HOH:O	1.94	0.85
1:F:307:ILE:HD11	1:F:334:MET:HE3	1.54	0.85
1:G:229:ARG:NH2	7:G:514:HOH:O	2.09	0.84
1:A:324:LYS:HD2	1:D:317:TYR:HB2	1.58	0.84
4:A:403:LMT:H3'	4:B:406:LMT:H4'	1.59	0.83
1:I:302:MET:HG3	1:J:302:MET:HE1	1.59	0.82
1:A:13:PRO:HG3	1:D:153:ARG:HD3	1.62	0.81
1:D:229:ARG:HG2	1:D:258:THR:HG23	1.63	0.80
1:G:140:GLN:HE22	1:G:145:ASP:HB3	1.45	0.80
1:A:307:ILE:HD11	1:A:334:MET:HG2	1.64	0.80
1:I:235:LEU:HD12	1:I:242:LEU:HD11	1.63	0.80
1:B:74:GLN:NE2	7:B:526:HOH:O	2.15	0.79
1:I:89:ASP:OD2	7:I:505:HOH:O	1.99	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:GLN:NE2	7:C:522:HOH:O	2.14	0.79
1:F:13:PRO:HG3	1:I:153:ARG:HD3	1.63	0.79
4:A:403:LMT:H12	4:B:406:LMT:H51	1.62	0.79
1:F:306:PHE:CE1	1:G:304:LEU:HB3	2.18	0.79
1:J:88:GLU:OE2	7:J:507:HOH:O	2.01	0.78
1:B:252:ARG:NH2	5:C:406:PEG:O4	2.15	0.78
1:F:307:ILE:CD1	1:F:334:MET:CE	2.57	0.78
1:I:326:GLY:HA2	1:I:327:TYR:HB3	1.65	0.78
1:D:48:GLU:OE2	7:D:510:HOH:O	2.01	0.78
1:I:184:LEU:HD21	1:I:221:LEU:HD11	1.65	0.78
1:J:218:LEU:HD21	1:J:268:PHE:HB3	1.66	0.78
1:D:54:ARG:NH1	1:D:79:PHE:O	2.17	0.77
3:C:403:CL:CL	7:C:503:HOH:O	2.39	0.77
4:A:403:LMT:O2'	4:B:406:LMT:O3'	2.01	0.77
1:D:199:VAL:HG13	1:D:279:TYR:HB2	1.66	0.77
1:G:41:GLU:OE2	1:G:155:ARG:NE	2.16	0.77
1:G:168:TYR:OH	3:G:406:CL:CL	2.39	0.76
1:G:74:GLN:HE22	5:G:409:PEG:H31	1.48	0.76
1:H:175:ASP:OD1	7:H:505:HOH:O	2.03	0.76
1:E:83:HIS:CD2	1:E:85:LEU:H	2.03	0.76
1:B:253:ASP:OD1	7:B:506:HOH:O	2.02	0.76
3:E:404:CL:CL	7:E:503:HOH:O	2.41	0.76
1:I:326:GLY:HA3	1:I:328:PRO:CD	2.14	0.76
1:C:192:ILE:HG12	1:C:214:LEU:HD21	1.68	0.76
1:I:325:TRP:HA	1:I:325:TRP:CE3	2.20	0.76
1:E:61:TRP:HB2	1:E:169:LEU:HD21	1.67	0.75
4:A:403:LMT:H12	4:B:406:LMT:C5	2.17	0.75
1:B:163:LYS:NZ	7:B:511:HOH:O	2.19	0.75
1:H:120:HIS:O	1:H:213:GLN:NE2	2.20	0.74
1:F:307:ILE:HG13	1:F:308:ALA:N	2.02	0.74
1:F:307:ILE:HD11	1:F:334:MET:HG2	1.69	0.74
1:H:195:LEU:HD21	1:H:211:THR:HA	1.68	0.74
1:D:73:VAL:HG21	1:D:91:LEU:HD21	1.68	0.74
1:G:232:LEU:HD13	1:G:254:VAL:HG12	1.68	0.74
4:A:403:LMT:C3'	4:B:406:LMT:O3'	2.36	0.73
1:D:140:GLN:HE22	1:D:145:ASP:HB3	1.52	0.73
1:I:63:ASN:HD22	1:I:151:ARG:HH22	1.32	0.73
1:F:311:TYR:HE2	1:F:330:VAL:HG21	1.53	0.73
1:F:301:PHE:C	1:F:303:PRO:HD2	2.13	0.73
1:I:327:TYR:HB2	1:J:315:PHE:HZ	1.53	0.73
1:I:331:LEU:O	1:I:334:MET:HB2	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:82:ILE:HG12	1:J:130:ILE:HD13	1.71	0.72
1:G:100:GLU:O	7:G:523:HOH:O	2.06	0.72
1:B:89:ASP:OD2	7:B:502:HOH:O	2.07	0.72
1:I:327:TYR:CD1	1:J:318:MET:HE3	2.24	0.72
1:J:229:ARG:NH1	7:J:518:HOH:O	2.22	0.72
1:I:222:ARG:NE	1:I:266:GLU:OE1	2.23	0.72
1:I:211:THR:HG21	1:I:276:LEU:HD13	1.73	0.71
1:H:61:TRP:HB2	1:H:169:LEU:HD21	1.72	0.71
1:E:200:LEU:HD12	1:E:201:GLU:HG3	1.73	0.71
1:F:32:MET:HE3	1:F:41:GLU:HB3	1.73	0.71
1:F:311:TYR:HB2	1:I:313:MET:HG2	1.72	0.71
1:E:327:TYR:HA	1:E:330:VAL:HB	1.72	0.71
1:H:125:GLU:HG3	1:H:141:GLU:HB2	1.72	0.71
1:D:61:TRP:HB2	1:D:169:LEU:HD21	1.73	0.71
1:B:198:GLU:OE1	1:B:210:ARG:NH1	2.24	0.71
1:G:61:TRP:HE1	1:G:138:MET:HE2	1.55	0.71
1:D:184:LEU:HD21	1:D:221:LEU:HD11	1.72	0.70
3:H:401:CL:CL	1:J:14:PRO:HD2	2.28	0.70
1:C:8:ALA:O	7:C:511:HOH:O	2.09	0.70
7:F:513:HOH:O	1:G:223:LYS:NZ	2.16	0.70
1:A:184:LEU:HD21	1:A:221:LEU:HD11	1.72	0.70
1:C:263:ASP:OD2	1:E:96[A]:ARG:NH1	2.21	0.70
1:A:314:ASN:ND2	1:B:314:ASN:OD1	2.25	0.70
1:C:200:LEU:HD12	1:C:201:GLU:HG3	1.72	0.70
1:E:83:HIS:HD2	1:E:85:LEU:H	1.40	0.69
1:I:307:ILE:HD11	1:I:334:MET:HG2	1.73	0.69
1:E:221:LEU:HG	1:E:225:ILE:HD12	1.74	0.69
1:B:232:LEU:HD13	1:B:254:VAL:HG12	1.75	0.69
1:C:83:HIS:ND1	1:C:84:PRO:HD2	2.08	0.69
1:G:272:VAL:O	7:G:515:HOH:O	2.10	0.69
1:A:256:ASP:OD2	7:A:518:HOH:O	2.09	0.69
1:E:120:HIS:ND1	1:E:191:GLU:OE2	2.26	0.69
1:A:99:VAL:HG22	1:A:231:VAL:HG13	1.74	0.69
4:B:407:LMT:O2'	4:B:407:LMT:H31	1.93	0.69
1:A:19:TYR:OH	1:A:141:GLU:OE1	2.09	0.68
1:F:301:PHE:CE2	1:I:303:PRO:HG3	2.23	0.68
4:B:407:LMT:H1B	4:B:407:LMT:O3'	1.91	0.68
1:E:195:LEU:HD21	1:E:211:THR:HA	1.76	0.68
1:H:200:LEU:HD12	1:H:201:GLU:HG3	1.76	0.68
1:B:153:ARG:HD3	1:C:13:PRO:HG3	1.74	0.68
1:D:222:ARG:HD2	1:D:266:GLU:OE1	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:253:ASP:OD1	7:J:512:HOH:O	2.11	0.67
1:A:291:MET:HE2	1:B:291:MET:HG2	1.75	0.67
1:J:228:LEU:HA	1:J:231:VAL:HB	1.76	0.67
1:H:105:TYR:HB3	1:H:132:THR:HB	1.76	0.66
1:C:316:GLU:HG2	1:E:321:LEU:CB	2.24	0.66
4:A:403:LMT:H3'	4:B:406:LMT:C4'	2.25	0.66
1:F:319:PRO:HB2	1:F:320:GLU:HA	1.77	0.66
1:G:318:MET:HG2	1:G:319:PRO:HD3	1.77	0.66
1:D:200:LEU:HD12	1:D:201:GLU:HG3	1.78	0.66
1:G:327:TYR:HB3	1:G:328:PRO:HD3	1.77	0.66
1:I:45:THR:O	7:I:509:HOH:O	2.14	0.66
1:I:326:GLY:CA	1:I:328:PRO:HD3	2.24	0.66
1:I:328:PRO:CD	1:I:329:VAL:H	2.08	0.66
1:J:88:GLU:OE1	7:J:501:HOH:O	2.14	0.66
1:F:264:THR:OG1	7:F:513:HOH:O	2.12	0.66
1:F:77:GLY:HA3	1:F:87:LEU:HD21	1.77	0.66
4:A:403:LMT:O3'	4:B:406:LMT:O3'	2.13	0.65
1:D:203:PRO:HB3	7:D:521:HOH:O	1.91	0.65
1:E:90:ILE:HD11	1:E:130:ILE:HD11	1.77	0.65
1:F:165:ARG:HH12	1:F:243:ILE:HG21	1.61	0.65
1:G:193:ASP:OD2	7:G:513:HOH:O	2.14	0.65
1:J:108:ILE:HD13	1:J:235:LEU:HD21	1.79	0.65
1:J:255:TYR:O	1:J:258:THR:HG22	1.96	0.65
1:H:308:ALA:N	1:H:309:GLY:HA3	2.11	0.65
1:A:153:ARG:HD3	1:B:13:PRO:HG3	1.78	0.65
1:B:27:PHE:CZ	1:B:72:VAL:HG21	2.32	0.65
1:F:61:TRP:HB2	1:F:169:LEU:HD21	1.79	0.65
1:A:3:GLU:N	1:D:186:GLU:OE1	2.30	0.65
1:J:83:HIS:ND1	1:J:84:PRO:HD2	2.12	0.65
1:A:90:ILE:HD11	1:A:130:ILE:HD11	1.79	0.65
1:A:331:LEU:HD22	1:A:334:MET:HE2	1.79	0.65
1:I:40:ARG:HH21	1:I:42:PHE:HE2	1.43	0.65
1:A:291:MET:HE1	1:B:294:LEU:HD22	1.78	0.65
1:B:316:GLU:HB2	1:C:324:LYS:HG2	1.79	0.64
1:E:337:ILE:HA	1:E:340:ILE:HG12	1.79	0.64
1:F:302:MET:HG3	1:I:302:MET:HE3	1.78	0.64
1:I:327:TYR:CE1	1:J:318:MET:CE	2.69	0.64
1:A:302:MET:HE1	1:B:302:MET:HG3	1.78	0.64
1:F:302:MET:HG3	1:I:302:MET:CE	2.28	0.64
1:I:125:GLU:OE1	1:I:140:GLN:NE2	2.25	0.64
1:G:233:SER:OG	1:G:237:ARG:NH2	2.31	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:303:PRO:HG3	1:H:301:PHE:CE2	2.33	0.64
1:D:29:ILE:HG21	1:D:50:VAL:HG11	1.78	0.64
1:J:12:LEU:O	7:J:503:HOH:O	2.14	0.64
1:C:82:ILE:HG12	1:C:130:ILE:HD13	1.80	0.64
1:C:29:ILE:HG21	1:C:50:VAL:HG11	1.80	0.64
1:C:308:ALA:N	1:C:309:GLY:HA3	2.13	0.64
1:J:147:PHE:HZ	1:J:177:LEU:HD12	1.63	0.64
1:G:221:LEU:HD23	1:G:265:VAL:HG21	1.80	0.63
1:J:33:ASN:ND2	1:J:60:THR:OG1	2.31	0.63
1:B:302:MET:HE1	1:C:298:ALA:HA	1.81	0.63
1:G:184:LEU:HD21	1:G:221:LEU:HD11	1.80	0.63
1:G:306:PHE:CZ	5:G:408:PEG:H41	2.33	0.63
1:A:83:HIS:HE2	1:A:85:LEU:HD12	1.63	0.63
1:A:253:ASP:OD1	7:A:504:HOH:O	2.15	0.63
1:I:325:TRP:HA	1:I:325:TRP:HE3	1.63	0.63
1:E:82:ILE:HG13	1:E:105:TYR:CE2	2.33	0.63
1:B:323:TRP:HB2	4:B:407:LMT:H4O1	1.63	0.63
1:E:185:LEU:HD11	1:E:261:ILE:HG23	1.80	0.63
1:E:231:VAL:HG12	1:E:232:LEU:HG	1.81	0.63
1:F:307:ILE:HD12	1:F:334:MET:HE3	1.80	0.63
1:A:95:GLN:HA	1:D:260:GLN:HE22	1.64	0.62
1:A:155:ARG:O	7:A:514:HOH:O	2.15	0.62
1:H:314:ASN:ND2	1:J:314:ASN:OD1	2.32	0.62
4:A:403:LMT:H3'	4:B:406:LMT:C3'	2.29	0.62
1:B:311:TYR:HE2	1:B:330:VAL:HG21	1.65	0.62
1:D:211:THR:HG21	1:D:276:LEU:HD13	1.80	0.62
1:I:40:ARG:NH1	7:I:520:HOH:O	2.23	0.62
1:B:324:LYS:HG2	1:B:325:TRP:H	1.63	0.62
1:E:236:TYR:CE1	1:E:252:ARG:HB2	2.34	0.62
1:F:192:ILE:HG12	1:F:214:LEU:HD21	1.81	0.62
1:F:200:LEU:HD13	1:G:209:GLN:HG2	1.81	0.62
1:G:315:PHE:HB3	1:H:327:TYR:HB2	1.82	0.62
1:H:115:TYR:HB2	1:H:184:LEU:HD11	1.82	0.62
1:I:327:TYR:HA	1:I:330:VAL:HB	1.81	0.62
1:B:112:MET:HE2	1:B:127:VAL:HG22	1.82	0.62
1:D:307:ILE:HD11	1:D:334:MET:HG2	1.82	0.62
1:G:30:GLU:HG3	1:G:43:LYS:HG2	1.80	0.62
1:A:168:TYR:OH	1:B:14:PRO:HG2	2.00	0.62
1:F:9:LYS:HB2	1:F:12:LEU:HD12	1.80	0.62
1:A:303:PRO:HG3	1:B:301:PHE:HE2	1.65	0.61
1:D:148:ASP:O	1:D:152:GLU:HG2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:MET:HE2	1:A:127:VAL:HG22	1.81	0.61
1:B:55:ASP:HB3	5:B:411:PEG:H11	1.82	0.61
1:D:348:LYS:HG2	1:D:349:LYS:H	1.66	0.61
1:I:320:GLU:C	1:I:322:ARG:H	2.07	0.61
1:J:70:THR:HG22	1:J:91:LEU:HD13	1.81	0.61
1:D:209:GLN:HG2	1:E:200:LEU:HD22	1.81	0.61
1:G:175:ASP:OD2	7:G:510:HOH:O	2.16	0.61
1:I:307:ILE:HD11	1:I:334:MET:CG	2.30	0.61
1:J:200:LEU:HD12	1:J:201:GLU:HG3	1.83	0.61
1:C:243:ILE:HG13	1:C:246:GLU:HB2	1.83	0.61
1:C:302:MET:HE1	1:E:302:MET:HG3	1.81	0.61
1:D:14:PRO:HD2	3:E:403:CL:CL	2.38	0.60
1:G:150:VAL:HG11	1:G:173:LEU:HD23	1.83	0.60
1:G:153:ARG:HD3	1:H:13:PRO:HG3	1.83	0.60
1:E:12:LEU:HD13	1:E:16:THR:HG21	1.83	0.60
1:F:29:ILE:HG21	1:F:50:VAL:HG11	1.83	0.60
1:C:83:HIS:CD2	1:C:85:LEU:HB2	2.36	0.60
1:D:175:ASP:OD2	7:D:501:HOH:O	2.17	0.60
1:G:36:ILE:HD13	1:G:163:LYS:HG3	1.83	0.60
1:G:310:ILE:HG22	1:H:334:MET:HE1	1.82	0.60
1:F:200:LEU:HD12	1:F:201:GLU:HG3	1.84	0.60
1:G:272:VAL:HA	1:G:275:LEU:HD22	1.83	0.60
1:D:130:ILE:HB	1:D:137:LEU:HB2	1.84	0.60
1:H:152:GLU:HB2	1:H:158:ARG:HH21	1.66	0.60
1:A:199:VAL:HG13	1:A:279:TYR:HB2	1.83	0.60
1:F:165:ARG:NH1	1:F:243:ILE:HG21	2.17	0.60
1:C:98:LYS:NZ	1:C:100:GLU:OE1	2.21	0.59
1:F:302:MET:HE1	1:G:298:ALA:HA	1.85	0.59
3:F:403:CL:CL	1:G:14:PRO:HD2	2.39	0.59
1:J:203:PRO:HG2	1:J:286:LYS:HE2	1.84	0.59
4:A:403:LMT:O3'	4:B:406:LMT:C4'	2.51	0.59
1:D:243:ILE:HG13	1:D:246:GLU:HB2	1.85	0.59
1:J:23:TYR:CE2	1:J:142:LYS:HD3	2.37	0.59
1:E:239:VAL:HA	1:E:242:LEU:HD12	1.82	0.59
1:F:312:GLY:O	1:I:314:ASN:ND2	2.35	0.59
1:H:112:MET:HG3	1:H:177:LEU:HD11	1.83	0.59
1:I:326:GLY:HA2	1:I:327:TYR:CB	2.31	0.59
1:I:165:ARG:NH2	1:I:243:ILE:HD12	2.18	0.59
1:C:34:TYR:O	1:C:59:PRO:HD2	2.02	0.59
1:G:195:LEU:HD21	1:G:211:THR:HA	1.84	0.59
1:F:5:ARG:O	1:F:5:ARG:NE	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:99:VAL:HG22	1:H:108:ILE:HG12	1.85	0.59
1:C:131:LEU:HD22	1:C:170:LEU:HD22	1.83	0.59
1:C:174:ILE:O	1:C:178:VAL:HG23	2.02	0.59
1:I:255:TYR:O	1:I:258:THR:HG22	2.03	0.59
1:I:27:PHE:CZ	1:I:72:VAL:HG21	2.38	0.59
1:B:33:ASN:HB2	1:B:60:THR:HG23	1.85	0.58
1:G:143:ILE:HD13	1:G:144:GLY:H	1.68	0.58
1:F:195:LEU:HD11	1:F:210:ARG:HB3	1.83	0.58
1:H:330:VAL:HA	1:H:333:VAL:HG12	1.84	0.58
4:A:403:LMT:O3'	4:B:406:LMT:H4'	2.03	0.58
1:B:140:GLN:HE22	1:B:145:ASP:HB3	1.67	0.58
1:B:306:PHE:CE1	1:C:304:LEU:HB3	2.38	0.58
1:B:324:LYS:O	1:B:326:GLY:N	2.36	0.58
1:J:225:ILE:HD12	1:J:228:LEU:HD23	1.84	0.58
1:A:323:TRP:CB	1:A:324:LYS:HA	2.28	0.58
1:D:120:HIS:H	1:D:120:HIS:CD2	2.19	0.58
1:F:288:ASN:HD21	1:F:292:LYS:HE3	1.69	0.58
1:I:308:ALA:HA	1:J:313:MET:HE3	1.84	0.58
1:B:274:GLY:O	1:B:278:VAL:HG23	2.04	0.58
1:E:22:LYS:HE3	1:E:23:TYR:CZ	2.37	0.58
1:E:229:ARG:NE	1:E:259:ILE:HG12	2.17	0.58
1:F:178:VAL:HG21	1:F:254:VAL:HG13	1.85	0.58
1:H:281:SER:HB3	1:J:279:TYR:HE2	1.68	0.58
1:H:326:GLY:O	1:H:329:VAL:HG12	2.03	0.58
1:E:157:ASN:CG	1:E:162:ARG:HG3	2.28	0.58
1:D:117:LYS:HE3	1:D:187:LYS:HG2	1.85	0.58
1:D:320:GLU:HB3	1:E:315:PHE:CE1	2.39	0.58
1:F:83:HIS:ND1	1:F:84:PRO:HD2	2.19	0.58
1:A:22:LYS:HE3	1:A:23:TYR:CE1	2.39	0.58
1:B:181:TYR:O	1:B:185:LEU:HG	2.04	0.58
1:B:236:TYR:CZ	1:B:252:ARG:HG3	2.39	0.58
1:C:232:LEU:HD13	1:C:254:VAL:HG12	1.86	0.58
1:D:195:LEU:HD23	1:D:275:LEU:HD23	1.86	0.58
1:I:61:TRP:HE1	1:I:138:MET:HE2	1.69	0.58
1:I:326:GLY:CA	1:I:327:TYR:HB3	2.33	0.58
1:B:34:TYR:OH	1:B:169:LEU:HD13	2.03	0.57
1:B:73:VAL:HG11	1:B:91:LEU:HD21	1.85	0.57
1:F:229:ARG:HA	1:F:258:THR:HG21	1.86	0.57
1:H:302:MET:HE1	1:J:298:ALA:HA	1.85	0.57
1:B:30:GLU:OE1	1:B:151:ARG:NH2	2.37	0.57
1:G:93:VAL:HA	1:G:126:GLN:OE1	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:LYS:H	1:E:346:LYS:HE3	1.69	0.57
1:J:311:TYR:HE2	1:J:330:VAL:HG21	1.69	0.57
5:E:405:PEG:H32	7:G:535:HOH:O	2.03	0.57
1:F:315:PHE:HD2	1:G:318:MET:HE2	1.70	0.57
1:D:222:ARG:HD3	1:D:269:ARG:HD2	1.87	0.57
3:G:406:CL:CL	7:G:533:HOH:O	2.54	0.57
1:J:221:LEU:O	1:J:225:ILE:HG22	2.04	0.57
1:A:108:ILE:HD12	1:A:170:LEU:HD11	1.86	0.57
1:F:307:ILE:HD11	1:F:334:MET:HG3	1.86	0.57
1:G:255:TYR:O	1:G:258:THR:HG22	2.04	0.57
1:H:299:THR:HG1	1:H:345:PHE:HZ	1.50	0.57
1:D:328:PRO:HG2	1:D:329:VAL:HG13	1.86	0.57
1:E:253:ASP:OD1	7:E:507:HOH:O	2.18	0.57
1:E:323:TRP:O	1:E:326:GLY:N	2.38	0.57
1:J:47:VAL:HG21	1:J:72:VAL:HG13	1.86	0.57
1:C:100:GLU:HB3	1:C:102:PHE:CE1	2.40	0.56
1:D:327:TYR:CE1	1:E:318:MET:HG3	2.40	0.56
1:H:292:LYS:HD3	1:H:348:LYS:HB3	1.87	0.56
1:D:298:ALA:HB1	1:D:302:MET:HE2	1.87	0.56
1:F:116:ASP:O	1:F:120:HIS:HA	2.04	0.56
1:F:312:GLY:HA2	1:I:314:ASN:HD22	1.68	0.56
1:G:140:GLN:NE2	1:G:145:ASP:HB3	2.17	0.56
1:I:10:LYS:HD3	5:J:405:PEG:O4	2.05	0.56
1:I:328:PRO:CG	1:I:329:VAL:H	2.18	0.56
1:B:153:ARG:HG2	1:B:158:ARG:HB2	1.87	0.56
1:B:336:VAL:O	1:B:340:ILE:HG23	2.06	0.56
1:E:17:LEU:HG	1:E:91:LEU:HD12	1.88	0.56
1:A:325:TRP:CE3	1:A:325:TRP:HA	2.39	0.56
1:H:300:ILE:O	1:H:303:PRO:HD2	2.05	0.56
1:C:316:GLU:CG	1:E:321:LEU:O	2.53	0.56
1:J:304:LEU:HD13	1:J:334:MET:HB3	1.86	0.56
1:D:327:TYR:HA	1:D:330:VAL:H	1.70	0.56
1:H:120:HIS:HB2	1:H:213:GLN:HE22	1.70	0.56
4:A:403:LMT:C3'	4:B:406:LMT:C4'	2.78	0.56
1:C:288:ASN:HD21	1:C:292:LYS:HE3	1.70	0.56
1:D:144:GLY:O	7:D:511:HOH:O	2.18	0.56
1:F:157:ASN:CG	1:F:162:ARG:HG3	2.31	0.56
1:F:229:ARG:HA	1:F:258:THR:CG2	2.35	0.56
1:J:178:VAL:HG21	1:J:232:LEU:HD11	1.88	0.56
1:H:252:ARG:NH2	7:H:509:HOH:O	2.39	0.56
1:A:200:LEU:HD13	1:B:209:GLN:HG2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:PHE:CD2	1:C:137:LEU:HD11	2.41	0.55
1:C:310:ILE:HD13	1:E:331:LEU:HD11	1.87	0.55
1:C:111:LYS:O	1:C:181:TYR:OH	2.20	0.55
1:B:129:LEU:CD2	1:B:138:MET:HG3	2.37	0.55
1:B:261:ILE:O	1:B:265:VAL:HG23	2.06	0.55
1:C:315:PHE:HA	1:E:321:LEU:HD22	1.87	0.55
1:H:313:MET:HA	1:J:312:GLY:HA2	1.89	0.55
1:H:319:PRO:HA	1:H:320:GLU:C	2.31	0.55
1:C:225:ILE:HD12	1:C:228:LEU:HB3	1.89	0.55
1:G:109:VAL:O	1:G:110:LEU:HD23	2.06	0.55
1:J:77:GLY:HA3	1:J:87:LEU:HD11	1.87	0.55
1:F:243:ILE:HG13	1:F:246:GLU:HB2	1.87	0.55
1:E:63:ASN:HA	1:E:138:MET:HB3	1.89	0.55
1:F:69:ARG:HB3	1:F:71:ASP:OD1	2.07	0.55
1:A:324:LYS:HE3	1:A:325:TRP:H	1.72	0.55
1:B:86:VAL:HG13	1:B:107:PHE:CD2	2.42	0.55
1:H:333:VAL:HA	1:H:336:VAL:HG12	1.88	0.55
1:C:308:ALA:HB2	1:C:334:MET:HE1	1.87	0.55
1:E:112:MET:HE2	1:E:127:VAL:HG22	1.89	0.55
1:F:167:ASP:HB2	1:F:242:LEU:HD23	1.88	0.55
1:I:311:TYR:HB2	1:J:313:MET:HE2	1.89	0.55
1:G:39:PHE:HE2	1:G:41:GLU:HG2	1.72	0.54
1:A:307:ILE:HA	1:A:310:ILE:HG12	1.87	0.54
1:B:252:ARG:NH2	1:C:100:GLU:HG2	2.21	0.54
1:D:208:VAL:HG13	1:D:276:LEU:HD11	1.88	0.54
1:F:310:ILE:HG23	1:F:311:TYR:CD1	2.42	0.54
1:H:222:ARG:HA	1:H:225:ILE:HG22	1.89	0.54
1:I:63:ASN:ND2	1:I:151:ARG:HH22	2.02	0.54
1:I:110:LEU:HD13	1:I:177:LEU:HD22	1.89	0.54
1:J:174:ILE:HG21	1:J:232:LEU:HD21	1.89	0.54
1:C:62:ILE:HD12	1:C:137:LEU:HD21	1.89	0.54
1:H:284:SER:HB3	1:J:283:VAL:HG11	1.87	0.54
1:A:334:MET:HE1	1:D:310:ILE:HD11	1.90	0.54
1:E:111:LYS:O	1:E:181:TYR:OH	2.19	0.54
1:H:270:ASP:OD2	1:J:215:LYS:HE2	2.07	0.54
1:B:310:ILE:HA	1:B:313:MET:HG3	1.89	0.54
1:D:325:TRP:O	1:D:328:PRO:HD3	2.07	0.54
1:I:61:TRP:HB2	1:I:169:LEU:HD21	1.90	0.54
1:B:195:LEU:HD21	1:B:211:THR:HA	1.88	0.54
1:E:327:TYR:O	1:E:331:LEU:N	2.36	0.54
1:F:301:PHE:O	1:F:302:MET:HB2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:188:ILE:HG23	1:J:214:LEU:HD11	1.90	0.54
1:A:111:LYS:NZ	1:A:126:GLN:OE1	2.41	0.54
1:A:317:TYR:CD1	1:A:317:TYR:N	2.76	0.54
4:A:403:LMT:H3'	4:B:406:LMT:H2'	1.89	0.54
1:C:63:ASN:OD1	1:C:138:MET:HG2	2.07	0.54
1:E:82:ILE:HD11	1:E:130:ILE:HG21	1.89	0.54
1:G:222:ARG:HA	1:G:225:ILE:HG22	1.90	0.54
1:H:192:ILE:HG12	1:H:214:LEU:HD21	1.90	0.54
1:C:228:LEU:O	1:C:231:VAL:HB	2.07	0.54
1:G:200:LEU:HD12	1:G:201:GLU:HG3	1.90	0.54
1:I:328:PRO:HD2	1:I:329:VAL:H	1.72	0.54
1:D:82:ILE:HG13	1:D:105:TYR:CZ	2.42	0.53
1:D:294:LEU:HD13	1:E:295:THR:HA	1.90	0.53
1:E:318:MET:HB3	1:E:320:GLU:N	2.23	0.53
1:F:250:TYR:O	1:F:253:ASP:HB3	2.07	0.53
1:J:230:GLU:O	1:J:234:SER:OG	2.22	0.53
1:A:326:GLY:O	1:A:329:VAL:N	2.40	0.53
1:B:166:ALA:O	1:B:169:LEU:HB3	2.09	0.53
1:C:330:VAL:O	1:C:334:MET:HG2	2.08	0.53
1:D:110:LEU:HD13	1:D:177:LEU:HD22	1.90	0.53
1:G:82:ILE:HG12	1:G:130:ILE:HD13	1.89	0.53
1:F:90:ILE:HD11	1:F:130:ILE:HD11	1.89	0.53
1:H:281:SER:HB3	1:J:279:TYR:CE2	2.43	0.53
1:A:149:PRO:HB3	1:B:11:GLY:HA2	1.91	0.53
1:D:110:LEU:HD11	1:D:174:ILE:HG12	1.91	0.53
1:D:327:TYR:CG	1:D:327:TYR:O	2.61	0.53
1:E:346:LYS:NZ	1:E:347:LYS:HG3	2.23	0.53
1:F:300:ILE:HG13	1:F:301:PHE:N	2.23	0.53
1:F:313:MET:SD	1:G:311:TYR:HB2	2.48	0.53
1:D:206:GLU:HG3	1:D:207:THR:N	2.24	0.53
1:D:212:HIS:NE2	1:E:196:GLU:OE1	2.39	0.53
1:A:195:LEU:HD21	1:A:211:THR:HA	1.91	0.53
1:D:239:VAL:HA	1:D:242:LEU:HD12	1.91	0.53
1:F:168:TYR:OH	1:G:14:PRO:HG2	2.09	0.53
1:H:99:VAL:HG23	1:H:231:VAL:HG22	1.91	0.53
1:J:99:VAL:HG23	1:J:231:VAL:HG22	1.90	0.53
1:J:108:ILE:HD12	1:J:174:ILE:HD11	1.91	0.53
1:B:19:TYR:CZ	1:B:21:GLY:HA3	2.44	0.53
1:F:186:GLU:OE2	1:G:7:SER:HB3	2.09	0.53
1:H:82:ILE:HG13	1:H:105:TYR:CE2	2.43	0.53
1:H:327:TYR:CZ	1:H:331:LEU:HD11	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LEU:HD21	1:C:228:LEU:HD13	1.91	0.52
1:F:293:VAL:HA	1:F:296:ILE:HG12	1.91	0.52
1:G:225:ILE:HD12	1:G:228:LEU:HD23	1.91	0.52
1:I:13:PRO:HG3	1:J:153:ARG:HD3	1.91	0.52
1:J:100:GLU:OE2	7:J:515:HOH:O	2.19	0.52
1:B:324:LYS:C	1:B:326:GLY:H	2.17	0.52
1:I:29:ILE:HG21	1:I:50:VAL:HG11	1.91	0.52
1:D:145:ASP:OD2	1:D:151:ARG:NH2	2.33	0.52
1:F:195:LEU:HD21	1:F:211:THR:HA	1.89	0.52
1:A:310:ILE:HG21	1:B:334:MET:HE1	1.91	0.52
1:D:125:GLU:HG3	1:D:141:GLU:HB2	1.90	0.52
1:E:165:ARG:NH2	1:E:243:ILE:HG21	2.24	0.52
1:I:63:ASN:HD22	1:I:151:ARG:NH2	2.03	0.52
1:I:148:ASP:O	1:I:152:GLU:HG2	2.08	0.52
1:I:328:PRO:HG2	1:I:329:VAL:H	1.74	0.52
1:B:296:ILE:HA	1:B:299:THR:HG22	1.90	0.52
1:B:311:TYR:CE2	1:B:330:VAL:HG21	2.43	0.52
1:B:312:GLY:H	1:B:313:MET:HB2	1.74	0.52
1:F:307:ILE:HD11	1:F:334:MET:SD	2.49	0.52
1:H:310:ILE:HD11	1:J:334:MET:HE1	1.92	0.52
1:J:147:PHE:CZ	1:J:177:LEU:HD12	2.42	0.52
1:B:301:PHE:O	1:B:305:THR:N	2.39	0.52
1:J:316:GLU:HG2	1:J:317:TYR:H	1.74	0.52
1:G:63:ASN:CG	1:G:138:MET:HE3	2.35	0.52
1:I:99:VAL:CG2	1:I:231:VAL:HG13	2.40	0.52
1:J:73:VAL:HG21	1:J:91:LEU:HD21	1.92	0.52
1:B:221:LEU:HG	1:B:225:ILE:HD12	1.91	0.52
1:E:44:THR:HG1	1:E:46:ASP:H	1.58	0.52
1:E:164:LYS:NZ	1:E:246:GLU:HB3	2.24	0.52
1:G:83:HIS:ND1	1:G:84:PRO:HD2	2.25	0.52
1:I:304:LEU:HD11	1:I:338:ALA:HB2	1.92	0.52
1:C:218:LEU:HD21	1:C:268:PHE:HB3	1.90	0.52
1:E:89:ASP:OD2	7:E:516:HOH:O	2.19	0.52
1:I:240:PRO:HB2	1:I:241:PRO:HD3	1.91	0.52
1:I:326:GLY:CA	1:I:327:TYR:CB	2.87	0.52
1:B:27:PHE:HZ	1:B:72:VAL:HG21	1.74	0.51
1:F:105:TYR:HB3	1:F:132:THR:HB	1.91	0.51
1:A:23:TYR:CE2	1:A:142:LYS:HD3	2.45	0.51
1:A:82:ILE:HG12	1:A:130:ILE:HD13	1.93	0.51
1:A:195:LEU:HD11	1:A:210:ARG:HB3	1.92	0.51
1:A:240:PRO:HB2	1:A:241:PRO:HD3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:301:PHE:HE2	1:I:303:PRO:CG	2.14	0.51
5:G:408:PEG:O1	5:G:408:PEG:H32	2.10	0.51
1:D:297:ILE:HG12	1:E:299:THR:OG1	2.10	0.51
1:G:12:LEU:HD13	1:G:16:THR:HG21	1.92	0.51
1:G:307:ILE:HD11	1:G:334:MET:SD	2.50	0.51
1:G:319:PRO:HG2	1:G:322:ARG:O	2.10	0.51
1:I:120:HIS:ND1	1:I:191:GLU:OE2	2.38	0.51
1:I:328:PRO:CG	1:I:329:VAL:N	2.73	0.51
1:A:65:THR:OG1	7:A:516:HOH:O	2.19	0.51
1:I:165:ARG:CZ	1:I:243:ILE:HD12	2.41	0.51
1:A:209:GLN:HG2	1:D:200:LEU:HD13	1.91	0.51
1:C:260:GLN:O	1:C:264:THR:OG1	2.16	0.51
1:D:198:GLU:O	1:D:202:ARG:N	2.43	0.51
1:D:323:TRP:O	1:D:325:TRP:N	2.44	0.51
1:H:295:THR:O	1:H:299:THR:HG23	2.11	0.51
1:B:303:PRO:HG3	1:C:301:PHE:CE2	2.45	0.51
5:B:408:PEG:H41	7:B:526:HOH:O	2.11	0.51
1:F:153:ARG:HD3	1:G:13:PRO:HG3	1.93	0.51
1:G:215:LYS:O	1:G:219:VAL:HG23	2.10	0.51
1:H:239:VAL:HG11	1:H:248:VAL:HG22	1.91	0.51
1:H:336:VAL:O	1:H:340:ILE:HG23	2.11	0.51
1:H:171:TYR:HE1	1:H:254:VAL:HG23	1.76	0.51
1:J:295:THR:O	1:J:299:THR:HG23	2.11	0.51
1:D:109:VAL:O	1:D:110:LEU:HD23	2.11	0.51
1:H:41:GLU:OE1	1:H:155:ARG:NH2	2.44	0.51
1:H:244:GLU:HA	1:H:248:VAL:HG23	1.93	0.51
1:A:320:GLU:OE2	4:A:403:LMT:H1B	2.09	0.51
1:E:83:HIS:CE1	1:E:84:PRO:HD2	2.45	0.51
1:G:113:PHE:HD2	1:G:181:TYR:HE1	1.59	0.51
1:G:330:VAL:O	1:G:334:MET:HG2	2.10	0.51
1:B:323:TRP:NE1	4:B:407:LMT:O6'	2.44	0.50
1:C:110:LEU:HD13	1:C:177:LEU:HD22	1.93	0.50
1:C:233:SER:OG	1:C:237:ARG:NH2	2.43	0.50
1:G:34:TYR:O	1:G:59:PRO:HD2	2.11	0.50
1:G:316:GLU:HG3	1:H:324:LYS:HB3	1.93	0.50
1:I:326:GLY:CA	1:I:328:PRO:CD	2.85	0.50
1:C:86:VAL:HG13	1:C:107:PHE:CE2	2.46	0.50
1:D:327:TYR:HE1	1:E:318:MET:HG3	1.76	0.50
1:F:307:ILE:CD1	1:F:334:MET:CG	2.83	0.50
1:G:146:VAL:HG21	1:G:177:LEU:HA	1.93	0.50
1:A:317:TYR:N	1:A:317:TYR:HD1	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ILE:HG12	1:B:64:ILE:HG12	1.93	0.50
1:I:125:GLU:HG3	1:I:141:GLU:HB2	1.94	0.50
1:I:195:LEU:HD21	1:I:211:THR:HA	1.94	0.50
1:A:14:PRO:HG3	1:D:171:TYR:OH	2.11	0.50
1:B:232:LEU:CD1	1:B:254:VAL:HG12	2.39	0.50
1:E:44:THR:OG1	1:E:45:THR:N	2.45	0.50
1:F:208:VAL:HG12	1:I:278:VAL:HG13	1.93	0.50
1:H:277:ASP:HB3	1:J:276:LEU:HD23	1.93	0.50
1:B:129:LEU:HD23	1:B:138:MET:HG3	1.94	0.50
1:D:167:ASP:OD2	1:D:243:ILE:N	2.31	0.50
1:D:239:VAL:HG11	1:D:248:VAL:HG22	1.94	0.50
1:E:73:VAL:HG21	1:E:91:LEU:HD21	1.93	0.50
1:E:93:VAL:HA	1:E:126:GLN:NE2	2.25	0.50
1:I:320:GLU:C	1:I:322:ARG:N	2.68	0.50
1:J:233:SER:OG	1:J:237:ARG:NH2	2.44	0.50
1:A:227:PRO:O	1:A:230:GLU:N	2.44	0.50
1:D:96:ARG:NH1	1:D:227:PRO:HB3	2.27	0.50
1:E:115:TYR:OH	1:E:120:HIS:HB3	2.12	0.50
1:F:222:ARG:HH11	1:F:222:ARG:CG	2.24	0.50
1:A:110:LEU:HD11	1:A:174:ILE:HG12	1.92	0.50
1:B:244:GLU:HA	1:B:248:VAL:HG23	1.94	0.50
1:C:228:LEU:HA	1:C:231:VAL:HB	1.93	0.50
1:E:29:ILE:HG21	1:E:50:VAL:HG11	1.94	0.50
1:E:51:LEU:N	1:E:52:PRO:HD2	2.26	0.50
1:F:99:VAL:HG22	1:F:108:ILE:HG12	1.94	0.50
1:G:270:ASP:O	1:G:273:SER:OG	2.22	0.50
1:I:46:ASP:O	1:I:49:SER:OG	2.26	0.50
1:I:112:MET:HE2	1:I:127:VAL:CG2	2.41	0.50
1:A:73:VAL:HG21	1:A:91:LEU:HD21	1.93	0.50
1:A:136:VAL:HG11	1:A:173:LEU:HD12	1.94	0.50
1:B:255:TYR:CE2	1:B:259:ILE:HD11	2.46	0.50
1:E:296:ILE:HG22	1:E:345:PHE:CE2	2.47	0.50
1:I:153:ARG:HG2	1:I:158:ARG:HB2	1.94	0.50
1:J:187:LYS:O	1:J:190:ASP:HB2	2.12	0.50
1:E:346:LYS:HZ2	1:E:347:LYS:HG3	1.77	0.50
1:F:315:PHE:HE1	1:G:327:TYR:HD2	1.59	0.50
1:G:229:ARG:HA	1:G:258:THR:HG21	1.94	0.50
1:H:188:ILE:O	1:H:192:ILE:HG13	2.11	0.50
1:B:255:TYR:CZ	1:B:259:ILE:HD11	2.47	0.49
1:D:253:ASP:O	1:D:256:ASP:N	2.44	0.49
1:E:255:TYR:O	1:E:258:THR:HG22	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:VAL:HG23	1:G:231:VAL:HG22	1.93	0.49
1:G:326:GLY:HA2	1:G:329:VAL:HG22	1.93	0.49
1:H:291:MET:HE3	1:J:290:VAL:HG12	1.94	0.49
1:I:73:VAL:HG21	1:I:91:LEU:HD21	1.94	0.49
1:B:34:TYR:O	1:B:58:THR:HB	2.12	0.49
1:C:167:ASP:OD2	1:C:243:ILE:N	2.43	0.49
1:E:336:VAL:O	1:E:340:ILE:HG23	2.12	0.49
1:F:306:PHE:HE1	1:G:304:LEU:HB3	1.71	0.49
1:G:74:GLN:NE2	5:G:409:PEG:H31	2.24	0.49
1:B:83:HIS:ND1	1:B:84:PRO:HD2	2.28	0.49
1:D:167:ASP:OD1	1:D:168:TYR:N	2.44	0.49
1:G:167:ASP:OD2	1:G:243:ILE:HG12	2.12	0.49
1:I:228:LEU:O	1:I:231:VAL:HB	2.12	0.49
1:J:95:GLN:HE22	1:J:98:LYS:HZ3	1.60	0.49
1:F:211:THR:HG21	1:F:276:LEU:HD13	1.94	0.49
1:G:239:VAL:HB	1:G:242:LEU:HB2	1.93	0.49
1:I:34:TYR:CE1	1:I:59:PRO:HB2	2.47	0.49
1:I:328:PRO:CD	1:I:329:VAL:N	2.72	0.49
1:C:88:GLU:HB3	7:C:504:HOH:O	2.11	0.49
1:C:272:VAL:HA	1:C:275:LEU:HD22	1.93	0.49
1:G:315:PHE:CD2	1:H:327:TYR:HA	2.47	0.49
1:A:303:PRO:HG3	1:B:301:PHE:CE2	2.45	0.49
1:E:192:ILE:HG12	1:E:214:LEU:HD21	1.92	0.49
1:G:246:GLU:OE1	5:G:411:PEG:C1	2.60	0.49
1:I:60:THR:HB	1:I:135:CYS:SG	2.52	0.49
1:I:328:PRO:O	1:I:331:LEU:N	2.45	0.49
1:J:195:LEU:O	1:J:199:VAL:HG23	2.12	0.49
1:J:333:VAL:O	1:J:336:VAL:HG12	2.12	0.49
1:A:222:ARG:HG3	1:A:226:TRP:CD1	2.47	0.49
1:B:315:PHE:HD2	1:C:327:TYR:HD1	1.59	0.49
7:B:506:HOH:O	1:C:89:ASP:OD2	2.20	0.49
1:C:165:ARG:NH2	1:C:243:ILE:HG21	2.28	0.49
1:F:257:HIS:O	1:F:260:GLN:N	2.45	0.49
1:G:35:SER:HB3	1:G:58:THR:HG21	1.95	0.49
1:J:230:GLU:HA	1:J:233:SER:HB3	1.95	0.49
1:E:83:HIS:ND1	1:E:84:PRO:HD2	2.28	0.49
1:H:51:LEU:N	1:H:52:PRO:HD2	2.28	0.49
1:H:239:VAL:HG21	1:H:244:GLU:HG3	1.93	0.49
1:J:47:VAL:O	1:J:50:VAL:HG22	2.12	0.49
1:B:300:ILE:O	1:B:304:LEU:HG	2.13	0.49
1:C:116:ASP:O	1:C:120:HIS:HA	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:THR:HG1	1:G:46:ASP:H	1.60	0.49
1:G:239:VAL:HG12	1:G:242:LEU:HD12	1.94	0.49
1:H:120:HIS:HB2	1:H:213:GLN:NE2	2.28	0.49
1:I:295:THR:O	1:I:299:THR:HG22	2.13	0.49
1:J:167:ASP:OD1	1:J:168:TYR:N	2.45	0.49
1:J:192:ILE:HG12	1:J:214:LEU:HD21	1.95	0.49
1:J:303:PRO:HG2	1:J:304:LEU:HD23	1.95	0.49
1:A:204:GLU:HG2	1:A:205:LYS:H	1.77	0.48
1:A:320:GLU:OE2	4:A:403:LMT:C1B	2.60	0.48
1:B:10:LYS:C	1:B:12:LEU:H	2.20	0.48
1:E:83:HIS:CG	1:E:84:PRO:HD2	2.47	0.48
1:C:101:PHE:H	5:C:406:PEG:C4	2.26	0.48
1:C:307:ILE:C	1:C:309:GLY:HA3	2.38	0.48
1:E:328:PRO:O	1:E:332:ALA:N	2.45	0.48
1:G:93:VAL:O	1:G:111:LYS:NZ	2.46	0.48
1:I:85:LEU:HD11	1:J:250:TYR:CD1	2.47	0.48
1:A:190:ASP:O	1:A:194:VAL:HG23	2.14	0.48
1:B:31:VAL:HG11	1:B:53:PHE:CE2	2.48	0.48
1:G:113:PHE:HE2	1:G:224:THR:HG21	1.78	0.48
1:D:51:LEU:N	1:D:52:PRO:HD2	2.28	0.48
1:D:160:ILE:HG22	1:D:164:LYS:HG2	1.96	0.48
1:D:299:THR:HG21	1:D:345:PHE:CZ	2.47	0.48
1:G:171:TYR:HE1	1:G:254:VAL:HG23	1.78	0.48
1:H:236:TYR:CD1	1:H:252:ARG:HB2	2.49	0.48
4:A:403:LMT:C3'	4:B:406:LMT:C3'	2.92	0.48
1:C:277:ASP:HB3	1:E:276:LEU:HD23	1.94	0.48
1:F:301:PHE:O	1:F:303:PRO:HD2	2.13	0.48
1:F:303:PRO:HG2	1:F:304:LEU:H	1.79	0.48
1:J:95:GLN:HE22	1:J:98:LYS:NZ	2.12	0.48
1:B:319:PRO:HA	1:B:320:GLU:C	2.38	0.48
1:C:24:ARG:HA	1:C:68:HIS:CD2	2.49	0.48
1:D:288:ASN:HD21	1:D:292:LYS:HE3	1.79	0.48
1:A:186:GLU:OE2	1:B:7:SER:HB3	2.12	0.48
1:J:330:VAL:O	1:J:334:MET:HG3	2.14	0.48
1:F:27:PHE:CD2	1:F:45:THR:HG22	2.48	0.48
1:I:36:ILE:HD13	1:I:163:LYS:HD2	1.95	0.48
1:I:330:VAL:HG13	1:J:313:MET:HE1	1.96	0.48
1:B:192:ILE:HG12	1:B:214:LEU:HD21	1.95	0.48
1:J:324:LYS:O	1:J:326:GLY:N	2.47	0.48
4:A:403:LMT:C3B	4:B:406:LMT:H6D	2.28	0.48
1:D:51:LEU:HD13	1:D:79:PHE:CD2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:TRP:O	1:E:325:TRP:N	2.47	0.48
1:A:129:LEU:HD13	1:A:170:LEU:HD12	1.96	0.47
1:D:128:SER:HB2	1:D:139:PHE:HB2	1.95	0.47
1:I:23:TYR:CD2	1:I:142:LYS:HD3	2.49	0.47
1:D:299:THR:HG21	1:D:345:PHE:CE2	2.49	0.47
1:F:336:VAL:O	1:F:340:ILE:HG23	2.15	0.47
1:B:51:LEU:HB3	1:B:79:PHE:CE2	2.49	0.47
1:C:12:LEU:HD22	1:C:16:THR:HG21	1.96	0.47
1:D:317:TYR:CG	1:D:318:MET:N	2.83	0.47
1:G:227:PRO:HA	7:G:521:HOH:O	2.13	0.47
1:H:51:LEU:HD22	1:H:79:PHE:CD2	2.50	0.47
1:J:292:LYS:HE2	1:J:348:LYS:O	2.14	0.47
1:A:5:ARG:O	1:A:5:ARG:NE	2.46	0.47
1:C:31:VAL:HG11	1:C:53:PHE:CE2	2.50	0.47
1:E:218:LEU:HD21	1:E:268:PHE:HB3	1.96	0.47
1:J:325:TRP:C	1:J:328:PRO:HD2	2.39	0.47
1:A:112:MET:HG3	1:A:177:LEU:HD11	1.97	0.47
1:D:327:TYR:HB2	1:D:330:VAL:HB	1.97	0.47
1:G:147:PHE:O	1:G:150:VAL:HB	2.15	0.47
1:H:271:ILE:HD13	1:J:216:ARG:NH1	2.30	0.47
1:I:68:HIS:CE1	1:I:69:ARG:HG2	2.50	0.47
1:I:80:PHE:CD2	1:I:137:LEU:HD11	2.50	0.47
1:I:239:VAL:HG11	1:I:248:VAL:HG22	1.97	0.47
1:I:314:ASN:O	1:I:316:GLU:N	2.45	0.47
1:C:167:ASP:HB2	1:C:242:LEU:HD23	1.97	0.47
1:C:319:PRO:CB	1:C:322:ARG:HB3	2.44	0.47
1:E:77:GLY:HA3	1:E:87:LEU:HD21	1.96	0.47
1:F:160:ILE:HG13	1:F:164:LYS:HG3	1.97	0.47
1:G:258:THR:HA	1:G:261:ILE:HD12	1.97	0.47
1:B:95:GLN:HG2	1:B:96:ARG:N	2.29	0.47
1:B:240:PRO:HB2	1:B:241:PRO:HD3	1.97	0.47
1:B:323:TRP:CE2	4:B:407:LMT:H6E	2.50	0.47
1:C:17:LEU:HG	1:C:91:LEU:HD12	1.97	0.47
1:C:196:GLU:OE1	1:E:212:HIS:NE2	2.46	0.47
1:C:236:TYR:CE1	1:C:252:ARG:HB2	2.50	0.47
1:F:311:TYR:CE2	1:F:330:VAL:HG21	2.40	0.47
1:G:308:ALA:HB2	1:G:334:MET:HE1	1.97	0.47
1:H:154:ILE:HG12	1:H:161:ILE:HD13	1.97	0.47
1:H:316:GLU:O	1:H:319:PRO:HD2	2.13	0.47
1:I:170:LEU:O	1:I:174:ILE:HG13	2.14	0.47
1:I:330:VAL:HG12	1:I:331:LEU:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:291:MET:HE3	1:J:291:MET:HB3	1.64	0.47
1:A:210:ARG:NH2	7:A:513:HOH:O	2.46	0.47
1:C:41:GLU:CD	1:C:155:ARG:HE	2.23	0.47
1:C:51:LEU:HD22	1:C:79:PHE:CG	2.50	0.47
1:C:101:PHE:H	5:C:406:PEG:H42	1.78	0.47
1:E:229:ARG:HA	1:E:258:THR:CG2	2.44	0.47
1:G:285:ASN:O	1:G:288:ASN:HB3	2.15	0.47
1:B:272:VAL:HA	1:B:275:LEU:HD22	1.97	0.47
1:D:19:TYR:CZ	1:D:21:GLY:HA3	2.50	0.47
1:F:13:PRO:HG3	1:I:153:ARG:CD	2.41	0.47
1:I:307:ILE:HG13	1:I:334:MET:HE2	1.97	0.47
1:J:39:PHE:HE2	1:J:41:GLU:HG2	1.80	0.47
1:A:32:MET:HE2	1:A:32:MET:HB3	1.67	0.47
1:C:288:ASN:ND2	1:C:292:LYS:HE3	2.30	0.47
1:E:232:LEU:HD22	1:E:254:VAL:CG1	2.44	0.47
1:G:182:PHE:O	1:G:186:GLU:HG3	2.15	0.47
1:A:111:LYS:O	1:A:177:LEU:HD21	2.15	0.46
1:C:62:ILE:HB	1:C:137:LEU:HD23	1.96	0.46
1:E:140:GLN:HE21	1:E:140:GLN:HB3	1.55	0.46
1:G:230:GLU:HB2	7:G:521:HOH:O	2.14	0.46
1:H:12:LEU:HD13	1:H:16:THR:HG21	1.97	0.46
1:H:310:ILE:HA	1:H:313:MET:SD	2.55	0.46
1:I:99:VAL:HG13	1:I:108:ILE:HG12	1.97	0.46
1:J:154:ILE:HG12	1:J:161:ILE:HD13	1.97	0.46
1:A:34:TYR:O	1:A:59:PRO:HD2	2.15	0.46
1:B:225:ILE:HD13	1:B:265:VAL:HG21	1.97	0.46
1:C:302:MET:HE2	1:C:302:MET:HB3	1.72	0.46
1:C:316:GLU:HG2	1:E:321:LEU:O	2.14	0.46
1:E:30:GLU:HG3	1:E:43:LYS:HG2	1.96	0.46
1:E:291:MET:HE3	1:E:291:MET:HB3	1.57	0.46
1:E:345:PHE:O	1:E:349:LYS:HA	2.15	0.46
1:G:62:ILE:HB	1:G:137:LEU:HD23	1.97	0.46
1:H:110:LEU:HD22	1:H:228:LEU:HD13	1.98	0.46
1:I:319:PRO:C	1:I:320:GLU:HG3	2.41	0.46
1:A:120:HIS:ND1	1:A:191:GLU:OE2	2.47	0.46
1:B:286:LYS:O	1:B:290:VAL:N	2.48	0.46
1:E:235:LEU:HD12	1:E:242:LEU:HD11	1.97	0.46
1:F:188:ILE:HG21	1:F:218:LEU:HD11	1.96	0.46
1:J:227:PRO:O	1:J:231:VAL:N	2.41	0.46
1:A:297:ILE:HG21	1:D:299:THR:HA	1.96	0.46
1:D:303:PRO:O	1:D:306:PHE:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:LYS:O	1:F:219:VAL:HG23	2.16	0.46
1:G:32:MET:HG2	1:G:41:GLU:HB2	1.96	0.46
1:I:328:PRO:HG2	1:I:329:VAL:N	2.30	0.46
1:A:323:TRP:HD1	1:A:324:LYS:O	1.98	0.46
1:D:116:ASP:O	1:D:120:HIS:HA	2.15	0.46
1:D:209:GLN:HE21	1:E:200:LEU:HD13	1.79	0.46
1:E:110:LEU:HD13	1:E:177:LEU:HD22	1.98	0.46
1:I:307:ILE:HA	1:I:310:ILE:HG22	1.97	0.46
1:J:86:VAL:HG13	1:J:107:PHE:CE2	2.51	0.46
1:C:225:ILE:HG12	1:C:261:ILE:HG22	1.97	0.46
1:D:304:LEU:HB3	1:E:306:PHE:CE1	2.51	0.46
1:F:82:ILE:HD11	1:F:130:ILE:HG21	1.97	0.46
1:A:69:ARG:HB3	1:A:71:ASP:OD1	2.16	0.46
1:D:320:GLU:H	1:D:322:ARG:N	2.13	0.46
1:F:271:ILE:HD11	1:G:216:ARG:HG2	1.97	0.46
1:G:65:THR:HG21	1:G:143:ILE:HA	1.98	0.46
1:I:115:TYR:OH	1:I:120:HIS:HB3	2.16	0.46
1:B:199:VAL:HG11	1:B:278:VAL:HB	1.98	0.46
1:C:232:LEU:HD13	1:C:254:VAL:CG1	2.46	0.46
1:D:300:ILE:O	1:D:303:PRO:HD2	2.15	0.46
1:E:113:PHE:HE2	1:E:224:THR:HG21	1.81	0.46
1:F:67:ILE:HG21	1:F:139:PHE:HB3	1.98	0.46
1:H:82:ILE:HG22	1:H:87:LEU:HG	1.98	0.46
1:I:89:ASP:OD2	1:I:98:LYS:NZ	2.32	0.46
1:A:145:ASP:HB2	1:A:147:PHE:HD2	1.81	0.46
1:E:131:LEU:HD22	1:E:170:LEU:HD22	1.98	0.46
1:E:164:LYS:HZ1	1:E:246:GLU:HB3	1.81	0.46
1:F:276:LEU:HD12	1:F:276:LEU:HA	1.56	0.46
1:I:65:THR:HG21	1:I:143:ILE:HA	1.98	0.46
1:I:314:ASN:HD21	1:J:314:ASN:ND2	2.14	0.46
1:J:185:LEU:HD11	1:J:261:ILE:HG23	1.98	0.46
1:A:165:ARG:NH2	1:A:243:ILE:HG21	2.31	0.46
1:B:324:LYS:CG	1:B:325:TRP:H	2.29	0.46
1:C:100:GLU:HB3	1:C:102:PHE:HE1	1.79	0.46
1:D:327:TYR:HB3	1:E:315:PHE:CD2	2.51	0.46
1:G:138:MET:SD	1:G:147:PHE:CE2	3.09	0.46
1:J:160:ILE:HG12	3:J:404:CL:CL	2.53	0.46
1:A:291:MET:SD	1:D:291:MET:HE1	2.57	0.45
1:B:325:TRP:O	1:B:329:VAL:HB	2.15	0.45
1:D:27:PHE:CD2	1:D:45:THR:HG22	2.51	0.45
1:E:22:LYS:HE3	1:E:23:TYR:OH	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:VAL:O	1:E:111:LYS:NZ	2.48	0.45
1:E:174:ILE:HG21	1:E:232:LEU:HD21	1.99	0.45
1:G:23:TYR:CE2	1:G:142:LYS:HD3	2.51	0.45
1:G:110:LEU:HD12	1:G:177:LEU:HD13	1.97	0.45
5:G:408:PEG:H22	1:H:331:LEU:HD22	1.98	0.45
1:H:148:ASP:O	1:H:152:GLU:HG2	2.17	0.45
1:A:280:LEU:HD23	1:B:280:LEU:HD21	1.97	0.45
1:A:302:MET:HE2	1:A:302:MET:HB3	1.75	0.45
4:A:403:LMT:H3'	4:B:406:LMT:C2'	2.46	0.45
1:B:30:GLU:HG3	1:B:43:LYS:HG2	1.98	0.45
1:C:231:VAL:HG12	1:C:232:LEU:HG	1.97	0.45
1:C:239:VAL:HA	1:C:242:LEU:HD12	1.98	0.45
1:F:200:LEU:HD13	1:G:209:GLN:HE21	1.81	0.45
1:F:240:PRO:HB2	1:F:241:PRO:CD	2.46	0.45
1:G:337:ILE:HA	1:G:340:ILE:HG12	1.99	0.45
1:D:102:PHE:CD2	1:D:105:TYR:CE2	3.05	0.45
1:F:73:VAL:HG21	1:F:91:LEU:HD21	1.97	0.45
1:H:153:ARG:HG3	1:H:153:ARG:HH11	1.80	0.45
1:I:225:ILE:HG13	1:I:262:ALA:HB2	1.98	0.45
1:J:274:GLY:O	1:J:278:VAL:HG23	2.17	0.45
1:C:36:ILE:HD13	1:C:163:LYS:HG3	1.98	0.45
1:C:120:HIS:CD2	1:C:120:HIS:H	2.34	0.45
1:D:276:LEU:HD12	1:D:276:LEU:HA	1.74	0.45
1:D:296:ILE:HA	1:D:299:THR:HG22	1.98	0.45
1:E:22:LYS:NZ	1:E:123:GLU:OE2	2.38	0.45
1:H:99:VAL:CG2	1:H:231:VAL:HG13	2.47	0.45
1:E:228:LEU:O	1:E:231:VAL:HB	2.17	0.45
1:I:23:TYR:CE2	1:I:142:LYS:HD3	2.51	0.45
1:J:221:LEU:HA	1:J:221:LEU:HD12	1.61	0.45
1:A:240:PRO:HB2	1:A:241:PRO:CD	2.47	0.45
1:B:87:LEU:HA	1:B:87:LEU:HD23	1.73	0.45
1:B:299:THR:OG1	1:C:297:ILE:HG12	2.16	0.45
1:E:131:LEU:HD12	1:E:136:VAL:HG22	1.99	0.45
1:E:232:LEU:HD22	1:E:254:VAL:HG12	1.98	0.45
1:G:9:LYS:O	1:G:9:LYS:HG3	2.16	0.45
1:I:298:ALA:HA	1:J:302:MET:HE2	1.99	0.45
1:A:276:LEU:HD12	1:A:276:LEU:HA	1.85	0.45
1:B:51:LEU:HD13	1:B:79:PHE:CG	2.51	0.45
1:D:275:LEU:HD12	1:D:275:LEU:HA	1.70	0.45
1:F:113:PHE:HB2	1:F:184:LEU:HD22	1.97	0.45
1:H:153:ARG:HD3	1:J:13:PRO:HG3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:56:SER:OG	1:I:58:THR:O	2.34	0.45
1:J:195:LEU:HD21	1:J:211:THR:HA	1.99	0.45
1:C:235:LEU:HD12	1:C:235:LEU:HA	1.86	0.45
1:D:296:ILE:HG13	1:D:297:ILE:HD12	1.98	0.45
1:I:328:PRO:C	1:I:330:VAL:N	2.73	0.45
1:A:87:LEU:HD23	1:A:87:LEU:HA	1.76	0.45
1:B:16:THR:HG22	1:B:18:VAL:HG23	1.99	0.45
1:E:51:LEU:HB3	1:E:79:PHE:CE2	2.52	0.45
1:G:171:TYR:CZ	1:G:250:TYR:HB3	2.52	0.45
1:H:128:SER:HB2	1:H:139:PHE:HB2	1.99	0.45
1:B:160:ILE:HG12	3:B:404:CL:CL	2.54	0.45
1:B:295:THR:O	1:B:299:THR:HG22	2.17	0.45
1:C:337:ILE:HA	1:C:340:ILE:HG12	1.99	0.45
1:F:216:ARG:HG2	1:I:271:ILE:HG12	1.97	0.45
1:G:291:MET:HB3	1:G:291:MET:HE3	1.54	0.45
1:H:140:GLN:HE22	1:H:145:ASP:HB3	1.82	0.45
1:H:185:LEU:HD23	1:H:185:LEU:HA	1.70	0.45
1:J:218:LEU:HD12	1:J:218:LEU:HA	1.74	0.45
1:B:43:LYS:NZ	5:B:410:PEG:H22	2.32	0.44
1:C:138:MET:HE1	1:C:147:PHE:CD2	2.53	0.44
1:D:23:TYR:CE2	1:D:142:LYS:HD3	2.52	0.44
1:D:225:ILE:HD13	1:D:265:VAL:HG21	1.97	0.44
1:D:295:THR:O	1:D:299:THR:HG22	2.16	0.44
1:E:48:GLU:HA	1:E:51:LEU:HD12	1.99	0.44
1:H:23:TYR:CE2	1:H:142:LYS:HD3	2.51	0.44
1:I:327:TYR:O	1:I:327:TYR:CD2	2.70	0.44
1:J:339:VAL:O	1:J:342:VAL:HB	2.17	0.44
1:B:228:LEU:HD12	1:B:228:LEU:O	2.16	0.44
1:B:312:GLY:H	1:B:313:MET:CB	2.30	0.44
1:C:34:TYR:CE2	1:C:154:ILE:HD13	2.53	0.44
1:D:241:PRO:HA	7:D:522:HOH:O	2.17	0.44
1:D:311:TYR:CE1	1:D:318:MET:HE1	2.53	0.44
1:F:99:VAL:HG23	1:F:231:VAL:HG22	1.99	0.44
1:F:307:ILE:CD1	1:F:334:MET:HG3	2.47	0.44
1:H:240:PRO:HB2	1:H:241:PRO:HD3	1.99	0.44
1:I:307:ILE:HD11	1:I:334:MET:CE	2.47	0.44
1:J:112:MET:HE2	1:J:127:VAL:CG2	2.47	0.44
1:B:16:THR:O	1:B:88:GLU:HG3	2.16	0.44
1:B:71:ASP:OD1	1:B:71:ASP:N	2.47	0.44
1:B:252:ARG:CZ	1:C:100:GLU:HG2	2.48	0.44
1:G:39:PHE:CZ	1:G:155:ARG:HG2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:337:ILE:HA	1:I:340:ILE:HG12	2.00	0.44
1:A:17:LEU:HD23	1:A:74:GLN:HB2	1.99	0.44
4:A:403:LMT:H1'	4:B:406:LMT:H32	1.99	0.44
4:A:403:LMT:C2'	4:B:406:LMT:O3'	2.65	0.44
1:B:103:GLU:HG2	7:B:508:HOH:O	2.16	0.44
1:B:318:MET:HE2	1:B:321:LEU:HD21	2.00	0.44
1:E:218:LEU:HD12	1:E:218:LEU:HA	1.74	0.44
1:H:167:ASP:HB2	1:H:242:LEU:HD23	1.99	0.44
1:H:199:VAL:HG13	1:H:279:TYR:HB2	1.99	0.44
1:J:261:ILE:O	1:J:265:VAL:HG23	2.18	0.44
1:A:22:LYS:HG3	1:A:23:TYR:CD1	2.53	0.44
1:A:301:PHE:CE2	1:D:303:PRO:HG3	2.52	0.44
1:D:288:ASN:ND2	1:D:292:LYS:HE3	2.32	0.44
1:E:16:THR:O	1:E:88:GLU:HG3	2.17	0.44
1:G:55:ASP:HA	7:G:527:HOH:O	2.18	0.44
1:G:157:ASN:ND2	1:G:162:ARG:HG3	2.32	0.44
1:G:236:TYR:CE1	1:G:252:ARG:HB2	2.53	0.44
1:G:296:ILE:HB	1:G:345:PHE:CE2	2.53	0.44
1:A:272:VAL:HA	1:A:275:LEU:HD22	2.00	0.44
1:B:77:GLY:HA3	1:B:87:LEU:HD11	1.99	0.44
1:B:248:VAL:N	1:B:249:PRO:HD2	2.33	0.44
1:D:330:VAL:HG12	1:D:334:MET:HE3	1.99	0.44
1:F:170:LEU:O	1:F:174:ILE:HG13	2.17	0.44
1:G:307:ILE:HA	1:G:310:ILE:HG12	1.99	0.44
1:H:185:LEU:HD23	1:H:188:ILE:HD12	1.99	0.44
1:I:222:ARG:HA	1:I:225:ILE:HG22	1.99	0.44
1:I:331:LEU:HA	1:I:331:LEU:HD23	1.74	0.44
1:A:221:LEU:HD12	1:A:221:LEU:HA	1.70	0.44
1:C:292:LYS:O	1:C:296:ILE:HG23	2.18	0.44
1:C:306:PHE:CE1	1:E:304:LEU:HD23	2.53	0.44
1:D:33:ASN:ND2	1:D:60:THR:OG1	2.50	0.44
1:D:298:ALA:O	1:D:302:MET:HB2	2.17	0.44
1:D:322:ARG:O	1:D:323:TRP:HB2	2.16	0.44
1:D:337:ILE:O	1:D:341:MET:HG2	2.17	0.44
1:E:185:LEU:HD23	1:E:185:LEU:HA	1.72	0.44
1:E:240:PRO:HB2	1:E:241:PRO:HD3	1.99	0.44
1:I:99:VAL:HG23	1:I:231:VAL:HG22	1.99	0.44
1:J:148:ASP:N	1:J:149:PRO:HD2	2.33	0.44
1:J:272:VAL:HA	1:J:275:LEU:HD22	2.00	0.44
1:C:34:TYR:O	1:C:58:THR:HB	2.17	0.44
1:C:240:PRO:HB2	1:C:241:PRO:HD3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:PHE:CE2	1:E:303:PRO:HG3	2.53	0.44
1:E:47:VAL:O	1:E:51:LEU:HG	2.18	0.44
1:F:222:ARG:HD2	1:F:226:TRP:HE1	1.83	0.44
1:H:119:LEU:H	1:H:119:LEU:HG	1.56	0.44
1:H:311:TYR:CD2	1:H:330:VAL:HG21	2.53	0.44
1:J:169:LEU:O	1:J:173:LEU:HG	2.17	0.44
1:J:345:PHE:O	1:J:348:LYS:HD3	2.18	0.44
1:A:225:ILE:O	1:A:228:LEU:HB3	2.17	0.44
1:B:55:ASP:HB3	5:B:411:PEG:H31	2.00	0.44
1:B:323:TRP:CZ3	1:B:325:TRP:HB2	2.53	0.44
1:G:206:GLU:HG3	1:G:207:THR:N	2.33	0.44
1:H:32:MET:HE3	1:H:41:GLU:HB3	2.00	0.44
1:H:214:LEU:HD23	1:H:272:VAL:HG21	1.99	0.44
1:C:125:GLU:HG3	1:C:141:GLU:HB2	2.00	0.43
1:I:307:ILE:HD11	1:I:334:MET:HE3	1.99	0.43
1:A:148:ASP:N	1:A:149:PRO:HD2	2.33	0.43
1:E:339:VAL:O	1:E:343:VAL:N	2.41	0.43
1:G:105:TYR:HB3	1:G:132:THR:HB	2.00	0.43
1:G:318:MET:SD	1:G:318:MET:N	2.92	0.43
1:H:15:GLY:O	1:H:17:LEU:HD13	2.18	0.43
1:H:82:ILE:HA	1:H:105:TYR:CE2	2.53	0.43
1:H:302:MET:HE2	1:J:301:PHE:HB2	2.00	0.43
1:J:100:GLU:HB3	1:J:102:PHE:HE1	1.84	0.43
1:J:244:GLU:HA	1:J:248:VAL:HG23	1.99	0.43
1:J:301:PHE:HA	1:J:304:LEU:HB2	1.99	0.43
1:B:6:LEU:HD13	1:B:20:THR:O	2.18	0.43
1:B:86:VAL:HG13	1:B:107:PHE:CG	2.53	0.43
1:B:113:PHE:CE1	1:B:124:SER:HB3	2.53	0.43
1:B:245:LYS:HD3	1:B:245:LYS:HA	1.63	0.43
1:C:252:ARG:O	1:C:252:ARG:HG2	2.18	0.43
1:C:296:ILE:HG22	1:C:345:PHE:CE2	2.53	0.43
1:E:257:HIS:O	1:E:261:ILE:HG13	2.19	0.43
1:F:307:ILE:CG1	1:F:334:MET:CE	2.97	0.43
1:G:222:ARG:HD3	1:G:269:ARG:CD	2.48	0.43
1:I:317:TYR:HD1	1:I:317:TYR:O	2.02	0.43
1:A:102:PHE:HD2	1:A:105:TYR:CZ	2.36	0.43
1:A:160:ILE:HG22	1:A:164:LYS:HG2	2.00	0.43
5:C:406:PEG:H12	5:C:406:PEG:H32	1.57	0.43
1:F:302:MET:HG3	1:I:302:MET:HE1	2.00	0.43
1:G:239:VAL:HG11	1:G:248:VAL:HG22	2.00	0.43
1:I:313:MET:HE2	1:I:313:MET:HB2	1.94	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:148:ASP:O	1:J:152:GLU:HG2	2.18	0.43
1:A:314:ASN:O	1:B:321:LEU:HD22	2.19	0.43
3:A:402:CL:CL	1:B:14:PRO:HD2	2.56	0.43
1:C:347:LYS:HE3	1:C:348:LYS:HB3	1.99	0.43
1:F:302:MET:CG	1:I:302:MET:HE3	2.48	0.43
1:H:226:TRP:CE2	1:H:229:ARG:NH2	2.87	0.43
1:I:247:THR:C	1:I:249:PRO:HD2	2.43	0.43
1:J:110:LEU:CD2	1:J:228:LEU:HD13	2.48	0.43
1:I:108:ILE:HD12	1:I:174:ILE:HD11	2.01	0.43
1:J:180:ASP:HB2	5:J:405:PEG:H41	2.00	0.43
1:A:95:GLN:HE22	1:A:98:LYS:CE	2.32	0.43
1:D:122:LEU:HD21	1:D:220:GLU:CD	2.44	0.43
1:F:178:VAL:HG21	1:F:254:VAL:CG1	2.48	0.43
1:G:51:LEU:HB3	1:G:79:PHE:CE2	2.54	0.43
1:G:260:GLN:OE1	1:H:95:GLN:HA	2.19	0.43
1:I:31:VAL:HG11	1:I:53:PHE:CE2	2.54	0.43
1:J:225:ILE:O	1:J:228:LEU:HB3	2.19	0.43
1:B:12:LEU:HA	1:B:13:PRO:HD3	1.91	0.43
1:B:23:TYR:CZ	1:B:142:LYS:HD3	2.54	0.43
1:B:297:ILE:HD12	1:B:297:ILE:HA	1.85	0.43
1:D:249:PRO:O	1:D:252:ARG:HB3	2.18	0.43
1:F:184:LEU:HD21	1:F:221:LEU:HD11	2.00	0.43
1:G:208:VAL:HG13	1:G:276:LEU:HD11	2.00	0.43
1:H:337:ILE:HA	1:H:340:ILE:HG12	2.01	0.43
1:I:200:LEU:HD12	1:I:201:GLU:HG3	2.01	0.43
1:I:218:LEU:HD12	1:I:218:LEU:HA	1.75	0.43
1:I:291:MET:HE3	1:I:291:MET:HB3	1.57	0.43
1:I:293:VAL:HA	1:I:296:ILE:HG12	2.00	0.43
1:A:99:VAL:HG13	1:A:108:ILE:HG12	2.01	0.43
1:A:233:SER:HB2	1:A:255:TYR:CE1	2.54	0.43
1:D:253:ASP:O	1:D:254:VAL:C	2.61	0.43
1:F:82:ILE:HG12	1:F:130:ILE:HD13	2.00	0.43
1:I:276:LEU:HA	1:I:276:LEU:HD12	1.59	0.43
1:J:185:LEU:HD13	1:J:264:THR:CG2	2.48	0.43
1:A:316:GLU:HA	1:A:317:TYR:HA	1.71	0.43
1:C:39:PHE:CZ	1:C:155:ARG:HA	2.54	0.43
1:D:337:ILE:HA	1:D:340:ILE:HG12	2.01	0.43
1:E:115:TYR:HH	1:E:120:HIS:HB3	1.84	0.43
1:F:233:SER:HB2	1:F:255:TYR:CE1	2.54	0.43
1:G:83:HIS:HD2	1:G:85:LEU:HB2	1.84	0.43
1:H:19:TYR:CE1	1:H:21:GLY:HA3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:LYS:HB2	1:I:12:LEU:HD12	2.00	0.43
1:I:316:GLU:CD	1:I:318:MET:HE3	2.44	0.43
1:J:111:LYS:O	1:J:177:LEU:HD21	2.19	0.43
1:A:324:LYS:CE	1:A:325:TRP:H	2.30	0.42
4:A:403:LMT:H12	4:B:406:LMT:H52	1.98	0.42
1:B:299:THR:HA	1:C:297:ILE:HG21	2.01	0.42
1:D:202:ARG:HA	1:D:203:PRO:HD3	1.82	0.42
1:E:51:LEU:O	1:E:79:PHE:HE2	2.02	0.42
1:E:202:ARG:HA	1:E:203:PRO:HD3	1.82	0.42
1:F:301:PHE:HB2	1:I:302:MET:HE2	2.01	0.42
1:H:89:ASP:OD1	7:H:502:HOH:O	2.21	0.42
1:I:100:GLU:HB3	1:I:102:PHE:CE1	2.53	0.42
1:J:41:GLU:OE2	1:J:155:ARG:NE	2.47	0.42
1:A:35:SER:HB3	1:A:58:THR:HG21	2.02	0.42
1:A:163:LYS:HD2	1:A:163:LYS:N	2.34	0.42
1:B:233:SER:HB2	1:B:255:TYR:CE1	2.54	0.42
1:C:41:GLU:OE2	1:C:155:ARG:NE	2.52	0.42
1:D:143:ILE:HD12	1:D:144:GLY:H	1.84	0.42
1:E:243:ILE:HG13	1:E:246:GLU:HB2	2.00	0.42
1:F:303:PRO:HG2	1:F:304:LEU:N	2.34	0.42
1:G:148:ASP:N	1:G:149:PRO:HD2	2.34	0.42
1:G:221:LEU:HD23	1:G:265:VAL:CG2	2.49	0.42
1:H:105:TYR:CB	1:H:132:THR:HB	2.46	0.42
1:B:129:LEU:HD21	1:B:138:MET:HG3	2.01	0.42
1:B:218:LEU:HD21	1:B:268:PHE:HB3	2.01	0.42
1:C:304:LEU:HD11	1:C:338:ALA:HB2	2.01	0.42
1:D:115:TYR:HE2	1:D:191:GLU:HG3	1.83	0.42
1:E:107:PHE:C	1:E:108:ILE:HG13	2.44	0.42
1:F:9:LYS:HB2	1:F:9:LYS:HE3	1.83	0.42
1:G:91:LEU:HA	1:G:91:LEU:HD23	1.71	0.42
1:I:94:HIS:O	1:J:260:GLN:NE2	2.53	0.42
1:C:339:VAL:O	1:C:343:VAL:HG23	2.19	0.42
1:H:103:GLU:H	1:H:103:GLU:HG2	1.59	0.42
1:H:115:TYR:OH	1:H:120:HIS:HB3	2.19	0.42
1:H:198:GLU:O	1:H:202:ARG:N	2.52	0.42
1:H:298:ALA:O	1:H:302:MET:HB2	2.19	0.42
1:J:347:LYS:HD3	1:J:349:LYS:HG3	2.01	0.42
1:C:12:LEU:HA	1:C:13:PRO:HD3	1.89	0.42
1:C:221:LEU:O	1:C:225:ILE:HG22	2.20	0.42
1:E:198:GLU:O	1:E:202:ARG:N	2.52	0.42
1:E:340:ILE:HA	1:E:343:VAL:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:LEU:N	1:F:52:PRO:HD2	2.34	0.42
1:F:111:LYS:HB2	1:F:224:THR:HG21	2.02	0.42
1:F:153:ARG:CD	1:G:13:PRO:HG3	2.49	0.42
1:G:199:VAL:HG12	1:G:278:VAL:HG12	2.02	0.42
1:H:232:LEU:HD13	1:H:254:VAL:HG12	2.02	0.42
1:I:80:PHE:CE2	1:I:137:LEU:HD21	2.55	0.42
1:I:328:PRO:O	1:I:332:ALA:N	2.53	0.42
1:A:295:THR:O	1:A:299:THR:N	2.42	0.42
1:A:315:PHE:HD2	1:B:321:LEU:HA	1.85	0.42
1:B:269:ARG:HB3	1:B:269:ARG:NH2	2.35	0.42
4:B:407:LMT:H31	4:B:407:LMT:H61	1.68	0.42
1:C:61:TRP:CZ3	1:C:151:ARG:HG2	2.55	0.42
1:D:83:HIS:HA	1:D:84:PRO:HD3	1.96	0.42
1:F:235:LEU:HD12	1:F:235:LEU:HA	1.96	0.42
1:I:34:TYR:O	1:I:59:PRO:HD2	2.19	0.42
1:C:276:LEU:HD12	1:C:276:LEU:HA	1.88	0.42
1:E:67:ILE:HG23	1:E:140:GLN:O	2.19	0.42
1:E:212:HIS:O	1:E:216:ARG:HG3	2.18	0.42
1:F:86:VAL:O	1:F:90:ILE:HG13	2.20	0.42
1:G:78:GLU:OE1	7:G:525:HOH:O	2.21	0.42
1:J:17:LEU:HD23	1:J:74:GLN:HB2	2.01	0.42
1:J:240:PRO:HB2	1:J:241:PRO:HD3	2.00	0.42
1:J:300:ILE:HG13	1:J:301:PHE:CD1	2.55	0.42
1:A:167:ASP:N	1:A:167:ASP:OD1	2.52	0.42
1:C:19:TYR:OH	1:C:141:GLU:OE1	2.32	0.42
1:C:181:TYR:N	1:C:181:TYR:CD1	2.88	0.42
1:C:225:ILE:O	1:C:228:LEU:HB3	2.19	0.42
1:C:291:MET:HE3	1:C:291:MET:HB3	1.82	0.42
1:D:272:VAL:O	1:D:275:LEU:HB2	2.20	0.42
1:E:306:PHE:O	1:E:310:ILE:HG12	2.19	0.42
1:G:153:ARG:HA	1:G:158:ARG:HB2	2.00	0.42
1:I:296:ILE:HG13	1:I:297:ILE:HD12	2.01	0.42
1:J:232:LEU:HD13	1:J:254:VAL:O	2.20	0.42
1:J:321:LEU:C	1:J:323:TRP:H	2.28	0.42
1:C:316:GLU:HG2	1:E:321:LEU:C	2.45	0.42
1:H:300:ILE:HG13	1:H:301:PHE:CD1	2.54	0.42
1:J:125:GLU:OE1	1:J:141:GLU:N	2.52	0.42
1:J:185:LEU:HD13	1:J:264:THR:HG21	2.01	0.42
1:B:55:ASP:OD1	7:B:519:HOH:O	2.21	0.42
1:C:275:LEU:HD12	1:C:275:LEU:HA	1.75	0.42
1:F:312:GLY:CA	1:I:314:ASN:HD22	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:ASP:HB2	1:G:147:PHE:CD2	2.55	0.42
1:G:276:LEU:HD12	1:G:276:LEU:HA	1.72	0.42
1:H:307:ILE:C	1:H:309:GLY:HA3	2.43	0.42
1:I:166:ALA:O	1:I:169:LEU:HB3	2.20	0.42
1:I:213:GLN:NE2	1:I:213:GLN:HA	2.35	0.42
1:A:30:GLU:HG2	1:A:43:LYS:HG2	2.02	0.41
1:B:165:ARG:N	1:B:165:ARG:HD2	2.35	0.41
1:G:12:LEU:HD13	1:G:16:THR:CG2	2.50	0.41
1:G:27:PHE:CZ	1:G:72:VAL:HG21	2.56	0.41
1:G:252:ARG:O	1:G:255:TYR:HB3	2.20	0.41
1:G:310:ILE:O	1:G:313:MET:HB3	2.20	0.41
1:I:316:GLU:HA	1:I:317:TYR:HB3	2.02	0.41
1:J:195:LEU:HD23	1:J:275:LEU:HD23	2.02	0.41
1:A:204:GLU:HG2	1:A:205:LYS:N	2.35	0.41
1:D:300:ILE:O	1:D:304:LEU:HG	2.21	0.41
1:F:61:TRP:HB2	1:F:169:LEU:CD2	2.47	0.41
1:F:236:TYR:CE1	1:F:252:ARG:HB2	2.55	0.41
1:G:211:THR:HG21	1:G:276:LEU:HD13	2.02	0.41
1:H:229:ARG:HA	1:H:258:THR:CG2	2.50	0.41
1:H:311:TYR:HD2	1:H:330:VAL:HG21	1.85	0.41
1:J:47:VAL:CG2	1:J:72:VAL:HG13	2.50	0.41
1:A:296:ILE:HG22	1:A:345:PHE:CZ	2.55	0.41
4:A:403:LMT:C4B	4:B:406:LMT:H6D	2.50	0.41
1:C:86:VAL:HG13	1:C:107:PHE:CZ	2.55	0.41
1:C:337:ILE:O	1:C:341:MET:HG2	2.20	0.41
1:D:165:ARG:CZ	1:D:243:ILE:HG21	2.50	0.41
1:F:24:ARG:HA	1:F:68:HIS:CD2	2.55	0.41
1:G:61:TRP:NE1	1:G:138:MET:HE2	2.31	0.41
1:G:115:TYR:OH	1:G:120:HIS:HB3	2.20	0.41
1:J:327:TYR:HB3	1:J:328:PRO:HD3	2.02	0.41
1:A:105:TYR:HB3	1:A:132:THR:HB	2.03	0.41
4:B:407:LMT:O2'	4:B:407:LMT:H61	2.20	0.41
1:C:130:ILE:HB	1:C:137:LEU:HB2	2.02	0.41
1:C:147:PHE:CZ	1:C:177:LEU:HD12	2.55	0.41
1:F:222:ARG:HD2	1:F:226:TRP:NE1	2.35	0.41
1:F:288:ASN:ND2	1:F:292:LYS:HE3	2.33	0.41
1:F:292:LYS:HG2	1:F:348:LYS:HD3	2.02	0.41
1:G:139:PHE:N	1:G:139:PHE:CD1	2.87	0.41
1:H:347:LYS:HG3	1:H:348:LYS:HD2	2.02	0.41
1:A:83:HIS:O	1:A:86:VAL:HB	2.21	0.41
1:A:149:PRO:CB	1:B:11:GLY:HA2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LYS:O	1:B:9:LYS:HG3	2.20	0.41
1:F:16:THR:O	1:F:88:GLU:HG3	2.21	0.41
1:F:188:ILE:O	1:F:192:ILE:HG13	2.20	0.41
1:G:240:PRO:HB2	1:G:241:PRO:CD	2.50	0.41
1:I:131:LEU:HD22	1:I:170:LEU:HB2	2.02	0.41
1:J:254:VAL:O	1:J:258:THR:HB	2.20	0.41
1:A:294:LEU:HD12	1:A:294:LEU:O	2.20	0.41
1:A:315:PHE:N	1:A:315:PHE:CD1	2.88	0.41
1:C:87:LEU:HD23	1:C:87:LEU:HA	1.90	0.41
1:D:77:GLY:HA3	1:D:87:LEU:HD21	2.02	0.41
1:E:280:LEU:HD12	1:E:280:LEU:HA	1.83	0.41
1:E:283:VAL:O	1:E:287:THR:N	2.49	0.41
1:G:75:ARG:HA	7:G:525:HOH:O	2.20	0.41
1:G:143:ILE:HD13	1:G:144:GLY:N	2.35	0.41
1:G:224:THR:O	1:G:227:PRO:HG2	2.20	0.41
1:G:244:GLU:HB3	1:G:245:LYS:HE2	2.03	0.41
1:I:136:VAL:CG2	1:I:169:LEU:HD23	2.50	0.41
1:C:347:LYS:CD	1:C:348:LYS:H	2.34	0.41
1:E:307:ILE:HD11	1:E:334:MET:HG2	2.02	0.41
1:F:86:VAL:HG13	1:F:107:PHE:CD2	2.55	0.41
1:F:111:LYS:O	1:F:181:TYR:OH	2.32	0.41
1:F:160:ILE:HD12	1:F:164:LYS:HE3	2.02	0.41
1:F:304:LEU:HD12	1:F:304:LEU:HA	1.85	0.41
1:G:32:MET:O	1:G:60:THR:HA	2.20	0.41
1:G:302:MET:HE1	1:H:302:MET:HG3	2.03	0.41
1:G:322:ARG:O	1:G:324:LYS:N	2.53	0.41
1:G:324:LYS:HD3	1:G:324:LYS:HA	1.87	0.41
1:H:328:PRO:HA	1:H:331:LEU:HB2	2.03	0.41
1:I:211:THR:O	1:I:214:LEU:N	2.54	0.41
1:J:23:TYR:CD2	1:J:142:LYS:HD3	2.55	0.41
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.85	0.41
1:A:255:TYR:O	1:A:258:THR:HG22	2.21	0.41
1:B:116:ASP:O	1:B:120:HIS:HA	2.20	0.41
4:B:406:LMT:H6'2	4:B:406:LMT:H1B	1.87	0.41
1:C:244:GLU:HA	1:C:248:VAL:HG23	2.03	0.41
1:F:257:HIS:O	1:F:260:GLN:HB3	2.21	0.41
1:G:164:LYS:HA	1:G:164:LYS:HD2	2.00	0.41
1:H:93:VAL:HA	1:H:126:GLN:OE1	2.21	0.41
1:H:164:LYS:NZ	1:H:246:GLU:HB3	2.36	0.41
1:I:148:ASP:N	1:I:149:PRO:HD2	2.36	0.41
1:A:71:ASP:OD1	1:A:72:VAL:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LEU:HD12	1:B:218:LEU:HA	1.75	0.41
1:C:54:ARG:HD3	1:C:80:PHE:HA	2.03	0.41
1:C:164:LYS:HE2	1:C:246:GLU:HB3	2.03	0.41
1:D:60:THR:HB	1:D:135:CYS:SG	2.61	0.41
1:D:321:LEU:HB3	1:D:322:ARG:H	1.60	0.41
1:E:165:ARG:CZ	1:E:243:ILE:HG21	2.51	0.41
1:F:82:ILE:HG22	1:F:87:LEU:HG	2.01	0.41
1:F:138:MET:SD	1:F:147:PHE:CE2	3.14	0.41
1:F:171:TYR:OH	1:G:14:PRO:HG3	2.21	0.41
1:F:272:VAL:O	1:F:275:LEU:HB2	2.20	0.41
1:F:311:TYR:O	1:I:314:ASN:N	2.49	0.41
1:G:93:VAL:HG21	1:G:141:GLU:OE1	2.21	0.41
1:G:333:VAL:O	1:G:337:ILE:HG22	2.21	0.41
1:J:185:LEU:HD23	1:J:185:LEU:HA	1.65	0.41
1:B:10:LYS:C	1:B:12:LEU:N	2.78	0.41
1:B:99:VAL:HG12	1:B:100:GLU:N	2.35	0.41
1:D:185:LEU:HD11	1:D:261:ILE:HG23	2.03	0.41
1:E:113:PHE:CE2	1:E:224:THR:HG21	2.56	0.41
1:E:229:ARG:HA	1:E:258:THR:HG23	2.03	0.41
1:J:300:ILE:HG22	1:J:341:MET:CB	2.51	0.41
1:A:239:VAL:HG23	1:A:239:VAL:O	2.22	0.40
1:D:229:ARG:HA	1:D:258:THR:HG23	2.03	0.40
1:G:204:GLU:HG2	1:G:205:LYS:H	1.87	0.40
1:H:23:TYR:CD2	1:H:142:LYS:HD3	2.56	0.40
1:I:264:THR:O	1:I:267:THR:HB	2.21	0.40
1:J:68:HIS:CE1	1:J:69:ARG:HG2	2.56	0.40
1:B:196:GLU:O	1:B:200:LEU:HG	2.22	0.40
1:B:199:VAL:HG21	1:B:275:LEU:HG	2.02	0.40
1:C:110:LEU:HB3	1:C:177:LEU:HD22	2.03	0.40
1:D:257:HIS:HE1	7:D:503:HOH:O	2.03	0.40
1:F:120:HIS:CD2	1:F:120:HIS:H	2.38	0.40
1:G:99:VAL:HG13	1:G:108:ILE:HG12	2.04	0.40
1:H:153:ARG:HG3	1:H:153:ARG:NH1	2.36	0.40
1:I:112:MET:HE3	1:I:112:MET:HB2	1.75	0.40
1:J:98:LYS:HE3	1:J:100:GLU:CD	2.45	0.40
1:G:30:GLU:OE1	1:G:151:ARG:NH2	2.54	0.40
1:G:278:VAL:HA	1:H:276:LEU:HD21	2.03	0.40
1:I:29:ILE:HG12	1:I:64:ILE:HG12	2.03	0.40
1:I:315:PHE:O	7:I:521:HOH:O	2.22	0.40
1:J:184:LEU:HD21	1:J:221:LEU:HD11	2.04	0.40
1:A:267:THR:O	1:A:271:ILE:HG13	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:TRP:HZ2	1:D:138:MET:HE1	1.87	0.40
1:F:95:GLN:HA	1:I:260:GLN:HE22	1.85	0.40
1:F:196:GLU:HB3	1:F:275:LEU:HD11	2.04	0.40
1:H:129:LEU:HD21	1:H:138:MET:SD	2.61	0.40
1:I:314:ASN:C	1:I:316:GLU:N	2.79	0.40
1:A:200:LEU:HD12	1:A:201:GLU:HG3	2.04	0.40
1:B:236:TYR:CE1	1:B:252:ARG:HG3	2.57	0.40
1:D:103:GLU:H	1:D:103:GLU:HG2	1.53	0.40
1:E:276:LEU:HA	1:E:276:LEU:HD12	1.63	0.40
1:F:236:TYR:CD1	1:F:252:ARG:HB2	2.56	0.40
1:F:315:PHE:CD2	1:G:318:MET:HE2	2.52	0.40
1:F:322:ARG:O	1:F:324:LYS:HA	2.21	0.40
1:F:342:VAL:O	1:F:345:PHE:N	2.55	0.40
1:J:177:LEU:HD23	1:J:177:LEU:O	2.22	0.40
1:J:236:TYR:OH	1:J:252:ARG:HD2	2.21	0.40
1:J:325:TRP:O	1:J:329:VAL:HG22	2.21	0.40
1:J:334:MET:HE2	1:J:334:MET:HB2	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	345/351 (98%)	323 (94%)	19 (6%)	3 (1%)	14	35
1	B	346/351 (99%)	320 (92%)	24 (7%)	2 (1%)	21	44
1	C	345/351 (98%)	321 (93%)	22 (6%)	2 (1%)	21	44
1	D	341/351 (97%)	316 (93%)	22 (6%)	3 (1%)	14	35
1	E	344/351 (98%)	321 (93%)	22 (6%)	1 (0%)	36	60
1	F	344/351 (98%)	318 (92%)	22 (6%)	4 (1%)	10	27
1	G	344/351 (98%)	317 (92%)	21 (6%)	6 (2%)	7	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	341/351 (97%)	322 (94%)	17 (5%)	2 (1%)	21	44
1	I	343/351 (98%)	315 (92%)	25 (7%)	3 (1%)	14	35
1	J	343/351 (98%)	322 (94%)	17 (5%)	4 (1%)	10	27
All	All	3436/3510 (98%)	3195 (93%)	211 (6%)	30 (1%)	14	35

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	302	MET
1	I	327	TYR
1	B	325	TRP
1	D	324	LYS
1	H	67	ILE
1	I	328	PRO
1	A	241	PRO
1	B	241	PRO
1	C	241	PRO
1	G	317	TYR
1	H	241	PRO
1	I	241	PRO
1	J	322	ARG
1	J	323	TRP
1	J	325	TRP
1	F	241	PRO
1	G	322	ARG
1	J	241	PRO
1	F	240	PRO
1	G	241	PRO
1	G	318	MET
1	A	325	TRP
1	D	240	PRO
1	D	241	PRO
1	F	319	PRO
1	A	240	PRO
1	E	241	PRO
1	C	240	PRO
1	G	319	PRO
1	G	240	PRO

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	326/330 (99%)	288 (88%)	38 (12%)	5	13
1	B	327/330 (99%)	295 (90%)	32 (10%)	7	19
1	C	323/330 (98%)	291 (90%)	32 (10%)	7	19
1	D	322/330 (98%)	281 (87%)	41 (13%)	4	11
1	E	320/330 (97%)	282 (88%)	38 (12%)	5	13
1	F	321/330 (97%)	277 (86%)	44 (14%)	3	9
1	G	319/330 (97%)	281 (88%)	38 (12%)	5	13
1	H	318/330 (96%)	280 (88%)	38 (12%)	5	13
1	I	320/330 (97%)	283 (88%)	37 (12%)	5	13
1	J	320/330 (97%)	287 (90%)	33 (10%)	7	18
All	All	3216/3300 (98%)	2845 (88%)	371 (12%)	5	14

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	6	LEU
1	A	40	ARG
1	A	58	THR
1	A	96	ARG
1	A	99	VAL
1	A	104	ASN
1	A	122	LEU
1	A	127	VAL
1	A	128	SER
1	A	143	ILE
1	A	161	ILE
1	A	192	ILE
1	A	195	LEU
1	A	200	LEU
1	A	206	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	215	LYS
1	A	218	LEU
1	A	223	LYS
1	A	229	ARG
1	A	234	SER
1	A	235	LEU
1	A	243	ILE
1	A	266	GLU
1	A	272	VAL
1	A	275	LEU
1	A	283	VAL
1	A	287	THR
1	A	299	THR
1	A	302	MET
1	A	315	PHE
1	A	317	TYR
1	A	324	LYS
1	A	325	TRP
1	A	329	VAL
1	A	331	LEU
1	A	333	VAL
1	A	339	VAL
1	B	4	LYS
1	B	26	ASP
1	B	36	ILE
1	B	60	THR
1	B	82	ILE
1	B	95	GLN
1	B	104	ASN
1	B	127	VAL
1	B	131	LEU
1	B	143	ILE
1	B	146	VAL
1	B	160	ILE
1	B	200	LEU
1	B	206	GLU
1	B	215	LYS
1	B	218	LEU
1	B	223	LYS
1	B	224	THR
1	B	239	VAL
1	B	243	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	252	ARG
1	B	258	THR
1	B	267	THR
1	B	270	ASP
1	B	275	LEU
1	B	290	VAL
1	B	291	MET
1	B	297	ILE
1	B	315	PHE
1	B	329	VAL
1	B	339	VAL
1	B	340	ILE
1	C	6	LEU
1	C	50	VAL
1	C	60	THR
1	C	109	VAL
1	C	118	ASN
1	C	120	HIS
1	C	123	GLU
1	C	128	SER
1	C	143	ILE
1	C	161	ILE
1	C	162	ARG
1	C	177	LEU
1	C	192	ILE
1	C	215	LYS
1	C	218	LEU
1	C	222	ARG
1	C	231	VAL
1	C	235	LEU
1	C	258	THR
1	C	265	VAL
1	C	273	SER
1	C	275	LEU
1	C	283	VAL
1	C	297	ILE
1	C	299	THR
1	C	307	ILE
1	C	321	LEU
1	C	322	ARG
1	C	331	LEU
1	C	336	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	339	VAL
1	C	347	LYS
1	D	39	PHE
1	D	44	THR
1	D	45	THR
1	D	50	VAL
1	D	82	ILE
1	D	94	HIS
1	D	99	VAL
1	D	103	GLU
1	D	106	VAL
1	D	114	THR
1	D	120	HIS
1	D	162	ARG
1	D	173	LEU
1	D	192	ILE
1	D	206	GLU
1	D	215	LYS
1	D	218	LEU
1	D	221	LEU
1	D	223	LYS
1	D	225	ILE
1	D	229	ARG
1	D	232	LEU
1	D	235	LEU
1	D	243	ILE
1	D	244	GLU
1	D	253	ASP
1	D	258	THR
1	D	265	VAL
1	D	267	THR
1	D	275	LEU
1	D	282	SER
1	D	290	VAL
1	D	291	MET
1	D	297	ILE
1	D	307	ILE
1	D	315	PHE
1	D	322	ARG
1	D	323	TRP
1	D	325	TRP
1	D	327	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	349	LYS
1	E	17	LEU
1	E	39	PHE
1	E	44	THR
1	E	50	VAL
1	E	60	THR
1	E	82	ILE
1	E	106	VAL
1	E	109	VAL
1	E	114	THR
1	E	118	ASN
1	E	120	HIS
1	E	127	VAL
1	E	128	SER
1	E	135	CYS
1	E	143	ILE
1	E	178	VAL
1	E	199	VAL
1	E	215	LYS
1	E	222	ARG
1	E	223	LYS
1	E	231	VAL
1	E	234	SER
1	E	235	LEU
1	E	244	GLU
1	E	258	THR
1	E	264	THR
1	E	265	VAL
1	E	267	THR
1	E	275	LEU
1	E	276	LEU
1	E	282	SER
1	E	286	LYS
1	E	287	THR
1	E	291	MET
1	E	300	ILE
1	E	304	LEU
1	E	346	LYS
1	E	347	LYS
1	F	5	ARG
1	F	9	LYS
1	F	10	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	40	ARG
1	F	45	THR
1	F	50	VAL
1	F	60	THR
1	F	70	THR
1	F	93	VAL
1	F	96	ARG
1	F	120	HIS
1	F	122	LEU
1	F	143	ILE
1	F	161	ILE
1	F	172	SER
1	F	195	LEU
1	F	200	LEU
1	F	202	ARG
1	F	213	GLN
1	F	215	LYS
1	F	218	LEU
1	F	222	ARG
1	F	223	LYS
1	F	231	VAL
1	F	235	LEU
1	F	243	ILE
1	F	248	VAL
1	F	258	THR
1	F	263	ASP
1	F	265	VAL
1	F	271	ILE
1	F	275	LEU
1	F	276	LEU
1	F	283	VAL
1	F	297	ILE
1	F	299	THR
1	F	304	LEU
1	F	313	MET
1	F	320	GLU
1	F	324	LYS
1	F	329	VAL
1	F	333	VAL
1	F	339	VAL
1	F	343	VAL
1	G	12	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	36	ILE
1	G	40	ARG
1	G	41	GLU
1	G	44	THR
1	G	50	VAL
1	G	67	ILE
1	G	114	THR
1	G	118	ASN
1	G	143	ILE
1	G	161	ILE
1	G	164	LYS
1	G	178	VAL
1	G	185	LEU
1	G	206	GLU
1	G	215	LYS
1	G	218	LEU
1	G	221	LEU
1	G	223	LYS
1	G	224	THR
1	G	229	ARG
1	G	235	LEU
1	G	246	GLU
1	G	247	THR
1	G	258	THR
1	G	265	VAL
1	G	267	THR
1	G	275	LEU
1	G	276	LEU
1	G	282	SER
1	G	283	VAL
1	G	291	MET
1	G	295	THR
1	G	296	ILE
1	G	297	ILE
1	G	307	ILE
1	G	318	MET
1	G	325	TRP
1	H	14	PRO
1	H	17	LEU
1	H	18	VAL
1	H	26	ASP
1	H	47	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	50	VAL
1	H	60	THR
1	H	69	ARG
1	H	82	ILE
1	H	103	GLU
1	H	106	VAL
1	H	114	THR
1	H	118	ASN
1	H	119	LEU
1	H	120	HIS
1	H	140	GLN
1	H	143	ILE
1	H	150	VAL
1	H	162	ARG
1	H	174	ILE
1	H	177	LEU
1	H	200	LEU
1	H	206	GLU
1	H	213	GLN
1	H	215	LYS
1	H	218	LEU
1	H	226	TRP
1	H	229	ARG
1	H	231	VAL
1	H	235	LEU
1	H	243	ILE
1	H	253	ASP
1	H	258	THR
1	H	276	LEU
1	H	287	THR
1	H	320	GLU
1	H	330	VAL
1	H	341	MET
1	I	10	LYS
1	I	17	LEU
1	I	18	VAL
1	I	36	ILE
1	I	50	VAL
1	I	106	VAL
1	I	114	THR
1	I	120	HIS
1	I	122	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	128	SER
1	I	150	VAL
1	I	204	GLU
1	I	213	GLN
1	I	218	LEU
1	I	222	ARG
1	I	223	LYS
1	I	231	VAL
1	I	233	SER
1	I	235	LEU
1	I	243	ILE
1	I	258	THR
1	I	260	GLN
1	I	267	THR
1	I	271	ILE
1	I	272	VAL
1	I	275	LEU
1	I	276	LEU
1	I	278	VAL
1	I	281	SER
1	I	307	ILE
1	I	313	MET
1	I	315	PHE
1	I	320	GLU
1	I	323	TRP
1	I	325	TRP
1	I	336	VAL
1	I	339	VAL
1	J	5	ARG
1	J	9	LYS
1	J	17	LEU
1	J	18	VAL
1	J	50	VAL
1	J	108	ILE
1	J	114	THR
1	J	124	SER
1	J	125	GLU
1	J	128	SER
1	J	143	ILE
1	J	164	LYS
1	J	177	LEU
1	J	200	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	204	GLU
1	J	215	LYS
1	J	218	LEU
1	J	222	ARG
1	J	231	VAL
1	J	234	SER
1	J	235	LEU
1	J	258	THR
1	J	275	LEU
1	J	291	MET
1	J	293	VAL
1	J	295	THR
1	J	296	ILE
1	J	304	LEU
1	J	315	PHE
1	J	320	GLU
1	J	330	VAL
1	J	337	ILE
1	J	348	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	157	ASN
1	B	63	ASN
1	B	74	GLN
1	B	140	GLN
1	B	213	GLN
1	B	257	HIS
1	B	288	ASN
1	C	94	HIS
1	C	126	GLN
1	C	209	GLN
1	C	288	ASN
1	D	33	ASN
1	D	63	ASN
1	D	95	GLN
1	D	140	GLN
1	D	209	GLN
1	D	288	ASN
1	D	314	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	74	GLN
1	E	83	HIS
1	E	126	GLN
1	E	157	ASN
1	E	209	GLN
1	E	260	GLN
1	F	33	ASN
1	F	118	ASN
1	F	288	ASN
1	G	33	ASN
1	G	63	ASN
1	G	74	GLN
1	G	94	HIS
1	G	95	GLN
1	G	118	ASN
1	G	126	GLN
1	G	140	GLN
1	G	157	ASN
1	G	209	GLN
1	H	63	ASN
1	H	120	HIS
1	H	140	GLN
1	H	213	GLN
1	H	288	ASN
1	H	314	ASN
1	I	63	ASN
1	I	74	GLN
1	I	213	GLN
1	I	260	GLN
1	I	314	ASN
1	J	33	ASN
1	J	68	HIS
1	J	95	GLN
1	J	140	GLN
1	J	260	GLN
1	J	314	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 62 ligands modelled in this entry, 37 are monoatomic - leaving 25 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	$\# Z > 2$
5	PEG	E	407	-	6,6,6	0.60	0	5,5,5	0.51	0
5	PEG	H	402	-	6,6,6	0.34	0	5,5,5	0.25	0
4	LMT	B	406	-	36,36,36	0.42	0	47,47,47	0.82	1 (2%)
5	PEG	G	411	-	6,6,6	0.37	0	5,5,5	0.28	0
5	PEG	B	409	-	6,6,6	0.36	0	5,5,5	0.44	0
5	PEG	B	411	-	6,6,6	0.56	0	5,5,5	1.35	1 (20%)
4	LMT	A	403	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
5	PEG	C	405	-	6,6,6	0.29	0	5,5,5	0.45	0
5	PEG	B	410	-	6,6,6	0.37	0	5,5,5	0.42	0
4	LMT	B	407	-	33,33,36	0.44	0	44,44,47	0.84	2 (4%)
5	PEG	G	412	-	6,6,6	0.58	0	5,5,5	1.11	0
5	PEG	E	405	-	6,6,6	0.61	0	5,5,5	0.60	0
5	PEG	J	406	-	6,6,6	0.59	0	5,5,5	0.77	0
5	PEG	J	405	-	6,6,6	0.51	0	5,5,5	0.78	0
5	PEG	I	404	-	6,6,6	0.58	0	5,5,5	0.70	0
6	PG0	E	409	-	7,7,7	0.42	0	6,6,6	1.10	1 (16%)
5	PEG	F	404	-	6,6,6	0.58	0	5,5,5	0.88	0
5	PEG	E	408	-	6,6,6	0.45	0	5,5,5	1.32	1 (20%)
5	PEG	G	408	-	6,6,6	0.57	0	5,5,5	0.70	0
5	PEG	C	406	-	6,6,6	0.65	0	5,5,5	0.93	0
5	PEG	E	406	-	6,6,6	0.56	0	5,5,5	1.29	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	G	410	-	6,6,6	0.34	0	5,5,5	0.45	0
5	PEG	B	408	-	6,6,6	0.56	0	5,5,5	0.72	0
5	PEG	G	409	-	6,6,6	0.55	0	5,5,5	0.87	0
5	PEG	D	405	-	6,6,6	0.39	0	5,5,5	0.99	0

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
5	PEG	E	407	-	-	2/4/4/4	-
5	PEG	H	402	-	-	2/4/4/4	-
4	LMT	B	406	-	-	13/21/61/61	0/2/2/2
5	PEG	G	411	-	-	2/4/4/4	-
5	PEG	B	409	-	-	2/4/4/4	-
5	PEG	B	411	-	-	4/4/4/4	-
4	LMT	A	403	-	-	12/21/61/61	0/2/2/2
5	PEG	C	405	-	-	3/4/4/4	-
5	PEG	B	410	-	-	3/4/4/4	-
4	LMT	B	407	-	-	9/18/58/61	0/2/2/2
5	PEG	G	412	-	-	2/4/4/4	-
5	PEG	E	405	-	-	1/4/4/4	-
5	PEG	J	406	-	-	1/4/4/4	-
5	PEG	J	405	-	-	2/4/4/4	-
5	PEG	I	404	-	-	3/4/4/4	-
6	PG0	E	409	-	-	2/5/5/5	-
5	PEG	F	404	-	-	1/4/4/4	-
5	PEG	E	408	-	-	1/4/4/4	-
5	PEG	G	408	-	-	3/4/4/4	-
5	PEG	C	406	-	-	1/4/4/4	-
5	PEG	E	406	-	-	2/4/4/4	-
5	PEG	G	410	-	-	2/4/4/4	-
5	PEG	B	408	-	-	4/4/4/4	-
5	PEG	G	409	-	-	4/4/4/4	-
5	PEG	D	405	-	-	2/4/4/4	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	408	PEG	C3-O2-C2	2.89	125.89	113.26
5	E	406	PEG	C3-O2-C2	2.77	125.37	113.26
4	A	403	LMT	C1B-O1B-C4'	-2.61	111.79	117.98
4	B	407	LMT	C1B-O1B-C4'	-2.60	111.82	117.98
4	B	406	LMT	C1B-O1B-C4'	-2.38	112.35	117.98
5	B	411	PEG	C3-O2-C2	2.24	123.07	113.26
6	E	409	PG0	C2-O1-C3	2.20	122.89	113.26
4	B	407	LMT	C3B-C4B-C5B	2.04	113.93	110.23

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	407	LMT	C2-C1-O1'-C1'
5	J	405	PEG	C1-C2-O2-C3
4	A	403	LMT	O5'-C5'-C6'-O6'
4	B	406	LMT	O5B-C5B-C6B-O6B
4	A	403	LMT	O5B-C5B-C6B-O6B
5	B	411	PEG	C1-C2-O2-C3
4	A	403	LMT	C4'-C5'-C6'-O6'
4	B	406	LMT	C4B-C5B-C6B-O6B
4	A	403	LMT	C4B-C5B-C6B-O6B
4	A	403	LMT	O5'-C1'-O1'-C1
4	B	407	LMT	O5'-C1'-O1'-C1
5	C	406	PEG	C1-C2-O2-C3
4	A	403	LMT	C2'-C1'-O1'-C1
4	B	407	LMT	C2'-C1'-O1'-C1
5	B	409	PEG	O2-C3-C4-O4
5	B	410	PEG	O1-C1-C2-O2
5	B	411	PEG	O1-C1-C2-O2
5	B	411	PEG	O2-C3-C4-O4
5	E	408	PEG	O2-C3-C4-O4
5	J	405	PEG	O1-C1-C2-O2
4	B	407	LMT	O5B-C5B-C6B-O6B
5	B	408	PEG	O1-C1-C2-O2
5	G	409	PEG	O1-C1-C2-O2
5	G	410	PEG	O1-C1-C2-O2
5	G	411	PEG	O2-C3-C4-O4
4	B	406	LMT	C3'-C4'-O1B-C1B
4	B	406	LMT	C5'-C4'-O1B-C1B
5	G	409	PEG	C1-C2-O2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	407	LMT	O1'-C1-C2-C3
4	A	403	LMT	C2-C3-C4-C5
4	B	406	LMT	C2-C1-O1'-C1'
4	A	403	LMT	O1'-C1-C2-C3
5	H	402	PEG	O1-C1-C2-O2
4	A	403	LMT	C4-C5-C6-C7
5	E	406	PEG	C1-C2-O2-C3
4	B	406	LMT	O1'-C1-C2-C3
4	B	406	LMT	C7-C8-C9-C10
5	B	410	PEG	C1-C2-O2-C3
4	A	403	LMT	C1-C2-C3-C4
4	B	406	LMT	C11-C10-C9-C8
4	B	406	LMT	C6-C7-C8-C9
5	F	404	PEG	O1-C1-C2-O2
5	G	409	PEG	O2-C3-C4-O4
5	G	410	PEG	O2-C3-C4-O4
5	G	411	PEG	O1-C1-C2-O2
5	I	404	PEG	O2-C3-C4-O4
4	B	407	LMT	C3'-C4'-O1B-C1B
5	B	410	PEG	C4-C3-O2-C2
4	B	407	LMT	C5'-C4'-O1B-C1B
5	E	405	PEG	O2-C3-C4-O4
4	B	406	LMT	C3-C4-C5-C6
4	B	407	LMT	C4-C5-C6-C7
4	B	406	LMT	C2'-C1'-O1'-C1
5	E	406	PEG	C4-C3-O2-C2
5	C	405	PEG	C4-C3-O2-C2
5	J	406	PEG	C4-C3-O2-C2
5	D	405	PEG	C4-C3-O2-C2
5	G	408	PEG	C4-C3-O2-C2
5	G	408	PEG	C1-C2-O2-C3
6	E	409	PG0	C1-C2-O1-C3
5	B	408	PEG	C1-C2-O2-C3
5	C	405	PEG	O1-C1-C2-O2
5	G	412	PEG	O2-C3-C4-O4
6	E	409	PG0	OTT-C1-C2-O1
5	B	408	PEG	O2-C3-C4-O4
5	H	402	PEG	C1-C2-O2-C3
5	C	405	PEG	C1-C2-O2-C3
5	E	407	PEG	O2-C3-C4-O4
5	B	409	PEG	C4-C3-O2-C2
4	A	403	LMT	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	406	LMT	C9-C10-C11-C12
4	A	403	LMT	C6-C7-C8-C9
5	I	404	PEG	C1-C2-O2-C3
5	B	408	PEG	C4-C3-O2-C2
5	G	409	PEG	C4-C3-O2-C2
5	G	412	PEG	C1-C2-O2-C3
5	I	404	PEG	O1-C1-C2-O2
4	B	407	LMT	C3-C4-C5-C6
5	D	405	PEG	C1-C2-O2-C3
5	E	407	PEG	C4-C3-O2-C2
4	B	406	LMT	C2-C3-C4-C5
5	B	411	PEG	C4-C3-O2-C2
5	G	408	PEG	O2-C3-C4-O4

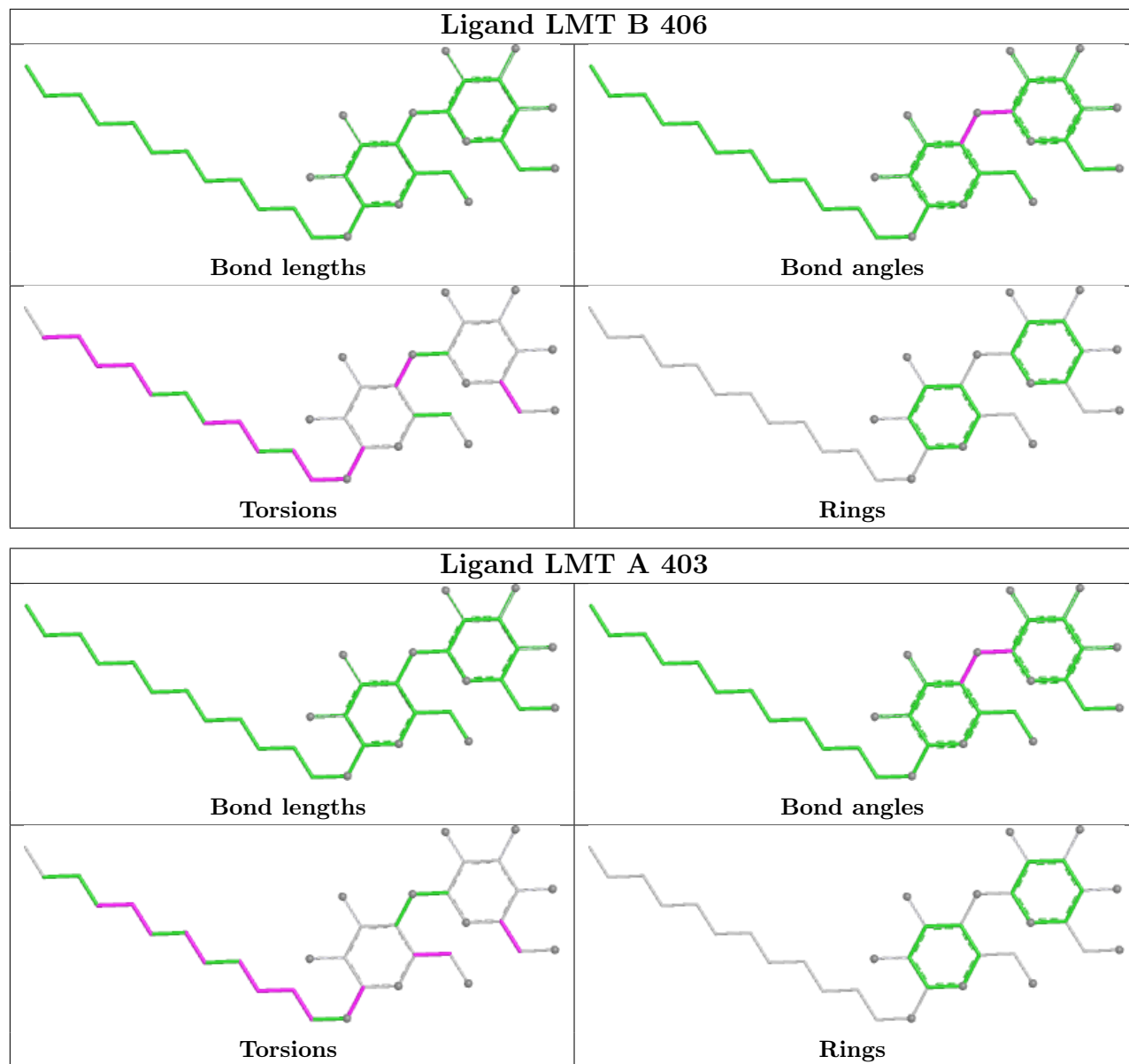
There are no ring outliers.

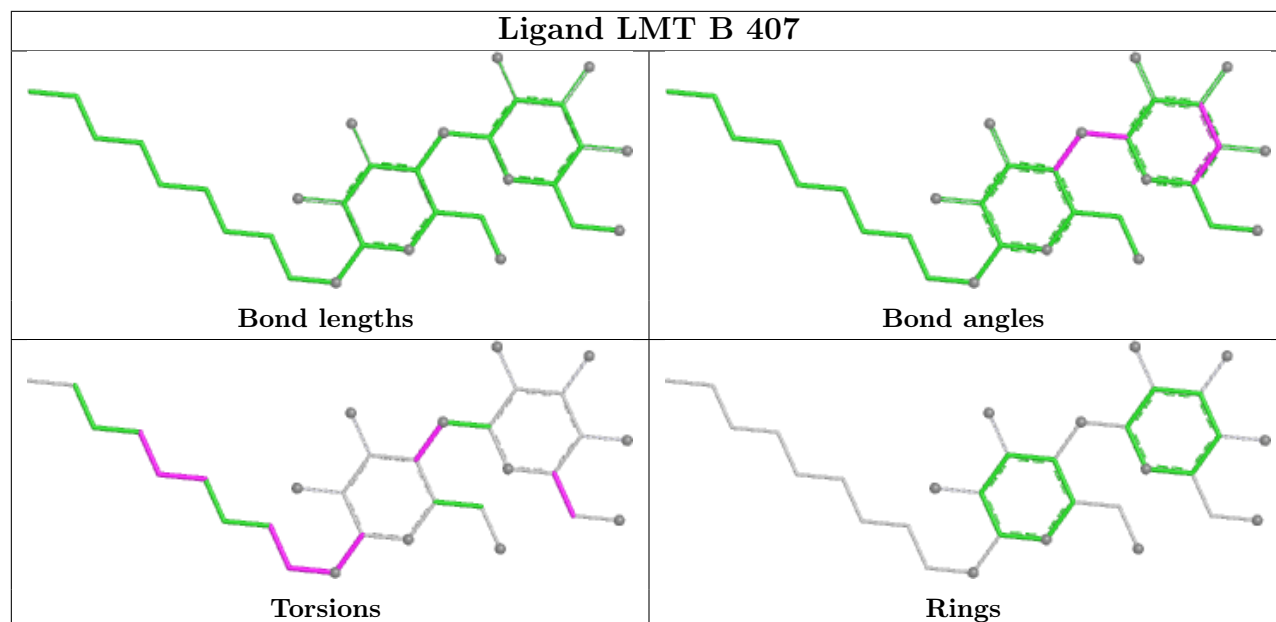
12 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	406	LMT	26	0
5	G	411	PEG	3	0
5	B	411	PEG	2	0
4	A	403	LMT	27	0
5	B	410	PEG	2	0
4	B	407	LMT	8	0
5	E	405	PEG	1	0
5	J	405	PEG	2	0
5	G	408	PEG	3	0
5	C	406	PEG	4	0
5	B	408	PEG	1	0
5	G	409	PEG	2	0

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

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [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	347/351 (98%)	-0.08	3 (0%) 81 80	33, 72, 122, 180	0
1	B	348/351 (99%)	-0.23	2 (0%) 85 85	27, 58, 126, 158	0
1	C	347/351 (98%)	-0.09	2 (0%) 85 85	25, 75, 145, 230	0
1	D	343/351 (97%)	-0.16	4 (1%) 76 75	40, 77, 133, 197	0
1	E	345/351 (98%)	-0.20	1 (0%) 90 89	35, 71, 149, 187	1 (0%)
1	F	346/351 (98%)	-0.26	0 100 100	32, 70, 135, 202	0
1	G	346/351 (98%)	-0.21	5 (1%) 73 72	30, 57, 141, 234	0
1	H	343/351 (97%)	-0.10	4 (1%) 76 75	30, 71, 127, 191	0
1	I	345/351 (98%)	-0.10	5 (1%) 73 72	38, 71, 143, 246	0
1	J	345/351 (98%)	-0.05	9 (2%) 57 54	32, 71, 151, 192	0
All	All	3455/3510 (98%)	-0.15	35 (1%) 79 78	25, 70, 140, 246	1 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	167	ASP	3.9
1	J	199	VAL	3.4
1	J	236	TYR	3.4
1	G	326	GLY	3.4
1	I	318	MET	3.0
1	I	200	LEU	2.9
1	H	50	VAL	2.9
1	D	193	ASP	2.9
1	C	278	VAL	2.8
1	J	93	VAL	2.8
1	H	326	GLY	2.6
1	C	315	PHE	2.5
1	I	301	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	152	GLU	2.4
1	A	152	GLU	2.4
1	J	317	TYR	2.4
1	G	314	ASN	2.4
1	H	256	ASP	2.4
1	A	219	VAL	2.3
1	I	321	LEU	2.3
1	G	325	TRP	2.2
1	J	208	VAL	2.2
1	G	312	GLY	2.2
1	I	330	VAL	2.2
1	H	325	TRP	2.1
1	J	33	ASN	2.1
1	B	321	LEU	2.1
1	D	317	TYR	2.1
1	G	315	PHE	2.1
1	E	323	TRP	2.1
1	A	199	VAL	2.1
1	J	238	ASP	2.0
1	D	314	ASN	2.0
1	B	308	ALA	2.0
1	D	283	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	G	411	7/7	0.37	0.13	203,214,221,223	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PG0	E	409	8/8	0.43	0.09	72,83,97,98	0
4	LMT	B	406	35/35	0.46	0.14	89,123,133,135	0
2	MG	J	401	1/1	0.53	0.19	107,107,107,107	0
4	LMT	A	403	35/35	0.63	0.11	72,129,136,142	35
4	LMT	B	407	32/35	0.64	0.11	114,176,197,203	0
5	PEG	D	405	7/7	0.64	0.08	62,80,92,108	0
5	PEG	F	404	7/7	0.67	0.08	92,113,123,126	0
5	PEG	E	408	7/7	0.72	0.09	67,71,77,82	0
5	PEG	J	405	7/7	0.73	0.12	49,53,59,63	0
5	PEG	G	408	7/7	0.73	0.08	91,103,105,109	0
5	PEG	C	405	7/7	0.74	0.08	79,82,95,100	0
5	PEG	E	407	7/7	0.77	0.07	77,83,87,96	0
5	PEG	B	409	7/7	0.78	0.09	67,87,95,95	0
5	PEG	G	412	7/7	0.78	0.09	72,74,87,90	0
2	MG	D	401	1/1	0.80	0.28	86,86,86,86	0
5	PEG	G	409	7/7	0.81	0.09	75,92,99,102	0
5	PEG	E	406	7/7	0.82	0.06	65,75,91,107	0
5	PEG	B	410	7/7	0.83	0.09	57,74,82,87	0
5	PEG	E	405	7/7	0.83	0.07	82,84,92,95	0
5	PEG	J	406	7/7	0.83	0.07	78,88,95,100	0
2	MG	D	403	1/1	0.83	0.12	57,57,57,57	0
5	PEG	I	404	7/7	0.84	0.06	77,82,84,89	0
3	CL	D	404	1/1	0.84	0.10	66,66,66,66	0
5	PEG	C	406	7/7	0.85	0.09	49,60,63,75	0
5	PEG	B	411	7/7	0.85	0.06	61,68,72,78	0
2	MG	G	402	1/1	0.85	0.05	69,69,69,69	0
5	PEG	G	410	7/7	0.87	0.08	98,101,110,114	0
5	PEG	H	402	7/7	0.87	0.09	73,84,92,97	0
3	CL	E	403	1/1	0.88	0.07	62,62,62,62	0
3	CL	B	405	1/1	0.89	0.29	50,50,50,50	0
3	CL	G	406	1/1	0.91	0.06	46,46,46,46	0
3	CL	G	407	1/1	0.91	0.08	65,65,65,65	0
5	PEG	B	408	7/7	0.91	0.05	64,77,83,85	0
3	CL	H	401	1/1	0.91	0.07	52,52,52,52	0
3	CL	J	404	1/1	0.91	0.15	46,46,46,46	0
2	MG	E	402	1/1	0.91	0.17	56,56,56,56	0
2	MG	A	401	1/1	0.92	0.11	65,65,65,65	0
3	CL	C	403	1/1	0.92	0.10	41,41,41,41	0
2	MG	G	401	1/1	0.92	0.14	61,61,61,61	0
3	CL	F	403	1/1	0.93	0.09	60,60,60,60	0
2	MG	C	401	1/1	0.93	0.10	53,53,53,53	0
3	CL	A	402	1/1	0.93	0.06	52,52,52,52	0

Continued on next page...

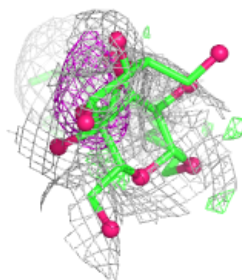
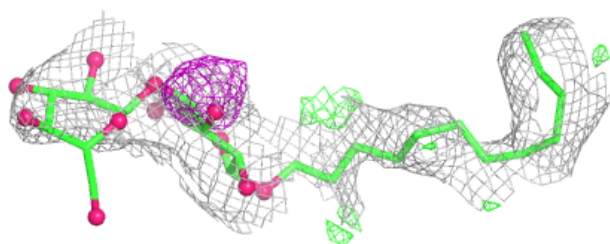
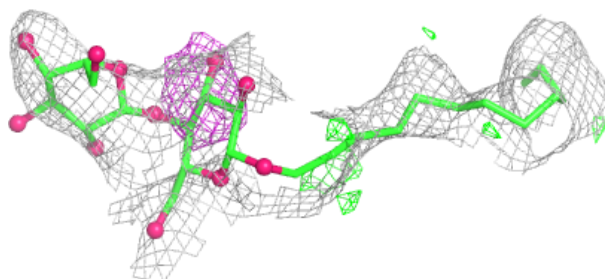
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	J	403	1/1	0.95	0.08	50,50,50,50	0
2	MG	I	403	1/1	0.95	0.10	45,45,45,45	0
2	MG	J	402	1/1	0.95	0.09	43,43,43,43	0
2	MG	B	401	1/1	0.96	0.09	45,45,45,45	0
2	MG	D	402	1/1	0.96	0.06	35,35,35,35	0
3	CL	C	404	1/1	0.96	0.04	44,44,44,44	0
2	MG	G	403	1/1	0.96	0.04	54,54,54,54	0
2	MG	F	401	1/1	0.96	0.12	42,42,42,42	0
3	CL	E	404	1/1	0.96	0.09	52,52,52,52	0
2	MG	G	405	1/1	0.97	0.13	39,39,39,39	0
2	MG	I	401	1/1	0.97	0.11	56,56,56,56	0
2	MG	E	401	1/1	0.97	0.05	34,34,34,34	0
3	CL	B	404	1/1	0.97	0.06	57,57,57,57	0
2	MG	B	403	1/1	0.97	0.06	45,45,45,45	0
2	MG	G	404	1/1	0.98	0.04	45,45,45,45	0
2	MG	F	402	1/1	0.98	0.11	57,57,57,57	0
2	MG	C	402	1/1	0.98	0.07	45,45,45,45	0
2	MG	B	402	1/1	0.99	0.05	39,39,39,39	0
2	MG	I	402	1/1	0.99	0.03	58,58,58,58	0

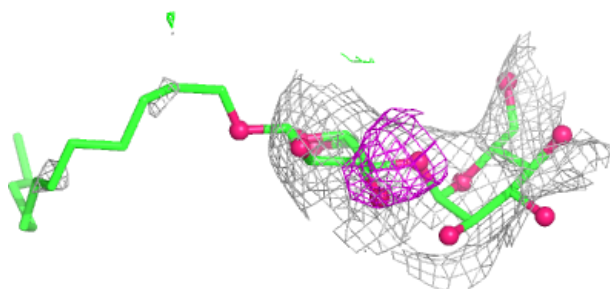
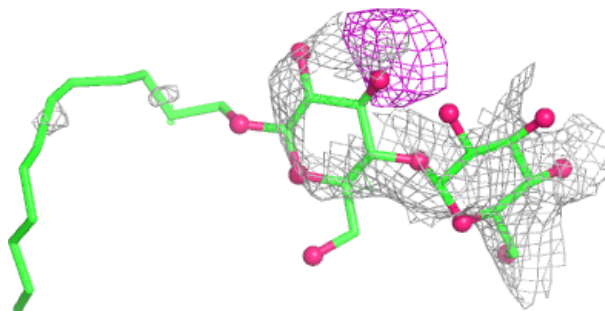
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

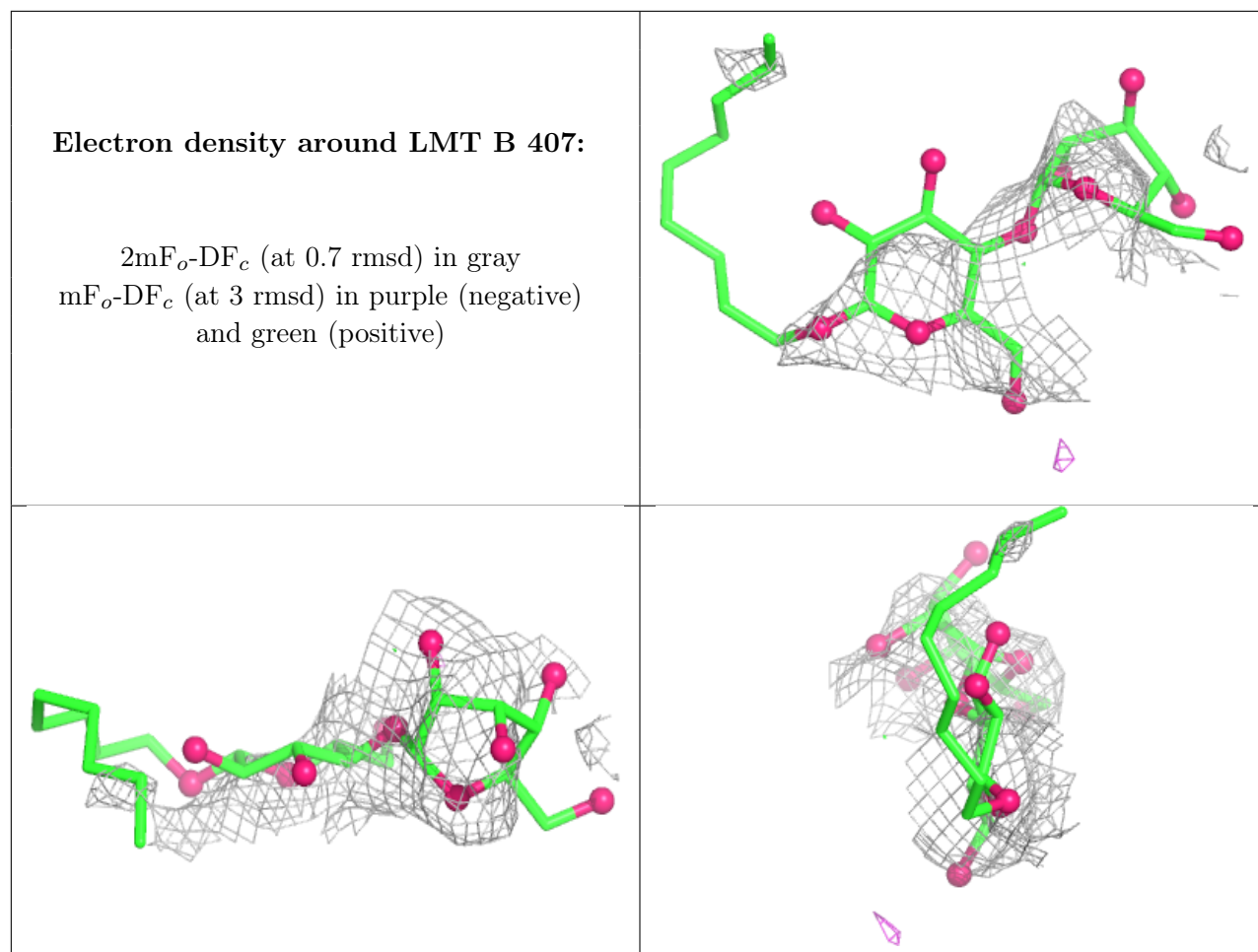
Electron density around LMT B 406:

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

**Electron density around LMT A 403:**

$2mF_o-DF_c$ (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.